Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 09:15 PM EDT

PDB ID	:	1WDW
Title	:	Structural basis of mutual activation of the tryptophan synthase a2b2 complex from a hyperthermophile, Pyrococcus furiosus
Authors	:	Lee, S.J.; Ogasahara, K.; Ma, J.; Nishio, K.; Ishida, M.; Yamagata, Y.; Tsukihara, T.; Yutani, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-19
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

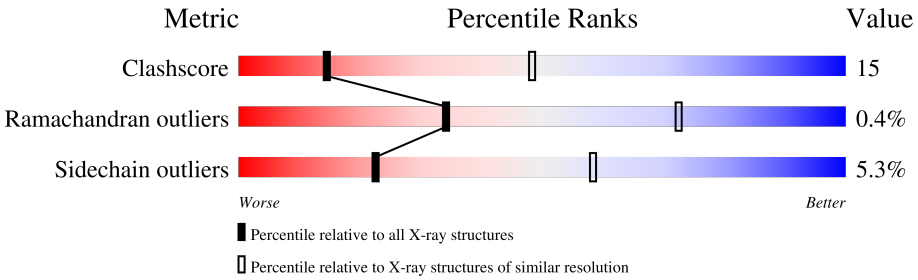
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	68% 28% • •
1	C	248	69% 27% • •
1	E	248	71% 27% •
1	G	248	71% 25% • •
1	I	248	70% 27% • •
1	K	248	68% 26% • 6%
2	B	385	70% 26% •
2	D	385	68% 28% •

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Mol	Chain	Length	Quality of chain
2	F	385	70% 26%
2	H	385	69% 28%
2	J	385	70% 27%
2	L	385	68% 30%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29563 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.

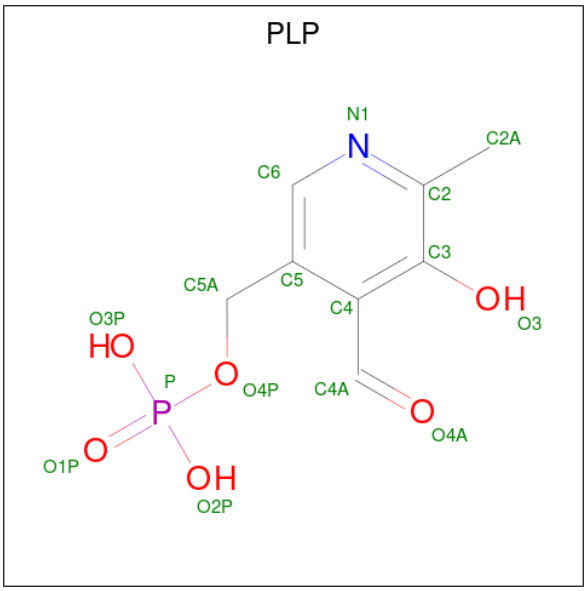
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1895	1224	321	346	4			
1	C	241	Total	C	N	O	S	0	0	0
			1895	1225	321	345	4			
1	E	248	Total	C	N	O	S	0	0	0
			1942	1251	331	356	4			
1	G	242	Total	C	N	O	S	0	0	0
			1904	1230	322	348	4			
1	I	244	Total	C	N	O	S	0	0	0
			1919	1238	327	350	4			
1	K	234	Total	C	N	O	S	0	0	0
			1835	1184	313	334	4			

- Molecule 2 is a protein called Tryptophan synthase beta chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	D	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	F	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	H	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	J	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			
2	L	385	Total	C	N	O	S	0	0	0
			2977	1902	512	551	12			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 15 8 1 5 1	0	0
3	D	1	Total C N O P 15 8 1 5 1	0	0
3	F	1	Total C N O P 15 8 1 5 1	0	0
3	H	1	Total C N O P 15 8 1 5 1	0	0
3	J	1	Total C N O P 15 8 1 5 1	0	0
3	L	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	23	Total O 23 23	0	0
4	C	2	Total O 2 2	0	0
4	D	23	Total O 23 23	0	0
4	E	4	Total O 4 4	0	0
4	F	33	Total O 33 33	0	0
4	G	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	36	Total O 36 36	0	0
4	I	13	Total O 13 13	0	0
4	J	43	Total O 43 43	0	0
4	L	35	Total O 35 35	0	0

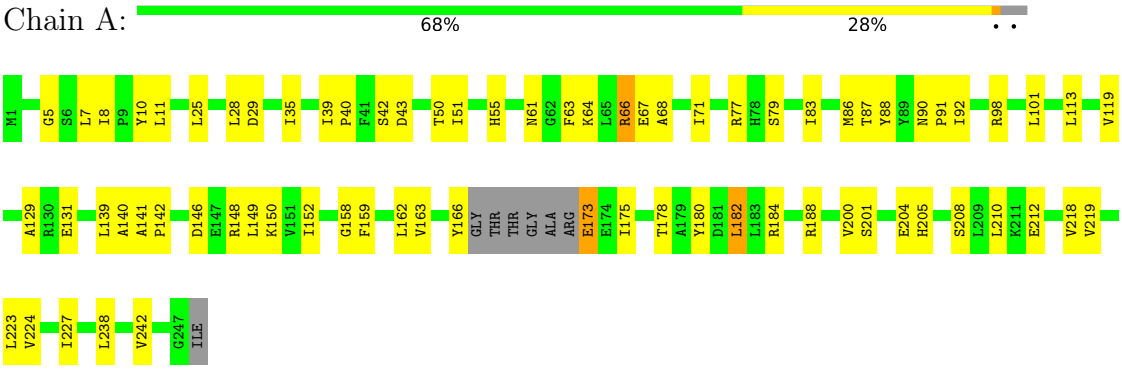
3 Residue-property plots (i)

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

Note EDS was not executed.

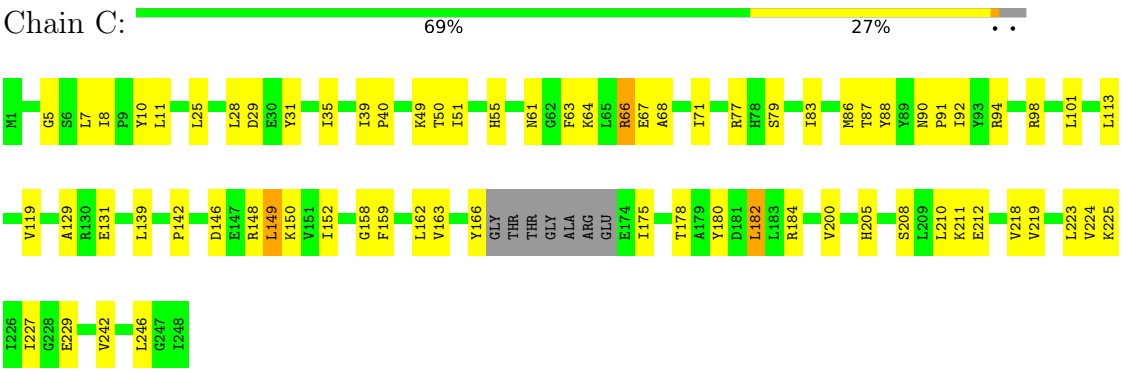
• Molecule 1: Tryptophan synthase alpha chain

Chain A:



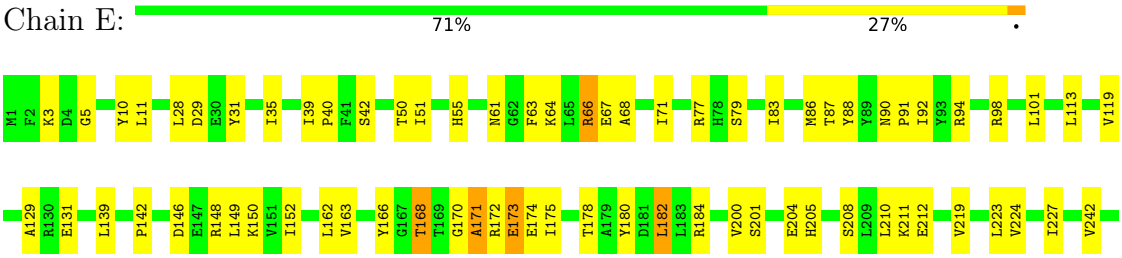
• Molecule 1: Tryptophan synthase alpha chain

Chain C:



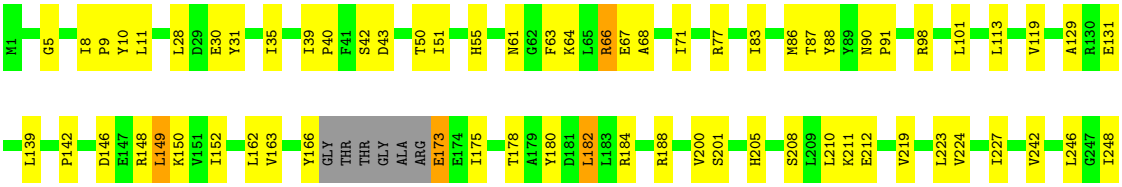
• Molecule 1: Tryptophan synthase alpha chain

Chain E:



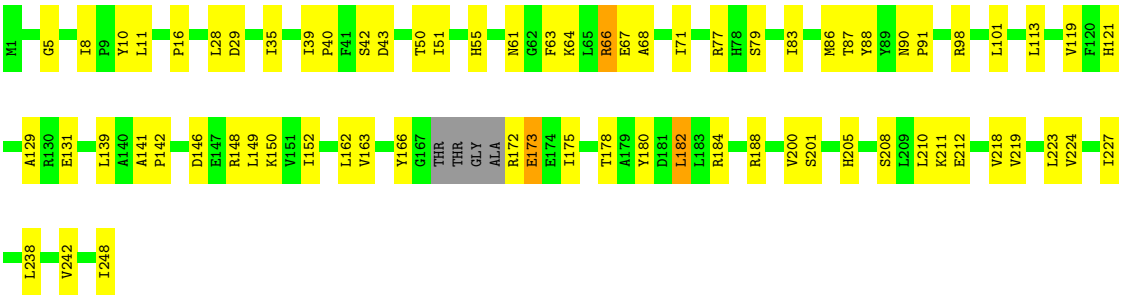
• Molecule 1: Tryptophan synthase alpha chain

Chain G:



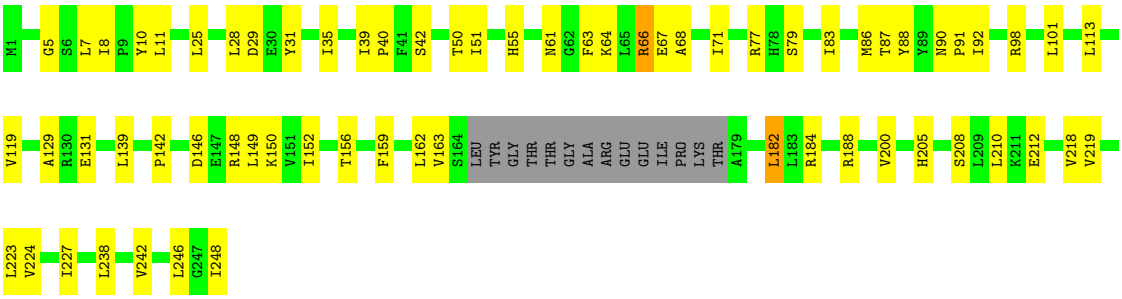
• Molecule 1: Tryptophan synthase alpha chain

Chain I:



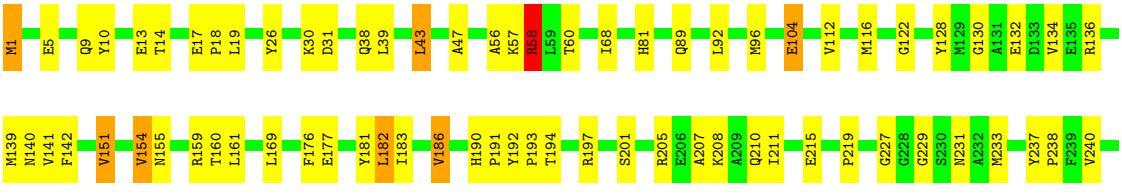
• Molecule 1: Tryptophan synthase alpha chain

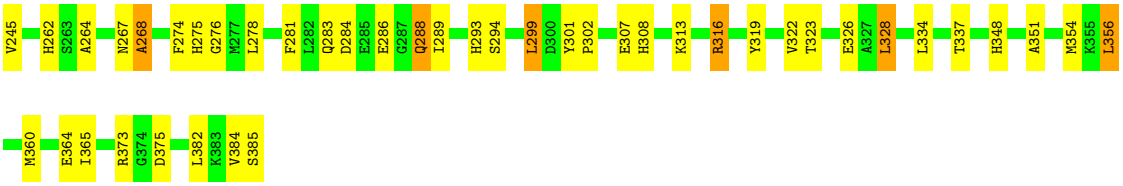
Chain K:



• Molecule 2: Tryptophan synthase beta chain 1

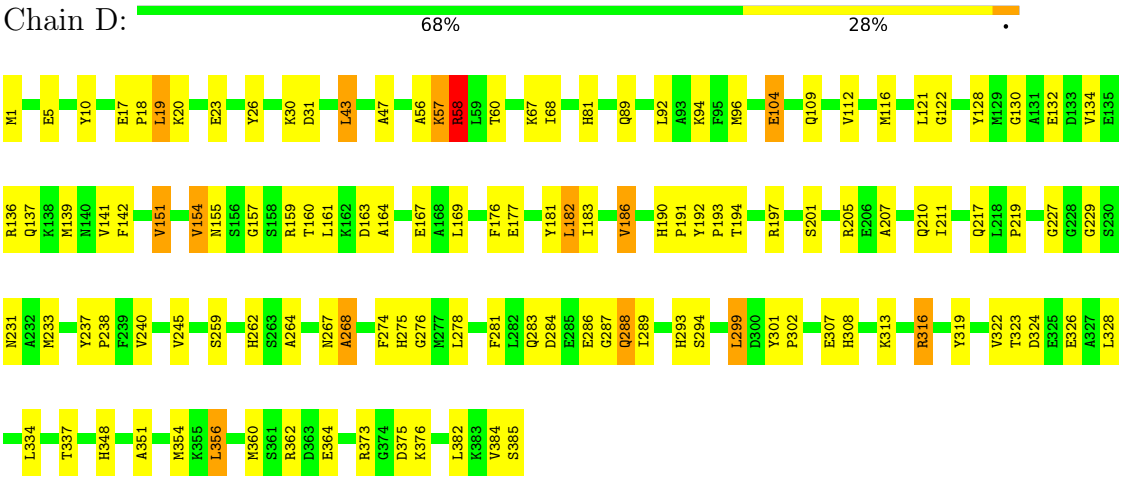
Chain B:





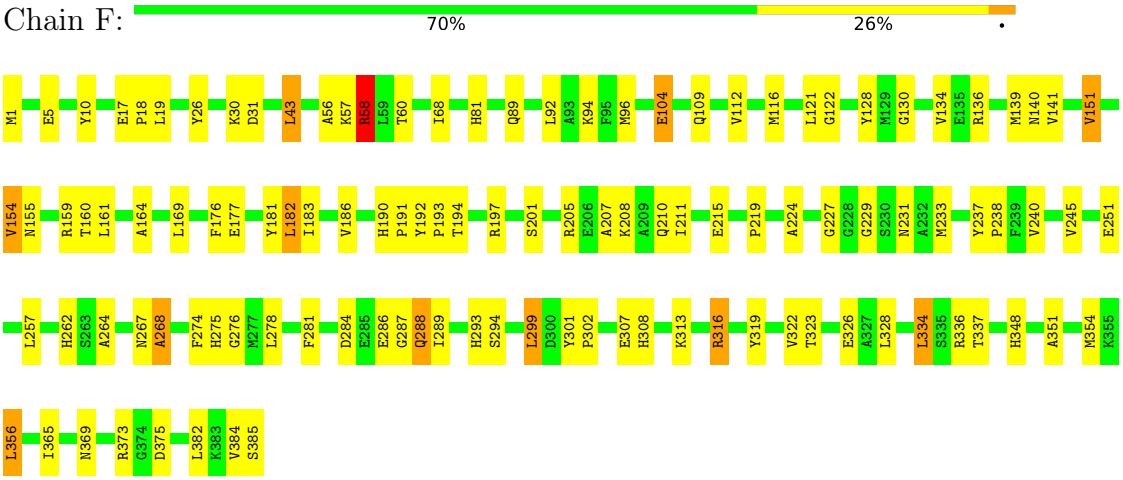
• Molecule 2: Tryptophan synthase beta chain 1

Chain D:



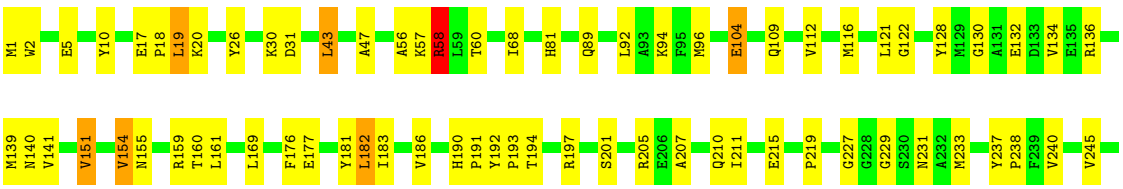
• Molecule 2: Tryptophan synthase beta chain 1

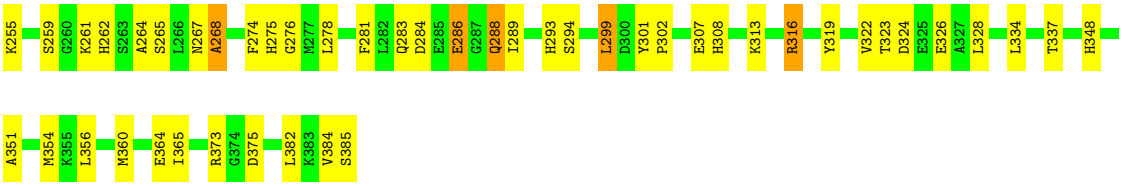
Chain F:



• Molecule 2: Tryptophan synthase beta chain 1

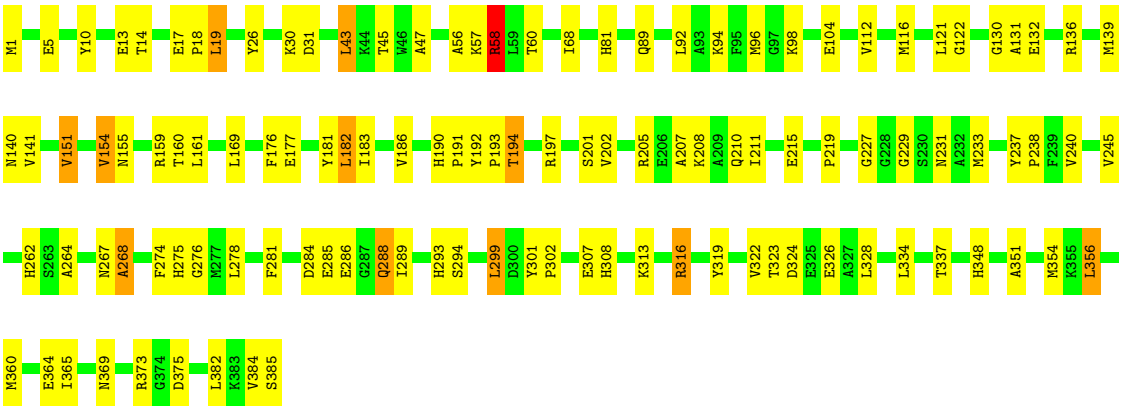
Chain H:





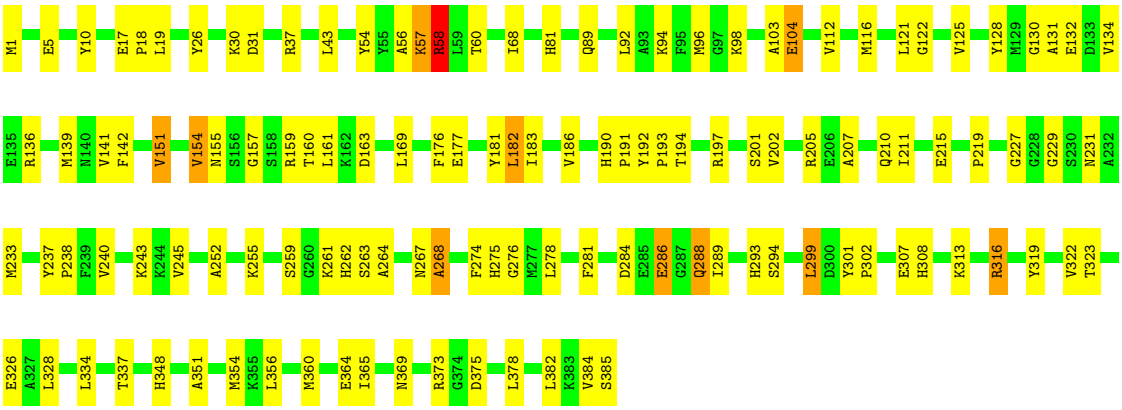
• Molecule 2: Tryptophan synthase beta chain 1

Chain J:



• Molecule 2: Tryptophan synthase beta chain 1

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.06Å 220.26Å 292.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.17 – 3.00	Depositor
% Data completeness (in resolution range)	97.7 (89.17-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29563	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

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: PLP

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	A	0.37	0/1931	0.59	0/2605
1	C	0.38	0/1931	0.58	0/2604
1	E	0.39	0/1979	0.59	0/2670
1	G	0.37	0/1940	0.57	0/2616
1	I	0.39	0/1955	0.58	0/2635
1	K	0.42	0/1869	0.57	0/2519
2	B	0.40	0/3038	0.65	2/4099 (0.0%)
2	D	0.40	0/3038	0.66	3/4099 (0.1%)
2	F	0.40	0/3038	0.65	3/4099 (0.1%)
2	H	0.40	0/3038	0.66	2/4099 (0.0%)
2	J	0.40	0/3038	0.65	3/4099 (0.1%)
2	L	0.40	0/3038	0.66	3/4099 (0.1%)
All	All	0.39	0/29833	0.63	16/40243 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	58	ARG	NE-CZ-NH2	-11.35	114.63	120.30
2	L	58	ARG	NE-CZ-NH2	-10.32	115.14	120.30
2	D	58	ARG	NE-CZ-NH2	-9.31	115.64	120.30
2	B	58	ARG	NE-CZ-NH2	-8.65	115.98	120.30
2	F	58	ARG	NE-CZ-NH2	-7.98	116.31	120.30
2	J	58	ARG	NE-CZ-NH2	-7.13	116.73	120.30
2	D	58	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	F	58	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	L	58	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	J	58	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	F	227	GLY	N-CA-C	-5.36	99.70	113.10
2	D	227	GLY	N-CA-C	-5.25	99.98	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	227	GLY	N-CA-C	-5.20	100.10	113.10
2	L	227	GLY	N-CA-C	-5.17	100.16	113.10
2	B	227	GLY	N-CA-C	-5.09	100.37	113.10
2	H	227	GLY	N-CA-C	-5.03	100.54	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1895	0	1948	55	0
1	C	1895	0	1953	54	0
1	E	1942	0	1998	60	0
1	G	1904	0	1959	54	1
1	I	1919	0	1975	57	0
1	K	1835	0	1889	51	0
2	B	2977	0	2999	109	0
2	D	2977	0	2999	120	0
2	F	2977	0	2999	102	0
2	H	2977	0	2999	103	0
2	J	2977	0	2999	111	0
2	L	2977	0	2999	120	1
3	B	15	0	7	0	0
3	D	15	0	7	0	0
3	F	15	0	6	1	0
3	H	15	0	7	0	0
3	J	15	0	7	0	0
3	L	15	0	7	0	0
4	B	23	0	0	2	0
4	C	2	0	0	0	0
4	D	23	0	0	4	0
4	E	4	0	0	1	0
4	F	33	0	0	6	0
4	G	9	0	0	1	0
4	H	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	13	0	0	3	0
4	J	43	0	0	5	0
4	L	35	0	0	9	0
All	All	29563	0	29757	909	1

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 15.

All (909) 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)
2:J:122:GLY:CA	2:L:58:ARG:HH22	1.25	1.49
2:F:122:GLY:CA	2:H:58:ARG:HH22	1.31	1.40
2:B:122:GLY:CA	2:D:58:ARG:HH22	1.44	1.30
2:F:122:GLY:HA2	2:H:58:ARG:NH2	1.45	1.27
2:B:58:ARG:HH22	2:D:122:GLY:CA	1.46	1.27
2:J:122:GLY:HA2	2:L:58:ARG:NH2	1.48	1.26
2:F:58:ARG:HH22	2:H:122:GLY:CA	1.58	1.15
1:E:168:THR:HG23	1:E:173:GLU:HA	1.23	1.15
2:J:122:GLY:CA	2:L:58:ARG:NH2	2.09	1.11
2:J:58:ARG:HH22	2:L:122:GLY:CA	1.69	1.05
2:B:58:ARG:HH22	2:D:122:GLY:HA2	1.20	1.05
2:F:58:ARG:HH22	2:H:122:GLY:HA2	1.15	1.05
1:E:168:THR:CG2	1:E:173:GLU:HA	1.86	1.04
2:B:122:GLY:HA3	2:D:58:ARG:HH22	1.19	1.04
2:J:122:GLY:HA2	2:L:58:ARG:HH22	0.91	1.03
2:B:122:GLY:HA2	2:D:58:ARG:NH2	1.74	1.02
2:B:58:ARG:NH2	2:D:122:GLY:HA2	1.73	1.02
2:B:122:GLY:CA	2:D:58:ARG:NH2	2.22	1.01
2:J:122:GLY:HA3	2:L:58:ARG:HH22	1.24	1.01
2:F:58:ARG:NH2	2:H:122:GLY:HA2	1.77	0.99
2:B:58:ARG:HH22	2:D:122:GLY:HA3	1.29	0.96
1:I:42:SER:HB3	2:J:288:GLN:HG3	1.46	0.95
1:A:42:SER:HB3	2:B:288:GLN:HG3	1.50	0.94
2:J:160:THR:HG22	2:J:161:LEU:H	1.31	0.94
2:B:58:ARG:NH2	2:D:122:GLY:CA	2.27	0.93
2:L:160:THR:HG22	2:L:161:LEU:H	1.33	0.93
2:D:160:THR:HG22	2:D:161:LEU:H	1.33	0.92
2:F:251:GLU:OE2	4:F:419:HOH:O	1.87	0.92
2:F:122:GLY:HA2	2:H:58:ARG:HH22	0.77	0.91
2:F:160:THR:HG22	2:F:161:LEU:H	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:HG22	2:B:161:LEU:H	1.32	0.90
2:H:160:THR:HG22	2:H:161:LEU:H	1.36	0.88
2:J:58:ARG:HH22	2:L:122:GLY:HA3	1.39	0.87
1:K:42:SER:HB3	2:L:288:GLN:HG3	1.55	0.87
2:J:58:ARG:HG3	2:J:58:ARG:HH11	1.40	0.86
1:G:42:SER:HB3	2:H:288:GLN:HG3	1.57	0.86
1:G:42:SER:H	2:H:288:GLN:HE21	1.24	0.85
2:F:58:ARG:HG3	2:F:58:ARG:HH11	1.41	0.85
2:D:58:ARG:HG3	2:D:58:ARG:HH11	1.40	0.84
2:D:58:ARG:HG3	2:D:58:ARG:NH1	1.93	0.83
2:F:337:THR:HA	4:F:423:HOH:O	1.76	0.83
2:L:58:ARG:HH11	2:L:58:ARG:HG3	1.43	0.82
2:L:58:ARG:HG3	2:L:58:ARG:NH1	1.95	0.82
1:A:42:SER:H	2:B:288:GLN:HE21	1.27	0.82
2:B:58:ARG:HG3	2:B:58:ARG:HH11	1.44	0.81
2:D:56:ALA:O	2:D:60:THR:HG23	1.79	0.81
2:H:58:ARG:HG3	2:H:58:ARG:HH11	1.44	0.81
2:F:122:GLY:CA	2:H:58:ARG:NH2	2.16	0.81
2:H:58:ARG:HG3	2:H:58:ARG:NH1	1.96	0.80
2:H:237:TYR:HB3	2:H:238:PRO:HD3	1.63	0.80
2:H:262:HIS:HD2	2:H:264:ALA:H	1.29	0.80
2:B:1:MET:HB3	2:B:190:HIS:HB2	1.64	0.80
2:J:58:ARG:NH2	2:L:122:GLY:HA2	1.97	0.79
2:J:58:ARG:HG3	2:J:58:ARG:NH1	1.95	0.79
2:H:60:THR:HG21	2:H:68:ILE:H	1.48	0.79
2:J:58:ARG:NH2	2:L:122:GLY:CA	2.46	0.78
2:D:262:HIS:HD2	2:D:264:ALA:H	1.29	0.78
2:F:58:ARG:HG3	2:F:58:ARG:NH1	1.95	0.78
2:B:56:ALA:O	2:B:60:THR:HG23	1.82	0.78
2:D:237:TYR:HB3	2:D:238:PRO:HD3	1.66	0.77
2:J:58:ARG:HH22	2:L:122:GLY:HA2	1.48	0.77
2:B:237:TYR:HB3	2:B:238:PRO:HD3	1.66	0.77
2:J:237:TYR:HB3	2:J:238:PRO:HD3	1.67	0.77
2:F:60:THR:HG21	2:F:68:ILE:H	1.50	0.77
2:F:237:TYR:HB3	2:F:238:PRO:HD3	1.66	0.76
2:B:58:ARG:HG3	2:B:58:ARG:NH1	1.97	0.76
2:B:262:HIS:HD2	2:B:264:ALA:H	1.30	0.76
2:F:262:HIS:HD2	2:F:264:ALA:H	1.32	0.76
2:J:202:VAL:HG23	4:J:410:HOH:O	1.85	0.76
2:L:60:THR:HG21	2:L:68:ILE:H	1.51	0.76
2:L:262:HIS:HD2	2:L:264:ALA:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:56:ALA:O	2:L:60:THR:HG23	1.86	0.75
2:J:58:ARG:HD3	2:J:337:THR:HG23	1.69	0.75
1:I:42:SER:H	2:J:288:GLN:HE21	1.32	0.75
2:J:262:HIS:HD2	2:J:264:ALA:H	1.31	0.75
2:L:237:TYR:HB3	2:L:238:PRO:HD3	1.66	0.74
2:D:58:ARG:CD	2:D:337:THR:HG23	2.17	0.74
2:D:58:ARG:HD3	2:D:337:THR:HG23	1.67	0.74
2:J:56:ALA:O	2:J:60:THR:HG23	1.87	0.74
1:K:28:LEU:HD22	1:K:242:VAL:HG21	1.68	0.74
2:L:202:VAL:HG23	4:L:427:HOH:O	1.87	0.74
2:F:56:ALA:O	2:F:60:THR:HG23	1.87	0.74
2:H:56:ALA:O	2:H:60:THR:HG23	1.88	0.73
2:J:58:ARG:CD	2:J:337:THR:HG23	2.18	0.73
2:J:60:THR:HG21	2:J:68:ILE:H	1.53	0.73
1:A:28:LEU:HD22	1:A:242:VAL:HG21	1.69	0.73
1:K:42:SER:H	2:L:288:GLN:HE21	1.36	0.73
2:F:122:GLY:HA3	2:H:58:ARG:HH22	1.49	0.73
2:B:60:THR:HG21	2:B:68:ILE:H	1.55	0.72
2:F:58:ARG:HD3	2:F:337:THR:HG23	1.71	0.72
2:L:58:ARG:HD3	2:L:337:THR:HG23	1.70	0.72
2:H:58:ARG:HD3	2:H:337:THR:HG23	1.72	0.72
2:F:58:ARG:CD	2:F:337:THR:HG23	2.20	0.71
2:L:58:ARG:CD	2:L:337:THR:HG23	2.20	0.71
1:E:28:LEU:HD22	1:E:242:VAL:HG21	1.72	0.71
1:C:28:LEU:HD22	1:C:242:VAL:HG21	1.73	0.71
2:D:362:ARG:NH2	1:E:248:ILE:HG23	2.05	0.71
1:G:248:ILE:O	1:G:248:ILE:HG22	1.91	0.70
2:F:284:ASP:HB3	2:F:288:GLN:H	1.57	0.70
2:B:58:ARG:HD3	2:B:337:THR:HG23	1.72	0.70
2:L:243:LYS:HG3	4:L:431:HOH:O	1.90	0.70
2:D:60:THR:HG21	2:D:68:ILE:H	1.55	0.70
2:B:58:ARG:HH11	2:B:58:ARG:CG	2.04	0.70
2:B:58:ARG:CD	2:B:337:THR:HG23	2.21	0.70
1:G:64:LYS:HA	2:H:286:GLU:OE2	1.91	0.70
1:I:28:LEU:HD22	1:I:242:VAL:HG21	1.74	0.70
2:F:58:ARG:NH2	2:H:122:GLY:CA	2.41	0.70
2:J:98:LYS:HE3	4:J:419:HOH:O	1.92	0.70
2:L:37:ARG:NH2	4:L:401:HOH:O	2.23	0.69
2:H:284:ASP:HB3	2:H:288:GLN:H	1.58	0.69
2:L:58:ARG:HH11	2:L:58:ARG:CG	2.05	0.69
2:J:1:MET:HE1	4:J:422:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ARG:HG3	2:B:136:ARG:HH11	1.58	0.69
2:H:112:VAL:O	2:H:116:MET:HG3	1.93	0.69
2:F:112:VAL:O	2:F:116:MET:HG3	1.93	0.69
2:D:58:ARG:HH11	2:D:58:ARG:CG	2.06	0.69
2:L:136:ARG:HG3	2:L:136:ARG:HH11	1.57	0.69
2:L:299:LEU:CD2	2:L:348:HIS:CD2	2.76	0.69
2:B:373:ARG:HD2	2:B:375:ASP:OD2	1.92	0.68
1:G:28:LEU:HD22	1:G:242:VAL:HG21	1.74	0.68
2:J:112:VAL:O	2:J:116:MET:HG3	1.93	0.68
2:F:299:LEU:CD2	2:F:348:HIS:CD2	2.77	0.68
2:J:240:VAL:O	2:J:316:ARG:NH1	2.27	0.68
2:B:284:ASP:HB3	2:B:288:GLN:H	1.58	0.68
1:G:42:SER:H	2:H:288:GLN:NE2	1.90	0.68
2:H:58:ARG:CD	2:H:337:THR:HG23	2.22	0.68
2:J:58:ARG:HH11	2:J:58:ARG:CG	2.06	0.68
2:J:384:VAL:HG23	2:J:385:SER:N	2.09	0.68
2:F:58:ARG:HH22	2:H:122:GLY:HA3	1.55	0.68
2:H:58:ARG:HH11	2:H:58:ARG:CG	2.05	0.68
2:J:284:ASP:HB3	2:J:288:GLN:H	1.58	0.68
2:F:58:ARG:HH11	2:F:58:ARG:CG	2.06	0.68
2:D:384:VAL:HG23	2:D:385:SER:N	2.08	0.68
2:F:384:VAL:HG23	2:F:385:SER:N	2.09	0.67
1:A:42:SER:H	2:B:288:GLN:NE2	1.92	0.67
1:E:3:LYS:HE2	4:E:250:HOH:O	1.92	0.67
2:H:240:VAL:O	2:H:316:ARG:NH1	2.27	0.67
2:H:301:TYR:CD1	2:H:302:PRO:HD2	2.30	0.67
1:G:64:LYS:HB3	2:H:286:GLU:OE1	1.93	0.67
2:D:284:ASP:HB3	2:D:288:GLN:H	1.59	0.67
2:H:373:ARG:HD2	2:H:375:ASP:OD2	1.95	0.67
2:J:197:ARG:HG3	2:J:233:MET:HG3	1.77	0.67
2:J:373:ARG:HD2	2:J:375:ASP:OD2	1.94	0.67
2:L:284:ASP:HB3	2:L:288:GLN:H	1.58	0.67
2:D:181:TYR:CE2	2:D:183:ILE:HD11	2.30	0.67
2:B:1:MET:SD	2:B:1:MET:N	2.53	0.67
1:I:42:SER:H	2:J:288:GLN:NE2	1.93	0.67
2:H:60:THR:CG2	2:H:68:ILE:H	2.08	0.66
2:L:384:VAL:HG23	2:L:385:SER:N	2.08	0.66
2:F:240:VAL:O	2:F:316:ARG:NH1	2.28	0.66
2:F:373:ARG:HD2	2:F:375:ASP:OD2	1.95	0.66
2:D:136:ARG:HH11	2:D:136:ARG:HG3	1.59	0.66
2:D:299:LEU:CD2	2:D:348:HIS:CD2	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:299:LEU:CD2	2:J:348:HIS:CD2	2.79	0.66
2:B:197:ARG:HG3	2:B:233:MET:HG3	1.76	0.66
2:B:384:VAL:HG23	2:B:385:SER:N	2.10	0.66
2:D:373:ARG:HD2	2:D:375:ASP:OD2	1.95	0.66
1:E:101:LEU:HD13	1:E:129:ALA:HA	1.78	0.66
2:L:10:TYR:O	2:L:276:GLY:HA2	1.96	0.66
2:H:384:VAL:HG23	2:H:385:SER:N	2.11	0.66
2:L:181:TYR:CE2	2:L:183:ILE:HD11	2.31	0.66
2:F:60:THR:CG2	2:F:68:ILE:H	2.09	0.65
1:I:173:GLU:HG3	1:I:201:SER:OG	1.96	0.65
2:B:10:TYR:O	2:B:276:GLY:HA2	1.97	0.65
2:B:181:TYR:CE2	2:B:183:ILE:HD11	2.32	0.65
1:A:50:THR:HG22	1:A:224:VAL:HG23	1.79	0.65
1:I:101:LEU:HD13	1:I:129:ALA:HA	1.77	0.65
2:J:136:ARG:HG3	2:J:136:ARG:HH11	1.62	0.65
2:J:181:TYR:CE2	2:J:183:ILE:HD11	2.32	0.65
2:F:301:TYR:CD1	2:F:302:PRO:HD2	2.31	0.65
2:L:197:ARG:HG3	2:L:233:MET:HG3	1.77	0.65
2:F:10:TYR:O	2:F:276:GLY:HA2	1.97	0.65
2:L:60:THR:CG2	2:L:68:ILE:H	2.10	0.65
2:L:240:VAL:O	2:L:316:ARG:NH1	2.29	0.64
1:E:168:THR:HG22	1:E:170:GLY:H	1.62	0.64
2:L:373:ARG:HD2	2:L:375:ASP:OD2	1.95	0.64
2:F:351:ALA:HA	2:F:354:MET:HE2	1.79	0.64
2:D:112:VAL:O	2:D:116:MET:HG3	1.97	0.64
1:G:42:SER:N	2:H:288:GLN:HE21	1.95	0.64
2:J:10:TYR:O	2:J:276:GLY:HA2	1.98	0.64
2:J:194:THR:HG22	4:J:413:HOH:O	1.97	0.64
2:B:240:VAL:O	2:B:316:ARG:NH1	2.30	0.64
1:A:173:GLU:HG3	1:A:201:SER:OG	1.98	0.64
2:B:122:GLY:HA3	2:D:58:ARG:NH2	2.00	0.64
1:G:173:GLU:HG3	1:G:201:SER:OG	1.98	0.63
2:L:301:TYR:CD1	2:L:302:PRO:HD2	2.33	0.63
1:A:101:LEU:HD13	1:A:129:ALA:HA	1.80	0.63
1:E:173:GLU:HG3	1:E:201:SER:OG	1.98	0.63
2:H:197:ARG:HG3	2:H:233:MET:HG3	1.80	0.63
1:K:42:SER:H	2:L:288:GLN:NE2	1.96	0.63
2:B:301:TYR:CD1	2:B:302:PRO:HD2	2.33	0.63
2:F:136:ARG:HG3	2:F:136:ARG:HH11	1.62	0.63
1:K:101:LEU:HD13	1:K:129:ALA:HA	1.80	0.63
2:D:240:VAL:O	2:D:316:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:181:TYR:CE2	2:H:183:ILE:HD11	2.33	0.63
1:K:50:THR:HG22	1:K:224:VAL:HG23	1.80	0.63
2:B:197:ARG:HD3	2:B:307:GLU:OE1	1.99	0.62
2:F:197:ARG:HG3	2:F:233:MET:HG3	1.81	0.62
1:G:50:THR:HG22	1:G:224:VAL:HG23	1.79	0.62
1:I:172:ARG:O	1:I:173:GLU:HG2	1.99	0.62
2:L:112:VAL:O	2:L:116:MET:HG3	1.99	0.62
2:J:197:ARG:HD3	2:J:307:GLU:OE1	1.99	0.62
2:D:10:TYR:O	2:D:276:GLY:HA2	1.99	0.62
2:L:308:HIS:HD2	2:L:319:TYR:OH	1.82	0.62
1:C:50:THR:HG22	1:C:224:VAL:HG23	1.81	0.62
2:D:301:TYR:CD1	2:D:302:PRO:HD2	2.34	0.62
1:E:64:LYS:HD3	1:E:66:ARG:NH2	2.14	0.62
1:E:98:ARG:NH2	1:E:131:GLU:OE2	2.33	0.62
1:C:98:ARG:NH2	1:C:131:GLU:OE2	2.32	0.62
2:H:136:ARG:HG3	2:H:136:ARG:HH11	1.63	0.62
2:J:351:ALA:HA	2:J:354:MET:HE2	1.81	0.62
2:B:112:VAL:O	2:B:116:MET:HG3	2.00	0.62
2:D:308:HIS:HD2	2:D:319:TYR:OH	1.83	0.62
2:F:181:TYR:CE2	2:F:183:ILE:HD11	2.35	0.62
1:I:51:ILE:HD13	1:I:224:VAL:HG21	1.82	0.62
1:E:50:THR:HG22	1:E:224:VAL:HG23	1.80	0.61
1:I:50:THR:HG22	1:I:224:VAL:HG23	1.81	0.61
2:B:60:THR:CG2	2:B:68:ILE:H	2.13	0.61
1:G:40:PRO:HA	1:G:55:HIS:ND1	2.15	0.61
2:B:1:MET:HG2	2:B:9:GLN:HB2	1.82	0.61
1:C:101:LEU:HD13	1:C:129:ALA:HA	1.81	0.61
2:D:60:THR:CG2	2:D:68:ILE:H	2.13	0.61
1:K:51:ILE:HD13	1:K:224:VAL:HG21	1.82	0.61
2:D:197:ARG:HG3	2:D:233:MET:HG3	1.83	0.61
1:K:40:PRO:HA	1:K:55:HIS:ND1	2.16	0.61
1:K:98:ARG:NH2	1:K:131:GLU:OE2	2.34	0.61
2:L:197:ARG:HD3	2:L:307:GLU:OE1	2.01	0.61
1:A:40:PRO:HA	1:A:55:HIS:ND1	2.16	0.61
1:A:51:ILE:HD13	1:A:224:VAL:HG21	1.83	0.61
2:B:58:ARG:NH2	2:D:122:GLY:HA3	2.08	0.60
2:D:20:LYS:NZ	4:D:410:HOH:O	2.33	0.60
1:G:101:LEU:HD13	1:G:129:ALA:HA	1.81	0.60
1:I:98:ARG:NH2	1:I:131:GLU:OE2	2.34	0.60
2:D:160:THR:HG22	2:D:161:LEU:N	2.13	0.60
1:G:64:LYS:HD3	1:G:66:ARG:NH2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:NH2	1:A:131:GLU:OE2	2.35	0.60
2:D:351:ALA:HA	2:D:354:MET:HE2	1.82	0.60
2:J:301:TYR:CD1	2:J:302:PRO:HD2	2.36	0.60
2:D:217:GLN:NE2	1:E:5:GLY:HA3	2.17	0.60
2:L:201:SER:HB2	2:L:205:ARG:HH21	1.65	0.60
2:D:197:ARG:HD3	2:D:307:GLU:OE1	2.02	0.60
1:G:98:ARG:NH2	1:G:131:GLU:OE2	2.35	0.60
2:L:136:ARG:HG3	2:L:136:ARG:NH1	2.15	0.60
2:J:308:HIS:HD2	2:J:319:TYR:OH	1.84	0.60
2:J:60:THR:CG2	2:J:68:ILE:H	2.14	0.59
2:B:328:LEU:HD21	2:B:384:VAL:HG21	1.85	0.59
1:C:94:ARG:HD3	2:D:287:GLY:HA3	1.84	0.59
1:C:40:PRO:HA	1:C:55:HIS:ND1	2.17	0.59
1:E:40:PRO:HA	1:E:55:HIS:ND1	2.17	0.59
1:A:88:TYR:O	1:A:91:PRO:HD2	2.02	0.59
2:F:60:THR:HG22	2:F:68:ILE:HB	1.84	0.59
2:L:351:ALA:HA	2:L:354:MET:HE2	1.83	0.59
1:C:88:TYR:O	1:C:91:PRO:HD2	2.03	0.59
2:L:160:THR:HG22	2:L:161:LEU:N	2.13	0.59
2:F:197:ARG:HD3	2:F:307:GLU:OE1	2.02	0.59
2:F:201:SER:HB2	2:F:205:ARG:HH21	1.68	0.59
2:B:351:ALA:HA	2:B:354:MET:HE2	1.84	0.58
1:C:64:LYS:HD3	1:C:66:ARG:NH2	2.18	0.58
2:D:262:HIS:CD2	2:D:264:ALA:H	2.17	0.58
2:H:197:ARG:HD3	2:H:307:GLU:OE1	2.02	0.58
2:H:233:MET:HE1	2:H:308:HIS:NE2	2.19	0.58
1:I:40:PRO:HA	1:I:55:HIS:ND1	2.18	0.58
1:C:51:ILE:HD13	1:C:224:VAL:HG21	1.85	0.58
2:H:10:TYR:O	2:H:276:GLY:HA2	2.03	0.58
2:L:103:ALA:HB1	4:L:403:HOH:O	2.02	0.58
2:L:262:HIS:CD2	2:L:264:ALA:H	2.18	0.58
2:L:322:VAL:HG13	2:L:326:GLU:HB2	1.85	0.58
2:F:160:THR:HG22	2:F:161:LEU:N	2.14	0.58
2:L:233:MET:HE1	2:L:308:HIS:NE2	2.18	0.58
2:D:60:THR:HG22	2:D:68:ILE:HB	1.86	0.58
1:A:90:ASN:HD21	2:B:283:GLN:NE2	2.01	0.58
2:L:26:TYR:O	2:L:30:LYS:HB2	2.03	0.58
1:E:172:ARG:O	1:E:173:GLU:HG2	2.03	0.58
1:E:173:GLU:N	1:E:173:GLU:OE1	2.37	0.58
2:H:308:HIS:HD2	2:H:319:TYR:OH	1.86	0.58
2:H:351:ALA:HA	2:H:354:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:VAL:HG13	2:B:326:GLU:HB2	1.86	0.57
2:D:136:ARG:HG3	2:D:136:ARG:NH1	2.17	0.57
2:H:245:VAL:O	2:H:316:ARG:NH2	2.37	0.57
1:I:88:TYR:O	1:I:91:PRO:HD2	2.04	0.57
2:H:160:THR:HG22	2:H:161:LEU:N	2.15	0.57
2:B:262:HIS:CD2	2:B:264:ALA:H	2.18	0.57
2:J:233:MET:HE1	2:J:308:HIS:NE2	2.18	0.57
2:F:308:HIS:HD2	2:F:319:TYR:OH	1.87	0.57
1:K:90:ASN:HB3	1:K:91:PRO:HD3	1.86	0.57
2:J:160:THR:HG22	2:J:161:LEU:N	2.11	0.57
2:L:1:MET:HB2	2:L:190:HIS:HB2	1.86	0.57
2:L:60:THR:HG22	2:L:68:ILE:HB	1.86	0.57
2:D:17:GLU:HB3	2:D:18:PRO:HD3	1.87	0.57
2:D:26:TYR:O	2:D:30:LYS:HB2	2.05	0.57
2:B:17:GLU:HB3	2:B:18:PRO:HD3	1.87	0.56
2:D:245:VAL:O	2:D:316:ARG:NH2	2.38	0.56
2:D:322:VAL:HG13	2:D:326:GLU:HB2	1.86	0.56
1:E:51:ILE:HD13	1:E:224:VAL:HG21	1.86	0.56
2:J:60:THR:HG22	2:J:68:ILE:HB	1.87	0.56
2:J:201:SER:HB2	2:J:205:ARG:HH21	1.69	0.56
1:K:64:LYS:HD3	1:K:66:ARG:NH2	2.19	0.56
2:F:245:VAL:O	2:F:316:ARG:NH2	2.38	0.56
2:H:322:VAL:HG13	2:H:326:GLU:HB2	1.87	0.56
2:B:26:TYR:O	2:B:30:LYS:HB2	2.04	0.56
2:B:136:ARG:HG3	2:B:136:ARG:NH1	2.16	0.56
2:B:233:MET:HE1	2:B:308:HIS:NE2	2.19	0.56
2:B:245:VAL:O	2:B:316:ARG:NH2	2.37	0.56
2:B:308:HIS:HD2	2:B:319:TYR:OH	1.88	0.56
2:F:136:ARG:HG3	2:F:136:ARG:NH1	2.19	0.56
1:G:66:ARG:H	1:G:66:ARG:HD3	1.69	0.56
1:G:88:TYR:O	1:G:91:PRO:HD2	2.04	0.56
1:I:64:LYS:HD3	1:I:66:ARG:NH2	2.20	0.56
1:I:90:ASN:HB3	1:I:91:PRO:HD3	1.86	0.56
2:J:322:VAL:HG13	2:J:326:GLU:HB2	1.87	0.56
2:J:328:LEU:HD21	2:J:384:VAL:HG21	1.87	0.56
2:L:17:GLU:HB3	2:L:18:PRO:HD3	1.87	0.56
1:E:168:THR:CG2	1:E:170:GLY:H	2.19	0.56
2:H:92:LEU:O	2:H:96:MET:HG3	2.05	0.56
1:K:88:TYR:O	1:K:91:PRO:HD2	2.05	0.56
1:I:141:ALA:HB2	2:J:14:THR:HG22	1.87	0.56
1:K:64:LYS:HB3	2:L:286:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HD3	1:A:66:ARG:NH2	2.20	0.56
2:B:5:GLU:OE2	2:B:313:LYS:HE2	2.05	0.56
2:B:201:SER:HB2	2:B:205:ARG:HH21	1.70	0.56
1:E:171:ALA:HB3	1:E:174:GLU:OE1	2.06	0.56
2:L:5:GLU:OE2	2:L:313:LYS:HE2	2.06	0.56
1:K:219:VAL:HG12	1:K:223:LEU:HG	1.88	0.56
1:A:219:VAL:HG12	1:A:223:LEU:HG	1.88	0.55
2:F:274:PHE:CE2	2:F:289:ILE:HG12	2.41	0.55
2:H:136:ARG:HG3	2:H:136:ARG:NH1	2.19	0.55
2:J:262:HIS:CD2	2:J:264:ALA:H	2.18	0.55
2:D:328:LEU:HD21	2:D:384:VAL:HG21	1.89	0.55
2:J:245:VAL:O	2:J:316:ARG:NH2	2.38	0.55
2:F:58:ARG:HD2	2:F:337:THR:HG23	1.89	0.55
2:F:328:LEU:HD21	2:F:384:VAL:HG21	1.87	0.55
2:J:5:GLU:OE2	2:J:313:LYS:HE2	2.07	0.55
2:L:384:VAL:CG2	2:L:385:SER:N	2.70	0.55
2:F:17:GLU:HB3	2:F:18:PRO:HD3	1.88	0.55
2:F:322:VAL:HG13	2:F:326:GLU:HB2	1.88	0.55
2:H:17:GLU:HB3	2:H:18:PRO:HD3	1.88	0.55
1:I:35:ILE:HB	1:I:83:ILE:HD13	1.89	0.55
1:A:90:ASN:HB3	1:A:91:PRO:HD3	1.88	0.55
2:F:26:TYR:O	2:F:30:LYS:HB2	2.06	0.55
2:F:262:HIS:CD2	2:F:264:ALA:H	2.19	0.55
2:J:26:TYR:O	2:J:30:LYS:HB2	2.06	0.55
1:A:173:GLU:OE1	1:A:173:GLU:N	2.40	0.55
2:L:89:GLN:OE1	2:L:182:LEU:HD13	2.07	0.55
2:L:328:LEU:HD21	2:L:384:VAL:HG21	1.89	0.55
2:F:384:VAL:CG2	2:F:385:SER:N	2.70	0.55
2:J:17:GLU:HB3	2:J:18:PRO:HD3	1.89	0.55
1:A:10:TYR:O	1:A:11:LEU:HD23	2.07	0.54
1:I:173:GLU:N	1:I:173:GLU:OE1	2.40	0.54
2:D:5:GLU:OE2	2:D:313:LYS:HE2	2.07	0.54
1:G:51:ILE:HD13	1:G:224:VAL:HG21	1.88	0.54
2:H:328:LEU:HD21	2:H:384:VAL:HG21	1.89	0.54
1:I:141:ALA:CB	2:J:14:THR:HG22	2.38	0.54
1:K:11:LEU:HD22	1:K:227:ILE:CD1	2.37	0.54
2:D:384:VAL:CG2	2:D:385:SER:N	2.70	0.54
1:E:66:ARG:H	1:E:66:ARG:HD3	1.73	0.54
2:F:5:GLU:OE2	2:F:313:LYS:HE2	2.07	0.54
1:G:173:GLU:N	1:G:173:GLU:OE1	2.41	0.54
2:J:136:ARG:HG3	2:J:136:ARG:NH1	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:384:VAL:CG2	2:J:385:SER:N	2.70	0.54
2:B:60:THR:HG22	2:B:68:ILE:HB	1.88	0.54
1:C:219:VAL:HG12	1:C:223:LEU:HG	1.90	0.54
2:H:60:THR:HG22	2:H:68:ILE:HB	1.90	0.54
1:I:142:PRO:HD3	1:I:163:VAL:O	2.08	0.54
1:A:35:ILE:HB	1:A:83:ILE:HD13	1.88	0.54
2:B:323:THR:OG1	2:B:326:GLU:HG3	2.08	0.54
1:C:11:LEU:HD22	1:C:227:ILE:CD1	2.38	0.54
1:I:248:ILE:O	1:I:248:ILE:HG13	2.07	0.54
2:L:125:VAL:N	4:L:425:HOH:O	2.41	0.54
1:C:90:ASN:HD21	2:D:283:GLN:NE2	2.05	0.54
1:E:90:ASN:HB3	1:E:91:PRO:HD3	1.88	0.54
1:E:175:ILE:HB	1:E:180:TYR:HE1	1.71	0.54
2:L:274:PHE:CE2	2:L:289:ILE:HG12	2.43	0.54
2:D:130:GLY:HA2	2:D:154:VAL:HG22	1.90	0.54
2:H:201:SER:HB2	2:H:205:ARG:HH21	1.72	0.54
1:E:142:PRO:HD3	1:E:163:VAL:O	2.08	0.54
1:K:142:PRO:HD3	1:K:163:VAL:O	2.07	0.54
2:H:264:ALA:HB1	2:H:267:ASN:HB2	1.90	0.53
2:D:58:ARG:HD2	2:D:337:THR:HG23	1.89	0.53
2:B:274:PHE:CE2	2:B:289:ILE:HG12	2.43	0.53
1:E:248:ILE:HG22	1:E:248:ILE:O	2.07	0.53
1:E:219:VAL:HG12	1:E:223:LEU:HG	1.90	0.53
2:H:5:GLU:OE2	2:H:313:LYS:HE2	2.08	0.53
2:D:233:MET:HE1	2:D:308:HIS:NE2	2.24	0.53
1:E:88:TYR:O	1:E:91:PRO:HD2	2.07	0.53
1:G:142:PRO:HD3	1:G:163:VAL:O	2.09	0.53
2:J:58:ARG:HD2	2:J:337:THR:HG23	1.88	0.53
2:L:58:ARG:HD2	2:L:337:THR:HG23	1.90	0.53
2:B:130:GLY:HA2	2:B:154:VAL:HG22	1.91	0.53
2:B:229:GLY:O	2:B:308:HIS:HE1	1.92	0.53
2:H:262:HIS:CD2	2:H:264:ALA:H	2.19	0.53
1:I:11:LEU:HD22	1:I:227:ILE:CD1	2.38	0.53
2:F:264:ALA:HB1	2:F:267:ASN:HB2	1.89	0.53
1:K:86:MET:CE	1:K:113:LEU:HD23	2.39	0.53
2:B:160:THR:HG22	2:B:161:LEU:N	2.12	0.53
2:L:130:GLY:HA2	2:L:154:VAL:HG22	1.90	0.53
2:B:58:ARG:HD2	2:B:337:THR:HG23	1.90	0.53
2:D:264:ALA:HB1	2:D:267:ASN:HB2	1.90	0.53
1:E:35:ILE:HB	1:E:83:ILE:HD13	1.91	0.53
1:E:175:ILE:HB	1:E:180:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ASN:HB3	1:G:91:PRO:HD3	1.90	0.53
2:B:384:VAL:CG2	2:B:385:SER:N	2.71	0.52
1:K:64:LYS:HA	2:L:286:GLU:OE2	2.09	0.52
1:C:35:ILE:HB	1:C:83:ILE:HD13	1.91	0.52
1:C:90:ASN:HB3	1:C:91:PRO:HD3	1.91	0.52
2:F:89:GLN:OE1	2:F:182:LEU:HD13	2.09	0.52
2:F:130:GLY:HA2	2:F:154:VAL:HG22	1.91	0.52
2:H:26:TYR:O	2:H:30:LYS:HB2	2.09	0.52
2:J:229:GLY:O	2:J:308:HIS:HE1	1.92	0.52
2:H:323:THR:OG1	2:H:326:GLU:HG3	2.09	0.52
2:D:201:SER:HB2	2:D:205:ARG:HH21	1.74	0.52
2:L:264:ALA:HB1	2:L:267:ASN:HB2	1.91	0.52
2:B:299:LEU:CD2	2:B:348:HIS:CD2	2.92	0.52
2:F:229:GLY:O	2:F:308:HIS:HE1	1.91	0.52
2:J:160:THR:CG2	2:J:161:LEU:H	2.13	0.52
1:A:86:MET:CE	1:A:113:LEU:HD23	2.40	0.52
2:H:384:VAL:CG2	2:H:385:SER:N	2.72	0.52
2:J:264:ALA:HB1	2:J:267:ASN:HB2	1.90	0.52
1:K:63:PHE:HZ	1:K:68:ALA:HB2	1.74	0.52
1:A:175:ILE:HB	1:A:180:TYR:HE1	1.75	0.52
1:E:11:LEU:HD22	1:E:227:ILE:CD1	2.40	0.52
1:E:63:PHE:HZ	1:E:68:ALA:HB2	1.75	0.52
1:G:11:LEU:HD22	1:G:227:ILE:CD1	2.39	0.52
1:K:35:ILE:HB	1:K:83:ILE:HD13	1.91	0.52
1:A:142:PRO:HD3	1:A:163:VAL:O	2.10	0.52
2:B:1:MET:HB3	2:B:190:HIS:CB	2.38	0.52
2:D:274:PHE:CE2	2:D:289:ILE:HG12	2.44	0.52
2:B:274:PHE:HB2	2:B:281:PHE:CE2	2.45	0.52
2:F:275:HIS:HD2	2:F:301:TYR:OH	1.93	0.52
1:I:162:LEU:HB3	1:I:182:LEU:HD13	1.92	0.52
2:J:274:PHE:CE2	2:J:289:ILE:HG12	2.44	0.52
1:I:219:VAL:HG12	1:I:223:LEU:HG	1.91	0.51
1:K:42:SER:N	2:L:288:GLN:HE21	2.08	0.51
1:C:66:ARG:HD3	1:C:66:ARG:H	1.73	0.51
1:K:66:ARG:H	1:K:66:ARG:HD3	1.76	0.51
1:G:42:SER:N	2:H:288:GLN:NE2	2.57	0.51
2:H:81:HIS:CD2	2:H:231:ASN:HB3	2.46	0.51
1:C:94:ARG:NE	2:D:287:GLY:HA2	2.25	0.51
2:H:229:GLY:O	2:H:308:HIS:HE1	1.92	0.51
2:F:92:LEU:O	2:F:96:MET:HG3	2.11	0.51
2:H:81:HIS:NE2	2:H:231:ASN:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:229:GLY:O	2:L:308:HIS:HE1	1.92	0.51
2:F:274:PHE:HB2	2:F:281:PHE:CE2	2.46	0.51
1:K:5:GLY:HA2	1:K:210:LEU:HD22	1.93	0.51
2:L:274:PHE:HB2	2:L:281:PHE:CE2	2.45	0.51
1:C:86:MET:CE	1:C:113:LEU:HD23	2.41	0.51
1:G:35:ILE:HB	1:G:83:ILE:HD13	1.93	0.51
1:K:10:TYR:O	1:K:11:LEU:HD23	2.11	0.51
2:L:89:GLN:CD	2:L:182:LEU:HD13	2.31	0.51
2:L:245:VAL:O	2:L:316:ARG:NH2	2.44	0.51
2:L:92:LEU:O	2:L:96:MET:HG3	2.10	0.51
1:K:31:TYR:CD2	1:K:248:ILE:HD11	2.46	0.51
2:H:58:ARG:HD2	2:H:337:THR:HG23	1.93	0.50
1:K:39:ILE:HD12	1:K:87:THR:HB	1.91	0.50
2:L:81:HIS:CD2	2:L:231:ASN:HB3	2.46	0.50
2:J:89:GLN:OE1	2:J:182:LEU:HD13	2.11	0.50
2:D:141:VAL:HG13	2:D:151:VAL:HG11	1.93	0.50
2:D:160:THR:CG2	2:D:161:LEU:H	2.14	0.50
2:H:20:LYS:NZ	4:H:417:HOH:O	2.44	0.50
2:L:18:PRO:HG3	2:L:176:PHE:CD2	2.46	0.50
2:F:233:MET:HE1	2:F:308:HIS:NE2	2.26	0.50
1:A:11:LEU:HD22	1:A:227:ILE:CD1	2.41	0.50
1:E:172:ARG:C	1:E:173:GLU:HG2	2.31	0.50
2:F:323:THR:OG1	2:F:326:GLU:HG3	2.12	0.50
1:G:219:VAL:HG12	1:G:223:LEU:HG	1.93	0.50
1:I:63:PHE:HZ	1:I:68:ALA:HB2	1.76	0.50
2:B:264:ALA:HB1	2:B:267:ASN:HB2	1.93	0.50
1:C:142:PRO:HD3	1:C:163:VAL:O	2.11	0.50
2:D:92:LEU:O	2:D:96:MET:HG3	2.11	0.50
1:G:90:ASN:HD21	2:H:283:GLN:NE2	2.10	0.50
2:J:130:GLY:HA2	2:J:154:VAL:HG22	1.94	0.50
2:D:229:GLY:O	2:D:308:HIS:HE1	1.94	0.50
2:L:263:SER:OG	2:L:301:TYR:O	2.29	0.50
1:I:42:SER:N	2:J:288:GLN:HE21	2.06	0.50
1:A:39:ILE:HD12	1:A:87:THR:HB	1.94	0.49
1:G:162:LEU:HB3	1:G:182:LEU:HD13	1.94	0.49
1:G:184:ARG:HG3	1:G:184:ARG:HH11	1.77	0.49
2:J:89:GLN:CD	2:J:182:LEU:HD13	2.31	0.49
1:A:42:SER:N	2:B:288:GLN:HE21	2.05	0.49
1:A:63:PHE:HZ	1:A:68:ALA:HB2	1.78	0.49
1:I:5:GLY:HA2	1:I:210:LEU:HD22	1.94	0.49
1:I:66:ARG:H	1:I:66:ARG:HD3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:275:HIS:HD2	2:L:301:TYR:OH	1.96	0.49
1:A:140:ALA:HA	2:B:13:GLU:HG2	1.94	0.49
2:F:160:THR:CG2	2:F:161:LEU:H	2.15	0.49
1:C:175:ILE:HB	1:C:180:TYR:HE1	1.77	0.49
2:D:323:THR:OG1	2:D:326:GLU:HG3	2.12	0.49
2:F:356:LEU:O	2:F:356:LEU:HD22	2.12	0.49
2:J:323:THR:OG1	2:J:326:GLU:HG3	2.12	0.49
1:K:162:LEU:HB3	1:K:182:LEU:HD13	1.94	0.49
1:E:119:VAL:HG21	1:E:152:ILE:HG12	1.95	0.49
1:C:5:GLY:HA2	1:C:210:LEU:HD22	1.94	0.49
1:C:184:ARG:HG3	1:C:184:ARG:HH11	1.78	0.49
2:D:274:PHE:HB2	2:D:281:PHE:CE2	2.47	0.49
2:L:98:LYS:HE3	4:L:415:HOH:O	2.13	0.49
1:E:10:TYR:O	1:E:11:LEU:HD23	2.12	0.49
2:H:233:MET:HE1	2:H:308:HIS:CD2	2.47	0.49
2:H:274:PHE:CE2	2:H:289:ILE:HG12	2.48	0.49
1:K:146:ASP:O	1:K:150:LYS:HG3	2.12	0.49
2:L:81:HIS:NE2	2:L:231:ASN:HB3	2.28	0.49
1:C:39:ILE:HD12	1:C:87:THR:HB	1.94	0.49
1:A:5:GLY:HA2	1:A:210:LEU:HD22	1.95	0.49
1:I:86:MET:CE	1:I:113:LEU:HD23	2.43	0.49
2:J:92:LEU:O	2:J:96:MET:HG3	2.13	0.49
1:C:11:LEU:HD22	1:C:227:ILE:HD11	1.95	0.49
2:D:1:MET:HE1	4:D:410:HOH:O	2.12	0.49
2:D:362:ARG:NH2	1:E:248:ILE:CG2	2.74	0.49
2:F:18:PRO:HG3	2:F:176:PHE:CD2	2.48	0.49
2:H:18:PRO:HG3	2:H:176:PHE:CD2	2.48	0.49
1:K:200:VAL:HG13	1:K:205:HIS:HB2	1.95	0.49
1:C:49:LYS:CE	2:D:167:GLU:OE2	2.60	0.48
1:K:119:VAL:HG21	1:K:152:ILE:HG12	1.95	0.48
1:G:39:ILE:HD12	1:G:87:THR:HB	1.95	0.48
1:A:66:ARG:H	1:A:66:ARG:HD3	1.78	0.48
1:E:86:MET:CE	1:E:113:LEU:HD23	2.43	0.48
2:F:89:GLN:CD	2:F:182:LEU:HD13	2.33	0.48
1:G:63:PHE:HZ	1:G:68:ALA:HB2	1.78	0.48
2:H:274:PHE:HB2	2:H:281:PHE:CE2	2.48	0.48
1:A:146:ASP:O	1:A:150:LYS:HG3	2.13	0.48
2:F:369:ASN:HB3	4:F:432:HOH:O	2.11	0.48
1:G:61:ASN:N	1:G:61:ASN:HD22	2.11	0.48
1:A:175:ILE:HB	1:A:180:TYR:CE1	2.47	0.48
1:I:175:ILE:HB	1:I:180:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:HIS:CD2	2:B:231:ASN:HB3	2.48	0.48
2:D:81:HIS:CD2	2:D:231:ASN:HB3	2.48	0.48
1:I:175:ILE:HB	1:I:180:TYR:HE1	1.78	0.48
1:C:94:ARG:NH2	2:D:284:ASP:O	2.46	0.48
1:E:42:SER:HB3	2:F:288:GLN:HG3	1.95	0.48
1:I:10:TYR:O	1:I:11:LEU:HD23	2.14	0.48
1:C:175:ILE:HB	1:C:180:TYR:CE1	2.49	0.48
1:K:31:TYR:HB3	1:K:246:LEU:CD1	2.43	0.48
1:G:119:VAL:HG21	1:G:152:ILE:HG12	1.96	0.48
2:H:130:GLY:HA2	2:H:154:VAL:HG22	1.96	0.48
1:I:67:GLU:O	1:I:71:ILE:HG13	2.14	0.48
1:K:11:LEU:HD22	1:K:227:ILE:HD11	1.94	0.48
1:K:61:ASN:HD22	1:K:61:ASN:N	2.11	0.48
1:K:184:ARG:HH11	1:K:184:ARG:HG3	1.79	0.48
1:E:162:LEU:HB3	1:E:182:LEU:HD13	1.96	0.47
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.79	0.47
1:I:11:LEU:HD22	1:I:227:ILE:HD11	1.96	0.47
2:J:192:TYR:HB2	2:J:193:PRO:HD3	1.96	0.47
2:J:274:PHE:HB2	2:J:281:PHE:CE2	2.49	0.47
2:L:215:GLU:HG3	2:L:365:ILE:HD13	1.96	0.47
2:B:356:LEU:HD22	2:B:356:LEU:O	2.14	0.47
1:A:11:LEU:HD22	1:A:227:ILE:HD11	1.96	0.47
2:D:18:PRO:HG3	2:D:176:PHE:CD2	2.50	0.47
1:G:86:MET:CE	1:G:113:LEU:HD23	2.44	0.47
2:J:81:HIS:CD2	2:J:231:ASN:HB3	2.49	0.47
2:J:155:ASN:HA	2:J:159:ARG:HD2	1.95	0.47
2:L:192:TYR:HB2	2:L:193:PRO:HD3	1.97	0.47
1:A:61:ASN:HD22	1:A:61:ASN:N	2.11	0.47
1:A:119:VAL:HG21	1:A:152:ILE:HG12	1.97	0.47
1:C:63:PHE:HZ	1:C:68:ALA:HB2	1.79	0.47
1:C:162:LEU:HB3	1:C:182:LEU:HD13	1.96	0.47
2:D:192:TYR:HB2	2:D:193:PRO:HD3	1.97	0.47
1:E:172:ARG:C	1:E:173:GLU:CG	2.83	0.47
1:G:11:LEU:HD22	1:G:227:ILE:HD11	1.97	0.47
1:G:30:GLU:HG2	4:G:252:HOH:O	2.14	0.47
1:G:175:ILE:HB	1:G:180:TYR:CE1	2.49	0.47
1:C:49:LYS:HE2	2:D:167:GLU:OE2	2.15	0.47
2:F:233:MET:HE1	2:F:308:HIS:CD2	2.50	0.47
1:A:184:ARG:HG3	1:A:184:ARG:HH11	1.79	0.47
2:B:142:PHE:CD1	2:D:382:LEU:HD23	2.50	0.47
2:B:192:TYR:HB2	2:B:193:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:HD12	1:E:87:THR:HB	1.96	0.47
1:G:10:TYR:O	1:G:11:LEU:HD23	2.13	0.47
2:J:132:GLU:HB2	2:J:159:ARG:O	2.15	0.47
2:J:233:MET:HE1	2:J:308:HIS:CD2	2.49	0.47
1:K:67:GLU:O	1:K:71:ILE:HG13	2.15	0.47
2:B:30:LYS:HE3	2:B:31:ASP:OD1	2.15	0.47
2:B:140:ASN:HD22	2:B:140:ASN:HA	1.58	0.47
2:H:130:GLY:O	2:H:134:VAL:HG23	2.15	0.47
2:L:233:MET:HE1	2:L:308:HIS:CD2	2.50	0.47
2:B:141:VAL:HG13	2:B:151:VAL:HG11	1.96	0.47
1:C:67:GLU:O	1:C:71:ILE:HG13	2.15	0.47
2:D:89:GLN:OE1	2:D:182:LEU:HD13	2.15	0.47
1:G:5:GLY:HA2	1:G:210:LEU:HD22	1.97	0.47
2:H:299:LEU:CD2	2:H:348:HIS:CD2	2.97	0.47
1:K:31:TYR:HB3	1:K:246:LEU:HD11	1.97	0.47
2:B:92:LEU:O	2:B:96:MET:HG3	2.14	0.47
2:D:89:GLN:CD	2:D:182:LEU:HD13	2.36	0.46
2:F:60:THR:HG22	2:F:68:ILE:CB	2.45	0.46
2:H:192:TYR:HB2	2:H:193:PRO:HD3	1.96	0.46
1:I:39:ILE:HD12	1:I:87:THR:HB	1.96	0.46
2:J:215:GLU:HG3	2:J:365:ILE:HD13	1.97	0.46
1:C:61:ASN:N	1:C:61:ASN:HD22	2.11	0.46
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.79	0.46
2:H:275:HIS:HD2	2:H:301:TYR:OH	1.98	0.46
1:I:172:ARG:C	1:I:173:GLU:HG2	2.35	0.46
2:L:141:VAL:HG13	2:L:151:VAL:HG11	1.96	0.46
1:C:119:VAL:HG21	1:C:152:ILE:HG12	1.97	0.46
1:C:146:ASP:O	1:C:150:LYS:HG3	2.15	0.46
2:H:160:THR:CG2	2:H:161:LEU:H	2.17	0.46
1:I:119:VAL:HG21	1:I:152:ILE:HG12	1.97	0.46
2:J:43:LEU:O	2:J:47:ALA:HB3	2.16	0.46
2:L:323:THR:OG1	2:L:326:GLU:HG3	2.15	0.46
2:D:207:ALA:HA	2:D:210:GLN:HE21	1.80	0.46
2:F:141:VAL:HG13	2:F:151:VAL:HG11	1.96	0.46
1:G:175:ILE:HB	1:G:180:TYR:HE1	1.79	0.46
1:E:11:LEU:HD22	1:E:227:ILE:HD11	1.97	0.46
2:F:30:LYS:HE3	2:F:31:ASP:OD1	2.16	0.46
2:F:81:HIS:CD2	2:F:231:ASN:HB3	2.51	0.46
1:G:67:GLU:O	1:G:71:ILE:HG13	2.16	0.46
1:G:200:VAL:HG13	1:G:205:HIS:HB2	1.96	0.46
2:H:89:GLN:OE1	2:H:182:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:PRO:HD2	1:I:63:PHE:CE1	2.51	0.46
1:A:67:GLU:O	1:A:71:ILE:HG13	2.14	0.46
2:B:89:GLN:OE1	2:B:182:LEU:HD13	2.16	0.46
1:E:61:ASN:N	1:E:61:ASN:HD22	2.12	0.46
1:E:200:VAL:HG13	1:E:205:HIS:HB2	1.97	0.46
1:I:200:VAL:HG13	1:I:205:HIS:HB2	1.98	0.46
2:J:18:PRO:HG3	2:J:176:PHE:CD2	2.51	0.46
2:J:30:LYS:HE3	2:J:31:ASP:OD1	2.16	0.46
1:A:162:LEU:HB3	1:A:182:LEU:HD13	1.97	0.46
1:A:200:VAL:HG13	1:A:205:HIS:HB2	1.97	0.46
2:B:275:HIS:HD2	2:B:301:TYR:OH	1.97	0.46
1:C:40:PRO:HD2	1:C:63:PHE:CE1	2.51	0.46
1:G:40:PRO:HD2	1:G:63:PHE:CE1	2.50	0.46
1:A:238:LEU:O	1:A:242:VAL:HG23	2.16	0.46
2:J:207:ALA:HA	2:J:210:GLN:HE21	1.81	0.46
2:L:155:ASN:HA	2:L:159:ARG:HD2	1.98	0.46
2:H:1:MET:HG3	2:H:2:TRP:CD1	2.51	0.46
2:L:30:LYS:HE3	2:L:31:ASP:OD1	2.15	0.46
2:L:382:LEU:C	2:L:382:LEU:HD13	2.37	0.46
2:F:293:HIS:CG	2:F:294:SER:N	2.84	0.45
1:K:86:MET:HE3	1:K:113:LEU:HD23	1.97	0.45
2:L:207:ALA:HA	2:L:210:GLN:HE21	1.80	0.45
2:L:267:ASN:O	2:L:268:ALA:HB2	2.16	0.45
2:J:159:ARG:HG3	2:J:159:ARG:HH11	1.82	0.45
2:J:211:ILE:HG21	2:J:219:PRO:HD3	1.97	0.45
1:K:208:SER:O	1:K:212:GLU:HG2	2.16	0.45
2:L:160:THR:CG2	2:L:161:LEU:H	2.14	0.45
2:B:233:MET:HE1	2:B:308:HIS:CD2	2.51	0.45
2:L:190:HIS:ND1	2:L:191:PRO:HA	2.32	0.45
1:A:40:PRO:HD2	1:A:63:PHE:CE1	2.51	0.45
1:E:40:PRO:HD2	1:E:63:PHE:CE1	2.51	0.45
2:F:207:ALA:HA	2:F:210:GLN:HE21	1.80	0.45
1:I:146:ASP:O	1:I:150:LYS:HG3	2.16	0.45
2:F:109:GLN:HB2	4:F:404:HOH:O	2.16	0.45
1:G:146:ASP:O	1:G:150:LYS:HG3	2.16	0.45
2:H:89:GLN:CD	2:H:182:LEU:HD13	2.37	0.45
2:H:215:GLU:HG3	2:H:365:ILE:HD13	1.98	0.45
2:H:237:TYR:HB3	2:H:238:PRO:CD	2.40	0.45
1:I:43:ASP:OD2	2:J:289:ILE:HG13	2.17	0.45
1:K:40:PRO:HD2	1:K:63:PHE:CE1	2.52	0.45
1:A:204:GLU:H	1:A:204:GLU:HG3	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:LEU:O	2:H:47:ALA:HB3	2.17	0.45
2:H:109:GLN:HB2	4:H:405:HOH:O	2.15	0.45
2:B:208:LYS:O	2:B:211:ILE:HG22	2.17	0.45
2:D:60:THR:HG22	2:D:68:ILE:CB	2.47	0.45
1:G:77:ARG:HG2	1:G:77:ARG:HH11	1.81	0.45
2:L:360:MET:HB3	2:L:364:GLU:OE2	2.15	0.45
2:D:211:ILE:HG21	2:D:219:PRO:HD3	1.97	0.45
2:L:284:ASP:N	2:L:288:GLN:O	2.47	0.45
2:L:323:THR:HB	4:L:434:HOH:O	2.17	0.45
1:A:43:ASP:OD2	2:B:289:ILE:HG13	2.17	0.45
1:C:10:TYR:O	1:C:11:LEU:HD23	2.17	0.45
2:D:67:LYS:NZ	1:E:246:LEU:O	2.25	0.45
2:J:356:LEU:O	2:J:356:LEU:HD22	2.17	0.45
2:B:81:HIS:NE2	2:B:231:ASN:HB3	2.32	0.45
2:D:81:HIS:NE2	2:D:231:ASN:HB3	2.32	0.45
1:I:61:ASN:N	1:I:61:ASN:HD22	2.13	0.45
1:I:148:ARG:HG3	1:I:148:ARG:HH11	1.81	0.45
1:I:184:ARG:HG3	1:I:184:ARG:HH11	1.82	0.45
2:J:275:HIS:HD2	2:J:301:TYR:OH	1.99	0.45
1:E:67:GLU:O	1:E:71:ILE:HG13	2.17	0.44
2:J:122:GLY:HA3	2:L:58:ARG:NH2	2.00	0.44
2:F:192:TYR:HB2	2:F:193:PRO:HD3	1.99	0.44
1:G:50:THR:HG22	1:G:224:VAL:CG2	2.45	0.44
1:I:238:LEU:O	1:I:242:VAL:HG23	2.18	0.44
2:J:360:MET:HB3	2:J:364:GLU:OE2	2.17	0.44
1:K:148:ARG:HG3	1:K:148:ARG:HH11	1.82	0.44
1:K:248:ILE:HG13	1:K:248:ILE:O	2.17	0.44
2:L:60:THR:HG22	2:L:68:ILE:CB	2.47	0.44
2:L:211:ILE:HG21	2:L:219:PRO:HD3	1.98	0.44
2:F:140:ASN:HD22	2:F:140:ASN:HA	1.58	0.44
2:J:141:VAL:HG13	2:J:151:VAL:HG11	1.98	0.44
2:B:237:TYR:HB3	2:B:238:PRO:CD	2.44	0.44
1:C:31:TYR:HB3	1:C:246:LEU:CD1	2.47	0.44
1:E:146:ASP:O	1:E:150:LYS:HG3	2.16	0.44
2:F:208:LYS:O	2:F:211:ILE:HG22	2.18	0.44
2:F:299:LEU:HD23	2:F:348:HIS:CD2	2.53	0.44
2:B:18:PRO:HG3	2:B:176:PHE:CD2	2.52	0.44
2:B:360:MET:HB3	2:B:364:GLU:OE2	2.18	0.44
2:D:190:HIS:ND1	2:D:191:PRO:HA	2.32	0.44
2:D:233:MET:HE1	2:D:308:HIS:CD2	2.53	0.44
1:K:50:THR:HG22	1:K:224:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:ASN:HA	2:D:159:ARG:HD2	1.99	0.44
2:D:159:ARG:HH11	2:D:159:ARG:HG3	1.83	0.44
2:F:81:HIS:NE2	2:F:231:ASN:HB3	2.32	0.44
1:K:77:ARG:HG2	1:K:77:ARG:HH11	1.82	0.44
2:L:231:ASN:ND2	4:L:429:HOH:O	2.51	0.44
2:B:104:GLU:HA	2:B:128:TYR:O	2.17	0.44
2:H:30:LYS:HE3	2:H:31:ASP:OD1	2.18	0.44
2:H:382:LEU:HD13	2:H:382:LEU:C	2.38	0.44
2:H:104:GLU:HA	2:H:128:TYR:O	2.18	0.44
2:H:190:HIS:ND1	2:H:191:PRO:HA	2.32	0.44
2:H:211:ILE:HG21	2:H:219:PRO:HD3	1.99	0.44
2:L:157:GLY:HA3	2:L:163:ASP:OD1	2.18	0.44
1:C:50:THR:HG22	1:C:224:VAL:CG2	2.47	0.44
1:E:50:THR:HG22	1:E:224:VAL:CG2	2.47	0.44
1:E:94:ARG:HD3	2:F:287:GLY:HA3	1.99	0.44
1:E:148:ARG:HG3	1:E:148:ARG:HH11	1.82	0.44
1:E:170:GLY:O	1:E:171:ALA:C	2.55	0.44
1:I:172:ARG:C	1:I:173:GLU:CG	2.86	0.44
2:L:1:MET:HB2	2:L:190:HIS:CB	2.48	0.44
2:L:299:LEU:HD23	2:L:348:HIS:CD2	2.51	0.44
1:C:200:VAL:HG13	1:C:205:HIS:HB2	2.00	0.43
1:C:208:SER:O	1:C:212:GLU:HG2	2.18	0.43
2:D:356:LEU:HD22	2:D:356:LEU:O	2.17	0.43
1:E:86:MET:HE3	1:E:113:LEU:HD23	2.00	0.43
2:H:293:HIS:CG	2:H:294:SER:N	2.86	0.43
1:K:29:ASP:OD1	1:K:79:SER:HB2	2.18	0.43
2:J:293:HIS:CG	2:J:294:SER:N	2.86	0.43
2:L:237:TYR:HB3	2:L:238:PRO:CD	2.44	0.43
1:A:50:THR:HG22	1:A:224:VAL:CG2	2.46	0.43
2:B:89:GLN:CD	2:B:182:LEU:HD13	2.38	0.43
2:B:190:HIS:ND1	2:B:191:PRO:HA	2.34	0.43
2:D:186:VAL:HB	4:D:402:HOH:O	2.18	0.43
1:E:77:ARG:HH11	1:E:77:ARG:HG2	1.83	0.43
2:F:267:ASN:O	2:F:268:ALA:HB2	2.18	0.43
2:H:60:THR:HG22	2:H:68:ILE:CB	2.49	0.43
2:J:284:ASP:OD2	2:J:285:GLU:N	2.50	0.43
2:L:190:HIS:CG	2:L:191:PRO:HA	2.53	0.43
1:A:86:MET:HE3	1:A:113:LEU:HD23	2.00	0.43
2:H:155:ASN:HA	2:H:159:ARG:HD2	2.00	0.43
1:K:238:LEU:O	1:K:242:VAL:HG23	2.18	0.43
2:L:293:HIS:CG	2:L:294:SER:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:ASN:O	2:D:268:ALA:HB2	2.19	0.43
2:F:211:ILE:HG21	2:F:219:PRO:HD3	2.00	0.43
1:A:208:SER:O	1:A:212:GLU:HG2	2.18	0.43
2:D:217:GLN:HE22	1:E:5:GLY:HA3	1.81	0.43
2:F:130:GLY:O	2:F:134:VAL:HG23	2.18	0.43
1:I:42:SER:N	2:J:288:GLN:NE2	2.63	0.43
1:I:77:ARG:HG2	1:I:77:ARG:HH11	1.83	0.43
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.84	0.43
2:B:323:THR:HB	4:B:414:HOH:O	2.18	0.43
2:D:132:GLU:HB2	2:D:159:ARG:O	2.19	0.43
2:F:190:HIS:ND1	2:F:191:PRO:HA	2.34	0.43
2:J:322:VAL:CG1	2:J:326:GLU:HB2	2.49	0.43
2:J:382:LEU:HD13	2:J:382:LEU:C	2.38	0.43
2:L:132:GLU:HB2	2:L:159:ARG:O	2.19	0.43
2:L:322:VAL:CG1	2:L:326:GLU:HB2	2.48	0.43
2:B:322:VAL:CG1	2:B:326:GLU:HB2	2.49	0.43
2:D:30:LYS:HE3	2:D:31:ASP:OD1	2.19	0.43
1:E:29:ASP:OD1	1:E:79:SER:HB2	2.19	0.43
2:F:257:LEU:HD23	2:F:257:LEU:HA	1.87	0.43
2:F:382:LEU:HD13	2:F:382:LEU:C	2.39	0.43
1:G:43:ASP:OD2	2:H:289:ILE:HG13	2.19	0.43
1:K:42:SER:N	2:L:288:GLN:NE2	2.65	0.43
2:L:130:GLY:O	2:L:134:VAL:HG23	2.19	0.43
1:C:148:ARG:HG3	1:C:148:ARG:HH11	1.84	0.43
1:G:31:TYR:HB3	1:G:246:LEU:CD1	2.49	0.43
2:H:140:ASN:HD22	2:H:140:ASN:HA	1.58	0.43
1:I:121:HIS:HE1	4:I:260:HOH:O	2.02	0.43
1:I:188:ARG:O	1:I:188:ARG:HG2	2.19	0.43
2:B:267:ASN:O	2:B:268:ALA:HB2	2.19	0.42
2:J:60:THR:HG22	2:J:68:ILE:CB	2.49	0.42
2:J:190:HIS:ND1	2:J:191:PRO:HA	2.34	0.42
1:K:7:LEU:HD22	1:K:246:LEU:HG	2.01	0.42
2:B:382:LEU:C	2:B:382:LEU:HD13	2.39	0.42
2:D:157:GLY:HA3	2:D:163:ASP:OD1	2.20	0.42
2:B:155:ASN:HA	2:B:159:ARG:HD2	2.01	0.42
1:C:29:ASP:OD1	1:C:79:SER:HB2	2.19	0.42
2:D:275:HIS:HD2	2:D:301:TYR:OH	2.02	0.42
1:E:5:GLY:HA2	1:E:210:LEU:HD22	2.00	0.42
2:F:155:ASN:HA	2:F:159:ARG:HD2	2.01	0.42
2:J:132:GLU:OE1	2:J:136:ARG:NH2	2.52	0.42
2:L:201:SER:HB2	2:L:205:ARG:NH2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD22	1:A:35:ILE:HG21	2.02	0.42
2:B:130:GLY:O	2:B:134:VAL:HG23	2.20	0.42
1:C:25:LEU:HD22	1:C:35:ILE:HG21	2.01	0.42
2:H:94:LYS:HE2	2:H:121:LEU:O	2.20	0.42
2:J:19:LEU:HD12	2:J:19:LEU:HA	1.88	0.42
2:J:140:ASN:HD22	2:J:140:ASN:HA	1.58	0.42
2:D:293:HIS:CG	2:D:294:SER:N	2.87	0.42
2:J:201:SER:HB2	2:J:205:ARG:NH2	2.34	0.42
2:L:18:PRO:HG3	2:L:176:PHE:CG	2.55	0.42
2:L:131:ALA:HB3	2:L:159:ARG:HE	1.84	0.42
2:D:43:LEU:O	2:D:47:ALA:HB3	2.19	0.42
2:D:299:LEU:HD23	2:D:348:HIS:CD2	2.54	0.42
2:D:322:VAL:CG1	2:D:326:GLU:HB2	2.49	0.42
2:F:94:LYS:HE2	2:F:121:LEU:O	2.20	0.42
2:H:267:ASN:O	2:H:268:ALA:HB2	2.18	0.42
1:K:25:LEU:HD22	1:K:35:ILE:HG21	2.00	0.42
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.84	0.42
2:D:58:ARG:NE	4:D:416:HOH:O	2.50	0.42
2:D:382:LEU:C	2:D:382:LEU:HD13	2.40	0.42
2:L:104:GLU:HA	2:L:128:TYR:O	2.20	0.42
1:G:208:SER:O	1:G:212:GLU:HG2	2.20	0.42
1:G:211:LYS:HB2	1:G:211:LYS:HE3	1.83	0.42
2:H:190:HIS:CG	2:H:191:PRO:HA	2.55	0.42
1:I:211:LYS:HE3	1:I:211:LYS:HB2	1.82	0.42
2:J:324:ASP:O	2:J:328:LEU:HB2	2.19	0.42
1:K:156:THR:HG21	1:K:159:PHE:C	2.40	0.42
2:B:181:TYR:CE2	2:B:183:ILE:CD1	3.03	0.42
2:D:324:ASP:O	2:D:328:LEU:HB2	2.20	0.42
2:H:159:ARG:HG3	2:H:159:ARG:HH11	1.85	0.42
1:I:8:ILE:O	1:I:218:VAL:HA	2.19	0.42
1:C:90:ASN:HD21	2:D:283:GLN:HE21	1.68	0.42
1:E:204:GLU:H	1:E:204:GLU:HG3	1.59	0.42
2:F:109:GLN:OE1	3:F:400:PLP:O3	2.37	0.42
2:J:267:ASN:O	2:J:268:ALA:HB2	2.18	0.42
1:K:8:ILE:O	1:K:218:VAL:HA	2.19	0.42
2:B:60:THR:HG22	2:B:68:ILE:CB	2.50	0.41
1:E:31:TYR:HB3	1:E:246:LEU:CD1	2.50	0.41
1:E:211:LYS:HB2	1:E:211:LYS:HE3	1.85	0.41
2:H:141:VAL:HG13	2:H:151:VAL:HG11	2.02	0.41
2:J:81:HIS:NE2	2:J:231:ASN:HB3	2.34	0.41
2:J:94:LYS:HE2	2:J:121:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159:ARG:HG3	2:L:159:ARG:HH11	1.85	0.41
2:L:328:LEU:HD12	2:L:328:LEU:HA	1.94	0.41
1:A:42:SER:N	2:B:288:GLN:NE2	2.64	0.41
2:B:211:ILE:HG21	2:B:219:PRO:HD3	2.01	0.41
2:B:293:HIS:CG	2:B:294:SER:N	2.88	0.41
1:C:31:TYR:HB3	1:C:246:LEU:HD11	2.02	0.41
2:H:207:ALA:HA	2:H:210:GLN:HE21	1.84	0.41
1:C:158:GLY:O	1:C:159:PHE:HB3	2.21	0.41
2:D:104:GLU:HA	2:D:128:TYR:O	2.20	0.41
2:F:336:ARG:O	4:F:423:HOH:O	2.22	0.41
2:L:132:GLU:OE1	2:L:136:ARG:NH2	2.53	0.41
2:B:207:ALA:HA	2:B:210:GLN:HE21	1.85	0.41
1:C:211:LYS:HB2	1:C:211:LYS:HE3	1.81	0.41
2:D:109:GLN:NE2	2:D:376:LYS:HD2	2.36	0.41
2:D:130:GLY:O	2:D:134:VAL:HG23	2.20	0.41
2:F:104:GLU:HA	2:F:128:TYR:O	2.20	0.41
2:F:215:GLU:HG3	2:F:365:ILE:HD13	2.02	0.41
2:F:369:ASN:HD22	2:F:369:ASN:HA	1.69	0.41
1:G:148:ARG:HH11	1:G:148:ARG:HG3	1.85	0.41
2:H:19:LEU:HD12	2:H:19:LEU:HA	1.91	0.41
1:A:8:ILE:O	1:A:218:VAL:HA	2.20	0.41
1:A:61:ASN:N	1:A:61:ASN:ND2	2.69	0.41
1:A:188:ARG:O	1:A:188:ARG:HG2	2.21	0.41
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.94	0.41
2:D:190:HIS:CG	2:D:191:PRO:HA	2.55	0.41
1:E:208:SER:O	1:E:212:GLU:HG2	2.21	0.41
2:F:43:LEU:HD12	2:F:43:LEU:HA	1.92	0.41
1:G:188:ARG:O	1:G:188:ARG:HG2	2.20	0.41
2:L:94:LYS:HE2	2:L:121:LEU:O	2.20	0.41
1:A:158:GLY:O	1:A:159:PHE:HB3	2.20	0.41
2:B:43:LEU:O	2:B:47:ALA:HB3	2.21	0.41
2:B:215:GLU:HG3	2:B:365:ILE:HD13	2.03	0.41
2:D:237:TYR:HB3	2:D:238:PRO:CD	2.44	0.41
1:G:149:LEU:HD23	1:G:149:LEU:HA	1.90	0.41
2:J:208:LYS:O	2:J:211:ILE:HG22	2.21	0.41
1:C:8:ILE:O	1:C:218:VAL:HA	2.20	0.41
2:H:132:GLU:OE1	2:H:136:ARG:NH2	2.54	0.41
2:H:324:ASP:O	2:H:328:LEU:HB2	2.19	0.41
2:L:252:ALA:HB1	4:L:406:HOH:O	2.20	0.41
1:A:7:LEU:HD12	1:A:7:LEU:HA	1.94	0.41
1:A:141:ALA:CB	2:B:14:THR:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:CG2	2:B:161:LEU:N	2.80	0.41
1:C:61:ASN:N	1:C:61:ASN:ND2	2.69	0.41
2:D:18:PRO:HG3	2:D:176:PHE:CG	2.56	0.41
2:D:67:LYS:HE2	1:E:248:ILE:HG13	2.03	0.41
2:D:181:TYR:CE2	2:D:183:ILE:CD1	3.03	0.41
1:I:50:THR:HG22	1:I:224:VAL:CG2	2.49	0.41
2:J:58:ARG:HD2	2:J:337:THR:CG2	2.50	0.41
1:K:188:ARG:O	1:K:188:ARG:HG2	2.20	0.41
2:B:38:GLN:HE21	2:B:38:GLN:HB3	1.66	0.41
2:B:186:VAL:HB	4:B:416:HOH:O	2.21	0.41
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.87	0.41
2:D:58:ARG:HD2	2:D:337:THR:CG2	2.50	0.41
2:D:137:GLN:HA	2:D:137:GLN:NE2	2.36	0.41
2:J:1:MET:HB2	2:J:190:HIS:CG	2.56	0.41
2:J:13:GLU:N	4:J:423:HOH:O	2.49	0.41
2:L:384:VAL:CG2	2:L:385:SER:H	2.34	0.41
2:B:382:LEU:HD23	2:D:142:PHE:CD1	2.56	0.40
1:C:49:LYS:HE3	2:D:167:GLU:OE2	2.21	0.40
1:C:94:ARG:HD2	2:D:283:GLN:HE22	1.86	0.40
2:D:132:GLU:OE1	2:D:136:ARG:NH2	2.54	0.40
2:D:154:VAL:HG11	2:D:164:ALA:HA	2.03	0.40
2:D:360:MET:HB3	2:D:364:GLU:OE2	2.20	0.40
2:F:18:PRO:HG3	2:F:176:PHE:CG	2.56	0.40
2:F:190:HIS:CG	2:F:191:PRO:HA	2.56	0.40
1:G:61:ASN:N	1:G:61:ASN:ND2	2.68	0.40
2:H:322:VAL:CG1	2:H:326:GLU:HB2	2.50	0.40
2:H:360:MET:HB3	2:H:364:GLU:OE2	2.21	0.40
2:J:160:THR:CG2	2:J:161:LEU:N	2.79	0.40
2:J:299:LEU:HD23	2:J:348:HIS:CD2	2.55	0.40
2:J:382:LEU:HB2	2:L:142:PHE:CE2	2.55	0.40
2:L:1:MET:CB	2:L:190:HIS:CG	3.03	0.40
2:L:378:LEU:HD23	2:L:378:LEU:HA	1.87	0.40
2:B:39:LEU:O	2:B:43:LEU:HD22	2.20	0.40
2:B:43:LEU:HD12	2:B:43:LEU:HA	1.97	0.40
2:D:19:LEU:O	2:D:23:GLU:HG3	2.21	0.40
2:D:57:LYS:HE3	2:D:57:LYS:HB3	1.92	0.40
2:F:224:ALA:HA	4:F:432:HOH:O	2.21	0.40
1:I:86:MET:HE3	1:I:113:LEU:HD23	2.02	0.40
2:J:45:THR:O	2:L:54:TYR:HB2	2.22	0.40
2:L:57:LYS:HE3	2:L:57:LYS:HB3	1.87	0.40
1:A:29:ASP:OD1	1:A:79:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:SER:HB2	2:F:205:ARG:NH2	2.34	0.40
2:F:237:TYR:HB3	2:F:238:PRO:CD	2.44	0.40
2:F:334:LEU:HD23	2:F:334:LEU:HA	1.96	0.40
1:I:16:PRO:HD3	4:I:254:HOH:O	2.22	0.40
1:I:121:HIS:CE1	4:I:260:HOH:O	2.74	0.40
2:J:131:ALA:HB3	2:J:159:ARG:HE	1.85	0.40
2:L:255:LYS:HB2	2:L:261:LYS:HB2	2.03	0.40
2:B:132:GLU:OE1	2:B:136:ARG:NH2	2.55	0.40
2:B:384:VAL:CG2	2:B:385:SER:H	2.35	0.40
1:C:225:LYS:O	1:C:229:GLU:HG3	2.21	0.40
2:F:1:MET:HB2	2:F:190:HIS:CG	2.56	0.40
2:F:154:VAL:HG11	2:F:164:ALA:HA	2.04	0.40
1:G:90:ASN:HD21	2:H:283:GLN:HE22	1.70	0.40
1:I:29:ASP:OD1	1:I:79:SER:HB2	2.21	0.40
2:D:94:LYS:HE2	2:D:121:LEU:O	2.22	0.40
1:G:8:ILE:HA	1:G:9:PRO:HD3	1.94	0.40
2:H:255:LYS:HB2	2:H:261:LYS:HB2	2.02	0.40
1:I:208:SER:O	1:I:212:GLU:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ARG:NH2	2:L:98:LYS:O[4_466]	2.11	0.09

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	A	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
1	C	237/248 (96%)	226 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	246/248 (99%)	230 (94%)	15 (6%)	1 (0%)	34	72
1	G	238/248 (96%)	228 (96%)	10 (4%)	0	100	100
1	I	240/248 (97%)	228 (95%)	12 (5%)	0	100	100
1	K	230/248 (93%)	219 (95%)	11 (5%)	0	100	100
2	B	383/385 (100%)	352 (92%)	29 (8%)	2 (0%)	29	68
2	D	383/385 (100%)	355 (93%)	25 (6%)	3 (1%)	19	57
2	F	383/385 (100%)	354 (92%)	27 (7%)	2 (0%)	29	68
2	H	383/385 (100%)	358 (94%)	22 (6%)	3 (1%)	19	57
2	J	383/385 (100%)	357 (93%)	24 (6%)	2 (0%)	29	68
2	L	383/385 (100%)	356 (93%)	24 (6%)	3 (1%)	19	57
All	All	3726/3798 (98%)	3489 (94%)	221 (6%)	16 (0%)	34	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	171	ALA
2	J	268	ALA
2	L	268	ALA
2	B	268	ALA
2	D	186	VAL
2	D	268	ALA
2	F	186	VAL
2	F	268	ALA
2	H	186	VAL
2	H	268	ALA
2	L	186	VAL
2	B	186	VAL
2	J	186	VAL
2	D	259	SER
2	H	259	SER
2	L	259	SER

5.3.2 Protein sidechains (i)

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	A	201/205 (98%)	193 (96%)	8 (4%)	31	68
1	C	201/205 (98%)	194 (96%)	7 (4%)	36	71
1	E	205/205 (100%)	196 (96%)	9 (4%)	28	65
1	G	202/205 (98%)	195 (96%)	7 (4%)	36	71
1	I	203/205 (99%)	196 (97%)	7 (3%)	37	72
1	K	194/205 (95%)	189 (97%)	5 (3%)	46	78
2	B	306/306 (100%)	285 (93%)	21 (7%)	15	48
2	D	306/306 (100%)	287 (94%)	19 (6%)	18	52
2	F	306/306 (100%)	287 (94%)	19 (6%)	18	52
2	H	306/306 (100%)	286 (94%)	20 (6%)	17	50
2	J	306/306 (100%)	286 (94%)	20 (6%)	17	50
2	L	306/306 (100%)	286 (94%)	20 (6%)	17	50
All	All	3042/3066 (99%)	2880 (95%)	162 (5%)	22	58

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	92	ILE
1	A	139	LEU
1	A	149	LEU
1	A	166	TYR
1	A	173	GLU
1	A	178	THR
1	A	182	LEU
2	B	1	MET
2	B	19	LEU
2	B	43	LEU
2	B	57	LYS
2	B	58	ARG
2	B	104	GLU
2	B	139	MET
2	B	151	VAL
2	B	154	VAL
2	B	169	LEU
2	B	177	GLU
2	B	182	LEU

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Mol	Chain	Res	Type
2	B	194	THR
2	B	278	LEU
2	B	286	GLU
2	B	288	GLN
2	B	299	LEU
2	B	316	ARG
2	B	328	LEU
2	B	334	LEU
2	B	356	LEU
1	C	66	ARG
1	C	92	ILE
1	C	139	LEU
1	C	149	LEU
1	C	166	TYR
1	C	178	THR
1	C	182	LEU
2	D	19	LEU
2	D	43	LEU
2	D	57	LYS
2	D	58	ARG
2	D	104	GLU
2	D	139	MET
2	D	151	VAL
2	D	154	VAL
2	D	169	LEU
2	D	177	GLU
2	D	182	LEU
2	D	194	THR
2	D	278	LEU
2	D	286	GLU
2	D	288	GLN
2	D	299	LEU
2	D	316	ARG
2	D	334	LEU
2	D	356	LEU
1	E	66	ARG
1	E	92	ILE
1	E	139	LEU
1	E	149	LEU
1	E	166	TYR
1	E	168	THR
1	E	173	GLU

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Mol	Chain	Res	Type
1	E	178	THR
1	E	182	LEU
2	F	19	LEU
2	F	43	LEU
2	F	57	LYS
2	F	58	ARG
2	F	104	GLU
2	F	139	MET
2	F	151	VAL
2	F	154	VAL
2	F	169	LEU
2	F	177	GLU
2	F	182	LEU
2	F	194	THR
2	F	278	LEU
2	F	286	GLU
2	F	288	GLN
2	F	299	LEU
2	F	316	ARG
2	F	334	LEU
2	F	356	LEU
1	G	66	ARG
1	G	139	LEU
1	G	149	LEU
1	G	166	TYR
1	G	173	GLU
1	G	178	THR
1	G	182	LEU
2	H	19	LEU
2	H	43	LEU
2	H	57	LYS
2	H	58	ARG
2	H	104	GLU
2	H	139	MET
2	H	151	VAL
2	H	154	VAL
2	H	169	LEU
2	H	177	GLU
2	H	182	LEU
2	H	194	THR
2	H	265	SER
2	H	278	LEU

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Mol	Chain	Res	Type
2	H	286	GLU
2	H	288	GLN
2	H	299	LEU
2	H	316	ARG
2	H	334	LEU
2	H	356	LEU
1	I	66	ARG
1	I	139	LEU
1	I	149	LEU
1	I	166	TYR
1	I	173	GLU
1	I	178	THR
1	I	182	LEU
2	J	19	LEU
2	J	43	LEU
2	J	57	LYS
2	J	58	ARG
2	J	104	GLU
2	J	139	MET
2	J	151	VAL
2	J	154	VAL
2	J	169	LEU
2	J	177	GLU
2	J	182	LEU
2	J	194	THR
2	J	278	LEU
2	J	286	GLU
2	J	288	GLN
2	J	299	LEU
2	J	316	ARG
2	J	334	LEU
2	J	356	LEU
2	J	369	ASN
1	K	66	ARG
1	K	92	ILE
1	K	139	LEU
1	K	149	LEU
1	K	182	LEU
2	L	19	LEU
2	L	43	LEU
2	L	57	LYS
2	L	58	ARG

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Mol	Chain	Res	Type
2	L	104	GLU
2	L	139	MET
2	L	151	VAL
2	L	154	VAL
2	L	169	LEU
2	L	177	GLU
2	L	182	LEU
2	L	194	THR
2	L	278	LEU
2	L	286	GLU
2	L	288	GLN
2	L	299	LEU
2	L	316	ARG
2	L	334	LEU
2	L	356	LEU
2	L	369	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	99	ASN
1	A	192	ASN
2	B	38	GLN
2	B	77	HIS
2	B	137	GLN
2	B	140	ASN
2	B	210	GLN
2	B	217	GLN
2	B	262	HIS
2	B	267	ASN
2	B	275	HIS
2	B	283	GLN
2	B	288	GLN
2	B	308	HIS
2	B	348	HIS
2	B	369	ASN
1	C	61	ASN
1	C	99	ASN
1	C	192	ASN
2	D	38	GLN
2	D	77	HIS

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Mol	Chain	Res	Type
2	D	137	GLN
2	D	140	ASN
2	D	166	ASN
2	D	210	GLN
2	D	217	GLN
2	D	262	HIS
2	D	267	ASN
2	D	275	HIS
2	D	283	GLN
2	D	288	GLN
2	D	308	HIS
2	D	348	HIS
2	D	369	ASN
1	E	61	ASN
1	E	99	ASN
1	E	192	ASN
2	F	38	GLN
2	F	77	HIS
2	F	109	GLN
2	F	137	GLN
2	F	140	ASN
2	F	210	GLN
2	F	217	GLN
2	F	262	HIS
2	F	267	ASN
2	F	275	HIS
2	F	283	GLN
2	F	288	GLN
2	F	308	HIS
2	F	348	HIS
2	F	369	ASN
1	G	61	ASN
1	G	99	ASN
1	G	192	ASN
2	H	38	GLN
2	H	77	HIS
2	H	137	GLN
2	H	140	ASN
2	H	210	GLN
2	H	217	GLN
2	H	262	HIS
2	H	267	ASN

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Mol	Chain	Res	Type
2	H	275	HIS
2	H	283	GLN
2	H	288	GLN
2	H	308	HIS
2	H	348	HIS
2	H	369	ASN
1	I	61	ASN
1	I	99	ASN
1	I	192	ASN
2	J	38	GLN
2	J	77	HIS
2	J	137	GLN
2	J	140	ASN
2	J	210	GLN
2	J	217	GLN
2	J	262	HIS
2	J	267	ASN
2	J	275	HIS
2	J	283	GLN
2	J	288	GLN
2	J	308	HIS
2	J	348	HIS
2	J	369	ASN
1	K	61	ASN
1	K	99	ASN
1	K	192	ASN
2	L	38	GLN
2	L	77	HIS
2	L	137	GLN
2	L	140	ASN
2	L	210	GLN
2	L	217	GLN
2	L	262	HIS
2	L	267	ASN
2	L	275	HIS
2	L	283	GLN
2	L	288	GLN
2	L	308	HIS
2	L	348	HIS
2	L	369	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	PLP	L	400	2	15,15,16	1.61	5 (33%)	20,22,23	1.97	5 (25%)
3	PLP	B	400	2	15,15,16	1.64	3 (20%)	20,22,23	1.95	4 (20%)
3	PLP	J	400	2	15,15,16	1.68	4 (26%)	20,22,23	1.91	3 (15%)
3	PLP	F	400	2	15,15,16	1.52	4 (26%)	20,22,23	1.98	4 (20%)
3	PLP	D	400	2	15,15,16	1.60	3 (20%)	20,22,23	2.07	5 (25%)
3	PLP	H	400	2	15,15,16	1.71	5 (33%)	20,22,23	1.93	6 (30%)

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
3	PLP	L	400	2	-	0/6/6/8	0/1/1/1
3	PLP	B	400	2	-	0/6/6/8	0/1/1/1
3	PLP	J	400	2	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	F	400	2	-	0/6/6/8	0/1/1/1
3	PLP	D	400	2	-	0/6/6/8	0/1/1/1
3	PLP	H	400	2	-	0/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	400	PLP	C5-C4	3.17	1.44	1.40
3	B	400	PLP	C5-C4	3.16	1.44	1.40
3	J	400	PLP	C2-N1	3.01	1.39	1.33
3	D	400	PLP	C2-N1	2.87	1.39	1.33
3	J	400	PLP	C5-C4	2.83	1.43	1.40
3	D	400	PLP	C3-C2	-2.71	1.38	1.40
3	L	400	PLP	C2-N1	2.67	1.38	1.33
3	H	400	PLP	C2-N1	2.63	1.38	1.33
3	L	400	PLP	C3-C2	-2.62	1.38	1.40
3	B	400	PLP	C2-N1	2.61	1.38	1.33
3	F	400	PLP	C5-C4	2.41	1.43	1.40
3	B	400	PLP	P-O3P	-2.40	1.45	1.54
3	H	400	PLP	P-O3P	-2.39	1.45	1.54
3	F	400	PLP	C2-N1	2.35	1.38	1.33
3	J	400	PLP	C3-C2	-2.34	1.38	1.40
3	F	400	PLP	P-O3P	-2.29	1.46	1.54
3	D	400	PLP	P-O3P	-2.25	1.46	1.54
3	L	400	PLP	P-O3P	-2.12	1.46	1.54
3	F	400	PLP	C6-N1	2.10	1.38	1.34
3	L	400	PLP	C4A-C4	2.07	1.55	1.51
3	H	400	PLP	C2A-C2	2.06	1.53	1.50
3	J	400	PLP	P-O3P	-2.06	1.46	1.54
3	H	400	PLP	C6-N1	2.05	1.38	1.34
3	L	400	PLP	C5-C4	2.04	1.42	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	400	PLP	O4P-C5A-C5	5.94	120.66	109.35
3	F	400	PLP	O4P-C5A-C5	5.78	120.36	109.35
3	L	400	PLP	O4P-C5A-C5	5.75	120.31	109.35
3	J	400	PLP	O4P-C5A-C5	5.58	119.99	109.35
3	H	400	PLP	O4P-C5A-C5	5.49	119.82	109.35
3	B	400	PLP	O4P-C5A-C5	5.38	119.60	109.35
3	D	400	PLP	C2A-C2-C3	4.05	125.89	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	PLP	C2A-C2-C3	3.95	125.76	120.89
3	L	400	PLP	C2A-C2-C3	3.93	125.75	120.89
3	F	400	PLP	C2A-C2-C3	3.79	125.57	120.89
3	H	400	PLP	C2A-C2-C3	3.74	125.50	120.89
3	J	400	PLP	C2A-C2-C3	3.67	125.42	120.89
3	F	400	PLP	C6-C5-C4	-2.77	115.97	118.16
3	B	400	PLP	C6-C5-C4	-2.67	116.06	118.16
3	J	400	PLP	C6-C5-C4	-2.61	116.11	118.16
3	L	400	PLP	C6-C5-C4	-2.44	116.24	118.16
3	H	400	PLP	C6-C5-C4	-2.39	116.28	118.16
3	D	400	PLP	C6-C5-C4	-2.34	116.32	118.16
3	D	400	PLP	C4-C3-C2	2.25	123.41	120.07
3	H	400	PLP	C3-C2-N1	-2.23	117.89	120.77
3	H	400	PLP	C4-C3-C2	2.20	123.33	120.07
3	L	400	PLP	C5A-C5-C6	-2.15	115.84	119.37
3	F	400	PLP	C4-C3-C2	2.11	123.19	120.07
3	H	400	PLP	C5A-C5-C6	-2.07	115.97	119.37
3	B	400	PLP	C5A-C5-C6	-2.06	115.99	119.37
3	L	400	PLP	C4-C3-C2	2.06	123.12	120.07
3	D	400	PLP	C5A-C5-C6	-2.02	116.05	119.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	400	PLP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.