



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:38 PM BST

PDB ID : 1Q5C
EMDB ID: : EMD-1052
Title : S-S-lambda-shaped TRANS and CIS interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

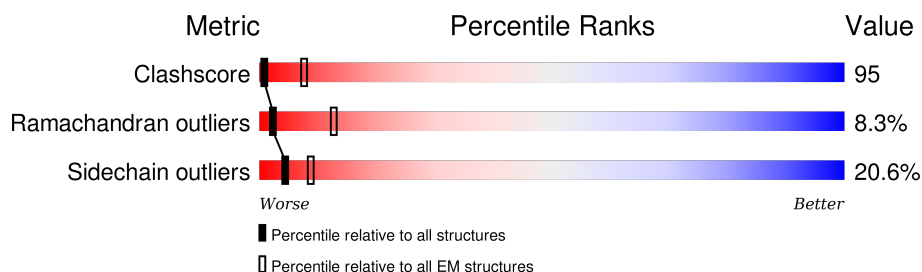
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	880	16% 30% 11% • 39%
1	B	880	16% 31% 11% • 39%
1	C	880	15% 31% 11% • 39%
1	D	880	15% 32% 11% • 39%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	904	-	-	X	-
2	NAG	C	801	-	-	X	-
2	NAG	C	805	X	-	-	-
2	NAG	C	806	X	-	X	-
2	NAG	C	807	-	-	X	-
2	NAG	C	809	-	-	X	-
2	NAG	C	810	-	-	X	-
2	NAG	C	904	-	-	X	-
2	NAG	D	801	-	-	X	-
2	NAG	D	805	X	-	X	-
2	NAG	D	806	X	-	X	-
2	NAG	D	807	-	-	X	-
2	NAG	D	809	-	-	X	-
2	NAG	D	810	-	-	X	-
2	NAG	D	904	-	-	X	-
3	NDG	A	902	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	B	902	-	-	X	-
3	NDG	C	902	-	-	X	-
3	NDG	D	811	-	-	X	-
3	NDG	D	902	-	-	X	-

2 Entry composition [i](#)

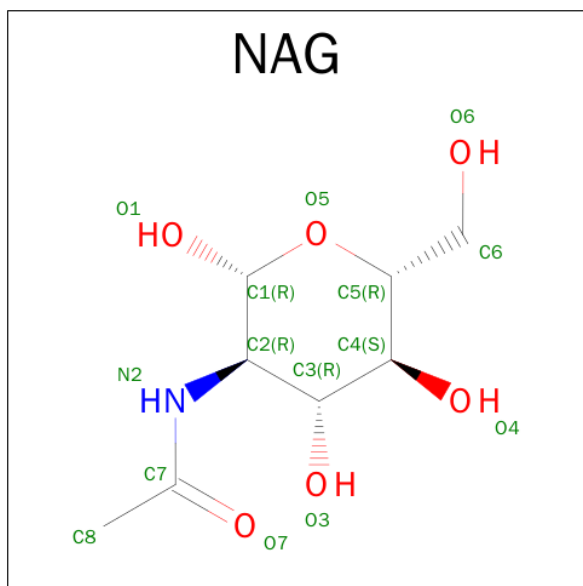
There are 4 unique types of molecules in this entry. The entry contains 17652 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	B	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	C	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	D	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	

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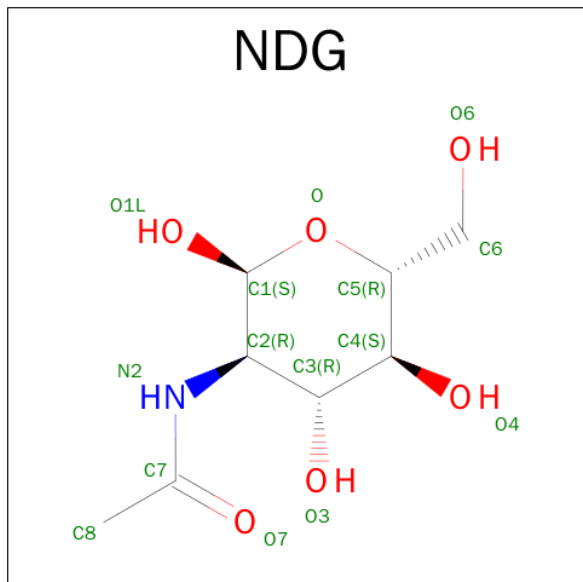
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	C	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	
2	D	1	Total	C	N	O	0
			154	88	11	55	

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	
3	C	1	Total	C	N	O	0
			56	32	4	20	

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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	
3	D	1	Total	C	N	O	0
			56	32	4	20	

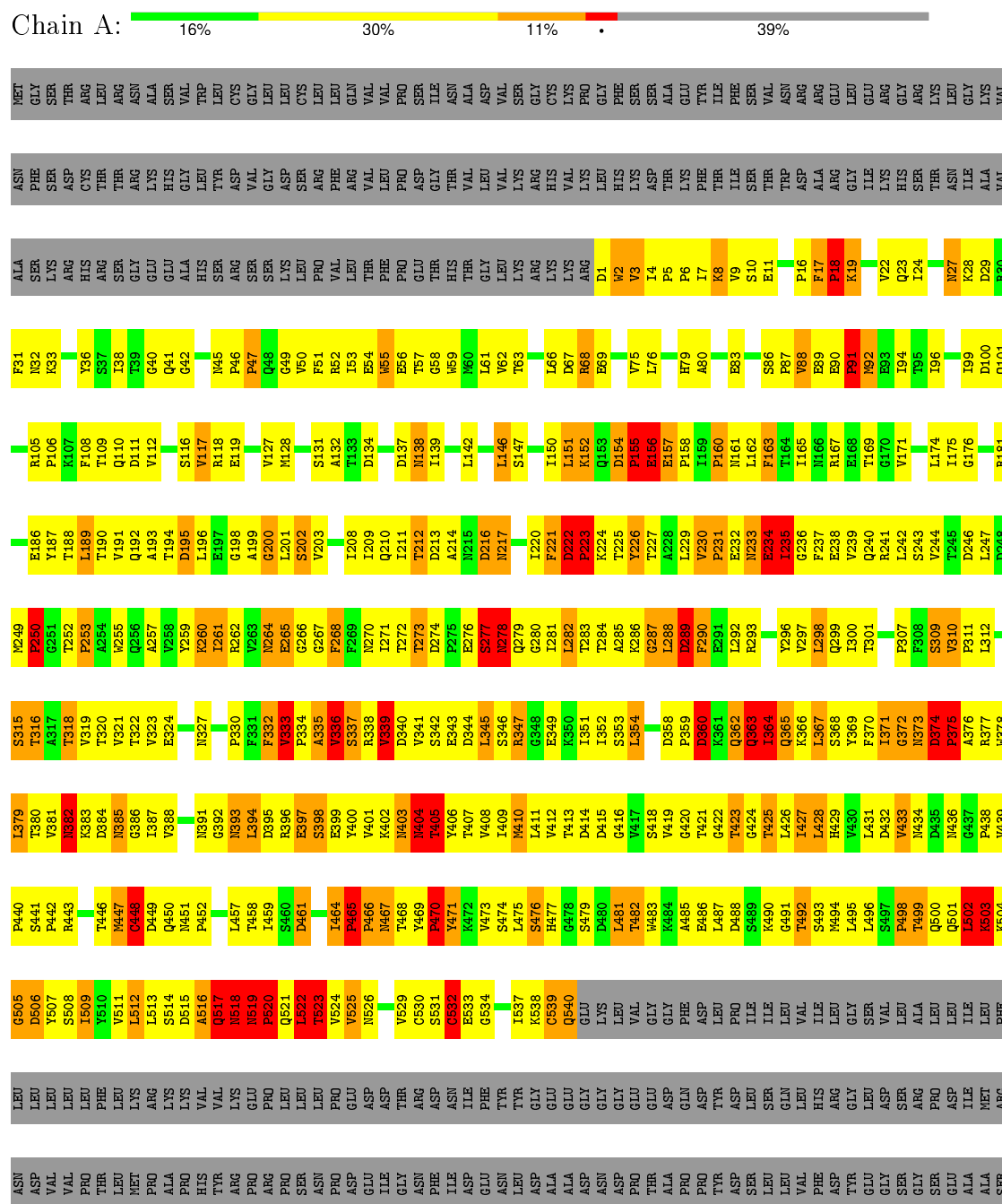
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	12	Total	Ca	0
			12	12	
4	A	12	Total	Ca	0
			12	12	
4	D	12	Total	Ca	0
			12	12	
4	C	12	Total	Ca	0
			12	12	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: EP-cadherin



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GLU
HIS
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LEU
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• Molecule 1: EP-cadherin

Chain B: 16% 31% 11% • 39%

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- Molecule 1: EP-cadherin

Chain D:

MET	GLY	SER	ARG	LEU	ARG	ASN	ALA	SER	VAL	TRP	LEU	CYS	GLY	LEU	CYS	LEU	LEU	CYS	LEU	LEU	GLN	VAL	VAL	PHE	ASP	VAL	SER	CYS	LVS	PRO	GLY	PHE	SER	SER	ALA	GLU	THR	ILE	PHE	VAL	ASN	ARG	ARG	GLU	LEU	GLU	ARG	GLY	LVS	LEU	GLY	LVS	VAL
ASN	PHE	SER	ASP	CYS	THR	ARG	LVS	HIS	GLY	LEU	THR	ASP	ASP	VAL	GLY	SER	ARG	PHE	ARG	VAL	LEU	PHE	LEU	VAL	VAL	LVS	ARG	HIS	VAL	LVS	LEU	HIS	LVS	ASP	THR	PHE	THR	ILE	ILE	SER	THR	THR	ASP	ALA	ARG	GLY	ILE	LVS	HIS	ILE	ALA	VAL	

SER	GLU	PRO	LEU	Q500	D435	D374	S309	V244	L174	I94	K33	ALA
GLU	ILE	ASP	LEU	Q501	M436	P375	V310	T245	I175	T95	V34	SER
ALA	LEU	ILE	LEU	L502	G437	A376	P311	D246	G176	I96	V35	LYS
ALA	LEU	MET	LEU	K503	P438	R377	L312	L247		N97	T36	ARG
SER	LEU	ARG	PHE	K504	V439	M378	S315	D248	R181	D100	S37	HIS
LEU	LEU	ASN	LEU	G505	P440	L379	L316	M249		Q101	I38	ARG
SER	LEU	ASP	LEU	D506	S441	T380	T317	P250	E186		T39	SER
SER	LEU	VAL	LEU	P442	R443	V381	T318	T251	T187		Q40	GLY
LEU	LEU	VAL	LEU	R443		M382	L383	T252	T188	R105	Q41	GLU
ASN	PRO	PRO	PHE	L509		K383	V319	P253	L189	K107	G42	GLU
SER	SER	THR	PHE	Y510	T446	D384	T320	A254	T190	F108	A43	ALA
SER	LEU	LEU	LEU	V511	M447	N385	V321	T255	V191	T109	D44	HIS
ASN	ASN	MET	LYS	L512	C448	N386	T322	Q256	Q192	Q110	N45	SER
SER	PRO	PRO	ARG	L513	D449	I387	V323	A257	A193		P46	ARG
ASN	ASN	ALA	LYS	L514	Q450	V388	E324	V258	T194	D111	P47	SER
ASP	ASP	PRO	LYS	D515	M451			T259	D195	Q48	Q48	SER
GLU	GLU	HIS	VAL	A516	P452	N391	N327	T260	L196	G49	V50	LYS
HIS	TYR	TYR	VAL	Q517		G392		I261	E197	S116	F51	LEU
ASP	ASP	ARG	LYS	M518	L457	N393	P330	R262	G198	V117	R52	PRO
TYR	TYR	PRO	GLU	M519	T458	L394	F331	V263	A199	R118	T53	VAL
ASN	ASN	ARG	PRO	P520	T459	D395	P332	R264	G200	E119	E54	LEU
TYR	TYR	PRO	LEU	Q521	S460	R396	V333	E265	L201		V127	THR
LEU	LEU	SER	LEU	L522	D461	E397	P334	G266	S202		M55	PHE
SER	SER	ASN	LEU	T523		S398	A335	G267	V203	M128	E56	PRO
ASP	ASP	PRO	PRO	V524	L464	E399	V336	F268		A129	T57	GLU
TRP	TRP	ASP	GLU	V525	P465	Y400	S337	F269	T208	V130	G58	THR
GLY	GLY	GLU	ASP	N526	P466	V401	R338		T209	M138	L66	LYS
SER	SER	ILE	ASP		M467	K402	V339	E276	Q210	I139	D67	LYS
ARG	ARG	GLY	THR	V529	T468	M403	D340	S277	T212		R68	ARG
PHE	PHE	ASN	THR	C530	Y469	M404	V341	T272	T211	T133	L61	GLY
ARG	ARG	PHE	ASN	S531	P470	T405	S342	T273	T212	D134	V62	LEU
LYS	LYS	ILE	ASN	G532	Y471	Y406	E343	F275	D213		T63	LYS
LEU	LEU	ASP	ILE	E533	T472	T407	D344	E276	A214	D137		ARG
ALA	ALA	GLU	PHE	G534	Y473	V408	L345	S278	R215	M138	L66	LYS
ASP	ASP	ASN	TYR		S474	M409	S346	T277	N217	I139	D68	LYS
ASP	ASP	LEU	TYR	I537	S475	M410	R347	Q279		L142	E69	ARG
GLU	GLU	PRO	GLY	K538	S476	L411	G348	G280	T220		V2	D1
GLU	GLU	ALA	GLU	G539	H477	V412	E349	I281	F221	L146	V3	V2
GLY	GLY	ALA	GLY	Q540	G478	T413	R350	L282	D222		I4	I4
ASP	ASP	ASP	GLY	LYS	S479	D414	L351	T283	P223	I150	K73	P6
ASP	ASP	ASN	GLY	VAL	D480	D415	L352	T284	K224	L151	V74	P6
GLU	GLU	PRO	GLY	VAL	L481	G416	S353	A285	T225	K152	V75	I7
GLU	GLU	THR	GLY	VAL	T482	V417	L354	G286	K286	Q153	L76	K8
GLU	GLY	THR	GLY	GLY	M483	S418		G287	T227	D154	S77	K8
ALA	GLY	ALA	ASP	PHE	K484	V419	D358	L288	A228	P155	S78	E11
PRO	PRO	PRO	GLN	LEU	A485	G420	P359	D289	L229	E156	H79	P16
PRO	PRO	TYR	ASP	ASP	E486	T421	D360	V290	V230	E157	A80	P16
TYR	TYR	TYR	TYR	LEU	L487	G422	G361	E291	P231	P158	V81	F17
ASP	ASP	ASP	ASP	PRO	D488	T423	D362	L292	E232	I159	S82	P18
SER	SER	SER	LEU	ILE	S489	G424	D363	R293	N233	P160	E83	K19
LEU	LEU	LEU	SER	ILE	K490	T425	L364		E234	N161	H84	V22
LEU	LEU	LEU	GLN	LEU	G491	L426	D365	Y296	I235	L162	G85	Q23
VAL	VAL	VAL	LEU	VAL	T492	I427	K366	V297	G236	F163	S86	Q23
PHE	PHE	HIS	HIS	ILE	S493	L428	L367	L298	F237	T164	P87	K27
ASP	ASP	ARG	ARG	LEU	M494	A429	S368	Q299	E238	I165	V88	N27
TYR	TYR	TYR	GLY	GLY	L495	V430	Y369	I300	V239	T169	E89	D29
GLU	GLU	GLU	LEU	SER	L496	L431	F370	T301	Q240	T169	E90	D29
GLY	GLY	GLY	ASP	VAL	S497	D432	I371		R241	G170	F91	R30
SER	SER	SER	SER	LEU	P498	V433	G372	P307	L242	V171	M92	F31
GLY	GLY	GLY	ARG	ALA	T499	M434	N373	F308	S243		E93	N32

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120000	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	50000	Depositor
Image detector	GATAN 794	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, NDG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.70	8/4276 (0.2%)	1.39	77/5839 (1.3%)
1	B	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	C	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
1	D	0.70	8/4276 (0.2%)	1.39	78/5839 (1.3%)
All	All	0.70	32/17104 (0.2%)	1.39	311/23356 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	ALA	CA-CB	-8.37	1.34	1.52
1	A	335	ALA	CA-CB	-8.36	1.34	1.52
1	D	335	ALA	CA-CB	-8.34	1.34	1.52
1	C	335	ALA	CA-CB	-8.29	1.35	1.52
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	A	539	CYS	CB-SG	8.15	1.96	1.82
1	C	539	CYS	CB-SG	8.14	1.96	1.82
1	D	539	CYS	CB-SG	8.13	1.96	1.82
1	A	223	PRO	CG-CD	7.02	1.73	1.50
1	B	223	PRO	CG-CD	7.00	1.73	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	PRO	CG-CD	7.00	1.73	1.50
1	D	223	PRO	CG-CD	6.98	1.73	1.50
1	D	523	THR	N-CA	-6.25	1.33	1.46
1	B	523	THR	N-CA	-6.25	1.33	1.46
1	C	523	THR	N-CA	-6.22	1.33	1.46
1	A	523	THR	N-CA	-6.22	1.33	1.46
1	B	522	LEU	N-CA	-5.99	1.34	1.46
1	C	522	LEU	N-CA	-5.98	1.34	1.46
1	A	522	LEU	N-CA	-5.98	1.34	1.46
1	D	18	PRO	N-CD	5.97	1.56	1.47
1	C	18	PRO	N-CD	5.95	1.56	1.47
1	D	522	LEU	N-CA	-5.95	1.34	1.46
1	B	18	PRO	N-CD	5.94	1.56	1.47
1	A	18	PRO	N-CD	5.90	1.56	1.47
1	A	530	CYS	CB-SG	5.51	1.91	1.82
1	C	530	CYS	CB-SG	5.49	1.91	1.82
1	D	530	CYS	CB-SG	5.49	1.91	1.82
1	B	530	CYS	CB-SG	5.46	1.91	1.82
1	C	499	THR	CA-CB	5.04	1.66	1.53
1	B	499	THR	CA-CB	5.02	1.66	1.53
1	A	499	THR	CA-CB	5.02	1.66	1.53
1	D	499	THR	CA-CB	5.01	1.66	1.53

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	520	PRO	CA-C-N	-13.29	87.95	117.20
1	B	520	PRO	CA-C-N	-13.27	88.00	117.20
1	C	520	PRO	CA-C-N	-13.27	88.00	117.20
1	A	520	PRO	CA-C-N	-13.25	88.04	117.20
1	D	235	ILE	N-CA-C	12.74	145.39	111.00
1	D	290	PHE	N-CA-C	12.74	145.39	111.00
1	A	290	PHE	N-CA-C	12.73	145.38	111.00
1	C	235	ILE	N-CA-C	12.73	145.38	111.00
1	B	235	ILE	N-CA-C	12.73	145.37	111.00
1	C	290	PHE	N-CA-C	12.73	145.37	111.00
1	B	290	PHE	N-CA-C	12.72	145.35	111.00
1	A	235	ILE	N-CA-C	12.71	145.32	111.00
1	B	374	ASP	N-CA-C	11.61	142.35	111.00
1	A	374	ASP	N-CA-C	11.60	142.32	111.00
1	C	374	ASP	N-CA-C	11.60	142.33	111.00
1	D	374	ASP	N-CA-C	11.60	142.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	PHE	C-N-CD	-11.54	95.21	120.60
1	C	17	PHE	C-N-CD	-11.54	95.22	120.60
1	A	17	PHE	C-N-CD	-11.53	95.24	120.60
1	D	17	PHE	C-N-CD	-11.53	95.25	120.60
1	B	398	SER	N-CA-C	11.37	141.71	111.00
1	D	398	SER	N-CA-C	11.38	141.71	111.00
1	A	398	SER	N-CA-C	11.37	141.69	111.00
1	C	398	SER	N-CA-C	11.36	141.66	111.00
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	C	465	PRO	C-N-CD	-11.04	96.31	120.60
1	D	465	PRO	C-N-CD	-11.04	96.32	120.60
1	A	465	PRO	C-N-CD	-11.01	96.38	120.60
1	D	222	ASP	CB-CG-OD2	10.09	127.38	118.30
1	C	222	ASP	CB-CG-OD2	10.06	127.36	118.30
1	B	222	ASP	CB-CG-OD2	10.04	127.33	118.30
1	A	222	ASP	CB-CG-OD2	10.02	127.31	118.30
1	A	236	GLY	N-CA-C	-9.99	88.13	113.10
1	B	236	GLY	N-CA-C	-9.99	88.14	113.10
1	D	236	GLY	N-CA-C	-9.97	88.17	113.10
1	B	230	VAL	C-N-CD	-9.97	98.66	120.60
1	C	236	GLY	N-CA-C	-9.97	88.18	113.10
1	C	230	VAL	C-N-CD	-9.94	98.72	120.60
1	D	230	VAL	C-N-CD	-9.94	98.74	120.60
1	A	230	VAL	C-N-CD	-9.94	98.74	120.60
1	A	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	B	376	ALA	N-CA-C	9.66	137.09	111.00
1	C	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	B	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	D	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	C	376	ALA	N-CA-C	9.65	137.07	111.00
1	D	376	ALA	N-CA-C	9.65	137.07	111.00
1	A	376	ALA	N-CA-C	9.65	137.05	111.00
1	B	522	LEU	CA-CB-CG	-9.38	93.73	115.30
1	A	522	LEU	CA-CB-CG	-9.38	93.74	115.30
1	D	522	LEU	CA-CB-CG	-9.37	93.75	115.30
1	C	522	LEU	CA-CB-CG	-9.36	93.78	115.30
1	A	520	PRO	N-CA-C	9.31	136.31	112.10
1	C	520	PRO	N-CA-C	9.31	136.30	112.10
1	A	223	PRO	N-CA-C	-9.30	87.92	112.10
1	B	520	PRO	N-CA-C	9.30	136.27	112.10
1	A	221	PHE	C-N-CA	-9.29	98.46	121.70
1	B	221	PHE	C-N-CA	-9.29	98.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	PHE	C-N-CA	-9.29	98.46	121.70
1	C	223	PRO	N-CA-C	-9.30	87.93	112.10
1	D	221	PHE	C-N-CA	-9.29	98.46	121.70
1	D	223	PRO	N-CA-C	-9.30	87.93	112.10
1	B	223	PRO	N-CA-C	-9.29	87.94	112.10
1	D	481	LEU	N-CA-C	-9.29	85.92	111.00
1	B	481	LEU	N-CA-C	-9.28	85.95	111.00
1	D	520	PRO	N-CA-C	9.28	136.23	112.10
1	C	481	LEU	N-CA-C	-9.28	85.96	111.00
1	A	481	LEU	N-CA-C	-9.26	85.99	111.00
1	D	481	LEU	CA-CB-CG	-8.76	95.14	115.30
1	B	481	LEU	CA-CB-CG	-8.76	95.15	115.30
1	A	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	C	481	LEU	CA-CB-CG	-8.74	95.19	115.30
1	D	289	ASP	C-N-CA	-8.44	100.61	121.70
1	B	289	ASP	C-N-CA	-8.43	100.63	121.70
1	C	289	ASP	C-N-CA	-8.43	100.64	121.70
1	A	289	ASP	C-N-CA	-8.42	100.65	121.70
1	C	516	ALA	N-CA-C	-8.36	88.42	111.00
1	A	516	ALA	N-CA-C	-8.35	88.45	111.00
1	B	516	ALA	N-CA-C	-8.35	88.45	111.00
1	D	516	ALA	N-CA-C	-8.35	88.46	111.00
1	C	222	ASP	C-N-CD	-8.20	102.56	120.60
1	A	222	ASP	C-N-CD	-8.20	102.56	120.60
1	B	222	ASP	C-N-CD	-8.19	102.58	120.60
1	D	222	ASP	C-N-CD	-8.19	102.58	120.60
1	B	290	PHE	CA-C-N	-8.19	99.19	117.20
1	A	290	PHE	CA-C-N	-8.18	99.20	117.20
1	D	290	PHE	CA-C-N	-8.18	99.21	117.20
1	C	290	PHE	CA-C-N	-8.17	99.22	117.20
1	B	46	PRO	C-N-CD	-8.05	102.89	120.60
1	A	46	PRO	C-N-CD	-8.03	102.94	120.60
1	D	46	PRO	C-N-CD	-8.03	102.94	120.60
1	C	46	PRO	C-N-CD	-8.02	102.95	120.60
1	C	233	ASN	N-CA-C	7.88	132.27	111.00
1	A	233	ASN	N-CA-C	7.87	132.26	111.00
1	D	233	ASN	N-CA-C	7.86	132.22	111.00
1	B	233	ASN	N-CA-C	7.86	132.21	111.00
1	D	336	VAL	N-CA-C	7.81	132.09	111.00
1	A	336	VAL	N-CA-C	7.81	132.09	111.00
1	B	336	VAL	N-CA-C	7.80	132.05	111.00
1	C	522	LEU	C-N-CA	-7.80	102.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LEU	C-N-CA	-7.79	102.23	121.70
1	C	336	VAL	N-CA-C	7.79	132.03	111.00
1	D	522	LEU	C-N-CA	-7.79	102.23	121.70
1	B	522	LEU	C-N-CA	-7.78	102.25	121.70
1	A	362	GLN	N-CA-C	-7.73	90.13	111.00
1	D	362	GLN	N-CA-C	-7.73	90.14	111.00
1	C	362	GLN	N-CA-C	-7.72	90.16	111.00
1	B	362	GLN	N-CA-C	-7.72	90.17	111.00
1	C	234	GLU	N-CA-C	-7.60	90.48	111.00
1	A	234	GLU	N-CA-C	-7.60	90.48	111.00
1	B	234	GLU	N-CA-C	-7.58	90.55	111.00
1	D	234	GLU	N-CA-C	-7.57	90.56	111.00
1	A	234	GLU	C-N-CA	7.43	140.28	121.70
1	D	234	GLU	C-N-CA	7.41	140.22	121.70
1	C	234	GLU	C-N-CA	7.40	140.21	121.70
1	B	234	GLU	C-N-CA	7.40	140.20	121.70
1	C	521	GLN	C-N-CA	-7.39	103.22	121.70
1	A	521	GLN	C-N-CA	-7.39	103.23	121.70
1	B	521	GLN	C-N-CA	-7.37	103.28	121.70
1	D	521	GLN	C-N-CA	-7.36	103.30	121.70
1	A	277	SER	N-CA-C	-7.21	91.53	111.00
1	D	277	SER	N-CA-C	-7.20	91.56	111.00
1	B	277	SER	N-CA-C	-7.19	91.59	111.00
1	C	277	SER	N-CA-C	-7.19	91.59	111.00
1	C	337	SER	N-CA-C	-7.19	91.59	111.00
1	D	337	SER	N-CA-C	-7.19	91.60	111.00
1	A	337	SER	N-CA-C	-7.18	91.62	111.00
1	B	337	SER	N-CA-C	-7.17	91.64	111.00
1	D	503	LYS	N-CA-C	7.03	129.97	111.00
1	C	503	LYS	N-CA-C	7.02	129.94	111.00
1	B	503	LYS	N-CA-C	7.01	129.92	111.00
1	A	503	LYS	N-CA-C	7.00	129.90	111.00
1	A	523	THR	N-CA-CB	-6.95	97.10	110.30
1	B	523	THR	N-CA-CB	-6.94	97.11	110.30
1	C	523	THR	N-CA-CB	-6.93	97.12	110.30
1	D	523	THR	N-CA-CB	-6.93	97.14	110.30
1	A	492	THR	N-CA-C	6.78	129.31	111.00
1	C	492	THR	N-CA-C	6.77	129.27	111.00
1	D	492	THR	N-CA-C	6.76	129.26	111.00
1	B	492	THR	N-CA-C	6.76	129.24	111.00
1	D	448	CYS	CA-CB-SG	-6.71	101.93	114.00
1	A	448	CYS	CA-CB-SG	-6.69	101.96	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	CYS	CA-CB-SG	-6.68	101.97	114.00
1	B	448	CYS	CA-CB-SG	-6.68	101.98	114.00
1	D	476	SER	N-CA-C	6.59	128.78	111.00
1	C	476	SER	N-CA-C	6.58	128.78	111.00
1	A	476	SER	N-CA-C	6.58	128.77	111.00
1	D	398	SER	C-N-CA	-6.58	105.24	121.70
1	A	398	SER	C-N-CA	-6.58	105.25	121.70
1	C	398	SER	C-N-CA	-6.58	105.25	121.70
1	B	398	SER	C-N-CA	-6.57	105.26	121.70
1	B	476	SER	N-CA-C	6.57	128.75	111.00
1	B	491	GLY	N-CA-C	6.55	129.47	113.10
1	D	491	GLY	N-CA-C	6.53	129.44	113.10
1	A	491	GLY	N-CA-C	6.53	129.41	113.10
1	C	525	VAL	N-CA-C	-6.53	93.38	111.00
1	C	491	GLY	N-CA-C	6.51	129.38	113.10
1	D	525	VAL	N-CA-C	-6.51	93.42	111.00
1	A	525	VAL	N-CA-C	-6.50	93.45	111.00
1	B	525	VAL	N-CA-C	-6.49	93.47	111.00
1	B	335	ALA	N-CA-C	-6.33	93.90	111.00
1	A	335	ALA	N-CA-C	-6.33	93.91	111.00
1	C	335	ALA	N-CA-C	-6.33	93.91	111.00
1	D	335	ALA	N-CA-C	-6.33	93.92	111.00
1	C	532	CYS	N-CA-C	6.32	128.06	111.00
1	D	532	CYS	N-CA-C	6.31	128.03	111.00
1	A	532	CYS	N-CA-C	6.30	128.00	111.00
1	B	532	CYS	N-CA-C	6.29	127.98	111.00
1	C	234	GLU	CA-C-N	-6.28	103.38	117.20
1	B	234	GLU	CA-C-N	-6.28	103.39	117.20
1	D	234	GLU	CA-C-N	-6.28	103.39	117.20
1	A	234	GLU	CA-C-N	-6.24	103.46	117.20
1	B	222	ASP	N-CA-C	6.16	127.64	111.00
1	A	222	ASP	N-CA-C	6.16	127.63	111.00
1	A	235	ILE	CA-C-N	-6.16	103.89	116.20
1	D	222	ASP	N-CA-C	6.16	127.62	111.00
1	C	222	ASP	N-CA-C	6.15	127.62	111.00
1	D	235	ILE	CA-C-N	-6.14	103.92	116.20
1	B	235	ILE	CA-C-N	-6.14	103.92	116.20
1	C	235	ILE	CA-C-N	-6.14	103.92	116.20
1	C	397	GLU	C-N-CA	-6.14	106.36	121.70
1	A	397	GLU	C-N-CA	-6.14	106.36	121.70
1	B	397	GLU	C-N-CA	-6.13	106.38	121.70
1	D	397	GLU	C-N-CA	-6.12	106.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	503	LYS	CB-CA-C	-6.11	98.19	110.40
1	B	18	PRO	CA-N-CD	-6.10	102.96	111.50
1	B	503	LYS	CB-CA-C	-6.09	98.22	110.40
1	C	18	PRO	CA-N-CD	-6.09	102.97	111.50
1	C	503	LYS	CB-CA-C	-6.09	98.22	110.40
1	A	503	LYS	CB-CA-C	-6.08	98.24	110.40
1	D	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	A	18	PRO	CA-N-CD	-6.08	102.99	111.50
1	D	502	LEU	N-CA-C	6.07	127.38	111.00
1	C	502	LEU	N-CA-C	6.06	127.36	111.00
1	B	502	LEU	N-CA-C	6.05	127.33	111.00
1	A	502	LEU	N-CA-C	6.05	127.33	111.00
1	A	2	TRP	N-CA-C	-6.03	94.71	111.00
1	D	2	TRP	N-CA-C	-6.03	94.73	111.00
1	B	2	TRP	N-CA-C	-6.01	94.76	111.00
1	C	2	TRP	N-CA-C	-6.01	94.76	111.00
1	D	374	ASP	C-N-CD	5.98	140.95	128.40
1	A	222	ASP	N-CA-CB	5.97	121.35	110.60
1	C	374	ASP	C-N-CD	5.97	140.94	128.40
1	D	222	ASP	N-CA-CB	5.96	121.33	110.60
1	A	374	ASP	C-N-CD	5.96	140.91	128.40
1	C	222	ASP	N-CA-CB	5.95	121.30	110.60
1	B	374	ASP	C-N-CD	5.94	140.88	128.40
1	B	222	ASP	N-CA-CB	5.94	121.29	110.60
1	C	364	ILE	N-CA-C	-5.92	95.00	111.00
1	A	364	ILE	N-CA-C	-5.92	95.03	111.00
1	D	364	ILE	N-CA-C	-5.91	95.04	111.00
1	B	364	ILE	N-CA-C	-5.91	95.05	111.00
1	D	382	ASN	N-CA-C	-5.84	95.22	111.00
1	C	376	ALA	CA-C-N	-5.84	104.35	117.20
1	B	382	ASN	N-CA-C	-5.84	95.24	111.00
1	A	376	ALA	CA-C-N	-5.83	104.36	117.20
1	D	376	ALA	CA-C-N	-5.83	104.37	117.20
1	A	382	ASN	N-CA-C	-5.83	95.27	111.00
1	C	382	ASN	N-CA-C	-5.83	95.27	111.00
1	B	376	ALA	CA-C-N	-5.81	104.42	117.20
1	B	471	TYR	N-CA-C	5.74	126.50	111.00
1	C	471	TYR	N-CA-C	5.73	126.47	111.00
1	D	471	TYR	N-CA-C	5.72	126.45	111.00
1	A	471	TYR	N-CA-C	5.72	126.45	111.00
1	B	481	LEU	CA-C-N	-5.70	104.65	117.20
1	C	481	LEU	CA-C-N	-5.70	104.65	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	LEU	CA-C-N	-5.70	104.66	117.20
1	D	481	LEU	CA-C-N	-5.70	104.67	117.20
1	D	374	ASP	C-N-CA	-5.67	98.17	122.00
1	C	374	ASP	C-N-CA	-5.67	98.19	122.00
1	B	374	ASP	C-N-CA	-5.67	98.21	122.00
1	A	374	ASP	C-N-CA	-5.66	98.21	122.00
1	A	403	ASN	N-CA-C	-5.64	95.78	111.00
1	B	403	ASN	N-CA-C	-5.63	95.80	111.00
1	D	403	ASN	N-CA-C	-5.63	95.80	111.00
1	C	403	ASN	N-CA-C	-5.63	95.81	111.00
1	B	221	PHE	CA-C-N	5.58	129.48	117.20
1	A	221	PHE	CA-C-N	5.57	129.46	117.20
1	D	505	GLY	N-CA-C	5.57	127.03	113.10
1	C	505	GLY	N-CA-C	5.57	127.03	113.10
1	C	221	PHE	CA-C-N	5.56	129.43	117.20
1	D	221	PHE	CA-C-N	5.56	129.43	117.20
1	B	505	GLY	N-CA-C	5.55	126.98	113.10
1	D	502	LEU	CB-CA-C	-5.54	99.67	110.20
1	A	505	GLY	N-CA-C	5.54	126.95	113.10
1	B	502	LEU	CB-CA-C	-5.54	99.68	110.20
1	A	502	LEU	CB-CA-C	-5.53	99.69	110.20
1	C	502	LEU	CB-CA-C	-5.53	99.69	110.20
1	D	157	GLU	C-N-CD	-5.47	108.56	120.60
1	A	157	GLU	C-N-CD	-5.47	108.57	120.60
1	C	157	GLU	C-N-CD	-5.47	108.57	120.60
1	B	157	GLU	C-N-CD	-5.45	108.60	120.60
1	B	519	ASN	N-CA-C	5.37	125.49	111.00
1	D	519	ASN	N-CA-C	5.36	125.48	111.00
1	C	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	519	ASN	N-CA-C	5.34	125.42	111.00
1	A	405	THR	N-CA-C	5.32	125.36	111.00
1	C	405	THR	N-CA-C	5.32	125.36	111.00
1	B	405	THR	N-CA-C	5.32	125.35	111.00
1	D	405	THR	N-CA-C	5.32	125.35	111.00
1	C	367	LEU	CA-CB-CG	-5.31	103.08	115.30
1	D	367	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	367	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	367	LEU	CA-CB-CG	-5.28	103.15	115.30
1	B	521	GLN	N-CA-C	-5.21	96.94	111.00
1	D	521	GLN	N-CA-C	-5.21	96.94	111.00
1	C	521	GLN	N-CA-C	-5.20	96.95	111.00
1	A	521	GLN	N-CA-C	-5.20	96.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	PHE	O-C-N	5.20	131.01	122.70
1	A	290	PHE	O-C-N	5.19	131.00	122.70
1	A	520	PRO	C-N-CA	5.18	134.65	121.70
1	B	290	PHE	O-C-N	5.17	130.98	122.70
1	C	532	CYS	N-CA-CB	-5.17	101.29	110.60
1	B	520	PRO	C-N-CA	5.17	134.62	121.70
1	C	290	PHE	O-C-N	5.17	130.97	122.70
1	C	520	PRO	C-N-CA	5.17	134.61	121.70
1	D	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	A	532	CYS	N-CA-CB	-5.15	101.33	110.60
1	D	520	PRO	C-N-CA	5.14	134.54	121.70
1	B	18	PRO	CA-CB-CG	-5.13	94.26	104.00
1	B	532	CYS	N-CA-CB	-5.13	101.37	110.60
1	A	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	B	339	VAL	N-CA-C	5.12	124.83	111.00
1	D	18	PRO	CA-CB-CG	-5.12	94.27	104.00
1	C	339	VAL	N-CA-C	5.12	124.82	111.00
1	C	522	LEU	N-CA-C	-5.12	97.18	111.00
1	A	522	LEU	N-CA-C	-5.12	97.19	111.00
1	B	522	LEU	N-CA-C	-5.12	97.19	111.00
1	A	339	VAL	N-CA-C	5.11	124.81	111.00
1	D	522	LEU	N-CA-C	-5.11	97.21	111.00
1	D	339	VAL	N-CA-C	5.10	124.77	111.00
1	C	18	PRO	CA-CB-CG	-5.09	94.32	104.00
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	C	16	PRO	C-N-CA	-5.07	109.03	121.70
1	B	16	PRO	C-N-CA	-5.07	109.03	121.70
1	D	16	PRO	C-N-CA	-5.06	109.06	121.70
1	C	470	PRO	N-CA-C	5.03	125.19	112.10
1	C	332	PHE	N-CA-C	-5.03	97.42	111.00
1	D	332	PHE	N-CA-C	-5.03	97.42	111.00
1	B	470	PRO	N-CA-C	5.03	125.17	112.10
1	A	332	PHE	N-CA-C	-5.03	97.42	111.00
1	C	221	PHE	N-CA-C	5.03	124.57	111.00
1	B	332	PHE	N-CA-C	-5.03	97.43	111.00
1	B	221	PHE	N-CA-C	5.02	124.56	111.00
1	A	221	PHE	N-CA-C	5.02	124.55	111.00
1	A	539	CYS	N-CA-C	5.02	124.55	111.00
1	D	470	PRO	N-CA-C	5.02	125.15	112.10
1	B	539	CYS	N-CA-C	5.01	124.54	111.00
1	D	539	CYS	N-CA-C	5.01	124.54	111.00
1	D	221	PHE	N-CA-C	5.01	124.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	539	CYS	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain
1	B	18	PRO	Mainchain
1	B	222	ASP	Mainchain
1	B	520	PRO	Mainchain
1	C	17	PHE	Sidechain
1	C	18	PRO	Mainchain
1	C	222	ASP	Mainchain
1	C	520	PRO	Mainchain
1	D	17	PHE	Sidechain
1	D	18	PRO	Mainchain
1	D	222	ASP	Mainchain
1	D	520	PRO	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4191	0	4089	794	0
1	B	4191	0	4081	861	0
1	C	4191	0	4078	1114	0
1	D	4191	0	4082	1110	0
2	A	154	0	142	84	0
2	B	154	0	142	81	0
2	C	154	0	143	83	0
2	D	154	0	143	83	0
3	A	56	0	52	16	0
3	B	56	0	52	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	56	0	52	15	0
3	D	56	0	52	17	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
4	D	12	0	0	0	0
All	All	17652	0	17108	3282	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 95.

All (3282) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HB	1:D:2:TRP:CE2	1.18	1.70
1:C:87:PRO:HG3	1:D:43:ALA:CB	1.22	1.65
1:C:87:PRO:CG	1:D:43:ALA:CB	1.77	1.61
1:C:87:PRO:HG3	1:D:43:ALA:CA	1.16	1.58
1:D:464:ILE:HD12	1:D:465:PRO:CD	1.29	1.58
1:C:81:VAL:HG21	1:D:45:ASN:CB	1.32	1.55
1:C:87:PRO:CA	1:D:43:ALA:HB2	1.12	1.55
1:C:81:VAL:CG2	1:D:45:ASN:CB	1.80	1.54
1:A:24:ILE:CB	1:D:2:TRP:CE2	1.91	1.54
1:B:83:GLU:HB2	1:C:25:LYS:CD	1.10	1.54
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.54
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.54
1:C:81:VAL:HG12	1:D:43:ALA:CB	1.33	1.53
1:C:83:GLU:HA	1:D:41:GLN:CD	1.24	1.53
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.53
1:C:81:VAL:CG1	1:D:43:ALA:HB3	1.40	1.52
1:B:31:PHE:HE1	1:D:75:VAL:CG1	1.22	1.50
1:C:1:ASP:HA	1:D:89:GLU:CD	1.21	1.48
1:B:83:GLU:CB	1:C:25:LYS:CD	1.87	1.48
1:B:33:LYS:N	1:C:25:LYS:HE2	1.26	1.47
1:C:27:ASN:HD22	1:D:93:GLU:CB	1.26	1.46
1:A:24:ILE:CB	1:D:2:TRP:NE1	1.77	1.46
1:C:32:ASN:H	1:D:75:VAL:CG2	1.24	1.45
1:C:79:HIS:CA	1:D:39:THR:HG21	1.24	1.45
1:A:1:ASP:N	1:B:94:ILE:HD11	1.18	1.45
1:C:87:PRO:CG	1:D:43:ALA:HA	1.38	1.43
1:B:31:PHE:N	1:C:30:ARG:HB2	1.31	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:ILE:CD1	1:C:465:PRO:HD2	1.50	1.42
1:C:79:HIS:HA	1:D:39:THR:CG2	1.09	1.41
1:A:2:TRP:CE2	1:B:80:ALA:CB	1.76	1.41
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.40
1:D:464:ILE:CD1	1:D:465:PRO:HD2	1.50	1.40
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.40
1:C:85:GLY:CA	1:D:42:GLY:N	1.83	1.38
1:B:31:PHE:HA	1:C:30:ARG:CA	1.54	1.38
1:C:81:VAL:CG2	1:D:45:ASN:HB2	0.91	1.37
1:C:83:GLU:HA	1:D:41:GLN:NE2	1.06	1.37
1:C:87:PRO:CD	1:D:43:ALA:HA	1.55	1.37
1:B:89:GLU:HA	1:D:1:ASP:CB	1.34	1.36
1:C:87:PRO:CA	1:D:43:ALA:CB	2.02	1.36
1:B:31:PHE:HA	1:C:30:ARG:N	1.38	1.35
1:A:9:VAL:C	1:D:30:ARG:HD3	1.44	1.35
1:C:1:ASP:N	1:D:28:LYS:HD3	1.37	1.34
1:C:83:GLU:CA	1:D:41:GLN:NE2	1.90	1.33
1:A:90:GLU:HB3	1:B:3:VAL:C	1.46	1.33
1:B:31:PHE:CE1	1:D:75:VAL:CG1	2.12	1.33
1:B:31:PHE:CE1	1:D:75:VAL:HG11	1.64	1.33
1:A:2:TRP:CD2	1:B:80:ALA:HB2	1.29	1.33
1:C:1:ASP:CA	1:D:89:GLU:CD	1.96	1.32
1:B:89:GLU:CA	1:D:1:ASP:CB	1.87	1.32
1:A:24:ILE:HB	1:D:2:TRP:NE1	1.02	1.32
1:C:90:GLU:HB3	1:D:79:HIS:O	1.28	1.31
1:C:1:ASP:O	1:D:28:LYS:NZ	1.63	1.31
1:C:87:PRO:CB	1:D:43:ALA:CB	2.09	1.31
1:C:27:ASN:ND2	1:D:93:GLU:CB	1.91	1.31
1:C:81:VAL:HG22	1:D:45:ASN:ND2	1.42	1.30
1:C:32:ASN:N	1:D:75:VAL:HG21	1.43	1.30
1:C:79:HIS:CB	1:D:44:ASP:OD1	1.81	1.29
1:C:85:GLY:HA2	1:D:42:GLY:N	1.40	1.28
1:C:32:ASN:N	1:D:75:VAL:CG2	1.92	1.27
1:A:2:TRP:CE2	1:B:80:ALA:HB2	0.95	1.27
1:A:4:ILE:CA	1:B:91:PRO:N	1.97	1.26
1:C:84:ASN:HB2	1:D:74:TYR:CE1	1.44	1.25
1:B:89:GLU:HA	1:D:1:ASP:CG	0.94	1.24
1:C:28:LYS:O	1:D:75:VAL:HG13	1.07	1.24
1:C:28:LYS:O	1:D:75:VAL:CG1	1.86	1.24
1:B:83:GLU:HB2	1:C:25:LYS:CG	1.53	1.23
1:A:91:PRO:N	1:B:3:VAL:HG22	1.51	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HA	1:B:91:PRO:N	1.20	1.23
1:B:30:ARG:C	1:C:30:ARG:HB2	1.58	1.23
1:C:4:ILE:CG2	1:D:87:PRO:HG2	1.69	1.23
1:C:87:PRO:N	1:D:43:ALA:HB2	1.52	1.22
1:C:90:GLU:OE1	1:D:53:ILE:CD1	1.85	1.22
1:B:33:LYS:H	1:C:25:LYS:CE	1.52	1.22
1:A:2:TRP:CD2	1:B:80:ALA:CB	2.04	1.22
1:A:4:ILE:HA	1:B:90:GLU:C	1.59	1.22
1:C:1:ASP:HA	1:D:89:GLU:OE2	1.37	1.21
1:C:85:GLY:CA	1:D:42:GLY:CA	1.77	1.21
1:C:540:GLN:CD	1:C:540:GLN:O	1.79	1.21
1:C:87:PRO:CG	1:D:43:ALA:CA	1.85	1.20
1:B:86:SER:CA	1:D:90:GLU:HG3	1.62	1.20
1:C:84:ASN:HB2	1:D:74:TYR:CZ	1.43	1.20
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.19
1:A:540:GLN:CD	1:A:540:GLN:O	1.79	1.19
1:C:31:PHE:HB2	1:D:95:THR:CG2	1.72	1.19
1:C:90:GLU:CA	1:D:79:HIS:H	1.53	1.19
1:B:32:ASN:HB2	1:C:29:ASP:OD2	1.41	1.19
1:B:83:GLU:N	1:C:25:LYS:HD3	1.56	1.19
1:C:84:ASN:CB	1:D:74:TYR:CE1	2.15	1.19
1:C:79:HIS:HB2	1:D:44:ASP:OD1	1.40	1.18
1:C:31:PHE:CB	1:D:95:THR:HG23	1.72	1.18
1:B:31:PHE:HE2	1:C:26:SER:O	1.25	1.18
1:D:450:GLN:HG2	1:D:532:CYS:O	1.43	1.18
1:C:450:GLN:HG2	1:C:532:CYS:O	1.43	1.18
1:D:540:GLN:CD	1:D:540:GLN:O	1.79	1.18
1:D:8:LYS:H	1:D:8:LYS:HD2	1.04	1.18
1:C:89:GLU:OE1	1:D:78:SER:OG	1.56	1.17
1:D:474:SER:HB2	1:D:512:LEU:HG	1.25	1.17
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.17
1:B:89:GLU:CA	1:D:1:ASP:HB2	1.41	1.16
1:D:482:THR:HG23	1:D:499:THR:CG2	1.75	1.16
1:D:423:THR:HB	2:D:810:NAG:C7	1.76	1.16
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.75	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.16
1:C:87:PRO:CD	1:D:43:ALA:CA	2.16	1.16
1:B:83:GLU:CB	1:C:25:LYS:HD2	1.55	1.16
1:C:1:ASP:N	1:D:88:VAL:HG12	1.61	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:THR:HG23	1:C:499:THR:CG2	1.75	1.16
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.16
1:D:234:GLU:H	1:D:235:ILE:HG23	1.08	1.16
1:C:35:TYR:O	1:D:45:ASN:ND2	1.76	1.15
1:D:338:ARG:HD3	1:D:352:ILE:HG22	1.26	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:C:469:TYR:CG	1:C:470:PRO:HD2	1.81	1.15
1:D:469:TYR:CG	1:D:470:PRO:HD2	1.80	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.43	1.15
1:C:83:GLU:CA	1:D:41:GLN:CD	2.11	1.15
1:C:91:PRO:CB	1:D:37:SER:OG	1.93	1.15
1:B:31:PHE:CA	1:C:30:ARG:N	2.08	1.14
1:C:87:PRO:CB	1:D:43:ALA:HB1	1.72	1.14
1:C:87:PRO:CB	1:D:43:ALA:HB2	1.75	1.14
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.14
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.14
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.13
1:C:8:LYS:HD2	1:C:8:LYS:H	1.04	1.13
1:B:30:ARG:C	1:C:30:ARG:CB	2.16	1.13
1:B:32:ASN:CB	1:C:29:ASP:OD2	1.96	1.13
1:C:81:VAL:HG23	1:D:45:ASN:HB2	1.28	1.13
1:C:84:ASN:CB	1:D:74:TYR:CZ	2.23	1.13
1:A:9:VAL:C	1:D:30:ARG:CD	2.18	1.13
1:B:89:GLU:CA	1:D:1:ASP:CG	1.90	1.12
1:B:84:ASN:OD1	1:C:26:SER:CA	1.85	1.12
1:C:93:GLU:OE2	1:D:85:GLY:HA2	1.43	1.12
1:C:27:ASN:ND2	1:D:93:GLU:HB3	1.58	1.12
1:C:79:HIS:CA	1:D:39:THR:CG2	1.84	1.12
1:D:32:ASN:HD21	1:D:83:GLU:HB2	0.98	1.12
1:A:8:LYS:HD2	1:A:8:LYS:H	1.04	1.12
1:C:31:PHE:HB2	1:D:95:THR:HG21	1.32	1.12
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.12
1:B:89:GLU:N	1:D:1:ASP:HB2	1.65	1.11
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.11
1:C:31:PHE:HB3	1:D:75:VAL:HG22	1.23	1.11
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.11
1:B:83:GLU:H	1:C:25:LYS:HD3	0.97	1.11
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.11
1:D:154:ASP:C	2:D:801:NAG:H82	1.70	1.11
1:A:1:ASP:N	1:B:94:ILE:CD1	2.13	1.11
1:A:90:GLU:HB3	1:B:3:VAL:CA	1.70	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:SER:HB2	1:C:512:LEU:HG	1.25	1.10
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.10
1:B:83:GLU:CG	1:C:25:LYS:HD2	1.82	1.10
1:A:90:GLU:HG3	1:B:3:VAL:HG23	1.24	1.10
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.10
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.10
1:C:90:GLU:OE2	1:D:53:ILE:CG2	2.00	1.09
1:C:91:PRO:CA	1:D:37:SER:OG	1.81	1.09
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.09
1:C:86:SER:N	1:D:42:GLY:HA3	0.97	1.09
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:C:222:ASP:O	1:C:222:ASP:OD1	1.69	1.09
1:B:86:SER:CA	1:D:90:GLU:CA	2.30	1.09
1:D:482:THR:HG23	1:D:499:THR:HG22	1.09	1.09
1:C:227:THR:HG21	2:C:807:NAG:C8	1.82	1.09
1:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.09
1:A:9:VAL:CA	1:D:30:ARG:HD3	1.83	1.09
1:C:482:THR:HG23	1:C:499:THR:HG22	1.09	1.09
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.09
1:C:32:ASN:HD21	1:C:83:GLU:HB2	0.98	1.08
1:D:227:THR:HG21	2:D:807:NAG:C8	1.82	1.08
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.08
1:C:234:GLU:H	1:C:235:ILE:HG23	1.08	1.08
1:C:31:PHE:CB	1:D:95:THR:CG2	2.29	1.08
1:B:8:LYS:HD2	1:B:8:LYS:H	1.04	1.08
1:D:222:ASP:OD1	1:D:222:ASP:O	1.69	1.08
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.08
1:D:301:THR:HG21	2:D:805:NAG:H82	1.29	1.08
1:B:33:LYS:N	1:C:25:LYS:CE	2.13	1.08
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.07
1:C:87:PRO:HA	1:D:43:ALA:HB2	1.11	1.07
1:C:31:PHE:CE2	1:D:74:TYR:N	2.21	1.07
1:C:90:GLU:OE1	1:D:53:ILE:HD13	0.90	1.07
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.07
1:B:31:PHE:CA	1:C:30:ARG:HB2	1.85	1.07
1:C:29:ASP:HA	1:D:75:VAL:HG11	1.31	1.07
1:C:450:GLN:CG	1:C:532:CYS:O	2.03	1.07
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.07
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.07
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.54	1.07
1:C:89:GLU:N	1:D:38:ILE:HG13	1.69	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PRO:HD3	1:D:43:ALA:HA	1.32	1.06
1:C:81:VAL:HG22	1:D:45:ASN:CG	1.74	1.06
1:A:450:GLN:CG	1:A:532:CYS:O	2.02	1.06
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.06
1:C:1:ASP:H2	1:D:88:VAL:CG1	1.66	1.06
1:B:450:GLN:CG	1:B:532:CYS:O	2.03	1.06
1:C:4:ILE:HG22	1:D:87:PRO:HB2	1.38	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:C:485:ALA:O	1:C:486:GLU:HG2	1.54	1.06
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.06
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.06
1:D:290:PHE:HB2	1:D:292:LEU:N	1.69	1.06
1:A:485:ALA:O	1:A:486:GLU:HG2	1.55	1.06
1:D:469:TYR:CD1	1:D:470:PRO:HD2	1.91	1.06
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:A:24:ILE:CA	1:D:2:TRP:CE2	2.23	1.05
1:C:84:ASN:C	1:D:74:TYR:CE2	2.28	1.05
1:D:450:GLN:CG	1:D:532:CYS:O	2.03	1.05
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.92	1.05
1:D:335:ALA:HB1	3:D:811:NDG:O6	1.54	1.05
1:B:485:ALA:O	1:B:486:GLU:HG2	1.55	1.05
1:C:81:VAL:HG21	1:D:45:ASN:CA	1.87	1.05
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.05
1:C:335:ALA:HB1	3:C:811:NDG:O6	1.54	1.05
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:C:31:PHE:HE2	1:D:73:LYS:C	1.50	1.04
1:A:8:LYS:HE3	1:D:28:LYS:HG3	1.39	1.04
1:C:82:SER:CB	1:D:75:VAL:H	1.70	1.04
1:A:3:VAL:HG22	1:B:78:SER:H	1.21	1.04
1:C:522:LEU:HD22	1:C:523:THR:HB	1.39	1.04
1:D:485:ALA:O	1:D:486:GLU:HG2	1.54	1.04
1:B:84:ASN:ND2	1:D:91:PRO:HB2	1.71	1.04
1:C:31:PHE:CG	1:D:95:THR:HG23	1.92	1.04
1:C:87:PRO:HG3	1:D:43:ALA:HB1	1.17	1.04
1:C:90:GLU:OE2	1:D:53:ILE:HG21	1.57	1.04
1:B:31:PHE:CE2	1:C:26:SER:O	2.09	1.04
1:C:90:GLU:CB	1:D:79:HIS:O	2.05	1.04
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.92	1.04
1:A:24:ILE:HA	1:D:2:TRP:CG	1.60	1.04
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.04
1:C:87:PRO:CG	1:D:43:ALA:HB1	1.61	1.04
1:D:464:ILE:CD1	1:D:465:PRO:CD	2.20	1.04
1:D:522:LEU:HD22	1:D:523:THR:HB	1.39	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:C:482:THR:HG21	1:C:499:THR:H	1.23	1.04
1:C:81:VAL:HG11	1:D:45:ASN:H	1.21	1.03
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.03
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	1.03
1:C:482:THR:CG2	1:C:499:THR:N	2.22	1.03
1:A:1:ASP:H2	1:B:94:ILE:HD11	1.20	1.02
1:B:84:ASN:OD1	1:C:26:SER:C	1.96	1.02
1:D:482:THR:CG2	1:D:499:THR:N	2.22	1.02
1:B:83:GLU:CB	1:C:25:LYS:HD3	1.76	1.02
1:C:90:GLU:N	1:D:79:HIS:N	2.07	1.02
1:C:450:GLN:HB2	1:C:533:GLU:HA	1.41	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:D:403:ASN:HB2	3:D:902:NDG:C8	1.90	1.02
1:C:403:ASN:HB2	3:C:902:NDG:C8	1.90	1.02
1:C:337:SER:HA	1:C:427:ILE:HG23	1.38	1.02
1:C:81:VAL:HG22	1:D:45:ASN:HD22	1.02	1.02
1:C:90:GLU:N	1:D:79:HIS:H	1.54	1.02
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.02
1:C:290:PHE:HB2	1:C:292:LEU:H	0.88	1.02
1:C:1:ASP:N	1:D:88:VAL:CG1	2.21	1.01
1:C:81:VAL:CG1	1:D:44:ASP:H	1.73	1.01
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.01
1:B:403:ASN:HB2	3:B:902:NDG:C8	1.90	1.01
1:C:81:VAL:HG11	1:D:44:ASP:N	1.75	1.01
1:C:82:SER:HB3	1:D:75:VAL:H	1.23	1.01
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.01
1:B:290:PHE:HB2	1:B:292:LEU:H	0.88	1.01
1:A:24:ILE:HB	1:D:2:TRP:CZ2	1.96	1.01
1:D:290:PHE:HB2	1:D:292:LEU:H	0.88	1.01
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:A:403:ASN:HB2	3:A:902:NDG:C8	1.90	1.01
1:C:79:HIS:CB	1:D:39:THR:CG2	2.37	1.01
1:C:89:GLU:OE1	1:D:78:SER:N	1.75	1.01
1:C:93:GLU:H	1:D:81:VAL:HG11	1.25	1.01
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ASP:O	1:D:278:ASN:HA	1.61	1.01
1:C:4:ILE:HG22	1:D:87:PRO:CB	1.90	1.00
1:C:32:ASN:N	1:D:75:VAL:HG23	1.76	1.00
1:B:31:PHE:N	1:C:30:ARG:CB	2.24	1.00
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.00
1:D:337:SER:HA	1:D:427:ILE:HG23	1.38	1.00
1:C:81:VAL:HG22	1:D:45:ASN:HB2	1.32	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:B:86:SER:HA	1:D:90:GLU:CA	1.39	1.00
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	1.00
1:A:523:THR:HG23	1:A:524:VAL:H	1.27	1.00
1:C:523:THR:HG23	1:C:524:VAL:H	1.26	1.00
1:D:432:ASP:OD2	1:D:464:ILE:HG22	1.60	1.00
1:C:1:ASP:H2	1:D:88:VAL:HG12	0.84	0.99
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	0.99
1:C:93:GLU:CB	1:D:81:VAL:HG11	1.92	0.99
1:B:31:PHE:HE2	1:C:26:SER:C	1.65	0.99
1:C:79:HIS:CB	1:D:39:THR:HG22	1.93	0.99
1:C:90:GLU:CB	1:D:79:HIS:H	1.74	0.99
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.99
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:C:4:ILE:CG2	1:D:87:PRO:CG	2.41	0.99
1:D:450:GLN:HB2	1:D:533:GLU:HA	1.41	0.99
1:D:188:THR:HG23	1:D:208:ILE:HG12	1.43	0.99
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.99
1:D:482:THR:HG21	1:D:499:THR:H	1.23	0.99
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.98
1:B:31:PHE:HA	1:C:30:ARG:CB	1.92	0.98
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	0.98
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.98
1:A:10:SER:N	1:D:30:ARG:CD	2.27	0.98
1:C:2:TRP:H	1:D:89:GLU:HA	1.23	0.98
1:C:1:ASP:N	1:D:28:LYS:CD	2.25	0.98
1:B:82:SER:HB3	1:C:27:ASN:HB3	1.44	0.98
1:D:482:THR:CG2	1:D:499:THR:H	1.76	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:C:91:PRO:HA	1:D:79:HIS:CD2	1.96	0.98
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.98
1:B:30:ARG:O	1:C:30:ARG:HG3	1.64	0.97
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:THR:HG23	1:D:524:VAL:H	1.26	0.97
1:C:31:PHE:CG	1:D:95:THR:CG2	2.47	0.97
1:D:8:LYS:H	1:D:8:LYS:CD	1.74	0.97
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.97
1:B:86:SER:CA	1:D:90:GLU:CG	2.20	0.97
1:C:8:LYS:CD	1:C:8:LYS:H	1.74	0.97
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	0.97
1:B:87:PRO:HG2	1:C:2:TRP:HB2	1.45	0.97
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.97
1:D:320:THR:HG21	2:D:807:NAG:N2	1.78	0.97
1:C:80:ALA:HB3	1:D:77:SER:HB3	1.45	0.97
1:D:366:LYS:HG3	1:D:367:LEU:H	1.28	0.97
1:C:4:ILE:HG23	1:D:87:PRO:HG2	1.45	0.96
1:C:81:VAL:HG22	1:D:45:ASN:CB	1.78	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:C:27:ASN:HD22	1:D:93:GLU:HB2	0.80	0.96
1:C:87:PRO:HA	1:D:43:ALA:CB	1.77	0.96
1:C:32:ASN:HD21	1:C:83:GLU:CB	1.79	0.96
1:C:86:SER:HA	1:D:42:GLY:C	1.83	0.96
1:C:81:VAL:HG13	1:D:44:ASP:OD2	1.64	0.96
1:D:482:THR:HG21	1:D:499:THR:N	1.81	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.96
1:C:81:VAL:CG1	1:D:44:ASP:N	2.27	0.96
1:A:3:VAL:HG22	1:B:78:SER:N	1.79	0.96
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.96
1:B:31:PHE:CA	1:C:30:ARG:H	1.75	0.96
1:C:27:ASN:ND2	1:D:93:GLU:H	1.62	0.96
1:C:320:THR:HG21	2:C:807:NAG:HN2	1.31	0.96
1:B:83:GLU:HB2	1:C:25:LYS:HD2	0.96	0.95
1:C:31:PHE:HE2	1:D:74:TYR:N	1.59	0.95
1:C:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:A:24:ILE:HB	1:D:2:TRP:HE1	1.28	0.95
1:B:31:PHE:CB	1:C:30:ARG:H	1.79	0.95
1:C:88:VAL:HG12	1:D:94:ILE:HB	1.47	0.95
1:C:88:VAL:O	1:D:94:ILE:HD12	1.65	0.95
1:C:81:VAL:HB	1:D:41:GLN:C	1.86	0.95
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.95
1:A:2:TRP:NE1	1:B:80:ALA:HB2	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ASP:H2	1:D:28:LYS:HD3	0.96	0.95
1:A:24:ILE:CA	1:D:2:TRP:CG	2.39	0.95
1:B:86:SER:N	1:D:90:GLU:HG3	1.44	0.95
1:A:90:GLU:CB	1:B:3:VAL:C	2.35	0.95
1:A:2:TRP:C	1:B:92:MET:HB2	1.79	0.95
1:A:90:GLU:CG	1:B:3:VAL:HG23	1.96	0.95
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.95
1:B:31:PHE:HE1	1:D:75:VAL:HG11	0.78	0.94
1:D:235:ILE:CG1	1:D:287:GLY:HA2	1.96	0.94
1:C:87:PRO:CA	1:D:76:LEU:HD22	1.96	0.94
1:A:24:ILE:HA	1:D:2:TRP:CD1	2.02	0.94
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.94
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:A:1:ASP:H3	1:B:94:ILE:CD1	1.73	0.94
1:A:4:ILE:CA	1:B:90:GLU:C	2.33	0.94
1:C:87:PRO:C	1:D:76:LEU:HD22	1.88	0.94
1:A:89:GLU:OE1	1:B:2:TRP:HB3	1.65	0.94
1:C:289:ASP:O	1:C:290:PHE:HB3	1.67	0.94
1:D:366:LYS:CG	1:D:367:LEU:H	1.80	0.94
1:B:83:GLU:CA	1:C:25:LYS:HD3	1.97	0.94
1:C:91:PRO:CA	1:D:79:HIS:CD2	2.50	0.94
1:C:90:GLU:HB3	1:D:79:HIS:C	1.87	0.94
1:D:290:PHE:CB	1:D:292:LEU:H	1.79	0.94
1:D:227:THR:HG21	2:D:807:NAG:H83	1.48	0.94
1:A:8:LYS:CD	1:A:8:LYS:H	1.74	0.94
1:D:32:ASN:HD21	1:D:83:GLU:CB	1.79	0.94
1:C:290:PHE:CB	1:C:292:LEU:H	1.79	0.94
1:C:366:LYS:HG3	1:C:367:LEU:H	1.28	0.94
1:C:27:ASN:HD22	1:C:28:LYS:N	1.66	0.93
1:A:99:ILE:HG21	1:D:30:ARG:HH12	1.29	0.93
1:C:91:PRO:HB2	1:D:37:SER:OG	1.65	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.93
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.93
1:D:352:ILE:HG13	1:D:388:VAL:HB	1.51	0.93
1:C:352:ILE:HG13	1:C:388:VAL:HB	1.51	0.93
1:C:87:PRO:HD3	1:D:43:ALA:CA	1.92	0.93
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.93
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.93
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.83	0.93
1:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.93
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.93
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.93
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:A:24:ILE:CB	1:D:2:TRP:CD1	2.52	0.93
1:A:1:ASP:HA	1:B:24:ILE:HG21	1.51	0.93
1:A:24:ILE:CG2	1:D:2:TRP:NE1	2.32	0.92
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.92
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.92
1:D:195:ASP:HB2	1:D:201:LEU:H	1.34	0.92
1:B:32:ASN:CA	1:C:29:ASP:OD2	2.17	0.92
1:C:27:ASN:ND2	1:D:93:GLU:HB2	1.65	0.92
1:D:464:ILE:HD12	1:D:465:PRO:HD2	0.94	0.92
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.92
1:A:90:GLU:C	1:B:3:VAL:HG22	1.85	0.92
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.92
1:C:81:VAL:HB	1:D:41:GLN:CA	1.86	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:C:404:ASN:O	1:C:404:ASN:ND2	2.03	0.92
1:D:289:ASP:O	1:D:290:PHE:HB3	1.67	0.92
1:D:320:THR:HG21	2:D:807:NAG:HN2	1.31	0.92
1:C:86:SER:N	1:D:41:GLN:O	2.01	0.92
1:B:403:ASN:HB2	3:B:902:NDG:C7	2.00	0.92
1:D:27:ASN:HD22	1:D:28:LYS:N	1.66	0.92
1:D:446:THR:HG23	1:D:539:CYS:SG	2.10	0.92
1:B:31:PHE:CA	1:C:30:ARG:CB	2.48	0.92
1:C:88:VAL:HG22	1:D:76:LEU:HD23	1.47	0.92
1:D:396:ARG:HH22	1:D:464:ILE:HB	1.33	0.92
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.92
1:D:227:THR:HG21	2:D:807:NAG:C7	1.99	0.92
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:C:195:ASP:HB2	1:C:201:LEU:H	1.34	0.92
1:C:87:PRO:HD3	1:D:42:GLY:O	1.69	0.92
1:C:446:THR:HG23	1:C:539:CYS:SG	2.10	0.92
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	1.99	0.91
1:C:1:ASP:H3	1:D:88:VAL:HB	1.35	0.91
1:B:446:THR:HG23	1:B:539:CYS:SG	2.10	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASN:ND2	1:D:83:GLU:HB2	1.84	0.91
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.91
1:C:86:SER:H	1:D:74:TYR:HD2	1.16	0.91
1:A:403:ASN:HB2	3:A:902:NDG:C7	2.00	0.91
1:A:404:ASN:ND2	1:A:404:ASN:O	2.03	0.91
1:C:517:GLN:O	1:C:519:ASN:N	2.03	0.91
1:D:335:ALA:CB	3:D:811:NDG:O6	2.18	0.91
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.91
1:B:83:GLU:H	1:C:25:LYS:CD	1.84	0.91
1:C:1:ASP:O	1:D:28:LYS:CE	2.19	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.91
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.91
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.91
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.91
1:A:10:SER:N	1:D:30:ARG:HD3	1.86	0.91
1:C:90:GLU:CD	1:D:53:ILE:HG21	1.89	0.91
1:C:396:ARG:HH22	1:C:464:ILE:HB	1.33	0.91
1:C:403:ASN:HB2	3:C:902:NDG:C7	2.00	0.91
1:D:403:ASN:HB2	3:D:902:NDG:C7	2.00	0.91
1:B:83:GLU:CG	1:C:25:LYS:CD	2.45	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	2.00	0.91
1:B:31:PHE:CE2	1:C:26:SER:C	2.45	0.90
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.90
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.90
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.90
1:B:30:ARG:C	1:C:30:ARG:CG	2.31	0.90
1:D:234:GLU:N	1:D:235:ILE:HG23	1.86	0.90
2:D:805:NAG:O5	2:D:806:NAG:H83	1.71	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:C:79:HIS:HB3	1:D:44:ASP:OD1	1.70	0.90
1:D:8:LYS:HD2	1:D:8:LYS:N	1.87	0.90
1:D:517:GLN:O	1:D:519:ASN:N	2.03	0.90
1:C:87:PRO:CD	1:D:43:ALA:CB	2.48	0.90
1:C:1:ASP:HA	1:D:89:GLU:OE1	1.68	0.90
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.90
2:D:805:NAG:H62	2:D:806:NAG:C7	1.99	0.90
1:A:24:ILE:CB	1:D:2:TRP:CZ2	2.54	0.90
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.90
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASP:HA	1:D:429:HIS:HB3	1.53	0.90
1:D:404:ASN:ND2	1:D:404:ASN:O	2.03	0.90
1:C:374:ASP:O	1:C:375:PRO:C	2.06	0.90
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.90
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.90
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.90
1:C:234:GLU:N	1:C:235:ILE:HG23	1.86	0.90
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	0.90
1:C:90:GLU:OE2	1:D:53:ILE:HG23	1.72	0.89
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.89
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.89
1:C:81:VAL:CG2	1:D:45:ASN:HD22	1.85	0.89
1:D:449:ASP:H	1:D:532:CYS:HB3	1.37	0.89
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	0.89
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.89
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.89
1:C:93:GLU:H	1:D:81:VAL:CG1	1.86	0.89
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.89
1:D:154:ASP:HB3	1:D:155:PRO:HD2	1.54	0.89
1:D:523:THR:HG23	1:D:524:VAL:CG2	2.03	0.89
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.89
1:C:371:ILE:CD1	1:C:381:VAL:HG11	2.03	0.89
1:D:338:ARG:HD3	1:D:352:ILE:CG2	2.02	0.89
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.89
1:A:8:LYS:CE	1:D:28:LYS:HG3	2.03	0.89
1:D:464:ILE:HD12	1:D:465:PRO:HD3	1.53	0.89
1:D:518:ASN:O	1:D:520:PRO:HD3	1.72	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.89
1:A:4:ILE:HA	1:B:91:PRO:CD	1.94	0.89
1:B:85:GLY:C	1:D:91:PRO:HD2	1.92	0.89
1:B:31:PHE:CA	1:C:30:ARG:CA	2.49	0.89
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.89
1:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.89
1:D:221:PHE:HE1	1:D:315:SER:O	1.56	0.89
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.89
1:A:24:ILE:HG22	1:D:2:TRP:CD1	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:C:318:THR:HG21	2:C:806:NAG:H5	1.55	0.88
1:C:89:GLU:OE1	1:D:78:SER:CB	2.21	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:C:31:PHE:HB3	1:D:75:VAL:CG2	2.02	0.88
1:C:81:VAL:HG13	1:D:40:GLY:H	1.38	0.88
1:D:396:ARG:NH2	1:D:464:ILE:CG2	2.35	0.88
1:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.88
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.88
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.88
1:A:3:VAL:HG23	1:B:91:PRO:HB3	1.55	0.88
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.88
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.88
1:C:464:ILE:HD11	1:C:465:PRO:HD2	1.53	0.88
1:A:91:PRO:HA	1:B:1:ASP:O	1.73	0.88
1:C:482:THR:HG21	1:C:499:THR:N	1.81	0.88
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.88
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.88
1:D:378:TRP:HB2	1:D:379:LEU:HD23	1.53	0.88
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.88
1:C:449:ASP:H	1:C:532:CYS:HB3	1.37	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.88
1:C:483:TRP:CZ3	1:C:498:PRO:HG3	2.09	0.88
1:C:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.88
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.88
1:C:89:GLU:OE1	1:D:78:SER:CA	2.22	0.88
1:D:464:ILE:HD11	1:D:465:PRO:HD2	1.53	0.88
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.88
1:D:371:ILE:CD1	1:D:381:VAL:HG11	2.03	0.88
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.87
1:D:483:TRP:CZ3	1:D:498:PRO:HG3	2.09	0.87
1:D:333:VAL:HB	1:D:334:PRO:HD3	1.56	0.87
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.87
1:C:90:GLU:CD	1:D:53:ILE:HD13	1.95	0.87
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.87
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.87
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.87
1:D:441:SER:OG	1:D:442:PRO:HD3	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.87
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.87
1:C:35:TYR:HD2	1:D:45:ASN:OD1	1.55	0.86
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.86
1:D:374:ASP:O	1:D:375:PRO:C	2.06	0.86
1:C:81:VAL:CG1	1:D:45:ASN:H	1.87	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:C:221:PHE:HE1	1:C:315:SER:O	1.56	0.86
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.86
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:C:82:SER:HB3	1:D:75:VAL:N	1.89	0.86
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.86
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.86
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.86
1:A:99:ILE:HG21	1:D:30:ARG:NH1	1.90	0.86
1:C:91:PRO:CA	1:D:79:HIS:HD2	1.89	0.86
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.86
1:D:486:GLU:HB2	1:D:495:LEU:HB2	1.56	0.86
1:C:87:PRO:HD2	1:D:51:PHE:HB2	1.57	0.86
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.57	0.86
1:C:31:PHE:HE1	1:D:97:ASN:OD1	1.58	0.86
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.86
1:C:441:SER:OG	1:C:442:PRO:HD3	1.75	0.85
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.58	0.85
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.85
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.85
1:D:440:PRO:CD	1:D:522:LEU:HD12	2.05	0.85
1:D:523:THR:HG23	1:D:524:VAL:N	1.90	0.85
1:C:85:GLY:CA	1:D:42:GLY:HA2	1.70	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.85
1:D:257:ALA:O	1:D:273:THR:HG21	1.74	0.85
1:C:91:PRO:HA	1:D:79:HIS:HD2	1.40	0.85
1:D:423:THR:CB	2:D:810:NAG:C7	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	0.85
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:D:343:GLU:HB3	1:D:433:VAL:HG21	1.55	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:A:4:ILE:HG22	1:B:91:PRO:O	1.76	0.85
1:C:451:ASN:N	1:C:533:GLU:O	2.10	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:D:318:THR:HG21	2:D:806:NAG:H5	1.56	0.85
1:C:81:VAL:HG12	1:D:43:ALA:CA	2.07	0.85
1:C:90:GLU:CA	1:D:79:HIS:N	2.38	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.85
1:B:30:ARG:O	1:C:30:ARG:HA	1.77	0.85
1:C:31:PHE:O	1:D:73:LYS:HD3	1.77	0.85
1:C:87:PRO:HB3	1:D:43:ALA:HB1	1.56	0.85
1:D:464:ILE:HD12	1:D:465:PRO:N	1.91	0.85
1:D:483:TRP:HZ2	1:D:507:TYR:CE1	1.95	0.85
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.85
1:D:320:THR:HG21	2:D:807:NAG:C2	2.05	0.85
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.84
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.84
1:C:423:THR:CB	2:C:810:NAG:C7	2.54	0.84
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.84
1:D:155:PRO:HB2	2:D:801:NAG:H81	1.60	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.84
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.84
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.84
1:D:375:PRO:HB3	1:D:400:TYR:CE2	2.12	0.84
1:C:1:ASP:H2	1:D:28:LYS:CD	1.86	0.84
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:D:396:ARG:NE	1:D:432:ASP:HB2	1.93	0.84
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.84
1:C:440:PRO:HD2	1:C:522:LEU:HD12	1.59	0.84
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.84
1:D:230:VAL:O	1:D:324:GLU:N	2.11	0.84
1:C:1:ASP:CA	1:D:28:LYS:HD3	2.08	0.84
1:C:1:ASP:CA	1:D:89:GLU:OE2	2.16	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.84
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.84
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.83
1:C:464:ILE:HD12	1:C:465:PRO:N	1.92	0.83
1:D:438:PRO:HB3	1:D:471:TYR:HE2	1.41	0.83
1:A:147:SER:OG	1:A:167:ARG:HD2	1.78	0.83
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.83
1:A:87:PRO:O	1:B:2:TRP:CZ2	2.30	0.83
1:D:423:THR:CB	2:D:810:NAG:N2	2.42	0.83
1:B:32:ASN:CB	1:C:27:ASN:HA	2.07	0.83
1:C:448:CYS:O	1:C:452:PRO:HG3	1.79	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:D:448:CYS:O	1:D:452:PRO:HG3	1.78	0.83
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.83
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.83
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.83
1:C:483:TRP:HZ2	1:C:507:TYR:HE1	1.24	0.83
1:D:28:LYS:HD3	1:D:88:VAL:HG12	1.61	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:D:469:TYR:CG	1:D:470:PRO:CD	2.61	0.83
1:D:440:PRO:HD2	1:D:522:LEU:HD12	1.59	0.83
1:C:32:ASN:ND2	1:C:83:GLU:H	1.77	0.83
1:C:85:GLY:C	1:D:41:GLN:C	2.34	0.83
1:C:80:ALA:CB	1:D:39:THR:OG1	2.25	0.83
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:D:446:THR:HG21	1:D:537:ILE:O	1.79	0.83
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.44	0.82
1:A:289:ASP:OD2	1:A:289:ASP:O	1.97	0.82
1:B:540:GLN:OE1	1:B:540:GLN:O	1.97	0.82
1:A:540:GLN:O	1:A:540:GLN:OE1	1.97	0.82
1:D:451:ASN:N	1:D:533:GLU:O	2.10	0.82
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.82
1:C:87:PRO:HD3	1:D:42:GLY:C	2.00	0.82
1:D:482:THR:HG21	1:D:500:GLN:N	1.94	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:GLN:O	1:C:540:GLN:OE1	1.97	0.82
1:C:482:THR:HG21	1:C:500:GLN:N	1.94	0.82
1:D:235:ILE:HG13	1:D:287:GLY:HA2	1.58	0.82
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.82
1:D:423:THR:HB	2:D:810:NAG:N2	1.93	0.82
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.82
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:C:469:TYR:CG	1:C:470:PRO:CD	2.61	0.82
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.82
1:D:483:TRP:HZ2	1:D:507:TYR:HE1	1.24	0.82
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.82
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.82
1:D:289:ASP:OD2	1:D:289:ASP:O	1.97	0.81
1:D:32:ASN:ND2	1:D:83:GLU:H	1.77	0.81
1:D:277:SER:C	1:D:278:ASN:HD22	1.83	0.81
1:A:3:VAL:N	1:B:78:SER:O	2.12	0.81
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.81
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.60	0.81
1:C:85:GLY:HA3	1:D:42:GLY:HA2	1.62	0.81
1:C:87:PRO:HG3	1:D:43:ALA:C	2.00	0.81
1:C:85:GLY:CA	1:D:41:GLN:C	2.47	0.81
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.81
1:B:289:ASP:OD2	1:B:289:ASP:O	1.97	0.81
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.45	0.81
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.44	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.81
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.81
1:C:31:PHE:CE1	1:D:97:ASN:OD1	2.33	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:D:540:GLN:OE1	1:D:540:GLN:O	1.97	0.81
1:D:154:ASP:HB3	2:D:801:NAG:N2	1.95	0.81
1:D:496:LEU:HD21	1:D:509:ILE:HD13	1.63	0.81
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.81
1:A:90:GLU:HB3	1:B:3:VAL:O	1.80	0.81
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.81
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:TYR:CD2	1:D:470:PRO:HD2	2.16	0.81
1:C:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.81
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.81
1:C:290:PHE:CE2	1:C:293:ARG:HB2	2.16	0.81
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.81
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.81
1:B:30:ARG:C	1:C:30:ARG:HG3	1.96	0.81
1:D:517:GLN:C	1:D:519:ASN:H	1.84	0.81
1:C:486:GLU:O	1:C:494:MET:HA	1.81	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.81
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.81
1:B:86:SER:N	1:D:91:PRO:HD2	1.96	0.80
1:C:79:HIS:HB3	1:D:39:THR:HG22	1.63	0.80
1:C:84:ASN:HA	1:D:71:TYR:CD2	2.16	0.80
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.80
1:D:486:GLU:O	1:D:494:MET:HA	1.81	0.80
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.80
1:B:30:ARG:O	1:C:30:ARG:CG	2.29	0.80
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.80
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.80
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.80
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.80
1:C:86:SER:CA	1:D:42:GLY:C	2.46	0.80
1:C:93:GLU:N	1:D:81:VAL:HG11	1.96	0.80
1:C:299:GLN:HG2	1:C:318:THR:HG23	1.62	0.80
1:D:406:TYR:CD1	2:D:808:NAG:H83	2.17	0.80
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.80
1:D:265:GLU:HB3	1:D:268:PHE:HE2	1.46	0.80
1:C:222:ASP:C	1:C:222:ASP:OD1	2.20	0.80
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.80
1:A:396:ARG:HD3	1:A:431:LEU:C	2.02	0.80
1:C:540:GLN:CG	1:C:540:GLN:O	2.30	0.80
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.80
1:C:265:GLU:HB3	1:C:268:PHE:HE2	1.46	0.80
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.80
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.80
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.80
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:D:371:ILE:HD11	1:D:381:VAL:HG11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.80
1:C:1:ASP:H3	1:D:88:VAL:CB	1.95	0.80
1:D:234:GLU:H	1:D:235:ILE:CG2	1.92	0.80
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.80
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.79
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:C:35:TYR:CD2	1:D:45:ASN:OD1	2.35	0.79
1:C:87:PRO:CD	1:D:43:ALA:HB2	2.12	0.79
1:D:396:ARG:HH21	1:D:464:ILE:HG22	1.46	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.79
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.79
1:C:83:GLU:OE1	1:D:41:GLN:NE2	2.12	0.79
1:C:1:ASP:CB	1:D:89:GLU:CD	2.37	0.79
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.79
1:B:396:ARG:HD3	1:B:431:LEU:C	2.03	0.79
1:D:449:ASP:HB3	1:D:532:CYS:H	1.47	0.79
1:D:540:GLN:O	1:D:540:GLN:CG	2.30	0.79
1:D:290:PHE:CE2	1:D:293:ARG:HB2	2.16	0.79
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.79
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.79
1:B:27:ASN:C	1:B:27:ASN:HD22	1.85	0.79
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.79
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	0.79
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.79
1:C:85:GLY:HA2	1:D:42:GLY:H	1.45	0.79
2:D:904:NAG:H3	2:D:904:NAG:O7	1.82	0.79
1:D:127:VAL:HG13	1:D:128:MET:H	1.46	0.79
1:A:7:ILE:HG23	1:D:27:ASN:OD1	1.83	0.79
1:D:482:THR:OG1	1:D:500:GLN:HG2	1.82	0.79
2:D:809:NAG:H61	2:D:810:NAG:H62	1.65	0.79
1:D:154:ASP:HB3	2:D:801:NAG:HN2	1.44	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:A:24:ILE:CG1	1:D:2:TRP:CZ2	2.66	0.79
1:B:32:ASN:HB3	1:C:27:ASN:HA	1.64	0.79
1:C:27:ASN:ND2	1:D:93:GLU:N	2.30	0.79
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.79
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.79
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.79
1:D:154:ASP:CB	1:D:155:PRO:HD2	2.13	0.79
1:D:299:GLN:HG2	1:D:318:THR:HG23	1.62	0.79
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.79
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.31	0.79
2:B:904:NAG:H3	2:B:904:NAG:O7	1.82	0.79
1:A:1:ASP:HA	1:B:24:ILE:HD13	1.63	0.79
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.79
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.79
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.78
1:A:540:GLN:CG	1:A:540:GLN:O	2.30	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.31	0.78
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.78
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78
1:C:90:GLU:CB	1:D:79:HIS:N	2.45	0.78
1:D:232:GLU:HG3	1:D:290:PHE:N	1.98	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:D:396:ARG:HD3	1:D:431:LEU:C	2.03	0.78
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.78
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.78
1:A:24:ILE:CA	1:D:2:TRP:CD1	2.61	0.78
1:B:88:VAL:O	1:D:1:ASP:CB	2.32	0.78
1:D:432:ASP:OD2	1:D:464:ILE:CG2	2.30	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.78
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.78
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.78
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.78
1:C:93:GLU:HB2	1:D:81:VAL:HG11	1.64	0.78
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:D:222:ASP:OD1	1:D:222:ASP:C	2.20	0.78
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:D:365:GLN:HG3	1:D:365:GLN:O	1.82	0.78
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	0.78
1:C:482:THR:OG1	1:C:500:GLN:HG2	1.82	0.78
1:D:155:PRO:C	1:D:157:GLU:H	1.86	0.78
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.78
1:C:81:VAL:HG13	1:D:40:GLY:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.78
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
1:D:238:GLU:HA	1:D:283:THR:HG22	1.66	0.78
1:A:10:SER:HB2	1:D:30:ARG:HG3	1.64	0.78
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.78
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.78
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.78
1:D:27:ASN:HD22	1:D:27:ASN:C	1.85	0.77
1:C:82:SER:N	1:D:41:GLN:O	2.17	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.77
1:A:147:SER:OG	1:A:167:ARG:CG	2.32	0.77
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.77
1:C:523:THR:CG2	1:C:524:VAL:H	1.94	0.77
1:C:365:GLN:O	1:C:365:GLN:HG3	1.82	0.77
1:A:2:TRP:CG	1:B:80:ALA:HB2	2.16	0.77
1:D:223:PRO:HD2	1:D:226:TYR:OH	1.85	0.77
1:C:524:VAL:CG2	2:C:904:NAG:H81	2.14	0.77
2:C:904:NAG:H3	2:C:904:NAG:O7	1.82	0.77
1:D:485:ALA:O	1:D:486:GLU:CG	2.30	0.77
1:A:147:SER:OG	1:A:167:ARG:CD	2.32	0.77
1:A:24:ILE:HG13	1:D:2:TRP:CZ2	2.19	0.77
1:C:35:TYR:HD2	1:D:45:ASN:CG	1.86	0.77
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.77
1:D:524:VAL:CG2	2:D:904:NAG:H81	2.14	0.77
1:D:194:THR:HB	1:D:198:GLY:HA2	1.66	0.77
1:A:2:TRP:O	1:B:92:MET:HB2	1.83	0.77
1:C:86:SER:HA	1:D:42:GLY:O	1.84	0.77
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.77
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.77
1:B:31:PHE:HZ	1:C:34:VAL:HG21	1.49	0.77
1:C:90:GLU:OE2	1:D:36:TYR:C	2.17	0.77
1:C:86:SER:HB3	1:D:76:LEU:HD11	1.66	0.77
1:D:290:PHE:HZ	1:D:296:TYR:HH	1.30	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:C:194:THR:HB	1:C:198:GLY:HA2	1.67	0.77
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.77
1:D:195:ASP:HB3	1:D:200:GLY:HA3	1.65	0.77
1:B:30:ARG:O	1:C:30:ARG:CB	2.31	0.77
1:C:81:VAL:HG11	1:D:45:ASN:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.33	0.77
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.77
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.77
1:B:540:GLN:CG	1:B:540:GLN:O	2.30	0.77
1:A:194:THR:HB	1:A:198:GLY:HA2	1.67	0.77
1:B:86:SER:HA	1:D:90:GLU:HA	1.62	0.76
1:C:31:PHE:HA	1:D:73:LYS:NZ	2.00	0.76
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.76
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.76
1:D:272:THR:HG22	1:D:273:THR:H	1.51	0.76
1:D:290:PHE:HD2	1:D:293:ARG:H	1.28	0.76
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.67	0.76
1:D:505:GLY:C	1:D:506:ASP:OD1	2.23	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.76
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.76
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.76
1:D:368:SER:HG	1:D:370:PHE:HE1	1.33	0.76
1:C:396:ARG:HH21	1:C:464:ILE:CG2	1.98	0.76
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.76
1:D:241:ARG:HE	1:D:281:ILE:HD12	1.51	0.76
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.76
1:C:88:VAL:CG1	1:D:94:ILE:HB	2.15	0.76
1:A:90:GLU:N	1:B:2:TRP:HE3	1.83	0.76
1:D:440:PRO:HB3	1:D:457:LEU:HD21	1.67	0.76
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.76
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.76
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.98	0.76
1:A:24:ILE:CG2	1:D:2:TRP:CD1	2.67	0.76
1:C:4:ILE:HG21	1:D:87:PRO:HG2	1.68	0.76
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.76
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.76
1:D:362:GLN:O	1:D:364:ILE:HG23	1.85	0.76
1:C:88:VAL:C	1:D:38:ILE:HG13	2.05	0.76
1:D:432:ASP:CG	1:D:464:ILE:HG22	2.05	0.76
1:D:366:LYS:CG	1:D:367:LEU:N	2.48	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:D:156:GLU:HG3	1:D:160:PRO:HB3	1.66	0.76
1:B:501:GLN:HG2	1:B:501:GLN:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:SER:CB	1:C:27:ASN:HB3	2.15	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.76
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.76
1:D:371:ILE:HD12	1:D:410:MET:HB3	1.68	0.76
1:A:91:PRO:CA	1:B:1:ASP:O	2.34	0.76
1:D:196:LEU:HB2	1:D:199:ALA:HB3	1.67	0.76
1:D:448:CYS:SG	1:D:537:ILE:HG22	2.26	0.76
1:C:501:GLN:O	1:C:501:GLN:HG2	1.84	0.76
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.75
1:B:84:ASN:HD22	1:D:91:PRO:HB2	1.49	0.75
1:C:301:THR:HG21	2:C:805:NAG:C8	2.13	0.75
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:B:88:VAL:HG13	1:C:27:ASN:OD1	1.87	0.75
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.75
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.75
1:C:272:THR:HG22	1:C:273:THR:H	1.50	0.75
1:D:501:GLN:O	1:D:501:GLN:HG2	1.84	0.75
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.75
1:B:31:PHE:CE2	1:C:29:ASP:CB	2.68	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.27	0.75
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.75
1:D:290:PHE:CD2	1:D:293:ARG:N	2.55	0.75
1:B:194:THR:HB	1:B:198:GLY:HA2	1.67	0.75
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:D:449:ASP:HB3	1:D:532:CYS:N	2.02	0.75
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.75
1:C:290:PHE:HD2	1:C:293:ARG:H	1.28	0.75
1:A:5:PRO:HD2	1:B:90:GLU:OE2	1.87	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.74
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.74
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.74
1:D:523:THR:HG23	1:D:524:VAL:HG22	1.67	0.74
1:C:2:TRP:N	1:D:89:GLU:HA	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.74
1:A:272:THR:HG22	1:A:273:THR:H	1.50	0.74
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.74
1:A:3:VAL:HG23	1:B:91:PRO:CB	2.17	0.74
1:D:450:GLN:HG3	1:D:533:GLU:OE2	1.88	0.74
1:D:188:THR:HG23	1:D:208:ILE:CG1	2.16	0.74
1:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	0.74
1:B:368:SER:HG	1:B:370:PHE:HE1	1.36	0.74
1:B:84:ASN:HD21	1:D:91:PRO:HB2	1.53	0.74
1:B:84:ASN:O	1:C:24:ILE:HB	1.87	0.74
1:C:90:GLU:C	1:D:79:HIS:H	1.78	0.74
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.99	0.74
1:A:79:HIS:HA	1:B:1:ASP:H2	1.53	0.74
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.74
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.88	0.74
1:C:88:VAL:HG22	1:D:76:LEU:CD2	1.96	0.74
1:C:80:ALA:HB3	1:D:39:THR:OG1	1.88	0.74
1:D:451:ASN:O	1:D:534:GLY:HA2	1.88	0.74
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	0.74
1:A:364:ILE:HG13	1:A:364:ILE:O	1.87	0.74
1:C:87:PRO:C	1:D:76:LEU:CD2	2.53	0.74
1:A:79:HIS:HA	1:B:1:ASP:N	2.03	0.74
1:C:290:PHE:HZ	1:C:296:TYR:HH	1.35	0.74
1:D:523:THR:CG2	1:D:524:VAL:N	2.46	0.74
1:A:298:LEU:HD23	1:A:298:LEU:N	2.03	0.74
1:C:31:PHE:CB	1:D:75:VAL:HG22	2.13	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:C:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.74
1:C:90:GLU:OE2	1:D:37:SER:CA	2.30	0.73
1:A:90:GLU:C	1:B:3:VAL:CG2	2.57	0.73
1:C:450:GLN:HG3	1:C:533:GLU:OE2	1.88	0.73
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.73
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.73
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.01	0.73
1:B:31:PHE:HA	1:C:30:ARG:HA	1.67	0.73
1:C:1:ASP:H1	1:D:28:LYS:HB2	1.53	0.73
1:C:26:SER:OG	1:D:77:SER:CB	2.36	0.73
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:D:320:THR:CG2	2:D:807:NAG:HN2	2.02	0.73
1:B:31:PHE:CE2	1:C:29:ASP:HB3	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.73
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.73
1:C:88:VAL:HG12	1:D:94:ILE:CB	2.18	0.73
1:C:4:ILE:HG22	1:D:87:PRO:CG	2.16	0.73
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:C:223:PRO:HB2	1:C:226:TYR:CE2	2.23	0.73
1:C:364:ILE:HG13	1:C:364:ILE:O	1.87	0.73
1:C:79:HIS:CG	1:D:44:ASP:OD1	2.41	0.73
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.73
1:D:223:PRO:HB2	1:D:226:TYR:CE2	2.23	0.73
1:D:364:ILE:O	1:D:364:ILE:HG13	1.87	0.73
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.73
1:C:91:PRO:C	1:D:37:SER:OG	2.26	0.73
1:C:1:ASP:H1	1:D:28:LYS:HD3	1.47	0.73
1:C:84:ASN:O	1:D:47:PRO:HG2	1.88	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:D:333:VAL:CB	1:D:334:PRO:HD3	2.18	0.73
1:B:298:LEU:HD23	1:B:298:LEU:N	2.03	0.73
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:D:373:ASN:ND2	1:D:374:ASP:H	1.87	0.73
1:C:290:PHE:HE2	1:C:293:ARG:HB2	1.52	0.73
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.73
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.73
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.73
1:D:301:THR:HG21	2:D:805:NAG:C8	2.12	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.73
1:D:298:LEU:N	1:D:298:LEU:HD23	2.03	0.73
1:D:396:ARG:HH21	1:D:464:ILE:CG2	1.98	0.73
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.73
1:B:364:ILE:O	1:B:364:ILE:CG1	2.37	0.73
1:D:364:ILE:CG1	1:D:364:ILE:O	2.37	0.73
1:C:511:VAL:HG23	1:C:523:THR:O	1.89	0.72
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.72
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.72
1:B:32:ASN:HA	1:C:29:ASP:OD2	1.87	0.72
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.72
1:C:1:ASP:N	1:D:88:VAL:CB	2.52	0.72
1:A:90:GLU:CB	1:B:3:VAL:O	2.34	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PHE:HE2	1:D:293:ARG:HB2	1.52	0.72
1:D:33:LYS:HB3	1:D:83:GLU:HG2	1.71	0.72
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.01	0.72
1:D:320:THR:CG2	2:D:807:NAG:N2	2.52	0.72
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.72
1:C:298:LEU:HD23	1:C:298:LEU:N	2.03	0.72
1:D:482:THR:CG2	1:D:499:THR:CG2	2.62	0.72
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.72
1:A:99:ILE:CG2	1:D:30:ARG:NH1	2.50	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:C:373:ASN:ND2	1:C:374:ASP:H	1.87	0.72
1:D:511:VAL:HG23	1:D:523:THR:O	1.89	0.72
1:D:273:THR:O	2:D:803:NAG:H82	1.89	0.72
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.72
1:C:333:VAL:CB	1:C:334:PRO:HD3	2.18	0.72
1:A:364:ILE:CG1	1:A:364:ILE:O	2.37	0.72
1:C:32:ASN:H	1:D:75:VAL:HG21	0.57	0.72
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.72
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.72
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.72
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.72
1:B:32:ASN:C	1:C:25:LYS:HE2	2.06	0.72
1:C:82:SER:HB2	1:D:75:VAL:H	1.52	0.72
1:D:276:GLU:HG3	1:D:277:SER:H	1.54	0.72
1:B:88:VAL:C	1:D:1:ASP:HB2	2.09	0.71
1:D:396:ARG:NH2	1:D:464:ILE:HB	2.02	0.71
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.71
1:D:342:SER:HA	1:D:431:LEU:HB2	1.71	0.71
1:A:4:ILE:C	1:B:91:PRO:HB2	2.10	0.71
1:B:394:LEU:HD12	1:B:394:LEU:N	2.05	0.71
1:C:90:GLU:HB3	1:D:79:HIS:N	2.05	0.71
1:C:342:SER:HA	1:C:431:LEU:HB2	1.71	0.71
1:C:227:THR:O	2:C:812:NAG:O5	2.09	0.71
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	0.71
1:D:414:ASP:HB3	1:D:420:GLY:HA3	1.73	0.71
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.71
1:D:229:LEU:HD23	1:D:322:THR:HB	1.73	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.71
1:D:438:PRO:HB3	1:D:471:TYR:CE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:C:90:GLU:HB3	1:D:79:HIS:CA	2.20	0.71
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.91	0.71
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.71
1:A:289:ASP:CG	1:A:289:ASP:O	2.29	0.71
1:A:403:ASN:CB	3:A:902:NDG:N2	2.54	0.71
1:B:30:ARG:O	1:C:30:ARG:CA	2.39	0.71
1:C:81:VAL:CG1	1:D:40:GLY:N	2.49	0.71
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.71
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.71
1:D:337:SER:CA	1:D:427:ILE:HG23	2.19	0.71
1:A:91:PRO:CA	1:B:3:VAL:HG22	2.21	0.71
1:C:93:GLU:OE2	1:D:85:GLY:CA	2.30	0.71
1:D:276:GLU:CG	1:D:277:SER:H	2.03	0.71
1:C:33:LYS:HB3	1:C:83:GLU:HG2	1.71	0.70
1:C:26:SER:OG	1:D:77:SER:HB2	1.90	0.70
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.70
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.02	0.70
1:D:394:LEU:N	1:D:394:LEU:HD12	2.05	0.70
1:B:33:LYS:H	1:C:25:LYS:HE2	0.84	0.70
1:C:85:GLY:N	1:D:74:TYR:CE2	2.59	0.70
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.70
1:D:187:TYR:HA	2:D:801:NAG:C7	2.21	0.70
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.70
1:A:290:PHE:CD2	1:A:293:ARG:N	2.54	0.70
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.70
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.70
1:D:434:ASN:OD1	1:D:467:ASN:HB3	1.91	0.70
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.70
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.70
1:D:227:THR:O	2:D:812:NAG:O5	2.09	0.70
1:D:316:THR:O	2:D:806:NAG:H82	1.91	0.70
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.70
1:A:1:ASP:HB3	1:B:92:MET:HB3	1.72	0.70
1:C:289:ASP:CG	1:C:289:ASP:O	2.29	0.70
1:A:3:VAL:CG2	1:B:78:SER:H	2.01	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:D:403:ASN:CB	3:D:902:NDG:N2	2.54	0.70
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:HB3	1:D:77:SER:CB	2.21	0.70
1:C:31:PHE:CD1	1:D:95:THR:CG2	2.75	0.70
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.73	0.70
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.70
1:A:485:ALA:C	1:A:486:GLU:HG2	2.12	0.70
1:B:83:GLU:N	1:C:25:LYS:CD	2.43	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.70
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.70
1:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.69
1:C:4:ILE:CG2	1:D:87:PRO:CB	2.68	0.69
1:D:474:SER:HB2	1:D:512:LEU:CG	2.15	0.69
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.69
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.69
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.69
1:C:1:ASP:H3	1:D:88:VAL:CG1	2.03	0.69
1:C:290:PHE:CD2	1:C:293:ARG:N	2.55	0.69
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.69
1:C:403:ASN:CB	3:C:902:NDG:N2	2.54	0.69
1:D:485:ALA:C	1:D:486:GLU:HG2	2.11	0.69
1:D:405:THR:OG1	1:D:406:TYR:N	2.22	0.69
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.69
1:C:1:ASP:C	1:D:28:LYS:NZ	2.44	0.69
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.69
1:D:1:ASP:CG	1:D:2:TRP:H	1.96	0.69
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.69
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.69
1:C:35:TYR:CD2	1:D:45:ASN:CG	2.65	0.69
1:C:82:SER:HB3	1:D:75:VAL:O	1.92	0.69
1:C:186:GLU:OE1	2:C:801:NAG:H62	1.93	0.69
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.69
1:B:83:GLU:HG2	1:C:25:LYS:CD	2.20	0.69
1:D:53:ILE:HG13	1:D:59:TRP:O	1.93	0.69
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.69
1:D:186:GLU:OE1	2:D:801:NAG:H62	1.93	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:C:79:HIS:HB3	1:D:39:THR:CG2	2.20	0.69
1:A:10:SER:N	1:D:30:ARG:HG3	2.08	0.69
1:C:90:GLU:HG2	1:D:36:TYR:CB	2.08	0.69
1:B:27:ASN:ND2	1:B:27:ASN:C	2.46	0.69
1:D:289:ASP:O	1:D:289:ASP:CG	2.29	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.69
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.69
1:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.69
1:B:403:ASN:CB	3:B:902:NDG:N2	2.54	0.69
1:B:83:GLU:O	1:C:25:LYS:N	2.17	0.69
1:C:83:GLU:CB	1:D:41:GLN:NE2	2.56	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.74	0.69
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.69
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.69
1:D:523:THR:HG23	1:D:524:VAL:HG23	1.74	0.69
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.69
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.69
1:A:1:ASP:HA	1:B:24:ILE:CD1	2.22	0.68
1:A:1:ASP:H3	1:B:94:ILE:HD11	0.87	0.68
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:B:81:VAL:HB	1:D:90:GLU:HG2	1.74	0.68
1:C:31:PHE:HB3	1:D:95:THR:HG23	1.72	0.68
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.68
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.68
1:D:396:ARG:HD3	1:D:431:LEU:O	1.94	0.68
1:B:289:ASP:O	1:B:289:ASP:CG	2.29	0.68
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.76	0.68
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.68
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.77	0.68
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.68
1:D:272:THR:HG22	1:D:273:THR:N	2.09	0.68
1:C:87:PRO:N	1:D:43:ALA:CB	2.35	0.68
1:A:396:ARG:HD3	1:A:431:LEU:O	1.93	0.68
1:D:242:LEU:HD12	1:D:280:GLY:O	1.93	0.68
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.68
1:C:282:LEU:HD23	1:C:283:THR:N	2.08	0.68
1:B:282:LEU:HD23	1:B:283:THR:H	1.59	0.68
1:C:87:PRO:HD3	1:D:43:ALA:N	2.08	0.68
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.68
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.68
1:C:84:ASN:HA	1:D:71:TYR:CG	2.28	0.68
1:B:396:ARG:HD3	1:B:431:LEU:O	1.94	0.68
1:A:482:THR:HG21	1:A:500:GLN:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:CA	1:D:38:ILE:HG13	2.24	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:C:517:GLN:C	1:C:519:ASN:N	2.46	0.68
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.68
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.68
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.68
1:B:88:VAL:C	1:D:1:ASP:CB	2.62	0.68
1:D:396:ARG:HE	1:D:432:ASP:HB2	1.57	0.68
1:C:4:ILE:HG23	1:D:87:PRO:CG	2.17	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.68
1:A:368:SER:HG	1:A:370:PHE:HE1	1.42	0.68
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.68
1:B:87:PRO:HG2	1:C:2:TRP:CB	2.21	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:C:396:ARG:HD3	1:C:431:LEU:O	1.94	0.68
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.68
1:C:1:ASP:CA	1:D:89:GLU:CG	2.57	0.68
1:C:93:GLU:HB3	1:D:81:VAL:HG11	1.73	0.68
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.68
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.68
1:C:371:ILE:CG2	1:C:372:GLY:N	2.57	0.68
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.68
1:D:347:ARG:CD	1:D:392:GLY:H	2.07	0.68
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.68
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.67
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.67
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.67
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.67
1:D:440:PRO:HA	1:D:458:THR:O	1.94	0.67
1:D:333:VAL:HB	1:D:334:PRO:CD	2.24	0.67
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:A:282:LEU:HD23	1:A:283:THR:H	1.58	0.67
1:D:282:LEU:HD23	1:D:283:THR:H	1.58	0.67
1:B:84:ASN:OD1	1:C:27:ASN:N	2.25	0.67
1:B:32:ASN:HB2	1:C:27:ASN:HA	1.74	0.67
1:D:396:ARG:HE	1:D:432:ASP:CB	2.07	0.67
1:D:423:THR:HB	2:D:810:NAG:C8	2.24	0.67
1:D:222:ASP:CG	1:D:222:ASP:O	2.32	0.67
1:D:195:ASP:HB2	1:D:201:LEU:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.67
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.67
1:D:137:ASP:OD2	1:D:139:ILE:HG22	1.94	0.67
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.67
1:C:91:PRO:C	1:D:79:HIS:CD2	2.66	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67
1:C:474:SER:CB	1:C:512:LEU:HG	2.14	0.67
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.67
1:C:90:GLU:HG2	1:D:36:TYR:HB3	1.75	0.67
1:D:27:ASN:C	1:D:27:ASN:ND2	2.46	0.67
1:A:24:ILE:C	1:D:2:TRP:CZ2	2.48	0.67
1:D:474:SER:CB	1:D:512:LEU:HG	2.14	0.67
1:D:483:TRP:CZ2	1:D:507:TYR:HE1	2.09	0.67
1:B:482:THR:HG21	1:B:500:GLN:H	1.59	0.67
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.67
1:D:524:VAL:HG21	2:D:904:NAG:H81	1.77	0.67
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.67
1:D:282:LEU:HD23	1:D:283:THR:N	2.08	0.67
1:D:396:ARG:NH2	1:D:464:ILE:CB	2.58	0.67
1:C:482:THR:HG21	1:C:500:GLN:H	1.58	0.67
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.76	0.67
1:D:187:TYR:HA	2:D:801:NAG:C8	2.25	0.67
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.67
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.76	0.67
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.67
1:C:396:ARG:HE	1:C:432:ASP:CB	2.07	0.67
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.67
1:A:90:GLU:N	1:B:2:TRP:CE3	2.60	0.67
1:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67
1:A:10:SER:N	1:D:30:ARG:CG	2.58	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.67
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.67
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.67
1:D:373:ASN:ND2	1:D:374:ASP:N	2.43	0.67
3:C:902:NDG:H3	3:C:902:NDG:O7	1.95	0.67
1:D:446:THR:CG2	1:D:537:ILE:O	2.43	0.67
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ARG:CG	1:D:392:GLY:H	2.08	0.67
1:C:32:ASN:CG	1:C:33:LYS:H	1.98	0.66
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:446:THR:CG2	1:B:537:ILE:O	2.43	0.66
1:D:401:VAL:HG13	1:D:405:THR:O	1.95	0.66
3:D:902:NDG:O7	3:D:902:NDG:H3	1.95	0.66
1:C:82:SER:CB	1:D:75:VAL:N	2.49	0.66
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.66
1:D:32:ASN:CG	1:D:33:LYS:H	1.99	0.66
1:C:27:ASN:ND2	1:D:93:GLU:CA	2.58	0.66
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.66
1:D:320:THR:HG21	2:D:807:NAG:H2	1.76	0.66
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.66
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.77	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.66
1:C:86:SER:CB	1:D:76:LEU:HD11	2.26	0.66
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.66
1:D:232:GLU:HG2	1:D:289:ASP:HA	1.77	0.66
1:D:290:PHE:HZ	1:D:296:TYR:OH	1.77	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
1:D:440:PRO:HD2	1:D:522:LEU:CD1	2.26	0.66
1:D:403:ASN:HB2	3:D:902:NDG:N2	2.10	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:D:371:ILE:CG2	1:D:372:GLY:N	2.57	0.66
1:A:36:TYR:CE2	1:D:2:TRP:HH2	2.13	0.66
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66
1:B:403:ASN:HB2	3:B:902:NDG:N2	2.10	0.66
1:C:440:PRO:HD2	1:C:522:LEU:CD1	2.26	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.66
1:C:90:GLU:OE1	1:D:53:ILE:HG21	1.95	0.66
1:D:464:ILE:O	1:D:467:ASN:HB2	1.96	0.66
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.66
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.66
1:C:373:ASN:ND2	1:C:374:ASP:N	2.43	0.66
1:D:347:ARG:HD2	1:D:392:GLY:H	1.60	0.66
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.66
1:A:8:LYS:HB2	1:D:30:ARG:HE	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.77	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.66
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.66
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.99	0.66
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.66
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.95	0.66
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	0.66
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.66
1:D:366:LYS:HG3	1:D:367:LEU:HG	1.77	0.66
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.66
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.66
1:D:482:THR:HG21	1:D:500:GLN:H	1.59	0.65
1:A:222:ASP:CG	1:A:222:ASP:O	2.32	0.65
2:C:805:NAG:C6	2:C:806:NAG:C7	2.74	0.65
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.65
1:A:403:ASN:HB2	3:A:902:NDG:N2	2.10	0.65
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.65
1:C:88:VAL:HG12	1:D:94:ILE:N	2.10	0.65
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.65
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.65
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.65
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.65
1:A:10:SER:HB2	1:D:30:ARG:CG	2.26	0.65
1:C:1:ASP:H1	1:D:28:LYS:CD	2.03	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:D:482:THR:OG1	1:D:500:GLN:CG	2.44	0.65
1:D:32:ASN:ND2	1:D:83:GLU:N	2.45	0.65
1:D:155:PRO:HB2	2:D:801:NAG:C8	2.24	0.65
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.65
1:A:403:ASN:HB2	3:A:902:NDG:H8C1	1.78	0.65
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.65
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.65
1:B:30:ARG:HH11	1:C:30:ARG:HG2	1.60	0.65
1:D:488:ASP:HB2	1:D:493:SER:OG	1.97	0.65
3:A:902:NDG:O7	3:A:902:NDG:H3	1.95	0.65
1:C:347:ARG:HD2	1:C:392:GLY:H	1.60	0.65
1:A:90:GLU:HG3	1:B:3:VAL:CG2	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.65
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.65
1:B:84:ASN:OD1	1:C:26:SER:HA	1.71	0.65
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.65
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.65
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.65
1:C:79:HIS:CG	1:D:39:THR:HG22	2.32	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
1:D:224:LYS:HE3	1:D:316:THR:O	1.95	0.65
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.65
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.65
1:B:31:PHE:CZ	1:C:34:VAL:HG21	2.32	0.65
1:A:89:GLU:OE1	1:B:2:TRP:CB	2.26	0.65
1:C:446:THR:CG2	1:C:537:ILE:O	2.44	0.65
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.65
1:B:403:ASN:HB2	3:B:902:NDG:H8C1	1.78	0.65
1:C:403:ASN:HB2	3:C:902:NDG:N2	2.10	0.65
1:A:2:TRP:CE2	1:B:79:HIS:O	2.43	0.65
1:C:88:VAL:HG23	1:D:39:THR:O	1.97	0.65
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.65
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.65
1:A:364:ILE:O	1:A:364:ILE:HD12	1.97	0.65
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
1:A:2:TRP:CE2	1:B:80:ALA:HB1	2.16	0.65
1:C:81:VAL:CG1	1:D:43:ALA:CA	2.70	0.65
2:D:809:NAG:C6	2:D:810:NAG:H62	2.26	0.65
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.65
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.65
1:C:32:ASN:ND2	1:C:83:GLU:N	2.45	0.64
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.64
1:B:364:ILE:HD12	1:B:364:ILE:O	1.97	0.64
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.64
1:C:31:PHE:HD2	1:D:75:VAL:HG23	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.64
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.64
2:C:904:NAG:C3	2:C:904:NAG:O7	2.45	0.64
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.64
1:D:482:THR:HG21	1:D:499:THR:CA	2.27	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:D:232:GLU:HG3	1:D:290:PHE:H	1.61	0.64
1:D:212:THR:HG22	1:D:213:ASP:H	1.62	0.64
1:D:265:GLU:HB3	1:D:268:PHE:CE2	2.31	0.64
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.64
3:B:902:NDG:H3	3:B:902:NDG:O7	1.95	0.64
1:D:524:VAL:HG23	2:D:904:NAG:H81	1.78	0.64
1:D:406:TYR:CE1	2:D:808:NAG:H83	2.32	0.64
1:C:364:ILE:O	1:C:364:ILE:HD12	1.97	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.64
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.64
1:D:409:ILE:HG12	1:D:425:THR:HG23	1.80	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.64
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.64
1:D:341:VAL:HG21	1:D:345:LEU:HD12	1.79	0.64
1:D:346:SER:OG	1:D:349:GLU:HG3	1.97	0.64
1:C:90:GLU:OE2	1:D:37:SER:HA	1.98	0.64
1:C:409:ILE:HG12	1:C:425:THR:HG23	1.80	0.64
1:C:81:VAL:HG21	1:D:45:ASN:HB2	0.64	0.64
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:C:347:ARG:HG3	1:C:392:GLY:H	1.62	0.64
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:D:375:PRO:HB3	1:D:400:TYR:CD2	2.33	0.64
1:D:347:ARG:HG3	1:D:392:GLY:H	1.62	0.64
1:A:364:ILE:CD1	1:A:364:ILE:O	2.46	0.64
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.64
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.64
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.64
2:D:904:NAG:O7	2:D:904:NAG:C3	2.45	0.64
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.64
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	0.64
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.63
1:D:327:ASN:HA	1:D:360:ASP:OD2	1.97	0.63
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:D:221:PHE:CE1	1:D:315:SER:O	2.45	0.63
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.63
1:D:440:PRO:HD3	1:D:522:LEU:HD12	1.78	0.63
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.63
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:C:142:LEU:HB3	1:C:196:LEU:HA	1.81	0.63
1:B:87:PRO:HD2	1:D:90:GLU:O	1.97	0.63
1:A:10:SER:HA	1:D:30:ARG:HD2	1.81	0.63
1:C:84:ASN:HB3	1:D:73:LYS:O	1.98	0.63
1:D:504:LYS:NZ	1:D:531:SER:OG	2.31	0.63
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.63
1:C:419:VAL:HG13	2:C:809:NAG:O7	1.98	0.63
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.63
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.63
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.81	0.63
1:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.63
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:C:1:ASP:N	1:D:88:VAL:HB	2.11	0.63
1:C:446:THR:CG2	1:C:539:CYS:SG	2.86	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.63
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.63
1:D:142:LEU:HB3	1:D:196:LEU:HA	1.81	0.63
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.63
1:D:364:ILE:O	1:D:364:ILE:CD1	2.46	0.63
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.63
1:C:90:GLU:CD	1:D:36:TYR:HB3	2.18	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	0.63
1:D:469:TYR:CE1	1:D:470:PRO:HD2	2.34	0.63
1:D:154:ASP:O	1:D:155:PRO:C	2.36	0.63
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:GLU:O	1:D:494:MET:CA	2.46	0.63
1:D:22:VAL:HG22	1:D:23:GLN:N	2.14	0.63
1:D:419:VAL:HG13	2:D:809:NAG:O7	1.98	0.63
1:C:403:ASN:CB	3:C:902:NDG:C7	2.76	0.63
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.63
1:D:364:ILE:HD12	1:D:364:ILE:O	1.97	0.63
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.63
1:C:154:ASP:CA	2:C:801:NAG:H82	2.29	0.63
1:D:371:ILE:HG22	1:D:372:GLY:N	2.14	0.63
1:C:127:VAL:HG22	1:C:128:MET:N	2.14	0.63
1:B:364:ILE:CD1	1:B:364:ILE:O	2.46	0.63
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.63
1:C:81:VAL:CG1	1:D:43:ALA:CB	2.26	0.62
1:A:3:VAL:CG2	1:B:78:SER:N	2.60	0.62
1:D:411:LEU:HD22	1:D:421:THR:HG23	1.81	0.62
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.62
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.62
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.62
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.62
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.62
1:C:90:GLU:OE2	1:D:36:TYR:O	2.15	0.62
1:D:343:GLU:HB3	1:D:433:VAL:CG2	2.27	0.62
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	0.62
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.62
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.62
1:D:508:SER:HB3	1:D:526:ASN:OD1	2.00	0.62
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.62
1:C:524:VAL:HG23	2:C:904:NAG:C8	2.29	0.62
1:D:524:VAL:HG23	2:D:904:NAG:C8	2.29	0.62
1:D:127:VAL:HG22	1:D:128:MET:N	2.14	0.62
1:C:87:PRO:O	1:D:38:ILE:HD11	2.00	0.62
1:A:89:GLU:O	1:B:1:ASP:O	2.18	0.62
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.62
1:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.62
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.62
1:B:88:VAL:O	1:D:1:ASP:OD2	2.17	0.62
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.62
2:D:805:NAG:C6	2:D:806:NAG:C7	2.74	0.62
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.62
1:A:403:ASN:CB	3:A:902:NDG:C7	2.76	0.62
1:D:518:ASN:O	1:D:520:PRO:CD	2.46	0.62
1:D:371:ILE:CG2	1:D:372:GLY:H	2.13	0.62
1:A:1:ASP:H2	1:B:94:ILE:CD1	1.98	0.62
1:B:33:LYS:H	1:C:25:LYS:NZ	1.97	0.62
1:B:83:GLU:HG2	1:C:25:LYS:HD2	1.79	0.62
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.62
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.62
1:A:147:SER:OG	1:A:167:ARG:HG3	1.99	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	1.99	0.62
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.62
1:C:482:THR:HG22	1:C:499:THR:N	2.13	0.62
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.62
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.31	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.62
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.62
1:D:154:ASP:CA	2:D:801:NAG:H82	2.29	0.62
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.62
1:A:91:PRO:CD	1:B:3:VAL:HG22	2.28	0.61
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.61
1:D:235:ILE:HG12	1:D:287:GLY:HA2	1.82	0.61
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.61
1:D:415:ASP:OD1	1:D:416:GLY:N	2.26	0.61
1:D:68:ARG:HD3	1:D:100:ASP:HA	1.82	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:C:1:ASP:H1	1:D:28:LYS:CB	2.13	0.61
1:C:81:VAL:HG11	1:D:43:ALA:C	2.21	0.61
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.61
1:D:403:ASN:O	1:D:405:THR:N	2.33	0.61
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLY:HA3	1:D:47:PRO:HB2	1.82	0.61
1:C:27:ASN:HD21	1:D:93:GLU:H	1.45	0.61
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:D:374:ASP:O	1:D:375:PRO:O	2.17	0.61
1:A:2:TRP:CD1	1:B:80:ALA:HB2	2.35	0.61
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.61
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.61
1:D:403:ASN:CB	3:D:902:NDG:C7	2.76	0.61
1:C:379:LEU:H	1:C:379:LEU:HD23	1.66	0.61
1:D:154:ASP:O	2:D:801:NAG:H82	1.98	0.61
1:D:524:VAL:CG2	2:D:904:NAG:C8	2.78	0.61
1:A:91:PRO:N	1:B:1:ASP:O	2.33	0.61
1:D:469:TYR:CD2	1:D:470:PRO:CD	2.80	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:D:475:LEU:O	1:D:479:SER:HB3	2.01	0.61
1:A:9:VAL:N	1:D:30:ARG:HD3	2.15	0.61
1:C:31:PHE:O	1:D:73:LYS:CD	2.47	0.61
1:D:212:THR:HG22	1:D:213:ASP:N	2.15	0.61
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:D:181:ARG:NE	1:D:213:ASP:OD1	2.34	0.61
1:A:379:LEU:H	1:A:379:LEU:HD23	1.66	0.61
1:D:379:LEU:H	1:D:379:LEU:HD23	1.66	0.61
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:C:368:SER:HG	1:C:370:PHE:HE1	1.48	0.61
1:D:449:ASP:H	1:D:532:CYS:CB	2.12	0.61
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.61
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:C:371:ILE:CG2	1:C:372:GLY:H	2.13	0.60
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.60
1:C:88:VAL:CA	1:D:38:ILE:HD11	2.31	0.60
1:D:189:LEU:HD23	1:D:189:LEU:N	2.16	0.60
1:C:189:LEU:HD23	1:C:189:LEU:N	2.16	0.60
1:A:9:VAL:C	1:D:30:ARG:HD2	2.16	0.60
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.60
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.60
1:C:81:VAL:H	1:D:45:ASN:HD22	1.48	0.60
1:C:90:GLU:CG	1:D:36:TYR:HB3	2.32	0.60
1:D:523:THR:CG2	1:D:524:VAL:H	1.94	0.60
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.60
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.60
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.60
1:D:227:THR:CG2	2:D:807:NAG:C7	2.76	0.60
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:A:189:LEU:N	1:A:189:LEU:HD23	2.16	0.60
1:A:2:TRP:CZ2	1:B:36:TYR:CD2	2.75	0.60
1:D:446:THR:CG2	1:D:539:CYS:SG	2.86	0.60
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.60
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	0.60
1:C:32:ASN:CB	1:D:75:VAL:HG23	2.31	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.60
1:C:403:ASN:HB2	3:C:902:NDG:H8C1	1.78	0.60
1:C:508:SER:HA	1:C:526:ASN:HA	1.84	0.60
1:C:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:B:88:VAL:O	1:D:1:ASP:CG	2.40	0.59
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.59
1:C:81:VAL:HG13	1:D:44:ASP:H	1.63	0.59
1:D:403:ASN:HB2	3:D:902:NDG:H8C1	1.78	0.59
1:D:367:LEU:CB	1:D:413:THR:O	2.51	0.59
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.59
1:C:1:ASP:C	1:D:28:LYS:HZ3	1.97	0.59
1:D:514:SER:HA	1:D:517:GLN:O	2.02	0.59
1:D:232:GLU:CG	1:D:290:PHE:N	2.64	0.59
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.59
1:D:116:SER:HA	1:D:210:GLN:O	2.02	0.59
1:D:146:LEU:HA	1:D:194:THR:O	2.02	0.59
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.59
1:D:239:VAL:HG13	1:D:240:GLN:H	1.67	0.59
1:D:49:GLY:O	1:D:63:THR:HG21	2.02	0.59
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.59
1:C:31:PHE:CB	1:D:95:THR:HG21	2.10	0.59
1:D:396:ARG:NH2	1:D:464:ILE:HG21	2.17	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.59
1:D:336:VAL:HB	1:D:426:LEU:HD23	1.84	0.59
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:C:443:ARG:HH11	1:C:443:ARG:HG3	1.67	0.59
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.59
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.59
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.59
1:C:239:VAL:HG13	1:C:240:GLN:H	1.67	0.59
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.59
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.59
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.59
1:C:286:LYS:O	1:C:287:GLY:O	2.21	0.59
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.59
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.59
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.84	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:C:28:LYS:HB3	1:D:76:LEU:O	2.03	0.59
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.59
1:A:90:GLU:CB	1:B:3:VAL:HG23	2.33	0.59
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.59
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.59
1:D:486:GLU:O	1:D:495:LEU:N	2.31	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.59
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.59
1:D:363:GLN:O	1:D:364:ILE:HG22	2.03	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:D:508:SER:HA	1:D:526:ASN:HA	1.84	0.59
1:D:289:ASP:O	1:D:290:PHE:CB	2.25	0.59
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.59
1:B:88:VAL:O	1:D:1:ASP:HB3	2.01	0.58
1:A:4:ILE:CG2	1:B:91:PRO:O	2.33	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.58
1:D:38:ILE:HG22	1:D:53:ILE:HG22	1.85	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.58
1:C:88:VAL:CG2	1:D:76:LEU:HD23	2.25	0.58
1:C:86:SER:N	1:D:74:TYR:HD2	1.94	0.58
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.58
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.58
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.58
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.58
1:B:403:ASN:CB	3:B:902:NDG:C7	2.76	0.58
1:D:443:ARG:HA	1:D:525:VAL:HG13	1.85	0.58
1:A:91:PRO:HA	1:B:1:ASP:C	2.23	0.58
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.58
1:D:286:LYS:O	1:D:287:GLY:O	2.21	0.58
1:D:232:GLU:HG2	1:D:289:ASP:CA	2.33	0.58
1:D:366:LYS:HG3	1:D:367:LEU:N	2.04	0.58
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.67	0.58
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.58
1:C:28:LYS:HD3	1:D:76:LEU:O	2.02	0.58
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.58
1:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:C:31:PHE:HA	1:D:73:LYS:HZ1	1.69	0.58
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58
1:D:221:PHE:HA	1:D:244:VAL:HG12	1.85	0.58
1:D:226:TYR:CE2	1:D:242:LEU:HD23	2.39	0.58
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.58
1:A:1:ASP:CA	1:B:24:ILE:HD13	2.33	0.58
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.58
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.58
1:D:522:LEU:CD2	1:D:523:THR:HB	2.26	0.58
1:D:406:TYR:HB3	1:D:428:LEU:CD2	2.33	0.58
1:D:537:ILE:HG12	1:D:538:LYS:N	2.19	0.58
1:D:443:ARG:HH11	1:D:443:ARG:HG3	1.67	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.58
1:D:473:VAL:HA	1:D:513:LEU:HD23	1.85	0.58
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.58
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.58
1:C:42:GLY:HA2	1:C:47:PRO:O	2.04	0.58
1:C:27:ASN:C	1:C:27:ASN:ND2	2.46	0.58
1:C:79:HIS:ND1	1:D:39:THR:HG22	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:TYR:HB2	1:D:321:VAL:HB	1.86	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.67	0.58
1:D:42:GLY:HA2	1:D:47:PRO:O	2.04	0.58
1:A:89:GLU:CD	1:B:2:TRP:CD1	2.51	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.58
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.58
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.58
1:B:87:PRO:CG	1:C:2:TRP:HB2	2.29	0.57
1:C:90:GLU:CG	1:D:79:HIS:O	2.51	0.57
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.86	0.57
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.57
1:C:84:ASN:O	1:D:74:TYR:CE2	2.57	0.57
1:C:88:VAL:CG1	1:D:94:ILE:O	2.52	0.57
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.57
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.57
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.84	0.57
1:D:268:PHE:HA	1:D:285:ALA:HB3	1.84	0.57
1:C:240:GLN:HG3	1:C:241:ARG:N	2.19	0.57
1:D:240:GLN:HG3	1:D:241:ARG:N	2.19	0.57
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.57
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.57
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.86	0.57
1:D:299:GLN:C	1:D:300:ILE:HD12	2.24	0.57
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.57
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.57
1:D:447:MET:HB2	1:D:529:VAL:HG22	1.84	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PRO:C	1:D:38:ILE:HD11	2.24	0.57
1:D:330:PRO:HD3	1:D:414:ASP:HB2	1.86	0.57
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.57
1:D:154:ASP:CB	1:D:155:PRO:CD	2.82	0.57
1:C:154:ASP:CB	2:C:801:NAG:HN2	2.16	0.57
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.57
1:C:79:HIS:HB3	1:D:44:ASP:CG	2.25	0.57
1:B:28:LYS:NZ	1:D:2:TRP:O	2.33	0.57
1:C:83:GLU:CB	1:D:41:GLN:HE22	2.16	0.57
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.57
1:A:2:TRP:CZ2	1:B:79:HIS:O	2.38	0.57
1:C:87:PRO:CD	1:D:43:ALA:N	2.65	0.57
1:D:482:THR:HG22	1:D:499:THR:N	2.13	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:D:32:ASN:HD22	1:D:83:GLU:H	1.51	0.57
1:D:195:ASP:CB	1:D:200:GLY:HA3	2.33	0.57
1:C:363:GLN:O	1:C:364:ILE:HG22	2.03	0.57
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.57
1:A:10:SER:CA	1:D:30:ARG:HD2	2.35	0.57
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.57
1:D:406:TYR:HB3	1:D:428:LEU:HD21	1.87	0.57
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.57
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.57
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.57
1:D:332:PHE:CD2	1:D:424:GLY:HA3	2.39	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:D:154:ASP:CB	2:D:801:NAG:HN2	2.16	0.57
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.57
1:C:505:GLY:HA2	1:C:529:VAL:H	1.69	0.57
1:C:89:GLU:N	1:D:38:ILE:CG1	2.58	0.57
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.57
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.57
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.57
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.57
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.57
1:D:369:TYR:HD1	1:D:383:LYS:O	1.88	0.57
1:C:26:SER:CB	1:D:77:SER:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.57
1:C:221:PHE:HA	1:C:244:VAL:HG12	1.85	0.57
1:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.57
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:D:335:ALA:HB1	3:D:811:NDG:C6	2.33	0.56
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.56
1:B:85:GLY:O	1:D:90:GLU:HA	2.05	0.56
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.56
1:D:68:ARG:HG3	1:D:69:GLU:N	2.19	0.56
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.56
1:C:82:SER:OG	1:D:74:TYR:HB3	2.05	0.56
1:C:27:ASN:HD21	1:D:93:GLU:HB3	1.60	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.56
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.56
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.56
1:D:189:LEU:HD21	1:D:209:ILE:HD12	1.87	0.56
1:D:309:SER:O	1:D:310:VAL:HG23	2.03	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.56
1:C:85:GLY:HA2	1:D:41:GLN:C	2.13	0.56
1:D:517:GLN:C	1:D:519:ASN:N	2.47	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:D:378:TRP:O	1:D:391:ASN:HB2	2.06	0.56
1:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.56
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.56
1:B:83:GLU:CG	1:C:25:LYS:HD3	2.25	0.56
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.56
1:A:5:PRO:N	1:B:91:PRO:HB2	2.21	0.56
1:D:222:ASP:N	1:D:243:SER:O	2.38	0.56
1:B:394:LEU:CD1	1:B:394:LEU:N	2.69	0.56
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.56
1:B:30:ARG:NH1	1:C:30:ARG:HB3	2.21	0.56
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.56
1:D:155:PRO:N	2:D:801:NAG:H82	2.20	0.56
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	0.56
1:C:415:ASP:OD1	1:C:416:GLY:N	2.26	0.56
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.56
1:C:108:PHE:CE1	1:C:203:VAL:HG23	2.40	0.56
1:D:32:ASN:CG	1:D:33:LYS:N	2.59	0.56
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:A:4:ILE:CA	1:B:91:PRO:CD	2.69	0.56
1:D:450:GLN:HB2	1:D:533:GLU:CA	2.26	0.56
1:C:365:GLN:CG	1:C:365:GLN:O	2.54	0.56
1:D:393:ASN:C	1:D:394:LEU:HD12	2.25	0.56
1:D:108:PHE:CE1	1:D:203:VAL:HG23	2.40	0.56
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.56
1:D:162:LEU:O	1:D:174:LEU:HD12	2.06	0.56
1:D:432:ASP:CG	1:D:464:ILE:CG2	2.74	0.56
1:C:118:ARG:HA	1:C:212:THR:HB	1.87	0.56
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.86	0.56
1:B:505:GLY:HA2	1:B:529:VAL:H	1.69	0.56
1:C:31:PHE:O	1:D:73:LYS:CE	2.54	0.56
1:C:88:VAL:HG13	1:D:94:ILE:O	2.05	0.56
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.56
1:D:336:VAL:HG12	1:D:338:ARG:HB2	1.87	0.56
1:C:222:ASP:N	1:C:243:SER:O	2.38	0.56
1:A:2:TRP:CH2	1:B:35:TYR:O	2.58	0.55
1:D:339:VAL:HG21	1:D:351:ILE:CG2	2.36	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:C:35:TYR:HB3	1:D:45:ASN:ND2	2.22	0.55
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:D:259:TYR:O	1:D:260:LYS:HB3	2.05	0.55
1:C:1:ASP:N	1:D:89:GLU:OE2	2.38	0.55
1:C:89:GLU:C	1:D:38:ILE:HG13	2.26	0.55
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.55
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.55
1:D:155:PRO:HG2	2:D:801:NAG:O7	2.07	0.55
1:D:505:GLY:HA2	1:D:529:VAL:H	1.70	0.55
1:C:79:HIS:HB3	1:D:39:THR:CB	2.36	0.55
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.37	0.55
1:D:118:ARG:HA	1:D:212:THR:HB	1.87	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.55
1:D:268:PHE:CD2	1:D:268:PHE:N	2.75	0.55
1:D:394:LEU:N	1:D:394:LEU:CD1	2.69	0.55
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.55
1:B:30:ARG:NH1	1:C:30:ARG:CG	2.69	0.55
1:D:28:LYS:HB3	1:D:88:VAL:HG11	1.89	0.55
1:C:278:ASN:N	1:C:278:ASN:HD22	2.05	0.55
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.55
1:C:79:HIS:N	1:D:39:THR:HG21	2.10	0.55
1:D:419:VAL:CG1	1:D:420:GLY:N	2.70	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:D:155:PRO:C	1:D:157:GLU:N	2.56	0.55
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.55
1:C:459:ILE:HG21	1:C:471:TYR:CE2	2.42	0.55
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.55
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.55
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.55
1:C:394:LEU:N	1:C:394:LEU:CD1	2.69	0.55
1:B:28:LYS:HE3	1:D:4:ILE:N	2.13	0.55
1:C:81:VAL:HG21	1:D:45:ASN:N	2.20	0.55
1:C:86:SER:O	1:D:41:GLN:O	2.25	0.55
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.55
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.55
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.55
1:D:154:ASP:CG	1:D:155:PRO:CD	2.75	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:B:83:GLU:CB	1:C:25:LYS:CG	2.37	0.55
1:C:82:SER:OG	1:D:74:TYR:CD2	2.60	0.55
1:C:83:GLU:CA	1:D:41:GLN:HE22	2.06	0.55
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.55
1:D:459:ILE:HG21	1:D:471:TYR:CE2	2.42	0.55
1:D:466:PRO:O	1:D:468:THR:N	2.40	0.55
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.55
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:D:278:ASN:N	1:D:278:ASN:HD22	2.05	0.55
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.55
1:A:10:SER:N	1:D:30:ARG:HD2	2.20	0.55
1:C:31:PHE:CB	1:D:75:VAL:CG2	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:THR:HG21	1:D:499:THR:C	2.27	0.55
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.55
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:D:333:VAL:CG2	1:D:334:PRO:HD3	2.36	0.55
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.55
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.54
1:B:32:ASN:C	1:C:25:LYS:CE	2.68	0.54
1:C:31:PHE:CD2	1:D:74:TYR:O	2.60	0.54
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.54
1:D:439:VAL:HG13	1:D:522:LEU:HD11	1.88	0.54
1:D:363:GLN:C	1:D:364:ILE:CG2	2.75	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.07	0.54
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.37	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.89	0.54
1:D:272:THR:CG2	1:D:273:THR:H	2.19	0.54
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.54
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.54
1:A:90:GLU:HB2	1:B:3:VAL:O	2.06	0.54
1:D:330:PRO:HB3	1:D:358:ASP:HB2	1.89	0.54
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.54
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.54
1:D:226:TYR:O	1:D:227:THR:CG2	2.55	0.54
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.08	0.54
1:A:490:LYS:HG2	1:A:490:LYS:O	2.08	0.54
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.54
1:C:419:VAL:CG1	1:C:420:GLY:N	2.70	0.54
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.54
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.54
1:D:117:VAL:O	1:D:211:ILE:HA	2.07	0.54
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.54
1:C:88:VAL:CG2	1:D:75:VAL:O	2.43	0.54
1:A:10:SER:CB	1:D:30:ARG:HG3	2.36	0.54
1:C:87:PRO:CG	1:D:43:ALA:HB2	1.86	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:LEU:C	1:D:367:LEU:HD12	2.28	0.54
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.54
1:C:268:PHE:N	1:C:268:PHE:CD2	2.75	0.54
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.54
1:D:490:LYS:HG2	1:D:490:LYS:O	2.08	0.54
1:C:1:ASP:N	1:D:28:LYS:CB	2.71	0.54
1:B:367:LEU:HD12	1:B:367:LEU:C	2.28	0.54
1:D:169:THR:OG1	1:D:171:VAL:HG23	2.07	0.54
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.54
1:C:26:SER:HG	1:D:77:SER:CB	2.19	0.54
1:C:330:PRO:HB3	1:C:358:ASP:HB2	1.89	0.54
1:C:93:GLU:HB3	1:D:81:VAL:CG1	2.37	0.54
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.54
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.54
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.54
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:D:332:PHE:HD2	1:D:424:GLY:HA3	1.73	0.54
1:D:217:ASN:ND2	1:D:217:ASN:N	2.56	0.54
1:D:438:PRO:HB2	1:D:513:LEU:HD12	1.89	0.54
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.54
1:A:272:THR:CG2	1:A:273:THR:H	2.18	0.54
1:D:241:ARG:NE	1:D:281:ILE:HD12	2.22	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.76	0.54
1:C:90:GLU:H	1:D:79:HIS:N	1.91	0.54
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	0.54
1:D:443:ARG:NH1	1:D:443:ARG:HG3	2.24	0.54
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.54
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	0.54
1:B:75:VAL:O	1:B:76:LEU:HD23	2.08	0.53
1:B:81:VAL:CB	1:D:90:GLU:HG2	2.37	0.53
1:B:86:SER:N	1:D:91:PRO:CD	2.70	0.53
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.53
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.53
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.53
1:C:85:GLY:N	1:D:74:TYR:CD2	2.77	0.53
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.91	0.53
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:C:79:HIS:CB	1:D:39:THR:CB	2.80	0.53
1:D:450:GLN:CB	1:D:532:CYS:O	2.56	0.53
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.53
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.53
1:D:373:ASN:HB3	1:D:409:ILE:H	1.73	0.53
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	0.53
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.23	0.53
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.53
1:D:105:ARG:HG3	1:D:106:PRO:HD2	1.91	0.53
1:C:88:VAL:C	1:D:38:ILE:CG1	2.76	0.53
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.53
1:C:154:ASP:C	2:C:801:NAG:C8	2.62	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:D:458:THR:HG22	1:D:493:SER:HB3	1.91	0.53
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.53
1:C:443:ARG:NH1	1:C:443:ARG:HG3	2.23	0.53
1:D:22:VAL:HG22	1:D:23:GLN:H	1.73	0.53
1:C:83:GLU:C	1:D:41:GLN:NE2	2.61	0.53
1:C:533:GLU:OE2	1:C:533:GLU:HA	2.09	0.53
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.53
1:D:367:LEU:HD13	1:D:412:VAL:HG23	1.91	0.53
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.53
1:C:490:LYS:O	1:C:490:LYS:HG2	2.08	0.53
1:D:75:VAL:O	1:D:76:LEU:HD23	2.08	0.53
1:A:320:THR:CG2	2:A:807:NAG:C2	2.77	0.53
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.53
1:C:272:THR:CG2	1:C:273:THR:H	2.18	0.53
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.53
1:D:242:LEU:O	1:D:279:GLN:HB3	2.09	0.53
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.53
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.53
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.53
1:D:249:MET:O	1:D:252:THR:HB	2.08	0.53
1:C:318:THR:CG2	2:C:806:NAG:H5	2.34	0.53
1:B:379:LEU:CD2	1:B:379:LEU:H	2.22	0.53
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.53
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.53
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.53
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.53
1:A:4:ILE:CB	1:B:90:GLU:C	2.76	0.53
1:D:403:ASN:C	1:D:405:THR:H	2.12	0.53
1:A:278:ASN:N	1:A:278:ASN:HD22	2.05	0.53
1:C:249:MET:O	1:C:252:THR:HB	2.08	0.53
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.90	0.53
1:C:1:ASP:O	1:D:28:LYS:CD	2.57	0.52
1:D:31:PHE:CD2	1:D:32:ASN:HB2	2.44	0.52
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.52
1:D:227:THR:CG2	2:D:807:NAG:H83	2.32	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.89	0.52
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.52
1:A:24:ILE:CG2	1:D:2:TRP:HE1	2.18	0.52
1:A:24:ILE:HA	1:D:2:TRP:CB	2.33	0.52
1:A:2:TRP:CZ2	1:B:36:TYR:HA	2.43	0.52
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.52
1:C:81:VAL:CG1	1:D:43:ALA:H	2.22	0.52
1:A:4:ILE:CA	1:B:91:PRO:CB	2.81	0.52
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.09	0.52
1:D:512:LEU:HD11	1:D:519:ASN:HD21	1.74	0.52
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.52
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.45	0.52
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.75	0.52
1:D:496:LEU:HD21	1:D:509:ILE:CD1	2.38	0.52
1:D:312:LEU:O	3:D:804:NDG:C8	2.57	0.52
1:A:2:TRP:HH2	1:B:35:TYR:O	1.92	0.52
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.45	0.52
1:C:91:PRO:N	1:D:79:HIS:HD2	2.03	0.52
1:C:379:LEU:H	1:C:379:LEU:CD2	2.22	0.52
1:D:272:THR:CG2	2:D:803:NAG:HN2	2.23	0.52
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.52
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.52
1:D:226:TYR:HB2	1:D:319:VAL:HG22	1.89	0.52
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.52
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.52
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.52
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.52
1:C:28:LYS:CB	1:D:76:LEU:O	2.57	0.52
1:B:30:ARG:NH1	1:C:30:ARG:HG2	2.25	0.52
1:D:396:ARG:NH2	1:D:464:ILE:HG22	2.12	0.52
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.52
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.75	0.52
1:D:318:THR:CG2	2:D:806:NAG:H5	2.34	0.52
1:C:194:THR:HG22	1:C:195:ASP:N	2.25	0.52
1:C:1:ASP:CA	1:D:89:GLU:OE1	2.39	0.52
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.52
1:D:338:ARG:HB3	1:D:339:VAL:HG22	1.92	0.52
1:C:93:GLU:CA	1:D:81:VAL:HG11	2.38	0.52
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.52
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.52
1:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.52
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	0.52
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.52
1:C:367:LEU:HD13	1:C:412:VAL:HG23	1.91	0.52
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.52
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:C:27:ASN:HD21	1:D:93:GLU:N	2.04	0.52
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.52
1:B:426:LEU:HD13	1:B:426:LEU:O	2.10	0.52
1:C:373:ASN:HB3	1:C:409:ILE:H	1.73	0.52
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.52
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.52
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.52
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.52
1:D:365:GLN:O	1:D:365:GLN:CG	2.54	0.52
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.52
1:B:89:GLU:N	1:D:1:ASP:CB	2.46	0.52
1:D:482:THR:CG2	1:D:499:THR:CA	2.87	0.52
1:D:155:PRO:CD	2:D:801:NAG:H82	2.40	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.52
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.52
1:D:138:ASN:HD22	1:D:138:ASN:C	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:THR:HG22	1:D:482:THR:O	2.09	0.52
1:D:221:PHE:HB3	1:D:223:PRO:O	2.10	0.52
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.52
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.52
1:D:347:ARG:HD2	1:D:392:GLY:N	2.25	0.52
1:D:371:ILE:HG23	1:D:372:GLY:H	1.73	0.52
1:D:505:GLY:O	1:D:506:ASP:OD1	2.28	0.52
1:D:252:THR:HG23	1:D:253:PRO:HD2	1.90	0.52
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.52
1:C:30:ARG:NH2	1:D:6:PRO:HG3	2.25	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:D:234:GLU:HB2	1:D:235:ILE:HG22	1.93	0.51
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.51
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:D:369:TYR:O	1:D:383:LYS:HG2	2.09	0.51
1:A:3:VAL:HG21	1:B:77:SER:OG	2.10	0.51
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.51
1:A:533:GLU:OE2	1:A:533:GLU:HA	2.09	0.51
1:C:514:SER:HB3	1:C:517:GLN:O	2.11	0.51
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.51
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.51
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.51
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.51
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.51
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.51
1:C:88:VAL:HG22	1:D:75:VAL:O	2.03	0.51
1:B:81:VAL:CG1	1:D:90:GLU:HG2	2.40	0.51
1:D:514:SER:HB3	1:D:517:GLN:O	2.10	0.51
1:D:426:LEU:O	1:D:426:LEU:HD13	2.09	0.51
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.51
1:C:426:LEU:O	1:C:426:LEU:HD13	2.10	0.51
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.51
1:C:403:ASN:HB2	3:C:902:NDG:H8C2	1.87	0.51
1:D:347:ARG:HG3	1:D:391:ASN:HA	1.91	0.51
1:D:333:VAL:CB	1:D:334:PRO:CD	2.88	0.51
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:C:88:VAL:CG1	1:D:94:ILE:N	2.73	0.51
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:CB	1:B:3:VAL:CA	2.60	0.51
1:A:426:LEU:HD13	1:A:426:LEU:O	2.09	0.51
1:D:336:VAL:O	1:D:426:LEU:HD22	2.10	0.51
1:D:33:LYS:HB3	1:D:83:GLU:CG	2.40	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.51
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.51
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.51
1:C:82:SER:HB2	1:D:74:TYR:HA	1.92	0.51
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.51
1:B:471:TYR:CD1	1:B:471:TYR:N	2.79	0.51
1:D:151:LEU:HD12	1:D:190:THR:O	2.11	0.51
1:C:151:LEU:HD12	1:C:190:THR:O	2.11	0.51
1:C:90:GLU:H	1:D:78:SER:HB2	1.74	0.51
1:C:82:SER:OG	1:D:74:TYR:HD2	1.93	0.51
1:C:90:GLU:H	1:D:78:SER:CB	1.92	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.51
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.51
1:C:138:ASN:C	1:C:138:ASN:HD22	2.13	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.51
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.51
1:C:31:PHE:CE2	1:D:73:LYS:C	2.36	0.51
1:A:4:ILE:HA	1:B:90:GLU:CA	2.37	0.51
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.51
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.51
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.51
1:D:268:PHE:C	1:D:285:ALA:HB3	2.30	0.51
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.51
1:C:25:LYS:NZ	1:C:29:ASP:OD2	2.40	0.51
1:C:31:PHE:CD1	1:D:95:THR:HG21	2.44	0.51
1:D:396:ARG:CZ	1:D:432:ASP:HB2	2.41	0.51
2:D:809:NAG:H61	2:D:810:NAG:C6	2.39	0.51
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLU:HB2	1:C:235:ILE:HG22	1.93	0.51
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.51
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.51
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.51
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.51
1:D:76:LEU:O	1:D:94:ILE:N	2.44	0.51
1:C:88:VAL:HG12	1:D:94:ILE:CA	2.40	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:D:352:ILE:HG13	1:D:388:VAL:CB	2.33	0.51
1:A:471:TYR:N	1:A:471:TYR:CD1	2.79	0.51
1:A:458:THR:HG22	1:A:493:SER:CB	2.41	0.51
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.51
1:D:276:GLU:HG3	1:D:277:SER:N	2.25	0.51
1:C:241:ARG:NE	1:C:281:ILE:HD12	2.22	0.51
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.51
1:B:32:ASN:HB2	1:C:26:SER:O	2.11	0.50
1:C:31:PHE:CA	1:D:73:LYS:NZ	2.72	0.50
1:D:80:ALA:O	1:D:88:VAL:HG23	2.11	0.50
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	0.50
1:A:513:LEU:C	1:A:514:SER:HG	2.14	0.50
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.50
1:D:458:THR:HA	1:D:493:SER:HA	1.93	0.50
1:D:194:THR:HG22	1:D:195:ASP:N	2.25	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.90	0.50
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.50
1:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.50
1:C:428:LEU:HD23	1:C:428:LEU:O	2.11	0.50
1:D:458:THR:HG22	1:D:493:SER:CB	2.42	0.50
1:D:217:ASN:HD22	1:D:217:ASN:N	2.09	0.50
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.50
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.50
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.93	0.50
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.50
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.50
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.50
1:D:297:VAL:CG2	2:D:807:NAG:H62	2.41	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:D:142:LEU:O	1:D:196:LEU:HD23	2.11	0.50
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.50
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.50
1:A:2:TRP:CD2	1:B:80:ALA:HB3	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLU:CD	1:D:37:SER:C	2.66	0.50
1:D:432:ASP:CB	1:D:464:ILE:CG2	2.89	0.50
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.50
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.50
1:D:403:ASN:HB2	3:D:902:NDG:H8C2	1.87	0.50
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.50
1:B:268:PHE:N	1:B:268:PHE:CD2	2.75	0.50
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50
1:D:382:ASN:OD1	1:D:385:ASN:N	2.45	0.50
1:D:471:TYR:CD1	1:D:471:TYR:N	2.79	0.50
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.50
1:B:403:ASN:HB2	3:B:902:NDG:H8C2	1.87	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.42	0.50
1:B:458:THR:HG22	1:B:493:SER:CB	2.42	0.50
1:D:428:LEU:O	1:D:428:LEU:HD23	2.11	0.50
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.50
1:B:217:ASN:HD22	1:B:217:ASN:N	2.09	0.50
1:D:450:GLN:CB	1:D:533:GLU:HA	2.29	0.50
1:C:482:THR:O	1:C:482:THR:HG22	2.09	0.50
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.50
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.50
1:C:471:TYR:CD1	1:C:471:TYR:N	2.79	0.50
1:D:363:GLN:C	1:D:364:ILE:HG23	2.32	0.50
1:D:11:GLU:OE2	1:D:69:GLU:OE1	2.30	0.50
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.50
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.44	0.50
1:D:261:ILE:HD11	1:D:264:ASN:HD22	1.77	0.50
1:A:1:ASP:HB3	1:B:92:MET:CB	2.40	0.50
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.50
1:C:87:PRO:C	1:D:38:ILE:CD1	2.80	0.50
1:C:88:VAL:HG21	1:D:75:VAL:O	2.07	0.50
1:B:482:THR:O	1:B:482:THR:HG22	2.09	0.50
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.93	0.50
1:A:423:THR:HB	2:A:810:NAG:H83	1.93	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:PRO:HG2	2:D:801:NAG:C7	2.42	0.50
1:D:320:THR:CG2	2:D:807:NAG:C2	2.77	0.50
1:C:496:LEU:HD21	1:C:509:ILE:CD1	2.38	0.50
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.50
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.50
1:C:87:PRO:N	1:D:43:ALA:CA	2.69	0.50
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.34	0.50
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.93	0.50
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.50
2:C:812:NAG:O7	2:C:812:NAG:C1	2.60	0.50
2:D:807:NAG:O7	2:D:807:NAG:H3	2.11	0.50
2:B:812:NAG:O7	2:B:812:NAG:C1	2.60	0.50
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.90	0.50
1:D:352:ILE:CG1	1:D:388:VAL:HB	2.33	0.50
1:D:373:ASN:ND2	1:D:374:ASP:OD1	2.45	0.50
1:B:366:LYS:HG2	1:B:367:LEU:H	1.74	0.50
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.50
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.50
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.50
1:A:1:ASP:CA	1:B:24:ILE:HG21	2.32	0.49
1:C:81:VAL:HB	1:D:43:ALA:H	1.76	0.49
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.49
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.49
1:C:335:ALA:CB	3:C:811:NDG:C6	2.90	0.49
1:D:457:LEU:HD23	1:D:494:MET:SD	2.52	0.49
1:D:367:LEU:HB2	1:D:413:THR:O	2.12	0.49
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.49
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.49
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:D:154:ASP:O	2:D:801:NAG:C8	2.60	0.49
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.49
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.34	0.49
1:C:373:ASN:ND2	1:C:374:ASP:OD1	2.45	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
1:A:10:SER:CA	1:D:30:ARG:CD	2.89	0.49
1:D:419:VAL:HG22	2:D:809:NAG:H81	1.93	0.49
2:B:807:NAG:H3	2:B:807:NAG:O7	2.11	0.49
1:D:335:ALA:CB	3:D:811:NDG:C6	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:THR:H	2:D:803:NAG:HN2	1.60	0.49
1:C:86:SER:N	1:D:74:TYR:CD2	2.73	0.49
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.41	0.49
1:D:451:ASN:O	1:D:534:GLY:CA	2.60	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.92	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:D:402:LYS:C	1:D:403:ASN:O	2.46	0.49
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:C:68:ARG:HD3	1:C:100:ASP:CA	2.43	0.49
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.49
1:C:151:LEU:HD12	1:C:151:LEU:H	1.77	0.49
1:D:397:GLU:OE1	1:D:397:GLU:N	2.45	0.49
1:C:423:THR:HB	2:C:810:NAG:H83	1.94	0.49
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.49
1:D:68:ARG:HD3	1:D:100:ASP:CA	2.43	0.49
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.49
1:D:252:THR:CG2	1:D:253:PRO:HD2	2.43	0.49
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.49
1:A:87:PRO:O	1:B:2:TRP:CH2	2.66	0.49
1:D:423:THR:HB	2:D:810:NAG:H83	1.94	0.49
1:D:336:VAL:CG1	1:D:338:ARG:HB2	2.43	0.49
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.49
1:D:226:TYR:C	1:D:227:THR:HG23	2.33	0.49
1:D:224:LYS:HE3	2:D:806:NAG:H82	1.95	0.49
1:D:276:GLU:CG	1:D:277:SER:N	2.71	0.49
1:A:272:THR:CG2	1:A:273:THR:N	2.76	0.49
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.49
1:A:217:ASN:N	1:A:217:ASN:HD22	2.09	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.49
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.49
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.49
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.49
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.49
1:B:151:LEU:H	1:B:151:LEU:HD12	1.77	0.49
1:D:310:VAL:HG12	1:D:312:LEU:HG	1.95	0.49
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.49
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:PHE:CD2	1:D:75:VAL:HG23	2.44	0.49
1:A:89:GLU:OE1	1:B:2:TRP:CG	2.62	0.49
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.49
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.49
1:C:512:LEU:HD11	1:C:519:ASN:ND2	2.28	0.49
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.49
1:B:365:GLN:CG	1:B:365:GLN:O	2.54	0.49
1:D:216:ASP:HB2	1:D:217:ASN:ND2	2.27	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.49
2:D:809:NAG:H62	2:D:810:NAG:O6	2.13	0.49
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.49
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.49
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.49
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:C:397:GLU:N	1:C:397:GLU:OE1	2.45	0.49
1:B:87:PRO:HG2	1:C:2:TRP:CD1	2.47	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:D:449:ASP:CB	1:D:532:CYS:H	2.22	0.49
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.49
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.49
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.49
1:D:186:GLU:OE1	2:D:801:NAG:C6	2.59	0.49
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.60	0.49
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.49
1:C:363:GLN:C	1:C:364:ILE:HG23	2.32	0.49
1:D:151:LEU:H	1:D:151:LEU:HD12	1.78	0.49
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.95	0.49
1:D:250:PRO:O	1:D:255:TRP:CE3	2.66	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:B:84:ASN:O	1:C:24:ILE:CB	2.57	0.48
1:D:432:ASP:CB	1:D:464:ILE:HG21	2.43	0.48
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.48
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.48
1:B:278:ASN:N	1:B:278:ASN:HD22	2.05	0.48
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.48
1:C:67:ASP:OD2	1:C:69:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
1:C:151:LEU:O	1:C:152:LYS:HB2	2.13	0.48
1:D:109:THR:HG22	1:D:110:GLN:HG3	1.94	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.48
1:C:80:ALA:O	1:C:88:VAL:HG23	2.11	0.48
1:C:432:ASP:CB	1:C:464:ILE:HG21	2.43	0.48
1:D:513:LEU:C	1:D:514:SER:HG	2.16	0.48
2:A:807:NAG:H3	2:A:807:NAG:O7	2.11	0.48
1:D:224:LYS:CE	2:D:806:NAG:C8	2.91	0.48
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.48
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.48
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.48
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.48
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.48
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:A:403:ASN:HB2	3:A:902:NDG:H8C2	1.86	0.48
1:D:367:LEU:HD13	1:D:412:VAL:CG2	2.43	0.48
1:C:367:LEU:HD13	1:C:412:VAL:CG2	2.43	0.48
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.48
1:D:368:SER:OG	1:D:370:PHE:HE1	1.94	0.48
1:D:327:ASN:OD1	1:D:360:ASP:OD1	2.30	0.48
1:D:151:LEU:O	1:D:152:LYS:HB2	2.13	0.48
1:C:192:GLN:HA	1:C:203:VAL:O	2.13	0.48
1:C:250:PRO:O	1:C:255:TRP:CE3	2.66	0.48
1:C:32:ASN:HB3	1:D:75:VAL:HG23	1.94	0.48
1:A:8:LYS:CB	1:D:30:ARG:HH21	2.26	0.48
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
2:C:807:NAG:O7	2:C:807:NAG:H3	2.11	0.48
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.48
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:C:81:VAL:CG1	1:D:43:ALA:C	2.80	0.48
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.48
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.48
1:D:117:VAL:O	1:D:212:THR:N	2.46	0.48
1:D:154:ASP:CG	1:D:155:PRO:HD2	2.33	0.48
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.48
1:D:448:CYS:SG	1:D:537:ILE:CG2	3.01	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:A:483:TRP:CZ2	1:A:507:TYR:CE1	2.87	0.48
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.48
1:D:192:GLN:HA	1:D:203:VAL:O	2.13	0.48
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.48
1:A:10:SER:H	1:D:30:ARG:HG3	1.75	0.48
1:B:31:PHE:CG	1:C:30:ARG:N	2.57	0.48
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.48
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.48
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.48
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.48
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.48
1:A:397:GLU:OE1	1:A:397:GLU:N	2.44	0.48
1:A:5:PRO:N	1:B:91:PRO:CB	2.75	0.48
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.48
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.48
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.48
1:C:225:THR:HA	1:C:318:THR:O	2.14	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:B:281:ILE:HG23	1:B:281:ILE:O	2.13	0.48
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.48
1:B:397:GLU:OE1	1:B:397:GLU:N	2.45	0.48
1:D:41:GLN:HA	1:D:45:ASN:HB2	1.95	0.48
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.48
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.48
1:C:418:SER:O	1:C:419:VAL:HG23	2.14	0.48
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48
2:D:812:NAG:C1	2:D:812:NAG:O7	2.60	0.48
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:THR:H	2:C:803:NAG:HN2	1.60	0.48
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.48
1:D:119:GLU:OE2	1:D:216:ASP:OD1	2.32	0.48
1:D:27:ASN:C	1:D:29:ASP:H	2.15	0.48
1:D:512:LEU:HD11	1:D:519:ASN:ND2	2.28	0.48
2:C:809:NAG:H62	2:C:810:NAG:O6	2.13	0.48
1:D:241:ARG:HE	1:D:281:ILE:CD1	2.24	0.48
1:D:281:ILE:HG23	1:D:281:ILE:O	2.13	0.48
1:C:41:GLN:HA	1:C:45:ASN:HB2	1.96	0.48
1:D:150:ILE:HD11	1:D:165:ILE:HB	1.96	0.48
1:D:450:GLN:CG	1:D:533:GLU:OE2	2.58	0.47
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.47
1:D:225:THR:HA	1:D:318:THR:O	2.14	0.47
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.47
1:D:300:ILE:HD12	1:D:300:ILE:N	2.29	0.47
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.47
1:D:537:ILE:CG1	1:D:538:LYS:N	2.77	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:D:365:GLN:HA	1:D:416:GLY:HA3	1.95	0.47
1:D:282:LEU:CD2	1:D:283:THR:N	2.76	0.47
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.47
1:C:76:LEU:O	1:C:94:ILE:N	2.44	0.47
1:D:261:ILE:CD1	1:D:264:ASN:ND2	2.77	0.47
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.47
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.95	0.47
1:D:514:SER:CA	1:D:517:GLN:O	2.62	0.47
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.47
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.47
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.47
1:C:301:THR:CG2	1:C:316:THR:HG23	2.45	0.47
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.47
1:D:109:THR:HG22	1:D:110:GLN:CG	2.42	0.47
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.47
1:B:28:LYS:HG3	1:D:3:VAL:HG21	1.87	0.47
1:C:32:ASN:CA	1:D:75:VAL:CG2	2.88	0.47
1:D:8:LYS:CD	1:D:8:LYS:N	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.47
1:C:320:THR:CB	2:C:807:NAG:N2	2.78	0.47
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.47
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	0.47
1:D:67:ASP:OD2	1:D:69:GLU:HB2	2.13	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:C:50:VAL:HB	1:C:51:PHE:CD1	2.50	0.47
1:C:92:MET:HG3	1:D:79:HIS:ND1	2.29	0.47
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:B:300:ILE:N	1:B:300:ILE:HD12	2.30	0.47
1:D:320:THR:CB	2:D:807:NAG:N2	2.78	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:A:250:PRO:O	1:A:255:TRP:CE3	2.67	0.47
1:D:246:ASP:C	1:D:247:LEU:HD12	2.35	0.47
1:B:33:LYS:N	1:C:25:LYS:NZ	2.61	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
1:B:226:TYR:O	1:B:227:THR:HG23	2.14	0.47
1:D:373:ASN:CG	1:D:374:ASP:H	2.18	0.47
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.47
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.47
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.47
2:D:809:NAG:C6	2:D:810:NAG:C6	2.92	0.47
2:A:812:NAG:C1	2:A:812:NAG:O7	2.60	0.47
1:C:186:GLU:OE1	2:C:801:NAG:C6	2.59	0.47
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.47
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.47
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.47
1:D:23:GLN:HB2	1:D:59:TRP:CE3	2.50	0.47
1:A:90:GLU:CB	1:B:3:VAL:CG2	2.93	0.47
1:C:537:ILE:CG1	1:C:538:LYS:N	2.77	0.47
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:C:300:ILE:N	1:C:300:ILE:HD12	2.30	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.47
1:C:81:VAL:HG12	1:D:43:ALA:HB3	0.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:CG1	1:D:43:ALA:N	2.77	0.47
1:D:50:VAL:HB	1:D:51:PHE:CD1	2.50	0.47
1:B:539:CYS:HB3	1:B:540:GLN:H	1.46	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.47
1:B:271:ILE:HG23	1:B:271:ILE:O	2.15	0.47
1:A:8:LYS:HB3	1:D:30:ARG:HH21	1.79	0.47
1:B:88:VAL:CG1	1:C:27:ASN:OD1	2.60	0.47
1:C:82:SER:OG	1:D:41:GLN:O	2.12	0.47
1:D:418:SER:O	1:D:419:VAL:HG23	2.14	0.47
1:C:514:SER:CA	1:C:517:GLN:O	2.62	0.47
1:D:226:TYR:O	1:D:227:THR:HG23	2.15	0.47
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.47
1:C:272:THR:CG2	1:C:273:THR:N	2.76	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:A:89:GLU:O	1:B:1:ASP:C	2.54	0.46
1:A:4:ILE:C	1:B:91:PRO:CB	2.82	0.46
1:D:482:THR:HG22	1:D:499:THR:H	1.70	0.46
1:D:301:THR:CG2	1:D:316:THR:HG23	2.45	0.46
1:A:300:ILE:HD12	1:A:300:ILE:N	2.30	0.46
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:D:268:PHE:CA	1:D:285:ALA:HB3	2.45	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:C:88:VAL:N	1:D:38:ILE:HG12	2.30	0.46
1:D:36:TYR:O	1:D:55:TRP:HA	2.15	0.46
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.46
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.46
1:B:408:VAL:O	1:B:426:LEU:N	2.48	0.46
1:D:272:THR:HG23	2:D:803:NAG:HN2	1.81	0.46
1:D:363:GLN:O	1:D:364:ILE:CG2	2.63	0.46
1:C:310:VAL:HG12	1:C:311:PRO:O	2.15	0.46
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.46
1:B:31:PHE:CD2	1:C:29:ASP:OD2	2.69	0.46
1:A:449:ASP:N	1:A:532:CYS:HB3	2.19	0.46
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.46
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.46
1:D:194:THR:CG2	1:D:195:ASP:N	2.79	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.46
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.46
1:C:81:VAL:H	1:D:45:ASN:ND2	2.10	0.46
1:A:87:PRO:O	1:B:2:TRP:HZ2	1.83	0.46
1:C:539:CYS:HB3	1:C:540:GLN:H	1.45	0.46
1:D:155:PRO:O	1:D:157:GLU:N	2.43	0.46
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.46
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.97	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:D:506:ASP:N	1:D:506:ASP:OD1	2.49	0.46
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.46
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.46
1:D:54:GLU:HB2	1:D:57:THR:OG1	2.16	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:D:459:ILE:HD12	1:D:459:ILE:N	2.31	0.46
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.46
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.46
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
1:D:310:VAL:HG12	1:D:311:PRO:O	2.15	0.46
1:A:8:LYS:HE2	1:D:28:LYS:HG3	1.94	0.46
1:A:79:HIS:CA	1:B:1:ASP:N	2.70	0.46
1:C:3:VAL:HB	1:D:87:PRO:HB2	1.97	0.46
1:C:421:THR:HG21	2:C:809:NAG:H61	1.98	0.46
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.46
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.46
1:D:187:TYR:HE1	1:D:211:ILE:HD11	1.81	0.46
1:A:374:ASP:OD1	1:A:374:ASP:N	2.49	0.46
1:D:374:ASP:N	1:D:374:ASP:OD1	2.49	0.46
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.80	0.46
1:C:272:THR:HG23	2:C:803:NAG:HN2	1.80	0.46
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:C:31:PHE:C	1:D:73:LYS:CE	2.83	0.46
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	0.46
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.46
1:D:339:VAL:HG11	1:D:351:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.46
1:C:374:ASP:OD1	1:C:374:ASP:N	2.49	0.46
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.46
1:C:415:ASP:CG	1:C:416:GLY:H	2.16	0.46
1:D:100:ASP:OD1	1:D:101:GLN:N	2.49	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:C:90:GLU:N	1:D:78:SER:C	2.30	0.46
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.46
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.46
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.46
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.46
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.46
1:B:506:ASP:OD1	1:B:506:ASP:N	2.49	0.46
1:A:363:GLN:O	1:A:364:ILE:CG2	2.63	0.46
1:D:270:ASN:OD1	1:D:271:ILE:N	2.49	0.46
1:C:1:ASP:CA	1:D:28:LYS:CD	2.88	0.46
1:D:290:PHE:CE2	1:D:293:ARG:CB	2.92	0.46
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.46
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.46
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.46
1:D:524:VAL:HG21	2:D:904:NAG:C8	2.44	0.46
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.46
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.46
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:D:109:THR:CB	1:D:131:SER:HB2	2.46	0.46
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.45
1:B:30:ARG:NH1	1:C:30:ARG:CB	2.78	0.45
1:C:32:ASN:CA	1:D:75:VAL:HG23	2.44	0.45
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.45
1:D:461:ASP:HB3	1:D:468:THR:CG2	2.46	0.45
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:D:227:THR:HG22	1:D:320:THR:HB	1.99	0.45
2:D:805:NAG:C5	2:D:806:NAG:H83	2.46	0.45
1:B:374:ASP:OD1	1:B:374:ASP:N	2.49	0.45
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ASP:CG	1:D:416:GLY:H	2.16	0.45
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.45
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.45
1:C:1:ASP:O	1:D:28:LYS:HD3	2.16	0.45
1:C:28:LYS:CG	1:D:93:GLU:HG2	2.11	0.45
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.45
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.48	0.45
1:D:408:VAL:O	1:D:426:LEU:N	2.49	0.45
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45
1:C:514:SER:HG	1:C:519:ASN:HA	1.81	0.45
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.45
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.45
1:C:371:ILE:HA	1:C:371:ILE:HD12	1.65	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.17	0.45
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.45
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.45
1:A:298:LEU:CD2	1:A:298:LEU:N	2.75	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:D:108:PHE:HE1	1:D:203:VAL:HG23	1.80	0.45
1:D:271:ILE:HG23	1:D:271:ILE:O	2.15	0.45
1:B:85:GLY:N	1:C:25:LYS:O	2.47	0.45
1:D:473:VAL:CG2	1:D:487:LEU:HD21	2.47	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:C:506:ASP:OD1	1:C:506:ASP:N	2.49	0.45
1:D:152:LYS:O	1:D:189:LEU:HA	2.17	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:C:1:ASP:C	1:D:28:LYS:HD3	2.37	0.45
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.45
1:C:187:TYR:HE1	1:C:211:ILE:HD11	1.81	0.45
1:B:8:LYS:N	1:B:8:LYS:CD	2.51	0.45
1:D:440:PRO:HB3	1:D:457:LEU:CD2	2.43	0.45
1:D:381:VAL:HA	1:D:387:ILE:O	2.17	0.45
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.45
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.45
1:D:421:THR:HG21	2:D:809:NAG:H61	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
1:C:93:GLU:CB	1:D:81:VAL:CG1	2.79	0.45
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.45
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.45
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:D:266:GLY:N	1:D:268:PHE:CE2	2.76	0.45
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.45
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.45
1:D:449:ASP:CB	1:D:532:CYS:N	2.74	0.45
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.45
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.45
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:A:367:LEU:HG	1:A:367:LEU:H	1.41	0.45
1:C:381:VAL:HA	1:C:387:ILE:O	2.17	0.45
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.45
1:A:481:LEU:HA	1:A:481:LEU:HD12	1.50	0.45
1:D:450:GLN:CB	1:D:533:GLU:OE2	2.64	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
1:A:426:LEU:HD13	1:A:426:LEU:C	2.37	0.45
1:D:336:VAL:HG11	1:D:338:ARG:HD2	1.99	0.45
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.45
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.45
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.45
1:C:298:LEU:CD2	1:C:298:LEU:N	2.75	0.45
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.45
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.45
1:C:426:LEU:C	1:C:426:LEU:HD13	2.37	0.45
1:C:117:VAL:O	1:C:212:THR:N	2.46	0.45
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	0.45
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.45
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.45
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.45
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.45
1:D:162:LEU:HB2	1:D:163:PHE:CE1	2.52	0.45
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.45
1:D:109:THR:HB	1:D:131:SER:HB2	1.99	0.45
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.45
1:A:1:ASP:OD1	1:B:24:ILE:HB	2.17	0.45
1:C:78:SER:O	1:D:39:THR:HG21	2.17	0.45
1:D:482:THR:O	1:D:483:TRP:CD2	2.70	0.45
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.45
1:D:262:ARG:HG3	1:D:299:GLN:HB2	1.97	0.45
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.45
1:C:31:PHE:O	1:D:73:LYS:NZ	2.47	0.45
1:D:286:LYS:C	1:D:287:GLY:O	2.55	0.45
1:D:469:TYR:CD2	1:D:470:PRO:N	2.85	0.45
1:D:187:TYR:CE1	1:D:211:ILE:HD11	2.52	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.45
1:D:485:ALA:O	1:D:486:GLU:OE1	2.35	0.45
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.45
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.45
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.45
1:A:36:TYR:CE2	1:D:2:TRP:CH2	3.00	0.44
1:C:79:HIS:HB3	1:D:39:THR:HB	1.96	0.44
1:C:3:VAL:CB	1:D:87:PRO:HB2	2.47	0.44
1:D:227:THR:N	2:D:812:NAG:H2	2.31	0.44
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.44
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.44
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.44
1:B:31:PHE:CE1	1:D:75:VAL:HG12	2.38	0.44
1:B:30:ARG:CZ	1:C:30:ARG:HB3	2.47	0.44
1:C:83:GLU:N	1:D:41:GLN:CD	2.66	0.44
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.44
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.44
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	0.44
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.44
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.47	0.44
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.44
1:D:312:LEU:O	3:D:804:NDG:H8C1	2.17	0.44
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.44
1:D:519:ASN:CG	1:D:519:ASN:O	2.55	0.44
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:439:VAL:HA	1:B:440:PRO:HD3	1.81	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:C:84:ASN:C	1:D:74:TYR:HE2	2.07	0.44
1:D:28:LYS:CD	1:D:88:VAL:HG12	2.38	0.44
1:A:86:SER:HA	1:A:87:PRO:HD3	1.83	0.44
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.44
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44
1:D:374:ASP:C	1:D:375:PRO:O	2.54	0.44
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.44
1:D:511:VAL:N	1:D:523:THR:O	2.46	0.44
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.44
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	0.44
1:B:31:PHE:O	1:C:29:ASP:C	2.56	0.44
1:C:85:GLY:CA	1:D:47:PRO:HD2	2.48	0.44
1:D:232:GLU:HA	1:D:288:LEU:HD12	1.99	0.44
1:D:224:LYS:HE3	2:D:806:NAG:C8	2.48	0.44
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:D:380:THR:CG2	1:D:381:VAL:N	2.79	0.44
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.44
1:D:67:ASP:OD1	1:D:69:GLU:HB2	2.18	0.44
1:A:252:THR:HA	1:A:253:PRO:HD3	1.81	0.44
1:D:421:THR:CG2	1:D:422:GLY:N	2.81	0.44
1:D:290:PHE:CD2	1:D:293:ARG:O	2.71	0.44
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.44
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.44
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.44
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.44
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.44
1:C:152:LYS:O	1:C:189:LEU:HA	2.17	0.44
1:C:220:ILE:O	1:C:220:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:HA	1:D:38:ILE:HD11	1.99	0.44
1:D:155:PRO:CB	2:D:801:NAG:C8	2.94	0.44
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.44
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.44
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.44
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.44
1:D:261:ILE:HD11	1:D:264:ASN:ND2	2.32	0.44
1:D:435:ASP:HB2	1:D:436:ASN:H	1.58	0.44
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.44
1:A:92:MET:HB2	1:B:1:ASP:CB	2.48	0.44
1:A:3:VAL:HG21	1:B:77:SER:HA	2.00	0.44
1:A:540:GLN:O	1:A:540:GLN:NE2	2.47	0.44
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.44
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.44
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.44
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.44
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.44
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.44
1:B:3:VAL:HB	1:B:4:ILE:H	1.51	0.43
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:C:469:TYR:CD2	1:C:470:PRO:N	2.85	0.43
1:D:468:THR:C	1:D:469:TYR:O	2.54	0.43
1:D:469:TYR:CE2	1:D:470:PRO:HB2	2.52	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.33	0.43
1:C:485:ALA:O	1:C:486:GLU:OE1	2.35	0.43
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.36	0.43
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.43
1:B:151:LEU:N	1:B:151:LEU:HD12	2.33	0.43
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.43
1:A:8:LYS:CB	1:D:30:ARG:HE	2.30	0.43
1:A:92:MET:CG	1:B:3:VAL:HG12	2.47	0.43
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.43
1:B:419:VAL:HG13	1:B:420:GLY:N	2.33	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
2:D:805:NAG:H62	2:D:806:NAG:N2	2.31	0.43
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.43
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.43
1:D:220:ILE:O	1:D:220:ILE:HG22	2.18	0.43
1:C:89:GLU:HB3	1:D:78:SER:O	2.01	0.43
1:D:426:LEU:C	1:D:426:LEU:HD13	2.37	0.43
1:B:232:GLU:HA	1:B:288:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLN:HG3	1:B:532:CYS:O	2.10	0.43
1:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.43
1:A:299:GLN:CG	1:A:318:THR:HG23	2.42	0.43
1:C:511:VAL:N	1:C:523:THR:O	2.46	0.43
1:A:335:ALA:HB3	3:A:811:NDG:O6	2.15	0.43
1:D:441:SER:CB	1:D:442:PRO:HD3	2.47	0.43
1:C:92:MET:CE	1:D:91:PRO:CG	2.97	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:C:290:PHE:CD2	1:C:293:ARG:O	2.71	0.43
1:C:441:SER:CB	1:C:442:PRO:HD3	2.47	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:C:128:MET:HB3	1:C:129:ALA:H	1.62	0.43
1:D:128:MET:HB3	1:D:129:ALA:H	1.62	0.43
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.43
1:A:247:LEU:N	1:A:247:LEU:HD12	2.33	0.43
1:D:419:VAL:HG13	1:D:420:GLY:N	2.33	0.43
1:D:461:ASP:HB3	1:D:468:THR:HG22	2.00	0.43
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.43
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.43
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.43
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.43
1:D:380:THR:HG22	1:D:381:VAL:N	2.32	0.43
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.43
1:D:247:LEU:N	1:D:247:LEU:HD12	2.33	0.43
1:D:3:VAL:HB	1:D:4:ILE:H	1.51	0.43
1:C:31:PHE:C	1:D:75:VAL:CG2	2.79	0.43
1:A:4:ILE:HB	1:B:90:GLU:HB3	1.48	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:D:335:ALA:HB3	3:D:811:NDG:O6	2.15	0.43
1:D:442:PRO:HD2	1:D:457:LEU:HD12	2.00	0.43
1:D:194:THR:HG23	1:D:201:LEU:O	2.18	0.43
1:D:368:SER:CB	1:D:370:PHE:HE1	2.31	0.43
1:D:249:MET:HA	1:D:250:PRO:HD3	1.85	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:B:32:ASN:HA	1:C:29:ASP:CG	2.36	0.43
1:B:83:GLU:HB3	1:C:25:LYS:HB2	1.45	0.43
1:B:540:GLN:NE2	1:B:540:GLN:O	2.47	0.43
1:D:450:GLN:HG3	1:D:532:CYS:O	2.10	0.43
1:C:155:PRO:CB	2:C:801:NAG:C8	2.94	0.43
1:D:134:ASP:HB2	1:D:146:LEU:HD11	1.99	0.43
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:CA	1:B:24:ILE:CD1	2.95	0.43
1:D:22:VAL:CG2	1:D:23:GLN:N	2.81	0.43
1:A:9:VAL:O	1:D:30:ARG:CD	2.62	0.43
1:A:79:HIS:CA	1:B:1:ASP:H1	2.30	0.43
1:D:32:ASN:HD22	1:D:83:GLU:N	2.13	0.43
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.43
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.43
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.43
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.43
1:C:344:ASP:CG	1:C:344:ASP:O	2.57	0.43
1:D:175:ILE:CG2	1:D:176:GLY:N	2.82	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:D:367:LEU:H	1:D:367:LEU:HG	1.41	0.43
1:D:371:ILE:HG13	1:D:410:MET:SD	2.59	0.43
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.43
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.43
1:A:24:ILE:O	1:D:2:TRP:CH2	2.58	0.43
1:C:519:ASN:O	1:C:519:ASN:CG	2.55	0.43
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.43
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.43
1:D:138:ASN:ND2	1:D:138:ASN:C	2.73	0.43
1:D:344:ASP:CG	1:D:344:ASP:O	2.57	0.43
1:D:354:LEU:HD12	1:D:386:GLY:O	2.18	0.43
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.42
1:D:339:VAL:HG21	1:D:351:ILE:HG22	2.01	0.42
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.42
1:C:524:VAL:HG21	2:C:904:NAG:C8	2.44	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.42
1:D:298:LEU:N	1:D:298:LEU:CD2	2.75	0.42
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.42
1:A:344:ASP:O	1:A:344:ASP:CG	2.57	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.42
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.42
1:D:518:ASN:C	1:D:520:PRO:CD	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.42
1:C:490:LYS:CG	1:C:490:LYS:O	2.67	0.42
1:C:261:ILE:HD13	1:C:261:ILE:H	1.85	0.42
1:B:435:ASP:HB2	1:B:436:ASN:H	1.58	0.42
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.72	0.42
1:C:450:GLN:HG3	1:C:532:CYS:O	2.10	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:C:88:VAL:O	1:D:94:ILE:CD1	2.50	0.42
1:A:92:MET:HG2	1:B:3:VAL:HG12	2.01	0.42
1:C:5:PRO:HA	1:C:6:PRO:HD3	1.85	0.42
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.42
1:D:409:ILE:HD13	3:D:811:NDG:H8C3	2.01	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.42
1:D:333:VAL:HG23	1:D:334:PRO:HD3	2.01	0.42
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42
1:C:247:LEU:N	1:C:247:LEU:HD12	2.33	0.42
1:C:515:ASP:OD1	1:C:516:ALA:N	2.53	0.42
1:C:88:VAL:N	1:D:38:ILE:CG1	2.82	0.42
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.85	0.42
1:D:482:THR:HG23	1:D:499:THR:HG23	1.88	0.42
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.42
1:D:448:CYS:C	1:D:452:PRO:HG3	2.40	0.42
1:D:347:ARG:HD2	1:D:392:GLY:CA	2.49	0.42
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.42
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.42
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.42
1:C:89:GLU:CD	1:D:92:MET:H	2.22	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42
1:D:469:TYR:CE2	1:D:470:PRO:HD2	2.54	0.42
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:D:195:ASP:HB3	1:D:196:LEU:HG	2.01	0.42
1:C:252:THR:HA	1:C:253:PRO:HD3	1.81	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:D:261:ILE:HD13	1:D:261:ILE:H	1.85	0.42
1:D:264:ASN:HB3	1:D:267:GLY:HA2	2.01	0.42
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.42
1:C:83:GLU:CA	1:D:41:GLN:OE1	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:THR:H	2:D:801:NAG:H83	1.84	0.42
1:D:297:VAL:HG21	2:D:807:NAG:H62	2.01	0.42
1:C:367:LEU:HG	1:C:367:LEU:H	1.41	0.42
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.42
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.42
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.42
1:D:250:PRO:HA	1:D:255:TRP:CG	2.54	0.42
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.42
1:B:502:LEU:HD23	1:B:502:LEU:HA	1.82	0.42
1:D:7:ILE:O	1:D:96:ILE:HG23	2.20	0.42
1:B:84:ASN:O	1:C:24:ILE:CA	2.68	0.42
1:B:87:PRO:CG	1:C:2:TRP:CB	2.94	0.42
1:B:87:PRO:HG2	1:D:90:GLU:H	1.82	0.42
1:D:483:TRP:CZ2	1:D:507:TYR:CE1	2.87	0.42
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.42
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.42
1:D:67:ASP:CG	1:D:69:GLU:HB2	2.40	0.42
1:D:151:LEU:N	1:D:151:LEU:HD12	2.33	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.42
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:B:344:ASP:CG	1:B:344:ASP:O	2.57	0.42
1:B:87:PRO:CG	1:C:2:TRP:CD1	3.03	0.42
1:D:231:PRO:O	1:D:288:LEU:HD12	2.20	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.42
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.42
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.42
1:B:31:PHE:CE2	1:C:27:ASN:N	2.78	0.42
1:C:90:GLU:HG2	1:D:36:TYR:HA	1.43	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:C:8:LYS:CD	1:C:8:LYS:N	2.51	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:C:366:LYS:HG2	1:C:367:LEU:H	1.74	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.42
1:D:490:LYS:CG	1:D:490:LYS:O	2.67	0.42
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.42
1:C:237:PHE:N	1:C:284:THR:OG1	2.42	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.52	0.42
1:B:81:VAL:HG12	1:D:90:GLU:HG2	2.02	0.41
1:A:5:PRO:HG3	1:B:91:PRO:HG2	1.22	0.41
2:D:810:NAG:C1	2:D:810:NAG:O7	2.67	0.41
1:A:212:THR:CG2	1:A:213:ASP:H	2.32	0.41
1:D:522:LEU:HB3	1:D:523:THR:H	1.57	0.41
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.41
1:C:250:PRO:HA	1:C:255:TRP:CG	2.54	0.41
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.41
1:D:4:ILE:HA	1:D:5:PRO:HD3	1.72	0.41
1:B:367:LEU:HG	1:B:367:LEU:H	1.41	0.41
1:D:272:THR:CG2	1:D:273:THR:N	2.76	0.41
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.41
1:B:250:PRO:HA	1:B:255:TRP:CG	2.54	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:A:4:ILE:HB	1:B:90:GLU:C	2.39	0.41
1:D:474:SER:N	1:D:512:LEU:O	2.53	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:B:212:THR:CG2	1:B:213:ASP:H	2.32	0.41
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.41
1:C:231:PRO:O	1:C:235:ILE:HD13	2.21	0.41
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.41
1:C:347:ARG:HG3	1:C:392:GLY:N	2.33	0.41
1:D:230:VAL:O	1:D:323:VAL:HA	2.20	0.41
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.41
1:C:502:LEU:HD22	1:C:503:LYS:H	1.85	0.41
1:A:515:ASP:OD1	1:A:516:ALA:N	2.52	0.41
1:C:1:ASP:HB2	1:D:89:GLU:HG2	1.11	0.41
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.41
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.41
2:A:810:NAG:C1	2:A:810:NAG:O7	2.67	0.41
1:C:231:PRO:O	1:C:288:LEU:HD12	2.20	0.41
1:C:522:LEU:HA	1:C:522:LEU:HD23	1.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.41
1:D:108:PHE:HA	1:D:132:ALA:CB	2.50	0.41
1:C:32:ASN:ND2	1:C:83:GLU:CB	2.62	0.41
1:D:23:GLN:HB2	1:D:59:TRP:CD2	2.55	0.41
1:D:231:PRO:O	1:D:235:ILE:HD13	2.21	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.41
1:D:347:ARG:HG3	1:D:392:GLY:N	2.33	0.41
1:D:371:ILE:HA	1:D:410:MET:HB3	2.02	0.41
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:D:108:PHE:HA	1:D:132:ALA:HB2	2.03	0.41
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.41
1:D:111:ASP:O	1:D:112:VAL:HG13	2.21	0.41
1:D:515:ASP:OD1	1:D:516:ALA:N	2.52	0.41
1:A:4:ILE:HD12	1:B:90:GLU:HB3	1.53	0.41
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.41
1:B:118:ARG:CA	1:B:212:THR:HB	2.51	0.41
1:D:118:ARG:CA	1:D:212:THR:HB	2.51	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.41
1:D:68:ARG:HD3	1:D:100:ASP:CB	2.51	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.41
1:C:88:VAL:N	1:D:38:ILE:HD11	2.36	0.41
1:C:474:SER:N	1:C:512:LEU:O	2.54	0.41
1:D:297:VAL:HG22	2:D:807:NAG:H62	2.03	0.41
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.41
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.41
1:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.41
1:A:62:VAL:HG13	1:A:62:VAL:O	2.21	0.41
1:A:36:TYR:CZ	1:D:2:TRP:HH2	2.39	0.41
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.41
1:C:540:GLN:NE2	1:C:540:GLN:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:CG2	1:C:213:ASP:H	2.32	0.41
1:C:274:ASP:HA	1:C:275:PRO:HD3	1.93	0.41
1:A:448:CYS:C	1:A:452:PRO:HG3	2.40	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:B:490:LYS:CG	1:B:490:LYS:O	2.67	0.41
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.41
1:C:33:LYS:NZ	1:C:56:GLU:OE1	2.42	0.41
1:D:432:ASP:CG	1:D:433:VAL:N	2.74	0.41
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.41
1:A:432:ASP:CG	1:A:433:VAL:N	2.74	0.41
1:D:449:ASP:HB2	1:D:531:SER:HA	2.03	0.41
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.41
1:C:297:VAL:HG22	2:C:807:NAG:H62	2.03	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.54	0.41
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.41
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.41
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.41
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.41
1:D:127:VAL:HG22	1:D:128:MET:HG3	2.03	0.41
1:C:239:VAL:HG13	1:C:240:GLN:N	2.33	0.41
1:D:239:VAL:HG11	1:D:282:LEU:HD22	2.02	0.41
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:D:119:GLU:CG	1:D:214:ALA:HB3	2.51	0.41
1:B:261:ILE:HD13	1:B:261:ILE:H	1.85	0.41
1:C:62:VAL:O	1:C:62:VAL:HG13	2.21	0.41
1:C:84:ASN:C	1:D:74:TYR:CZ	2.90	0.41
1:B:249:MET:O	1:B:252:THR:CB	2.69	0.41
1:C:252:THR:O	1:C:255:TRP:N	2.54	0.41
1:D:62:VAL:O	1:D:62:VAL:HG13	2.21	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
2:C:810:NAG:C1	2:C:810:NAG:O7	2.67	0.40
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.40
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.40
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.40
1:D:522:LEU:HD23	1:D:522:LEU:HA	1.36	0.40
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.40
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:GLY:H	1:D:529:VAL:HB	1.85	0.40
1:D:259:TYR:O	1:D:260:LYS:CB	2.69	0.40
1:A:490:LYS:CG	1:A:490:LYS:O	2.67	0.40
1:B:119:GLU:CG	1:B:214:ALA:HB3	2.51	0.40
1:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.40
1:D:138:ASN:HD22	1:D:138:ASN:N	2.19	0.40
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.40
1:D:502:LEU:HD22	1:D:503:LYS:H	1.85	0.40
1:D:316:THR:OG1	2:D:806:NAG:H83	2.21	0.40
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.40
1:C:400:TYR:O	1:C:401:VAL:C	2.59	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:D:108:PHE:CZ	1:D:191:VAL:HG23	2.56	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:D:252:THR:HA	1:D:253:PRO:HD3	1.81	0.40
1:B:19:LYS:HB3	1:B:62:VAL:CG1	2.52	0.40
1:A:19:LYS:HB3	1:A:62:VAL:HG12	2.03	0.40
1:C:79:HIS:CB	1:D:39:THR:HB	2.35	0.40
1:D:23:GLN:HA	1:D:58:GLY:O	2.21	0.40
1:D:154:ASP:HB3	2:D:801:NAG:C7	2.48	0.40
1:C:290:PHE:CG	1:C:292:LEU:HB2	2.56	0.40
1:D:299:GLN:CG	1:D:318:THR:HG23	2.42	0.40
1:A:272:THR:O	1:A:281:ILE:HG22	2.22	0.40
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.40
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.40
1:C:249:MET:O	1:C:252:THR:CB	2.69	0.40
1:C:249:MET:HA	1:C:250:PRO:HD3	1.85	0.40
1:D:249:MET:O	1:D:252:THR:CB	2.69	0.40
1:C:34:VAL:CG1	1:C:80:ALA:HB1	2.52	0.40
1:D:34:VAL:CG1	1:D:80:ALA:HB1	2.52	0.40
1:C:90:GLU:HB3	1:D:79:HIS:H	1.59	0.40
1:C:396:ARG:HH21	1:C:432:ASP:CG	2.25	0.40
1:C:469:TYR:CE2	1:C:470:PRO:HD2	2.54	0.40
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.40
1:C:329:ALA:HA	1:C:330:PRO:HD3	1.87	0.40
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.40
1:D:409:ILE:HD13	3:D:811:NDG:C8	2.51	0.40
1:B:274:ASP:HA	1:B:275:PRO:HD3	1.93	0.40
1:D:230:VAL:HG23	1:D:323:VAL:HA	2.03	0.40
1:D:345:LEU:HD22	1:D:349:GLU:HB2	2.03	0.40
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ASN:ND2	1:C:385:ASN:O	2.55	0.40
1:D:385:ASN:ND2	1:D:385:ASN:O	2.55	0.40
1:A:261:ILE:H	1:A:261:ILE:HD13	1.85	0.40
1:D:19:LYS:HB3	1:D:62:VAL:HG12	2.03	0.40
1:D:193:ALA:O	1:D:202:SER:HA	2.21	0.40
1:C:87:PRO:O	1:D:38:ILE:CD1	2.68	0.40
1:A:396:ARG:HH21	1:A:432:ASP:CG	2.25	0.40
1:A:482:THR:HG22	1:A:499:THR:H	1.70	0.40
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.40
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
1:C:259:TYR:O	1:C:260:LYS:CB	2.69	0.40
1:A:249:MET:O	1:A:252:THR:CB	2.69	0.40
1:B:385:ASN:ND2	1:B:385:ASN:O	2.55	0.40
1:D:19:LYS:HB3	1:D:62:VAL:CG1	2.52	0.40
1:C:445:PHE:CD2	1:C:445:PHE:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/880 (61%)	402 (75%)	91 (17%)	45 (8%)	1	18
1	B	538/880 (61%)	401 (74%)	93 (17%)	44 (8%)	1	18
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
1	D	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
All	All	2152/3520 (61%)	1605 (75%)	368 (17%)	179 (8%)	2	18

All (179) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	B	91	PRO
1	B	155	PRO
1	B	235	ILE
1	B	347	ARG
1	B	363	GLN
1	B	364	ILE
1	B	374	ASP
1	B	404	ASN
1	B	467	ASN
1	B	476	SER
1	B	502	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	C	91	PRO
1	C	155	PRO
1	C	235	ILE
1	C	347	ARG
1	C	363	GLN
1	C	364	ILE
1	C	374	ASP
1	C	404	ASN
1	C	467	ASN
1	C	476	SER
1	C	502	LEU
1	C	517	GLN
1	C	518	ASN
1	C	519	ASN
1	D	91	PRO

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Mol	Chain	Res	Type
1	D	155	PRO
1	D	235	ILE
1	D	347	ARG
1	D	363	GLN
1	D	364	ILE
1	D	374	ASP
1	D	404	ASN
1	D	467	ASN
1	D	476	SER
1	D	502	LEU
1	D	517	GLN
1	D	518	ASN
1	D	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	B	3	VAL
1	B	156	GLU
1	B	260	LYS
1	B	287	GLY
1	B	470	PRO
1	B	503	LYS
1	C	3	VAL
1	C	156	GLU
1	C	260	LYS
1	C	287	GLY
1	C	470	PRO
1	C	503	LYS
1	D	3	VAL
1	D	156	GLU
1	D	260	LYS
1	D	287	GLY
1	D	470	PRO
1	D	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP

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Mol	Chain	Res	Type
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP
1	B	55	TRP
1	B	212	THR
1	B	250	PRO
1	B	333	VAL
1	B	360	ASP
1	B	372	GLY
1	B	377	ARG
1	B	506	ASP
1	C	55	TRP
1	C	212	THR
1	C	250	PRO
1	C	333	VAL
1	C	360	ASP
1	C	372	GLY
1	C	377	ARG
1	C	506	ASP
1	D	55	TRP
1	D	212	THR
1	D	250	PRO
1	D	333	VAL
1	D	360	ASP
1	D	372	GLY
1	D	377	ARG
1	D	506	ASP
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	B	152	LYS
1	B	223	PRO
1	B	359	PRO
1	B	375	PRO
1	C	152	LYS
1	C	223	PRO
1	C	359	PRO
1	C	375	PRO
1	D	152	LYS
1	D	223	PRO
1	D	359	PRO

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Mol	Chain	Res	Type
1	D	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN
1	A	289	ASP
1	A	482	THR
1	B	160	PRO
1	B	265	GLU
1	B	278	ASN
1	B	289	ASP
1	B	482	THR
1	C	160	PRO
1	C	265	GLU
1	C	278	ASN
1	C	289	ASP
1	C	482	THR
1	D	160	PRO
1	D	265	GLU
1	D	278	ASN
1	D	289	ASP
1	D	482	THR
1	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	C	498	PRO
1	C	523	THR
1	D	498	PRO
1	D	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP
1	B	307	PRO
1	C	154	ASP
1	C	307	PRO
1	D	154	ASP
1	D	307	PRO
1	A	222	ASP
1	B	222	ASP
1	C	222	ASP
1	D	222	ASP
1	A	200	GLY

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Mol	Chain	Res	Type
1	B	200	GLY
1	C	200	GLY
1	D	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	C	47	PRO
1	C	158	PRO
1	D	47	PRO
1	D	158	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	C	480/779 (62%)	381 (79%)	99 (21%)	1	10
1	D	480/779 (62%)	381 (79%)	99 (21%)	1	10
All	All	1920/3116 (62%)	1524 (79%)	396 (21%)	4	10

All (396) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET

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Mol	Chain	Res	Type
1	A	117	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	156	GLU
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	250	PRO
1	A	253	PRO
1	A	261	ILE
1	A	264	ASN
1	A	268	PHE
1	A	273	THR
1	A	277	SER
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU
1	A	309	SER
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU
1	A	353	SER

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Mol	Chain	Res	Type
1	A	354	LEU
1	A	360	ASP
1	A	363	GLN
1	A	364	ILE
1	A	365	GLN
1	A	371	ILE
1	A	373	ASN
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	385	ASN
1	A	393	ASN
1	A	394	LEU
1	A	395	ASP
1	A	398	SER
1	A	399	GLU
1	A	404	ASN
1	A	405	THR
1	A	407	THR
1	A	410	MET
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	428	LEU
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	461	ASP
1	A	464	ILE
1	A	465	PRO
1	A	466	PRO
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	520	PRO

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Mol	Chain	Res	Type
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	540	GLN
1	B	8	LYS
1	B	18	PRO
1	B	19	LYS
1	B	27	ASN
1	B	52	ARG
1	B	61	LEU
1	B	66	LEU
1	B	68	ARG
1	B	88	VAL
1	B	91	PRO
1	B	92	MET
1	B	117	VAL
1	B	138	ASN
1	B	146	LEU
1	B	151	LEU
1	B	155	PRO
1	B	156	GLU
1	B	161	ASN
1	B	163	PHE
1	B	189	LEU
1	B	195	ASP
1	B	202	SER
1	B	216	ASP
1	B	217	ASN
1	B	223	PRO
1	B	226	TYR
1	B	231	PRO
1	B	233	ASN
1	B	234	GLU
1	B	235	ILE
1	B	237	PHE
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE
1	B	264	ASN
1	B	268	PHE
1	B	273	THR
1	B	277	SER

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Mol	Chain	Res	Type
1	B	278	ASN
1	B	282	LEU
1	B	284	THR
1	B	288	LEU
1	B	298	LEU
1	B	309	SER
1	B	310	VAL
1	B	315	SER
1	B	316	THR
1	B	318	THR
1	B	333	VAL
1	B	336	VAL
1	B	339	VAL
1	B	345	LEU
1	B	353	SER
1	B	354	LEU
1	B	360	ASP
1	B	363	GLN
1	B	364	ILE
1	B	365	GLN
1	B	371	ILE
1	B	373	ASN
1	B	375	PRO
1	B	379	LEU
1	B	382	ASN
1	B	384	ASP
1	B	385	ASN
1	B	393	ASN
1	B	394	LEU
1	B	395	ASP
1	B	398	SER
1	B	399	GLU
1	B	404	ASN
1	B	405	THR
1	B	407	THR
1	B	410	MET
1	B	423	THR
1	B	425	THR
1	B	427	ILE
1	B	428	LEU
1	B	433	VAL
1	B	436	ASN

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Mol	Chain	Res	Type
1	B	447	MET
1	B	448	CYS
1	B	461	ASP
1	B	464	ILE
1	B	465	PRO
1	B	466	PRO
1	B	470	PRO
1	B	477	HIS
1	B	492	THR
1	B	509	ILE
1	B	512	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	B	520	PRO
1	B	522	LEU
1	B	523	THR
1	B	532	CYS
1	B	540	GLN
1	C	8	LYS
1	C	18	PRO
1	C	19	LYS
1	C	27	ASN
1	C	52	ARG
1	C	61	LEU
1	C	66	LEU
1	C	68	ARG
1	C	88	VAL
1	C	91	PRO
1	C	92	MET
1	C	117	VAL
1	C	138	ASN
1	C	146	LEU
1	C	151	LEU
1	C	155	PRO
1	C	156	GLU
1	C	161	ASN
1	C	163	PHE
1	C	189	LEU
1	C	195	ASP
1	C	202	SER
1	C	216	ASP

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Mol	Chain	Res	Type
1	C	217	ASN
1	C	223	PRO
1	C	226	TYR
1	C	231	PRO
1	C	233	ASN
1	C	234	GLU
1	C	235	ILE
1	C	237	PHE
1	C	250	PRO
1	C	253	PRO
1	C	261	ILE
1	C	264	ASN
1	C	268	PHE
1	C	273	THR
1	C	277	SER
1	C	278	ASN
1	C	282	LEU
1	C	284	THR
1	C	288	LEU
1	C	298	LEU
1	C	309	SER
1	C	310	VAL
1	C	315	SER
1	C	316	THR
1	C	318	THR
1	C	333	VAL
1	C	336	VAL
1	C	339	VAL
1	C	345	LEU
1	C	353	SER
1	C	354	LEU
1	C	360	ASP
1	C	363	GLN
1	C	364	ILE
1	C	365	GLN
1	C	371	ILE
1	C	373	ASN
1	C	375	PRO
1	C	379	LEU
1	C	382	ASN
1	C	384	ASP
1	C	385	ASN

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Mol	Chain	Res	Type
1	C	393	ASN
1	C	394	LEU
1	C	395	ASP
1	C	398	SER
1	C	399	GLU
1	C	404	ASN
1	C	405	THR
1	C	407	THR
1	C	410	MET
1	C	423	THR
1	C	425	THR
1	C	427	ILE
1	C	428	LEU
1	C	433	VAL
1	C	436	ASN
1	C	447	MET
1	C	448	CYS
1	C	461	ASP
1	C	464	ILE
1	C	465	PRO
1	C	466	PRO
1	C	470	PRO
1	C	477	HIS
1	C	492	THR
1	C	509	ILE
1	C	512	LEU
1	C	517	GLN
1	C	518	ASN
1	C	519	ASN
1	C	520	PRO
1	C	522	LEU
1	C	523	THR
1	C	532	CYS
1	C	540	GLN
1	D	8	LYS
1	D	18	PRO
1	D	19	LYS
1	D	27	ASN
1	D	52	ARG
1	D	61	LEU
1	D	66	LEU
1	D	68	ARG

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Mol	Chain	Res	Type
1	D	88	VAL
1	D	91	PRO
1	D	92	MET
1	D	117	VAL
1	D	138	ASN
1	D	146	LEU
1	D	151	LEU
1	D	155	PRO
1	D	156	GLU
1	D	161	ASN
1	D	163	PHE
1	D	189	LEU
1	D	195	ASP
1	D	202	SER
1	D	216	ASP
1	D	217	ASN
1	D	223	PRO
1	D	226	TYR
1	D	231	PRO
1	D	233	ASN
1	D	234	GLU
1	D	235	ILE
1	D	237	PHE
1	D	250	PRO
1	D	253	PRO
1	D	261	ILE
1	D	264	ASN
1	D	268	PHE
1	D	273	THR
1	D	277	SER
1	D	278	ASN
1	D	282	LEU
1	D	284	THR
1	D	288	LEU
1	D	298	LEU
1	D	309	SER
1	D	310	VAL
1	D	315	SER
1	D	316	THR
1	D	318	THR
1	D	333	VAL
1	D	336	VAL

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Mol	Chain	Res	Type
1	D	339	VAL
1	D	345	LEU
1	D	353	SER
1	D	354	LEU
1	D	360	ASP
1	D	363	GLN
1	D	364	ILE
1	D	365	GLN
1	D	371	ILE
1	D	373	ASN
1	D	375	PRO
1	D	379	LEU
1	D	382	ASN
1	D	384	ASP
1	D	385	ASN
1	D	393	ASN
1	D	394	LEU
1	D	395	ASP
1	D	398	SER
1	D	399	GLU
1	D	404	ASN
1	D	405	THR
1	D	407	THR
1	D	410	MET
1	D	423	THR
1	D	425	THR
1	D	427	ILE
1	D	428	LEU
1	D	433	VAL
1	D	436	ASN
1	D	447	MET
1	D	448	CYS
1	D	461	ASP
1	D	464	ILE
1	D	465	PRO
1	D	466	PRO
1	D	470	PRO
1	D	477	HIS
1	D	492	THR
1	D	509	ILE
1	D	512	LEU
1	D	517	GLN

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Mol	Chain	Res	Type
1	D	518	ASN
1	D	519	ASN
1	D	520	PRO
1	D	522	LEU
1	D	523	THR
1	D	532	CYS
1	D	540	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	32	ASN
1	A	45	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN
1	A	233	ASN
1	A	240	GLN
1	A	264	ASN
1	A	278	ASN
1	A	299	GLN
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	393	ASN
1	A	404	ASN
1	A	455	GLN
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	45	ASN
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
1	B	217	ASN

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Mol	Chain	Res	Type
1	B	233	ASN
1	B	240	GLN
1	B	264	ASN
1	B	278	ASN
1	B	299	GLN
1	B	373	ASN
1	B	385	ASN
1	B	391	ASN
1	B	393	ASN
1	B	404	ASN
1	B	455	GLN
1	B	467	ASN
1	B	517	GLN
1	B	519	ASN
1	C	12	ASN
1	C	27	ASN
1	C	32	ASN
1	C	45	ASN
1	C	104	ASN
1	C	110	GLN
1	C	122	GLN
1	C	138	ASN
1	C	217	ASN
1	C	233	ASN
1	C	240	GLN
1	C	264	ASN
1	C	278	ASN
1	C	299	GLN
1	C	373	ASN
1	C	385	ASN
1	C	391	ASN
1	C	393	ASN
1	C	404	ASN
1	C	455	GLN
1	C	467	ASN
1	C	517	GLN
1	C	519	ASN
1	D	12	ASN
1	D	27	ASN
1	D	32	ASN
1	D	79	HIS
1	D	104	ASN

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Mol	Chain	Res	Type
1	D	110	GLN
1	D	122	GLN
1	D	138	ASN
1	D	217	ASN
1	D	233	ASN
1	D	240	GLN
1	D	264	ASN
1	D	278	ASN
1	D	299	GLN
1	D	373	ASN
1	D	385	ASN
1	D	391	ASN
1	D	393	ASN
1	D	404	ASN
1	D	455	GLN
1	D	467	ASN
1	D	517	GLN
1	D	519	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 48 are monoatomic - leaving 60 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.65	0	15,19,21	0.89	0
2	NAG	A	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	A	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.19	2 (13%)
3	NDG	A	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.69	0	15,19,21	1.17	1 (6%)
2	NAG	A	806	1	14,14,15	0.54	0	15,19,21	1.41	2 (13%)
2	NAG	A	807	1	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
2	NAG	A	808	1	14,14,15	0.67	0	15,19,21	0.70	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	A	810	1	14,14,15	0.64	0	15,19,21	1.09	1 (6%)
3	NDG	A	811	1	14,14,15	0.82	0	15,19,21	2.16	1 (6%)
2	NAG	A	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	A	902	1	14,14,15	1.09	1 (7%)	15,19,21	0.96	0
3	NDG	A	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	A	904	1,2	14,14,15	0.76	1 (7%)	15,19,21	0.79	1 (6%)
2	NAG	B	801	1	14,14,15	0.64	0	15,19,21	0.88	0
2	NAG	B	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	B	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	B	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	B	805	1	14,14,15	0.69	0	15,19,21	1.17	1 (6%)
2	NAG	B	806	1	14,14,15	0.54	0	15,19,21	1.42	2 (13%)
2	NAG	B	807	1	14,14,15	0.64	0	15,19,21	1.15	1 (6%)
2	NAG	B	808	1	14,14,15	0.66	0	15,19,21	0.70	0
2	NAG	B	809	1	14,14,15	0.75	0	15,19,21	0.96	1 (6%)
2	NAG	B	810	1	14,14,15	0.64	0	15,19,21	1.09	2 (13%)
3	NDG	B	811	1	14,14,15	0.81	0	15,19,21	2.16	1 (6%)
2	NAG	B	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	B	902	1	14,14,15	1.07	1 (7%)	15,19,21	0.96	0
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.65	0
2	NAG	B	904	1,2	14,14,15	0.75	1 (7%)	15,19,21	0.77	1 (6%)
2	NAG	C	801	1	14,14,15	0.64	0	15,19,21	0.88	0
2	NAG	C	802	1	14,14,15	0.72	0	15,19,21	0.82	1 (6%)
2	NAG	C	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	C	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	C	805	1	14,14,15	0.69	0	15,19,21	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	806	1	14,14,15	0.55	0	15,19,21	1.41	2 (13%)
2	NAG	C	807	1	14,14,15	0.63	0	15,19,21	1.13	1 (6%)
2	NAG	C	808	1	14,14,15	0.67	0	15,19,21	0.70	0
2	NAG	C	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	C	810	1	14,14,15	0.62	0	15,19,21	1.09	2 (13%)
3	NDG	C	811	1	14,14,15	0.82	0	15,19,21	2.16	1 (6%)
2	NAG	C	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.96	0
3	NDG	C	903	1	14,14,15	0.52	0	15,19,21	0.64	0
2	NAG	C	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	D	801	1	14,14,15	0.64	0	15,19,21	0.88	0
2	NAG	D	802	1	14,14,15	0.73	0	15,19,21	0.82	1 (6%)
2	NAG	D	803	1	14,14,15	0.92	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	D	804	1	14,14,15	0.62	0	15,19,21	0.82	0
2	NAG	D	805	1	14,14,15	0.69	0	15,19,21	1.16	1 (6%)
2	NAG	D	806	1	14,14,15	0.54	0	15,19,21	1.40	2 (13%)
2	NAG	D	807	1	14,14,15	0.64	0	15,19,21	1.13	1 (6%)
2	NAG	D	808	1	14,14,15	0.66	0	15,19,21	0.70	0
2	NAG	D	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	D	810	1	14,14,15	0.63	0	15,19,21	1.08	1 (6%)
3	NDG	D	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	D	812	1	14,14,15	0.83	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	D	902	1	14,14,15	1.07	1 (7%)	15,19,21	0.96	0
3	NDG	D	903	1	14,14,15	0.51	0	15,19,21	0.63	0
2	NAG	D	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.78	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NDG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	A	812	1	-	0/6/23/26	0/1/1/1
3	NDG	A	902	1	-	0/6/23/26	0/1/1/1
3	NDG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	807	1	-	0/6/23/26	0/1/1/1
2	NAG	B	808	1	-	0/6/23/26	0/1/1/1
2	NAG	B	809	1	-	0/6/23/26	0/1/1/1
2	NAG	B	810	1	-	0/6/23/26	0/1/1/1
3	NDG	B	811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1	-	0/6/23/26	0/1/1/1
3	NDG	B	902	1	-	0/6/23/26	0/1/1/1
3	NDG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	B	904	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	802	1	-	0/6/23/26	0/1/1/1
2	NAG	C	803	1	-	0/6/23/26	0/1/1/1
3	NDG	C	804	1	-	0/6/23/26	0/1/1/1
2	NAG	C	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	807	1	-	0/6/23/26	0/1/1/1
2	NAG	C	808	1	-	0/6/23/26	0/1/1/1
2	NAG	C	809	1	-	0/6/23/26	0/1/1/1
2	NAG	C	810	1	-	0/6/23/26	0/1/1/1
3	NDG	C	811	1	-	0/6/23/26	0/1/1/1
2	NAG	C	812	1	-	0/6/23/26	0/1/1/1
3	NDG	C	902	1	-	0/6/23/26	0/1/1/1
3	NDG	C	903	1	-	0/6/23/26	0/1/1/1
2	NAG	C	904	1	-	0/6/23/26	0/1/1/1
2	NAG	D	801	1	-	0/6/23/26	0/1/1/1
2	NAG	D	802	1	-	0/6/23/26	0/1/1/1
2	NAG	D	803	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	D	804	1	-	0/6/23/26	0/1/1/1
2	NAG	D	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	807	1	-	0/6/23/26	0/1/1/1
2	NAG	D	808	1	-	0/6/23/26	0/1/1/1
2	NAG	D	809	1	-	0/6/23/26	0/1/1/1
2	NAG	D	810	1	-	0/6/23/26	0/1/1/1
3	NDG	D	811	1	-	0/6/23/26	0/1/1/1
2	NAG	D	812	1	-	0/6/23/26	0/1/1/1
3	NDG	D	902	1	-	0/6/23/26	0/1/1/1
3	NDG	D	903	1	-	0/6/23/26	0/1/1/1
2	NAG	D	904	1	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	904	NAG	C1-C2	-2.43	1.49	1.52
2	C	904	NAG	C1-C2	-2.40	1.49	1.52
2	A	904	NAG	C1-C2	-2.39	1.49	1.52
2	B	904	NAG	C1-C2	-2.38	1.49	1.52
2	A	812	NAG	C1-C2	-2.34	1.49	1.52
2	C	812	NAG	C1-C2	-2.30	1.49	1.52
2	D	812	NAG	C1-C2	-2.28	1.49	1.52
2	B	812	NAG	C1-C2	-2.26	1.49	1.52
2	D	809	NAG	C1-C2	-2.06	1.49	1.52
2	C	809	NAG	C1-C2	-2.05	1.49	1.52
2	A	809	NAG	C1-C2	-2.03	1.49	1.52
2	A	803	NAG	O5-C5	2.31	1.48	1.43
2	B	803	NAG	O5-C5	2.31	1.48	1.43
2	D	803	NAG	O5-C5	2.33	1.48	1.43
2	C	803	NAG	O5-C5	2.34	1.48	1.43
3	D	902	NDG	C1-C2	3.12	1.56	1.52
3	B	902	NDG	C1-C2	3.12	1.56	1.52
3	C	902	NDG	C1-C2	3.15	1.56	1.52
3	A	902	NDG	C1-C2	3.20	1.57	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	811	NDG	C2-N2-C7	-7.81	112.94	123.11
3	A	811	NDG	C2-N2-C7	-7.81	112.95	123.11
3	B	811	NDG	C2-N2-C7	-7.80	112.95	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	811	NDG	C2-N2-C7	-7.80	112.97	123.11
2	B	806	NAG	C2-N2-C7	-3.92	118.01	123.11
2	C	806	NAG	C2-N2-C7	-3.89	118.04	123.11
2	A	806	NAG	C2-N2-C7	-3.86	118.08	123.11
2	D	806	NAG	C2-N2-C7	-3.85	118.10	123.11
2	C	805	NAG	C2-N2-C7	-3.43	118.64	123.11
2	A	805	NAG	C2-N2-C7	-3.42	118.65	123.11
2	B	805	NAG	C2-N2-C7	-3.41	118.67	123.11
2	D	805	NAG	C2-N2-C7	-3.39	118.69	123.11
2	B	807	NAG	C2-N2-C7	-3.34	118.77	123.11
2	D	807	NAG	C2-N2-C7	-3.32	118.79	123.11
2	A	807	NAG	C2-N2-C7	-3.31	118.80	123.11
2	C	807	NAG	C2-N2-C7	-3.29	118.82	123.11
2	C	803	NAG	C2-N2-C7	-3.26	118.87	123.11
2	B	803	NAG	C2-N2-C7	-3.25	118.88	123.11
2	D	803	NAG	C2-N2-C7	-3.25	118.88	123.11
2	A	803	NAG	C2-N2-C7	-3.22	118.91	123.11
2	B	810	NAG	C4-C3-C2	-2.54	107.40	111.34
2	A	806	NAG	C4-C3-C2	-2.53	107.41	111.34
2	C	810	NAG	C4-C3-C2	-2.53	107.41	111.34
2	A	810	NAG	C4-C3-C2	-2.52	107.42	111.34
2	D	810	NAG	C4-C3-C2	-2.52	107.42	111.34
2	B	806	NAG	C4-C3-C2	-2.52	107.42	111.34
2	D	806	NAG	C4-C3-C2	-2.51	107.44	111.34
2	C	806	NAG	C4-C3-C2	-2.50	107.46	111.34
2	C	812	NAG	C2-N2-C7	-2.40	119.98	123.11
2	A	812	NAG	C2-N2-C7	-2.40	119.98	123.11
2	B	812	NAG	C2-N2-C7	-2.38	120.00	123.11
2	D	812	NAG	C2-N2-C7	-2.34	120.06	123.11
2	A	904	NAG	C2-N2-C7	-2.26	120.17	123.11
2	C	904	NAG	C2-N2-C7	-2.25	120.17	123.11
2	D	904	NAG	C2-N2-C7	-2.25	120.17	123.11
2	C	809	NAG	O5-C5-C4	-2.24	106.42	110.13
2	A	809	NAG	O5-C5-C4	-2.24	106.42	110.13
2	B	809	NAG	O5-C5-C4	-2.23	106.44	110.13
2	D	809	NAG	O5-C5-C4	-2.23	106.44	110.13
2	B	904	NAG	C2-N2-C7	-2.22	120.22	123.11
2	A	802	NAG	C2-N2-C7	-2.19	120.25	123.11
2	D	802	NAG	C2-N2-C7	-2.18	120.27	123.11
2	C	802	NAG	C2-N2-C7	-2.17	120.28	123.11
2	B	802	NAG	C2-N2-C7	-2.17	120.29	123.11
2	B	810	NAG	C1-O5-C5	-2.03	109.16	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	810	NAG	C1-O5-C5	-2.02	109.18	112.14
2	D	803	NAG	C1-O5-C5	2.24	115.43	112.14
2	A	803	NAG	C1-O5-C5	2.27	115.48	112.14
2	B	803	NAG	C1-O5-C5	2.28	115.49	112.14
2	C	803	NAG	C1-O5-C5	2.28	115.49	112.14

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	805	NAG	C1
2	A	806	NAG	C1
2	D	805	NAG	C1
2	D	806	NAG	C1
2	B	805	NAG	C1
2	C	806	NAG	C1
2	B	806	NAG	C1
2	A	805	NAG	C1

There are no torsion outliers.

There are no ring outliers.

52 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	20	0
2	A	803	NAG	4	0
3	A	804	NDG	2	0
2	A	805	NAG	7	0
2	A	806	NAG	12	0
2	A	807	NAG	17	0
2	A	808	NAG	2	0
2	A	809	NAG	8	0
2	A	810	NAG	13	0
3	A	811	NDG	6	0
2	A	812	NAG	3	0
3	A	902	NDG	8	0
2	A	904	NAG	8	0
2	B	801	NAG	19	0
2	B	803	NAG	4	0
3	B	804	NDG	2	0
2	B	805	NAG	7	0
2	B	806	NAG	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	807	NAG	16	0
2	B	808	NAG	2	0
2	B	809	NAG	8	0
2	B	810	NAG	12	0
3	B	811	NDG	7	0
2	B	812	NAG	3	0
3	B	902	NDG	8	0
2	B	904	NAG	8	0
2	C	801	NAG	21	0
2	C	803	NAG	4	0
3	C	804	NDG	2	0
2	C	805	NAG	6	0
2	C	806	NAG	10	0
2	C	807	NAG	17	0
2	C	808	NAG	2	0
2	C	809	NAG	8	0
2	C	810	NAG	13	0
3	C	811	NDG	5	0
2	C	812	NAG	3	0
3	C	902	NDG	8	0
2	C	904	NAG	8	0
2	D	801	NAG	20	0
2	D	803	NAG	4	0
3	D	804	NDG	2	0
2	D	805	NAG	7	0
2	D	806	NAG	12	0
2	D	807	NAG	17	0
2	D	808	NAG	2	0
2	D	809	NAG	8	0
2	D	810	NAG	12	0
3	D	811	NDG	7	0
2	D	812	NAG	3	0
3	D	902	NDG	8	0
2	D	904	NAG	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.