



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3NBY
Title : Crystal structure of the PKI NES-CRM1-RanGTP nuclear export complex
Authors : Guttler, T.; Madl, T.; Neumann, P.; Deichsel, D.; Corsini, L.; Monecke, T.;
Ficner, R.; Sattler, M.; Gorlich, D.
Deposited on : 2010-06-04
Resolution : 3.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

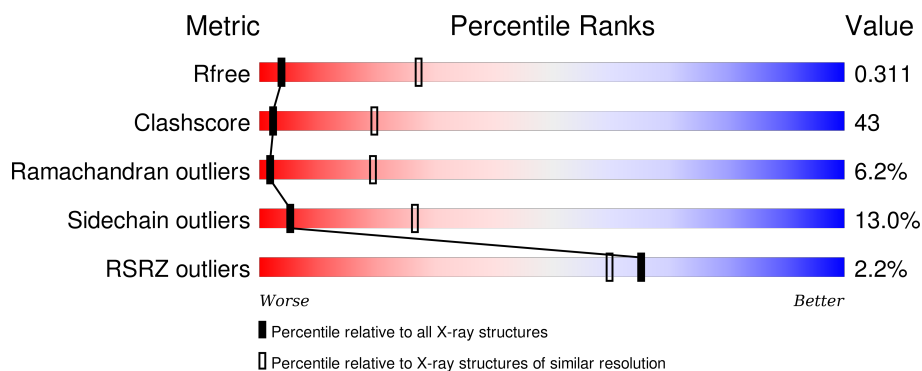
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	361	
1	E	361	
2	C	176	
2	F	176	
3	A	1073	

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Mol	Chain	Length	Quality of chain
3	D	1073	<div><div></div><div>3%</div><div>32%</div><div>53%</div><div>11%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24084 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	272	Total	C	N	O	S	0	0	0
			2193	1398	376	405	14			
1	E	277	Total	C	N	O	S	0	0	0
			2221	1416	380	410	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
B	1	LEU	-	expression tag	UNP O95149
B	2	ASN	-	expression tag	UNP O95149
B	3	GLU	-	expression tag	UNP O95149
B	4	LEU	-	expression tag	UNP O95149
B	5	ALA	-	expression tag	UNP O95149
B	6	LEU	-	expression tag	UNP O95149
B	7	LYS	-	expression tag	UNP O95149
B	8	LEU	-	expression tag	UNP O95149
B	9	ALA	-	expression tag	UNP O95149
B	10	GLY	-	expression tag	UNP O95149
B	11	LEU	-	expression tag	UNP O95149
B	12	ASP	-	expression tag	UNP O95149
B	13	ILE	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149
E	1	LEU	-	expression tag	UNP O95149
E	2	ASN	-	expression tag	UNP O95149
E	3	GLU	-	expression tag	UNP O95149
E	4	LEU	-	expression tag	UNP O95149
E	5	ALA	-	expression tag	UNP O95149
E	6	LEU	-	expression tag	UNP O95149
E	7	LYS	-	expression tag	UNP O95149
E	8	LEU	-	expression tag	UNP O95149

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Chain	Residue	Modelled	Actual	Comment	Reference
E	9	ALA	-	expression tag	UNP O95149
E	10	GLY	-	expression tag	UNP O95149
E	11	LEU	-	expression tag	UNP O95149
E	12	ASP	-	expression tag	UNP O95149
E	13	ILE	-	expression tag	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered	UNP P62826
F	69	LEU	GLN	engineered	UNP P62826

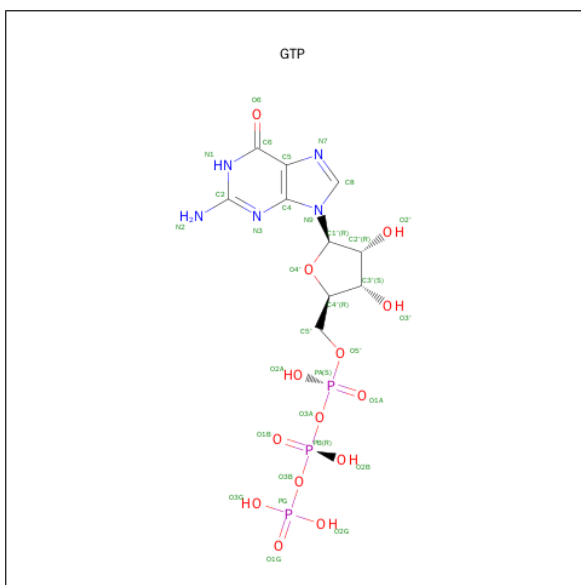
- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			
3	D	1041	Total	C	N	O	S	0	0	0
			8413	5397	1413	1549	54			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	F	1	Total 32	C 10	N 5	O 14	P 3	0	0

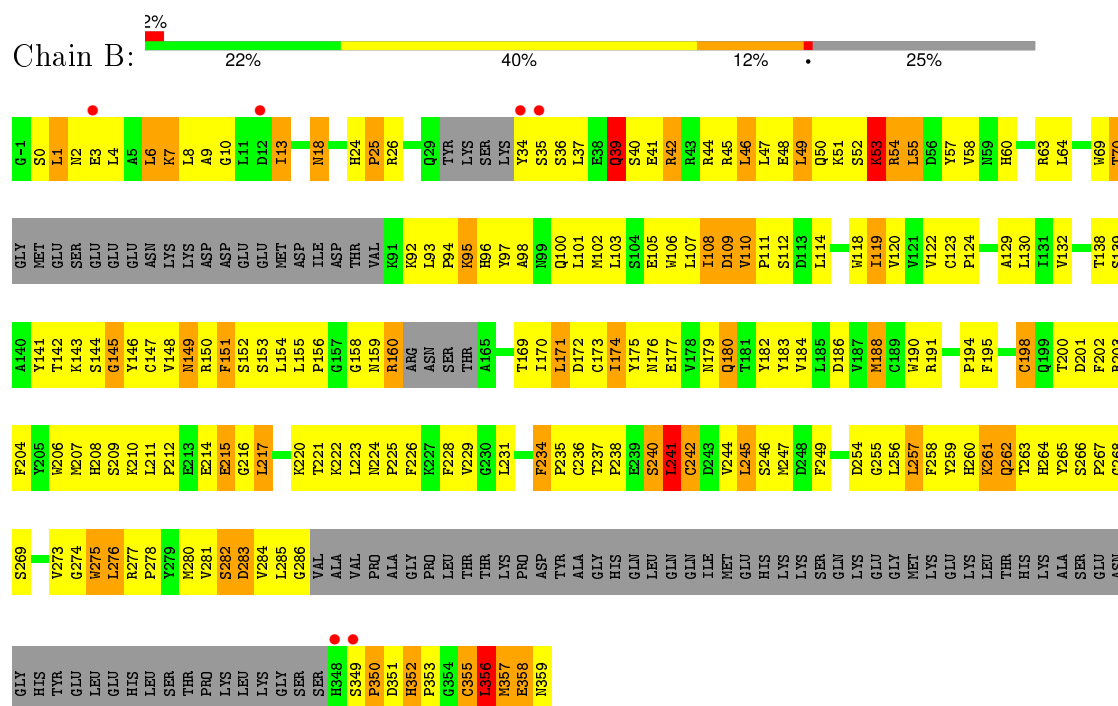
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

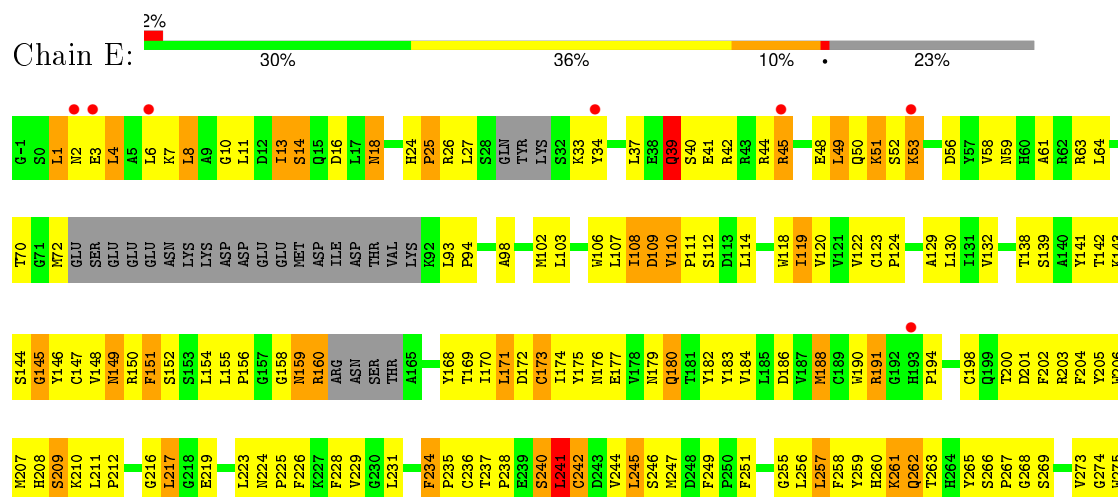
3 Residue-property plots

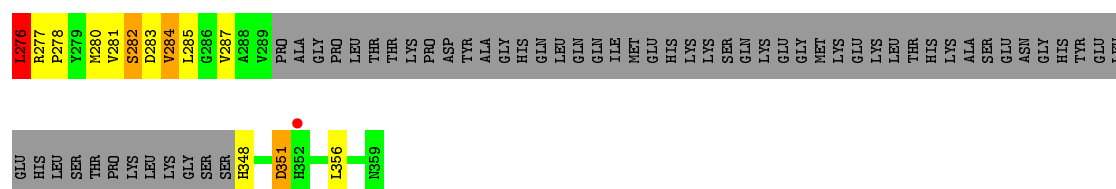
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Snurportin-1

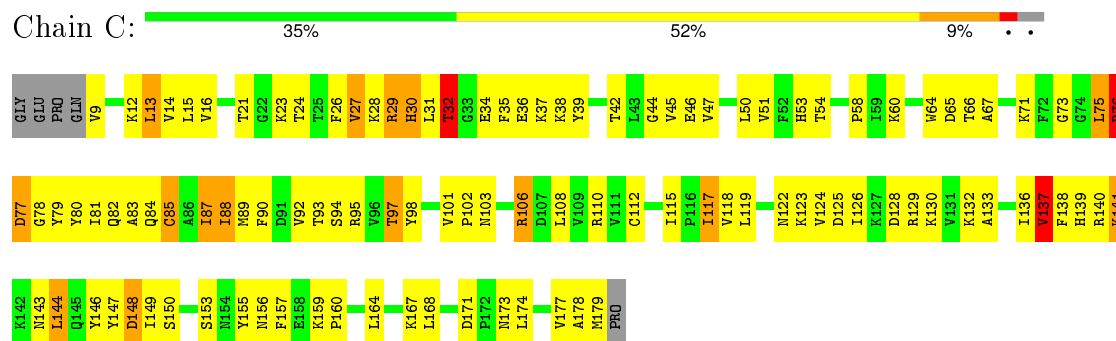


• Molecule 1: Snurportin-1

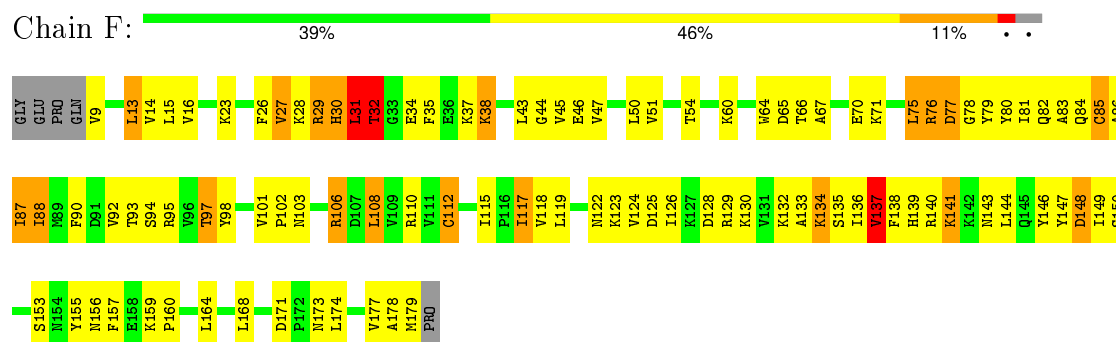




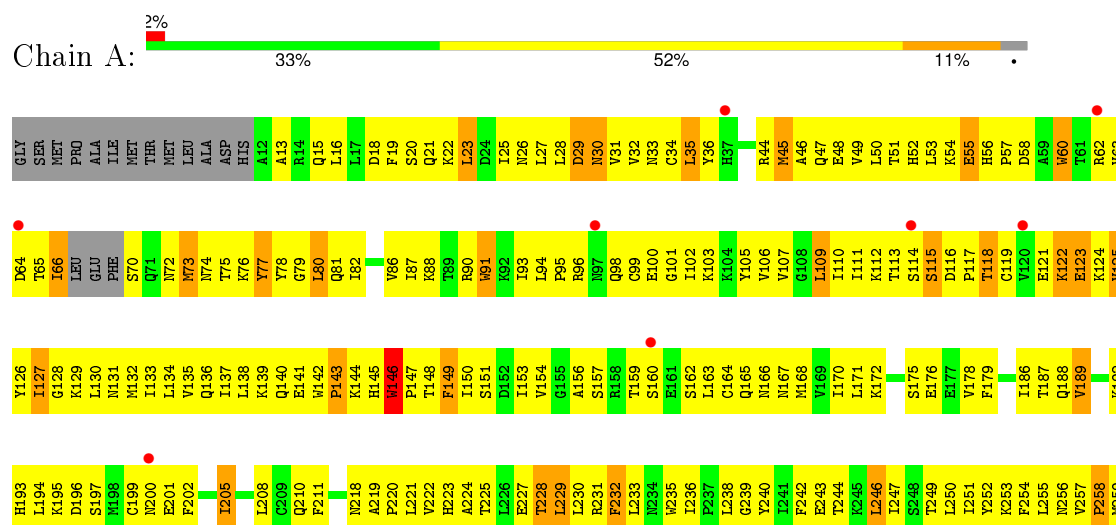
• Molecule 2: GTP-binding nuclear protein Ran

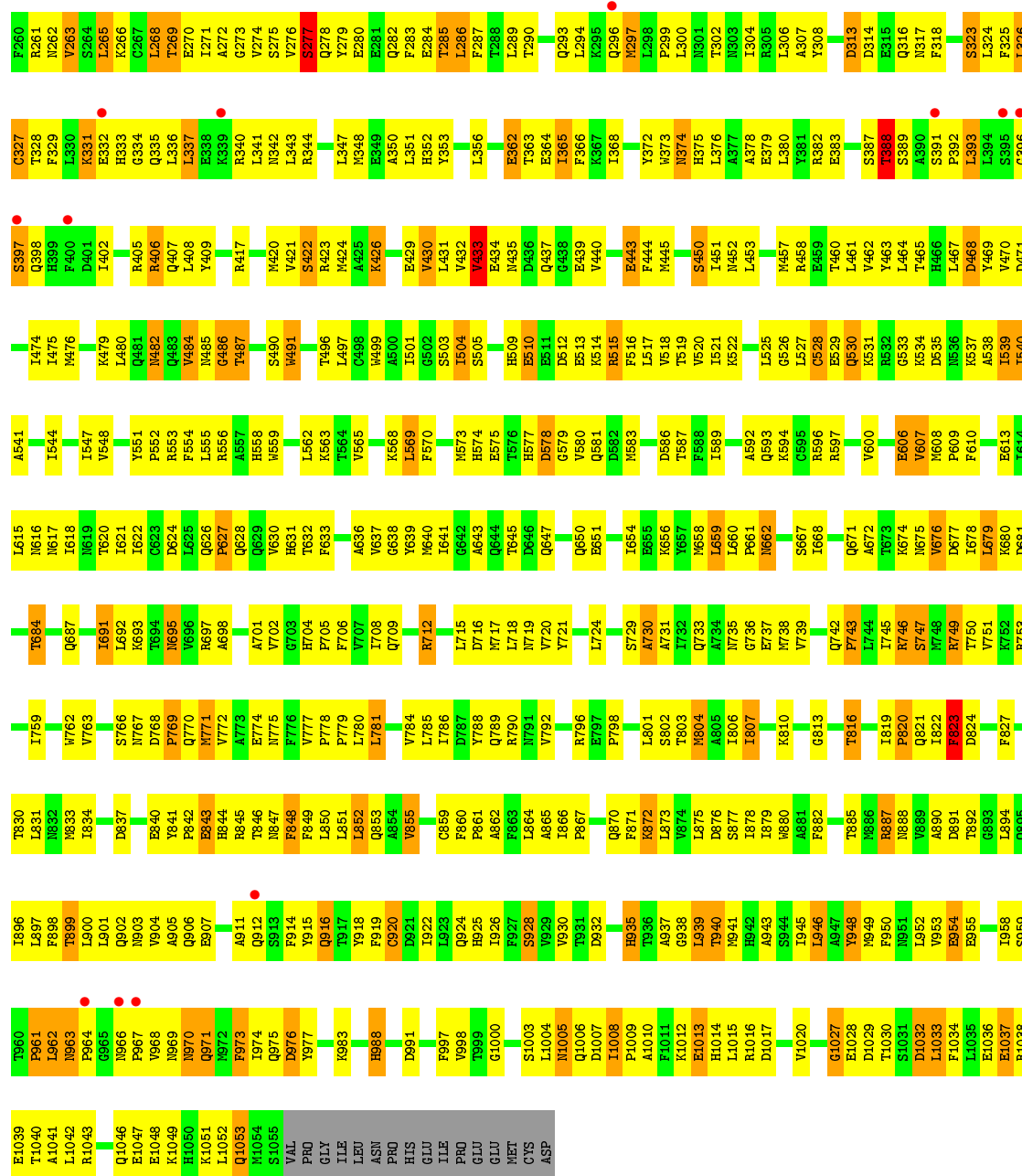


• Molecule 2: GTP-binding nuclear protein Ran

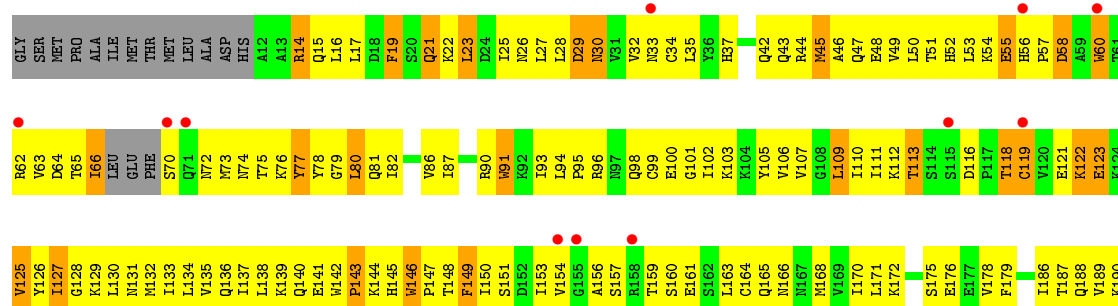


• Molecule 3: Exportin-1





• Molecule 3: Exportin-1



A1026	Y953	4890	P823	W751	L679	F610	K534	T465	L394	F325	P258	L191
G1027	B954	D891	F827	K752	K680	1611	D535	F466	S395	L326	M259	K192
E1028	B955	T892	F827	F753	P682	D612	M536	L467	G396	C327	F260	H193
D1029	Y958	L894	F754	T755	P682	E613	K537	D468	S397	T328	R261	L194
T1030	S959	L895	T755	T755	T684	L615	A538	Y469	Q398	F329	M262	K195
S1031	T960	T896	T755	T759	T684	L616	A539	Y470	Q399	L330	Y263	D196
D1032	P961	L897	T759	T759	T684	N617	I540	D471	F400	K331	S264	S197
L1033	P962	M833	T762	T762	T684	1618	A541	L474	D401	E532	L285	H198
F1034	P963	T899	T763	T763	L692	T620	I544	M476	L402	H333	K286	C199
T1035	P964	L900	T766	T766	K693	1621	I547	K479	R405	L288	T269	E201
E1036	G965	L901	T767	T767	T694	1622	V548	L480	R406	L336	E270	S202
E1037	G966	Q902	T768	T768	N695	E623	Y551	Q481	Q407	L337	I271	Q204
R1038	P967	N903	T769	T769	V696	D624	P552	M482	L408	R340	A272	L205
A1041	Y968	Y904	T770	T770	A698	L625	P552	Y491	Y409	L341	A273	L208
L1042	N970	A905	T771	T771	A698	Q626	R553	Q486	Q407	N342	G273	C209
R1043	Q971	Q906	T772	T772	A698	Q627	F554	Y494	Q407	L343	S275	Q210
Q1044	N972	E907	T773	T773	A701	Q628	L555	M485	R417	R344	V276	L208
E1047	F973	A911	T774	T774	V702	Q629	R556	Q486	M420	L347	S277	Q217
E1048	Y974	Q912	T775	T775	G703	Q630	A557	T487	V421	M348	Y279	M218
K1049	Q975	S913	T776	T776	H704	H631	M558	Y497	S422	E349	Y279	M219
H1050	D976	F914	T777	T777	P705	T632	M559	S490	R423	E280	E281	P220
L1051	Y977	Y915	T778	T778	P706	F633	W559	W491	M424	A350	E282	L221
L1052	N980	Q916	T779	T779	V707	V634	L562	T496	L425	L351	Q282	V222
Q1053	N981	T917	L780	L780	I708	E635	K563	T497	K426	H562	F283	H223
S1055	K983	Y918	L781	L781	Q709	A636	T564	Q498	Q427	L286	E284	A224
VAL	H988	F919	L782	L782	R712	V637	K568	C498	S428	L287	S277	L226
PRO	L989	Q920	L783	L783	A730	Q638	L569	A500	V430	F287	E227	E227
GLY	L990	L922	L784	L784	V784	Q639	F570	A500	L431	T363	T228	T228
ILE	Q990	L923	L785	L785	L715	N640	E571	G502	V432	E364	L229	L229
LEU	D991	Q924	L786	L786	D716	1641	F572	G503	V433	I365	L230	R231
ASN	L996	H925	L787	L787	M717	Q642	F572	S502	E434	F366	L294	F232
PRO	F997	H926	L788	L788	L718	A643	H574	S505	M435	K367	Q295	L233
HIS	G1000	I927	L789	L789	W720	T645	E575	H509	D436	I368	Q296	L233
GLU	L1001	S928	L790	L790	Y721	D646	T576	E510	Q437	E362	M297	W234
ILE	F1002	Y930	L791	L791	K722	Q647	H577	E511	G438	T363	L298	W235
GLU	S1003	V931	L792	L792	C723	Q650	D578	D512	E439	E371	P299	L238
GLU	L1004	D932	L793	L793	L724	B651	G579	E513	Y440	Y372	P299	G239
MET	N1005	H935	L794	L794	S729	K656	Q581	K514	V441	N374	L300	L240
CYS	D1006	T936	L795	L795	A730	Y657	D586	R515	E443	H375	T302	T241
ASP	D1007	A937	L796	L796	I732	M658	T587	F516	F444	L376	N303	L241
	P1009	G938	L797	L797	Q733	L659	F588	L517	A377	A378	I304	F242
	A1010	L939	L798	L798	T733	L660	I589	T519	E379	E379	R305	E243
	F1011	T940	L799	L799	G736	P661	L589	V520	S450	L380	L306	T244
	K1012	H941	L800	L800	E737	N662	A592	T521	S450	A307	L245	K245
	E1013	H942	L801	L801	N738	1662	Q593	I521	Y451	Y381	L247	L247
	H1014	A943	L802	L802	W739	S667	K594	K522	M452	R382	K312	S246
	L1015	S944	L803	L803	P743	1668	C595	L525	L453	E383	D314	T249
	R1016	T945	L804	L804	L744	Q671	R596	G526	M457	S387	D314	L250
	D1017	A947	L805	L805	I745	A672	R597	L527	R458	E315	E315	L251
	Y1020	Y948	L806	L806	T746	N675	V600	E529	T459	T388	Q316	Y252
	Q1021	H949	L807	L807	S747	1676	E806	Q530	T460	S389	N317	F254
	L1022	F950	L808	L808	M748	1677	V607	R531	L461	A390	F318	L256
	K1023	L952	L809	L809	T750	1678	E807	R532	Y463	S391	S323	M256
			L810	L810						P392	L394	L394
			L811	L811								
			L812	L812								
			L813	L813								
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			L815	L815								
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.09 Å 223.73 Å 163.06 Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	38.63 – 3.42 38.63 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.63-3.42) 88.9 (38.63-2.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.95 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.258 , 0.315 0.252 , 0.311	Depositor DCC
R_{free} test set	3408 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 6.6	EDS
Estimated twinning fraction	0.115 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 104746 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	24084	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG

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 > 5$	RMSZ	# $ Z > 5$
1	B	0.62	0/2250	0.85	3/3046 (0.1%)
1	E	0.59	1/2278 (0.0%)	0.81	4/3084 (0.1%)
2	C	0.58	0/1423	0.74	0/1921
2	F	0.57	0/1423	0.74	1/1921 (0.1%)
3	A	0.56	2/8584 (0.0%)	0.73	1/11627 (0.0%)
3	D	0.57	0/8584	0.74	0/11627
All	All	0.58	3/24542 (0.0%)	0.76	9/33226 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	CYS	CB-SG	-5.71	1.72	1.81
3	A	491	TRP	NE1-CE2	5.53	1.44	1.37
3	A	528	CYS	CB-SG	-5.08	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	42	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	B	42	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	B	42	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	E	42	ARG	NE-CZ-NH2	10.83	125.72	120.30
2	F	31	LEU	CA-CB-CG	5.93	128.93	115.30
1	B	42	ARG	CD-NE-CZ	5.78	131.69	123.60
1	E	42	ARG	CD-NE-CZ	5.34	131.07	123.60
3	A	393	LEU	CA-CB-CG	5.28	127.44	115.30
1	E	276	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

There are no planarity outliers.

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	B	2193	0	2138	241	0
1	E	2221	0	2170	208	0
2	C	1389	0	1419	128	0
2	F	1389	0	1419	121	0
3	A	8413	0	8480	753	0
3	D	8413	0	8480	731	0
4	C	32	0	12	8	0
4	F	32	0	12	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	24084	0	24130	2091	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 43.

All (2091) 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)
3:A:328:THR:HA	3:A:331:LYS:HD3	1.27	1.14
3:D:328:THR:HA	3:D:331:LYS:HD3	1.33	1.09
3:D:961:PRO:HG2	3:D:973:PHE:HD2	1.16	1.09
1:B:3:GLU:O	1:B:7:LYS:HB2	1.53	1.07
3:D:996:LEU:HD13	3:D:1035:LEU:HD12	1.37	1.06
1:B:159:ASN:HB2	1:B:223:LEU:HD21	1.36	1.06
3:A:528:CYS:HB2	3:A:540:ILE:HG21	1.38	1.06
3:D:528:CYS:HB2	3:D:540:ILE:HG21	1.40	1.04
3:A:962:LEU:HB3	3:A:964:PRO:HD2	1.41	1.02
1:E:4:LEU:HA	1:E:7:LYS:CB	1.89	1.01
1:B:255:GLY:HA2	1:B:278:PRO:HD3	1.42	1.01
1:E:180:GLN:HE22	3:D:684:THR:HG22	1.25	1.01
3:D:892:THR:O	3:D:896:ILE:HG13	1.61	1.01
3:A:482:ASN:HA	3:A:486:GLY:HA3	1.43	1.00
3:A:107:VAL:O	3:A:111:ILE:HG12	1.61	1.00
1:E:4:LEU:HA	1:E:7:LYS:HB2	1.01	1.00
1:B:159:ASN:OD1	1:B:160:ARG:HD2	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:961:PRO:HG2	3:D:973:PHE:CD2	1.98	0.98
3:A:892:THR:O	3:A:896:ILE:HG13	1.63	0.97
1:B:1:LEU:HD13	3:A:558:HIS:HD2	1.26	0.97
3:D:482:ASN:HA	3:D:486:GLY:HA3	1.42	0.97
1:E:40:SER:HB2	1:E:109:ASP:HB2	1.45	0.96
1:E:4:LEU:CA	1:E:7:LYS:HB2	1.94	0.96
1:E:4:LEU:O	1:E:8:LEU:N	1.97	0.96
3:D:287:PHE:CE2	3:D:337:LEU:HD11	2.00	0.96
3:A:484:VAL:HG13	3:A:530:GLN:OE1	1.66	0.95
3:D:107:VAL:O	3:D:111:ILE:HG12	1.66	0.95
3:A:900:LEU:O	3:A:904:VAL:HG23	1.66	0.95
1:E:255:GLY:HA2	1:E:278:PRO:HD3	1.47	0.95
2:C:148:ASP:HB3	2:C:155:TYR:HE2	1.31	0.94
2:C:32:THR:OG1	2:C:34:GLU:HG2	1.68	0.94
3:A:746:ARG:HH11	3:A:746:ARG:HG2	1.28	0.94
2:C:94:SER:O	2:C:97:THR:HG23	1.67	0.93
1:B:40:SER:HB2	1:B:109:ASP:HB2	1.48	0.93
3:A:287:PHE:CE2	3:A:337:LEU:HD11	2.04	0.93
3:A:887:ARG:HD3	3:A:937:ALA:HB3	1.50	0.93
3:D:484:VAL:HG13	3:D:530:GLN:OE1	1.69	0.92
2:F:94:SER:O	2:F:97:THR:HG23	1.69	0.92
3:A:337:LEU:HD13	3:A:347:LEU:HD12	1.52	0.92
3:D:900:LEU:O	3:D:904:VAL:HG23	1.69	0.91
2:F:148:ASP:HB3	2:F:155:TYR:HE2	1.34	0.91
3:D:337:LEU:HD22	3:D:347:LEU:HB2	1.52	0.91
2:F:77:ASP:HA	2:F:80:TYR:CD2	2.05	0.91
2:F:31:LEU:HD12	2:F:32:THR:HG22	1.50	0.91
1:B:41:GLU:HG3	1:B:109:ASP:HB3	1.52	0.91
3:A:337:LEU:HD22	3:A:347:LEU:HB2	1.51	0.91
3:A:672:ALA:HB2	3:A:678:ILE:HD11	1.53	0.91
1:B:4:LEU:O	1:B:8:LEU:N	2.03	0.91
3:D:672:ALA:HB2	3:D:678:ILE:HD11	1.53	0.91
1:B:124:PRO:HD3	1:B:231:LEU:HD11	1.52	0.91
3:D:746:ARG:HH11	3:D:746:ARG:HG2	1.34	0.90
2:C:93:THR:HG21	2:C:126:ILE:HD12	1.54	0.90
3:A:434:GLU:HB2	3:A:439:GLU:O	1.72	0.89
3:A:1047:GLU:O	3:A:1051:LYS:HD3	1.72	0.88
1:B:4:LEU:HD11	3:A:518:VAL:HG13	1.56	0.88
1:E:41:GLU:HG3	1:E:109:ASP:HB3	1.54	0.88
1:B:64:LEU:HD23	1:B:170:ILE:HD13	1.57	0.88
3:D:887:ARG:HD3	3:D:937:ALA:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:LEU:HD23	3:D:564:THR:HG22	1.54	0.87
3:D:650:GLN:HE22	3:D:705:PRO:HG2	1.39	0.87
1:E:124:PRO:HD3	1:E:231:LEU:HD11	1.54	0.87
3:A:650:GLN:HE22	3:A:705:PRO:HG2	1.41	0.86
1:B:55:LEU:H	1:B:55:LEU:HD12	1.38	0.86
3:A:899:THR:HG22	3:A:903:ASN:HD21	1.40	0.86
1:B:124:PRO:HD2	1:B:174:ILE:HD12	1.57	0.84
3:D:14:ARG:HG3	3:D:14:ARG:HH11	1.43	0.84
3:D:899:THR:HG22	3:D:903:ASN:HD21	1.43	0.84
1:B:190:TRP:CD1	1:B:191:ARG:HG3	2.12	0.84
1:E:209:SER:C	1:E:210:LYS:HD2	1.97	0.83
3:D:633:PHE:O	3:D:636:ALA:HB3	1.78	0.83
1:B:160:ARG:HA	1:B:160:ARG:NE	1.93	0.83
1:E:244:VAL:HG13	1:E:245:LEU:HD13	1.59	0.83
1:B:46:LEU:CD2	1:B:50:GLN:HE21	1.90	0.83
2:C:32:THR:HG1	2:C:34:GLU:HG2	1.44	0.83
1:B:160:ARG:HA	1:B:160:ARG:HE	1.42	0.83
2:C:77:ASP:HA	2:C:80:TYR:CD2	2.12	0.83
1:B:244:VAL:HG13	1:B:245:LEU:HD13	1.59	0.82
1:E:64:LEU:HD23	1:E:170:ILE:HD13	1.62	0.82
1:E:175:TYR:HB2	1:E:182:TYR:CE1	2.13	0.82
3:A:771:MET:HG2	3:A:775:ASN:HD22	1.44	0.82
3:D:941:MET:O	3:D:945:ILE:HG13	1.79	0.82
3:D:225:THR:HA	3:D:228:THR:HG22	1.62	0.82
1:B:63:ARG:HH12	1:B:70:THR:HB	1.43	0.82
3:A:736:GLY:O	3:A:739:VAL:HG23	1.80	0.82
1:E:51:LYS:NZ	1:E:263:THR:HA	1.94	0.82
2:F:93:THR:HG21	2:F:126:ILE:HD12	1.62	0.81
1:B:1:LEU:HD13	3:A:558:HIS:CD2	2.13	0.81
1:E:258:PHE:HD2	1:E:274:GLY:O	1.61	0.81
3:A:533:GLY:O	3:A:537:LYS:HG3	1.80	0.81
3:D:788:TYR:CE1	3:D:796:ARG:HB3	2.15	0.81
3:D:771:MET:HG2	3:D:775:ASN:HD22	1.44	0.81
3:A:33:ASN:HB3	3:A:44:ARG:HG3	1.63	0.81
1:B:282:SER:HA	1:B:286:GLY:HA2	1.60	0.81
1:E:129:ALA:HA	1:E:141:TYR:O	1.81	0.81
1:B:172:ASP:HB2	1:B:188:MET:HE1	1.61	0.81
1:B:258:PHE:HD2	1:B:274:GLY:O	1.64	0.81
1:B:110:VAL:HG11	1:B:285:LEU:HD13	1.62	0.81
3:A:73:MET:HB2	3:A:122:LYS:HE3	1.61	0.80
3:A:823:PHE:HZ	3:A:852:LEU:HD13	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:633:PHE:O	3:A:636:ALA:HB3	1.82	0.80
1:E:175:TYR:HE2	1:E:177:GLU:HG2	1.45	0.80
1:B:129:ALA:HA	1:B:141:TYR:O	1.82	0.79
3:A:225:THR:HA	3:A:228:THR:HG22	1.64	0.79
1:E:190:TRP:CD1	1:E:191:ARG:HG3	2.17	0.79
3:A:575:GLU:HG2	3:A:580:VAL:HG11	1.63	0.79
3:A:926:ILE:O	3:A:930:VAL:HG23	1.82	0.79
1:B:37:LEU:HB2	1:B:39:GLN:NE2	1.97	0.79
3:A:899:THR:CG2	3:A:903:ASN:HD21	1.96	0.79
1:B:102:MET:HG3	1:B:266:SER:O	1.83	0.79
1:B:13:ILE:HG21	3:A:575:GLU:CD	2.02	0.78
3:A:586:ASP:O	3:A:589:ILE:HG22	1.83	0.78
3:D:996:LEU:CD1	3:D:1035:LEU:HD12	2.12	0.78
3:D:476:MET:HE3	3:D:501:ILE:HG12	1.64	0.78
3:A:899:THR:HG22	3:A:903:ASN:ND2	1.99	0.78
3:A:569:LEU:HD21	3:A:587:THR:HG22	1.63	0.78
2:C:28:LYS:O	2:C:32:THR:HG23	1.82	0.78
3:A:485:ASN:O	3:A:487:THR:N	2.16	0.78
3:D:225:THR:HA	3:D:228:THR:CG2	2.13	0.78
3:A:834:ILE:HG22	3:A:845:ARG:HG2	1.65	0.78
3:D:337:LEU:HD13	3:D:347:LEU:HD12	1.65	0.78
3:D:990:GLN:HB3	3:D:1028:GLU:HG2	1.64	0.78
3:A:219:ALA:HB3	3:A:220:PRO:HD3	1.65	0.78
3:D:219:ALA:HB3	3:D:220:PRO:HD3	1.66	0.78
3:D:569:LEU:HD21	3:D:587:THR:HG22	1.64	0.77
3:D:823:PHE:HZ	3:D:852:LEU:HD13	1.48	0.77
3:D:899:THR:HG22	3:D:903:ASN:ND2	2.00	0.77
1:E:37:LEU:HB2	1:E:39:GLN:NE2	1.99	0.77
3:D:586:ASP:O	3:D:589:ILE:HG22	1.84	0.77
1:E:160:ARG:HH11	1:E:160:ARG:CG	1.97	0.77
3:D:819:ILE:O	3:D:823:PHE:HB2	1.84	0.77
3:D:899:THR:CG2	3:D:903:ASN:HD21	1.98	0.77
3:D:926:ILE:O	3:D:930:VAL:HG23	1.84	0.77
1:B:144:SER:O	1:B:146:TYR:N	2.18	0.77
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.67	0.77
3:D:433:VAL:HG12	3:D:441:VAL:HG23	1.65	0.77
1:B:209:SER:C	1:B:210:LYS:HD2	2.06	0.76
1:E:119:ILE:HD11	1:E:259:TYR:HB2	1.68	0.76
3:A:819:ILE:O	3:A:823:PHE:HB2	1.85	0.76
3:D:340:ARG:HB3	3:D:342:ASN:OD1	1.85	0.76
3:A:340:ARG:HB3	3:A:342:ASN:OD1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:575:GLU:HG2	3:D:580:VAL:HG11	1.67	0.75
3:A:866:ILE:HB	3:A:867:PRO:HD2	1.68	0.75
3:D:706:PHE:CZ	3:D:709:GLN:HG2	2.21	0.75
3:D:632:THR:HA	3:D:697:ARG:HH22	1.51	0.75
3:D:123:GLU:O	3:D:127:ILE:HD13	1.85	0.75
1:B:119:ILE:HD11	1:B:259:TYR:HB2	1.68	0.75
3:A:337:LEU:CD2	3:A:347:LEU:HB2	2.17	0.75
3:A:274:VAL:HG12	3:A:275:SER:H	1.51	0.75
1:B:4:LEU:HA	1:B:7:LYS:HB2	1.68	0.75
3:A:518:VAL:O	3:A:522:LYS:HB2	1.86	0.74
1:E:56:ASP:OD1	1:E:59:ASN:HB2	1.85	0.74
1:B:175:TYR:HB2	1:B:182:TYR:CE1	2.21	0.74
2:C:122:ASN:O	2:C:123:LYS:HB2	1.87	0.74
2:F:177:VAL:HG22	2:F:178:ALA:H	1.52	0.74
3:D:238:LEU:HD22	3:D:242:PHE:HE2	1.52	0.74
1:B:55:LEU:HD13	1:B:57:TYR:CE2	2.22	0.74
1:B:175:TYR:HE2	1:B:177:GLU:HG2	1.51	0.74
1:E:102:MET:HG3	1:E:266:SER:O	1.87	0.74
3:A:225:THR:HA	3:A:228:THR:CG2	2.18	0.74
3:A:479:LYS:HE2	3:A:479:LYS:HA	1.69	0.74
3:D:555:LEU:HB3	3:D:562:LEU:HD13	1.68	0.74
3:A:941:MET:O	3:A:945:ILE:HG13	1.87	0.74
3:A:970:ASN:N	3:A:970:ASN:HD22	1.84	0.74
3:D:479:LYS:HE2	3:D:479:LYS:HA	1.68	0.74
3:D:996:LEU:HD13	3:D:1035:LEU:CD1	2.17	0.73
3:A:238:LEU:HD22	3:A:242:PHE:HE2	1.52	0.73
3:D:518:VAL:O	3:D:522:LYS:HB2	1.88	0.73
3:D:570:PHE:O	3:D:573:MET:HB2	1.87	0.73
3:A:681:ASP:HB3	3:A:684:THR:HG23	1.69	0.73
2:F:126:ILE:HG22	2:F:128:ASP:H	1.54	0.73
3:A:424:MET:HA	3:A:457:MET:HE2	1.71	0.73
1:B:119:ILE:HD13	1:B:259:TYR:O	1.87	0.73
2:F:110:ARG:NH2	3:D:176:GLU:OE1	2.20	0.73
1:E:175:TYR:CE2	1:E:177:GLU:HG2	2.24	0.72
3:D:763:VAL:O	3:D:810:LYS:HG2	1.88	0.72
1:B:4:LEU:CD1	3:A:518:VAL:HG13	2.19	0.72
3:A:706:PHE:CZ	3:A:709:GLN:HG2	2.24	0.72
3:A:471:ASP:O	3:A:475:ILE:HG13	1.89	0.72
2:F:90:PHE:HB2	2:F:97:THR:OG1	1.88	0.72
1:B:13:ILE:HD11	3:A:538:ALA:HA	1.71	0.72
2:C:90:PHE:HB2	2:C:97:THR:OG1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:970:ASN:HD22	3:D:970:ASN:N	1.86	0.72
3:D:834:ILE:O	3:D:845:ARG:NH2	2.23	0.72
1:E:124:PRO:HD2	1:E:174:ILE:HD12	1.71	0.72
1:B:46:LEU:HD22	1:B:50:GLN:HE21	1.53	0.72
3:D:23:LEU:HD11	3:D:26:ASN:HB2	1.72	0.72
3:A:541:ALA:HA	3:A:544:ILE:HD12	1.71	0.72
3:A:106:VAL:O	3:A:110:ILE:HG13	1.90	0.72
3:D:274:VAL:HG12	3:D:275:SER:H	1.54	0.72
3:D:121:GLU:C	3:D:123:GLU:H	1.91	0.71
3:A:25:ILE:H	3:A:25:ILE:HD12	1.54	0.71
3:D:105:TYR:O	3:D:109:LEU:HD12	1.91	0.71
2:C:14:VAL:HG21	2:C:80:TYR:CD1	2.25	0.71
1:B:63:ARG:HH11	1:B:95:LYS:HZ2	1.36	0.71
3:D:698:ALA:O	3:D:702:VAL:HG23	1.90	0.71
3:A:327:CYS:O	3:A:331:LYS:HB3	1.90	0.71
1:B:24:HIS:HE1	1:B:108:ILE:HG23	1.56	0.71
3:D:224:ALA:O	3:D:228:THR:HG22	1.90	0.71
3:A:788:TYR:CE1	3:A:796:ARG:HB3	2.26	0.71
1:E:172:ASP:HB2	1:E:188:MET:HE1	1.72	0.71
3:D:533:GLY:O	3:D:537:LYS:HG3	1.91	0.71
2:C:44:GLY:HA3	3:A:45:MET:HE3	1.72	0.71
2:C:54:THR:HB	2:C:174:LEU:HD11	1.72	0.71
3:D:293:GLN:O	3:D:297:MET:HG3	1.90	0.71
1:E:8:LEU:CD2	3:D:564:THR:HG22	2.20	0.71
3:A:575:GLU:CG	3:A:580:VAL:HG11	2.20	0.71
2:F:44:GLY:HA3	3:D:45:MET:CE	2.20	0.71
1:B:357:MET:HG3	3:A:719:ASN:ND2	2.05	0.71
1:E:211:LEU:HB2	1:E:212:PRO:HD3	1.73	0.71
2:C:126:ILE:HG22	2:C:128:ASP:H	1.56	0.71
1:E:144:SER:O	1:E:146:TYR:N	2.24	0.71
1:B:107:LEU:HB2	1:B:274:GLY:HA3	1.73	0.71
1:B:13:ILE:HG21	3:A:575:GLU:OE1	1.90	0.70
1:B:241:LEU:O	1:B:244:VAL:HG12	1.91	0.70
3:D:497:LEU:O	3:D:501:ILE:HG13	1.91	0.70
2:F:54:THR:HB	2:F:174:LEU:HD11	1.72	0.70
3:D:106:VAL:O	3:D:110:ILE:HG13	1.91	0.70
3:D:681:ASP:HB3	3:D:684:THR:HG23	1.72	0.70
3:A:50:LEU:O	3:A:53:LEU:HG	1.92	0.70
1:E:119:ILE:HD13	1:E:259:TYR:O	1.91	0.70
3:A:698:ALA:O	3:A:702:VAL:HG23	1.91	0.70
2:F:14:VAL:HG21	2:F:80:TYR:CD1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:141:GLU:HB2	3:A:145:HIS:HB2	1.73	0.70
3:A:770:GLN:O	3:A:774:GLU:HG3	1.92	0.69
3:A:632:THR:HA	3:A:697:ARG:HH22	1.57	0.69
2:C:93:THR:HG21	2:C:126:ILE:CD1	2.21	0.69
3:A:23:LEU:HD11	3:A:26:ASN:HB2	1.74	0.69
3:D:846:THR:HG23	3:D:888:ASN:HD22	1.58	0.69
1:E:241:LEU:O	1:E:244:VAL:HG12	1.91	0.69
2:F:122:ASN:O	2:F:123:LYS:HB2	1.92	0.69
3:D:116:ASP:C	3:D:118:THR:H	1.96	0.69
3:D:179:PHE:CE1	3:D:195:LYS:HG3	2.26	0.69
3:A:763:VAL:O	3:A:810:LYS:HG2	1.92	0.69
3:A:804:MET:SD	3:A:807:ILE:HD11	2.33	0.69
1:E:282:SER:HB3	1:E:287:VAL:HA	1.74	0.69
3:A:497:LEU:O	3:A:501:ILE:HG13	1.91	0.69
3:A:823:PHE:CZ	3:A:852:LEU:HD13	2.27	0.69
1:B:151:PHE:N	1:B:151:PHE:HD1	1.91	0.69
3:D:50:LEU:O	3:D:53:LEU:HG	1.93	0.69
3:D:25:ILE:H	3:D:25:ILE:HD12	1.57	0.69
3:D:373:TRP:HA	3:D:373:TRP:CE3	2.28	0.69
2:F:31:LEU:HB3	2:F:50:LEU:HD21	1.74	0.68
3:A:224:ALA:O	3:A:228:THR:HG22	1.93	0.68
1:B:24:HIS:O	1:B:26:ARG:N	2.26	0.68
3:D:866:ILE:HB	3:D:867:PRO:HD2	1.73	0.68
3:D:17:LEU:HD23	3:D:22:LYS:NZ	2.08	0.68
1:E:160:ARG:HH11	1:E:160:ARG:HG2	1.55	0.68
2:F:103:ASN:O	2:F:106:ARG:HB3	1.94	0.68
3:A:45:MET:O	3:A:49:VAL:HG23	1.93	0.68
1:E:63:ARG:NH1	1:E:72:MET:HB2	2.07	0.68
3:A:658:MET:O	3:A:662:ASN:HB2	1.93	0.68
3:D:766:SER:H	3:D:810:LYS:NZ	1.91	0.68
3:D:471:ASP:O	3:D:475:ILE:HG13	1.93	0.68
3:A:109:LEU:O	3:A:113:THR:HG23	1.94	0.68
3:D:424:MET:HA	3:D:457:MET:HE2	1.76	0.68
3:A:834:ILE:O	3:A:845:ARG:NH2	2.27	0.68
3:D:916:GLN:HE22	3:D:959:SER:HB2	1.58	0.68
1:E:24:HIS:HE1	1:E:108:ILE:HG23	1.59	0.68
3:D:337:LEU:CD2	3:D:347:LEU:HB2	2.21	0.68
3:D:14:ARG:CG	3:D:14:ARG:HH11	2.06	0.68
3:A:555:LEU:HB3	3:A:562:LEU:HD13	1.75	0.68
1:B:260:HIS:CE1	1:B:262:GLN:HG3	2.28	0.68
3:D:627:PRO:O	3:D:630:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:759:ILE:HD13	3:D:780:LEU:HD21	1.75	0.68
2:F:139:HIS:HB2	2:F:144:LEU:O	1.94	0.68
2:F:77:ASP:HB2	3:D:77:TYR:OH	1.94	0.67
3:A:678:ILE:HD12	3:A:679:LEU:N	2.10	0.67
3:A:179:PHE:CE1	3:A:195:LYS:HG3	2.27	0.67
1:E:107:LEU:HB2	1:E:274:GLY:HA3	1.76	0.67
1:E:1:LEU:HG	1:E:2:ASN:N	2.10	0.67
1:B:175:TYR:CE2	1:B:177:GLU:HG2	2.30	0.67
3:D:834:ILE:HG22	3:D:845:ARG:HG2	1.76	0.67
3:D:823:PHE:CZ	3:D:852:LEU:HD13	2.29	0.67
3:D:631:HIS:CE1	3:D:693:LYS:HB2	2.29	0.67
1:E:24:HIS:ND1	1:E:25:PRO:HD2	2.09	0.67
3:A:284:GLU:HG3	3:A:343:LEU:HD21	1.77	0.67
3:A:164:CYS:SG	3:A:221:LEU:HD11	2.35	0.67
3:A:973:PHE:C	3:A:973:PHE:CD1	2.66	0.67
3:A:179:PHE:HE1	3:A:195:LYS:HG3	1.59	0.67
1:E:217:LEU:HG	1:E:228:PHE:HB2	1.76	0.67
3:A:105:TYR:O	3:A:109:LEU:HD12	1.95	0.67
3:D:45:MET:O	3:D:49:VAL:HG23	1.94	0.67
3:D:770:GLN:O	3:D:774:GLU:HG3	1.95	0.67
3:A:528:CYS:HB2	3:A:540:ILE:CG2	2.21	0.67
2:C:14:VAL:HG21	2:C:80:TYR:HD1	1.60	0.67
1:E:160:ARG:HG2	1:E:160:ARG:NH1	2.06	0.67
3:A:615:LEU:HD23	3:A:618:ILE:HD11	1.77	0.67
1:E:151:PHE:HD1	1:E:151:PHE:N	1.93	0.67
1:B:42:ARG:O	1:B:45:ARG:HB2	1.93	0.67
3:A:704:HIS:CD2	3:A:767:ASN:H	2.13	0.66
3:A:293:GLN:O	3:A:297:MET:HG3	1.94	0.66
3:D:593:GLN:HG3	3:D:639:TYR:CD2	2.29	0.66
3:D:131:ASN:HD21	3:D:166:ASN:HD21	1.42	0.66
2:C:75:LEU:N	2:C:75:LEU:HD12	2.10	0.66
3:A:570:PHE:O	3:A:573:MET:HB2	1.95	0.66
3:A:819:ILE:HD12	3:A:855:VAL:CG2	2.25	0.66
3:D:678:ILE:HD12	3:D:679:LEU:N	2.11	0.66
3:D:179:PHE:HE1	3:D:195:LYS:HG3	1.59	0.66
3:A:902:GLN:O	3:A:906:GLN:NE2	2.28	0.66
3:A:916:GLN:HE22	3:A:959:SER:HB2	1.60	0.66
3:A:1040:THR:HA	3:A:1043:ARG:HG2	1.76	0.66
1:E:51:LYS:HZ3	1:E:263:THR:HA	1.59	0.66
3:A:150:ILE:HG23	3:A:151:SER:H	1.60	0.66
1:B:211:LEU:HB2	1:B:212:PRO:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:LEU:HD22	3:D:558:HIS:HD2	1.60	0.66
1:E:260:HIS:CE1	1:E:262:GLN:HG3	2.30	0.66
3:D:997:PHE:HD1	3:D:1014:HIS:CE1	2.14	0.66
2:F:15:LEU:HD22	2:F:23:LYS:HB3	1.77	0.66
3:D:902:GLN:O	3:D:906:GLN:NE2	2.29	0.66
1:B:154:LEU:HG	1:B:224:ASN:HB2	1.76	0.66
3:D:769:PRO:HG2	3:D:770:GLN:H	1.61	0.66
3:A:286:LEU:O	3:A:286:LEU:HD12	1.95	0.66
3:A:509:HIS:O	3:A:512:ASP:HB2	1.96	0.66
3:D:819:ILE:HD12	3:D:855:VAL:CG2	2.25	0.66
2:F:14:VAL:HG21	2:F:80:TYR:HD1	1.60	0.66
2:C:44:GLY:HA3	3:A:45:MET:CE	2.24	0.66
1:E:277:ARG:NH2	3:D:620:THR:HG21	2.11	0.66
3:A:759:ILE:HD13	3:A:780:LEU:HD21	1.77	0.66
3:A:78:TYR:O	3:A:81:GLN:HB2	1.96	0.65
3:D:509:HIS:O	3:D:512:ASP:HB2	1.96	0.65
3:D:373:TRP:HA	3:D:373:TRP:HE3	1.61	0.65
3:A:131:ASN:HD21	3:A:166:ASN:HD21	1.44	0.65
3:D:327:CYS:O	3:D:331:LYS:HB3	1.96	0.65
1:E:147:CYS:SG	1:E:150:ARG:NH2	2.69	0.65
3:D:76:LYS:O	3:D:80:LEU:HD22	1.96	0.65
2:C:139:HIS:HB2	2:C:144:LEU:O	1.97	0.65
3:A:762:TRP:HH2	3:A:772:VAL:HG22	1.61	0.65
3:D:736:GLY:O	3:D:739:VAL:HG22	1.96	0.65
1:B:24:HIS:ND1	1:B:25:PRO:HD2	2.11	0.65
1:E:24:HIS:O	1:E:26:ARG:N	2.27	0.65
3:D:905:ALA:HB3	3:D:906:GLN:NE2	2.11	0.65
3:A:373:TRP:CE3	3:A:373:TRP:HA	2.32	0.65
3:A:900:LEU:HA	3:A:903:ASN:HD22	1.61	0.65
3:D:541:ALA:HA	3:D:544:ILE:HD12	1.79	0.65
1:E:1:LEU:O	1:E:4:LEU:HD12	1.97	0.65
1:B:175:TYR:CE2	1:B:177:GLU:HA	2.32	0.65
3:D:266:LYS:O	3:D:270:GLU:HG2	1.96	0.65
3:D:658:MET:O	3:D:662:ASN:HB2	1.96	0.65
2:C:103:ASN:O	2:C:106:ARG:HB3	1.97	0.65
2:F:124:VAL:HG22	2:F:150:SER:HB2	1.77	0.65
3:D:788:TYR:O	3:D:796:ARG:HG2	1.97	0.65
3:D:150:ILE:HG23	3:D:151:SER:H	1.62	0.65
2:F:44:GLY:HA3	3:D:45:MET:HE3	1.78	0.65
1:B:138:THR:HG22	1:B:151:PHE:CE1	2.32	0.65
2:C:148:ASP:HB3	2:C:155:TYR:CE2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:93:THR:HG21	2:F:126:ILE:CD1	2.26	0.65
3:D:1035:LEU:O	3:D:1036:GLU:C	2.35	0.64
3:A:30:ASN:HB3	3:A:47:GLN:NE2	2.12	0.64
1:B:63:ARG:NH1	1:B:95:LYS:NZ	2.45	0.64
3:A:766:SER:H	3:A:810:LYS:NZ	1.94	0.64
2:F:64:TRP:CE3	2:F:79:TYR:HB3	2.33	0.64
3:D:528:CYS:HB2	3:D:540:ILE:CG2	2.23	0.64
1:B:281:VAL:HG13	1:B:282:SER:H	1.63	0.64
1:E:175:TYR:CE2	1:E:177:GLU:HA	2.33	0.64
3:D:30:ASN:HB3	3:D:47:GLN:NE2	2.13	0.64
1:E:186:ASP:OD1	1:E:203:ARG:HD2	1.96	0.64
1:B:159:ASN:HB2	1:B:223:LEU:CD2	2.21	0.64
3:D:434:GLU:HG3	3:D:439:GLU:O	1.96	0.64
2:F:178:ALA:O	2:F:179:MET:HB2	1.97	0.64
1:B:351:ASP:HB2	1:B:352:HIS:ND1	2.12	0.64
1:B:3:GLU:O	1:B:7:LYS:CB	2.39	0.64
3:A:823:PHE:O	3:A:827:PHE:CB	2.45	0.64
3:A:1038:ARG:HA	3:A:1041:ALA:HB3	1.79	0.64
2:F:92:VAL:HG13	2:F:122:ASN:O	1.98	0.64
3:A:56:HIS:N	3:A:57:PRO:HD3	2.13	0.64
1:B:349:SER:HB3	1:B:350:PRO:HD2	1.80	0.64
3:D:336:LEU:O	3:D:336:LEU:HD12	1.96	0.64
3:D:804:MET:SD	3:D:807:ILE:HD11	2.38	0.64
1:B:186:ASP:OD1	1:B:203:ARG:HD2	1.97	0.64
1:B:4:LEU:HD11	3:A:518:VAL:HA	1.80	0.64
3:A:336:LEU:HD12	3:A:336:LEU:O	1.96	0.64
1:B:151:PHE:CD1	1:B:151:PHE:N	2.63	0.64
2:C:87:ILE:HA	2:C:118:VAL:O	1.97	0.64
3:D:463:TYR:O	3:D:467:LEU:HG	1.98	0.64
3:A:949:MET:O	3:A:953:VAL:HG23	1.97	0.64
3:A:299:PRO:HD2	3:A:302:THR:HG21	1.77	0.64
2:F:101:VAL:HB	2:F:102:PRO:HD3	1.80	0.64
3:A:860:PHE:N	3:A:861:PRO:HD2	2.13	0.64
3:D:622:ILE:HG21	3:D:633:PHE:CD2	2.33	0.64
3:D:485:ASN:O	3:D:487:THR:N	2.30	0.64
1:B:217:LEU:HG	1:B:228:PHE:HB2	1.79	0.64
1:B:63:ARG:HH11	1:B:95:LYS:NZ	1.96	0.64
3:A:56:HIS:C	3:A:58:ASP:H	2.02	0.63
2:C:77:ASP:HB2	3:A:77:TYR:OH	1.97	0.63
3:D:434:GLU:HA	3:D:439:GLU:O	1.98	0.63
3:A:290:THR:O	3:A:293:GLN:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:ILE:O	2:C:115:ILE:HG13	1.98	0.63
3:D:798:PRO:HG3	3:D:844:HIS:CE1	2.32	0.63
1:B:111:PRO:HD2	1:B:114:LEU:HD13	1.79	0.63
3:D:78:TYR:O	3:D:81:GLN:HB2	1.99	0.63
3:A:82:ILE:O	3:A:86:VAL:HG23	1.98	0.63
3:D:575:GLU:CG	3:D:580:VAL:HG11	2.27	0.63
3:D:650:GLN:NE2	3:D:705:PRO:HG2	2.12	0.63
3:D:960:THR:HG22	3:D:963:ASN:H	1.62	0.63
3:D:261:ARG:HD2	3:D:318:PHE:CG	2.33	0.63
3:D:628:GLN:NE2	3:D:628:GLN:H	1.96	0.63
3:D:1008:ILE:HD12	3:D:1008:ILE:O	1.98	0.63
3:D:949:MET:O	3:D:953:VAL:HG23	1.98	0.63
1:B:6:LEU:O	1:B:9:ALA:HB3	1.98	0.63
3:D:528:CYS:CB	3:D:540:ILE:HG21	2.24	0.63
3:A:841:TYR:O	3:A:845:ARG:HG3	1.99	0.63
3:A:127:ILE:HG22	3:A:131:ASN:ND2	2.12	0.63
1:B:120:VAL:HA	1:B:257:LEU:O	1.99	0.63
3:D:1048:GLU:O	3:D:1052:LEU:HG	1.99	0.63
3:D:860:PHE:N	3:D:861:PRO:HD2	2.14	0.63
3:D:900:LEU:HA	3:D:903:ASN:HD22	1.64	0.63
3:D:476:MET:CE	3:D:501:ILE:HG12	2.28	0.62
3:A:1043:ARG:HA	3:A:1043:ARG:NH1	2.13	0.62
3:A:762:TRP:CH2	3:A:772:VAL:HG22	2.34	0.62
3:A:132:MET:HE3	3:A:135:VAL:HB	1.80	0.62
1:E:151:PHE:N	1:E:151:PHE:CD1	2.64	0.62
1:B:154:LEU:HD13	1:B:215:GLU:HG2	1.81	0.62
3:A:997:PHE:HD1	3:A:1014:HIS:CE1	2.18	0.62
3:A:516:PHE:CE1	3:A:520:VAL:HG21	2.34	0.62
3:A:568:LYS:HA	3:A:568:LYS:HE2	1.79	0.62
3:D:299:PRO:HD2	3:D:302:THR:HG21	1.79	0.62
3:A:769:PRO:HG2	3:A:770:GLN:H	1.63	0.62
2:F:87:ILE:HA	2:F:118:VAL:O	1.99	0.62
3:A:627:PRO:O	3:A:630:VAL:HG12	1.99	0.62
1:E:154:LEU:HG	1:E:224:ASN:HB2	1.79	0.62
3:A:115:SER:HB3	3:A:162:SER:CB	2.28	0.62
2:C:92:VAL:HG13	2:C:122:ASN:O	2.00	0.62
3:D:860:PHE:HE1	3:D:900:LEU:HG	1.64	0.62
3:D:56:HIS:N	3:D:57:PRO:HD3	2.15	0.62
2:F:32:THR:OG1	2:F:34:GLU:HG2	2.00	0.62
1:B:4:LEU:HD22	3:A:521:ILE:HD11	1.81	0.62
3:A:153:ILE:HA	3:A:156:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:804:MET:HB3	3:A:851:LEU:HD13	1.82	0.62
1:B:260:HIS:O	1:B:263:THR:HG22	2.00	0.62
1:B:277:ARG:NH2	3:A:620:THR:HG21	2.15	0.62
3:D:513:GLU:HA	3:D:516:PHE:HB3	1.80	0.62
3:D:637:VAL:O	3:D:641:ILE:HD12	1.99	0.62
3:D:286:LEU:HD12	3:D:286:LEU:O	1.99	0.62
3:D:516:PHE:CE1	3:D:520:VAL:HG21	2.35	0.62
3:A:607:VAL:HG22	3:A:608:MET:SD	2.40	0.62
3:D:141:GLU:HB2	3:D:145:HIS:HB2	1.82	0.62
3:A:337:LEU:HD22	3:A:347:LEU:CB	2.26	0.62
2:F:148:ASP:HB3	2:F:155:TYR:CE2	2.26	0.62
3:A:627:PRO:O	3:A:631:HIS:CD2	2.53	0.62
3:D:421:VAL:HG11	3:D:476:MET:HG2	1.81	0.62
3:D:30:ASN:N	3:D:30:ASN:ND2	2.48	0.62
2:C:64:TRP:CE3	2:C:79:TYR:HB3	2.35	0.62
1:B:204:PHE:O	1:B:207:MET:HB2	2.00	0.62
3:D:940:THR:OG1	3:D:1012:LYS:HE3	2.00	0.62
3:A:513:GLU:HA	3:A:516:PHE:HB3	1.81	0.62
3:A:266:LYS:O	3:A:270:GLU:HG2	1.98	0.62
1:E:7:LYS:HB3	3:D:525:LEU:HD23	1.82	0.62
3:D:82:ILE:O	3:D:86:VAL:HG23	2.00	0.62
1:B:258:PHE:CD2	1:B:274:GLY:O	2.51	0.62
3:D:399:HIS:HB3	3:D:401:ASP:H	1.64	0.62
1:E:180:GLN:NE2	3:D:684:THR:HG22	2.06	0.61
3:A:484:VAL:HG22	3:A:527:LEU:HB2	1.81	0.61
3:D:484:VAL:HG22	3:D:527:LEU:HB2	1.81	0.61
3:D:54:LYS:O	3:D:55:GLU:HB2	2.00	0.61
3:A:30:ASN:ND2	3:A:30:ASN:N	2.48	0.61
3:A:74:ASN:O	3:A:77:TYR:HB3	2.00	0.61
3:A:193:HIS:O	3:A:197:SER:HB2	2.00	0.61
1:B:147:CYS:SG	1:B:150:ARG:NH2	2.72	0.61
1:E:111:PRO:HD2	1:E:114:LEU:HD13	1.82	0.61
3:A:846:THR:HG23	3:A:888:ASN:HD22	1.65	0.61
1:E:260:HIS:O	1:E:263:THR:HG22	2.00	0.61
1:B:51:LYS:HZ2	1:B:264:HIS:HB2	1.65	0.61
1:E:98:ALA:HB2	1:E:145:GLY:N	2.15	0.61
3:A:192:LYS:HE3	3:A:192:LYS:HA	1.82	0.61
1:B:40:SER:O	1:B:44:ARG:HG3	2.00	0.61
1:E:258:PHE:CD2	1:E:274:GLY:O	2.49	0.61
1:B:110:VAL:HG11	1:B:285:LEU:CD1	2.30	0.61
3:D:615:LEU:HD23	3:D:618:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:996:LEU:HD22	3:D:1033:LEU:HD11	1.82	0.61
3:A:650:GLN:NE2	3:A:705:PRO:HG2	2.14	0.61
1:B:63:ARG:NH1	1:B:70:THR:H	1.98	0.61
1:E:190:TRP:O	1:E:191:ARG:C	2.39	0.61
3:A:788:TYR:O	3:A:796:ARG:HG2	2.00	0.61
3:D:192:LYS:HA	3:D:192:LYS:HE3	1.83	0.61
2:C:153:SER:O	3:A:433:VAL:HG21	2.00	0.61
3:A:388:THR:OG1	3:A:402:ILE:HD13	2.00	0.61
1:B:46:LEU:HD23	1:B:50:GLN:HG3	1.82	0.61
1:B:98:ALA:HB2	1:B:145:GLY:N	2.16	0.61
1:B:225:PRO:HB2	1:B:226:PHE:CD2	2.36	0.61
3:D:153:ILE:HA	3:D:156:ALA:HB3	1.82	0.61
2:F:13:LEU:HD12	2:F:13:LEU:C	2.21	0.61
3:A:628:GLN:H	3:A:628:GLN:NE2	1.99	0.61
3:A:628:GLN:HA	3:A:631:HIS:HD2	1.66	0.61
1:B:349:SER:HB3	1:B:350:PRO:CD	2.31	0.61
3:A:877:SER:O	3:A:880:TRP:HB3	2.01	0.61
1:E:40:SER:O	1:E:44:ARG:HG3	2.01	0.60
3:D:846:THR:HG23	3:D:888:ASN:ND2	2.16	0.60
3:A:127:ILE:O	3:A:130:LEU:N	2.32	0.60
2:F:115:ILE:O	2:F:115:ILE:HG13	2.01	0.60
3:D:1044:GLN:O	3:D:1044:GLN:HG3	2.00	0.60
3:D:337:LEU:HD23	3:D:343:LEU:HB3	1.83	0.60
3:A:966:ASN:N	3:A:967:PRO:HD2	2.15	0.60
1:B:130:LEU:HG	1:B:132:VAL:HG23	1.83	0.60
3:D:132:MET:HE3	3:D:135:VAL:HB	1.82	0.60
3:D:43:GLN:HA	3:D:46:ALA:HB3	1.83	0.60
3:A:373:TRP:HE3	3:A:373:TRP:HA	1.66	0.60
3:D:945:ILE:O	3:D:949:MET:HG3	2.02	0.60
3:A:99:CYS:HA	3:A:102:ILE:HD12	1.83	0.60
3:A:33:ASN:CB	3:A:44:ARG:HG3	2.31	0.60
3:D:704:HIS:HD2	3:D:766:SER:CB	2.13	0.60
3:D:96:ARG:HH22	3:D:145:HIS:HB3	1.65	0.60
3:D:164:CYS:SG	3:D:221:LEU:HD11	2.42	0.60
3:A:116:ASP:HB2	3:A:119:CYS:HB2	1.83	0.60
1:B:1:LEU:CD1	3:A:558:HIS:HD2	2.08	0.60
1:E:146:TYR:CD1	1:E:148:VAL:HG22	2.36	0.60
3:D:1008:ILE:HD12	3:D:1008:ILE:C	2.22	0.60
3:A:1014:HIS:O	3:A:1017:ASP:HB3	2.02	0.60
3:A:178:VAL:HG11	3:A:194:LEU:HB3	1.84	0.60
3:A:344:ARG:O	3:A:348:MET:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:961:PRO:HD3	3:A:970:ASN:OD1	2.02	0.60
3:A:823:PHE:O	3:A:827:PHE:HB2	2.01	0.60
1:E:284:VAL:HG12	1:E:285:LEU:CD1	2.31	0.60
3:D:362:GLU:O	3:D:364:GLU:N	2.32	0.60
3:A:274:VAL:HG12	3:A:275:SER:N	2.17	0.60
1:B:358:GLU:O	1:B:359:ASN:O	2.19	0.60
1:B:103:LEU:HD13	1:B:268:GLY:HA2	1.84	0.60
3:D:568:LYS:HE2	3:D:568:LYS:HA	1.84	0.60
3:A:746:ARG:NH1	3:A:746:ARG:HG2	2.09	0.60
3:A:25:ILE:HD12	3:A:25:ILE:N	2.17	0.60
3:D:290:THR:O	3:D:293:GLN:HB2	2.02	0.60
3:A:265:LEU:O	3:A:268:LEU:N	2.35	0.60
3:A:1008:ILE:O	3:A:1008:ILE:HD12	2.02	0.60
2:C:124:VAL:HG22	2:C:150:SER:HB2	1.83	0.60
1:B:146:TYR:CD1	1:B:148:VAL:HG22	2.37	0.60
3:A:218:ASN:C	3:A:218:ASN:OD1	2.40	0.60
3:A:938:GLY:O	3:A:941:MET:N	2.35	0.59
3:D:74:ASN:O	3:D:77:TYR:HB3	2.02	0.59
3:D:833:MET:HB3	3:D:841:TYR:CD1	2.37	0.59
3:D:116:ASP:HB2	3:D:119:CYS:HB2	1.84	0.59
1:E:138:THR:HG22	1:E:151:PHE:CE1	2.37	0.59
3:D:1000:GLY:HA2	3:D:1042:LEU:HD13	1.84	0.59
3:D:484:VAL:HA	3:D:527:LEU:HD13	1.84	0.59
1:E:51:LYS:HZ1	1:E:263:THR:HA	1.64	0.59
1:E:159:ASN:O	1:E:160:ARG:HG2	2.02	0.59
3:D:733:GLN:HB2	3:D:792:VAL:HG11	1.85	0.59
3:A:639:TYR:N	3:A:701:ALA:HB1	2.17	0.59
1:E:120:VAL:HA	1:E:257:LEU:O	2.03	0.59
1:E:4:LEU:HD22	3:D:521:ILE:HD11	1.84	0.59
1:E:255:GLY:C	1:E:256:LEU:HD23	2.23	0.59
2:F:159:LYS:HB2	2:F:160:PRO:HD3	1.83	0.59
1:E:280:MET:O	1:E:284:VAL:HG23	2.02	0.59
3:D:150:ILE:HG21	3:D:201:GLU:CD	2.23	0.59
3:A:285:THR:O	3:A:289:LEU:HB2	2.03	0.59
3:A:925:HIS:O	3:A:928:SER:HB3	2.02	0.59
3:D:515:ARG:HG3	3:D:515:ARG:HH11	1.68	0.59
3:A:529:GLU:O	3:A:530:GLN:C	2.39	0.59
2:F:81:ILE:HD11	3:D:77:TYR:CD1	2.38	0.59
3:D:678:ILE:HD12	3:D:679:LEU:HG	1.84	0.59
3:D:420:MET:HB2	3:D:461:LEU:HD13	1.83	0.59
3:D:804:MET:HB3	3:D:851:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1048:GLU:O	3:A:1052:LEU:HG	2.02	0.59
3:D:337:LEU:HD22	3:D:347:LEU:CB	2.30	0.59
3:A:632:THR:CA	3:A:697:ARG:HH22	2.16	0.59
3:D:638:GLY:HA3	3:D:701:ALA:HB3	1.85	0.59
3:D:208:LEU:HD23	3:D:208:LEU:C	2.23	0.59
1:B:282:SER:HA	1:B:286:GLY:CA	2.30	0.59
2:C:13:LEU:HD12	2:C:13:LEU:C	2.22	0.59
3:A:833:MET:HB3	3:A:841:TYR:CD1	2.38	0.59
1:B:210:LYS:N	1:B:210:LYS:HD2	2.18	0.59
3:D:704:HIS:CD2	3:D:767:ASN:H	2.21	0.59
1:E:225:PRO:HB2	1:E:226:PHE:CD2	2.38	0.59
3:D:95:PRO:HG2	3:D:98:GLN:HE21	1.68	0.59
3:A:631:HIS:CE1	3:A:693:LYS:HB2	2.37	0.59
1:B:4:LEU:HA	1:B:7:LYS:CB	2.32	0.59
1:E:11:LEU:HG	3:D:572:PHE:HZ	1.68	0.59
2:F:139:HIS:O	2:F:143:ASN:N	2.35	0.59
2:F:84:GLN:O	2:F:85:CYS:HB3	2.03	0.59
3:A:973:PHE:HD1	3:A:974:ILE:N	2.01	0.58
3:D:56:HIS:C	3:D:58:ASP:H	2.06	0.58
3:D:621:ILE:HG22	3:D:622:ILE:HG23	1.85	0.58
3:D:762:TRP:CH2	3:D:772:VAL:HG22	2.38	0.58
1:E:50:GLN:O	1:E:52:SER:N	2.31	0.58
3:A:988:HIS:H	3:A:988:HIS:CD2	2.20	0.58
3:D:823:PHE:O	3:D:827:PHE:CB	2.51	0.58
3:D:168:MET:HE2	3:D:171:LEU:HD12	1.84	0.58
1:B:206:TRP:O	1:B:210:LYS:HB2	2.03	0.58
2:F:75:LEU:N	2:F:75:LEU:HD12	2.18	0.58
3:D:961:PRO:HD3	3:D:970:ASN:OD1	2.03	0.58
1:E:107:LEU:HD23	1:E:276:LEU:HD22	1.85	0.58
3:D:193:HIS:O	3:D:197:SER:HB2	2.03	0.58
3:A:208:LEU:HD23	3:A:208:LEU:C	2.24	0.58
3:D:639:TYR:N	3:D:701:ALA:HB1	2.18	0.58
3:D:252:TYR:O	3:D:256:ASN:ND2	2.36	0.58
1:B:58:VAL:HA	1:B:194:PRO:HG2	1.84	0.58
3:A:769:PRO:CG	3:A:770:GLN:H	2.16	0.58
3:D:803:THR:O	3:D:807:ILE:HG12	2.02	0.58
3:A:121:GLU:O	3:A:123:GLU:N	2.36	0.58
1:E:130:LEU:HG	1:E:132:VAL:HG23	1.85	0.58
3:D:529:GLU:O	3:D:530:GLN:C	2.41	0.58
1:B:146:TYR:CE2	3:A:626:GLN:NE2	2.71	0.58
3:A:569:LEU:HD11	3:A:587:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:115:SER:HB3	3:A:162:SER:HB3	1.84	0.58
3:D:996:LEU:CD2	3:D:1033:LEU:HD11	2.33	0.58
3:D:528:CYS:HA	3:D:540:ILE:HD13	1.84	0.58
3:D:963:ASN:N	3:D:964:PRO:HD3	2.19	0.58
2:C:137:VAL:HG12	2:C:140:ARG:NH1	2.19	0.58
3:A:202:PHE:O	3:A:205:ILE:HG23	2.04	0.58
3:D:534:LYS:HE2	3:D:577:HIS:HB2	1.86	0.58
3:A:897:LEU:O	3:A:901:LEU:HG	2.03	0.58
3:A:93:ILE:CG2	3:A:1027:GLY:HA3	2.33	0.58
1:B:190:TRP:O	1:B:191:ARG:C	2.42	0.57
2:F:88:ILE:HD11	2:F:117:ILE:CD1	2.34	0.57
3:D:344:ARG:O	3:D:348:MET:HG2	2.04	0.57
3:A:256:ASN:OD1	3:A:257:VAL:HG23	2.04	0.57
3:D:1003:SER:C	3:D:1005:ASN:H	2.06	0.57
2:C:39:TYR:HE1	4:C:217:GTP:O2B	1.86	0.57
1:E:356:LEU:O	3:D:719:ASN:ND2	2.37	0.57
3:A:515:ARG:HG3	3:A:515:ARG:HH11	1.69	0.57
1:B:146:TYR:HD1	1:B:148:VAL:HG22	1.67	0.57
2:F:177:VAL:HG22	2:F:178:ALA:N	2.19	0.57
3:A:252:TYR:O	3:A:256:ASN:ND2	2.37	0.57
2:F:138:PHE:HA	2:F:141:LYS:NZ	2.19	0.57
3:A:54:LYS:O	3:A:55:GLU:HB2	2.04	0.57
3:D:769:PRO:CG	3:D:770:GLN:H	2.16	0.57
3:A:261:ARG:HD2	3:A:318:PHE:CG	2.39	0.57
3:A:521:ILE:CG2	3:A:547:ILE:HG21	2.34	0.57
3:A:123:GLU:C	3:A:125:VAL:H	2.06	0.57
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.85	0.57
3:D:964:PRO:HG2	3:D:968:VAL:HB	1.86	0.57
2:F:134:LYS:HE3	2:F:135:SER:OG	2.04	0.57
3:A:746:ARG:CG	3:A:746:ARG:HH11	2.09	0.57
3:A:678:ILE:HD12	3:A:679:LEU:HG	1.86	0.57
1:B:258:PHE:O	1:B:273:VAL:HA	2.03	0.57
3:D:131:ASN:ND2	3:D:166:ASN:HD21	2.02	0.57
3:A:150:ILE:HG21	3:A:201:GLU:CD	2.25	0.57
3:A:304:ILE:CG1	3:A:356:LEU:HB3	2.35	0.57
3:D:274:VAL:HG12	3:D:275:SER:N	2.20	0.57
3:D:25:ILE:N	3:D:25:ILE:HD12	2.20	0.57
3:A:195:LYS:C	3:A:197:SER:H	2.07	0.57
3:A:463:TYR:O	3:A:467:LEU:HG	2.04	0.57
3:D:877:SER:O	3:D:880:TRP:HB3	2.05	0.57
3:A:1030:THR:HG23	3:A:1032:ASP:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:ILE:HG22	2:C:156:ASN:O	2.03	0.57
1:E:206:TRP:O	1:E:210:LYS:HB2	2.05	0.57
1:E:260:HIS:O	1:E:261:LYS:C	2.41	0.57
3:D:943:ALA:HB2	3:D:1015:LEU:HD12	1.85	0.57
2:C:75:LEU:O	2:C:78:GLY:N	2.35	0.57
3:A:846:THR:HG23	3:A:888:ASN:ND2	2.19	0.57
1:E:103:LEU:HD13	1:E:268:GLY:HA2	1.87	0.57
2:C:31:LEU:C	2:C:32:THR:HG22	2.25	0.57
3:D:823:PHE:O	3:D:827:PHE:HB2	2.04	0.57
3:D:265:LEU:O	3:D:268:LEU:N	2.38	0.57
2:F:88:ILE:HD11	2:F:117:ILE:HD11	1.87	0.57
3:D:871:PHE:CZ	3:D:875:LEU:HD11	2.40	0.57
3:A:637:VAL:O	3:A:641:ILE:HD12	2.05	0.57
3:A:134:LEU:O	3:A:138:LEU:HG	2.05	0.57
3:A:113:THR:HG21	3:A:126:TYR:HE2	1.69	0.57
3:A:875:LEU:O	3:A:878:ILE:N	2.37	0.57
3:A:434:GLU:CB	3:A:439:GLU:O	2.51	0.57
3:A:574:HIS:HD2	3:A:624:ASP:HB2	1.69	0.57
1:B:49:LEU:O	1:B:49:LEU:HG	2.05	0.57
3:D:304:ILE:CG1	3:D:356:LEU:HB3	2.35	0.57
3:D:202:PHE:O	3:D:205:ILE:HG23	2.05	0.57
1:E:244:VAL:CG1	1:E:245:LEU:HD13	2.33	0.56
1:B:98:ALA:HA	1:B:145:GLY:H	1.69	0.56
3:A:866:ILE:HB	3:A:867:PRO:CD	2.35	0.56
3:A:1008:ILE:C	3:A:1008:ILE:HD12	2.25	0.56
1:E:10:GLY:HA3	1:E:34:TYR:CZ	2.40	0.56
3:A:484:VAL:HA	3:A:527:LEU:HD13	1.86	0.56
3:A:875:LEU:HD21	3:A:914:PHE:CE1	2.40	0.56
3:D:62:ARG:NH2	3:D:79:GLY:HA2	2.19	0.56
2:F:44:GLY:HA3	3:D:45:MET:HE1	1.86	0.56
1:E:284:VAL:HG12	1:E:285:LEU:HD13	1.87	0.56
3:A:1000:GLY:HA2	3:A:1042:LEU:HD13	1.87	0.56
3:A:593:GLN:HG3	3:A:639:TYR:CD2	2.39	0.56
3:A:76:LYS:O	3:A:80:LEU:HD22	2.05	0.56
1:E:146:TYR:HD1	1:E:148:VAL:HG22	1.68	0.56
3:A:74:ASN:O	3:A:77:TYR:CB	2.54	0.56
1:B:107:LEU:HD23	1:B:276:LEU:HD22	1.87	0.56
3:A:480:LEU:HB2	3:A:497:LEU:HD21	1.87	0.56
3:A:476:MET:CE	3:A:501:ILE:HG12	2.35	0.56
3:A:420:MET:HB2	3:A:461:LEU:HD13	1.88	0.56
3:D:30:ASN:H	3:D:30:ASN:ND2	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:528:CYS:HA	3:A:540:ILE:HD13	1.87	0.56
2:F:149:ILE:HG22	2:F:156:ASN:O	2.05	0.56
3:D:938:GLY:O	3:D:941:MET:N	2.35	0.56
3:D:116:ASP:HB2	3:D:119:CYS:SG	2.46	0.56
3:D:195:LYS:C	3:D:197:SER:H	2.08	0.56
3:A:905:ALA:HB3	3:A:906:GLN:NE2	2.20	0.56
3:A:1052:LEU:HD12	3:A:1053:GLN:HB2	1.86	0.56
3:D:762:TRP:HH2	3:D:772:VAL:HG22	1.68	0.56
1:B:58:VAL:HG22	1:B:194:PRO:HG2	1.88	0.56
3:A:261:ARG:HD2	3:A:318:PHE:CD2	2.40	0.56
3:D:975:GLN:HG2	3:D:1002:PHE:CE1	2.40	0.56
3:D:847:ASN:O	3:D:848:PHE:C	2.42	0.56
2:C:138:PHE:HA	2:C:141:LYS:NZ	2.21	0.56
3:A:821:GLN:HA	3:D:597:ARG:HH21	1.71	0.56
3:D:55:GLU:HG2	3:D:56:HIS:ND1	2.21	0.56
3:A:70:SER:C	3:A:72:ASN:H	2.09	0.56
3:A:622:ILE:HG21	3:A:633:PHE:CD2	2.40	0.56
3:D:632:THR:HA	3:D:697:ARG:NH2	2.20	0.56
1:E:18:ASN:CG	1:E:108:ILE:HD11	2.26	0.56
3:D:1004:LEU:HD21	3:D:1042:LEU:HD22	1.86	0.56
3:A:372:TYR:O	3:A:373:TRP:C	2.43	0.56
3:D:256:ASN:OD1	3:D:257:VAL:HG23	2.05	0.56
3:D:178:VAL:HG11	3:D:194:LEU:HB3	1.88	0.56
2:C:66:THR:HG22	2:C:67:ALA:N	2.21	0.56
3:A:362:GLU:O	3:A:364:GLU:N	2.36	0.56
3:A:798:PRO:HG3	3:A:844:HIS:CE1	2.40	0.56
3:A:116:ASP:C	3:A:118:THR:H	2.09	0.56
1:B:244:VAL:CG1	1:B:245:LEU:HD13	2.34	0.56
3:A:534:LYS:HE2	3:A:577:HIS:HB2	1.87	0.56
3:D:134:LEU:O	3:D:138:LEU:HG	2.06	0.56
3:A:594:LYS:HA	3:A:594:LYS:HE2	1.87	0.56
3:A:962:LEU:HD13	3:A:968:VAL:HB	1.87	0.56
3:A:62:ARG:NH2	3:A:79:GLY:HA2	2.20	0.56
3:D:632:THR:CA	3:D:697:ARG:HH22	2.17	0.56
1:B:202:PHE:O	1:B:203:ARG:C	2.43	0.56
3:D:983:LYS:HE2	3:D:991:ASP:HA	1.87	0.56
3:A:117:PRO:O	3:A:118:THR:OG1	2.22	0.56
3:A:30:ASN:ND2	3:A:30:ASN:H	2.02	0.56
2:C:45:VAL:HG22	2:C:46:GLU:N	2.21	0.56
3:A:95:PRO:HG2	3:A:98:GLN:HE21	1.71	0.56
2:C:81:ILE:HD11	3:A:77:TYR:CD1	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:77:TYR:O	3:A:78:TYR:C	2.44	0.55
1:B:63:ARG:CZ	1:B:70:THR:H	2.19	0.55
3:D:847:ASN:O	3:D:849:PHE:N	2.39	0.55
1:E:110:VAL:HB	1:E:285:LEU:HD11	1.88	0.55
3:D:261:ARG:HD2	3:D:318:PHE:CD2	2.41	0.55
1:E:45:ARG:NH1	1:E:49:LEU:CD2	2.69	0.55
3:D:227:GLU:HG2	3:D:263:VAL:CG1	2.36	0.55
3:D:704:HIS:HD2	3:D:766:SER:CA	2.19	0.55
3:A:46:ALA:O	3:A:50:LEU:HD12	2.06	0.55
3:A:290:THR:HG21	3:A:325:PHE:CE2	2.41	0.55
3:A:637:VAL:HG12	3:A:641:ILE:HD12	1.88	0.55
1:E:58:VAL:HG22	1:E:194:PRO:HG2	1.88	0.55
1:E:4:LEU:HD23	3:D:522:LYS:HG3	1.87	0.55
3:A:421:VAL:HG11	3:A:476:MET:HG2	1.87	0.55
3:A:704:HIS:HD2	3:A:766:SER:CA	2.20	0.55
3:A:142:TRP:CZ3	3:A:197:SER:HB3	2.42	0.55
3:D:925:HIS:O	3:D:928:SER:HB3	2.06	0.55
3:D:99:CYS:HA	3:D:102:ILE:HD12	1.87	0.55
3:A:914:PHE:CE1	3:A:918:TYR:HD1	2.24	0.55
2:C:155:TYR:HE1	3:A:429:GLU:OE2	1.90	0.55
3:D:859:CYS:C	3:D:861:PRO:HD2	2.27	0.55
3:A:672:ALA:HB1	3:A:679:LEU:HD11	1.89	0.55
1:B:107:LEU:HB3	1:B:276:LEU:HD13	1.89	0.55
1:B:152:SER:O	1:B:225:PRO:CD	2.54	0.55
3:A:95:PRO:HG2	3:A:98:GLN:HB3	1.89	0.55
1:E:240:SER:O	1:E:241:LEU:C	2.43	0.55
3:A:56:HIS:O	3:A:58:ASP:N	2.40	0.55
1:B:260:HIS:O	1:B:261:LYS:C	2.43	0.55
3:D:972:MET:O	3:D:976:ASP:HB2	2.07	0.55
3:A:30:ASN:HB3	3:A:47:GLN:HE21	1.69	0.55
1:B:98:ALA:CA	1:B:145:GLY:H	2.19	0.55
1:B:351:ASP:O	3:A:715:LEU:HD12	2.06	0.55
3:D:747:SER:O	3:D:750:THR:HB	2.07	0.55
3:D:594:LYS:HE2	3:D:594:LYS:HA	1.88	0.55
3:A:790:ARG:NH1	3:D:647:GLN:HB2	2.21	0.55
3:A:962:LEU:CD1	3:A:968:VAL:HB	2.36	0.55
2:C:84:GLN:O	2:C:85:CYS:HB3	2.07	0.55
3:D:66:ILE:HG22	3:D:76:LYS:HD2	1.86	0.55
3:D:552:PRO:O	3:D:556:ARG:HG3	2.07	0.55
3:D:247:ILE:O	3:D:251:ILE:HG13	2.05	0.55
3:A:128:GLY:O	3:A:132:MET:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:HD12	1:E:118:TRP:CG	2.41	0.55
3:D:515:ARG:HH11	3:D:515:ARG:CG	2.19	0.55
1:E:204:PHE:O	1:E:207:MET:HB2	2.07	0.55
3:A:1003:SER:C	3:A:1005:ASN:H	2.09	0.55
3:D:432:VAL:O	3:D:432:VAL:HG23	2.06	0.55
2:C:122:ASN:HA	2:C:149:ILE:O	2.07	0.55
2:F:28:LYS:O	2:F:32:THR:HG23	2.07	0.55
3:D:225:THR:CA	3:D:228:THR:HG22	2.34	0.55
3:D:179:PHE:CE2	3:D:235:TRP:CE2	2.95	0.55
2:C:139:HIS:O	2:C:143:ASN:N	2.40	0.55
3:D:737:GLU:OE1	3:D:794:ALA:HB1	2.07	0.55
3:D:383:GLU:OE1	3:D:405:ARG:HB2	2.07	0.55
3:A:638:GLY:HA3	3:A:701:ALA:HB3	1.89	0.55
3:D:559:TRP:HH2	3:D:610:PHE:HB2	1.72	0.55
3:A:55:GLU:HG2	3:A:56:HIS:ND1	2.22	0.55
3:D:17:LEU:HD23	3:D:22:LYS:HZ1	1.71	0.55
3:D:616:ASN:OD1	3:D:656:LYS:HE3	2.06	0.55
3:A:616:ASN:OD1	3:A:656:LYS:HE3	2.06	0.55
3:D:870:GLN:O	3:D:873:LEU:N	2.39	0.55
2:F:66:THR:HG22	2:F:67:ALA:N	2.22	0.55
1:B:352:HIS:N	1:B:352:HIS:ND1	2.49	0.54
1:E:13:ILE:HD11	3:D:572:PHE:CZ	2.42	0.54
3:D:866:ILE:HB	3:D:867:PRO:CD	2.37	0.54
3:D:962:LEU:O	3:D:963:ASN:HB3	2.07	0.54
3:D:521:ILE:CG2	3:D:547:ILE:HG21	2.36	0.54
3:A:515:ARG:CG	3:A:515:ARG:HH11	2.19	0.54
3:A:816:THR:HG23	3:A:859:CYS:SG	2.47	0.54
3:A:280:GLU:HG3	3:A:336:LEU:CD1	2.37	0.54
3:D:280:GLU:HG3	3:D:336:LEU:CD1	2.37	0.54
3:A:639:TYR:CE1	3:A:701:ALA:HA	2.42	0.54
1:E:152:SER:O	1:E:225:PRO:CD	2.54	0.54
2:C:101:VAL:HB	2:C:102:PRO:HD3	1.89	0.54
3:D:95:PRO:HG2	3:D:98:GLN:HB3	1.90	0.54
3:A:276:VAL:CG2	3:A:280:GLU:HA	2.37	0.54
3:A:26:ASN:O	3:A:29:ASP:HB2	2.07	0.54
1:B:351:ASP:OD2	3:A:712:ARG:HA	2.08	0.54
3:D:26:ASN:O	3:D:29:ASP:HB2	2.07	0.54
2:F:98:TYR:HA	2:F:101:VAL:HG23	1.88	0.54
1:B:255:GLY:C	1:B:256:LEU:HD23	2.28	0.54
1:E:237:THR:O	1:E:238:PRO:C	2.45	0.54
2:F:81:ILE:HG22	2:F:82:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:676:VAL:HG12	3:A:676:VAL:O	2.07	0.54
3:D:626:GLN:HB2	3:D:627:PRO:HD2	1.89	0.54
1:E:175:TYR:HB2	1:E:182:TYR:CD1	2.42	0.54
3:D:417:ARG:NE	3:D:464:LEU:O	2.34	0.54
3:A:378:ALA:O	3:A:382:ARG:HG3	2.07	0.54
3:A:383:GLU:OE1	3:A:405:ARG:HB2	2.07	0.54
3:D:271:ILE:O	3:D:274:VAL:HG23	2.07	0.54
3:D:306:LEU:O	3:D:308:TYR:N	2.40	0.54
3:A:940:THR:OG1	3:A:1012:LYS:HE3	2.08	0.54
3:D:988:HIS:H	3:D:988:HIS:CD2	2.24	0.54
1:B:4:LEU:HD22	3:A:521:ILE:CD1	2.38	0.54
2:F:159:LYS:N	2:F:160:PRO:CD	2.71	0.54
1:E:159:ASN:HB2	1:E:223:LEU:HD11	1.90	0.54
2:C:110:ARG:NH2	3:A:176:GLU:OE1	2.40	0.54
3:A:983:LYS:HE2	3:A:991:ASP:HA	1.89	0.54
2:F:146:TYR:CD2	2:F:146:TYR:C	2.81	0.54
1:E:14:SER:HB2	1:E:16:ASP:OD2	2.07	0.54
3:A:517:LEU:O	3:A:518:VAL:C	2.43	0.54
1:E:4:LEU:O	1:E:7:LYS:N	2.40	0.54
3:D:287:PHE:CD2	3:D:337:LEU:HD11	2.42	0.54
1:E:209:SER:O	1:E:210:LYS:HD2	2.06	0.54
3:A:704:HIS:HD2	3:A:766:SER:CB	2.21	0.54
1:E:202:PHE:O	1:E:203:ARG:C	2.46	0.54
3:D:227:GLU:HG2	3:D:263:VAL:HG11	1.90	0.54
3:A:239:GLY:O	3:A:244:THR:HG23	2.08	0.54
3:A:337:LEU:HD23	3:A:343:LEU:HB3	1.89	0.54
3:D:433:VAL:HG13	3:D:434:GLU:N	2.22	0.54
3:D:378:ALA:O	3:D:382:ARG:HG3	2.07	0.54
3:A:847:ASN:O	3:A:850:LEU:N	2.41	0.54
2:F:29:ARG:HB3	2:F:157:PHE:HZ	1.73	0.54
1:E:142:THR:HG23	1:E:148:VAL:HG21	1.88	0.54
3:A:178:VAL:CG1	3:A:194:LEU:HB3	2.37	0.54
3:A:632:THR:HA	3:A:697:ARG:NH2	2.22	0.54
3:A:127:ILE:HG22	3:A:131:ASN:HD21	1.72	0.54
3:A:405:ARG:O	3:A:408:LEU:HB2	2.08	0.54
2:C:15:LEU:HD22	2:C:23:LYS:HB3	1.89	0.54
3:A:304:ILE:HG13	3:A:356:LEU:HB3	1.90	0.54
3:A:20:SER:HB2	3:A:22:LYS:HD3	1.90	0.54
3:A:131:ASN:ND2	3:A:166:ASN:HD21	2.05	0.53
3:D:30:ASN:HB3	3:D:47:GLN:HE21	1.71	0.53
1:E:348:HIS:CD2	3:D:708:ILE:O	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:668:ILE:HG22	3:D:668:ILE:O	2.08	0.53
3:A:973:PHE:C	3:A:973:PHE:HD1	2.10	0.53
3:A:819:ILE:N	3:A:820:PRO:HD2	2.22	0.53
2:F:156:ASN:HB3	2:F:159:LYS:HG3	1.88	0.53
3:D:133:ILE:O	3:D:136:GLN:HB2	2.08	0.53
3:A:964:PRO:HD2	3:A:968:VAL:HG21	1.91	0.53
3:A:819:ILE:HD12	3:A:855:VAL:HG21	1.89	0.53
3:A:569:LEU:HD21	3:A:587:THR:CG2	2.34	0.53
2:C:75:LEU:N	2:C:75:LEU:CD1	2.72	0.53
3:A:871:PHE:CZ	3:A:875:LEU:HD11	2.44	0.53
3:D:746:ARG:HH11	3:D:746:ARG:CG	2.12	0.53
3:A:293:GLN:O	3:A:296:GLN:HB3	2.08	0.53
3:D:905:ALA:HB3	3:D:906:GLN:HE22	1.72	0.53
3:A:218:ASN:OD1	3:A:218:ASN:O	2.27	0.53
3:A:1033:LEU:O	3:A:1034:PHE:C	2.47	0.53
3:D:304:ILE:HG13	3:D:356:LEU:HB3	1.91	0.53
1:E:173:CYS:SG	1:E:184:VAL:HG22	2.49	0.53
2:C:146:TYR:CD2	2:C:146:TYR:C	2.82	0.53
3:A:247:ILE:O	3:A:251:ILE:HG13	2.07	0.53
3:D:1047:GLU:O	3:D:1051:LYS:HE2	2.08	0.53
3:D:574:HIS:HD2	3:D:624:ASP:HB2	1.73	0.53
3:A:953:VAL:HG11	3:A:974:ILE:HD13	1.89	0.53
3:D:272:ALA:HB1	3:D:329:PHE:HD1	1.74	0.53
3:A:859:CYS:C	3:A:861:PRO:HD2	2.29	0.53
3:A:179:PHE:CE2	3:A:235:TRP:CE2	2.96	0.53
3:D:819:ILE:HD12	3:D:855:VAL:HG21	1.91	0.53
3:A:238:LEU:HD22	3:A:242:PHE:CE2	2.40	0.53
3:D:1014:HIS:O	3:D:1017:ASP:HB3	2.08	0.53
2:F:85:CYS:HB2	2:F:164:LEU:HD22	1.91	0.53
3:D:914:PHE:CE1	3:D:918:TYR:HD1	2.26	0.53
3:A:51:THR:O	3:A:51:THR:HG22	2.09	0.53
1:B:3:GLU:HB3	3:A:522:LYS:NZ	2.24	0.53
1:E:1:LEU:HD13	3:D:558:HIS:CD2	2.43	0.53
2:F:155:TYR:HE1	3:D:429:GLU:OE2	1.92	0.53
3:D:628:GLN:HA	3:D:631:HIS:HD2	1.74	0.53
2:C:81:ILE:HG22	2:C:82:GLN:HG3	1.91	0.53
3:A:168:MET:HE2	3:A:171:LEU:HD12	1.90	0.53
3:D:16:LEU:C	3:D:17:LEU:HD12	2.29	0.53
1:B:51:LYS:NZ	1:B:264:HIS:HB2	2.23	0.53
3:A:35:LEU:O	3:A:36:TYR:HD1	1.91	0.53
3:A:615:LEU:CD2	3:A:618:ILE:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:LEU:HD22	3:D:242:PHE:CE2	2.40	0.53
3:A:1004:LEU:HD21	3:A:1042:LEU:HD22	1.90	0.53
3:A:417:ARG:NE	3:A:464:LEU:O	2.36	0.53
1:E:4:LEU:HD11	3:D:518:VAL:HG13	1.89	0.53
3:A:733:GLN:HB2	3:A:792:VAL:HG11	1.92	0.53
1:E:258:PHE:O	1:E:273:VAL:HA	2.08	0.53
3:A:943:ALA:HB2	3:A:1015:LEU:HD12	1.89	0.53
1:B:24:HIS:C	1:B:26:ARG:H	2.11	0.53
2:F:137:VAL:HG12	2:F:140:ARG:NH1	2.24	0.53
3:D:749:ARG:O	3:D:753:ARG:HG3	2.09	0.53
2:C:36:GLU:OE2	2:C:38:LYS:HE2	2.08	0.53
3:D:1034:PHE:O	3:D:1035:LEU:O	2.27	0.52
3:D:517:LEU:HD11	3:D:551:TYR:CG	2.44	0.52
3:A:66:ILE:HG22	3:A:76:LYS:HD2	1.90	0.52
3:D:819:ILE:N	3:D:820:PRO:HD2	2.23	0.52
1:B:106:TRP:HZ3	1:B:276:LEU:HA	1.74	0.52
3:D:46:ALA:O	3:D:50:LEU:HD12	2.09	0.52
3:D:997:PHE:CD1	3:D:1014:HIS:NE2	2.77	0.52
2:C:92:VAL:CG2	2:C:129:ARG:HG3	2.39	0.52
2:F:15:LEU:CD2	2:F:23:LYS:HG2	2.39	0.52
3:A:821:GLN:HA	3:D:597:ARG:NH2	2.24	0.52
3:A:20:SER:O	3:A:22:LYS:N	2.42	0.52
3:A:860:PHE:HE1	3:A:900:LEU:HG	1.74	0.52
3:D:77:TYR:O	3:D:78:TYR:C	2.48	0.52
1:B:46:LEU:HD22	1:B:50:GLN:NE2	2.23	0.52
3:A:388:THR:O	3:A:389:SER:C	2.47	0.52
2:C:35:PHE:HE2	2:C:37:LYS:HG2	1.74	0.52
3:A:249:THR:O	3:A:253:LYS:HB3	2.10	0.52
1:B:183:TYR:HA	1:B:229:VAL:O	2.10	0.52
3:D:389:SER:C	3:D:391:SER:H	2.10	0.52
1:B:4:LEU:O	1:B:7:LYS:N	2.42	0.52
3:A:860:PHE:N	3:A:861:PRO:CD	2.71	0.52
1:B:119:ILE:CD1	1:B:259:TYR:HB2	2.37	0.52
1:E:98:ALA:HA	1:E:145:GLY:H	1.73	0.52
3:A:953:VAL:CG1	3:A:974:ILE:HD13	2.39	0.52
3:A:970:ASN:N	3:A:970:ASN:ND2	2.56	0.52
3:A:974:ILE:O	3:A:975:GLN:C	2.47	0.52
3:D:103:LYS:HE3	3:D:146:TRP:CD1	2.44	0.52
1:E:237:THR:O	1:E:240:SER:N	2.42	0.52
3:A:276:VAL:O	3:A:277:SER:C	2.47	0.52
3:A:56:HIS:C	3:A:58:ASP:N	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:168:MET:SD	3:D:225:THR:HG23	2.49	0.52
3:D:128:GLY:O	3:D:132:MET:HB2	2.10	0.52
3:D:293:GLN:O	3:D:296:GLN:HB3	2.10	0.52
3:D:324:LEU:CD2	3:D:368:ILE:HD13	2.40	0.52
3:A:870:GLN:O	3:A:873:LEU:N	2.42	0.52
3:D:615:LEU:HA	3:D:618:ILE:HG13	1.89	0.52
1:B:169:THR:HG22	1:B:171:LEU:HD21	1.91	0.52
3:D:816:THR:HG23	3:D:859:CYS:SG	2.49	0.52
2:F:75:LEU:O	2:F:78:GLY:N	2.40	0.52
1:E:98:ALA:CA	1:E:145:GLY:H	2.22	0.52
3:A:271:ILE:O	3:A:274:VAL:HG23	2.09	0.52
3:A:1052:LEU:HD12	3:A:1053:GLN:N	2.25	0.52
3:D:28:LEU:O	3:D:32:VAL:HG23	2.09	0.52
3:D:56:HIS:O	3:D:58:ASP:N	2.43	0.52
3:D:678:ILE:C	3:D:680:LYS:H	2.12	0.52
1:E:146:TYR:CE2	3:D:626:GLN:NE2	2.78	0.52
3:D:434:GLU:O	3:D:435:ASN:O	2.28	0.52
2:C:119:LEU:HD23	2:C:146:TYR:HD1	1.74	0.52
3:D:95:PRO:HG2	3:D:98:GLN:CB	2.40	0.52
3:D:1004:LEU:HD21	3:D:1042:LEU:CD2	2.39	0.52
3:D:134:LEU:O	3:D:134:LEU:HD12	2.10	0.52
3:D:882:PHE:HA	3:D:890:ALA:HA	1.91	0.52
3:A:210:GLN:O	3:A:211:PHE:C	2.49	0.52
3:D:948:TYR:CD1	3:D:948:TYR:C	2.83	0.52
3:A:133:ILE:O	3:A:136:GLN:HB2	2.10	0.51
3:A:95:PRO:HG2	3:A:98:GLN:CB	2.40	0.51
3:D:74:ASN:O	3:D:77:TYR:CB	2.58	0.51
3:A:30:ASN:HB2	3:A:48:GLU:OE2	2.10	0.51
3:A:621:ILE:HG22	3:A:622:ILE:HG23	1.92	0.51
3:D:417:ARG:O	3:D:421:VAL:HG23	2.10	0.51
3:A:695:ASN:HD21	3:A:709:GLN:HE21	1.58	0.51
3:D:29:ASP:O	3:D:33:ASN:ND2	2.43	0.51
3:A:798:PRO:HG2	3:A:843:GLU:OE1	2.09	0.51
3:D:163:LEU:O	3:D:163:LEU:HD23	2.10	0.51
3:D:860:PHE:N	3:D:861:PRO:CD	2.72	0.51
1:B:237:THR:O	1:B:240:SER:N	2.43	0.51
1:E:107:LEU:HB3	1:E:276:LEU:HD13	1.92	0.51
3:A:833:MET:HB3	3:A:841:TYR:HD1	1.75	0.51
3:A:406:ARG:O	3:A:407:GLN:C	2.48	0.51
3:A:882:PHE:HA	3:A:890:ALA:HA	1.91	0.51
1:E:6:LEU:C	1:E:6:LEU:HD23	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:LEU:O	2:C:31:LEU:HG	2.10	0.51
1:B:357:MET:CG	3:A:719:ASN:HD21	2.23	0.51
1:E:58:VAL:HA	1:E:194:PRO:HG2	1.91	0.51
1:B:234:PHE:CD1	1:B:234:PHE:N	2.78	0.51
3:A:647:GLN:O	3:A:651:GLU:HG3	2.10	0.51
3:D:600:VAL:HG11	3:D:640:MET:O	2.11	0.51
2:C:92:VAL:HG23	2:C:129:ARG:HG3	1.92	0.51
1:E:175:TYR:CD2	1:E:175:TYR:C	2.83	0.51
3:D:768:ASP:HB3	3:D:771:MET:HE3	1.92	0.51
1:E:63:ARG:HH22	1:E:70:THR:HG23	1.76	0.51
2:C:42:THR:OG1	4:C:217:GTP:O1G	2.25	0.51
3:D:430:VAL:CG1	3:D:430:VAL:O	2.58	0.51
3:A:521:ILE:HG22	3:A:547:ILE:HG21	1.92	0.51
1:B:4:LEU:HD11	3:A:518:VAL:CG1	2.35	0.51
2:F:31:LEU:C	2:F:32:THR:HG22	2.31	0.51
2:C:13:LEU:HB2	2:C:85:CYS:SG	2.51	0.51
1:B:142:THR:HG23	1:B:148:VAL:HG21	1.91	0.51
3:A:509:HIS:HB2	3:A:512:ASP:OD2	2.11	0.51
3:D:804:MET:HA	3:D:807:ILE:HG12	1.93	0.51
1:B:280:MET:O	1:B:284:VAL:HG23	2.10	0.51
3:A:306:LEU:O	3:A:308:TYR:N	2.43	0.51
3:D:517:LEU:O	3:D:518:VAL:C	2.46	0.51
3:D:347:LEU:O	3:D:351:LEU:HB2	2.09	0.51
3:A:74:ASN:O	3:A:77:TYR:N	2.44	0.51
1:B:215:GLU:HG2	1:B:216:GLY:H	1.75	0.51
2:C:117:ILE:HG23	2:C:144:LEU:HD22	1.91	0.51
3:A:406:ARG:HA	3:A:409:TYR:HD2	1.74	0.51
3:A:223:HIS:NE2	3:A:263:VAL:HG21	2.25	0.51
3:A:678:ILE:C	3:A:680:LYS:H	2.12	0.51
1:B:240:SER:O	1:B:241:LEU:C	2.47	0.51
2:F:98:TYR:HE1	2:F:136:ILE:HG23	1.75	0.51
2:C:47:VAL:HG23	2:C:47:VAL:O	2.09	0.51
3:D:238:LEU:CD2	3:D:242:PHE:HE2	2.23	0.51
1:B:357:MET:HG3	3:A:719:ASN:HD21	1.75	0.51
3:A:157:SER:HB3	3:A:164:CYS:HB2	1.92	0.51
3:A:432:VAL:O	3:A:433:VAL:HB	2.10	0.51
3:A:914:PHE:CD1	3:A:918:TYR:HD1	2.28	0.51
1:B:41:GLU:HG3	1:B:109:ASP:CB	2.35	0.51
3:D:672:ALA:HB1	3:D:679:LEU:HD11	1.93	0.51
3:A:654:ILE:HG22	3:A:654:ILE:O	2.10	0.51
1:E:119:ILE:CD1	1:E:259:TYR:HB2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:MET:CG	3:A:719:ASN:ND2	2.74	0.51
3:D:906:GLN:NE2	3:D:906:GLN:N	2.58	0.51
3:D:871:PHE:CE2	3:D:875:LEU:HD11	2.46	0.51
3:D:875:LEU:HD21	3:D:914:PHE:CE1	2.46	0.51
3:A:912:GLN:OE1	3:A:958:ILE:HG12	2.11	0.51
3:D:51:THR:HG22	3:D:51:THR:O	2.11	0.51
3:A:1006:GLN:HB2	3:A:1049:LYS:HG2	1.91	0.51
3:D:970:ASN:ND2	3:D:970:ASN:N	2.58	0.51
3:A:1038:ARG:HA	3:A:1041:ALA:CB	2.40	0.51
3:D:134:LEU:HD23	3:D:170:ILE:HD12	1.94	0.51
3:D:491:TRP:CH2	3:D:535:ASP:HB3	2.46	0.50
3:D:95:PRO:CG	3:D:98:GLN:HE21	2.24	0.50
1:E:281:VAL:HG13	1:E:282:SER:H	1.76	0.50
1:B:175:TYR:CD2	1:B:175:TYR:C	2.84	0.50
3:A:299:PRO:HD2	3:A:302:THR:CG2	2.41	0.50
3:D:30:ASN:N	3:D:30:ASN:HD22	2.07	0.50
3:D:44:ARG:O	3:D:47:GLN:HG2	2.11	0.50
3:A:257:VAL:HG12	3:A:257:VAL:O	2.11	0.50
3:D:912:GLN:OE1	3:D:958:ILE:HG12	2.11	0.50
3:A:123:GLU:C	3:A:125:VAL:N	2.63	0.50
3:A:103:LYS:HE3	3:A:146:TRP:CD1	2.46	0.50
3:A:95:PRO:CG	3:A:98:GLN:HE21	2.24	0.50
1:E:122:VAL:HG22	1:E:256:LEU:HD22	1.93	0.50
3:A:44:ARG:O	3:A:47:GLN:HG2	2.11	0.50
3:A:225:THR:CA	3:A:228:THR:HG22	2.39	0.50
1:B:180:GLN:OE1	3:A:684:THR:HG22	2.10	0.50
3:D:150:ILE:O	3:D:154:VAL:HG23	2.11	0.50
3:D:436:ASP:O	3:D:436:ASP:OD2	2.28	0.50
2:F:122:ASN:HA	2:F:149:ILE:O	2.12	0.50
1:B:98:ALA:HB1	1:B:144:SER:HA	1.93	0.50
3:D:841:TYR:O	3:D:845:ARG:HG3	2.12	0.50
3:A:803:THR:O	3:A:807:ILE:HG12	2.11	0.50
1:B:234:PHE:HB3	1:B:235:PRO:HD2	1.94	0.50
3:D:139:LYS:HD2	3:D:186:ILE:HD11	1.93	0.50
3:A:823:PHE:O	3:A:827:PHE:HB3	2.11	0.50
3:D:569:LEU:HD11	3:D:587:THR:HG21	1.94	0.50
3:A:378:ALA:HB1	3:A:382:ARG:NH1	2.26	0.50
2:F:132:LYS:O	2:F:135:SER:N	2.38	0.50
3:D:249:THR:O	3:D:253:LYS:HB3	2.11	0.50
3:A:101:GLY:O	3:A:105:TYR:HB2	2.10	0.50
3:A:280:GLU:HG3	3:A:336:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:GLU:C	3:D:125:VAL:H	2.13	0.50
3:D:142:TRP:CZ3	3:D:197:SER:HB3	2.46	0.50
1:B:138:THR:HG22	1:B:151:PHE:CZ	2.45	0.50
3:A:1043:ARG:HA	3:A:1043:ARG:CZ	2.41	0.50
2:C:117:ILE:CG1	2:C:118:VAL:N	2.74	0.50
1:B:152:SER:O	1:B:225:PRO:HD3	2.12	0.50
3:D:178:VAL:CG1	3:D:194:LEU:HB3	2.41	0.50
3:A:28:LEU:O	3:A:32:VAL:HG23	2.11	0.50
3:D:539:ILE:HG22	3:D:540:ILE:N	2.27	0.50
2:F:31:LEU:HB3	2:F:50:LEU:CD2	2.39	0.50
3:A:736:GLY:C	3:A:738:MET:N	2.64	0.50
3:D:569:LEU:HD21	3:D:587:THR:CG2	2.38	0.50
3:D:709:GLN:O	3:D:712:ARG:HB3	2.11	0.50
1:B:351:ASP:HB2	1:B:352:HIS:CE1	2.46	0.50
2:F:38:LYS:HD2	3:D:840:GLU:HA	1.92	0.50
3:D:290:THR:HG21	3:D:325:PHE:CE2	2.46	0.50
3:A:406:ARG:C	3:A:408:LEU:N	2.62	0.50
3:D:870:GLN:O	3:D:873:LEU:HB3	2.11	0.50
3:A:552:PRO:O	3:A:556:ARG:HG3	2.11	0.50
3:D:1038:ARG:O	3:D:1041:ALA:HB3	2.12	0.50
1:E:1:LEU:CD2	3:D:558:HIS:HD2	2.24	0.50
3:A:168:MET:SD	3:A:225:THR:HG23	2.51	0.50
3:D:123:GLU:HA	3:D:123:GLU:OE1	2.11	0.50
3:A:1046:GLN:HE22	3:A:1049:LYS:NZ	2.10	0.50
1:E:41:GLU:HG3	1:E:109:ASP:CB	2.36	0.50
2:C:31:LEU:C	2:C:32:THR:CG2	2.80	0.50
2:C:31:LEU:O	2:C:32:THR:HG22	2.12	0.50
1:B:39:GLN:HG2	1:B:39:GLN:O	2.11	0.50
1:B:357:MET:CB	3:A:719:ASN:HD21	2.24	0.50
2:F:47:VAL:HG12	2:F:64:TRP:CG	2.47	0.50
3:A:749:ARG:O	3:A:753:ARG:HG3	2.12	0.50
1:E:176:ASN:OD1	1:E:179:ASN:HB2	2.12	0.50
1:B:122:VAL:HG22	1:B:256:LEU:HD22	1.94	0.50
3:A:615:LEU:HA	3:A:618:ILE:HG13	1.92	0.50
3:D:1004:LEU:HD12	3:D:1014:HIS:HB2	1.93	0.50
3:D:962:LEU:O	3:D:963:ASN:CB	2.59	0.50
3:D:879:ILE:HD12	3:D:879:ILE:N	2.27	0.50
3:D:393:LEU:HD23	3:D:394:LEU:H	1.77	0.50
1:E:234:PHE:HB3	1:E:235:PRO:HD2	1.94	0.50
3:A:276:VAL:HG23	3:A:283:PHE:CD2	2.46	0.49
3:D:676:VAL:O	3:D:676:VAL:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:974:ILE:HD12	3:D:974:ILE:N	2.27	0.49
1:E:234:PHE:N	1:E:234:PHE:CD1	2.79	0.49
3:A:924:GLN:NE2	3:A:977:TYR:OH	2.45	0.49
3:A:15:GLN:HG2	3:A:16:LEU:O	2.12	0.49
3:D:300:LEU:HB3	3:D:352:HIS:CE1	2.47	0.49
3:A:129:LYS:O	3:A:133:ILE:HG13	2.12	0.49
3:A:72:ASN:O	3:A:75:THR:N	2.44	0.49
1:B:106:TRP:CZ3	1:B:276:LEU:HA	2.46	0.49
1:B:119:ILE:HD11	1:B:259:TYR:CB	2.40	0.49
3:D:142:TRP:N	3:D:143:PRO:HD2	2.27	0.49
2:F:117:ILE:CG1	2:F:118:VAL:N	2.75	0.49
3:D:963:ASN:N	3:D:964:PRO:CD	2.75	0.49
3:D:637:VAL:HG12	3:D:641:ILE:HD12	1.93	0.49
2:F:45:VAL:HG22	2:F:46:GLU:N	2.27	0.49
3:D:716:ASP:O	3:D:717:MET:C	2.51	0.49
3:D:276:VAL:O	3:D:276:VAL:HG13	2.10	0.49
3:A:948:TYR:CD1	3:A:948:TYR:C	2.85	0.49
3:A:528:CYS:CB	3:A:540:ILE:HG21	2.26	0.49
3:A:945:ILE:O	3:A:949:MET:HG3	2.12	0.49
3:A:526:GLY:O	3:A:530:GLN:HG3	2.12	0.49
3:A:56:HIS:N	3:A:57:PRO:CD	2.75	0.49
3:D:63:VAL:O	3:D:76:LYS:HE3	2.13	0.49
3:A:96:ARG:HH22	3:A:145:HIS:HB3	1.76	0.49
3:A:697:ARG:HG3	3:A:697:ARG:NH2	2.26	0.49
1:B:149:ASN:HD22	1:B:150:ARG:H	1.60	0.49
3:A:559:TRP:HH2	3:A:610:PHE:HB2	1.77	0.49
3:A:424:MET:HA	3:A:457:MET:CE	2.41	0.49
3:D:865:ALA:O	3:D:866:ILE:HG23	2.11	0.49
1:E:25:PRO:HG2	1:E:108:ILE:HD13	1.95	0.49
3:D:28:LEU:O	3:D:28:LEU:HD23	2.11	0.49
3:D:526:GLY:O	3:D:530:GLN:HG3	2.13	0.49
3:A:739:VAL:O	3:A:742:GLN:HG2	2.12	0.49
1:B:18:ASN:CG	1:B:108:ILE:HD11	2.33	0.49
2:C:75:LEU:HD11	3:A:49:VAL:HG22	1.95	0.49
3:A:163:LEU:O	3:A:163:LEU:HD23	2.13	0.49
3:A:547:ILE:HG22	3:A:548:VAL:N	2.26	0.49
3:A:514:LYS:O	3:A:515:ARG:C	2.49	0.49
3:A:329:PHE:CE1	3:A:333:HIS:HD2	2.30	0.49
3:A:29:ASP:O	3:A:33:ASN:ND2	2.45	0.49
1:E:106:TRP:CZ3	1:E:276:LEU:HA	2.48	0.49
3:A:997:PHE:CD1	3:A:1014:HIS:NE2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:966:ASN:HB3	3:D:967:PRO:HD3	1.94	0.49
3:A:313:ASP:HA	3:A:316:GLN:HG3	1.94	0.49
3:D:1035:LEU:O	3:D:1037:GLU:N	2.46	0.49
1:B:69:TRP:HB3	1:B:95:LYS:HE3	1.94	0.49
3:A:709:GLN:O	3:A:712:ARG:HB3	2.12	0.49
1:B:155:LEU:HG	1:B:217:LEU:HD11	1.95	0.49
3:D:962:LEU:C	3:D:964:PRO:HD3	2.33	0.49
1:B:220:LYS:C	1:B:221:THR:HG23	2.33	0.49
3:A:1036:GLU:O	3:A:1037:GLU:C	2.51	0.49
3:D:365:ILE:HG22	3:D:366:PHE:N	2.28	0.49
3:A:552:PRO:HA	3:A:555:LEU:HD12	1.95	0.49
3:D:639:TYR:CE1	3:D:701:ALA:HA	2.48	0.49
3:A:1004:LEU:HD21	3:A:1042:LEU:CD2	2.42	0.49
3:D:157:SER:HB3	3:D:164:CYS:HB2	1.94	0.49
1:B:160:ARG:CA	1:B:160:ARG:NE	2.68	0.49
3:A:153:ILE:HA	3:A:156:ALA:CB	2.43	0.49
2:C:123:LYS:C	2:C:125:ASP:H	2.15	0.49
3:D:676:VAL:HG13	3:D:679:LEU:HD12	1.94	0.49
3:A:650:GLN:O	3:A:654:ILE:HG13	2.12	0.49
3:A:30:ASN:N	3:A:30:ASN:HD22	2.09	0.49
3:A:766:SER:H	3:A:810:LYS:HZ3	1.60	0.49
3:A:255:LEU:HD12	3:A:268:LEU:CD1	2.42	0.49
2:F:70:GLU:OE2	3:D:1023:LYS:NZ	2.43	0.49
3:A:450:SER:O	3:A:453:LEU:N	2.46	0.49
3:A:146:TRP:CE3	3:A:149:PHE:HB2	2.47	0.49
3:A:276:VAL:O	3:A:278:GLN:N	2.46	0.49
3:D:297:MET:O	3:D:299:PRO:HD3	2.13	0.49
3:A:804:MET:HA	3:A:807:ILE:HG12	1.95	0.49
3:A:1008:ILE:HG13	3:A:1009:PRO:HD3	1.94	0.49
3:D:875:LEU:O	3:D:878:ILE:N	2.45	0.49
3:A:458:ARG:HG3	3:A:503:SER:HB2	1.94	0.49
3:A:279:TYR:O	3:A:283:PHE:CD2	2.66	0.48
1:E:210:LYS:HD2	1:E:210:LYS:N	2.22	0.48
1:E:11:LEU:HG	3:D:572:PHE:CZ	2.48	0.48
3:D:299:PRO:HD2	3:D:302:THR:CG2	2.43	0.48
3:A:127:ILE:CG2	3:A:131:ASN:HD21	2.26	0.48
3:A:962:LEU:HB3	3:A:964:PRO:CD	2.30	0.48
1:E:1:LEU:HG	1:E:2:ASN:HD22	1.78	0.48
2:C:156:ASN:HB3	2:C:159:LYS:HG3	1.93	0.48
1:B:236:CYS:HA	1:B:241:LEU:HD21	1.94	0.48
1:E:106:TRP:HZ3	1:E:276:LEU:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:178:ALA:O	2:F:179:MET:CB	2.61	0.48
3:D:833:MET:HB3	3:D:841:TYR:HD1	1.75	0.48
3:D:406:ARG:NH2	3:D:467:LEU:O	2.46	0.48
2:C:47:VAL:HG12	2:C:64:TRP:CG	2.48	0.48
3:D:897:LEU:O	3:D:901:LEU:HG	2.13	0.48
3:D:400:PHE:O	3:D:400:PHE:CD1	2.66	0.48
3:D:279:TYR:O	3:D:283:PHE:CD2	2.65	0.48
2:F:77:ASP:HA	2:F:80:TYR:CE2	2.45	0.48
3:A:672:ALA:HA	3:A:675:ASN:O	2.12	0.48
1:E:39:GLN:O	1:E:39:GLN:HG2	2.12	0.48
3:D:420:MET:O	3:D:424:MET:HB2	2.14	0.48
3:D:284:GLU:CG	3:D:336:LEU:HD11	2.42	0.48
3:D:218:ASN:O	3:D:222:VAL:HG23	2.13	0.48
3:D:1021:GLN:HE22	3:D:1033:LEU:HD13	1.79	0.48
3:D:1035:LEU:O	3:D:1038:ARG:N	2.46	0.48
3:A:672:ALA:CB	3:A:678:ILE:HD11	2.37	0.48
3:D:840:GLU:O	3:D:845:ARG:NH1	2.46	0.48
3:A:286:LEU:C	3:A:286:LEU:HD12	2.32	0.48
3:D:405:ARG:O	3:D:408:LEU:HB2	2.13	0.48
3:D:879:ILE:HG12	3:D:925:HIS:CD2	2.48	0.48
3:A:1036:GLU:O	3:A:1039:GLU:N	2.46	0.48
1:E:351:ASP:N	1:E:351:ASP:OD2	2.40	0.48
3:A:786:ILE:HD13	3:D:645:THR:HG21	1.94	0.48
2:C:159:LYS:N	2:C:160:PRO:CD	2.77	0.48
2:C:13:LEU:HD12	2:C:14:VAL:O	2.12	0.48
1:E:130:LEU:HD11	1:E:170:ILE:CG2	2.43	0.48
2:C:75:LEU:CD1	3:A:49:VAL:HG22	2.44	0.48
3:D:15:GLN:C	3:D:16:LEU:HD12	2.34	0.48
3:D:424:MET:HA	3:D:457:MET:CE	2.41	0.48
2:F:117:ILE:HG23	2:F:144:LEU:HD22	1.94	0.48
3:D:334:GLY:C	3:D:336:LEU:H	2.16	0.48
3:A:879:ILE:HG12	3:A:925:HIS:CD2	2.48	0.48
3:A:988:HIS:N	3:A:988:HIS:CD2	2.81	0.48
3:D:1003:SER:O	3:D:1005:ASN:N	2.47	0.48
4:C:217:GTP:O1A	4:C:217:GTP:O3B	2.32	0.48
3:A:134:LEU:HD23	3:A:170:ILE:HD12	1.96	0.48
3:A:430:VAL:O	3:A:430:VAL:CG1	2.61	0.48
3:D:272:ALA:HB1	3:D:329:PHE:CD1	2.49	0.48
3:A:334:GLY:C	3:A:336:LEU:H	2.16	0.48
3:A:232:PHE:O	3:A:236:ILE:HG23	2.14	0.48
3:A:324:LEU:CD2	3:A:368:ILE:HD13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:LEU:H	1:B:1:LEU:HD23	1.79	0.48
2:C:81:ILE:HD11	3:A:77:TYR:CG	2.49	0.48
3:D:188:GLN:NE2	3:D:1013:GLU:HG3	2.29	0.48
3:A:188:GLN:NE2	3:A:1013:GLU:HG3	2.28	0.48
3:A:551:TYR:O	3:A:554:PHE:HB3	2.14	0.48
3:A:894:LEU:HA	3:A:894:LEU:HD23	1.48	0.48
3:D:122:LYS:O	3:D:123:GLU:O	2.32	0.48
3:A:769:PRO:CG	3:A:770:GLN:N	2.77	0.48
3:A:259:MET:C	3:A:261:ARG:H	2.16	0.48
3:D:1022:ILE:CG1	3:D:1023:LYS:N	2.76	0.48
3:D:611:ILE:O	3:D:614:ILE:HB	2.14	0.48
3:D:802:SER:O	3:D:806:ILE:HG13	2.13	0.48
3:A:962:LEU:O	3:A:963:ASN:HB2	2.14	0.48
1:E:146:TYR:C	1:E:146:TYR:CD1	2.88	0.48
3:D:280:GLU:HG3	3:D:336:LEU:HD13	1.94	0.48
3:A:383:GLU:OE2	3:A:405:ARG:HG3	2.14	0.48
2:C:29:ARG:HB3	2:C:157:PHE:HZ	1.79	0.48
3:A:600:VAL:HG11	3:A:640:MET:O	2.14	0.48
3:D:924:GLN:NE2	3:D:977:TYR:OH	2.47	0.48
3:A:517:LEU:HD11	3:A:551:TYR:CG	2.49	0.48
1:B:1:LEU:HD22	3:A:514:LYS:NZ	2.28	0.48
3:A:329:PHE:CE1	3:A:333:HIS:CD2	3.02	0.48
3:A:334:GLY:C	3:A:336:LEU:N	2.66	0.48
2:C:24:THR:OG1	4:C:217:GTP:O1G	2.32	0.48
1:B:60:HIS:CE1	1:B:100:GLN:HE22	2.32	0.48
3:A:139:LYS:HD2	3:A:186:ILE:HD11	1.96	0.48
3:A:376:LEU:HG	3:A:380:LEU:HD12	1.95	0.48
3:D:504:ILE:HD12	3:D:504:ILE:O	2.14	0.48
3:D:329:PHE:CE1	3:D:333:HIS:HD2	2.30	0.47
3:D:127:ILE:HG22	3:D:128:GLY:N	2.29	0.47
3:A:271:ILE:C	3:A:273:GLY:H	2.17	0.47
3:A:150:ILE:O	3:A:154:VAL:HG23	2.14	0.47
3:D:157:SER:HB3	3:D:164:CYS:CB	2.44	0.47
1:B:58:VAL:HA	1:B:194:PRO:CG	2.44	0.47
3:A:831:LEU:HD13	3:A:848:PHE:CZ	2.49	0.47
3:A:687:GLN:O	3:A:691:ILE:HB	2.14	0.47
3:D:102:ILE:O	3:D:105:TYR:N	2.47	0.47
3:D:56:HIS:N	3:D:57:PRO:CD	2.77	0.47
3:D:62:ARG:HH12	3:D:82:ILE:HD13	1.79	0.47
3:A:56:HIS:HB3	3:A:82:ILE:CG2	2.44	0.47
3:D:894:LEU:HB3	3:D:941:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:736:GLY:C	3:A:738:MET:H	2.16	0.47
1:B:142:THR:C	1:B:144:SER:N	2.67	0.47
3:A:865:ALA:O	3:A:866:ILE:HG23	2.13	0.47
2:F:138:PHE:O	2:F:141:LYS:HD2	2.14	0.47
3:A:246:LEU:O	3:A:249:THR:N	2.46	0.47
3:D:578:ASP:OD2	3:D:578:ASP:N	2.47	0.47
3:D:491:TRP:CD2	3:D:539:ILE:HD12	2.49	0.47
3:D:547:ILE:HG22	3:D:548:VAL:N	2.28	0.47
1:B:55:LEU:H	1:B:55:LEU:CD1	2.09	0.47
1:B:98:ALA:CB	1:B:144:SER:HA	2.44	0.47
3:A:268:LEU:O	3:A:269:THR:C	2.53	0.47
3:A:964:PRO:O	3:A:968:VAL:HG22	2.13	0.47
3:A:871:PHE:CE2	3:A:875:LEU:HD11	2.49	0.47
3:A:55:GLU:HB3	3:A:57:PRO:HD3	1.97	0.47
1:B:247:MET:HB2	1:B:249:PHE:CE1	2.49	0.47
3:A:768:ASP:HB3	3:A:771:MET:HE3	1.96	0.47
3:D:129:LYS:O	3:D:133:ILE:HG13	2.14	0.47
3:D:80:LEU:HB3	3:D:133:ILE:HD11	1.95	0.47
1:B:18:ASN:ND2	1:B:36:SER:OG	2.47	0.47
1:E:284:VAL:CG1	1:E:285:LEU:HD13	2.44	0.47
3:D:615:LEU:CD2	3:D:618:ILE:HD11	2.43	0.47
3:A:239:GLY:HA2	3:A:243:GLU:OE2	2.13	0.47
3:A:975:GLN:HG3	3:A:998:VAL:CG1	2.44	0.47
2:F:123:LYS:C	2:F:125:ASP:H	2.17	0.47
3:D:887:ARG:CD	3:D:937:ALA:HB3	2.37	0.47
1:B:48:GLU:C	1:B:50:GLN:H	2.16	0.47
3:D:179:PHE:CE2	3:D:235:TRP:CD2	3.02	0.47
3:D:50:LEU:C	3:D:52:HIS:H	2.18	0.47
2:C:88:ILE:HD11	2:C:117:ILE:CD1	2.44	0.47
2:C:88:ILE:HD11	2:C:117:ILE:HD11	1.97	0.47
3:D:30:ASN:HB2	3:D:48:GLU:OE2	2.15	0.47
3:A:1004:LEU:HD12	3:A:1014:HIS:HB2	1.96	0.47
3:D:1003:SER:C	3:D:1005:ASN:N	2.67	0.47
3:D:376:LEU:HG	3:D:380:LEU:HD12	1.96	0.47
3:A:491:TRP:CH2	3:A:535:ASP:HB3	2.49	0.47
3:A:898:PHE:HD2	3:A:945:ILE:HG12	1.80	0.47
3:D:153:ILE:HA	3:D:156:ALA:CB	2.45	0.47
3:A:875:LEU:HD21	3:A:914:PHE:HE1	1.80	0.47
3:D:484:VAL:CG1	3:D:530:GLN:OE1	2.54	0.47
3:D:860:PHE:CE1	3:D:900:LEU:HG	2.47	0.47
3:D:56:HIS:C	3:D:58:ASP:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:THR:OG1	1:E:263:THR:HG23	2.14	0.47
1:E:119:ILE:HD11	1:E:259:TYR:CB	2.43	0.47
2:F:16:VAL:HG23	2:F:88:ILE:HA	1.95	0.47
1:B:155:LEU:HD11	1:B:228:PHE:CZ	2.49	0.47
3:D:1049:LYS:C	3:D:1051:LYS:H	2.18	0.47
3:D:313:ASP:HA	3:D:316:GLN:HG3	1.96	0.47
3:D:282:GLN:OE1	3:D:282:GLN:N	2.47	0.47
3:A:973:PHE:CD1	3:A:974:ILE:N	2.81	0.47
3:A:100:GLU:O	3:A:103:LYS:HB3	2.15	0.47
3:A:146:TRP:N	3:A:147:PRO:CD	2.77	0.47
3:A:122:LYS:O	3:A:123:GLU:O	2.32	0.47
1:E:244:VAL:HG13	1:E:245:LEU:CD1	2.39	0.47
1:E:122:VAL:HG11	1:E:249:PHE:CE2	2.49	0.47
2:F:124:VAL:HG21	2:F:155:TYR:CD2	2.50	0.47
1:B:13:ILE:CG2	3:A:575:GLU:OE1	2.59	0.47
3:D:344:ARG:NE	3:D:408:LEU:HD21	2.30	0.47
3:D:406:ARG:HA	3:D:409:TYR:HD2	1.78	0.47
2:F:140:ARG:NH2	3:D:371:GLU:OE1	2.39	0.47
3:A:656:LYS:O	3:A:656:LYS:HG2	2.13	0.47
2:C:98:TYR:HE1	2:C:136:ILE:HG23	1.79	0.47
3:D:1047:GLU:HA	3:D:1050:HIS:NE2	2.29	0.47
3:A:668:ILE:HG22	3:A:668:ILE:O	2.14	0.47
1:E:183:TYR:HA	1:E:229:VAL:O	2.14	0.47
3:D:915:TYR:HA	3:D:919:PHE:HB2	1.96	0.47
3:A:63:VAL:O	3:A:76:LYS:HE3	2.15	0.47
1:B:1:LEU:HG	1:B:2:ASN:N	2.30	0.47
3:A:731:ALA:HB1	3:A:739:VAL:HG11	1.95	0.47
3:D:704:HIS:HD2	3:D:766:SER:HA	1.80	0.47
3:D:847:ASN:O	3:D:850:LEU:N	2.47	0.47
3:D:23:LEU:HD11	3:D:26:ASN:CB	2.44	0.47
1:E:13:ILE:HD11	3:D:572:PHE:CE2	2.49	0.47
3:D:255:LEU:O	3:D:255:LEU:HD23	2.14	0.47
1:E:25:PRO:HG2	1:E:108:ILE:CD1	2.45	0.47
3:D:769:PRO:CG	3:D:770:GLN:N	2.78	0.47
3:D:239:GLY:O	3:D:244:THR:HG23	2.15	0.47
3:D:100:GLU:OE2	3:D:103:LYS:HD3	2.14	0.47
3:D:146:TRP:CE3	3:D:149:PHE:HB2	2.49	0.47
1:B:63:ARG:NH1	1:B:95:LYS:HZ2	2.05	0.47
1:B:146:TYR:C	1:B:146:TYR:CD1	2.89	0.47
3:A:168:MET:HE2	3:A:168:MET:HA	1.97	0.47
3:D:127:ILE:O	3:D:130:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:LYS:O	2:F:27:VAL:HG13	2.15	0.47
3:A:378:ALA:HB1	3:A:382:ARG:HH12	1.79	0.47
3:D:257:VAL:O	3:D:257:VAL:HG12	2.15	0.47
3:D:458:ARG:O	3:D:462:VAL:HG23	2.15	0.47
3:A:578:ASP:OD2	3:A:578:ASP:N	2.48	0.47
2:C:138:PHE:O	2:C:141:LYS:HD2	2.15	0.47
2:C:26:PHE:CZ	2:C:30:HIS:CE1	3.03	0.47
3:D:718:LEU:HD23	3:D:718:LEU:HA	1.56	0.47
3:D:102:ILE:O	3:D:103:LYS:C	2.54	0.46
2:C:155:TYR:O	2:C:156:ASN:C	2.54	0.46
1:B:188:MET:HE3	1:B:265:TYR:CE1	2.50	0.46
3:D:123:GLU:C	3:D:125:VAL:N	2.68	0.46
1:B:352:HIS:HA	1:B:353:PRO:HD3	1.79	0.46
3:A:142:TRP:HH2	3:A:197:SER:C	2.19	0.46
3:D:378:ALA:HB1	3:D:382:ARG:NH1	2.30	0.46
1:B:114:LEU:HD12	1:B:118:TRP:CG	2.50	0.46
3:D:258:PRO:O	3:D:261:ARG:HB3	2.15	0.46
1:E:52:SER:O	1:E:53:LYS:C	2.54	0.46
3:A:747:SER:O	3:A:750:THR:HB	2.15	0.46
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.62	0.46
3:A:918:TYR:O	3:A:922:ILE:HG13	2.15	0.46
3:A:351:LEU:HA	3:A:351:LEU:HD23	1.55	0.46
1:B:63:ARG:NH1	1:B:95:LYS:HZ1	2.10	0.46
1:B:142:THR:C	1:B:144:SER:H	2.18	0.46
3:A:840:GLU:O	3:A:845:ARG:NH1	2.47	0.46
3:A:704:HIS:CD2	3:A:767:ASN:N	2.83	0.46
3:D:660:LEU:O	3:D:661:PRO:C	2.51	0.46
3:A:952:LEU:O	3:A:952:LEU:HD23	2.15	0.46
3:D:521:ILE:HG22	3:D:547:ILE:HG21	1.97	0.46
3:A:66:ILE:HD13	3:A:66:ILE:H	1.80	0.46
3:D:101:GLY:O	3:D:105:TYR:HB2	2.14	0.46
3:A:287:PHE:CD2	3:A:337:LEU:HD11	2.50	0.46
2:F:155:TYR:O	2:F:156:ASN:C	2.54	0.46
2:F:81:ILE:HD11	3:D:77:TYR:CG	2.51	0.46
3:D:627:PRO:O	3:D:631:HIS:CD2	2.69	0.46
3:A:219:ALA:CB	3:A:220:PRO:HD3	2.43	0.46
3:A:93:ILE:HG23	3:A:1027:GLY:HA3	1.96	0.46
2:C:98:TYR:HA	2:C:101:VAL:HG23	1.96	0.46
3:A:240:TYR:O	3:A:244:THR:HG21	2.15	0.46
3:A:28:LEU:O	3:A:28:LEU:HD23	2.15	0.46
3:D:752:LYS:O	3:D:755:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:LYS:HG2	2:C:12:LYS:O	2.15	0.46
3:A:935:HIS:N	3:A:935:HIS:ND1	2.63	0.46
3:A:875:LEU:O	3:A:876:ASP:C	2.53	0.46
1:E:240:SER:O	1:E:242:CYS:N	2.49	0.46
3:A:272:ALA:HB1	3:A:329:PHE:HD1	1.80	0.46
1:B:25:PRO:HG2	1:B:108:ILE:CD1	2.45	0.46
2:F:75:LEU:N	2:F:75:LEU:CD1	2.79	0.46
3:A:906:GLN:N	3:A:906:GLN:NE2	2.63	0.46
2:F:64:TRP:HE3	2:F:79:TYR:HB3	1.78	0.46
3:D:406:ARG:C	3:D:408:LEU:N	2.65	0.46
2:F:83:ALA:O	2:F:115:ILE:HG21	2.15	0.46
2:C:45:VAL:HG22	2:C:46:GLU:H	1.79	0.46
3:A:240:TYR:O	3:A:244:THR:CG2	2.63	0.46
3:D:660:LEU:HD12	3:D:660:LEU:N	2.30	0.46
3:A:465:THR:O	3:A:469:TYR:HB3	2.16	0.46
2:C:50:LEU:O	2:C:60:LYS:HA	2.16	0.46
2:C:124:VAL:HG21	2:C:155:TYR:CD2	2.51	0.46
2:F:31:LEU:O	2:F:32:THR:HG22	2.15	0.46
3:D:286:LEU:C	3:D:286:LEU:HD12	2.35	0.46
3:A:189:VAL:HG11	3:A:1038:ARG:HG3	1.97	0.46
2:C:83:ALA:O	2:C:115:ILE:HG21	2.16	0.46
1:B:277:ARG:HG2	1:B:280:MET:HE3	1.98	0.46
3:A:269:THR:HG22	3:A:270:GLU:N	2.29	0.46
3:D:246:LEU:O	3:D:249:THR:N	2.47	0.46
3:A:964:PRO:HB2	3:A:968:VAL:CG1	2.46	0.46
3:A:813:GLY:HA2	3:A:816:THR:OG1	2.16	0.46
3:D:894:LEU:HD23	3:D:894:LEU:HA	1.48	0.46
3:A:297:MET:O	3:A:299:PRO:HD3	2.16	0.46
3:D:317:ASN:O	3:D:318:PHE:C	2.52	0.46
3:A:724:LEU:HD12	3:A:751:VAL:HB	1.97	0.46
3:A:938:GLY:O	3:A:939:LEU:C	2.53	0.46
3:A:87:ILE:HG23	3:A:91:TRP:CE3	2.50	0.46
3:D:87:ILE:HG23	3:D:91:TRP:CE3	2.51	0.46
3:A:819:ILE:N	3:A:820:PRO:CD	2.79	0.46
3:A:914:PHE:CE1	3:A:918:TYR:CD1	3.04	0.46
2:C:156:ASN:ND2	2:C:159:LYS:HE3	2.31	0.46
3:D:816:THR:HG23	3:D:859:CYS:CB	2.46	0.46
3:A:718:LEU:HA	3:A:718:LEU:HD23	1.48	0.46
3:A:25:ILE:H	3:A:25:ILE:CD1	2.25	0.46
3:D:467:LEU:O	3:D:468:ASP:HB2	2.16	0.46
3:D:259:MET:C	3:D:261:ARG:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:LEU:CD2	2:C:23:LYS:HG2	2.45	0.46
3:A:229:LEU:O	3:A:233:LEU:HG	2.15	0.46
3:D:56:HIS:HB3	3:D:82:ILE:CG2	2.45	0.46
3:A:676:VAL:HG13	3:A:679:LEU:HD12	1.97	0.46
1:E:13:ILE:HG22	3:D:537:LYS:CB	2.45	0.46
3:D:144:LYS:HB2	3:D:145:HIS:CD2	2.50	0.46
2:C:153:SER:HB2	3:A:431:LEU:HD21	1.98	0.46
3:A:167:ASN:HA	3:A:170:ILE:HG13	1.98	0.46
3:D:879:ILE:H	3:D:879:ILE:HD12	1.81	0.46
3:D:973:PHE:O	3:D:973:PHE:HD1	1.99	0.46
1:E:238:PRO:HA	1:E:241:LEU:HD12	1.96	0.46
3:D:887:ARG:O	3:D:891:ASP:HB2	2.16	0.46
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.79	0.46
3:A:142:TRP:N	3:A:143:PRO:HD2	2.31	0.46
3:D:378:ALA:HA	3:D:463:TYR:CE2	2.51	0.46
3:A:402:ILE:HG12	3:A:402:ILE:H	1.48	0.46
3:A:1007:ASP:OD1	3:A:1010:ALA:HB2	2.16	0.46
2:C:73:GLY:HA3	2:C:76:ARG:NH2	2.31	0.46
3:A:109:LEU:O	3:A:112:LYS:HG3	2.16	0.46
1:E:247:MET:HB2	1:E:249:PHE:CE1	2.51	0.46
3:D:269:THR:HG22	3:D:270:GLU:N	2.30	0.46
3:A:258:PRO:O	3:A:261:ARG:HB3	2.16	0.46
3:D:223:HIS:O	3:D:223:HIS:HD2	1.99	0.46
2:F:146:TYR:CD2	2:F:147:TYR:N	2.84	0.46
3:D:950:PHE:O	3:D:953:VAL:HB	2.16	0.45
3:D:480:LEU:HB2	3:D:497:LEU:HD21	1.98	0.45
3:A:704:HIS:HD2	3:A:766:SER:HA	1.80	0.45
1:B:280:MET:O	1:B:283:ASP:HB2	2.14	0.45
2:C:42:THR:OG1	4:C:217:GTP:PG	2.74	0.45
2:C:45:VAL:CG2	2:C:46:GLU:H	2.29	0.45
2:F:45:VAL:CG2	2:F:46:GLU:N	2.78	0.45
1:B:93:LEU:HA	1:B:94:PRO:HD3	1.74	0.45
3:D:801:LEU:HD11	3:D:830:THR:HG21	1.97	0.45
3:A:282:GLN:OE1	3:A:282:GLN:N	2.48	0.45
3:A:107:VAL:O	3:A:111:ILE:CG1	2.50	0.45
3:D:55:GLU:HB3	3:D:57:PRO:HD3	1.98	0.45
3:D:675:ASN:ND2	3:D:677:ASP:HB2	2.31	0.45
1:B:107:LEU:HB2	1:B:274:GLY:CA	2.44	0.45
3:D:195:LYS:O	3:D:197:SER:N	2.49	0.45
2:F:139:HIS:ND1	2:F:139:HIS:N	2.64	0.45
3:A:150:ILE:HG23	3:A:151:SER:N	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:ARG:HH22	3:D:620:THR:HG21	1.80	0.45
3:D:964:PRO:HG2	3:D:968:VAL:CB	2.46	0.45
3:A:467:LEU:O	3:A:468:ASP:HB2	2.16	0.45
1:B:60:HIS:HE1	1:B:100:GLN:HE22	1.63	0.45
3:A:102:ILE:O	3:A:105:TYR:N	2.49	0.45
3:D:329:PHE:CE1	3:D:333:HIS:CD2	3.05	0.45
3:D:675:ASN:C	3:D:677:ASP:H	2.20	0.45
3:D:1008:ILE:HG13	3:D:1009:PRO:HD3	1.97	0.45
1:B:154:LEU:HD13	1:B:215:GLU:CG	2.46	0.45
3:D:334:GLY:C	3:D:336:LEU:N	2.68	0.45
3:D:378:ALA:HB1	3:D:382:ARG:HH12	1.80	0.45
3:A:1032:ASP:OD1	3:A:1032:ASP:N	2.49	0.45
3:A:1003:SER:C	3:A:1005:ASN:N	2.69	0.45
3:D:656:LYS:HG2	3:D:656:LYS:O	2.16	0.45
3:A:559:TRP:O	3:A:559:TRP:CG	2.69	0.45
3:D:1022:ILE:HG13	3:D:1023:LYS:N	2.31	0.45
2:F:71:LYS:HE2	3:D:932:ASP:OD1	2.17	0.45
3:D:819:ILE:N	3:D:820:PRO:CD	2.80	0.45
3:D:746:ARG:NH1	3:D:746:ARG:HG2	2.15	0.45
3:A:930:VAL:HG11	3:A:1015:LEU:HD22	1.97	0.45
3:D:130:LEU:O	3:D:131:ASN:C	2.54	0.45
3:D:113:THR:HG22	3:D:119:CYS:SG	2.57	0.45
3:D:785:LEU:HD11	3:D:804:MET:HG2	1.97	0.45
3:A:344:ARG:NE	3:A:408:LEU:HD21	2.32	0.45
3:D:647:GLN:O	3:D:651:GLU:HG3	2.16	0.45
3:A:1003:SER:O	3:A:1005:ASN:N	2.50	0.45
1:E:348:HIS:NE2	3:D:708:ILE:O	2.49	0.45
3:D:715:LEU:O	3:D:718:LEU:HB2	2.17	0.45
2:F:153:SER:HB2	3:D:431:LEU:HD21	1.99	0.45
3:A:103:LYS:O	3:A:107:VAL:HG23	2.15	0.45
3:A:946:LEU:HD12	3:A:946:LEU:HA	1.61	0.45
3:D:172:LYS:O	3:D:175:SER:HB3	2.16	0.45
3:D:271:ILE:C	3:D:273:GLY:H	2.19	0.45
2:F:171:ASP:C	2:F:171:ASP:OD1	2.55	0.45
3:A:966:ASN:N	3:A:967:PRO:CD	2.80	0.45
1:E:152:SER:O	1:E:225:PRO:HD2	2.16	0.45
2:F:84:GLN:O	2:F:168:LEU:HD21	2.17	0.45
1:B:281:VAL:HG13	1:B:282:SER:N	2.30	0.45
3:A:122:LYS:HD2	3:A:122:LYS:HA	1.59	0.45
1:B:245:LEU:HD12	1:B:245:LEU:HA	1.55	0.45
2:F:106:ARG:O	2:F:110:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:632:THR:N	3:A:697:ARG:HH22	2.15	0.45
3:A:378:ALA:HA	3:A:463:TYR:CE2	2.52	0.45
3:A:406:ARG:NH2	3:A:467:LEU:O	2.50	0.45
3:A:847:ASN:O	3:A:849:PHE:N	2.50	0.45
3:A:458:ARG:O	3:A:462:VAL:HG23	2.16	0.45
3:A:691:ILE:CG2	3:A:692:LEU:N	2.79	0.45
1:E:1:LEU:O	1:E:4:LEU:CD1	2.64	0.45
3:A:118:THR:HG22	3:A:121:GLU:HG3	1.99	0.45
1:B:54:ARG:H	1:B:55:LEU:HD12	1.82	0.45
3:A:837:ASP:O	3:A:845:ARG:NH2	2.49	0.45
3:D:837:ASP:O	3:D:845:ARG:NH2	2.49	0.45
3:A:195:LYS:C	3:A:197:SER:N	2.69	0.45
3:D:736:GLY:C	3:D:738:MET:N	2.69	0.45
3:D:406:ARG:O	3:D:407:GLN:C	2.54	0.45
1:B:277:ARG:CG	1:B:280:MET:HE3	2.47	0.45
3:A:847:ASN:O	3:A:848:PHE:C	2.55	0.45
3:A:563:LYS:HE2	3:A:606:GLU:OE2	2.16	0.45
3:A:950:PHE:O	3:A:953:VAL:HB	2.16	0.45
1:B:107:LEU:O	1:B:276:LEU:HD11	2.17	0.45
3:D:121:GLU:C	3:D:123:GLU:N	2.61	0.45
3:A:50:LEU:C	3:A:52:HIS:H	2.21	0.45
1:E:277:ARG:CG	1:E:280:MET:HE3	2.47	0.45
3:D:509:HIS:HB2	3:D:512:ASP:OD2	2.17	0.45
3:A:372:TYR:O	3:A:375:HIS:N	2.50	0.45
3:D:918:TYR:O	3:D:922:ILE:HG13	2.17	0.45
3:D:988:HIS:N	3:D:988:HIS:CD2	2.84	0.45
3:D:551:TYR:O	3:D:554:PHE:HB3	2.17	0.45
3:D:351:LEU:HA	3:D:351:LEU:HD23	1.47	0.45
3:A:628:GLN:O	3:A:631:HIS:HB2	2.17	0.45
3:D:843:GLU:O	3:D:844:HIS:C	2.54	0.45
1:B:284:VAL:HG12	1:B:284:VAL:O	2.17	0.45
3:D:914:PHE:CD1	3:D:918:TYR:HD1	2.34	0.45
3:D:304:ILE:HG12	3:D:356:LEU:HB3	1.99	0.45
3:A:300:LEU:HB3	3:A:352:HIS:CE1	2.52	0.45
3:A:396:GLY:O	3:A:397:SER:O	2.34	0.45
3:A:250:LEU:HD23	3:A:250:LEU:HA	1.71	0.45
3:A:60:TRP:N	3:A:60:TRP:CD1	2.76	0.45
3:D:19:PHE:C	3:D:19:PHE:CD1	2.89	0.45
3:A:27:LEU:HA	3:A:30:ASN:OD1	2.16	0.45
1:B:69:TRP:CE3	1:B:95:LYS:HD3	2.52	0.45
3:A:729:SER:OG	3:A:792:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:930:VAL:HG11	3:D:1015:LEU:HD22	1.98	0.45
3:A:423:ARG:O	3:A:424:MET:C	2.53	0.45
3:D:66:ILE:HD13	3:D:66:ILE:H	1.82	0.45
3:D:116:ASP:HB2	3:D:119:CYS:CB	2.45	0.45
3:D:195:LYS:C	3:D:197:SER:N	2.70	0.45
1:B:111:PRO:CD	1:B:114:LEU:HD13	2.45	0.45
3:A:268:LEU:HD23	3:A:268:LEU:HA	1.80	0.45
3:D:559:TRP:CG	3:D:559:TRP:O	2.70	0.45
3:D:952:LEU:O	3:D:952:LEU:HD23	2.17	0.45
3:A:223:HIS:O	3:A:223:HIS:HD2	2.00	0.45
3:D:186:ILE:HG22	3:D:187:THR:O	2.17	0.45
3:D:898:PHE:HD2	3:D:945:ILE:HG12	1.83	0.44
1:E:152:SER:O	1:E:225:PRO:HD3	2.16	0.44
2:F:26:PHE:CZ	2:F:30:HIS:CE1	3.05	0.44
2:F:108:LEU:CD1	2:F:112:CYS:SG	3.05	0.44
3:D:60:TRP:CD1	3:D:60:TRP:N	2.76	0.44
3:A:539:ILE:HG22	3:A:540:ILE:N	2.33	0.44
3:A:515:ARG:CG	3:A:515:ARG:NH1	2.79	0.44
3:D:337:LEU:CD2	3:D:343:LEU:HB3	2.46	0.44
1:B:41:GLU:CG	1:B:109:ASP:HB3	2.36	0.44
2:F:94:SER:HB3	2:F:97:THR:CG2	2.47	0.44
1:B:237:THR:O	1:B:238:PRO:C	2.55	0.44
3:A:834:ILE:HG21	3:A:845:ARG:HA	1.99	0.44
3:A:1007:ASP:O	3:A:1010:ALA:HB3	2.18	0.44
3:A:304:ILE:HG12	3:A:356:LEU:HB3	1.99	0.44
3:D:190:LYS:O	3:D:194:LEU:HD13	2.16	0.44
3:A:362:GLU:C	3:A:364:GLU:H	2.19	0.44
2:C:45:VAL:CG2	2:C:46:GLU:N	2.80	0.44
2:F:45:VAL:CG2	2:F:46:GLU:H	2.30	0.44
3:A:643:ALA:O	3:A:645:THR:HG23	2.17	0.44
3:D:503:SER:O	3:D:505:SER:N	2.49	0.44
3:D:721:TYR:CE2	3:D:784:VAL:HG22	2.52	0.44
3:A:332:GLU:O	3:A:332:GLU:HG3	2.17	0.44
3:A:102:ILE:HG13	3:A:102:ILE:H	1.55	0.44
3:A:855:VAL:O	3:A:859:CYS:HB2	2.17	0.44
3:D:680:LYS:HE2	3:D:680:LYS:HB3	1.86	0.44
2:C:85:CYS:HB2	2:C:164:LEU:HD22	1.99	0.44
1:E:260:HIS:O	1:E:262:GLN:N	2.50	0.44
3:D:129:LYS:O	3:D:132:MET:HB3	2.16	0.44
3:A:19:PHE:O	3:A:20:SER:OG	2.33	0.44
1:E:4:LEU:HD22	3:D:521:ILE:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:103:LYS:O	3:D:107:VAL:HG23	2.16	0.44
3:D:78:TYR:CE2	3:D:82:ILE:HD11	2.52	0.44
1:E:142:THR:C	1:E:144:SER:H	2.19	0.44
3:A:736:GLY:O	3:A:738:MET:N	2.51	0.44
1:B:172:ASP:HB2	1:B:188:MET:CE	2.39	0.44
3:D:255:LEU:HD12	3:D:268:LEU:CD1	2.47	0.44
1:B:211:LEU:N	1:B:212:PRO:CD	2.80	0.44
3:D:509:HIS:O	3:D:510:GLU:C	2.56	0.44
3:D:72:ASN:O	3:D:75:THR:N	2.50	0.44
3:D:974:ILE:O	3:D:975:GLN:C	2.54	0.44
3:D:223:HIS:NE2	3:D:263:VAL:HG21	2.32	0.44
3:D:592:ALA:O	3:D:596:ARG:HB3	2.17	0.44
3:A:915:TYR:HA	3:A:919:PHE:HB2	1.98	0.44
3:A:116:ASP:C	3:A:118:THR:N	2.71	0.44
2:C:122:ASN:O	2:C:123:LYS:CB	2.60	0.44
3:A:329:PHE:CD1	3:A:333:HIS:HD2	2.35	0.44
3:D:900:LEU:HD23	3:D:900:LEU:C	2.37	0.44
3:D:831:LEU:HD12	3:D:834:ILE:HD11	1.99	0.44
3:A:157:SER:HB3	3:A:164:CYS:CB	2.47	0.44
3:D:879:ILE:HA	3:D:882:PHE:CE2	2.52	0.44
3:D:55:GLU:CG	3:D:56:HIS:H	2.31	0.44
2:F:50:LEU:O	2:F:60:LYS:HA	2.17	0.44
3:D:887:ARG:HA	3:D:887:ARG:HD2	1.76	0.44
3:A:654:ILE:CG2	3:A:654:ILE:O	2.64	0.44
1:E:142:THR:C	1:E:144:SER:N	2.70	0.44
3:A:735:ASN:HB2	3:A:739:VAL:CG2	2.48	0.44
3:A:179:PHE:CE2	3:A:235:TRP:CD2	3.05	0.44
1:E:277:ARG:HG2	1:E:280:MET:HE3	2.00	0.44
2:C:88:ILE:HD13	2:C:88:ILE:N	2.33	0.44
3:A:870:GLN:O	3:A:873:LEU:HB3	2.18	0.44
3:D:912:GLN:H	3:D:912:GLN:HG2	1.57	0.44
3:A:963:ASN:N	3:A:964:PRO:CD	2.80	0.44
1:E:1:LEU:HD22	3:D:558:HIS:CD2	2.45	0.44
3:A:98:GLN:O	3:A:102:ILE:HG13	2.18	0.44
3:A:279:TYR:O	3:A:283:PHE:HD2	2.01	0.44
2:F:92:VAL:CG2	2:F:129:ARG:HG3	2.47	0.44
3:D:672:ALA:CB	3:D:678:ILE:HD11	2.38	0.44
3:D:515:ARG:NH1	3:D:515:ARG:CG	2.79	0.44
3:A:426:LYS:HG3	3:A:499:TRP:CH2	2.53	0.44
3:A:659:LEU:HD23	3:A:659:LEU:HA	1.77	0.44
3:D:465:THR:O	3:D:469:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:172:LYS:O	3:D:176:GLU:HG3	2.18	0.44
1:E:211:LEU:N	1:E:212:PRO:CD	2.81	0.44
1:B:200:THR:OG1	1:B:263:THR:HG23	2.17	0.44
2:C:138:PHE:O	2:C:139:HIS:C	2.56	0.44
2:C:139:HIS:ND1	2:C:139:HIS:N	2.66	0.44
3:A:786:ILE:O	3:A:789:GLN:HB3	2.17	0.44
3:A:801:LEU:HD11	3:A:830:THR:HG21	1.99	0.44
3:A:88:LYS:HE2	3:A:136:GLN:NE2	2.33	0.44
2:C:171:ASP:OD1	2:C:171:ASP:C	2.56	0.44
1:E:114:LEU:HD12	1:E:118:TRP:CD1	2.53	0.44
3:A:879:ILE:HD12	3:A:879:ILE:N	2.33	0.44
3:D:137:ILE:O	3:D:140:GLN:HB2	2.18	0.44
3:A:32:VAL:O	3:A:36:TYR:HB2	2.17	0.44
3:D:643:ALA:O	3:D:645:THR:HG23	2.18	0.44
3:D:920:CYS:HB3	3:D:977:TYR:HE2	1.81	0.44
3:A:721:TYR:CE2	3:A:784:VAL:HG22	2.53	0.44
1:B:1:LEU:HD22	3:A:514:LYS:HE3	2.00	0.43
3:D:672:ALA:HA	3:D:675:ASN:O	2.17	0.43
1:E:149:ASN:HD22	1:E:150:ARG:H	1.66	0.43
3:A:735:ASN:HB2	3:A:739:VAL:HG22	1.99	0.43
3:A:622:ILE:HD13	3:A:630:VAL:HG23	2.00	0.43
1:E:103:LEU:HD21	1:E:143:LYS:HD3	2.00	0.43
3:D:138:LEU:C	3:D:140:GLN:H	2.19	0.43
3:D:973:PHE:CD1	3:D:973:PHE:C	2.92	0.43
3:A:552:PRO:O	3:A:553:ARG:C	2.55	0.43
3:A:962:LEU:HA	3:A:973:PHE:HE2	1.84	0.43
1:E:236:CYS:HA	1:E:241:LEU:HD21	2.00	0.43
3:A:833:MET:HE3	3:A:841:TYR:CE1	2.53	0.43
3:A:516:PHE:O	3:A:519:THR:HB	2.18	0.43
2:C:132:LYS:O	2:C:133:ALA:C	2.54	0.43
3:A:504:ILE:O	3:A:504:ILE:HD12	2.19	0.43
2:F:29:ARG:HB3	2:F:157:PHE:CZ	2.53	0.43
1:E:124:PRO:HB3	1:E:251:PHE:CD2	2.53	0.43
1:E:146:TYR:CE1	1:E:147:CYS:O	2.72	0.43
3:A:44:ARG:HD3	3:A:44:ARG:HA	1.81	0.43
1:B:63:ARG:NH1	1:B:70:THR:N	2.66	0.43
1:E:13:ILE:HG22	3:D:537:LYS:HB3	2.00	0.43
1:B:214:GLU:O	1:B:215:GLU:C	2.57	0.43
1:E:202:PHE:O	1:E:205:TYR:N	2.51	0.43
3:A:379:GLU:OE2	3:A:382:ARG:NH2	2.37	0.43
2:C:23:LYS:HE3	4:C:217:GTP:O1B	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:592:ALA:O	3:A:596:ARG:HB3	2.18	0.43
3:D:450:SER:O	3:D:453:LEU:N	2.51	0.43
3:D:25:ILE:H	3:D:25:ILE:CD1	2.27	0.43
3:A:134:LEU:HD12	3:A:134:LEU:O	2.18	0.43
3:D:559:TRP:CH2	3:D:610:PHE:HB2	2.53	0.43
3:A:229:LEU:O	3:A:229:LEU:HD22	2.17	0.43
3:A:822:ILE:O	3:A:824:ASP:N	2.51	0.43
1:B:278:PRO:O	1:B:281:VAL:HG12	2.18	0.43
3:A:816:THR:HG23	3:A:859:CYS:CB	2.48	0.43
3:A:62:ARG:HH12	3:A:82:ILE:HD13	1.84	0.43
3:D:946:LEU:HD12	3:D:946:LEU:HA	1.57	0.43
1:B:175:TYR:HB2	1:B:182:TYR:CD1	2.53	0.43
2:C:171:ASP:OD1	2:C:174:LEU:N	2.52	0.43
3:D:516:PHE:O	3:D:519:THR:HB	2.19	0.43
3:D:384:SER:CB	3:D:403:PRO:HG2	2.48	0.43
3:A:1007:ASP:OD2	3:A:1009:PRO:HD2	2.18	0.43
2:F:119:LEU:HD23	2:F:146:TYR:HD1	1.84	0.43
3:A:22:LYS:HA	3:A:22:LYS:HD2	1.64	0.43
3:A:503:SER:O	3:A:505:SER:N	2.50	0.43
2:C:53:HIS:HB2	2:C:179:MET:O	2.18	0.43
3:D:217:GLN:HG3	3:D:217:GLN:H	1.70	0.43
3:A:887:ARG:CD	3:A:937:ALA:HB3	2.35	0.43
1:B:98:ALA:CB	1:B:145:GLY:H	2.32	0.43
1:E:158:GLY:O	1:E:159:ASN:HB3	2.18	0.43
3:D:635:GLU:OE1	3:D:697:ARG:HD2	2.19	0.43
3:D:247:ILE:H	3:D:247:ILE:HG13	1.63	0.43
3:A:142:TRP:HZ3	3:A:197:SER:HB3	1.83	0.43
2:C:138:PHE:HA	2:C:141:LYS:HZ1	1.84	0.43
3:D:150:ILE:HG23	3:D:151:SER:N	2.30	0.43
3:A:516:PHE:CE1	3:A:520:VAL:CG2	3.00	0.43
3:D:516:PHE:CE1	3:D:520:VAL:CG2	3.01	0.43
3:A:954:GLU:O	3:A:955:GLU:HG3	2.19	0.43
3:D:778:PRO:O	3:D:781:LEU:HB2	2.19	0.43
3:A:894:LEU:HB3	3:A:941:MET:HE2	2.01	0.43
3:A:904:VAL:CG1	3:A:911:ALA:HA	2.49	0.43
3:A:926:ILE:HG21	3:A:946:LEU:HD13	2.01	0.43
1:E:138:THR:HG22	1:E:151:PHE:CZ	2.53	0.43
3:D:997:PHE:CD1	3:D:1014:HIS:CE1	3.01	0.43
3:A:879:ILE:HA	3:A:882:PHE:CE2	2.53	0.43
3:A:259:MET:C	3:A:261:ARG:N	2.72	0.43
2:F:134:LYS:HG3	2:F:135:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:138:LEU:C	3:A:140:GLN:H	2.20	0.43
3:D:448:THR:O	3:D:449:ASP:C	2.57	0.43
3:A:899:THR:HG23	3:A:903:ASN:HD21	1.81	0.43
3:A:287:PHE:HB2	3:A:329:PHE:CE2	2.54	0.43
3:D:823:PHE:O	3:D:827:PHE:HB3	2.18	0.43
3:A:730:ALA:O	3:A:731:ALA:C	2.57	0.43
3:D:831:LEU:HD13	3:D:848:PHE:CZ	2.54	0.43
3:D:777:VAL:O	3:D:780:LEU:HB2	2.18	0.43
3:D:30:ASN:CB	3:D:47:GLN:NE2	2.79	0.43
2:C:23:LYS:O	2:C:27:VAL:HG13	2.19	0.43
3:D:935:HIS:N	3:D:935:HIS:ND1	2.67	0.43
3:A:962:LEU:HD13	3:A:968:VAL:CB	2.48	0.43
3:D:100:GLU:O	3:D:103:LYS:HB3	2.19	0.43
1:E:278:PRO:O	1:E:281:VAL:HG12	2.18	0.43
3:D:55:GLU:HG2	3:D:56:HIS:H	1.84	0.43
1:B:55:LEU:HD13	1:B:57:TYR:HE2	1.76	0.43
3:A:30:ASN:CB	3:A:47:GLN:NE2	2.80	0.43
1:B:238:PRO:HA	1:B:241:LEU:HD12	1.99	0.43
1:B:350:PRO:HB2	1:B:351:ASP:H	1.61	0.43
2:F:47:VAL:HG11	2:F:64:TRP:CE2	2.54	0.43
1:B:103:LEU:CD1	1:B:268:GLY:HA2	2.49	0.43
3:A:317:ASN:O	3:A:318:PHE:C	2.55	0.43
3:A:186:ILE:HG22	3:A:187:THR:O	2.19	0.43
3:D:625:LEU:HB3	3:D:629:GLN:HB2	2.01	0.43
3:A:802:SER:O	3:A:806:ILE:HG13	2.18	0.43
1:B:173:CYS:SG	1:B:184:VAL:HG22	2.59	0.43
1:B:34:TYR:HB3	1:B:35:SER:H	1.74	0.43
3:A:778:PRO:N	3:A:779:PRO:CD	2.82	0.43
3:A:823:PHE:HA	3:A:823:PHE:HD1	1.72	0.43
1:B:240:SER:O	1:B:242:CYS:N	2.52	0.43
3:A:420:MET:O	3:A:424:MET:HB2	2.19	0.43
3:A:238:LEU:CD2	3:A:242:PHE:HE2	2.27	0.43
3:D:17:LEU:HD23	3:D:22:LYS:HZ2	1.84	0.43
3:A:137:ILE:O	3:A:140:GLN:HB2	2.19	0.43
3:D:306:LEU:C	3:D:308:TYR:N	2.72	0.43
1:B:195:PHE:HA	1:B:198:CYS:SG	2.59	0.43
1:B:7:LYS:HD2	3:A:522:LYS:CG	2.49	0.42
3:A:964:PRO:HB2	3:A:968:VAL:HG11	2.00	0.42
1:E:240:SER:C	1:E:242:CYS:N	2.73	0.42
2:F:156:ASN:HB3	2:F:159:LYS:CG	2.48	0.42
3:D:1007:ASP:OD1	3:D:1010:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:372:TYR:O	3:D:373:TRP:C	2.57	0.42
1:E:155:LEU:HG	1:E:217:LEU:HD11	2.01	0.42
3:A:286:LEU:HD12	3:A:290:THR:HG1	1.84	0.42
3:A:509:HIS:O	3:A:510:GLU:C	2.58	0.42
2:C:64:TRP:HE3	2:C:79:TYR:HB3	1.82	0.42
3:D:875:LEU:O	3:D:876:ASP:C	2.57	0.42
3:A:443:GLU:HA	3:A:443:GLU:OE1	2.19	0.42
3:A:323:SER:O	3:A:327:CYS:HB3	2.19	0.42
3:D:525:LEU:HD12	3:D:525:LEU:HA	1.82	0.42
1:E:1:LEU:HD21	1:E:2:ASN:ND2	2.35	0.42
3:A:66:ILE:HG22	3:A:76:LYS:NZ	2.33	0.42
3:A:27:LEU:HD23	3:A:75:THR:HG23	2.01	0.42
1:B:69:TRP:CD2	1:B:95:LYS:O	2.73	0.42
3:D:575:GLU:O	3:D:581:GLN:HG3	2.19	0.42
3:D:697:ARG:O	3:D:698:ALA:C	2.57	0.42
3:D:841:TYR:O	3:D:842:PRO:C	2.56	0.42
3:D:362:GLU:C	3:D:364:GLU:H	2.22	0.42
3:A:637:VAL:HG12	3:A:641:ILE:CD1	2.49	0.42
3:A:365:ILE:HG22	3:A:366:PHE:N	2.34	0.42
3:D:563:LYS:HE2	3:D:606:GLU:OE2	2.18	0.42
3:D:443:GLU:OE1	3:D:443:GLU:HA	2.19	0.42
3:A:887:ARG:O	3:A:891:ASP:HB2	2.19	0.42
3:A:715:LEU:O	3:A:718:LEU:HB2	2.19	0.42
3:A:195:LYS:O	3:A:197:SER:N	2.53	0.42
3:D:222:VAL:HG11	3:D:254:PHE:HE1	1.84	0.42
2:C:26:PHE:CE1	2:C:30:HIS:CE1	3.07	0.42
1:E:122:VAL:HG11	1:E:249:PHE:CZ	2.54	0.42
3:A:675:ASN:C	3:A:677:ASP:H	2.23	0.42
3:D:938:GLY:O	3:D:939:LEU:C	2.57	0.42
3:D:228:THR:O	3:D:232:PHE:CD2	2.72	0.42
3:D:265:LEU:HD11	3:D:325:PHE:HB2	2.02	0.42
3:D:142:TRP:HH2	3:D:197:SER:C	2.23	0.42
2:F:15:LEU:HD22	2:F:23:LYS:CB	2.49	0.42
3:D:27:LEU:HA	3:D:30:ASN:OD1	2.18	0.42
2:C:35:PHE:CE2	2:C:37:LYS:HG2	2.54	0.42
3:D:914:PHE:CE1	3:D:918:TYR:CD1	3.07	0.42
2:C:73:GLY:HA3	2:C:76:ARG:CZ	2.50	0.42
3:D:470:VAL:O	3:D:474:ILE:HG13	2.18	0.42
3:A:565:VAL:O	3:A:565:VAL:CG1	2.63	0.42
3:A:80:LEU:HD21	3:A:126:TYR:CE1	2.54	0.42
1:E:245:LEU:HD12	1:E:245:LEU:HA	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:55:GLU:CG	3:A:56:HIS:H	2.33	0.42
2:C:84:GLN:O	2:C:168:LEU:HD21	2.19	0.42
3:D:1007:ASP:O	3:D:1010:ALA:HB3	2.20	0.42
1:B:63:ARG:NH1	1:B:70:THR:HB	2.24	0.42
1:E:107:LEU:O	1:E:276:LEU:HD11	2.20	0.42
3:A:579:GLY:C	3:A:581:GLN:N	2.72	0.42
3:D:704:HIS:CD2	3:D:766:SER:HA	2.55	0.42
2:F:75:LEU:HD11	3:D:49:VAL:HG22	2.02	0.42
3:D:962:LEU:HD23	3:D:968:VAL:HG11	2.00	0.42
3:D:279:TYR:O	3:D:283:PHE:HD2	2.02	0.42
3:D:611:ILE:HG23	3:D:612:ASP:N	2.32	0.42
2:C:21:THR:HG21	2:C:89:MET:HB3	2.01	0.42
3:D:422:SER:O	3:D:496:THR:HG21	2.20	0.42
3:D:724:LEU:HD12	3:D:751:VAL:HB	2.00	0.42
1:B:52:SER:O	1:B:53:LYS:C	2.57	0.42
3:A:939:LEU:HD21	3:A:1016:ARG:HH11	1.83	0.42
3:A:80:LEU:HB3	3:A:133:ILE:HD11	2.00	0.42
3:A:272:ALA:HB1	3:A:329:PHE:CD1	2.55	0.42
3:A:862:ALA:O	3:A:865:ALA:N	2.52	0.42
3:D:766:SER:H	3:D:810:LYS:HZ3	1.65	0.42
3:A:785:LEU:HD11	3:A:804:MET:HG2	2.01	0.42
3:A:127:ILE:O	3:A:130:LEU:HB2	2.20	0.42
2:F:47:VAL:O	2:F:47:VAL:HG23	2.18	0.42
3:D:637:VAL:HG12	3:D:641:ILE:CD1	2.50	0.42
3:A:433:VAL:O	3:A:433:VAL:CG1	2.66	0.42
3:A:843:GLU:O	3:A:844:HIS:C	2.57	0.42
3:D:138:LEU:C	3:D:140:GLN:N	2.72	0.42
3:D:430:VAL:HG13	3:D:430:VAL:O	2.20	0.42
3:A:920:CYS:HB3	3:A:977:TYR:HE2	1.84	0.42
3:D:500:ALA:O	3:D:503:SER:OG	2.32	0.42
3:A:222:VAL:HG11	3:A:254:PHE:HE1	1.85	0.42
3:D:1029:ASP:HB3	3:D:1030:THR:H	1.63	0.42
2:C:177:VAL:HG22	2:C:178:ALA:N	2.35	0.42
1:E:3:GLU:O	1:E:7:LYS:HB2	2.20	0.42
3:A:78:TYR:CE2	3:A:82:ILE:HD11	2.54	0.42
3:D:127:ILE:N	3:D:127:ILE:HD12	2.35	0.42
3:D:133:ILE:O	3:D:136:GLN:N	2.52	0.42
1:E:155:LEU:HD11	1:E:228:PHE:CZ	2.55	0.42
2:C:117:ILE:HG12	2:C:118:VAL:N	2.34	0.42
3:A:1038:ARG:HH21	3:A:1042:LEU:CD2	2.33	0.42
3:A:255:LEU:C	3:A:257:VAL:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:401:ASP:O	3:D:403:PRO:HD3	2.20	0.42
3:A:406:ARG:O	3:A:408:LEU:N	2.52	0.42
1:B:96:HIS:HB3	1:B:97:TYR:H	1.65	0.42
3:A:470:VAL:O	3:A:474:ILE:HG13	2.19	0.42
3:A:970:ASN:O	3:A:971:GLN:C	2.58	0.42
1:E:4:LEU:C	1:E:7:LYS:H	2.23	0.42
3:A:102:ILE:O	3:A:103:LYS:C	2.58	0.42
3:A:94:LEU:HB2	3:A:99:CYS:SG	2.60	0.42
3:D:146:TRP:N	3:D:147:PRO:CD	2.82	0.42
2:C:155:TYR:CD1	3:A:445:MET:SD	3.12	0.42
3:D:16:LEU:HB3	3:D:17:LEU:H	1.62	0.42
2:F:132:LYS:O	2:F:133:ALA:C	2.56	0.42
2:C:38:LYS:HA	3:A:842:PRO:CG	2.50	0.42
3:A:716:ASP:O	3:A:717:MET:C	2.58	0.42
1:B:153:SER:N	1:B:158:GLY:O	2.44	0.42
3:D:687:GLN:O	3:D:691:ILE:HB	2.20	0.42
3:D:681:ASP:HA	3:D:682:PRO:HD3	1.95	0.42
3:A:149:PHE:CZ	3:A:153:ILE:HD13	2.54	0.42
3:D:98:GLN:O	3:D:102:ILE:HG13	2.19	0.42
3:A:887:ARG:HA	3:A:887:ARG:HD2	1.79	0.42
1:B:241:LEU:HA	1:B:244:VAL:HG12	2.02	0.42
3:D:953:VAL:O	3:D:955:GLU:N	2.53	0.42
1:B:24:HIS:C	1:B:26:ARG:N	2.72	0.42
3:A:704:HIS:CD2	3:A:766:SER:HA	2.55	0.42
1:E:18:ASN:ND2	1:E:108:ILE:HD11	2.35	0.42
2:C:42:THR:H	4:C:217:GTP:PG	2.43	0.42
3:D:178:VAL:HG12	3:D:178:VAL:O	2.20	0.42
1:E:58:VAL:HA	1:E:194:PRO:CG	2.50	0.42
2:F:146:TYR:CG	2:F:147:TYR:N	2.87	0.42
3:A:850:LEU:O	3:A:853:GLN:HB3	2.20	0.42
3:D:722:LYS:HD3	3:D:783:ALA:HA	2.02	0.42
1:E:93:LEU:HA	1:E:94:PRO:HD3	1.61	0.42
3:A:422:SER:O	3:A:496:THR:HG21	2.20	0.42
3:A:939:LEU:HD12	3:A:939:LEU:HA	1.80	0.42
3:A:125:VAL:O	3:A:126:TYR:C	2.58	0.42
1:E:41:GLU:CG	1:E:109:ASP:HB3	2.38	0.42
1:E:122:VAL:HG12	1:E:122:VAL:O	2.19	0.42
2:F:13:LEU:HD12	2:F:14:VAL:O	2.18	0.42
3:D:926:ILE:HG21	3:D:946:LEU:HD13	2.02	0.42
3:D:695:ASN:HA	3:D:695:ASN:HD22	1.54	0.42
2:C:44:GLY:HA3	3:A:45:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:777:VAL:O	3:A:780:LEU:HB2	2.20	0.42
3:A:1032:ASP:O	3:A:1034:PHE:CE1	2.73	0.42
3:A:306:LEU:C	3:A:308:TYR:N	2.73	0.42
1:B:60:HIS:CD2	1:B:93:LEU:HB3	2.55	0.42
1:B:101:LEU:HD23	1:B:101:LEU:N	2.34	0.42
1:E:48:GLU:HG2	1:E:48:GLU:H	1.55	0.42
3:A:531:LYS:HD3	3:A:531:LYS:HA	1.81	0.42
1:B:8:LEU:O	1:B:8:LEU:HG	2.20	0.41
3:A:91:TRP:CZ3	3:A:102:ILE:HD13	2.55	0.41
1:B:1:LEU:HD22	3:A:514:LYS:CE	2.50	0.41
3:A:334:GLY:O	3:A:337:LEU:N	2.50	0.41
3:D:732:ILE:HA	3:D:739:VAL:HG21	2.02	0.41
1:E:111:PRO:CD	1:E:114:LEU:HD13	2.48	0.41
3:D:729:SER:OG	3:D:792:VAL:HG13	2.20	0.41
3:D:514:LYS:O	3:D:515:ARG:C	2.58	0.41
1:E:10:GLY:HA3	1:E:34:TYR:CE1	2.55	0.41
3:D:707:VAL:CG1	3:D:708:ILE:N	2.83	0.41
3:D:970:ASN:O	3:D:971:GLN:C	2.58	0.41
3:D:287:PHE:HB2	3:D:329:PHE:CE2	2.55	0.41
2:F:28:LYS:O	2:F:29:ARG:C	2.58	0.41
1:E:175:TYR:O	1:E:175:TYR:CD2	2.73	0.41
3:D:168:MET:CE	3:D:171:LEU:HD12	2.49	0.41
3:A:575:GLU:O	3:A:581:GLN:HG3	2.20	0.41
3:D:125:VAL:O	3:D:126:TYR:C	2.58	0.41
3:A:695:ASN:HA	3:A:695:ASN:HD22	1.57	0.41
3:A:165:GLN:HA	3:A:221:LEU:HD13	2.01	0.41
3:A:608:MET:HA	3:A:609:PRO:HD3	1.62	0.41
3:A:255:LEU:HD12	3:A:268:LEU:HD12	2.02	0.41
3:A:262:ASN:OD1	3:A:318:PHE:HA	2.20	0.41
3:A:1029:ASP:O	3:A:1030:THR:C	2.58	0.41
3:A:534:LYS:CE	3:A:577:HIS:HB2	2.48	0.41
3:D:423:ARG:HH11	3:D:423:ARG:HG3	1.86	0.41
3:A:90:ARG:O	3:A:91:TRP:C	2.59	0.41
3:D:329:PHE:CD1	3:D:333:HIS:HD2	2.37	0.41
1:B:105:GLU:O	1:B:106:TRP:C	2.59	0.41
3:D:80:LEU:HD21	3:D:126:TYR:CE1	2.55	0.41
3:D:330:LEU:HB2	3:D:372:TYR:CE1	2.55	0.41
1:B:260:HIS:O	1:B:262:GLN:N	2.53	0.41
3:A:1038:ARG:HH21	3:A:1042:LEU:HD21	1.83	0.41
2:F:98:TYR:CE1	2:F:136:ILE:HG23	2.54	0.41
1:B:111:PRO:CG	1:B:114:LEU:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:964:PRO:HG2	3:D:968:VAL:CG1	2.50	0.41
3:A:607:VAL:HG22	3:A:608:MET:HG2	2.02	0.41
2:C:167:LYS:HD2	2:C:167:LYS:HA	1.92	0.41
3:A:962:LEU:HB2	3:A:973:PHE:HD2	1.85	0.41
3:A:133:ILE:O	3:A:136:GLN:N	2.53	0.41
3:D:347:LEU:HD23	3:D:347:LEU:C	2.41	0.41
3:D:90:ARG:O	3:D:91:TRP:C	2.59	0.41
3:D:91:TRP:CZ3	3:D:102:ILE:HD13	2.55	0.41
1:E:244:VAL:HA	1:E:247:MET:HG3	2.02	0.41
3:D:813:GLY:HA2	3:D:816:THR:OG1	2.21	0.41
3:D:939:LEU:HD21	3:D:1016:ARG:HH11	1.84	0.41
3:D:954:GLU:O	3:D:955:GLU:HG3	2.20	0.41
2:F:132:LYS:O	2:F:134:LYS:N	2.53	0.41
3:D:388:THR:HG21	3:D:402:ILE:HD13	2.02	0.41
3:A:551:TYR:N	3:A:552:PRO:CD	2.83	0.41
2:C:77:ASP:HA	2:C:80:TYR:CE2	2.52	0.41
1:B:244:VAL:HA	1:B:247:MET:HG3	2.03	0.41
1:B:244:VAL:HG13	1:B:245:LEU:CD1	2.40	0.41
3:A:742:GLN:HB2	3:A:743:PRO:HD2	2.03	0.41
1:E:119:ILE:HD13	1:E:119:ILE:H	1.85	0.41
3:D:695:ASN:HD21	3:D:709:GLN:HE21	1.67	0.41
1:B:103:LEU:HD21	1:B:143:LYS:HD3	2.03	0.41
2:F:141:LYS:HD2	2:F:141:LYS:H	1.86	0.41
3:A:244:THR:C	3:A:246:LEU:H	2.24	0.41
3:D:667:SER:O	3:D:671:GLN:HG3	2.21	0.41
3:D:427:PRO:HD3	3:D:499:TRP:CD2	2.55	0.41
1:B:176:ASN:OD1	1:B:179:ASN:N	2.54	0.41
3:A:864:LEU:HD23	3:A:864:LEU:HA	1.81	0.41
3:A:227:GLU:O	3:A:230:LEU:HB3	2.20	0.41
3:D:622:ILE:HD13	3:D:630:VAL:HG23	2.03	0.41
2:C:13:LEU:HD12	2:C:13:LEU:O	2.20	0.41
3:D:1008:ILE:C	3:D:1008:ILE:CD1	2.86	0.41
3:A:626:GLN:HB2	3:A:627:PRO:HD2	2.02	0.41
3:D:552:PRO:O	3:D:553:ARG:C	2.58	0.41
3:A:144:LYS:C	3:A:145:HIS:CD2	2.94	0.41
2:C:141:LYS:H	2:C:141:LYS:HD2	1.85	0.41
3:D:259:MET:C	3:D:261:ARG:N	2.74	0.41
1:E:98:ALA:CB	1:E:145:GLY:H	2.34	0.41
1:E:226:PHE:HZ	3:D:683:GLU:OE1	2.03	0.41
2:F:66:THR:HG22	2:F:67:ALA:H	1.84	0.41
1:E:348:HIS:N	3:D:707:VAL:HG13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430:VAL:HG13	3:A:430:VAL:O	2.20	0.41
3:A:721:TYR:CD2	3:A:784:VAL:HG22	2.56	0.41
2:F:35:PHE:CE2	2:F:37:LYS:HG2	2.55	0.41
3:A:871:PHE:O	3:A:872:LYS:C	2.57	0.41
1:E:245:LEU:HD21	1:E:281:VAL:HG11	2.03	0.41
3:D:631:HIS:CE1	3:D:693:LYS:CB	3.02	0.41
3:A:1015:LEU:HD23	3:A:1015:LEU:HA	1.82	0.41
3:A:1040:THR:HA	3:A:1043:ARG:CG	2.49	0.41
3:D:911:ALA:O	3:D:914:PHE:HB3	2.21	0.41
3:A:594:LYS:HE2	3:A:594:LYS:CA	2.49	0.41
2:C:71:LYS:HE2	3:A:932:ASP:OD1	2.20	0.41
3:D:744:LEU:O	3:D:744:LEU:HD12	2.21	0.41
3:A:949:MET:O	3:A:952:LEU:HB3	2.20	0.41
3:D:823:PHE:HA	3:D:823:PHE:HD1	1.72	0.41
1:B:130:LEU:HD11	1:B:170:ILE:CG2	2.51	0.41
1:E:262:GLN:HE21	1:E:262:GLN:HB2	1.66	0.41
3:D:697:ARG:HG3	3:D:697:ARG:NH2	2.35	0.41
2:F:86:ALA:C	2:F:87:ILE:HG13	2.41	0.41
3:D:997:PHE:HD1	3:D:1014:HIS:NE2	2.18	0.41
3:D:906:GLN:CD	3:D:906:GLN:N	2.72	0.41
3:A:372:TYR:O	3:A:374:ASN:N	2.53	0.41
3:D:93:ILE:CG2	3:D:1027:GLY:HA3	2.51	0.41
3:A:172:LYS:O	3:A:175:SER:HB3	2.20	0.41
3:A:975:GLN:HG3	3:A:998:VAL:HG12	2.03	0.41
3:A:445:MET:HB3	3:A:445:MET:HE2	1.96	0.41
3:A:23:LEU:HD11	3:A:26:ASN:CB	2.46	0.41
3:A:72:ASN:O	3:A:74:ASN:N	2.54	0.41
3:D:1007:ASP:OD2	3:D:1009:PRO:HD2	2.21	0.41
3:A:168:MET:HG3	3:A:225:THR:OG1	2.21	0.41
3:A:421:VAL:HG22	3:A:461:LEU:HD21	2.03	0.41
3:D:552:PRO:HA	3:D:555:LEU:HD12	2.03	0.41
3:D:853:GLN:O	3:D:857:SER:OG	2.36	0.41
3:D:847:ASN:C	3:D:849:PHE:N	2.75	0.41
3:D:850:LEU:O	3:D:853:GLN:HB3	2.21	0.41
2:C:44:GLY:CA	3:A:45:MET:HE3	2.48	0.41
2:F:171:ASP:OD1	2:F:174:LEU:N	2.54	0.41
2:C:106:ARG:O	2:C:110:ARG:HG3	2.20	0.41
3:D:27:LEU:CD2	3:D:75:THR:HG23	2.51	0.41
1:E:154:LEU:HA	1:E:154:LEU:HD23	1.82	0.41
3:D:516:PHE:O	3:D:520:VAL:HG23	2.21	0.41
3:D:161:GLU:O	3:D:164:CYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:198:MET:O	3:D:202:PHE:HB2	2.21	0.41
2:C:66:THR:HG22	2:C:67:ALA:H	1.84	0.41
3:D:983:LYS:HE2	3:D:991:ASP:OD1	2.21	0.41
2:C:146:TYR:CD2	2:C:147:TYR:N	2.89	0.41
3:D:391:SER:HA	3:D:392:PRO:HD3	1.73	0.41
3:D:240:TYR:O	3:D:244:THR:CG2	2.69	0.41
3:A:667:SER:O	3:A:671:GLN:HG3	2.21	0.41
1:E:61:ALA:HB1	1:E:168:TYR:HE1	1.86	0.41
3:D:531:LYS:HD3	3:D:531:LYS:HA	1.84	0.41
1:E:2:ASN:N	1:E:2:ASN:HD22	2.19	0.41
3:A:911:ALA:O	3:A:914:PHE:HB3	2.21	0.41
1:E:122:VAL:HG21	1:E:249:PHE:CZ	2.56	0.41
3:A:746:ARG:CG	3:A:746:ARG:NH1	2.76	0.41
3:D:55:GLU:HG2	3:D:56:HIS:N	2.36	0.41
3:D:14:ARG:NH1	3:D:14:ARG:CG	2.75	0.41
1:B:48:GLU:C	1:B:50:GLN:N	2.73	0.41
1:B:25:PRO:HG2	1:B:108:ILE:HD13	2.03	0.41
3:D:247:ILE:HG21	3:D:286:LEU:HB2	2.03	0.41
1:E:63:ARG:NH1	1:E:72:MET:CB	2.81	0.41
3:A:164:CYS:O	3:A:165:GLN:C	2.59	0.41
3:D:615:LEU:HA	3:D:618:ILE:CG1	2.51	0.41
3:D:165:GLN:HA	3:D:221:LEU:HD13	2.03	0.41
3:A:247:ILE:HG13	3:A:247:ILE:H	1.59	0.41
2:F:35:PHE:HE2	2:F:37:LYS:HG2	1.86	0.41
1:B:355:CYS:O	1:B:356:LEU:CB	2.69	0.41
3:D:229:LEU:O	3:D:233:LEU:HG	2.21	0.41
3:A:660:LEU:HB2	3:A:661:PRO:HD3	2.03	0.41
3:A:583:MET:C	3:A:583:MET:SD	3.00	0.41
2:C:9:VAL:HG22	2:C:58:PRO:O	2.21	0.41
3:A:970:ASN:O	3:A:973:PHE:HB3	2.21	0.40
3:D:287:PHE:HZ	3:D:350:ALA:CB	2.34	0.40
3:D:149:PHE:CZ	3:D:153:ILE:HD13	2.56	0.40
1:E:255:GLY:O	1:E:256:LEU:HD23	2.20	0.40
3:A:347:LEU:O	3:A:351:LEU:HB2	2.20	0.40
2:F:156:ASN:ND2	2:F:159:LYS:HE3	2.36	0.40
3:D:588:PHE:CE2	3:D:636:ALA:HB1	2.56	0.40
3:D:839:GLU:O	3:D:840:GLU:C	2.59	0.40
1:E:13:ILE:HD12	1:E:13:ILE:HG21	1.85	0.40
3:D:268:LEU:O	3:D:269:THR:C	2.59	0.40
1:E:63:ARG:NH1	1:E:70:THR:H	2.19	0.40
3:A:138:LEU:C	3:A:140:GLN:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:948:TYR:CE1	3:D:952:LEU:HD12	2.56	0.40
1:E:216:GLY:O	1:E:219:GLU:N	2.54	0.40
1:B:208:HIS:N	1:B:208:HIS:CD2	2.90	0.40
1:E:169:THR:HG22	1:E:171:LEU:HD21	2.02	0.40
1:E:208:HIS:CD2	1:E:208:HIS:N	2.90	0.40
3:D:855:VAL:O	3:D:859:CYS:HB2	2.21	0.40
3:D:672:ALA:O	3:D:676:VAL:HG22	2.22	0.40
1:B:240:SER:C	1:B:242:CYS:N	2.75	0.40
1:B:241:LEU:C	1:B:244:VAL:HG12	2.42	0.40
3:D:938:GLY:O	3:D:940:THR:N	2.54	0.40
1:B:105:GLU:O	1:B:274:GLY:HA2	2.20	0.40
3:A:219:ALA:HB3	3:A:220:PRO:CD	2.41	0.40
3:D:127:ILE:O	3:D:130:LEU:HB2	2.21	0.40
1:E:102:MET:SD	1:E:265:TYR:HA	2.61	0.40
2:F:75:LEU:CD1	3:D:49:VAL:HG22	2.51	0.40
3:A:130:LEU:O	3:A:131:ASN:C	2.59	0.40
3:A:997:PHE:CD1	3:A:1014:HIS:CE1	3.05	0.40
3:D:594:LYS:CA	3:D:594:LYS:HE2	2.50	0.40
3:D:1013:GLU:OE1	3:D:1013:GLU:HA	2.14	0.40
3:D:786:ILE:O	3:D:789:GLN:HB3	2.21	0.40
3:A:326:LEU:HA	3:A:326:LEU:HD23	1.89	0.40
1:B:7:LYS:HD2	3:A:522:LYS:HG3	2.04	0.40
3:A:287:PHE:HZ	3:A:350:ALA:CB	2.35	0.40
2:C:13:LEU:HD12	2:C:14:VAL:C	2.42	0.40
1:B:257:LEU:CD1	1:B:275:TRP:HB2	2.52	0.40
3:D:164:CYS:O	3:D:165:GLN:C	2.59	0.40
2:F:164:LEU:HA	2:F:164:LEU:HD23	1.91	0.40
2:C:37:LYS:HA	4:C:217:GTP:O2'	2.21	0.40
2:F:138:PHE:HA	2:F:141:LYS:HZ2	1.86	0.40
3:D:227:GLU:HG2	3:D:263:VAL:HG13	2.03	0.40
3:D:402:ILE:HG12	3:D:402:ILE:H	1.56	0.40
3:D:328:THR:HG23	3:D:331:LYS:NZ	2.35	0.40
3:A:973:PHE:O	3:A:976:ASP:CB	2.69	0.40
3:D:94:LEU:HB2	3:D:99:CYS:SG	2.62	0.40
3:A:672:ALA:O	3:A:676:VAL:HG22	2.22	0.40
3:A:55:GLU:HG2	3:A:56:HIS:H	1.86	0.40
3:D:219:ALA:HB3	3:D:220:PRO:CD	2.41	0.40
3:D:704:HIS:CD2	3:D:766:SER:CB	3.00	0.40
3:D:251:ILE:HG22	3:D:293:GLN:HG3	2.04	0.40
2:F:135:SER:O	2:F:137:VAL:HG22	2.21	0.40
2:C:38:LYS:HA	3:A:842:PRO:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:660:LEU:O	3:A:661:PRO:C	2.57	0.40
3:D:102:ILE:HG13	3:D:102:ILE:H	1.60	0.40
2:F:92:VAL:HG23	2:F:129:ARG:HG3	2.03	0.40
3:A:437:GLN:HB2	3:A:439:GLU:HG3	2.02	0.40
3:D:1008:ILE:O	3:D:1012:LYS:HB2	2.21	0.40
3:A:729:SER:O	3:A:730:ALA:C	2.59	0.40
1:E:107:LEU:HB2	1:E:274:GLY:CA	2.47	0.40
1:B:24:HIS:HA	1:B:25:PRO:HD3	1.97	0.40
3:D:15:GLN:O	3:D:16:LEU:HD12	2.21	0.40
1:B:260:HIS:CE1	1:B:262:GLN:CG	3.00	0.40
2:C:16:VAL:HG23	2:C:88:ILE:HA	2.03	0.40
3:D:736:GLY:O	3:D:737:GLU:C	2.60	0.40
3:D:27:LEU:HD23	3:D:75:THR:HG23	2.04	0.40
3:A:997:PHE:HD1	3:A:1014:HIS:NE2	2.19	0.40
3:D:383:GLU:OE2	3:D:405:ARG:HG3	2.21	0.40
3:D:407:GLN:HB3	3:D:407:GLN:HE21	1.66	0.40
1:B:254:ASP:O	1:B:277:ARG:NE	2.49	0.40
3:A:255:LEU:HD23	3:A:255:LEU:O	2.21	0.40
1:B:51:LYS:HZ1	1:B:264:HIS:N	2.19	0.40
3:A:958:ILE:HG13	3:A:958:ILE:O	2.21	0.40
3:A:232:PHE:HD2	3:A:232:PHE:HA	1.71	0.40
3:D:745:ILE:HA	3:D:745:ILE:HD13	1.83	0.40
3:D:1043:ARG:HA	3:D:1043:ARG:HD2	1.72	0.40
3:A:745:ILE:HD13	3:A:745:ILE:HA	1.84	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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	262/361 (73%)	206 (79%)	38 (14%)	18 (7%)	1 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	267/361 (74%)	211 (79%)	39 (15%)	17 (6%)	2	18
2	C	169/176 (96%)	139 (82%)	23 (14%)	7 (4%)	3	32
2	F	169/176 (96%)	138 (82%)	24 (14%)	7 (4%)	3	32
3	A	1037/1073 (97%)	760 (73%)	206 (20%)	71 (7%)	1	17
3	D	1037/1073 (97%)	755 (73%)	220 (21%)	62 (6%)	2	20
All	All	2941/3220 (91%)	2209 (75%)	550 (19%)	182 (6%)	2	19

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	B	145	GLY
1	B	180	GLN
1	B	217	LEU
2	C	76	ARG
3	A	55	GLU
3	A	114	SER
3	A	123	GLU
3	A	127	ILE
3	A	200	ASN
3	A	326	LEU
3	A	397	SER
3	A	433	VAL
3	A	450	SER
3	A	468	ASP
3	A	486	GLY
3	A	939	LEU
3	A	963	ASN
3	A	1028	GLU
1	E	39	GLN
1	E	145	GLY
1	E	180	GLN
1	E	217	LEU
2	F	76	ARG
3	D	42	GLN
3	D	55	GLU
3	D	123	GLU
3	D	127	ILE
3	D	200	ASN
3	D	326	LEU

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Mol	Chain	Res	Type
3	D	363	THR
3	D	392	PRO
3	D	435	ASN
3	D	450	SER
3	D	468	ASP
3	D	627	PRO
3	D	848	PHE
3	D	939	LEU
3	D	963	ASN
3	D	1029	ASP
3	D	1035	LEU
3	D	1036	GLU
1	B	53	LYS
2	C	32	THR
2	C	87	ILE
3	A	115	SER
3	A	118	THR
3	A	125	VAL
3	A	269	THR
3	A	277	SER
3	A	297	MET
3	A	307	ALA
3	A	388	THR
3	A	435	ASN
3	A	504	ILE
3	A	627	PRO
3	A	674	LYS
3	A	730	ALA
3	A	743	PRO
3	A	769	PRO
3	A	823	PHE
3	A	843	GLU
3	A	848	PHE
3	A	1027	GLY
3	A	1037	GLU
1	E	25	PRO
1	E	51	LYS
1	E	159	ASN
3	D	269	THR
3	D	297	MET
3	D	307	ALA
3	D	486	GLY

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Mol	Chain	Res	Type
3	D	504	ILE
3	D	712	ARG
3	D	737	GLU
3	D	769	PRO
3	D	965	GLY
1	B	10	GLY
1	B	25	PRO
1	B	156	PRO
1	B	261	LYS
1	B	350	PRO
2	C	65	ASP
2	C	106	ARG
3	A	13	ALA
3	A	64	ASP
3	A	122	LYS
3	A	143	PRO
3	A	149	PHE
3	A	362	GLU
3	A	363	THR
3	A	530	GLN
3	A	712	ARG
3	A	737	GLU
3	A	781	LEU
3	A	954	GLU
1	E	53	LYS
1	E	156	PRO
2	F	32	THR
2	F	106	ARG
3	D	64	ASP
3	D	125	VAL
3	D	143	PRO
3	D	530	GLN
3	D	730	ALA
3	D	743	PRO
3	D	823	PHE
3	D	843	GLU
3	D	954	GLU
1	B	49	LEU
1	B	240	SER
3	A	124	LYS
3	A	246	LEU
3	A	268	LEU

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Mol	Chain	Res	Type
3	A	392	PRO
3	A	679	LEU
3	A	961	PRO
1	E	191	ARG
1	E	240	SER
1	E	242	CYS
1	E	261	LYS
2	F	87	ILE
3	D	21	GLN
3	D	65	THR
3	D	77	TYR
3	D	122	LYS
3	D	149	PHE
3	D	196	ASP
3	D	217	GLN
3	D	246	LEU
3	D	268	LEU
3	D	362	GLU
3	D	679	LEU
3	D	781	LEU
3	D	820	PRO
1	B	241	LEU
1	B	242	CYS
1	B	356	LEU
1	B	358	GLU
2	C	85	CYS
3	A	21	GLN
3	A	65	THR
3	A	77	TYR
3	A	91	TRP
3	A	341	LEU
3	A	510	GLU
3	A	807	ILE
3	A	820	PRO
3	A	899	THR
3	A	971	GLN
3	A	1005	ASN
1	E	18	ASN
2	F	85	CYS
3	D	91	TRP
3	D	341	LEU
3	D	510	GLU

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Mol	Chain	Res	Type
3	D	899	THR
3	D	1037	GLU
1	B	18	ASN
1	B	267	PRO
3	A	482	ASN
1	E	241	LEU
1	E	267	PRO
2	F	65	ASP
3	D	235	TRP
3	D	335	GLN
3	A	258	PRO
3	A	484	VAL
3	A	540	ILE
3	D	807	ILE
3	D	961	PRO
3	D	1027	GLY
1	E	284	VAL
3	D	258	PRO
3	D	540	ILE
3	D	451	ILE
3	A	146	TRP
2	F	137	VAL
2	C	137	VAL
3	A	31	VAL
3	A	451	ILE
3	A	676	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	244/323 (76%)	199 (82%)	45 (18%)	2	10
1	E	247/323 (76%)	210 (85%)	37 (15%)	3	20
2	C	150/154 (97%)	129 (86%)	21 (14%)	4	23
2	F	150/154 (97%)	125 (83%)	25 (17%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	945/973 (97%)	838 (89%)	107 (11%)	7	33
3	D	945/973 (97%)	831 (88%)	114 (12%)	6	29
All	All	2681/2900 (92%)	2332 (87%)	349 (13%)	5	26

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	SER
1	B	1	LEU
1	B	6	LEU
1	B	7	LYS
1	B	13	ILE
1	B	39	GLN
1	B	46	LEU
1	B	53	LYS
1	B	54	ARG
1	B	55	LEU
1	B	70	THR
1	B	92	LYS
1	B	95	LYS
1	B	108	ILE
1	B	109	ASP
1	B	110	VAL
1	B	112	SER
1	B	119	ILE
1	B	123	CYS
1	B	139	SER
1	B	149	ASN
1	B	151	PHE
1	B	160	ARG
1	B	171	LEU
1	B	174	ILE
1	B	188	MET
1	B	198	CYS
1	B	201	ASP
1	B	215	GLU
1	B	222	LYS
1	B	234	PHE
1	B	241	LEU
1	B	245	LEU
1	B	246	SER

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Mol	Chain	Res	Type
1	B	257	LEU
1	B	262	GLN
1	B	269	SER
1	B	275	TRP
1	B	276	LEU
1	B	282	SER
1	B	283	ASP
1	B	352	HIS
1	B	355	CYS
1	B	356	LEU
1	B	357	MET
2	C	13	LEU
2	C	27	VAL
2	C	29	ARG
2	C	30	HIS
2	C	32	THR
2	C	51	VAL
2	C	75	LEU
2	C	76	ARG
2	C	77	ASP
2	C	88	ILE
2	C	95	ARG
2	C	97	THR
2	C	108	LEU
2	C	112	CYS
2	C	117	ILE
2	C	130	LYS
2	C	137	VAL
2	C	141	LYS
2	C	144	LEU
2	C	148	ASP
2	C	173	ASN
3	A	18	ASP
3	A	23	LEU
3	A	29	ASP
3	A	30	ASN
3	A	34	CYS
3	A	35	LEU
3	A	45	MET
3	A	60	TRP
3	A	66	ILE
3	A	73	MET

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Mol	Chain	Res	Type
3	A	80	LEU
3	A	109	LEU
3	A	146	TRP
3	A	148	THR
3	A	159	THR
3	A	160	SER
3	A	189	VAL
3	A	196	ASP
3	A	199	CYS
3	A	205	ILE
3	A	228	THR
3	A	229	LEU
3	A	231	ARG
3	A	232	PHE
3	A	263	VAL
3	A	265	LEU
3	A	277	SER
3	A	285	THR
3	A	286	LEU
3	A	294	LEU
3	A	313	ASP
3	A	314	ASP
3	A	323	SER
3	A	327	CYS
3	A	331	LYS
3	A	335	GLN
3	A	337	LEU
3	A	353	TYR
3	A	365	ILE
3	A	374	ASN
3	A	387	SER
3	A	388	THR
3	A	391	SER
3	A	393	LEU
3	A	398	GLN
3	A	406	ARG
3	A	422	SER
3	A	426	LYS
3	A	430	VAL
3	A	433	VAL
3	A	440	VAL
3	A	443	GLU

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Mol	Chain	Res	Type
3	A	444	PHE
3	A	452	ASN
3	A	460	THR
3	A	487	THR
3	A	490	SER
3	A	515	ARG
3	A	525	LEU
3	A	539	ILE
3	A	569	LEU
3	A	578	ASP
3	A	597	ARG
3	A	606	GLU
3	A	607	VAL
3	A	613	GLU
3	A	617	ASN
3	A	659	LEU
3	A	662	ASN
3	A	684	THR
3	A	691	ILE
3	A	695	ASN
3	A	708	ILE
3	A	720	VAL
3	A	746	ARG
3	A	747	SER
3	A	749	ARG
3	A	771	MET
3	A	781	LEU
3	A	804	MET
3	A	816	THR
3	A	823	PHE
3	A	852	LEU
3	A	855	VAL
3	A	872	LYS
3	A	885	THR
3	A	887	ARG
3	A	907	GLU
3	A	916	GLN
3	A	920	CYS
3	A	928	SER
3	A	935	HIS
3	A	940	THR
3	A	946	LEU

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Mol	Chain	Res	Type
3	A	948	TYR
3	A	962	LEU
3	A	969	ASN
3	A	970	ASN
3	A	973	PHE
3	A	976	ASP
3	A	988	HIS
3	A	1008	ILE
3	A	1013	GLU
3	A	1020	VAL
3	A	1032	ASP
3	A	1033	LEU
3	A	1053	GLN
1	E	1	LEU
1	E	4	LEU
1	E	8	LEU
1	E	13	ILE
1	E	14	SER
1	E	27	LEU
1	E	33	LYS
1	E	39	GLN
1	E	45	ARG
1	E	49	LEU
1	E	108	ILE
1	E	109	ASP
1	E	110	VAL
1	E	112	SER
1	E	119	ILE
1	E	123	CYS
1	E	139	SER
1	E	149	ASN
1	E	151	PHE
1	E	160	ARG
1	E	171	LEU
1	E	188	MET
1	E	198	CYS
1	E	201	ASP
1	E	209	SER
1	E	234	PHE
1	E	241	LEU
1	E	245	LEU
1	E	246	SER

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Mol	Chain	Res	Type
1	E	257	LEU
1	E	262	GLN
1	E	269	SER
1	E	275	TRP
1	E	276	LEU
1	E	282	SER
1	E	283	ASP
1	E	351	ASP
2	F	9	VAL
2	F	13	LEU
2	F	27	VAL
2	F	29	ARG
2	F	30	HIS
2	F	31	LEU
2	F	32	THR
2	F	38	LYS
2	F	43	LEU
2	F	51	VAL
2	F	75	LEU
2	F	76	ARG
2	F	77	ASP
2	F	88	ILE
2	F	95	ARG
2	F	97	THR
2	F	108	LEU
2	F	112	CYS
2	F	117	ILE
2	F	130	LYS
2	F	134	LYS
2	F	137	VAL
2	F	141	LYS
2	F	148	ASP
2	F	173	ASN
3	D	14	ARG
3	D	19	PHE
3	D	21	GLN
3	D	23	LEU
3	D	29	ASP
3	D	30	ASN
3	D	34	CYS
3	D	35	LEU
3	D	37	HIS

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Mol	Chain	Res	Type
3	D	45	MET
3	D	58	ASP
3	D	60	TRP
3	D	66	ILE
3	D	70	SER
3	D	73	MET
3	D	80	LEU
3	D	109	LEU
3	D	112	LYS
3	D	113	THR
3	D	118	THR
3	D	119	CYS
3	D	146	TRP
3	D	148	THR
3	D	159	THR
3	D	160	SER
3	D	189	VAL
3	D	199	CYS
3	D	205	ILE
3	D	210	GLN
3	D	229	LEU
3	D	231	ARG
3	D	263	VAL
3	D	265	LEU
3	D	277	SER
3	D	286	LEU
3	D	294	LEU
3	D	313	ASP
3	D	314	ASP
3	D	323	SER
3	D	327	CYS
3	D	331	LYS
3	D	335	GLN
3	D	336	LEU
3	D	337	LEU
3	D	353	TYR
3	D	365	ILE
3	D	374	ASN
3	D	387	SER
3	D	389	SER
3	D	393	LEU
3	D	395	SER

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Mol	Chain	Res	Type
3	D	401	ASP
3	D	402	ILE
3	D	406	ARG
3	D	422	SER
3	D	426	LYS
3	D	430	VAL
3	D	433	VAL
3	D	437	GLN
3	D	443	GLU
3	D	444	PHE
3	D	452	ASN
3	D	460	THR
3	D	485	ASN
3	D	490	SER
3	D	515	ARG
3	D	525	LEU
3	D	539	ILE
3	D	569	LEU
3	D	578	ASP
3	D	606	GLU
3	D	607	VAL
3	D	613	GLU
3	D	617	ASN
3	D	659	LEU
3	D	662	ASN
3	D	684	THR
3	D	691	ILE
3	D	695	ASN
3	D	708	ILE
3	D	720	VAL
3	D	739	VAL
3	D	743	PRO
3	D	746	ARG
3	D	747	SER
3	D	749	ARG
3	D	771	MET
3	D	781	LEU
3	D	804	MET
3	D	823	PHE
3	D	852	LEU
3	D	855	VAL
3	D	857	SER

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Mol	Chain	Res	Type
3	D	872	LYS
3	D	885	THR
3	D	887	ARG
3	D	907	GLU
3	D	916	GLN
3	D	928	SER
3	D	935	HIS
3	D	940	THR
3	D	946	LEU
3	D	948	TYR
3	D	970	ASN
3	D	973	PHE
3	D	976	ASP
3	D	988	HIS
3	D	1008	ILE
3	D	1013	GLU
3	D	1020	VAL
3	D	1030	THR
3	D	1031	SER
3	D	1050	HIS
3	D	1053	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	50	GLN
1	B	60	HIS
1	B	149	ASN
1	B	180	GLN
1	B	199	GLN
1	B	208	HIS
1	B	262	GLN
2	C	30	HIS
2	C	103	ASN
2	C	156	ASN
3	A	26	ASN
3	A	30	ASN
3	A	47	GLN
3	A	98	GLN
3	A	131	ASN
3	A	204	GLN

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Mol	Chain	Res	Type
3	A	317	ASN
3	A	321	ASN
3	A	333	HIS
3	A	335	GLN
3	A	374	ASN
3	A	399	HIS
3	A	407	GLN
3	A	437	GLN
3	A	543	ASN
3	A	574	HIS
3	A	617	ASN
3	A	626	GLN
3	A	628	GLN
3	A	631	HIS
3	A	650	GLN
3	A	695	ASN
3	A	704	HIS
3	A	719	ASN
3	A	727	ASN
3	A	742	GLN
3	A	767	ASN
3	A	775	ASN
3	A	853	GLN
3	A	858	HIS
3	A	888	ASN
3	A	903	ASN
3	A	906	GLN
3	A	916	GLN
3	A	924	GLN
3	A	963	ASN
3	A	970	ASN
3	A	988	HIS
3	A	993	GLN
3	A	1006	GLN
3	A	1046	GLN
1	E	2	ASN
1	E	18	ASN
1	E	60	HIS
1	E	149	ASN
1	E	199	GLN
1	E	208	HIS
1	E	260	HIS

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Mol	Chain	Res	Type
1	E	262	GLN
2	F	103	ASN
2	F	156	ASN
3	D	26	ASN
3	D	30	ASN
3	D	43	GLN
3	D	47	GLN
3	D	98	GLN
3	D	131	ASN
3	D	145	HIS
3	D	204	GLN
3	D	210	GLN
3	D	223	HIS
3	D	317	ASN
3	D	321	ASN
3	D	333	HIS
3	D	335	GLN
3	D	407	GLN
3	D	437	GLN
3	D	483	GLN
3	D	574	HIS
3	D	617	ASN
3	D	626	GLN
3	D	628	GLN
3	D	631	HIS
3	D	695	ASN
3	D	704	HIS
3	D	742	GLN
3	D	767	ASN
3	D	775	ASN
3	D	853	GLN
3	D	858	HIS
3	D	888	ASN
3	D	903	ASN
3	D	906	GLN
3	D	916	GLN
3	D	924	GLN
3	D	970	ASN
3	D	988	HIS
3	D	993	GLN
3	D	1006	GLN
3	D	1021	GLN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	GTP	C	217	5	25,34,34	0.98	1 (4%)	34,54,54	2.28	10 (29%)
4	GTP	F	217	5	25,34,34	0.96	1 (4%)	34,54,54	2.09	9 (26%)

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
4	GTP	C	217	5	-	0/18/38/38	0/3/3/3
4	GTP	F	217	5	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	217	GTP	C6-N1	2.77	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	217	GTP	C6-N1	2.82	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	217	GTP	PA-O3A-PB	-5.74	116.60	132.73
4	C	217	GTP	PA-O3A-PB	-5.27	117.93	132.73
4	C	217	GTP	C4-C5-N7	-5.05	104.83	109.48
4	F	217	GTP	N3-C2-N1	-4.75	120.22	127.44
4	C	217	GTP	N3-C2-N1	-4.43	120.69	127.44
4	C	217	GTP	C5-C6-N1	-4.08	118.00	123.59
4	F	217	GTP	C1'-N9-C4	-3.75	121.29	126.94
4	F	217	GTP	PB-O3B-PG	-3.68	120.32	132.67
4	F	217	GTP	C5-C6-N1	-3.29	119.09	123.59
4	C	217	GTP	O4'-C1'-N9	-2.94	101.95	108.10
4	C	217	GTP	O2'-C2'-C3'	-2.80	102.73	111.83
4	F	217	GTP	C4-C5-N7	-2.50	107.18	109.48
4	C	217	GTP	PB-O3B-PG	-2.08	125.70	132.67
4	F	217	GTP	C4'-O4'-C1'	-2.07	107.44	109.72
4	C	217	GTP	C4'-O4'-C1'	2.06	111.98	109.72
4	F	217	GTP	N2-C2-N1	2.07	120.63	117.20
4	C	217	GTP	C6-N1-C2	2.81	119.84	115.94
4	F	217	GTP	C6-N1-C2	3.14	120.30	115.94
4	C	217	GTP	C2'-C1'-N9	5.22	122.27	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	217	GTP	8	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	272/361 (75%)	0.01	6 (2%) 65 60	7, 30, 72, 91	4 (1%)
1	E	277/361 (76%)	0.05	8 (2%) 55 49	7, 30, 80, 111	7 (2%)
2	C	171/176 (97%)	-0.12	0 100 100	10, 28, 58, 84	1 (0%)
2	F	171/176 (97%)	-0.23	0 100 100	10, 27, 56, 80	0
3	A	1041/1073 (97%)	0.01	20 (1%) 70 64	4, 35, 90, 141	6 (0%)
3	D	1041/1073 (97%)	0.03	30 (2%) 55 49	5, 35, 89, 147	13 (1%)
All	All	2973/3220 (92%)	-0.00	64 (2%) 65 60	4, 32, 85, 147	31 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	70	SER	8.8
3	A	967	PRO	8.7
3	A	966	ASN	7.7
3	D	966	ASN	5.3
3	D	397	SER	5.1
3	D	965	GLY	4.5
1	E	352	HIS	4.4
3	D	71	GLN	4.2
3	D	1052	LEU	4.1
3	D	154	VAL	3.9
3	A	339	LYS	3.8
3	D	1032	ASP	3.7
1	E	45	ARG	3.7
3	A	391	SER	3.6
3	D	398	GLN	3.5
1	E	34	TYR	3.5
1	B	3	GLU	3.2
3	D	1026	ALA	3.1
3	D	155	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	332	GLU	3.0
3	A	397	SER	3.0
3	A	296	GLN	3.0
3	D	62	ARG	3.0
3	A	400	PHE	3.0
3	A	395	SER	2.9
3	D	395	SER	2.8
3	A	964	PRO	2.8
1	E	2	ASN	2.8
3	D	158	ARG	2.8
3	A	120	VAL	2.7
1	B	349	SER	2.7
3	D	1027	GLY	2.7
3	D	312	LYS	2.6
3	A	37	HIS	2.6
3	D	967	PRO	2.6
3	D	1021	GLN	2.6
3	D	487	THR	2.5
3	A	114	SER	2.5
1	E	3	GLU	2.5
3	D	119	CYS	2.5
3	D	980	ASN	2.4
3	D	56	HIS	2.4
3	A	200	ASN	2.3
1	E	6	LEU	2.3
3	A	64	ASP	2.3
3	D	203	SER	2.3
3	A	396	GLY	2.3
1	B	35	SER	2.3
1	E	53	LYS	2.3
3	D	33	ASN	2.2
3	A	62	ARG	2.2
3	D	60	TRP	2.2
3	A	160	SER	2.2
1	E	193	HIS	2.1
3	D	976	ASP	2.1
1	B	348	HIS	2.1
3	D	969	ASN	2.1
3	A	912	GLN	2.1
3	D	204	GLN	2.1
3	D	115	SER	2.0
3	A	97	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	D	1053	GLN	2.0
1	B	12	ASP	2.0
1	B	34	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GTP	C	217	32/32	0.94	0.19	-0.50	10,21,47,63	0
5	MG	C	218	1/1	0.96	0.19	-0.57	0,0,0,0	0
4	GTP	F	217	32/32	0.96	0.17	-0.71	7,18,30,35	0
5	MG	F	218	1/1	0.96	0.13	-2.05	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.