



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:39 PM BST

PDB ID : 1Q5B
EMDB ID: : EMD-1052
Title : 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

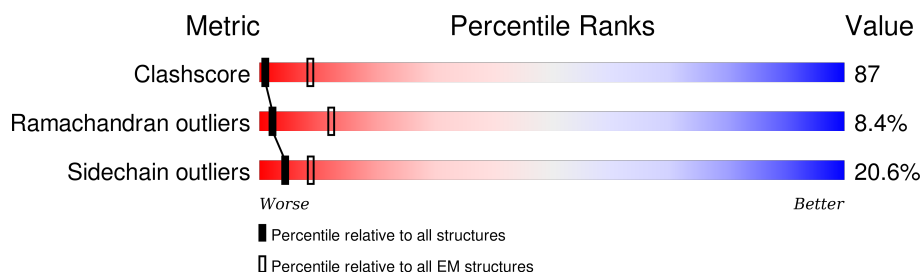
1 Overall quality at a glance

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% 31% 10% . 39%
1	B	880	16% 31% 11% . 39%
1	C	880	16% 31% 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	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	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	-
3	NDG	A	902	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	B	902	-	-	X	-
3	NDG	C	902	-	-	X	-

2 Entry composition [i](#)

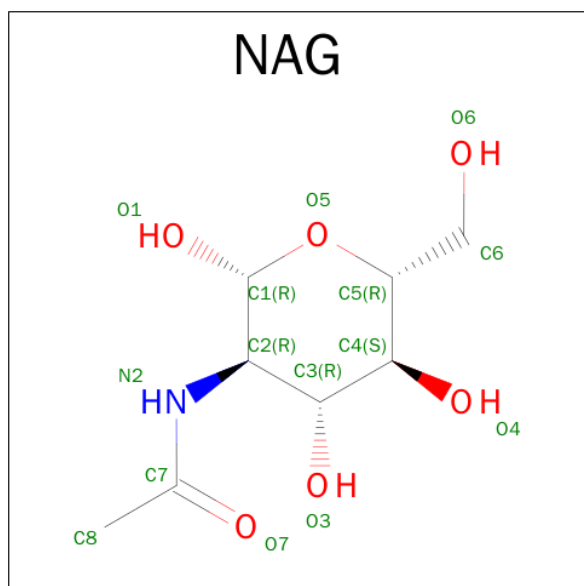
There are 4 unique types of molecules in this entry. The entry contains 13239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		

- 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	
2	A	1	Total	C	N	O	0
			154	88	11	55	

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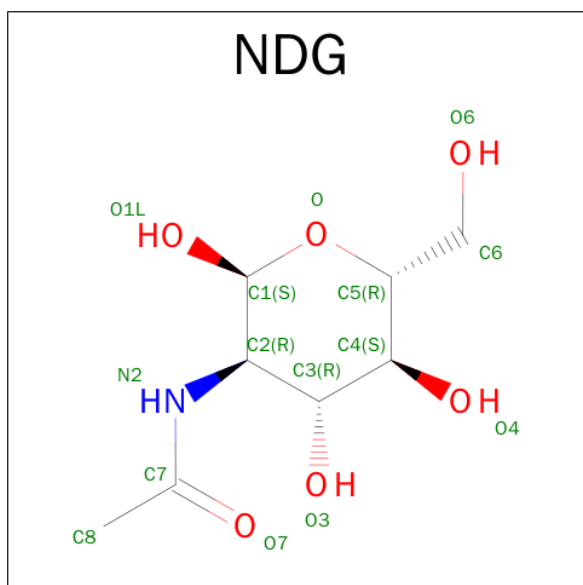
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1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

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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	

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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	

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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	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	

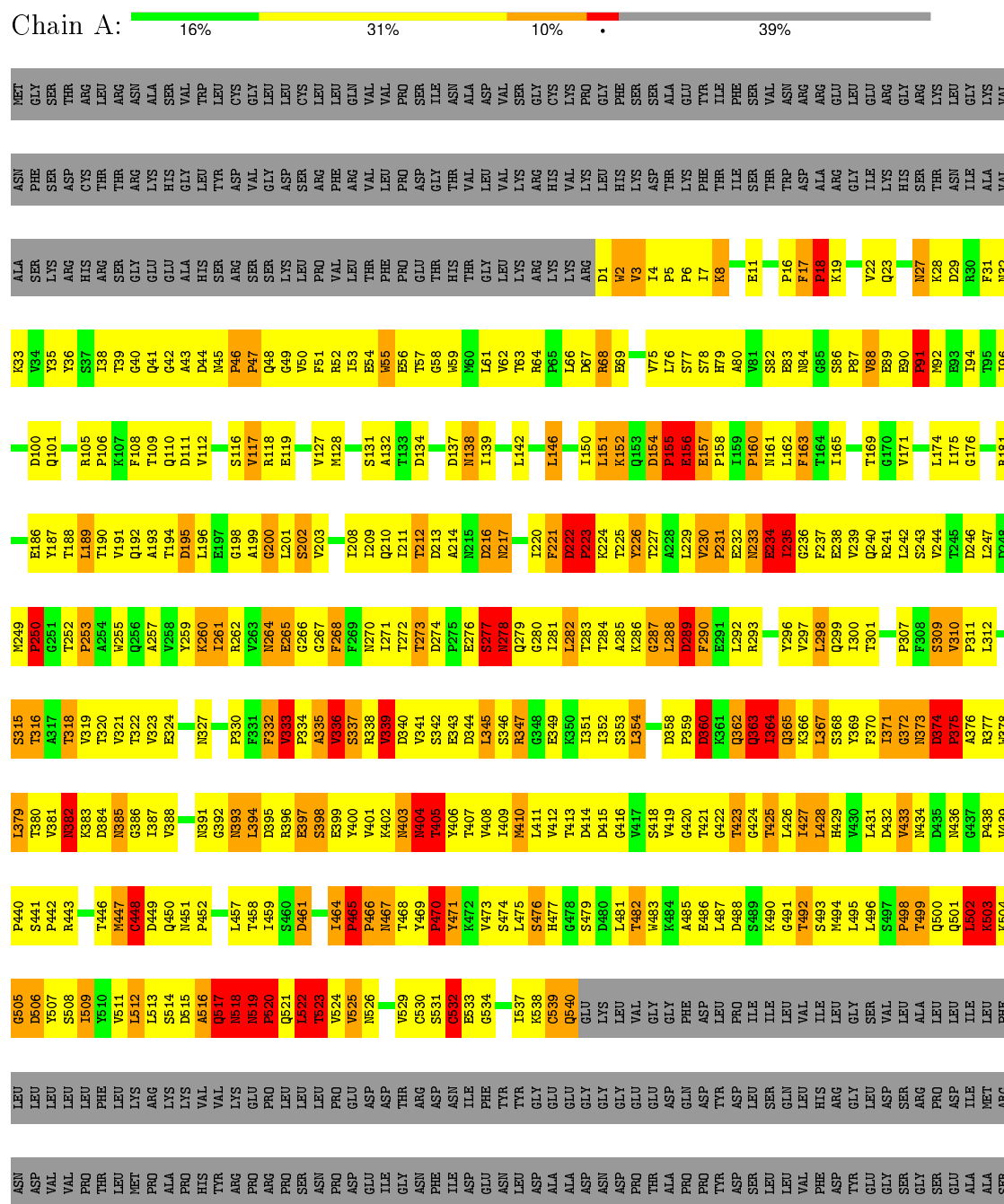
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

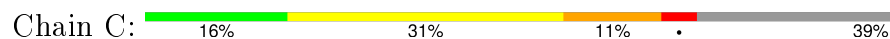
3 Residue-property plots

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



Chain B:



GLU	ALA	ASP	LEU	Q501	G437	A376	P311	D246	G176	D100	F31	ALA	ASN	MET
ALA	SER	ILE	ILE	L502	P438	R377	L312	L247	G176	Q101	N32	SER	PHE	GLY
SER	ARG	PHE	PHE	R503	P439	L379	S315	D248	R181	Q101	R33	LYS	ASP	SER
LEU	ASN	ARG	LEU	G505	P440	T380	T316	D249	R181	Q101	G34	ARG	THR	THR
SER	ASP	LEU	LEU	S441	P442	T381	G317	G251	E186	R105	Y35	HIS	CYS	ARG
SER	VAL	LEU	LEU	P443	R443	R382	T318	T252	T188	P106	Y36	ARG	THR	LEU
LEU	VAL	LEU	LEU	T444	T444	K383	T319	P253	L189	F107	S37	SER	THR	ARG
ASN	PRO	THR	LEU	F445	T446	D384	T320	A254	L189	F108	L38	GLY	ARG	ASN
SER	THR	THR	PHE	T447	T447	N385	T321	T255	T190	T109	T39	LYS	LYS	ALA
SER	SER	LEU	LEU	N447	N447	G386	T322	G256	Q192	Q110	G40	HIS	SER	SER
ASN	ASN	MET	LYS	G448	G448	I387	T323	A257	A193	Q111	Q41	ALA	GLY	VAL
SER	SER	PRO	ARG	D449	D449	I387	T324	G258	T194	V112	G42	HIS	LEU	TRP
ASN	ASN	ALA	LYS	Q450	Q450	R388	E324	Y259	D195	S116	D44	ARG	ASP	CYS
ASP	PRO	PRO	LYS	D451	P452	G391	N327	K260	L196	V117	N45	SER	VAL	GLY
GLU	GLU	HIS	VAL	A451	A452	N392	G327	L261	L197	R118	P46	SER	GLY	LEU
ASP	ASP	TYR	VAL	Q517	L457	N393	P330	R262	G198	E119	P47	LYS	ASP	LEU
ASP	ASP	ARG	LYS	R518	T458	L394	F331	G263	A199	V127	G48	LEU	SER	CYS
TYR	TYR	PRO	GLU	R519	T459	D395	F332	R264	G200	M128	G49	ARG	ARG	LEU
ASN	ASN	ARG	PRO	R520	T459	R396	F333	E265	L201	F51	V50	VAL	PHE	LEU
LEU	LEU	PRO	LEU	Q521	S460	G397	F334	G266	S202	S131	F51	LEU	ARG	GLN
SER	SER	SER	LEU	L522	D461	S398	A335	G267	G200	A132	I53	VAL	LEU	VAL
SER	SER	ASN	LEU	T523	G461	E399	V336	F268	V203	D133	I54	PHE	LEU	VAL
PRO	PRO	PRO	PRO	V524	T464	Y400	S337	F269	T208	T133	E54	VAL	PRO	PRO
ASP	ASP	ASP	GLU	V525	P465	V401	R338	T270	T209	D134	R55	ARG	ASP	SER
GLU	GLU	GLU	ASP	N526	P466	K402	F338	T271	Q210	L146	T63	LYS	GLY	ILE
SER	SER	ILE	ASP	V529	T467	N403	D340	Q279	T220	S147	L66	VAL	THR	ASN
ARG	ARG	GLY	THR	T468	T468	T404	V341	G280	F221	T150	D67	LYS	THR	ALA
PHE	PHE	ASN	ARG	G530	Y469	T405	S342	T273	T212	L151	R68	HIS	VAL	ALA
ARG	ARG	PHE	ASP	S531	P470	Y406	S343	D274	D213	K152	E69	LYS	LEU	ASP
LYS	LYS	ILE	ASN	G532	Y471	T407	D344	G275	D214	Q153	V75	LYS	VAL	VAL
LEU	LEU	ASP	ILE	E533	T472	V408	L345	T276	N215	P155	L76	LYS	LEU	SER
ALA	GLU	GLU	PHE	G534	V473	V408	L346	S277	D216	E156	S77	PHE	THR	GLY
ASP	ASP	ASN	TYR	V537	V474	I409	S346	R278	N217	P158	S78	ILE	THR	GLY
MET	MET	LEU	TYR	K538	L475	M410	R347	G280	T220	I159	H79	ILE	THR	CYS
TYR	TYR	GLY	GLY	S476	L475	L411	G348	T281	F222	P160	A80	SER	VAL	LYS
GLY	GLY	ALA	GLU	S477	H477	T412	K350	I282	D223	L162	V81	HIS	LYS	PRO
GLY	GLY	ALA	GLU	G539	G478	T413	L351	T283	P223	K152	R68	LYS	THR	GLY
ASP	ASP	ASP	GLY	Q540	S479	D415	L352	T284	K224	Q153	E69	LYS	ASP	PHE
ASP	ASP	ASN	GLY	GLU	D480	D416	S353	A285	T225	L162	E89	LYS	THR	GLY
GLU	GLU	PRO	GLY	LEU	L481	V417	L354	G286	Y226	E156	S77	LYS	ALA	ALA
GLU	GLU	VAL	VAL	VAL	T482	S418	L354	G287	T227	P155	S77	LYS	ARG	ARG
GLY	GLY	GLY	ASP	GLY	N483	V419	D358	T288	A228	F163	S86	ARG	GLU	GLU
ASP	ASP	ASP	GLN	PHE	T484	G420	P359	D289	L229	T164	P87	GLY	LEU	LEU
PRO	PRO	PRO	ASP	GLY	A485	T421	R360	F290	V230	I165	V88	ILE	GLU	GLU
PRO	PRO	TYR	ASP	ASP	E486	G422	K361	E291	E232	N161	E89	LYS	GLU	ARG
TYR	TYR	TYR	TYR	LEU	L487	T423	Q362	T292	E232	R167	E90	HIS	ARG	ARG
ASP	ASP	ASP	ASP	PRO	D488	G424	Q363	R293	R233	L162	E89	LYS	THR	LYS
SER	SER	SER	LEU	ILE	S489	T425	L364	G296	E234	F163	P91	SER	THR	LYS
LEU	LEU	LEU	SER	ILE	K490	L426	Q365	Y296	L235	T164	S86	LYS	ASN	LYS
LEU	LEU	LEU	GLN	LEU	G491	I427	K366	T297	G236	I165	P87	LYS	ASN	LYS
VAL	VAL	VAL	LEU	VAL	T492	L428	L367	O298	F237	N166	V88	LYS	ASN	LYS
PHE	PHE	PHE	HIS	ILE	S493	H429	S368	Q299	E238	R167	E89	LYS	ASN	LYS
ASP	ASP	ASP	ARG	LEU	N494	V430	T369	I300	V239	E168	E90	LYS	ASN	LYS
TYR	TYR	TYR	GLY	GLY	L495	L431	F370	T301	Q240	G170	P91	LYS	ASN	LYS
GLY	GLY	GLY	LEU	SER	L496	D432	L371	T301	R241	T171	E93	LYS	ASN	LYS
ASP	ASP	ASP	ASP	VAL	S497	V433	G372	P307	L242	V171	E93	LYS	ASN	LYS
SER	SER	SER	SER	LEU	P498	N434	R373	F308	S243	L174	T95	LYS	ASN	LYS
GLY	GLY	GLY	ARG	ALA	T499	D435	R374	S309	V244	L174	T95	LYS	ASN	LYS
SER	SER	SER	PRO	LEU	Q500	N436	P375	V310	T245	I175	I96	VAL	VAL	VAL

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%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
1	C	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	24/12828 (0.2%)	1.41	239/17517 (1.4%)

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	1	4
1	B	0	4
1	C	0	4
All	All	1	12

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	C	335	ALA	CA-CB	-8.35	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	C	539	CYS	CB-SG	8.18	1.96	1.82
1	A	539	CYS	CB-SG	8.17	1.96	1.82
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	B	223	PRO	CG-CD	7.02	1.73	1.50
1	A	223	PRO	CG-CD	7.00	1.73	1.50
1	C	223	PRO	CG-CD	7.00	1.73	1.50
1	A	523	THR	N-CA	-6.26	1.33	1.46
1	C	523	THR	N-CA	-6.25	1.33	1.46
1	B	523	THR	N-CA	-6.24	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	LEU	N-CA	-5.98	1.34	1.46
1	A	18	PRO	N-CD	5.97	1.56	1.47
1	C	18	PRO	N-CD	5.97	1.56	1.47
1	B	522	LEU	N-CA	-5.97	1.34	1.46
1	C	522	LEU	N-CA	-5.96	1.34	1.46
1	B	18	PRO	N-CD	5.91	1.56	1.47
1	A	530	CYS	CB-SG	5.53	1.91	1.82
1	C	530	CYS	CB-SG	5.49	1.91	1.82
1	B	530	CYS	CB-SG	5.46	1.91	1.82
1	A	499	THR	CA-CB	5.05	1.66	1.53
1	C	499	THR	CA-CB	5.04	1.66	1.53
1	B	499	THR	CA-CB	5.02	1.66	1.53

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20
1	C	520	PRO	CA-C-N	-13.29	87.97	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	C	290	PHE	N-CA-C	12.74	145.39	111.00
1	B	290	PHE	N-CA-C	12.73	145.38	111.00
1	C	235	ILE	N-CA-C	12.72	145.35	111.00
1	A	235	ILE	N-CA-C	12.72	145.34	111.00
1	B	235	ILE	N-CA-C	12.72	145.34	111.00
1	A	290	PHE	N-CA-C	12.71	145.32	111.00
1	C	374	ASP	N-CA-C	11.61	142.36	111.00
1	B	374	ASP	N-CA-C	11.61	142.35	111.00
1	A	374	ASP	N-CA-C	11.61	142.34	111.00
1	A	17	PHE	C-N-CD	-11.55	95.19	120.60
1	C	17	PHE	C-N-CD	-11.54	95.20	120.60
1	B	17	PHE	C-N-CD	-11.54	95.22	120.60
1	C	398	SER	N-CA-C	11.38	141.74	111.00
1	B	398	SER	N-CA-C	11.37	141.70	111.00
1	A	398	SER	N-CA-C	11.36	141.68	111.00
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	A	465	PRO	C-N-CD	-11.03	96.33	120.60
1	C	465	PRO	C-N-CD	-11.03	96.33	120.60
1	C	222	ASP	CB-CG-OD2	10.07	127.36	118.30
1	B	222	ASP	CB-CG-OD2	10.06	127.35	118.30
1	A	222	ASP	CB-CG-OD2	10.03	127.33	118.30
1	A	236	GLY	N-CA-C	-9.99	88.11	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	GLY	N-CA-C	-9.98	88.15	113.10
1	C	236	GLY	N-CA-C	-9.97	88.16	113.10
1	C	230	VAL	C-N-CD	-9.94	98.72	120.60
1	A	230	VAL	C-N-CD	-9.94	98.73	120.60
1	B	230	VAL	C-N-CD	-9.92	98.77	120.60
1	A	374	ASP	CB-CA-C	-9.67	91.05	110.40
1	C	374	ASP	CB-CA-C	-9.67	91.06	110.40
1	B	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	C	376	ALA	N-CA-C	9.66	137.08	111.00
1	B	376	ALA	N-CA-C	9.65	137.04	111.00
1	A	376	ALA	N-CA-C	9.64	137.04	111.00
1	C	522	LEU	CA-CB-CG	-9.39	93.71	115.30
1	B	522	LEU	CA-CB-CG	-9.38	93.74	115.30
1	A	522	LEU	CA-CB-CG	-9.36	93.77	115.30
1	C	223	PRO	N-CA-C	-9.31	87.89	112.10
1	B	223	PRO	N-CA-C	-9.30	87.91	112.10
1	B	520	PRO	N-CA-C	9.30	136.28	112.10
1	A	221	PHE	C-N-CA	-9.30	98.46	121.70
1	B	221	PHE	C-N-CA	-9.29	98.46	121.70
1	A	223	PRO	N-CA-C	-9.29	87.94	112.10
1	A	520	PRO	N-CA-C	9.29	136.25	112.10
1	B	481	LEU	N-CA-C	-9.29	85.92	111.00
1	C	221	PHE	C-N-CA	-9.28	98.50	121.70
1	C	481	LEU	N-CA-C	-9.28	85.94	111.00
1	A	481	LEU	N-CA-C	-9.27	85.97	111.00
1	C	520	PRO	N-CA-C	9.27	136.19	112.10
1	C	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	B	481	LEU	CA-CB-CG	-8.76	95.16	115.30
1	A	481	LEU	CA-CB-CG	-8.75	95.17	115.30
1	A	289	ASP	C-N-CA	-8.43	100.62	121.70
1	B	289	ASP	C-N-CA	-8.42	100.66	121.70
1	C	289	ASP	C-N-CA	-8.41	100.67	121.70
1	A	516	ALA	N-CA-C	-8.35	88.47	111.00
1	B	516	ALA	N-CA-C	-8.35	88.46	111.00
1	C	516	ALA	N-CA-C	-8.35	88.46	111.00
1	C	222	ASP	C-N-CD	-8.22	102.51	120.60
1	B	222	ASP	C-N-CD	-8.21	102.54	120.60
1	A	290	PHE	CA-C-N	-8.20	99.16	117.20
1	B	290	PHE	CA-C-N	-8.19	99.18	117.20
1	A	222	ASP	C-N-CD	-8.19	102.59	120.60
1	C	290	PHE	CA-C-N	-8.17	99.22	117.20
1	A	46	PRO	C-N-CD	-8.05	102.89	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	PRO	C-N-CD	-8.03	102.92	120.60
1	B	46	PRO	C-N-CD	-8.03	102.93	120.60
1	B	233	ASN	N-CA-C	7.88	132.28	111.00
1	C	233	ASN	N-CA-C	7.87	132.26	111.00
1	A	233	ASN	N-CA-C	7.86	132.22	111.00
1	A	336	VAL	N-CA-C	7.82	132.10	111.00
1	B	336	VAL	N-CA-C	7.81	132.09	111.00
1	C	336	VAL	N-CA-C	7.80	132.05	111.00
1	B	522	LEU	C-N-CA	-7.79	102.21	121.70
1	C	522	LEU	C-N-CA	-7.78	102.25	121.70
1	A	522	LEU	C-N-CA	-7.78	102.25	121.70
1	B	362	GLN	N-CA-C	-7.71	90.18	111.00
1	C	362	GLN	N-CA-C	-7.71	90.19	111.00
1	A	362	GLN	N-CA-C	-7.71	90.20	111.00
1	A	234	GLU	N-CA-C	-7.59	90.51	111.00
1	B	234	GLU	N-CA-C	-7.58	90.52	111.00
1	C	234	GLU	N-CA-C	-7.58	90.53	111.00
1	A	234	GLU	C-N-CA	7.42	140.24	121.70
1	C	234	GLU	C-N-CA	7.41	140.22	121.70
1	B	234	GLU	C-N-CA	7.41	140.22	121.70
1	C	521	GLN	C-N-CA	-7.38	103.24	121.70
1	A	521	GLN	C-N-CA	-7.38	103.25	121.70
1	B	521	GLN	C-N-CA	-7.38	103.26	121.70
1	A	490	LYS	CB-CA-C	7.32	125.04	110.40
1	C	277	SER	N-CA-C	-7.21	91.53	111.00
1	B	277	SER	N-CA-C	-7.21	91.54	111.00
1	A	277	SER	N-CA-C	-7.20	91.56	111.00
1	A	337	SER	N-CA-C	-7.19	91.59	111.00
1	C	337	SER	N-CA-C	-7.18	91.62	111.00
1	B	337	SER	N-CA-C	-7.16	91.67	111.00
1	B	503	LYS	N-CA-C	7.01	129.94	111.00
1	A	503	LYS	N-CA-C	7.00	129.91	111.00
1	C	503	LYS	N-CA-C	7.00	129.89	111.00
1	C	523	THR	N-CA-CB	-6.95	97.09	110.30
1	B	523	THR	N-CA-CB	-6.95	97.10	110.30
1	A	523	THR	N-CA-CB	-6.93	97.13	110.30
1	C	492	THR	N-CA-C	6.78	129.31	111.00
1	A	492	THR	N-CA-C	6.78	129.30	111.00
1	B	492	THR	N-CA-C	6.75	129.23	111.00
1	B	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	C	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	A	448	CYS	CA-CB-SG	-6.68	101.98	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	SER	C-N-CA	-6.57	105.27	121.70
1	A	398	SER	C-N-CA	-6.57	105.29	121.70
1	B	476	SER	N-CA-C	6.57	128.72	111.00
1	A	476	SER	N-CA-C	6.56	128.72	111.00
1	C	476	SER	N-CA-C	6.56	128.70	111.00
1	B	491	GLY	N-CA-C	6.55	129.47	113.10
1	B	398	SER	C-N-CA	-6.55	105.33	121.70
1	A	491	GLY	N-CA-C	6.53	129.43	113.10
1	C	491	GLY	N-CA-C	6.51	129.38	113.10
1	C	525	VAL	N-CA-C	-6.51	93.42	111.00
1	B	525	VAL	N-CA-C	-6.50	93.46	111.00
1	A	525	VAL	N-CA-C	-6.48	93.50	111.00
1	C	335	ALA	N-CA-C	-6.32	93.92	111.00
1	A	335	ALA	N-CA-C	-6.32	93.95	111.00
1	B	335	ALA	N-CA-C	-6.31	93.96	111.00
1	B	532	CYS	N-CA-C	6.30	128.01	111.00
1	A	532	CYS	N-CA-C	6.30	128.00	111.00
1	C	532	CYS	N-CA-C	6.29	128.00	111.00
1	B	234	GLU	CA-C-N	-6.28	103.38	117.20
1	A	234	GLU	CA-C-N	-6.28	103.39	117.20
1	C	234	GLU	CA-C-N	-6.27	103.40	117.20
1	A	222	ASP	N-CA-C	6.17	127.64	111.00
1	C	222	ASP	N-CA-C	6.17	127.65	111.00
1	B	222	ASP	N-CA-C	6.15	127.61	111.00
1	A	235	ILE	CA-C-N	-6.14	103.91	116.20
1	A	397	GLU	C-N-CA	-6.14	106.35	121.70
1	C	235	ILE	CA-C-N	-6.14	103.93	116.20
1	B	235	ILE	CA-C-N	-6.13	103.94	116.20
1	B	397	GLU	C-N-CA	-6.12	106.40	121.70
1	C	397	GLU	C-N-CA	-6.11	106.42	121.70
1	A	18	PRO	CA-N-CD	-6.11	102.94	111.50
1	C	18	PRO	CA-N-CD	-6.10	102.97	111.50
1	B	503	LYS	CB-CA-C	-6.09	98.21	110.40
1	A	503	LYS	CB-CA-C	-6.07	98.25	110.40
1	B	18	PRO	CA-N-CD	-6.07	103.00	111.50
1	B	502	LEU	N-CA-C	6.07	127.40	111.00
1	C	503	LYS	CB-CA-C	-6.07	98.25	110.40
1	A	502	LEU	N-CA-C	6.04	127.31	111.00
1	C	502	LEU	N-CA-C	6.03	127.29	111.00
1	A	2	TRP	N-CA-C	-6.03	94.72	111.00
1	C	2	TRP	N-CA-C	-6.02	94.75	111.00
1	B	2	TRP	N-CA-C	-6.01	94.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	ASP	C-N-CD	5.97	140.95	128.40
1	C	374	ASP	C-N-CD	5.97	140.94	128.40
1	B	222	ASP	N-CA-CB	5.96	121.32	110.60
1	C	222	ASP	N-CA-CB	5.96	121.32	110.60
1	A	374	ASP	C-N-CD	5.95	140.90	128.40
1	A	222	ASP	N-CA-CB	5.95	121.31	110.60
1	C	364	ILE	N-CA-C	-5.93	94.99	111.00
1	A	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	376	ALA	CA-C-N	-5.85	104.33	117.20
1	A	376	ALA	CA-C-N	-5.83	104.36	117.20
1	C	376	ALA	CA-C-N	-5.83	104.36	117.20
1	A	382	ASN	N-CA-C	-5.83	95.27	111.00
1	C	382	ASN	N-CA-C	-5.82	95.28	111.00
1	B	382	ASN	N-CA-C	-5.81	95.31	111.00
1	B	471	TYR	N-CA-C	5.74	126.51	111.00
1	C	471	TYR	N-CA-C	5.74	126.49	111.00
1	A	471	TYR	N-CA-C	5.73	126.46	111.00
1	C	481	LEU	CA-C-N	-5.70	104.66	117.20
1	A	481	LEU	CA-C-N	-5.67	104.72	117.20
1	B	481	LEU	CA-C-N	-5.67	104.72	117.20
1	A	374	ASP	C-N-CA	-5.67	98.20	122.00
1	B	374	ASP	C-N-CA	-5.67	98.20	122.00
1	C	374	ASP	C-N-CA	-5.66	98.24	122.00
1	B	403	ASN	N-CA-C	-5.63	95.81	111.00
1	C	403	ASN	N-CA-C	-5.62	95.81	111.00
1	A	403	ASN	N-CA-C	-5.62	95.83	111.00
1	C	221	PHE	CA-C-N	5.58	129.49	117.20
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	A	505	GLY	N-CA-C	5.57	127.02	113.10
1	B	505	GLY	N-CA-C	5.54	126.96	113.10
1	B	502	LEU	CB-CA-C	-5.54	99.67	110.20
1	C	505	GLY	N-CA-C	5.54	126.94	113.10
1	A	502	LEU	CB-CA-C	-5.52	99.71	110.20
1	C	502	LEU	CB-CA-C	-5.51	99.72	110.20
1	A	157	GLU	C-N-CD	-5.48	108.54	120.60
1	B	157	GLU	C-N-CD	-5.47	108.57	120.60
1	C	157	GLU	C-N-CD	-5.46	108.58	120.60
1	B	519	ASN	N-CA-C	5.35	125.45	111.00
1	C	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	519	ASN	N-CA-C	5.35	125.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	THR	N-CA-C	5.33	125.40	111.00
1	C	405	THR	N-CA-C	5.33	125.39	111.00
1	B	405	THR	N-CA-C	5.32	125.35	111.00
1	A	367	LEU	CA-CB-CG	-5.31	103.08	115.30
1	C	367	LEU	CA-CB-CG	-5.30	103.11	115.30
1	B	367	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	521	GLN	N-CA-C	-5.21	96.93	111.00
1	C	521	GLN	N-CA-C	-5.21	96.93	111.00
1	B	521	GLN	N-CA-C	-5.21	96.94	111.00
1	A	290	PHE	O-C-N	5.19	131.01	122.70
1	C	290	PHE	O-C-N	5.18	130.99	122.70
1	C	532	CYS	N-CA-CB	-5.18	101.28	110.60
1	C	520	PRO	C-N-CA	5.17	134.63	121.70
1	A	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	B	290	PHE	O-C-N	5.16	130.96	122.70
1	B	520	PRO	C-N-CA	5.15	134.58	121.70
1	B	532	CYS	N-CA-CB	-5.14	101.35	110.60
1	A	520	PRO	C-N-CA	5.13	134.54	121.70
1	A	18	PRO	CA-CB-CG	-5.13	94.25	104.00
1	B	522	LEU	N-CA-C	-5.12	97.17	111.00
1	A	522	LEU	N-CA-C	-5.11	97.19	111.00
1	B	18	PRO	CA-CB-CG	-5.11	94.28	104.00
1	A	339	VAL	N-CA-C	5.11	124.80	111.00
1	C	18	PRO	CA-CB-CG	-5.11	94.29	104.00
1	B	339	VAL	N-CA-C	5.10	124.77	111.00
1	C	339	VAL	N-CA-C	5.10	124.77	111.00
1	C	522	LEU	N-CA-C	-5.10	97.23	111.00
1	B	16	PRO	C-N-CA	-5.09	108.98	121.70
1	C	16	PRO	C-N-CA	-5.08	109.00	121.70
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	332	PHE	N-CA-C	-5.04	97.39	111.00
1	C	332	PHE	N-CA-C	-5.04	97.40	111.00
1	B	234	GLU	O-C-N	5.03	130.75	122.70
1	B	332	PHE	N-CA-C	-5.03	97.43	111.00
1	A	470	PRO	N-CA-C	5.02	125.16	112.10
1	B	221	PHE	N-CA-C	5.02	124.56	111.00
1	C	234	GLU	O-C-N	5.01	130.72	122.70
1	C	539	CYS	N-CA-C	5.01	124.53	111.00
1	A	539	CYS	N-CA-C	5.01	124.53	111.00
1	B	470	PRO	N-CA-C	5.01	125.13	112.10
1	B	539	CYS	N-CA-C	5.01	124.53	111.00
1	C	221	PHE	N-CA-C	5.01	124.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	PHE	N-CA-C	5.01	124.52	111.00
1	A	234	GLU	O-C-N	5.00	130.71	122.70
1	C	470	PRO	N-CA-C	5.00	125.11	112.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

All (12) 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

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	4081	822	0
1	B	4191	0	4087	811	0
1	C	4191	0	4085	858	0
2	A	154	0	143	85	0
2	B	154	0	143	84	0
2	C	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
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
All	All	13239	0	12838	2266	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 87.

All (2266) 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:46:PRO:HB2	1:C:35:TYR:CE2	1.24	1.62
1:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:C:464:ILE:HD12	1:C:465:PRO:CD	1.30	1.56
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54
1:B:81:VAL:O	1:C:2:TRP:CD2	1.68	1.44
1:A:43:ALA:HB1	1:C:79:HIS:CE1	1.32	1.44
1:C:464:ILE:CD1	1:C:465:PRO:HD2	1.50	1.41
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.41
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.37
1:B:86:SER:CB	1:C:4:ILE:N	1.87	1.36
1:A:87:PRO:CG	1:B:89:GLU:CB	2.03	1.36
1:B:82:SER:N	1:C:2:TRP:CA	1.86	1.36
1:A:46:PRO:CB	1:C:35:TYR:CE2	2.10	1.34
1:A:40:GLY:O	1:C:79:HIS:CB	1.74	1.33
1:A:82:SER:O	1:B:91:PRO:HD2	1.18	1.32
1:B:82:SER:N	1:C:2:TRP:HA	1.03	1.32
1:A:75:VAL:O	1:C:87:PRO:CG	1.80	1.29
1:B:81:VAL:C	1:C:2:TRP:HA	1.48	1.29
1:B:86:SER:HB2	1:C:3:VAL:C	1.50	1.29
1:A:40:GLY:O	1:C:79:HIS:HB3	1.21	1.29
1:A:43:ALA:CB	1:C:79:HIS:CE1	1.82	1.28
1:A:82:SER:OG	1:B:91:PRO:CB	1.79	1.28
1:A:43:ALA:HB3	1:C:79:HIS:ND1	1.45	1.27
1:A:43:ALA:O	1:C:39:THR:HG23	1.30	1.25
1:A:31:PHE:HB2	1:B:93:GLU:OE2	1.08	1.25
1:A:82:SER:OG	1:B:91:PRO:HB2	1.12	1.23
1:C:540:GLN:CD	1:C:540:GLN:O	1.79	1.21
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:HG3	1:B:89:GLU:CB	1.66	1.19
1:A:540:GLN:CD	1:A:540:GLN:O	1.79	1.19
1:A:31:PHE:CB	1:B:93:GLU:OE2	1.90	1.18
1:A:43:ALA:CB	1:C:79:HIS:ND1	2.00	1.18
1:B:81:VAL:O	1:C:2:TRP:CG	1.96	1.18
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.18
1:B:86:SER:HB3	1:C:4:ILE:N	1.54	1.18
1:C:474:SER:HB2	1:C:512:LEU:HG	1.25	1.18
1:A:84:ASN:HB2	1:B:79:HIS:CE1	1.77	1.17
1:A:46:PRO:HB2	1:C:35:TYR:CD2	1.79	1.17
1:C:482:THR:HG23	1:C:499:THR:CG2	1.75	1.17
1:C:8:LYS:HD2	1:C:8:LYS:H	1.04	1.17
1:A:49:GLY:C	1:C:44:ASP:OD1	1.83	1.16
1:A:43:ALA:O	1:C:39:THR:CG2	1.91	1.16
1:A:75:VAL:O	1:C:87:PRO:HG2	1.35	1.16
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.74	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:C:450:GLN:HG2	1:C:532:CYS:O	1.44	1.16
1:B:86:SER:CB	1:C:3:VAL:C	2.12	1.15
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.44	1.15
1:C:469:TYR:CG	1:C:470:PRO:HD2	1.81	1.15
1:A:8:LYS:HD2	1:A:8:LYS:H	1.04	1.15
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.15
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.14
1:C:423:THR:HB	2:C:810:NAG:C7	1.76	1.13
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.13
1:B:8:LYS:HD2	1:B:8:LYS:H	1.04	1.13
1:B:81:VAL:CA	1:C:1:ASP:O	1.94	1.13
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.12
1:A:38:ILE:O	1:C:91:PRO:HB2	1.46	1.12
1:B:30:ARG:HH12	1:C:25:LYS:C	1.30	1.12
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.12
1:C:154:ASP:C	2:C:801:NAG:H82	1.70	1.12
1:A:38:ILE:O	1:C:91:PRO:CB	1.73	1.11
1:A:89:GLU:OE1	1:B:1:ASP:C	1.88	1.11
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.11
1:A:75:VAL:CG1	1:C:87:PRO:HD2	1.81	1.11
1:C:222:ASP:OD1	1:C:222:ASP:O	1.69	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.10
1:A:46:PRO:CB	1:C:35:TYR:HE2	1.53	1.10
1:A:41:GLN:HB2	1:C:81:VAL:HG11	1.22	1.10
1:A:75:VAL:HG12	1:C:87:PRO:HD2	1.30	1.10
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.10
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.10
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.10
1:C:227:THR:HG21	2:C:807:NAG:C8	1.82	1.10
1:C:32:ASN:HD21	1:C:83:GLU:HB2	0.98	1.10
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.09
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:A:75:VAL:HB	1:C:87:PRO:HD3	1.31	1.09
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.09
1:C:338:ARG:HD3	1:C:352:ILE:HG22	1.26	1.09
1:C:234:GLU:H	1:C:235:ILE:HG23	1.08	1.09
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.09
1:A:90:GLU:O	1:B:1:ASP:OD1	1.70	1.08
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:B:32:ASN:HD21	1:B:83:GLU:HB2	0.98	1.07
1:B:83:GLU:OE2	1:C:2:TRP:CZ2	2.07	1.07
1:C:450:GLN:CG	1:C:532:CYS:O	2.02	1.07
1:A:485:ALA:O	1:A:486:GLU:HG2	1.54	1.07
1:B:450:GLN:CG	1:B:532:CYS:O	2.02	1.07
1:B:82:SER:HB3	1:C:2:TRP:HB3	1.36	1.07
1:A:450:GLN:CG	1:A:532:CYS:O	2.03	1.07
1:C:301:THR:HG21	2:C:805:NAG:H82	1.29	1.07
1:B:485:ALA:O	1:B:486:GLU:HG2	1.54	1.07
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.06
1:C:464:ILE:CD1	1:C:465:PRO:CD	2.20	1.06
1:C:485:ALA:O	1:C:486:GLU:HG2	1.54	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.06
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.55	1.06
1:A:44:ASP:C	1:C:79:HIS:N	1.86	1.06
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.06
1:C:290:PHE:HB2	1:C:292:LEU:N	1.69	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:C:335:ALA:HB1	3:C:811:NDG:O6	1.54	1.05
1:A:90:GLU:HB2	1:B:2:TRP:HB2	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:C:337:SER:HA	1:C:427:ILE:HG23	1.38	1.05
1:B:81:VAL:O	1:C:2:TRP:CE2	2.08	1.05
1:A:87:PRO:CD	1:B:89:GLU:HB3	1.86	1.05
1:C:482:THR:HG23	1:C:499:THR:HG22	1.09	1.05
1:B:290:PHE:HB2	1:B:292:LEU:H	0.89	1.05
1:C:290:PHE:HB2	1:C:292:LEU:H	0.88	1.04
1:A:75:VAL:C	1:C:87:PRO:HG2	1.78	1.04
1:A:84:ASN:CB	1:B:79:HIS:HE1	1.70	1.04
1:B:86:SER:OG	1:C:5:PRO:N	1.90	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.91	1.03
1:C:469:TYR:CD1	1:C:470:PRO:HD2	1.91	1.03
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.03
1:A:77:SER:C	1:C:90:GLU:OE2	1.95	1.03
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.03
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.03
1:C:482:THR:CG2	1:C:499:THR:N	2.22	1.03
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.03
1:A:84:ASN:HB2	1:B:79:HIS:HE1	0.91	1.03
1:A:39:THR:OG1	1:C:90:GLU:CA	2.00	1.02
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.02
1:C:403:ASN:HB2	3:C:902:NDG:C8	1.90	1.02
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.02
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:B:403:ASN:HB2	3:B:902:NDG:C8	1.90	1.02
1:A:49:GLY:CA	1:C:44:ASP:OD1	2.08	1.01
1:A:49:GLY:O	1:C:44:ASP:OD1	1.77	1.01
1:A:403:ASN:HB2	3:A:902:NDG:C8	1.90	1.01
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	1.01
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	1.01
1:C:274:ASP:O	1:C:278:ASN:HA	1.61	1.01
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	1.00
1:A:82:SER:HG	1:B:91:PRO:CB	1.61	1.00
1:B:81:VAL:HA	1:C:1:ASP:O	1.22	1.00
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.00
1:A:40:GLY:O	1:C:79:HIS:CG	2.13	1.00
1:A:41:GLN:H	1:C:81:VAL:CG1	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	0.99
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.99
1:A:523:THR:HG23	1:A:524:VAL:H	1.26	0.99
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.99
1:C:432:ASP:OD2	1:C:464:ILE:HG22	1.60	0.99
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:C:320:THR:HG21	2:C:807:NAG:N2	1.78	0.99
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.99
1:C:482:THR:HG21	1:C:499:THR:H	1.23	0.99
1:A:40:GLY:C	1:C:79:HIS:HB3	1.82	0.98
1:C:188:THR:HG23	1:C:208:ILE:HG12	1.43	0.98
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.98
1:A:78:SER:N	1:C:90:GLU:OE2	1.97	0.98
1:B:83:GLU:HA	1:C:2:TRP:CH2	1.99	0.98
1:A:35:TYR:OH	1:C:93:GLU:OE2	1.80	0.98
1:C:450:GLN:HB2	1:C:533:GLU:HA	1.41	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:C:522:LEU:HD22	1:C:523:THR:HB	1.39	0.98
1:B:33:LYS:O	1:C:2:TRP:CE2	2.17	0.98
1:A:41:GLN:N	1:C:81:VAL:HG13	1.78	0.98
1:A:82:SER:O	1:B:91:PRO:CD	2.12	0.97
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.97
1:C:366:LYS:HG3	1:C:367:LEU:H	1.28	0.97
1:C:523:THR:HG23	1:C:524:VAL:H	1.26	0.97
1:B:86:SER:HB2	1:C:4:ILE:N	1.59	0.97
1:A:8:LYS:CD	1:A:8:LYS:H	1.74	0.97
1:C:482:THR:CG2	1:C:499:THR:H	1.76	0.96
1:A:39:THR:OG1	1:C:89:GLU:O	1.82	0.96
1:B:89:GLU:H	1:C:1:ASP:N	1.62	0.96
1:C:8:LYS:CD	1:C:8:LYS:H	1.74	0.96
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.96
1:B:82:SER:CB	1:C:2:TRP:HB3	1.90	0.96
1:A:41:GLN:CB	1:C:81:VAL:HG11	1.88	0.96
1:A:75:VAL:O	1:C:87:PRO:HG3	1.65	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:B:32:ASN:HD21	1:B:83:GLU:CB	1.79	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:A:48:GLN:NE2	1:C:53:ILE:HG21	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.96
1:B:89:GLU:N	1:C:1:ASP:HB2	1.80	0.95
1:A:39:THR:OG1	1:C:90:GLU:HA	1.66	0.95
1:A:78:SER:CA	1:C:90:GLU:OE2	2.15	0.95
1:B:81:VAL:C	1:C:2:TRP:CA	2.22	0.95
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.95
1:C:235:ILE:CG1	1:C:287:GLY:HA2	1.96	0.95
1:A:82:SER:OG	1:B:91:PRO:CA	2.14	0.94
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.94
1:A:91:PRO:HB3	1:C:90:GLU:OE1	1.66	0.94
1:C:290:PHE:CB	1:C:292:LEU:H	1.79	0.94
1:C:366:LYS:CG	1:C:367:LEU:H	1.80	0.94
1:A:44:ASP:C	1:C:79:HIS:H	1.51	0.94
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.94
1:B:81:VAL:C	1:C:2:TRP:CG	2.31	0.94
1:A:49:GLY:HA3	1:C:44:ASP:OD1	1.67	0.94
1:C:32:ASN:HD21	1:C:83:GLU:CB	1.79	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:C:227:THR:HG21	2:C:807:NAG:H83	1.48	0.94
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.93
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.93
1:C:396:ARG:HH22	1:C:464:ILE:HB	1.33	0.93
1:C:320:THR:HG21	2:C:807:NAG:HN2	1.31	0.93
1:C:482:THR:HG21	1:C:499:THR:N	1.81	0.93
1:A:41:GLN:CB	1:C:81:VAL:CG1	2.46	0.93
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.93
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.93
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:B:86:SER:HB3	1:C:3:VAL:CB	1.98	0.93
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.92
1:A:87:PRO:HG2	1:B:89:GLU:CB	2.00	0.92
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.92
1:A:87:PRO:HG2	1:B:89:GLU:HB3	1.49	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.92
2:C:805:NAG:H62	2:C:806:NAG:C7	2.00	0.92
1:C:446:THR:HG23	1:C:539:CYS:SG	2.09	0.92
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:THR:HG23	1:B:539:CYS:SG	2.09	0.92
1:C:403:ASN:HB2	3:C:902:NDG:C7	2.00	0.92
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.92
1:A:43:ALA:HB1	1:C:79:HIS:HE1	1.18	0.92
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.92
1:B:403:ASN:HB2	3:B:902:NDG:C7	2.00	0.92
1:C:404:ASN:O	1:C:404:ASN:ND2	2.03	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:C:289:ASP:O	1:C:290:PHE:HB3	1.67	0.92
1:C:335:ALA:CB	3:C:811:NDG:O6	2.18	0.92
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.91
1:C:227:THR:HG21	2:C:807:NAG:C7	1.99	0.91
1:C:195:ASP:HB2	1:C:201:LEU:H	1.34	0.91
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.91
1:C:27:ASN:HD22	1:C:28:LYS:N	1.66	0.91
1:C:352:ILE:HG13	1:C:388:VAL:HB	1.51	0.91
1:B:32:ASN:ND2	1:B:83:GLU:HB2	1.84	0.91
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.91
1:C:32:ASN:ND2	1:C:83:GLU:HB2	1.84	0.91
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	1.99	0.91
1:A:403:ASN:HB2	3:A:902:NDG:C7	2.00	0.91
1:C:340:ASP:HA	1:C:429:HIS:HB3	1.53	0.91
1:A:404:ASN:ND2	1:A:404:ASN:O	2.03	0.91
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.91
1:C:464:ILE:HD11	1:C:465:PRO:HD2	1.53	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.91
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
2:C:805:NAG:O5	2:C:806:NAG:H83	1.71	0.91
1:A:90:GLU:HB2	1:B:2:TRP:CB	2.00	0.90
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.90
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.90
1:B:86:SER:OG	1:C:4:ILE:C	2.08	0.90
1:B:82:SER:H	1:C:2:TRP:HA	1.12	0.90
1:B:30:ARG:NH1	1:C:25:LYS:C	2.00	0.90
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.90
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.90
1:A:45:ASN:HA	1:C:37:SER:N	1.87	0.90
1:C:518:ASN:O	1:C:520:PRO:HD3	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:C:464:ILE:HD12	1:C:465:PRO:HD2	0.94	0.90
1:B:89:GLU:H	1:C:1:ASP:H3	1.16	0.90
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.90
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.90
1:C:517:GLN:O	1:C:519:ASN:N	2.03	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.90
1:C:464:ILE:HD12	1:C:465:PRO:HD3	1.53	0.89
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.89
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.89
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.89
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.89
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.89
1:C:234:GLU:N	1:C:235:ILE:HG23	1.86	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:C:523:THR:HG23	1:C:524:VAL:CG2	2.03	0.89
1:C:378:TRP:HB2	1:C:379:LEU:HD23	1.53	0.89
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.89
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.89
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.89
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.89
1:C:371:ILE:CD1	1:C:381:VAL:HG11	2.03	0.89
1:C:396:ARG:NH2	1:C:464:ILE:CG2	2.35	0.89
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.89
1:C:221:PHE:HE1	1:C:315:SER:O	1.56	0.89
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:C:154:ASP:HB3	1:C:155:PRO:HD2	1.54	0.89
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:C:343:GLU:HB3	1:C:433:VAL:HG21	1.55	0.88
1:C:338:ARG:HD3	1:C:352:ILE:CG2	2.02	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.88
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	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:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.88
1:A:87:PRO:CD	1:B:89:GLU:CB	2.46	0.87
1:C:8:LYS:HD2	1:C:8:LYS:N	1.87	0.87
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.87
1:B:86:SER:HB3	1:C:4:ILE:H	1.35	0.87
1:C:483:TRP:CZ3	1:C:498:PRO:HG3	2.09	0.87
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.87
1:C:257:ALA:O	1:C:273:THR:HG21	1.74	0.87
1:A:75:VAL:CG1	1:C:87:PRO:CD	2.53	0.87
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.87
1:C:320:THR:HG21	2:C:807:NAG:C2	2.05	0.87
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.87
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.87
1:C:486:GLU:HB2	1:C:495:LEU:HB2	1.56	0.87
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.87
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.87
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.87
1:A:49:GLY:HA3	1:C:44:ASP:CG	1.95	0.87
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.87
1:A:75:VAL:HG12	1:C:87:PRO:CD	2.05	0.86
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.86
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:A:82:SER:HG	1:B:91:PRO:HB2	0.90	0.86
1:C:235:ILE:HG13	1:C:287:GLY:HA2	1.58	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.86
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.86
1:C:441:SER:OG	1:C:442:PRO:HD3	1.75	0.86
1:A:90:GLU:CB	1:B:2:TRP:HB2	2.06	0.86
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.86
1:C:523:THR:HG23	1:C:524:VAL:N	1.90	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:C:318:THR:HG21	2:C:806:NAG:H5	1.55	0.86
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:PRO:CD	1:C:522:LEU:HD12	2.05	0.85
1:C:438:PRO:HB3	1:C:471:TYR:HE2	1.41	0.85
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	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:N	1.91	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:C:374:ASP:O	1:C:375:PRO:C	2.06	0.85
1:C:333:VAL:HB	1:C:334:PRO:HD3	1.56	0.85
1:C:483:TRP:HZ2	1:C:507:TYR:CE1	1.95	0.85
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:C:423:THR:CB	2:C:810:NAG:C7	2.54	0.84
1:A:87:PRO:HG2	1:B:89:GLU:CG	2.06	0.84
1:C:440:PRO:HD2	1:C:522:LEU:HD12	1.59	0.84
1:C:375:PRO:HB3	1:C:400:TYR:CE2	2.12	0.84
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.84
1:B:84:ASN:ND2	1:C:5:PRO:HD3	1.92	0.84
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.84
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.84
1:A:89:GLU:OE2	1:B:3:VAL:HG13	1.76	0.84
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.84
1:C:464:ILE:HD12	1:C:465:PRO:N	1.91	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:C:155:PRO:HB2	2:C:801:NAG:H81	1.59	0.84
1:C:396:ARG:NE	1:C:432:ASP:HB2	1.93	0.84
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.84
1:B:86:SER:CB	1:C:4:ILE:CA	2.56	0.83
1:A:44:ASP:OD2	1:C:79:HIS:ND1	1.98	0.83
1:A:48:GLN:NE2	1:C:53:ILE:CG2	2.39	0.83
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.83
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.83
1:C:448:CYS:O	1:C:452:PRO:HG3	1.79	0.83
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.83
1:B:147:SER:OG	1:B:167:ARG:HD2	1.78	0.83
1:C:451:ASN:N	1:C:533:GLU:O	2.10	0.83
1:C:32:ASN:ND2	1:C:83:GLU:H	1.76	0.83
1:C:28:LYS:HD3	1:C:88:VAL:HG12	1.61	0.83
1:B:81:VAL:HA	1:C:1:ASP:C	1.98	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.83
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.83
1:C:147:SER:OG	1:C:167:ARG:HD2	1.78	0.83
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.83
1:A:43:ALA:HB3	1:C:79:HIS:CG	2.09	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:A:89:GLU:OE1	1:B:1:ASP:CA	2.09	0.83
1:B:289:ASP:OD2	1:B:289:ASP:O	1.97	0.83
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.83
1:A:289:ASP:OD2	1:A:289:ASP:O	1.97	0.83
1:A:87:PRO:HD3	1:B:89:GLU:HB2	1.61	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.82
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.82
1:C:469:TYR:CG	1:C:470:PRO:CD	2.61	0.82
1:B:88:VAL:H	1:C:1:ASP:CA	1.92	0.82
1:B:83:GLU:OE2	1:C:2:TRP:HZ2	1.59	0.82
1:C:446:THR:HG21	1:C:537:ILE:O	1.79	0.82
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.82
1:A:540:GLN:OE1	1:A:540:GLN:O	1.97	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.45	0.82
1:A:87:PRO:HD3	1:B:89:GLU:CB	2.10	0.82
1:C:230:VAL:O	1:C:324:GLU:N	2.11	0.82
1:A:44:ASP:HA	1:C:77:SER:O	1.79	0.82
1:C:423:THR:CB	2:C:810:NAG:N2	2.42	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.44	0.82
1:A:75:VAL:HB	1:C:87:PRO:CD	2.10	0.81
1:C:482:THR:HG21	1:C:500:GLN:N	1.94	0.81
1:C:423:THR:HB	2:C:810:NAG:N2	1.93	0.81
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:C:154:ASP:HB3	2:C:801:NAG:N2	1.95	0.81
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.81
1:C:277:SER:C	1:C:278:ASN:HD22	1.84	0.81
1:C:540:GLN:OE1	1:C:540:GLN:O	1.97	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81
1:C:289:ASP:O	1:C:289:ASP:OD2	1.97	0.81
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.81
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.81
1:C:290:PHE:CE2	1:C:293:ARG:HB2	2.16	0.81
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.81
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:C:396:ARG:HH21	1:C:464:ILE:HG22	1.46	0.81
1:C:154:ASP:HB3	2:C:801:NAG:HN2	1.45	0.81
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.81
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.81
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.80
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:C:517:GLN:C	1:C:519:ASN:H	1.84	0.80
1:B:81:VAL:CA	1:C:2:TRP:HA	2.10	0.80
1:B:30:ARG:NH1	1:C:25:LYS:HG2	1.95	0.80
1:B:540:GLN:OE1	1:B:540:GLN:O	1.97	0.80
1:C:299:GLN:HG2	1:C:318:THR:HG23	1.62	0.80
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.80
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.80
1:A:77:SER:O	1:C:90:GLU:OE2	1.97	0.80
1:A:84:ASN:CG	1:B:77:SER:OG	2.19	0.80
1:C:234:GLU:H	1:C:235:ILE:CG2	1.92	0.80
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.80
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.80
1:C:265:GLU:HB3	1:C:268:PHE:HE2	1.46	0.80
1:C:486:GLU:O	1:C:494:MET:HA	1.81	0.80
2:C:904:NAG:H3	2:C:904:NAG:O7	1.82	0.80
1:C:127:VAL:HG13	1:C:128:MET:H	1.46	0.80
1:B:30:ARG:NH2	1:C:25:LYS:O	2.01	0.80
1:C:469:TYR:CD2	1:C:470:PRO:HD2	2.16	0.80
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.80
1:C:290:PHE:HZ	1:C:296:TYR:HH	1.30	0.80
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.80
1:B:396:ARG:HD3	1:B:431:LEU:C	2.02	0.79
1:A:82:SER:C	1:B:91:PRO:HD2	2.01	0.79
1:B:540:GLN:CG	1:B:540:GLN:O	2.31	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.79
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.79
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.79
1:C:290:PHE:HD2	1:C:293:ARG:H	1.28	0.79
1:C:406:TYR:CD1	2:C:808:NAG:H83	2.17	0.79
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.79
1:C:449:ASP:HB3	1:C:532:CYS:H	1.47	0.79
1:B:86:SER:HB2	1:C:3:VAL:O	1.82	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.79
1:C:432:ASP:OD2	1:C:464:ILE:CG2	2.30	0.79
1:B:27:ASN:C	1:B:27:ASN:HD22	1.85	0.79
1:A:44:ASP:O	1:C:38:ILE:HA	1.83	0.79
1:C:155:PRO:C	1:C:157:GLU:H	1.86	0.79
2:B:904:NAG:H3	2:B:904:NAG:O7	1.82	0.79
1:C:496:LEU:HD21	1:C:509:ILE:HD13	1.63	0.79
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.79
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.79
1:C:483:TRP:HZ2	1:C:507:TYR:HE1	1.24	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.30	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.79
2:C:809:NAG:H61	2:C:810:NAG:H62	1.65	0.79
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.79
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.79
1:C:232:GLU:HG3	1:C:290:PHE:N	1.98	0.79
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.79
1:B:365:GLN:HG3	1:B:365:GLN:O	1.82	0.79
1:C:396:ARG:HD3	1:C:431:LEU:C	2.03	0.79
1:C:482:THR:OG1	1:C:500:GLN:HG2	1.82	0.79
1:A:222:ASP:OD1	1:A:222:ASP:C	2.20	0.79
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.79
1:A:78:SER:C	1:C:90:GLU:OE2	2.21	0.78
1:B:30:ARG:CZ	1:C:25:LYS:O	2.30	0.78
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:C:238:GLU:HA	1:C:283:THR:HG22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.78
1:A:396:ARG:HD3	1:A:431:LEU:C	2.03	0.78
1:C:156:GLU:HG3	1:C:160:PRO:HB3	1.66	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:C:154:ASP:CB	1:C:155:PRO:HD2	2.13	0.78
1:C:485:ALA:O	1:C:486:GLU:CG	2.30	0.78
1:B:86:SER:HB2	1:C:4:ILE:CA	2.14	0.78
1:B:30:ARG:HA	1:C:27:ASN:OD1	1.82	0.78
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.78
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.78
1:C:222:ASP:C	1:C:222:ASP:OD1	2.20	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.30	0.78
1:B:147:SER:OG	1:B:167:ARG:CG	2.32	0.78
1:C:147:SER:OG	1:C:167:ARG:CD	2.32	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.78
1:C:147:SER:OG	1:C:167:ARG:CG	2.32	0.78
1:A:75:VAL:CB	1:C:87:PRO:HD3	2.10	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
1:B:147:SER:OG	1:B:167:ARG:CD	2.32	0.78
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.78
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.78
1:B:89:GLU:N	1:C:1:ASP:CB	2.47	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:A:89:GLU:OE1	1:B:2:TRP:N	2.18	0.77
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.77
1:B:30:ARG:NH1	1:C:25:LYS:O	2.15	0.77
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.31	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:B:33:LYS:O	1:C:2:TRP:NE1	2.09	0.77
1:A:540:GLN:CG	1:A:540:GLN:O	2.30	0.77
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.77
1:C:289:ASP:O	1:C:290:PHE:CB	2.25	0.77
1:C:371:ILE:HD11	1:C:381:VAL:HG11	1.64	0.77
1:B:501:GLN:HG2	1:B:501:GLN:O	1.84	0.77
1:B:82:SER:N	1:C:2:TRP:CB	2.35	0.77
1:A:89:GLU:CD	1:B:1:ASP:H3	1.86	0.77
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.77
1:A:41:GLN:N	1:C:81:VAL:CG1	2.41	0.77
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.77
1:C:365:GLN:HG3	1:C:365:GLN:O	1.82	0.77
1:C:27:ASN:HD22	1:C:27:ASN:C	1.85	0.77
1:C:540:GLN:CG	1:C:540:GLN:O	2.30	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.77
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.77
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	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:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.77
1:C:524:VAL:CG2	2:C:904:NAG:H81	2.14	0.77
1:B:194:THR:HB	1:B:198:GLY:HA2	1.66	0.77
1:C:505:GLY:C	1:C:506:ASP:OD1	2.23	0.77
1:C:195:ASP:HB3	1:C:200:GLY:HA3	1.65	0.77
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:C:440:PRO:HB3	1:C:457:LEU:HD21	1.67	0.76
1:C:523:THR:HG23	1:C:524:VAL:HG22	1.67	0.76
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.76
1:C:196:LEU:HB2	1:C:199:ALA:HB3	1.67	0.76
1:C:194:THR:HB	1:C:198:GLY:HA2	1.67	0.76
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.76
1:C:362:GLN:O	1:C:364:ILE:HG23	1.85	0.76
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.76
1:B:82:SER:HB3	1:C:2:TRP:CB	2.14	0.76
1:C:501:GLN:O	1:C:501:GLN:HG2	1.84	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.76
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.76
1:A:194:THR:HB	1:A:198:GLY:HA2	1.66	0.76
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.76
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.76
1:B:82:SER:CA	1:C:2:TRP:CA	2.62	0.76
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.76
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.76
1:C:432:ASP:CG	1:C:464:ILE:HG22	2.05	0.76
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:C:223:PRO:HD2	1:C:226:TYR:OH	1.85	0.75
1:C:366:LYS:CG	1:C:367:LEU:N	2.48	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:HE	1:C:281:ILE:HD12	1.51	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.75
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.75
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.75
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.68	0.75
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.75
1:B:80:ALA:CB	1:C:1:ASP:HA	2.17	0.75
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.75
1:A:90:GLU:HB3	1:B:2:TRP:HD1	1.52	0.75
1:C:482:THR:CG2	1:C:499:THR:CG2	2.62	0.75
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.75
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.75
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.75
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.75
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:C:272:THR:HG22	1:C:273:THR:H	1.51	0.75
1:A:87:PRO:HG3	1:B:89:GLU:HB3	0.75	0.75
1:C:396:ARG:HH21	1:C:464:ILE:CG2	1.99	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:C:301:THR:HG21	2:C:805:NAG:C8	2.12	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:A:90:GLU:C	1:B:1:ASP:OD1	2.26	0.75
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.75
1:A:84:ASN:HD22	1:B:79:HIS:CE1	2.04	0.75
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.87	0.74
1:C:448:CYS:SG	1:C:537:ILE:HG22	2.27	0.74
1:C:449:ASP:HB3	1:C:532:CYS:N	2.02	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.74
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:C:188:THR:HG23	1:C:208:ILE:CG1	2.16	0.74
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.74
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.99	0.74
1:C:451:ASN:O	1:C:534:GLY:HA2	1.88	0.74
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.74
1:A:364:ILE:HG13	1:A:364:ILE:O	1.86	0.74
1:C:450:GLN:HG3	1:C:533:GLU:OE2	1.88	0.74
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.74
1:C:290:PHE:CD2	1:C:293:ARG:N	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:HD23	1:B:298:LEU:N	2.03	0.74
1:A:87:PRO:HG2	1:B:89:GLU:HG3	1.67	0.73
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.73
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.73
1:C:298:LEU:N	1:C:298:LEU:HD23	2.03	0.73
1:C:371:ILE:HD12	1:C:410:MET:HB3	1.68	0.73
1:B:81:VAL:O	1:C:2:TRP:CD1	2.42	0.73
1:C:223:PRO:HB2	1:C:226:TYR:CE2	2.23	0.73
1:C:320:THR:CG2	2:C:807:NAG:HN2	2.01	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:C:373:ASN:ND2	1:C:374:ASP:H	1.87	0.73
1:C:33:LYS:HB3	1:C:83:GLU:HG2	1.71	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.73
1:B:86:SER:HB3	1:C:3:VAL:HB	1.71	0.73
1:A:75:VAL:CB	1:C:87:PRO:CD	2.67	0.73
1:C:511:VAL:HG23	1:C:523:THR:O	1.89	0.73
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.73
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.73
1:C:364:ILE:O	1:C:364:ILE:CG1	2.37	0.73
1:C:396:ARG:NH2	1:C:464:ILE:HB	2.02	0.72
1:C:320:THR:CG2	2:C:807:NAG:N2	2.52	0.72
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.72
1:C:368:SER:HG	1:C:370:PHE:HE1	1.37	0.72
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.98	0.72
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.72
1:C:333:VAL:CB	1:C:334:PRO:HD3	2.18	0.72
1:A:35:TYR:HB3	1:B:90:GLU:OE1	1.89	0.72
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.72
1:C:342:SER:HA	1:C:431:LEU:HB2	1.71	0.72
1:C:290:PHE:HE2	1:C:293:ARG:HB2	1.52	0.72
1:A:298:LEU:HD23	1:A:298:LEU:N	2.03	0.72
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.72
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:CG	1:B:89:GLU:CG	2.67	0.72
1:C:474:SER:CB	1:C:512:LEU:HG	2.14	0.72
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.72
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.72
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.72
1:C:366:LYS:HG3	1:C:367:LEU:N	2.04	0.72
1:B:394:LEU:N	1:B:394:LEU:HD12	2.05	0.72
1:C:364:ILE:O	1:C:364:ILE:HG13	1.87	0.72
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.72
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.72
1:C:273:THR:O	2:C:803:NAG:H82	1.89	0.72
1:B:80:ALA:HB3	1:C:1:ASP:HA	1.71	0.71
1:A:90:GLU:HB3	1:B:2:TRP:CD1	2.25	0.71
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.71
1:C:276:GLU:HG3	1:C:277:SER:H	1.54	0.71
1:A:28:LYS:NZ	1:B:4:ILE:H	1.87	0.71
1:C:474:SER:HB2	1:C:512:LEU:CG	2.15	0.71
1:A:364:ILE:CG1	1:A:364:ILE:O	2.37	0.71
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.71
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.71
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.71
1:C:227:THR:O	2:C:812:NAG:O5	2.09	0.71
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.02	0.71
1:C:276:GLU:CG	1:C:277:SER:H	2.03	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:C:229:LEU:HD23	1:C:322:THR:HB	1.73	0.71
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.71
1:B:364:ILE:CG1	1:B:364:ILE:O	2.37	0.71
1:C:394:LEU:HD12	1:C:394:LEU:N	2.05	0.71
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.71
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.71
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.71
1:C:316:THR:O	2:C:806:NAG:H82	1.91	0.71
1:C:434:ASN:OD1	1:C:467:ASN:HB3	1.91	0.71
1:B:35:TYR:N	1:C:2:TRP:CE2	2.56	0.71
1:A:48:GLN:HE22	1:C:53:ILE:CG2	2.03	0.71
1:A:48:GLN:HE22	1:C:53:ILE:HG21	1.54	0.71
1:C:337:SER:CA	1:C:427:ILE:HG23	2.20	0.71
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.71
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.71
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.71
1:C:187:TYR:HA	2:C:801:NAG:C7	2.21	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.71
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.71
1:A:368:SER:HG	1:A:370:PHE:HE1	1.39	0.71
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.70
1:C:403:ASN:CB	3:C:902:NDG:N2	2.54	0.70
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.70
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.90	0.70
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.70
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.70
1:B:403:ASN:CB	3:B:902:NDG:N2	2.54	0.70
1:B:83:GLU:OE2	1:C:2:TRP:CH2	2.44	0.70
1:C:485:ALA:C	1:C:486:GLU:HG2	2.11	0.70
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.70
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:C:396:ARG:HE	1:C:432:ASP:HB2	1.57	0.70
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.02	0.70
1:A:403:ASN:CB	3:A:902:NDG:N2	2.54	0.70
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.70
1:C:483:TRP:CZ2	1:C:507:TYR:HE1	2.09	0.70
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:A:46:PRO:HB2	1:C:35:TYR:HE2	0.91	0.69
1:A:289:ASP:CG	1:A:289:ASP:O	2.29	0.69
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.69
1:B:27:ASN:ND2	1:B:27:ASN:C	2.46	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:A:485:ALA:C	1:A:486:GLU:HG2	2.11	0.69
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.69
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.69
1:B:289:ASP:O	1:B:289:ASP:CG	2.30	0.69
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.69
1:C:289:ASP:O	1:C:289:ASP:CG	2.30	0.69
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.69
1:C:414:ASP:HB3	1:C:420:GLY:HA3	1.73	0.69
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.69
1:C:186:GLU:OE1	2:C:801:NAG:H62	1.93	0.69
1:C:405:THR:OG1	1:C:406:TYR:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.69
1:C:438:PRO:HB3	1:C:471:TYR:CE2	2.26	0.69
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.69
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.69
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.69
1:B:396:ARG:HD3	1:B:431:LEU:O	1.93	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.68
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.68
1:C:195:ASP:HB2	1:C:201:LEU:N	2.08	0.68
1:C:242:LEU:HD12	1:C:280:GLY:O	1.93	0.68
1:B:88:VAL:H	1:C:1:ASP:C	1.97	0.68
1:A:48:GLN:HG3	1:C:37:SER:HB2	1.76	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:C:53:ILE:HG13	1:C:59:TRP:O	1.93	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:C:482:THR:HG21	1:C:500:GLN:H	1.58	0.68
1:C:371:ILE:CG2	1:C:372:GLY:N	2.57	0.68
1:C:347:ARG:CD	1:C:392:GLY:H	2.07	0.68
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:B:87:PRO:HA	1:C:1:ASP:O	1.94	0.68
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.77	0.68
1:C:155:PRO:HB2	2:C:801:NAG:C8	2.24	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:A:282:LEU:HD23	1:A:283:THR:H	1.59	0.68
1:C:396:ARG:HD3	1:C:431:LEU:O	1.94	0.68
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.68
1:C:282:LEU:HD23	1:C:283:THR:N	2.08	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:C:232:GLU:HG2	1:C:289:ASP:HA	1.76	0.67
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67
1:C:401:VAL:HG13	1:C:405:THR:O	1.95	0.67
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.67
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.67
1:C:221:PHE:CE1	1:C:315:SER:O	2.45	0.67
1:C:137:ASP:OD2	1:C:139:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ARG:NH2	1:C:464:ILE:CB	2.58	0.67
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.67
1:C:423:THR:HB	2:C:810:NAG:C8	2.24	0.67
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.67
1:C:523:THR:HG23	1:C:524:VAL:HG23	1.74	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.67
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.67
1:C:440:PRO:HA	1:C:458:THR:O	1.94	0.67
3:A:902:NDG:O7	3:A:902:NDG:H3	1.95	0.67
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.67
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.67
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.67
1:C:224:LYS:HE3	1:C:316:THR:O	1.95	0.67
1:A:403:ASN:HB2	3:A:902:NDG:N2	2.10	0.67
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.67
1:C:272:THR:HG22	1:C:273:THR:N	2.09	0.67
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.67
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.67
1:C:320:THR:HG21	2:C:807:NAG:H2	1.76	0.67
1:C:282:LEU:HD23	1:C:283:THR:H	1.58	0.67
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.67
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.67
1:B:403:ASN:HB2	3:B:902:NDG:N2	2.10	0.67
1:A:396:ARG:HD3	1:A:431:LEU:O	1.94	0.67
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.67
1:C:524:VAL:HG21	2:C:904:NAG:H81	1.76	0.67
1:C:347:ARG:HD2	1:C:392:GLY:H	1.60	0.67
1:C:464:ILE:O	1:C:467:ASN:HB2	1.96	0.66
1:B:87:PRO:C	1:C:3:VAL:N	2.48	0.66
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:482:THR:HG21	1:B:500:GLN:H	1.58	0.66
1:C:187:TYR:HA	2:C:801:NAG:C8	2.25	0.66
1:C:290:PHE:HZ	1:C:296:TYR:OH	1.76	0.66
1:A:222:ASP:CG	1:A:222:ASP:O	2.32	0.66
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ARG:HE	1:C:432:ASP:CB	2.07	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
3:B:902:NDG:H3	3:B:902:NDG:O7	1.95	0.66
1:C:403:ASN:HB2	3:C:902:NDG:N2	2.10	0.66
1:A:46:PRO:HB3	1:C:35:TYR:CE2	2.26	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.96	0.66
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.66
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.66
1:C:373:ASN:ND2	1:C:374:ASP:N	2.43	0.66
1:B:282:LEU:HD23	1:B:283:THR:H	1.58	0.66
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.66
3:C:902:NDG:O7	3:C:902:NDG:H3	1.95	0.66
1:A:88:VAL:HA	1:B:92:MET:HG2	1.76	0.66
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.66
1:C:440:PRO:HD2	1:C:522:LEU:CD1	2.26	0.66
1:C:524:VAL:HG23	2:C:904:NAG:H81	1.78	0.66
1:B:88:VAL:N	1:C:1:ASP:CA	2.58	0.66
2:C:809:NAG:C6	2:C:810:NAG:H62	2.26	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:C:366:LYS:HG3	1:C:367:LEU:HG	1.77	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:B:32:ASN:CG	1:B:33:LYS:H	1.98	0.66
1:A:82:SER:OG	1:B:91:PRO:C	2.33	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.98	0.66
1:C:446:THR:CG2	1:C:537:ILE:O	2.44	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.66
1:C:232:GLU:HG3	1:C:290:PHE:H	1.61	0.66
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.66
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.65
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.77	0.65
1:C:265:GLU:HB3	1:C:268:PHE:CE2	2.31	0.65
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.65
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.65
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:HG22	1:C:213:ASP:H	1.62	0.65
1:C:32:ASN:CG	1:C:33:LYS:H	1.99	0.65
1:A:28:LYS:NZ	1:B:4:ILE:N	2.38	0.65
1:B:86:SER:HB3	1:C:3:VAL:C	1.99	0.65
1:C:488:ASP:HB2	1:C:493:SER:OG	1.97	0.65
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.65
1:C:32:ASN:ND2	1:C:83:GLU:N	2.44	0.65
1:C:403:ASN:HB2	3:C:902:NDG:H8C1	1.78	0.65
1:C:341:VAL:HG21	1:C:345:LEU:HD12	1.79	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:C:222:ASP:O	1:C:222:ASP:CG	2.32	0.65
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.65
1:C:347:ARG:CG	1:C:392:GLY:H	2.08	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
1:C:327:ASN:HA	1:C:360:ASP:OD2	1.97	0.65
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.65
1:C:333:VAL:HB	1:C:334:PRO:CD	2.24	0.65
1:B:88:VAL:N	1:C:1:ASP:C	2.50	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65
1:C:440:PRO:HD3	1:C:522:LEU:HD12	1.78	0.65
2:C:805:NAG:C6	2:C:806:NAG:C7	2.74	0.64
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.64
1:C:364:ILE:O	1:C:364:ILE:HD12	1.97	0.64
1:A:364:ILE:HD12	1:A:364:ILE:O	1.97	0.64
1:C:482:THR:OG1	1:C:500:GLN:CG	2.44	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:B:403:ASN:HB2	3:B:902:NDG:H8C1	1.78	0.64
1:B:364:ILE:HD12	1:B:364:ILE:O	1.98	0.64
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.64
1:C:469:TYR:CD2	1:C:470:PRO:CD	2.81	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.64
1:B:446:THR:CG2	1:B:537:ILE:O	2.44	0.64
1:C:346:SER:OG	1:C:349:GLU:HG3	1.97	0.64
1:B:33:LYS:O	1:C:2:TRP:CD1	2.46	0.64
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.64
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.64
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.64
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.64
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.64
1:B:35:TYR:HB2	1:C:2:TRP:CZ2	2.33	0.64
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.64
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.64
1:C:406:TYR:CE1	2:C:808:NAG:H83	2.32	0.64
1:C:415:ASP:OD1	1:C:416:GLY:N	2.27	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.64
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.64
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:C:375:PRO:HB3	1:C:400:TYR:CD2	2.33	0.64
1:C:364:ILE:O	1:C:364:ILE:CD1	2.46	0.64
1:A:403:ASN:HB2	3:A:902:NDG:H8C1	1.78	0.64
1:A:40:GLY:N	1:C:79:HIS:HD1	1.96	0.63
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.63
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:B:364:ILE:CD1	1:B:364:ILE:O	2.46	0.63
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.63
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.63
1:C:371:ILE:HG22	1:C:372:GLY:N	2.14	0.63
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.63
1:A:43:ALA:O	1:C:39:THR:HG21	1.92	0.63
1:C:419:VAL:HG13	2:C:809:NAG:O7	1.98	0.63
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.63
1:C:409:ILE:HG12	1:C:425:THR:HG23	1.80	0.63
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.63
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.63
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.63
1:A:40:GLY:O	1:C:79:HIS:HB2	1.94	0.63
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.63
1:C:154:ASP:O	2:C:801:NAG:H82	1.98	0.63
2:C:904:NAG:C3	2:C:904:NAG:O7	2.45	0.63
1:C:504:LYS:NZ	1:C:531:SER:OG	2.31	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:C:411:LEU:HD22	1:C:421:THR:HG23	1.81	0.63
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.63
1:C:142:LEU:HB3	1:C:196:LEU:HA	1.81	0.63
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.63
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.63
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.63
1:C:482:THR:HG21	1:C:499:THR:CA	2.27	0.63
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.63
1:C:154:ASP:CA	2:C:801:NAG:H82	2.29	0.63
1:B:403:ASN:CB	3:B:902:NDG:C7	2.76	0.63
1:A:87:PRO:CD	1:B:89:GLU:HB2	2.22	0.63
1:C:22:VAL:HG22	1:C:23:GLN:N	2.14	0.63
1:C:469:TYR:CE1	1:C:470:PRO:HD2	2.34	0.63
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.63
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.63
1:A:40:GLY:H	1:C:79:HIS:HD1	1.47	0.62
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.62
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.62
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.62
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.80	0.62
1:C:127:VAL:HG22	1:C:128:MET:N	2.14	0.62
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.62
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.62
1:A:39:THR:CB	1:C:89:GLU:O	2.46	0.62
1:C:486:GLU:O	1:C:494:MET:CA	2.46	0.62
1:C:147:SER:OG	1:C:167:ARG:HG3	1.99	0.62
1:C:446:THR:CG2	1:C:539:CYS:SG	2.86	0.62
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.62
1:A:31:PHE:CG	1:B:93:GLU:OE2	2.52	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.62
1:B:81:VAL:CA	1:C:1:ASP:C	2.62	0.62
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.62
1:B:368:SER:HG	1:B:370:PHE:HE1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASP:O	1:C:38:ILE:CA	2.44	0.62
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.62
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:C:374:ASP:O	1:C:375:PRO:O	2.17	0.62
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.62
1:C:486:GLU:O	1:C:495:LEU:N	2.31	0.62
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.62
1:B:147:SER:OG	1:B:167:ARG:HG3	1.99	0.62
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.62
1:C:343:GLU:HB3	1:C:433:VAL:CG2	2.28	0.62
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.32	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	2.00	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62
1:C:524:VAL:HG23	2:C:904:NAG:C8	2.29	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.61
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:C:403:ASN:O	1:C:405:THR:N	2.33	0.61
1:B:81:VAL:CA	1:C:2:TRP:CA	2.76	0.61
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.61
1:C:524:VAL:CG2	2:C:904:NAG:C8	2.78	0.61
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.61
1:B:83:GLU:CA	1:C:2:TRP:CH2	2.65	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:C:154:ASP:O	1:C:155:PRO:C	2.36	0.61
1:C:181:ARG:NE	1:C:213:ASP:OD1	2.34	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:C:235:ILE:HG12	1:C:287:GLY:HA2	1.82	0.61
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.61
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.61
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.61
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.61
1:A:89:GLU:CD	1:B:3:VAL:HG13	2.20	0.61
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.61
1:C:27:ASN:C	1:C:27:ASN:ND2	2.46	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.61
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:C:482:THR:HG22	1:C:499:THR:N	2.13	0.61
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
1:C:212:THR:HG22	1:C:213:ASP:N	2.15	0.61
1:C:68:ARG:HD3	1:C:100:ASP:HA	1.82	0.61
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:C:508:SER:HB3	1:C:526:ASN:OD1	2.00	0.60
1:C:189:LEU:HD23	1:C:189:LEU:N	2.16	0.60
1:C:517:GLN:C	1:C:519:ASN:N	2.46	0.60
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.60
1:A:379:LEU:H	1:A:379:LEU:HD23	1.66	0.60
1:B:30:ARG:HH12	1:C:25:LYS:HG2	1.59	0.60
1:C:379:LEU:H	1:C:379:LEU:HD23	1.66	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.60
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:A:403:ASN:CB	3:A:902:NDG:C7	2.76	0.60
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.60
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.60
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:C:475:LEU:O	1:C:479:SER:HB3	2.01	0.60
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.60
1:C:371:ILE:CG2	1:C:372:GLY:H	2.13	0.60
1:B:86:SER:CB	1:C:3:VAL:CA	2.79	0.60
1:C:227:THR:CG2	2:C:807:NAG:C7	2.76	0.60
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.60
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.60
1:C:146:LEU:HA	1:C:194:THR:O	2.02	0.60
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.60
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.60
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.60
1:C:116:SER:HA	1:C:210:GLN:O	2.02	0.60
1:B:81:VAL:C	1:C:2:TRP:CB	2.70	0.59
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.59
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.59
1:C:514:SER:HA	1:C:517:GLN:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ARG:HH11	1:C:443:ARG:HG3	1.68	0.59
1:A:189:LEU:HD23	1:A:189:LEU:N	2.17	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.59
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.59
1:C:268:PHE:HA	1:C:285:ALA:HB3	1.85	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:C:518:ASN:O	1:C:520:PRO:CD	2.46	0.59
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:C:508:SER:HA	1:C:526:ASN:HA	1.84	0.59
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.85	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:C:309:SER:O	1:C:310:VAL:HG23	2.03	0.59
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.59
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.59
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.59
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:B:33:LYS:O	1:C:2:TRP:CD2	2.56	0.58
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.58
1:C:335:ALA:HB1	3:C:811:NDG:C6	2.33	0.58
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:C:38:ILE:HG22	1:C:53:ILE:HG22	1.85	0.58
1:C:32:ASN:HD22	1:C:83:GLU:H	1.51	0.58
1:C:403:ASN:CB	3:C:902:NDG:C7	2.76	0.58
1:C:367:LEU:CB	1:C:413:THR:O	2.51	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:C:449:ASP:H	1:C:532:CYS:CB	2.12	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:C:406:TYR:HB3	1:C:428:LEU:CD2	2.33	0.58
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.58
1:C:447:MET:HB2	1:C:529:VAL:HG22	1.84	0.58
1:C:363:GLN:O	1:C:364:ILE:HG22	2.03	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.58
1:A:48:GLN:HG3	1:C:37:SER:CA	2.31	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.58
1:C:473:VAL:HA	1:C:513:LEU:HD23	1.85	0.58
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.58
1:C:232:GLU:HG2	1:C:289:ASP:CA	2.33	0.58
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.58
1:C:42:GLY:HA2	1:C:47:PRO:O	2.04	0.58
1:C:221:PHE:HA	1:C:244:VAL:HG12	1.85	0.58
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.58
1:C:232:GLU:CG	1:C:290:PHE:N	2.64	0.58
1:C:332:PHE:CD2	1:C:424:GLY:HA3	2.39	0.58
1:C:226:TYR:CE2	1:C:242:LEU:HD23	2.39	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:C:299:GLN:C	1:C:300:ILE:HD12	2.24	0.58
1:C:195:ASP:CB	1:C:200:GLY:HA3	2.33	0.58
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.67	0.58
1:C:49:GLY:O	1:C:63:THR:HG21	2.02	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.58
1:C:537:ILE:HG12	1:C:538:LYS:N	2.19	0.58
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:C:239:VAL:HG13	1:C:240:GLN:H	1.67	0.58
1:C:240:GLN:HG3	1:C:241:ARG:N	2.19	0.58
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:C:443:ARG:HA	1:C:525:VAL:HG13	1.85	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:48:GLN:NE2	1:C:37:SER:O	2.24	0.57
1:C:154:ASP:CB	1:C:155:PRO:CD	2.82	0.57
1:C:336:VAL:HB	1:C:426:LEU:HD23	1.84	0.57
1:C:286:LYS:O	1:C:287:GLY:O	2.21	0.57
1:A:45:ASN:CA	1:C:37:SER:N	2.56	0.57
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.57
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.57
1:C:406:TYR:HB3	1:C:428:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.57
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.67	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.57
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.57
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:C:396:ARG:NH2	1:C:464:ILE:HG21	2.17	0.57
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.57
1:B:505:GLY:HA2	1:B:529:VAL:H	1.70	0.57
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.57
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.57
1:C:330:PRO:HD3	1:C:414:ASP:HB2	1.86	0.57
1:C:68:ARG:HG3	1:C:69:GLU:N	2.19	0.57
1:C:189:LEU:HD21	1:C:209:ILE:HD12	1.87	0.57
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.57
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.57
1:C:108:PHE:CE1	1:C:203:VAL:HG23	2.40	0.57
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:C:320:THR:CG2	2:C:807:NAG:C2	2.76	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:B:82:SER:HB3	1:C:2:TRP:C	2.25	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.56
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.56
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.56
1:C:155:PRO:N	2:C:801:NAG:H82	2.20	0.56
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.56
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.86	0.56
1:C:505:GLY:HA2	1:C:529:VAL:H	1.70	0.56
1:C:393:ASN:C	1:C:394:LEU:HD12	2.25	0.56
1:C:369:TYR:HD1	1:C:383:LYS:O	1.88	0.56
1:B:32:ASN:CG	1:B:33:LYS:N	2.59	0.56
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.56
1:C:222:ASP:N	1:C:243:SER:O	2.38	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.56
1:C:118:ARG:HA	1:C:212:THR:HB	1.87	0.56
1:B:394:LEU:CD1	1:B:394:LEU:N	2.69	0.56
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.56
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.56
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.56
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:B:32:ASN:HD22	1:B:83:GLU:H	1.51	0.56
1:A:48:GLN:NE2	1:C:53:ILE:HG22	2.20	0.56
1:A:76:LEU:HA	1:C:87:PRO:HG2	1.88	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:B:86:SER:HB3	1:C:3:VAL:CA	2.36	0.56
1:B:86:SER:CB	1:C:3:VAL:CB	2.79	0.56
1:C:32:ASN:CG	1:C:33:LYS:N	2.59	0.56
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.56
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.56
1:B:30:ARG:CA	1:C:27:ASN:OD1	2.36	0.56
1:C:336:VAL:HG12	1:C:338:ARG:HB2	1.87	0.56
1:C:378:TRP:O	1:C:391:ASN:HB2	2.06	0.56
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.56
1:C:333:VAL:CG2	1:C:334:PRO:HD3	2.36	0.56
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.55
1:C:439:VAL:HG13	1:C:522:LEU:HD11	1.88	0.55
1:B:365:GLN:CG	1:B:365:GLN:O	2.54	0.55
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:C:339:VAL:HG21	1:C:351:ILE:CG2	2.37	0.55
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.55
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.55
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.55
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.55
1:C:155:PRO:HG2	2:C:801:NAG:O7	2.07	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.87	0.55
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.55
1:C:394:LEU:CD1	1:C:394:LEU:N	2.69	0.55
1:C:432:ASP:CG	1:C:464:ILE:CG2	2.74	0.55
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.55
1:C:117:VAL:O	1:C:211:ILE:HA	2.07	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.55
1:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.55
1:C:459:ILE:HG21	1:C:471:TYR:CE2	2.42	0.55
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.55
1:C:482:THR:HG21	1:C:499:THR:C	2.27	0.55
1:C:403:ASN:HB2	3:C:902:NDG:H8C2	1.87	0.55
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.55
1:C:28:LYS:HB3	1:C:88:VAL:HG11	1.89	0.55
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.55
1:C:162:LEU:O	1:C:174:LEU:HD12	2.06	0.55
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.55
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.55
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.55
1:C:226:TYR:O	1:C:227:THR:CG2	2.55	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:A:41:GLN:CB	1:C:81:VAL:HG13	2.35	0.55
1:A:45:ASN:ND2	1:C:79:HIS:CA	2.40	0.55
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:C:154:ASP:CG	1:C:155:PRO:CD	2.75	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:C:363:GLN:C	1:C:364:ILE:CG2	2.75	0.55
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.55
1:C:259:TYR:O	1:C:260:LYS:HB3	2.05	0.55
1:B:75:VAL:O	1:B:76:LEU:HD23	2.07	0.55
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.54
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.54
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.90	0.54
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.54
1:C:268:PHE:N	1:C:268:PHE:CD2	2.75	0.54
1:A:49:GLY:HA3	1:C:44:ASP:OD2	2.05	0.54
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.54
1:B:403:ASN:HB2	3:B:902:NDG:H8C2	1.87	0.54
1:A:367:LEU:HD12	1:A:367:LEU:C	2.28	0.54
1:A:84:ASN:ND2	1:B:77:SER:OG	2.41	0.54
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.75	0.54
1:C:75:VAL:O	1:C:76:LEU:HD23	2.08	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.08	0.54
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.54
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.54
1:C:419:VAL:CG1	1:C:420:GLY:N	2.70	0.54
1:B:88:VAL:H	1:C:1:ASP:N	2.05	0.54
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.54
1:C:154:ASP:CB	2:C:801:NAG:HN2	2.16	0.54
1:B:367:LEU:HD12	1:B:367:LEU:C	2.28	0.54
1:C:241:ARG:NE	1:C:281:ILE:HD12	2.22	0.54
1:C:466:PRO:O	1:C:468:THR:N	2.40	0.54
1:C:226:TYR:HB2	1:C:319:VAL:HG22	1.89	0.54
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.54
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.54
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.54
1:A:82:SER:OG	1:B:91:PRO:N	2.40	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.54
1:C:169:THR:OG1	1:C:171:VAL:HG23	2.07	0.54
1:C:490:LYS:O	1:C:490:LYS:HG2	2.08	0.54
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.54
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.54
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.54
1:C:276:GLU:CG	1:C:277:SER:N	2.71	0.54
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:B:84:ASN:HD22	1:C:5:PRO:HD3	1.73	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:C:438:PRO:HB2	1:C:513:LEU:HD12	1.89	0.54
1:C:332:PHE:HD2	1:C:424:GLY:HA3	1.73	0.54
1:A:84:ASN:ND2	1:B:79:HIS:CE1	2.76	0.53
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.53
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.53
1:C:458:THR:HG22	1:C:493:SER:HB3	1.90	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:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53
1:C:371:ILE:HG23	1:C:372:GLY:H	1.73	0.53
1:C:272:THR:CG2	1:C:273:THR:H	2.19	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.90	0.53
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.53
1:B:268:PHE:N	1:B:268:PHE:CD2	2.75	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:A:48:GLN:HG3	1:C:37:SER:CB	2.37	0.53
1:C:330:PRO:HB3	1:C:358:ASP:HB2	1.89	0.53
1:C:318:THR:CG2	2:C:806:NAG:H5	2.34	0.53
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.53
1:C:365:GLN:O	1:C:365:GLN:CG	2.54	0.53
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.53
1:A:75:VAL:HG11	1:C:87:PRO:HD2	1.84	0.53
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.53
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.53
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.53
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.53
1:A:533:GLU:OE2	1:A:533:GLU:HA	2.09	0.53
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.53
1:C:367:LEU:C	1:C:367:LEU:HD12	2.28	0.53
1:C:249:MET:O	1:C:252:THR:HB	2.09	0.53
1:C:105:ARG:HG3	1:C:106:PRO:HD2	1.91	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53
1:A:44:ASP:CB	1:C:77:SER:C	2.68	0.53
1:C:482:THR:CG2	1:C:499:THR:CA	2.87	0.53
1:C:31:PHE:CD2	1:C:32:ASN:HB2	2.44	0.53
1:C:312:LEU:O	3:C:804:NDG:C8	2.57	0.53
1:C:217:ASN:N	1:C:217:ASN:ND2	2.56	0.53
1:A:45:ASN:ND2	1:C:79:HIS:CB	2.69	0.53
1:A:88:VAL:HA	1:B:92:MET:CG	2.39	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.53
1:C:252:THR:HG23	1:C:253:PRO:HD2	1.90	0.53
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.53
1:C:450:GLN:CB	1:C:532:CYS:O	2.56	0.53
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:C:373:ASN:HB3	1:C:409:ILE:H	1.74	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.53
1:C:443:ARG:NH1	1:C:443:ARG:HG3	2.23	0.53
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.53
1:C:512:LEU:HD11	1:C:519:ASN:HD21	1.74	0.53
1:A:84:ASN:CG	1:B:77:SER:HG	2.12	0.53
1:B:482:THR:O	1:B:482:THR:HG22	2.09	0.53
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.74	0.53
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.33	0.53
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.74	0.53
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.53
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.53
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.53
1:B:426:LEU:HD13	1:B:426:LEU:O	2.10	0.52
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.52
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.52
1:C:242:LEU:O	1:C:279:GLN:HB3	2.09	0.52
1:C:403:ASN:C	1:C:405:THR:H	2.12	0.52
1:C:268:PHE:C	1:C:285:ALA:HB3	2.30	0.52
1:C:155:PRO:C	1:C:157:GLU:N	2.56	0.52
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:A:217:ASN:N	1:A:217:ASN:ND2	2.56	0.52
1:C:22:VAL:HG22	1:C:23:GLN:H	1.73	0.52
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.52
1:A:82:SER:O	1:B:90:GLU:OE2	2.25	0.52
1:C:227:THR:CG2	2:C:807:NAG:H83	2.32	0.52
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.52
1:B:86:SER:OG	1:C:4:ILE:CA	2.57	0.52
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.52
1:C:369:TYR:O	1:C:383:LYS:HG2	2.09	0.52
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.52
1:B:89:GLU:N	1:C:1:ASP:H3	1.98	0.52
1:C:28:LYS:CD	1:C:88:VAL:HG12	2.38	0.52
1:C:221:PHE:HB3	1:C:223:PRO:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.52
1:C:278:ASN:HD22	1:C:278:ASN:N	2.05	0.52
1:C:533:GLU:OE2	1:C:533:GLU:HA	2.09	0.52
1:C:290:PHE:CE2	1:C:293:ARG:CB	2.92	0.52
1:C:367:LEU:HD13	1:C:412:VAL:HG23	1.91	0.52
1:C:347:ARG:HD2	1:C:392:GLY:N	2.25	0.52
1:C:272:THR:CG2	2:C:803:NAG:HN2	2.23	0.52
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.40	0.52
1:A:90:GLU:CB	1:B:2:TRP:CD1	2.92	0.52
1:A:379:LEU:CD2	1:A:379:LEU:H	2.22	0.52
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.52
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.91	0.52
1:C:138:ASN:HD22	1:C:138:ASN:C	2.13	0.52
1:B:88:VAL:CG2	1:C:2:TRP:O	2.47	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.44	0.52
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.52
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.52
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.52
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.52
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.51
1:A:45:ASN:ND2	1:C:79:HIS:HB3	2.25	0.51
1:A:41:GLN:CA	1:C:81:VAL:HG13	2.38	0.51
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.51
1:A:403:ASN:HB2	3:A:902:NDG:H8C2	1.87	0.51
1:C:347:ARG:HG3	1:C:391:ASN:HA	1.91	0.51
1:C:505:GLY:O	1:C:506:ASP:OD1	2.28	0.51
1:A:45:ASN:CG	1:C:79:HIS:CB	2.49	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:C:450:GLN:CG	1:C:533:GLU:OE2	2.58	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.51
1:B:8:LYS:N	1:B:8:LYS:CD	2.51	0.51
1:C:155:PRO:CD	2:C:801:NAG:H82	2.40	0.51
1:C:426:LEU:O	1:C:426:LEU:HD13	2.09	0.51
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.51
1:C:336:VAL:O	1:C:426:LEU:HD22	2.10	0.51
1:C:194:THR:HG22	1:C:195:ASP:N	2.25	0.51
1:A:471:TYR:N	1:A:471:TYR:CD1	2.79	0.51
1:C:450:GLN:HB2	1:C:533:GLU:CA	2.26	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:C:396:ARG:CZ	1:C:432:ASP:HB2	2.41	0.51
1:A:75:VAL:C	1:C:87:PRO:CG	2.53	0.51
1:C:514:SER:HB3	1:C:517:GLN:O	2.10	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:C:352:ILE:HG13	1:C:388:VAL:CB	2.33	0.51
1:A:426:LEU:HD13	1:A:426:LEU:O	2.10	0.51
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.51
1:C:151:LEU:HD12	1:C:190:THR:O	2.11	0.51
1:A:38:ILE:O	1:C:91:PRO:HB3	1.94	0.51
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.51
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.51
1:C:297:VAL:CG2	2:C:807:NAG:H62	2.41	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.51
1:B:471:TYR:CD1	1:B:471:TYR:N	2.79	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:B:81:VAL:HA	1:C:2:TRP:CA	2.41	0.51
1:B:154:ASP:C	2:B:801:NAG:C8	2.62	0.51
1:A:365:GLN:O	1:A:365:GLN:CG	2.54	0.51
1:C:80:ALA:O	1:C:88:VAL:HG23	2.11	0.51
1:C:33:LYS:HB3	1:C:83:GLU:CG	2.40	0.51
1:B:458:THR:HG22	1:B:493:SER:CB	2.41	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.51
1:C:142:LEU:O	1:C:196:LEU:HD23	2.11	0.51
1:C:217:ASN:N	1:C:217:ASN:HD22	2.09	0.51
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.50
1:C:458:THR:HG22	1:C:493:SER:CB	2.42	0.50
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.50
1:B:397:GLU:OE1	1:B:397:GLU:N	2.44	0.50
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.50
1:B:88:VAL:HG22	1:C:2:TRP:O	1.63	0.50
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.50
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.50
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASP:O	2:C:801:NAG:C8	2.60	0.50
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.50
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.09	0.50
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.50
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.50
1:B:82:SER:CB	1:C:2:TRP:CA	2.89	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.50
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.50
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.50
1:C:338:ARG:HB3	1:C:339:VAL:HG22	1.92	0.50
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.50
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.50
1:C:458:THR:HA	1:C:493:SER:HA	1.93	0.50
1:A:278:ASN:N	1:A:278:ASN:HD22	2.05	0.50
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.50
1:C:471:TYR:N	1:C:471:TYR:CD1	2.79	0.50
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.50
1:C:419:VAL:HG22	2:C:809:NAG:H81	1.93	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.94	0.50
1:C:155:PRO:O	1:C:157:GLU:N	2.43	0.50
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.50
1:C:522:LEU:CD2	1:C:523:THR:HB	2.26	0.50
1:C:276:GLU:HG3	1:C:277:SER:N	2.25	0.50
1:C:432:ASP:CB	1:C:464:ILE:CG2	2.89	0.50
1:A:84:ASN:CB	1:B:79:HIS:CE1	2.62	0.50
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.50
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.50
1:C:234:GLU:HB2	1:C:235:ILE:HG22	1.93	0.50
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.50
1:C:373:ASN:ND2	1:C:374:ASP:OD1	2.45	0.50
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.50
1:C:333:VAL:CB	1:C:334:PRO:CD	2.88	0.50
1:C:363:GLN:C	1:C:364:ILE:HG23	2.32	0.50
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.50
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.50
1:C:109:THR:HG22	1:C:110:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASN:OD1	1:C:385:ASN:N	2.45	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.89	0.50
1:A:39:THR:OG1	1:C:89:GLU:C	2.47	0.50
1:C:449:ASP:CB	1:C:532:CYS:H	2.22	0.50
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.50
2:B:807:NAG:H3	2:B:807:NAG:O7	2.11	0.50
1:A:458:THR:HG22	1:A:493:SER:CB	2.42	0.50
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.50
1:C:428:LEU:HD23	1:C:428:LEU:O	2.11	0.50
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.50
1:C:241:ARG:HE	1:C:281:ILE:CD1	2.24	0.50
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.50
1:C:327:ASN:OD1	1:C:360:ASP:OD1	2.30	0.50
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.24	0.50
1:A:217:ASN:HD22	1:A:217:ASN:N	2.10	0.50
1:C:109:THR:HG22	1:C:110:GLN:CG	2.42	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.50
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.49
1:A:44:ASP:CG	1:C:79:HIS:ND1	2.63	0.49
1:C:27:ASN:C	1:C:29:ASP:H	2.16	0.49
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.49
1:C:155:PRO:HG2	2:C:801:NAG:C7	2.42	0.49
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.49
1:C:457:LEU:HD23	1:C:494:MET:SD	2.52	0.49
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.94	0.49
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.49
1:B:151:LEU:H	1:B:151:LEU:HD12	1.78	0.49
1:C:216:ASP:HB2	1:C:217:ASN:ND2	2.27	0.49
1:C:397:GLU:N	1:C:397:GLU:OE1	2.44	0.49
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.61	0.49
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.49
1:A:82:SER:H	1:B:90:GLU:C	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.49
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.49
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.49
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.49
1:C:252:THR:CG2	1:C:253:PRO:HD2	2.43	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.93	0.49
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.49
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.49
1:C:367:LEU:HB2	1:C:413:THR:O	2.12	0.49
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.49
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.49
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:482:THR:HG22	1:A:482:THR:O	2.09	0.49
1:C:273:THR:H	2:C:803:NAG:HN2	1.61	0.49
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.49
1:C:76:LEU:O	1:C:94:ILE:N	2.44	0.49
1:C:512:LEU:HD11	1:C:519:ASN:ND2	2.28	0.49
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.49
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.49
1:C:226:TYR:C	1:C:227:THR:HG23	2.33	0.49
2:A:807:NAG:H3	2:A:807:NAG:O7	2.11	0.49
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.49
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.49
1:B:281:ILE:HG23	1:B:281:ILE:O	2.13	0.49
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.49
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.95	0.49
1:B:82:SER:HB3	1:C:2:TRP:CA	2.42	0.49
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.49
1:C:336:VAL:CG1	1:C:338:ARG:HB2	2.43	0.49
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.49
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.49
1:C:192:GLN:HA	1:C:203:VAL:O	2.13	0.49
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
1:C:449:ASP:CB	1:C:532:CYS:N	2.74	0.49
2:C:812:NAG:O7	2:C:812:NAG:C1	2.60	0.49
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ILE:HG23	1:C:281:ILE:O	2.13	0.49
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:C:151:LEU:H	1:C:151:LEU:HD12	1.78	0.49
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:A:423:THR:HB	2:A:810:NAG:H83	1.94	0.49
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.49
1:C:224:LYS:HE3	2:C:806:NAG:H82	1.95	0.49
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.49
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.49
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.48
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
1:C:266:GLY:N	1:C:268:PHE:CE2	2.76	0.48
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.48
1:C:68:ARG:HD3	1:C:100:ASP:CA	2.43	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
2:C:809:NAG:H62	2:C:810:NAG:O6	2.13	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
1:C:371:ILE:HA	1:C:371:ILE:HD12	1.65	0.48
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.48
1:C:365:GLN:HA	1:C:416:GLY:HA3	1.95	0.48
1:C:368:SER:OG	1:C:370:PHE:HE1	1.94	0.48
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.96	0.48
1:A:89:GLU:OE2	1:B:3:VAL:CG1	2.55	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.48
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.48
2:C:807:NAG:H3	2:C:807:NAG:O7	2.11	0.48
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.48
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.48
1:C:250:PRO:O	1:C:255:TRP:CE3	2.66	0.48
1:C:261:ILE:HD11	1:C:264:ASN:HD22	1.77	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:A:43:ALA:HB3	1:C:79:HIS:HD1	1.63	0.48
1:C:186:GLU:OE1	2:C:801:NAG:C6	2.59	0.48
1:C:119:GLU:OE2	1:C:216:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLU:OE2	1:C:69:GLU:OE1	2.30	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:C:432:ASP:CB	1:C:464:ILE:HG21	2.43	0.48
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:C:41:GLN:HA	1:C:45:ASN:HB2	1.95	0.48
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.48
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.48
1:A:46:PRO:CB	1:C:35:TYR:CD2	2.72	0.48
1:C:154:ASP:CG	1:C:155:PRO:HD2	2.33	0.48
2:B:812:NAG:O7	2:B:812:NAG:C1	2.60	0.48
1:C:224:LYS:CE	2:C:806:NAG:C8	2.91	0.48
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.48
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:A:79:HIS:HD1	1:A:91:PRO:HG3	1.79	0.48
1:C:514:SER:CA	1:C:517:GLN:O	2.62	0.48
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.48
1:C:366:LYS:HG2	1:C:367:LEU:H	1.75	0.48
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.48
1:A:48:GLN:CG	1:C:37:SER:CB	2.92	0.48
1:C:482:THR:O	1:C:482:THR:HG22	2.08	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:C:335:ALA:CB	3:C:811:NDG:C6	2.90	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:C:150:ILE:HD11	1:C:165:ILE:HB	1.96	0.48
1:B:81:VAL:HA	1:C:2:TRP:HA	1.96	0.47
1:C:8:LYS:CD	1:C:8:LYS:N	2.51	0.47
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.47
1:A:366:LYS:HG2	1:A:367:LEU:H	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.47
1:C:67:ASP:OD2	1:C:69:GLU:HB2	2.13	0.47
1:C:451:ASN:O	1:C:534:GLY:CA	2.60	0.47
2:C:809:NAG:C6	2:C:810:NAG:C6	2.92	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.47
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47
1:A:82:SER:C	1:B:90:GLU:HG3	2.21	0.47
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.47
1:C:151:LEU:O	1:C:152:LYS:HB2	2.13	0.47
1:A:77:SER:OG	1:C:90:GLU:OE1	2.30	0.47
1:A:76:LEU:N	1:C:87:PRO:HG2	2.26	0.47
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:A:514:SER:HG	1:A:519:ASN:HA	1.79	0.47
1:B:300:ILE:N	1:B:300:ILE:HD12	2.29	0.47
1:C:226:TYR:O	1:C:227:THR:HG23	2.15	0.47
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.47
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.47
1:C:367:LEU:HD13	1:C:412:VAL:CG2	2.43	0.47
1:C:261:ILE:CD1	1:C:264:ASN:ND2	2.77	0.47
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.47
1:A:117:VAL:O	1:A:212:THR:N	2.46	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:B:80:ALA:HB3	1:C:1:ASP:CA	2.40	0.47
1:C:23:GLN:HB2	1:C:59:TRP:CE3	2.50	0.47
1:A:44:ASP:HB3	1:C:77:SER:C	2.32	0.47
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
1:C:423:THR:HB	2:C:810:NAG:H83	1.93	0.47
2:A:812:NAG:C1	2:A:812:NAG:O7	2.60	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ILE:CG1	1:C:388:VAL:HB	2.33	0.47
1:C:300:ILE:N	1:C:300:ILE:HD12	2.30	0.47
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.47
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.47
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:C:50:VAL:HB	1:C:51:PHE:CD1	2.50	0.47
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.47
1:C:225:THR:HA	1:C:318:THR:O	2.14	0.47
1:C:282:LEU:CD2	1:C:283:THR:N	2.76	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:C:481:LEU:HD12	1:C:481:LEU:HA	1.50	0.47
1:C:36:TYR:O	1:C:55:TRP:HA	2.15	0.47
1:A:39:THR:HA	1:C:79:HIS:HD1	1.79	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.47
1:C:246:ASP:C	1:C:247:LEU:HD12	2.35	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:C:448:CYS:SG	1:C:537:ILE:CG2	3.01	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:301:THR:CG2	1:C:316:THR:HG23	2.45	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:C:496:LEU:HD21	1:C:509:ILE:CD1	2.38	0.47
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.47
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.47
1:B:226:TYR:O	1:B:227:THR:HG23	2.15	0.46
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:C:402:LYS:C	1:C:403:ASN:O	2.46	0.46
1:B:379:LEU:CD2	1:B:379:LEU:H	2.22	0.46
1:A:41:GLN:CA	1:C:81:VAL:CG1	2.92	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.81	0.46
1:C:272:THR:HG23	2:C:803:NAG:HN2	1.80	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
2:C:809:NAG:H61	2:C:810:NAG:C6	2.39	0.46
1:C:408:VAL:O	1:C:426:LEU:N	2.49	0.46
1:C:374:ASP:OD1	1:C:374:ASP:N	2.49	0.46
1:A:27:ASN:ND2	1:A:28:LYS:N	2.50	0.46
1:C:268:PHE:CA	1:C:285:ALA:HB3	2.45	0.46
1:C:100:ASP:OD1	1:C:101:GLN:N	2.49	0.46
1:C:271:ILE:HG23	1:C:271:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.46
1:C:54:GLU:HB2	1:C:57:THR:OG1	2.16	0.46
1:C:421:THR:HG21	2:C:809:NAG:H61	1.98	0.46
1:C:373:ASN:CG	1:C:374:ASP:H	2.18	0.46
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.46
1:C:363:GLN:O	1:C:364:ILE:CG2	2.63	0.46
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.46
1:A:76:LEU:CA	1:C:87:PRO:HG2	2.45	0.46
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.46
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.92	0.46
1:C:187:TYR:HE1	1:C:211:ILE:HD11	1.81	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:A:374:ASP:OD1	1:A:374:ASP:N	2.49	0.46
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.81	0.46
1:C:506:ASP:OD1	1:C:506:ASP:N	2.49	0.46
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.46
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.46
1:B:374:ASP:OD1	1:B:374:ASP:N	2.49	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:A:64:ARG:HH12	1:C:44:ASP:HB2	1.80	0.46
1:C:117:VAL:O	1:C:212:THR:N	2.46	0.46
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.46
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.46
1:B:371:ILE:HD13	1:B:381:VAL:HG11	1.95	0.46
1:B:459:ILE:N	1:B:459:ILE:HD12	2.31	0.46
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.46
1:B:415:ASP:CG	1:B:416:GLY:H	2.17	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.46
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:C:374:ASP:C	1:C:375:PRO:O	2.54	0.46
1:B:271:ILE:HG23	1:B:271:ILE:O	2.15	0.46
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.86	0.46
1:A:40:GLY:CA	1:C:79:HIS:HB3	2.45	0.46
1:A:84:ASN:O	1:B:79:HIS:CE1	2.69	0.46
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.46
1:C:227:THR:N	2:C:812:NAG:H2	2.31	0.46
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ILE:HD12	1:C:459:ILE:N	2.31	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:C:310:VAL:HG12	1:C:311:PRO:O	2.15	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:C:514:SER:HG	1:C:519:ASN:HA	1.81	0.46
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.46
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.46
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.46
1:C:109:THR:CB	1:C:131:SER:HB2	2.46	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.45
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.45
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.45
1:C:272:THR:CG2	1:C:273:THR:N	2.76	0.45
1:C:473:VAL:CG2	1:C:487:LEU:HD21	2.47	0.45
1:C:270:ASN:OD1	1:C:271:ILE:N	2.49	0.45
1:A:44:ASP:OD1	1:C:91:PRO:HA	2.16	0.45
1:C:79:HIS:HD1	1:C:91:PRO:HG3	1.79	0.45
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:B:506:ASP:N	1:B:506:ASP:OD1	2.49	0.45
1:A:363:GLN:O	1:A:364:ILE:CG2	2.64	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.45
1:C:262:ARG:HG3	1:C:299:GLN:HB2	1.98	0.45
1:A:459:ILE:HD12	1:A:459:ILE:N	2.31	0.45
1:C:155:PRO:CB	2:C:801:NAG:C8	2.94	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.45
1:C:469:TYR:CD2	1:C:470:PRO:N	2.85	0.45
1:C:152:LYS:O	1:C:189:LEU:HA	2.17	0.45
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.45
1:C:450:GLN:CB	1:C:533:GLU:OE2	2.64	0.45
1:C:336:VAL:HG11	1:C:338:ARG:HD2	1.99	0.45
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:B:88:VAL:H	1:C:1:ASP:H3	1.62	0.45
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:C:461:ASP:HB3	1:C:468:THR:CG2	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.16	0.45
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.45
1:A:44:ASP:O	1:C:78:SER:HA	2.17	0.45
1:C:482:THR:O	1:C:483:TRP:CD2	2.70	0.45
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.45
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45
1:B:408:VAL:O	1:B:426:LEU:N	2.49	0.45
1:C:227:THR:HG22	1:C:320:THR:HB	1.98	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.45
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.45
1:C:450:GLN:CB	1:C:533:GLU:HA	2.29	0.45
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:C:286:LYS:C	1:C:287:GLY:O	2.55	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
2:C:805:NAG:C5	2:C:806:NAG:H83	2.46	0.45
1:C:380:THR:CG2	1:C:381:VAL:N	2.79	0.45
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.45
1:C:162:LEU:HB2	1:C:163:PHE:CE1	2.52	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:C:519:ASN:O	1:C:519:ASN:CG	2.55	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:C:468:THR:C	1:C:469:TYR:O	2.54	0.45
1:C:469:TYR:CE2	1:C:470:PRO:HB2	2.52	0.45
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.45
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.44
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.44
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.44
1:C:426:LEU:C	1:C:426:LEU:HD13	2.37	0.44
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.44
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.44
1:B:80:ALA:HB3	1:C:1:ASP:N	2.32	0.44
1:B:82:SER:H	1:C:2:TRP:CA	1.92	0.44
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.44
1:C:440:PRO:HB3	1:C:457:LEU:CD2	2.43	0.44
1:C:194:THR:CG2	1:C:195:ASP:N	2.79	0.44
1:C:67:ASP:OD1	1:C:69:GLU:HB2	2.18	0.44
1:C:312:LEU:O	3:C:804:NDG:H8C1	2.17	0.44
1:C:108:PHE:HE1	1:C:203:VAL:HG23	1.80	0.44
1:C:261:ILE:HD11	1:C:264:ASN:ND2	2.32	0.44
1:B:32:ASN:ND2	1:B:83:GLU:CB	2.62	0.44
1:A:45:ASN:HA	1:C:37:SER:O	2.18	0.44
1:A:64:ARG:NH1	1:C:44:ASP:HB2	2.33	0.44
1:B:299:GLN:CG	1:B:318:THR:HG23	2.42	0.44
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.44
1:C:232:GLU:HA	1:C:288:LEU:HD12	1.99	0.44
1:C:442:PRO:HD2	1:C:457:LEU:HD12	2.00	0.44
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.44
1:B:232:GLU:HA	1:B:288:LEU:HD12	1.99	0.44
1:C:187:TYR:CE1	1:C:211:ILE:HD11	2.52	0.44
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:C:485:ALA:O	1:C:486:GLU:OE1	2.35	0.44
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.44
1:C:339:VAL:HG11	1:C:351:ILE:HG23	1.98	0.44
1:C:224:LYS:HE3	2:C:806:NAG:C8	2.48	0.44
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.44
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.44
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.44
1:C:151:LEU:HD12	1:C:151:LEU:N	2.33	0.44
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.44
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.44
1:B:86:SER:HA	1:B:87:PRO:HD3	1.83	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.44
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.44
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.72	0.44
1:B:396:ARG:NH2	1:B:464:ILE:HG22	2.12	0.44
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.44
1:C:134:ASP:HB2	1:C:146:LEU:HD11	1.99	0.44
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.44
1:C:381:VAL:HA	1:C:387:ILE:O	2.17	0.44
1:C:380:THR:HG22	1:C:381:VAL:N	2.32	0.44
1:B:151:LEU:N	1:B:151:LEU:HD12	2.33	0.44
1:A:49:GLY:HA2	1:C:39:THR:HB	0.85	0.44
1:C:461:ASP:HB3	1:C:468:THR:HG22	2.00	0.44
1:A:426:LEU:HD13	1:A:426:LEU:C	2.38	0.44
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.44
1:C:27:ASN:ND2	1:C:28:LYS:N	2.50	0.44
1:A:45:ASN:HA	1:C:37:SER:C	2.37	0.44
1:C:86:SER:HA	1:C:87:PRO:HD3	1.83	0.44
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.44
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.44
1:C:194:THR:HG23	1:C:201:LEU:O	2.18	0.44
1:C:109:THR:HB	1:C:131:SER:HB2	1.99	0.44
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.44
1:C:354:LEU:HD12	1:C:386:GLY:O	2.18	0.44
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.43
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.43
1:C:371:ILE:HD13	1:C:381:VAL:HG11	1.95	0.43
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.43
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.43
1:B:34:VAL:HG22	1:C:2:TRP:HB2	2.00	0.43
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.43
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.43
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.43
1:B:366:LYS:HG2	1:B:367:LEU:H	1.75	0.43
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.43
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.43
1:B:247:LEU:N	1:B:247:LEU:HD12	2.33	0.43
1:B:502:LEU:HD23	1:B:502:LEU:HA	1.82	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.43
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.43
1:C:260:LYS:HB3	1:C:260:LYS:HE3	1.81	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:C:247:LEU:N	1:C:247:LEU:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.43
1:A:35:TYR:HB3	1:B:90:GLU:CD	2.38	0.43
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:A:82:SER:HG	1:B:91:PRO:C	2.19	0.43
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.43
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:B:4:ILE:HA	1:B:5:PRO:HD3	1.72	0.43
1:C:220:ILE:HG22	1:C:220:ILE:O	2.18	0.43
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.43
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.43
1:C:539:CYS:HB3	1:C:540:GLN:H	1.45	0.43
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	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:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.43
1:C:368:SER:CB	1:C:370:PHE:HE1	2.31	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:344:ASP:CG	1:A:344:ASP:O	2.57	0.43
1:A:46:PRO:HD2	1:C:35:TYR:O	2.19	0.43
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.43
1:B:239:VAL:HG13	1:B:240:GLN:N	2.34	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.34	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:C:239:VAL:HG13	1:C:240:GLN:N	2.33	0.43
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.43
1:A:48:GLN:O	1:C:44:ASP:HB3	2.18	0.43
1:C:421:THR:CG2	1:C:422:GLY:N	2.81	0.43
1:B:419:VAL:HG13	1:B:420:GLY:N	2.34	0.43
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.43
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.43
1:B:367:LEU:HG	1:B:367:LEU:H	1.41	0.43
1:C:333:VAL:HG23	1:C:334:PRO:HD3	2.01	0.43
1:C:175:ILE:CG2	1:C:176:GLY:N	2.82	0.43
1:C:22:VAL:CG2	1:C:23:GLN:N	2.81	0.42
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:LEU:HA	1:C:522:LEU:HD23	1.36	0.42
1:C:409:ILE:HD13	3:C:811:NDG:H8C3	2.01	0.42
1:C:195:ASP:HB3	1:C:196:LEU:HG	2.01	0.42
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.42
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:C:344:ASP:CG	1:C:344:ASP:O	2.57	0.42
1:B:32:ASN:HD22	1:B:83:GLU:N	2.13	0.42
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:89:GLU:CD	1:B:1:ASP:N	2.37	0.42
1:A:32:ASN:ND2	1:A:83:GLU:CB	2.62	0.42
1:C:419:VAL:HG13	1:C:420:GLY:N	2.33	0.42
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.42
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.42
1:C:90:GLU:O	1:C:91:PRO:O	2.37	0.42
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.42
1:A:450:GLN:HG3	1:A:532:CYS:O	2.10	0.42
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.42
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.42
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.42
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:C:371:ILE:HG13	1:C:410:MET:SD	2.59	0.42
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.42
1:C:127:VAL:HG13	1:C:128:MET:N	2.25	0.42
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.42
1:C:138:ASN:C	1:C:138:ASN:ND2	2.73	0.42
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.42
1:B:261:ILE:H	1:B:261:ILE:HD13	1.85	0.42
1:B:88:VAL:HG21	1:C:2:TRP:HB2	1.85	0.42
1:B:30:ARG:HH12	1:C:25:LYS:CG	2.31	0.42
1:B:482:THR:HG22	1:B:499:THR:H	1.70	0.42
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.42
1:C:230:VAL:O	1:C:323:VAL:HA	2.20	0.42
1:A:298:LEU:CD2	1:A:298:LEU:N	2.75	0.42
1:C:250:PRO:HA	1:C:255:TRP:CG	2.55	0.42
1:C:515:ASP:OD1	1:C:516:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.42
1:A:84:ASN:O	1:B:79:HIS:ND1	2.53	0.42
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:C:67:ASP:CG	1:C:69:GLU:HB2	2.40	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:B:83:GLU:CD	1:C:2:TRP:CH2	2.93	0.42
1:A:44:ASP:C	1:C:38:ILE:HA	2.38	0.42
2:C:805:NAG:H62	2:C:806:NAG:N2	2.31	0.42
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.42
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:C:40:GLY:O	1:C:45:ASN:HB2	2.19	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42
1:B:235:ILE:HG21	1:B:235:ILE:HD13	1.84	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.42
1:C:415:ASP:CG	1:C:416:GLY:H	2.16	0.42
1:B:250:PRO:HA	1:B:255:TRP:CG	2.55	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.53	0.42
1:C:7:ILE:O	1:C:96:ILE:HG23	2.20	0.42
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.72	0.42
1:A:539:CYS:HB3	1:A:540:GLN:H	1.45	0.42
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.42
1:C:188:THR:H	2:C:801:NAG:H83	1.84	0.42
1:C:32:ASN:HD22	1:C:83:GLU:N	2.13	0.42
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.42
1:C:439:VAL:HA	1:C:440:PRO:HD3	1.81	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:C:347:ARG:HD2	1:C:392:GLY:CA	2.50	0.42
1:C:239:VAL:HG11	1:C:282:LEU:HD22	2.02	0.42
1:C:505:GLY:H	1:C:529:VAL:HB	1.85	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.42
1:A:3:VAL:HB	1:A:4:ILE:H	1.51	0.42
1:A:45:ASN:CA	1:C:37:SER:C	2.88	0.42
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42
1:C:261:ILE:HD13	1:C:261:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:B:344:ASP:O	1:B:344:ASP:CG	2.57	0.42
1:A:35:TYR:CZ	1:C:93:GLU:OE2	2.69	0.41
1:C:449:ASP:N	1:C:532:CYS:HB3	2.19	0.41
1:B:514:SER:HG	1:B:519:ASN:HA	1.85	0.41
1:C:367:LEU:HG	1:C:367:LEU:H	1.41	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.41
1:C:108:PHE:HA	1:C:132:ALA:CB	2.50	0.41
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.41
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.41
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.41
1:C:264:ASN:HB3	1:C:267:GLY:HA2	2.01	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
2:A:810:NAG:C1	2:A:810:NAG:O7	2.67	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.41
1:C:231:PRO:O	1:C:288:LEU:HD12	2.20	0.41
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:B:127:VAL:HG13	1:B:128:MET:N	2.25	0.41
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.41
1:A:48:GLN:CG	1:C:37:SER:HB2	2.45	0.41
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:B:154:ASP:HB3	2:B:801:NAG:C7	2.48	0.41
1:C:154:ASP:HB3	2:C:801:NAG:C7	2.48	0.41
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.41
1:A:86:SER:HB3	1:B:92:MET:HB2	1.39	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.41
1:B:33:LYS:O	1:C:2:TRP:CG	2.73	0.41
1:C:297:VAL:HG21	2:C:807:NAG:H62	2.01	0.41
1:C:518:ASN:C	1:C:520:PRO:CD	2.87	0.41
1:C:230:VAL:HG23	1:C:323:VAL:HA	2.03	0.41
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.41
1:C:3:VAL:HB	1:C:4:ILE:H	1.51	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:C:119:GLU:CG	1:C:214:ALA:HB3	2.51	0.41
1:B:502:LEU:HD22	1:B:503:LYS:H	1.85	0.41
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
2:C:810:NAG:C1	2:C:810:NAG:O7	2.67	0.41
1:C:319:VAL:CG1	1:C:320:THR:N	2.84	0.41
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.41
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.41
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.41
1:C:502:LEU:HD22	1:C:503:LYS:H	1.85	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.41
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:C:62:VAL:O	1:C:62:VAL:HG13	2.21	0.41
1:C:23:GLN:HB2	1:C:59:TRP:CD2	2.55	0.41
1:A:82:SER:OG	1:B:91:PRO:CD	2.68	0.41
1:C:423:THR:CG2	2:C:810:NAG:N2	2.84	0.41
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:A:261:ILE:H	1:A:261:ILE:HD13	1.85	0.41
1:B:25:LYS:NZ	1:B:29:ASP:OD2	2.39	0.41
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.43	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:C:23:GLN:HA	1:C:58:GLY:O	2.21	0.41
1:B:449:ASP:HB2	1:B:531:SER:HA	2.03	0.41
1:C:483:TRP:CZ2	1:C:507:TYR:CE1	2.87	0.41
1:C:469:TYR:CE2	1:C:470:PRO:HD2	2.54	0.41
1:A:290:PHE:CG	1:A:292:LEU:HB2	2.56	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HG21	1.84	0.41
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.41
1:C:339:VAL:HG21	1:C:351:ILE:HG22	2.01	0.41
1:C:336:VAL:H	1:C:336:VAL:HG23	1.52	0.41
1:C:231:PRO:O	1:C:235:ILE:HD13	2.21	0.41
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.41
1:B:448:CYS:C	1:B:452:PRO:HG3	2.40	0.41
1:C:345:LEU:HD22	1:C:349:GLU:HB2	2.03	0.41
1:A:345:LEU:HD22	1:A:349:GLU:HB2	2.03	0.41
1:C:108:PHE:HA	1:C:132:ALA:HB2	2.03	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:138:ASN:N	1:A:138:ASN:HD22	2.19	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG13	1:A:62:VAL:O	2.21	0.41
1:A:45:ASN:ND2	1:C:80:ALA:C	2.48	0.41
1:C:448:CYS:C	1:C:452:PRO:HG3	2.40	0.41
1:C:118:ARG:CA	1:C:212:THR:HB	2.51	0.41
1:B:319:VAL:CG1	1:B:320:THR:N	2.84	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:C:290:PHE:CG	1:C:292:LEU:HB2	2.56	0.41
1:C:127:VAL:HG22	1:C:128:MET:HG3	2.03	0.41
1:C:68:ARG:HD3	1:C:100:ASP:CB	2.51	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:193:ALA:O	1:B:202:SER:HA	2.21	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:C:111:ASP:O	1:C:112:VAL:HG13	2.21	0.41
1:C:474:SER:N	1:C:512:LEU:O	2.53	0.40
1:C:449:ASP:HB2	1:C:531:SER:HA	2.03	0.40
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.40
1:C:226:TYR:O	1:C:227:THR:HG22	2.21	0.40
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40
1:C:274:ASP:O	1:C:278:ASN:CA	2.51	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
1:C:438:PRO:HB2	1:C:513:LEU:CD1	2.51	0.40
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.40
1:C:138:ASN:HD22	1:C:138:ASN:N	2.19	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:B:540:GLN:NE2	1:B:540:GLN:O	2.47	0.40
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.40
1:C:297:VAL:HG22	2:C:807:NAG:H62	2.03	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.51	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:C:19:LYS:HB3	1:C:62:VAL:HG12	2.03	0.40
1:C:445:PHE:CD2	1:C:445:PHE:N	2.89	0.40
1:C:432:ASP:CG	1:C:433:VAL:N	2.74	0.40
1:A:466:PRO:O	1:A:469:TYR:N	2.46	0.40
1:C:212:THR:CG2	1:C:213:ASP:N	2.83	0.40
1:C:223:PRO:HB2	1:C:226:TYR:CZ	2.56	0.40
1:C:316:THR:OG1	2:C:806:NAG:H83	2.21	0.40
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.40
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.40
1:C:371:ILE:HA	1:C:410:MET:HB3	2.02	0.40
1:B:239:VAL:HG11	1:B:282:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:THR:O	1:B:281:ILE:HG22	2.21	0.40
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.40
1:C:108:PHE:CZ	1:C:191:VAL:HG23	2.56	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:C:193:ALA:O	1:C:202:SER:HA	2.21	0.40
1:B:396:ARG:HH21	1:B:432:ASP:CG	2.25	0.40
1:A:78:SER:C	1:C:90:GLU:CD	2.79	0.40
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.40
1:B:423:THR:CG2	2:B:810:NAG:N2	2.84	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:28:LYS:NZ	1:B:4:ILE:HG22	2.37	0.40
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.65	0.40
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.40
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.40
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.40
1:C:42:GLY:CA	1:C:47:PRO:O	2.69	0.40
1:C:490:LYS:CG	1:C:490:LYS:O	2.67	0.40
1:A:249:MET:HA	1:A:250:PRO:HD3	1.85	0.40
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.40
1:C:235:ILE:CD1	1:C:287:GLY:HA2	2.50	0.40
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.40
1:C:400:TYR:O	1:C:401:VAL:C	2.59	0.40
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	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%)	401 (74%)	92 (17%)	45 (8%)	1	18
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	18
All	All	1614/2640 (61%)	1203 (74%)	276 (17%)	135 (8%)	2	18

All (135) 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

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Mol	Chain	Res	Type
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	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	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
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

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Mol	Chain	Res	Type
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	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	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	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	C	498	PRO
1	C	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP

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Mol	Chain	Res	Type
1	B	307	PRO
1	C	154	ASP
1	C	307	PRO
1	A	222	ASP
1	B	222	ASP
1	C	222	ASP
1	A	200	GLY
1	B	200	GLY
1	C	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	B	158	PRO
1	C	47	PRO
1	C	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
All	All	1440/2337 (62%)	1143 (79%)	297 (21%)	4	10

All (297) 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

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Mol	Chain	Res	Type
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
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

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Mol	Chain	Res	Type
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU
1	A	353	SER
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

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Mol	Chain	Res	Type
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	520	PRO
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

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Mol	Chain	Res	Type
1	B	264	ASN
1	B	268	PHE
1	B	273	THR
1	B	277	SER
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

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Mol	Chain	Res	Type
1	B	427	ILE
1	B	428	LEU
1	B	433	VAL
1	B	436	ASN
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

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Mol	Chain	Res	Type
1	C	189	LEU
1	C	195	ASP
1	C	202	SER
1	C	216	ASP
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

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Mol	Chain	Res	Type
1	C	379	LEU
1	C	382	ASN
1	C	384	ASP
1	C	385	ASN
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) 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	48	GLN
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	32	ASN
1	B	45	ASN
1	B	79	HIS
1	B	84	ASN
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
1	B	217	ASN
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

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Mol	Chain	Res	Type
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	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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 81 ligands modelled in this entry, 36 are monoatomic - leaving 45 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	0.64	0	15,19,21	0.88	0
2	NAG	A	802	1	14,14,15	0.71	0	15,19,21	0.82	1 (6%)
2	NAG	A	803	1	14,14,15	0.91	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	0.68	0	15,19,21	1.17	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.41	2 (13%)
2	NAG	A	807	1	14,14,15	0.64	0	15,19,21	1.14	1 (6%)
2	NAG	A	808	1	14,14,15	0.65	0	15,19,21	0.70	0
2	NAG	A	809	1	14,14,15	0.74	0	15,19,21	0.96	1 (6%)
2	NAG	A	810	1	14,14,15	0.63	0	15,19,21	1.08	2 (13%)
3	NDG	A	811	1	14,14,15	0.83	0	15,19,21	2.16	1 (6%)
2	NAG	A	812	1	14,14,15	0.82	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	A	902	1	14,14,15	1.07	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	14,14,15	0.75	1 (7%)	15,19,21	0.78	1 (6%)
2	NAG	B	801	1	14,14,15	0.64	0	15,19,21	0.89	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	0.91	1 (7%)	15,19,21	1.19	2 (13%)
3	NDG	B	804	1	14,14,15	0.61	0	15,19,21	0.82	0
2	NAG	B	805	1	14,14,15	0.68	0	15,19,21	1.18	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.42	2 (13%)
2	NAG	B	807	1	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
2	NAG	B	808	1	14,14,15	0.67	0	15,19,21	0.70	0
2	NAG	B	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.96	1 (6%)
2	NAG	B	810	1	14,14,15	0.63	0	15,19,21	1.09	2 (13%)
3	NDG	B	811	1	14,14,15	0.82	0	15,19,21	2.17	1 (6%)
2	NAG	B	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.51	0	15,19,21	0.64	0
2	NAG	B	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.79	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	0.91	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%)
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	1.14	1 (6%)
2	NAG	C	808	1	14,14,15	0.66	0	15,19,21	0.69	0
2	NAG	C	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	C	810	1	14,14,15	0.63	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	0.83	1 (7%)	15,19,21	0.76	1 (6%)
3	NDG	C	902	1	14,14,15	1.08	1 (7%)	15,19,21	0.97	0
3	NDG	C	903	1	14,14,15	0.51	0	15,19,21	0.64	0
2	NAG	C	904	1	14,14,15	0.76	1 (7%)	15,19,21	0.79	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
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	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	NAG	C1-C2	-2.41	1.49	1.52
2	B	904	NAG	C1-C2	-2.39	1.49	1.52
2	A	904	NAG	C1-C2	-2.37	1.49	1.52
2	C	812	NAG	C1-C2	-2.34	1.49	1.52
2	B	812	NAG	C1-C2	-2.33	1.49	1.52
2	A	812	NAG	C1-C2	-2.32	1.49	1.52
2	C	809	NAG	C1-C2	-2.03	1.49	1.52
2	B	809	NAG	C1-C2	-2.01	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	C	803	NAG	O5-C5	2.33	1.48	1.43
3	B	902	NDG	C1-C2	3.09	1.56	1.52
3	C	902	NDG	C1-C2	3.16	1.56	1.52
3	A	902	NDG	C1-C2	3.16	1.57	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-7.83	112.92	123.11
3	A	811	NDG	C2-N2-C7	-7.80	112.95	123.11
3	C	811	NDG	C2-N2-C7	-7.80	112.96	123.11
2	A	806	NAG	C2-N2-C7	-3.89	118.04	123.11
2	B	806	NAG	C2-N2-C7	-3.89	118.05	123.11
2	C	806	NAG	C2-N2-C7	-3.87	118.07	123.11
2	B	805	NAG	C2-N2-C7	-3.45	118.61	123.11
2	A	805	NAG	C2-N2-C7	-3.42	118.66	123.11
2	C	805	NAG	C2-N2-C7	-3.40	118.68	123.11
2	C	807	NAG	C2-N2-C7	-3.33	118.78	123.11
2	B	807	NAG	C2-N2-C7	-3.30	118.81	123.11
2	A	807	NAG	C2-N2-C7	-3.30	118.82	123.11
2	C	803	NAG	C2-N2-C7	-3.25	118.87	123.11
2	A	803	NAG	C2-N2-C7	-3.21	118.93	123.11
2	B	803	NAG	C2-N2-C7	-3.20	118.94	123.11
2	C	810	NAG	C4-C3-C2	-2.53	107.41	111.34
2	B	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	A	806	NAG	C4-C3-C2	-2.52	107.43	111.34
2	B	806	NAG	C4-C3-C2	-2.51	107.44	111.34
2	C	806	NAG	C4-C3-C2	-2.50	107.45	111.34
2	A	812	NAG	C2-N2-C7	-2.38	120.01	123.11
2	C	812	NAG	C2-N2-C7	-2.36	120.03	123.11
2	B	812	NAG	C2-N2-C7	-2.36	120.04	123.11
2	B	809	NAG	O5-C5-C4	-2.26	106.39	110.13
2	A	809	NAG	O5-C5-C4	-2.26	106.39	110.13
2	C	904	NAG	C2-N2-C7	-2.26	120.17	123.11
2	B	904	NAG	C2-N2-C7	-2.25	120.17	123.11
2	A	904	NAG	C2-N2-C7	-2.24	120.19	123.11
2	C	809	NAG	O5-C5-C4	-2.22	106.45	110.13
2	A	802	NAG	C2-N2-C7	-2.18	120.27	123.11
2	B	802	NAG	C2-N2-C7	-2.16	120.30	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	NAG	C2-N2-C7	-2.16	120.30	123.11
2	B	810	NAG	C1-O5-C5	-2.02	109.17	112.14
2	C	810	NAG	C1-O5-C5	-2.02	109.17	112.14
2	A	810	NAG	C1-O5-C5	-2.00	109.19	112.14
2	A	803	NAG	C1-O5-C5	2.24	115.44	112.14
2	B	803	NAG	C1-O5-C5	2.25	115.45	112.14
2	C	803	NAG	C1-O5-C5	2.28	115.49	112.14

All (6) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 300 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	21	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	21	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	13	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	20	0
2	C	803	NAG	4	0
3	C	804	NDG	2	0
2	C	805	NAG	7	0
2	C	806	NAG	12	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	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.