Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 AM GMT

PDB ID	:	2QJP
Title	:	Crystal structure of wild type rhodobacter sphaeroides with stigmatellin and antimycin inhibited
Authors	:	Esser, L.; Xia, D.
Deposited on	:	2007-07-08
Resolution	:	2.60 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:

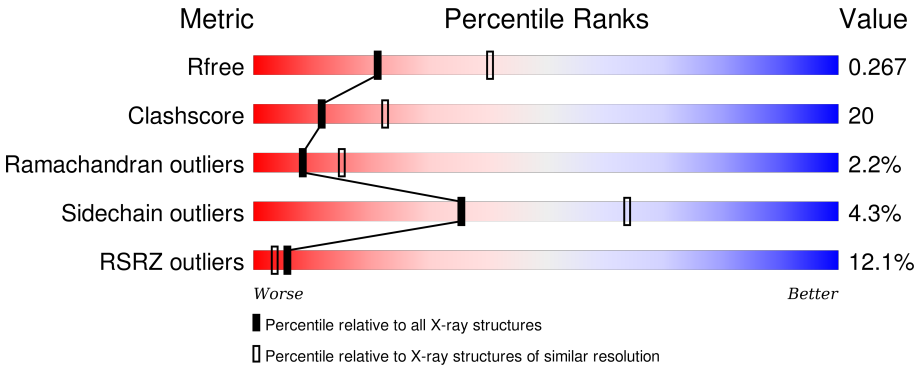
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	A	428	6% 65% 32% ·
1	D	428	7% 63% 35% ·
1	G	428	4% 64% 34% ·
1	J	428	4% 69% 29% ·
2	B	256	16% 61% 36% ·

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Mol	Chain	Length	Quality of chain
2	E	256	24% 58% 38%
2	H	256	15% 54% 42%
2	K	256	20% 61% 35%
3	C	179	14% 60% 35% 5%
3	F	179	25% 54% 41% 5%
3	I	179	12% 58% 39%
3	L	179	24% 56% 37% 6%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28227 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 Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			
1	D	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			
1	G	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			
1	J	428	Total	C	N	O	S	0	0	0
			3435	2319	545	556	15			

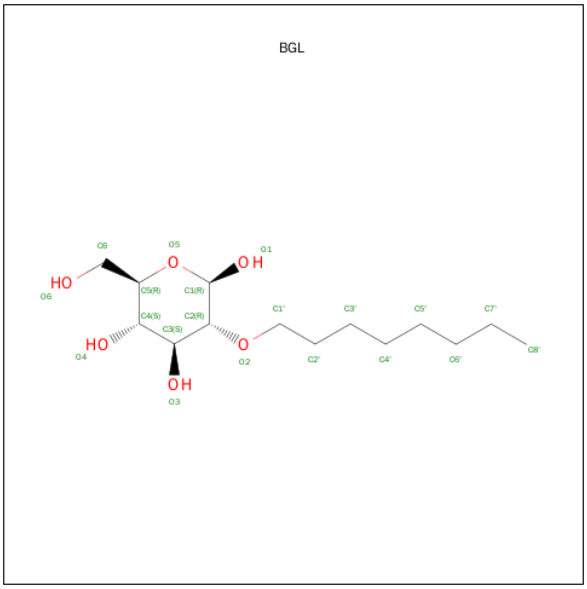
- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	E	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	H	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			
2	K	256	Total	C	N	O	S	0	0	0
			1953	1240	326	374	13			

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			
3	F	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			
3	I	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			
3	L	179	Total	C	N	O	S	0	0	0
			1341	845	237	253	6			

- Molecule 4 is Lauryl-oleoyl-phosphatidyl ethanolamine (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).

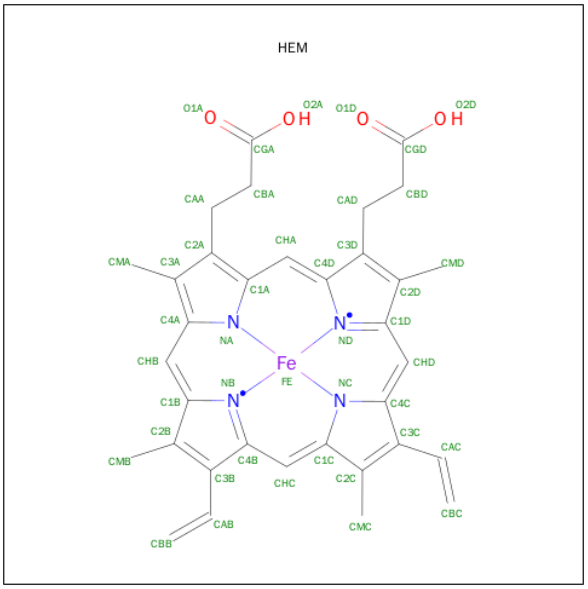


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0
4	E	1	Total C O 20 14 6	0	0
4	G	1	Total C O 20 14 6	0	0
4	J	1	Total C O 20 14 6	0	0

- Molecule 5 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

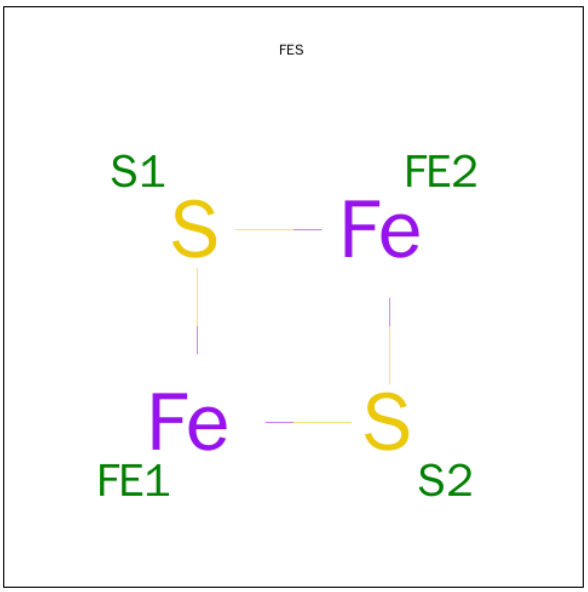
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Sr 1 1	0	0
5	J	1	Total Sr 1 1	0	0
5	K	1	Total Sr 1 1	0	0
5	E	1	Total Sr 1 1	0	0
5	H	1	Total Sr 1 1	0	0
5	B	1	Total Sr 1 1	0	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



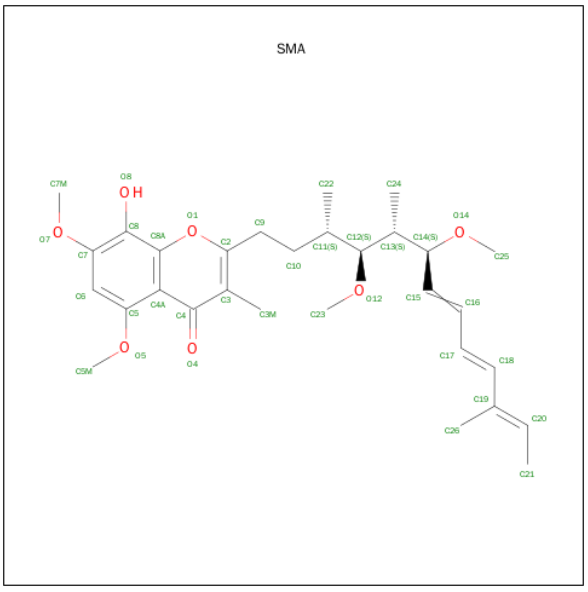
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



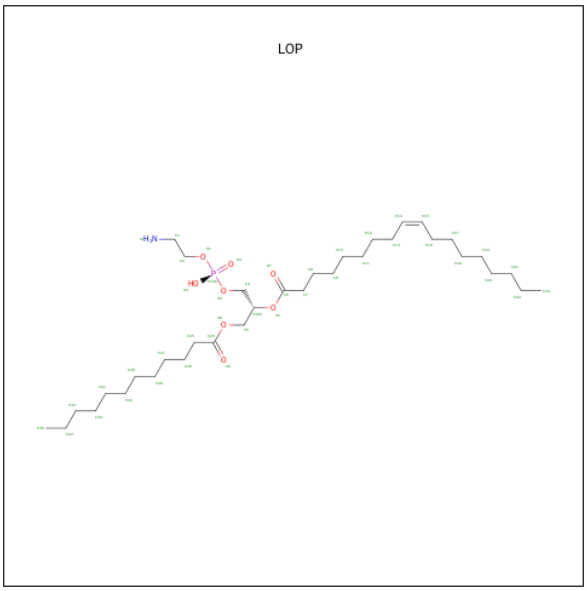
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Fe S 4 2 2	0	0
7	F	1	Total Fe S 4 2 2	0	0
7	I	1	Total Fe S 4 2 2	0	0
7	L	1	Total Fe S 4 2 2	0	0

- Molecule 8 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



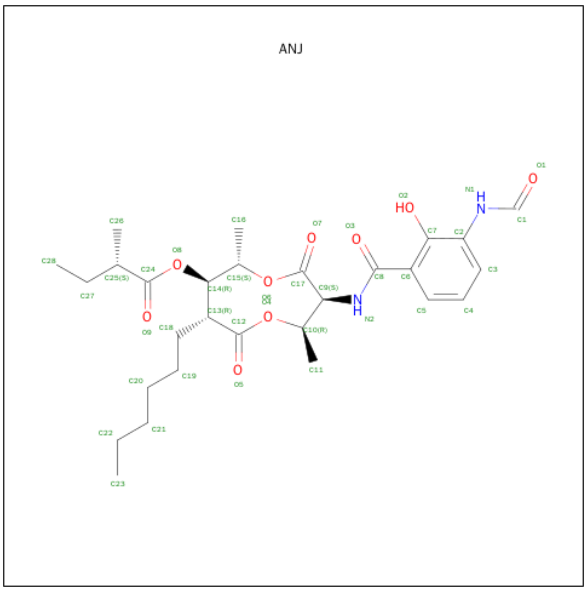
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 37 30 7	0	0
8	D	1	Total C O 37 30 7	0	0
8	G	1	Total C O 37 30 7	0	0
8	J	1	Total C O 37 30 7	0	0

- Molecule 9 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: $C_{35}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	J	1	Total C N O P 45 35 1 8 1	0	0
9	A	1	Total C N O P 45 35 1 8 1	0	0
9	D	1	Total C N O P 45 35 1 8 1	0	0
9	G	1	Total C N O P 45 35 1 8 1	0	0

- Molecule 10 is (2R,3S,6S,7R,8R)-3-{[3-(FORMYLAMINO)-2-HYDROXYBENZOYL]AMINO}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (three-letter code: ANJ) (formula: $C_{28}H_{40}N_2O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O 39 28 2 9	0	0
10	D	1	Total C N O 39 28 2 9	0	0
10	G	1	Total C N O 39 28 2 9	0	0
10	J	1	Total C N O 39 28 2 9	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	36	Total O 36 36	0	0
11	B	7	Total O 7 7	0	0
11	C	13	Total O 13 13	0	0
11	D	41	Total O 41 41	0	0
11	E	3	Total O 3 3	0	0
11	F	13	Total O 13 13	0	0
11	G	41	Total O 41 41	0	0
11	H	4	Total O 4 4	0	0

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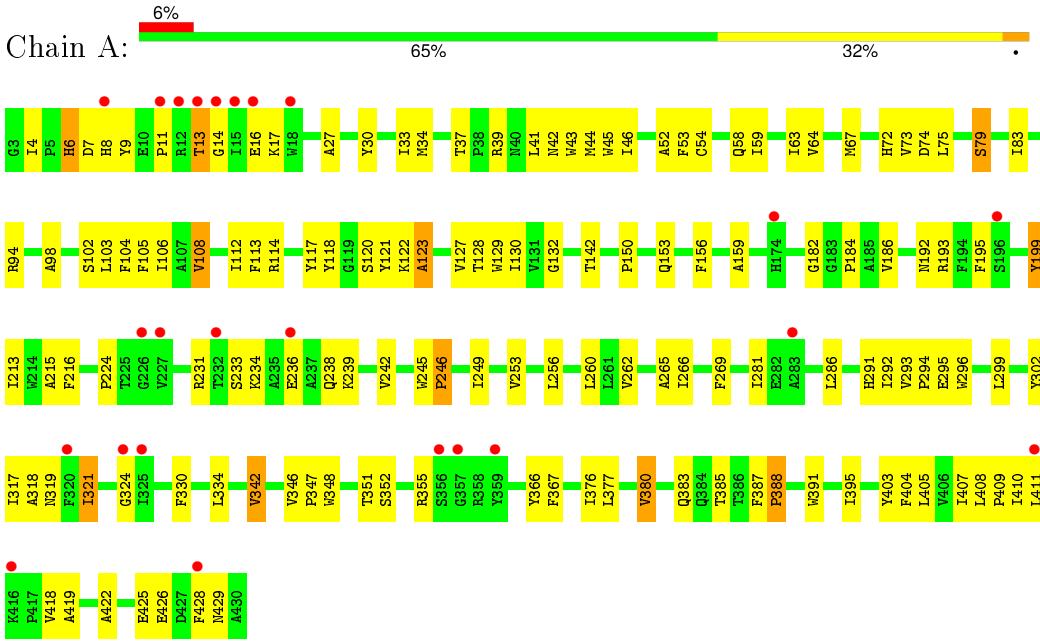
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	I	14	Total O 14 14	0	0
11	J	23	Total O 23 23	0	0
11	K	3	Total O 3 3	0	0
11	L	11	Total O 11 11	0	0

3 Residue-property plots (i)

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.

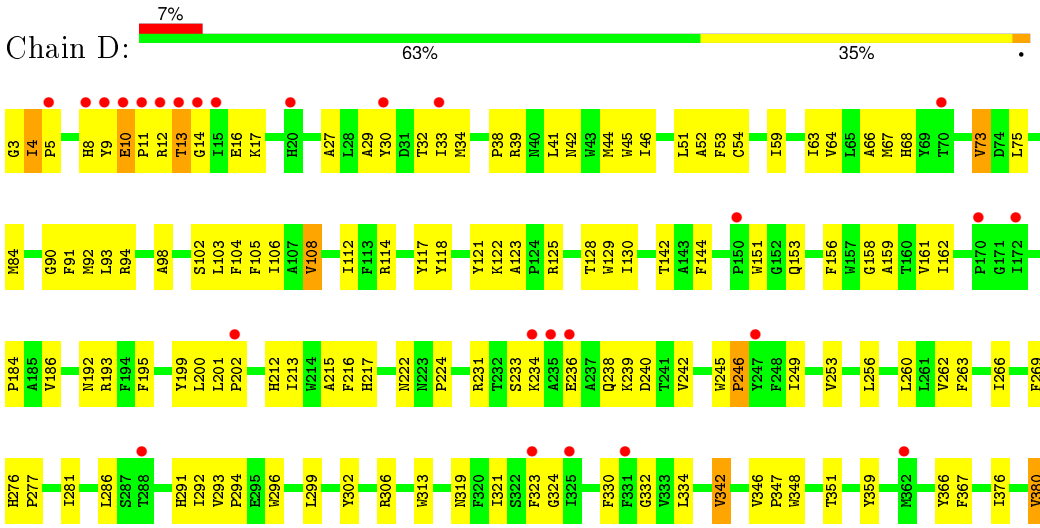
- Molecule 1: Cytochrome b

Chain A:



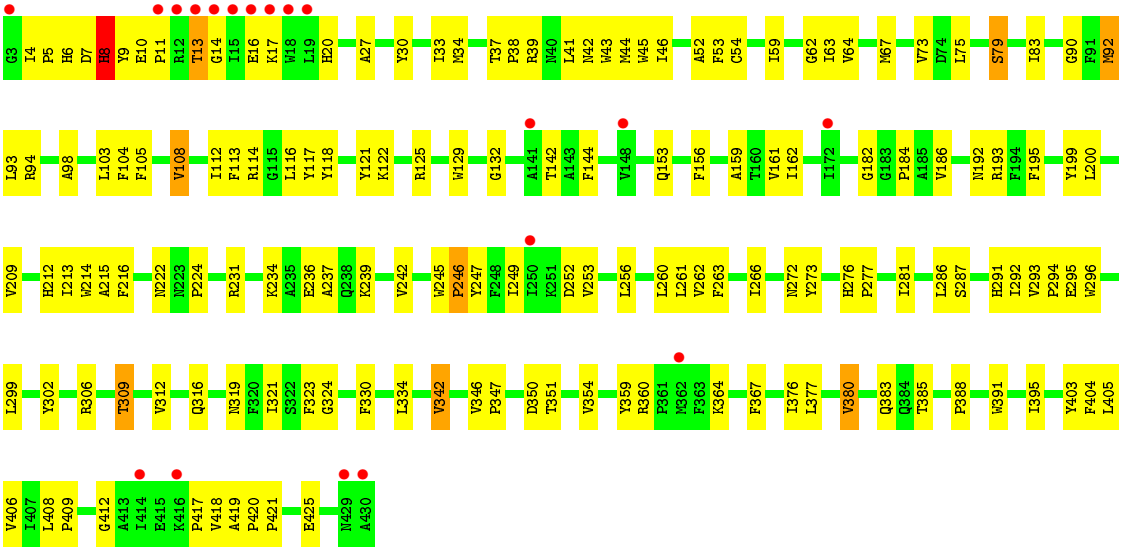
- Molecule 1: Cytochrome b

Chain D:



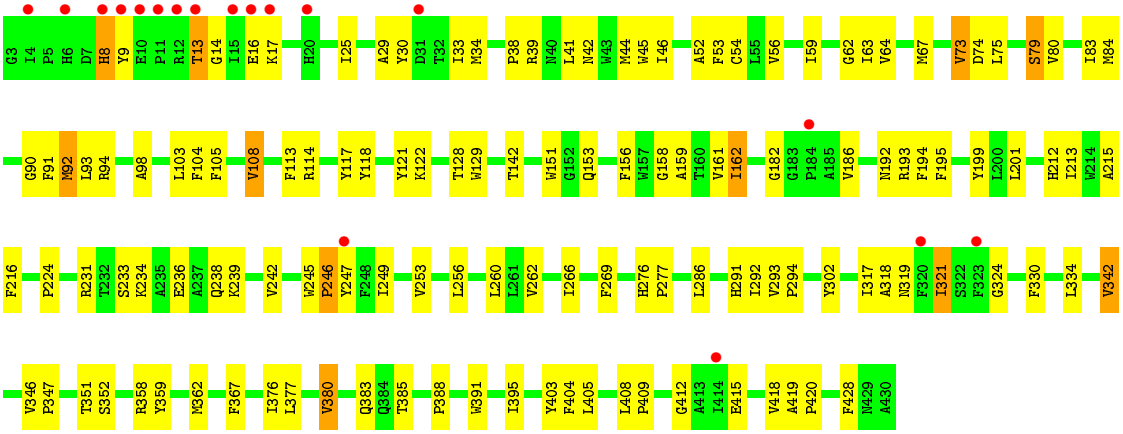
• Molecule 1: Cytochrome b

Chain G:



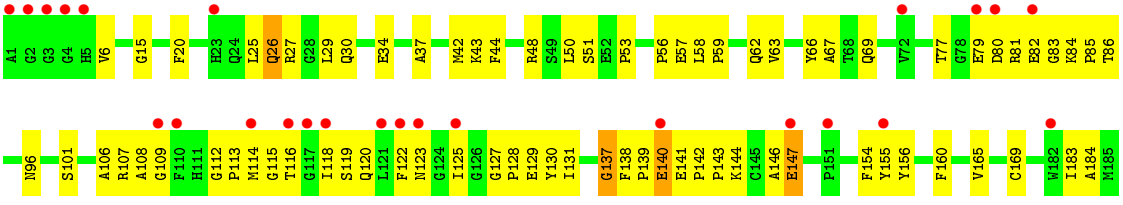
• Molecule 1: Cytochrome b

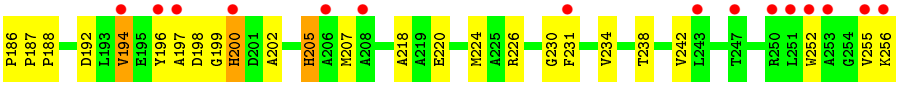
Chain J:



• Molecule 2: Cytochrome c1

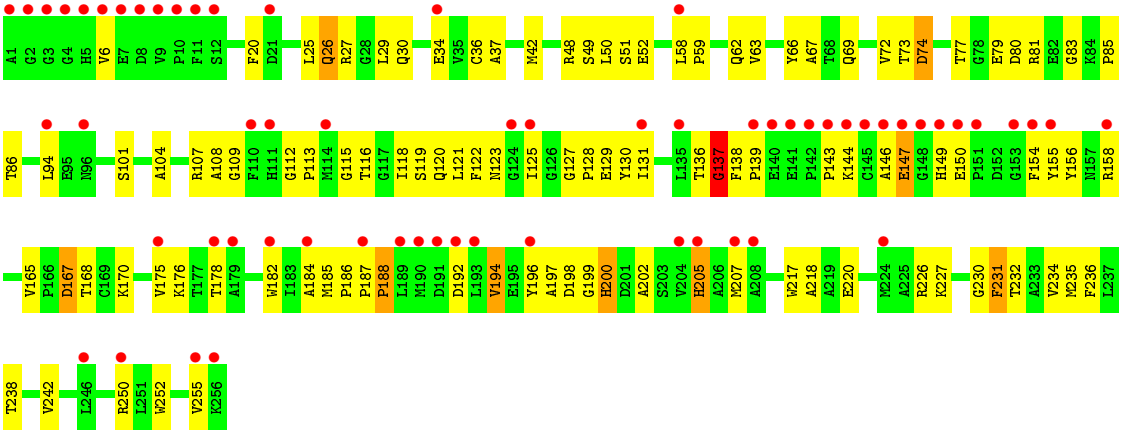
Chain B:





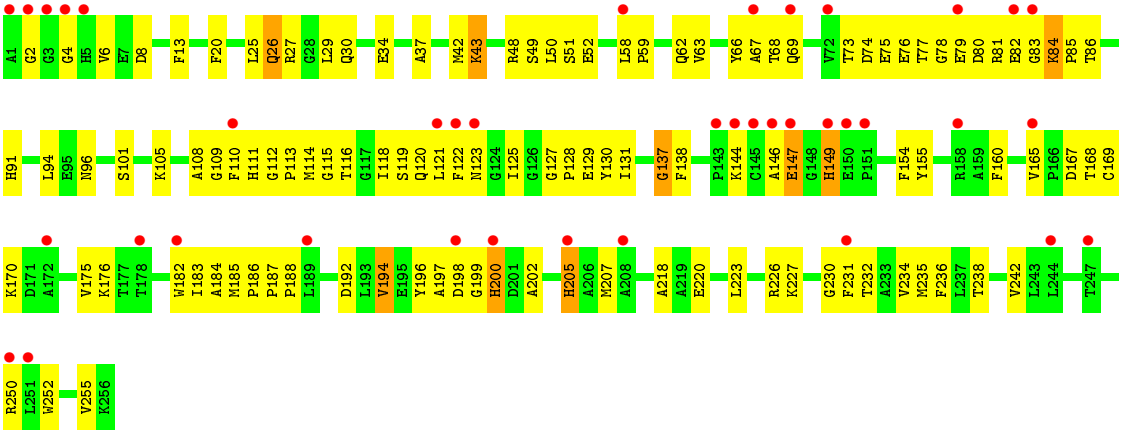
• Molecule 2: Cytochrome c1

Chain E:



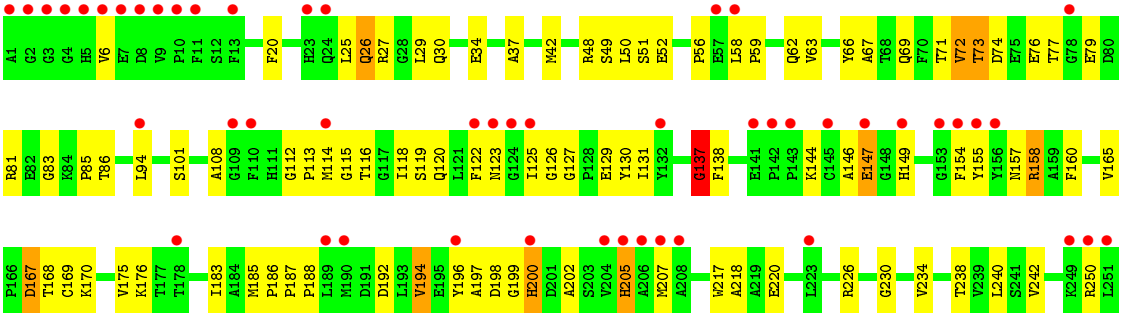
• Molecule 2: Cytochrome c1

Chain H:



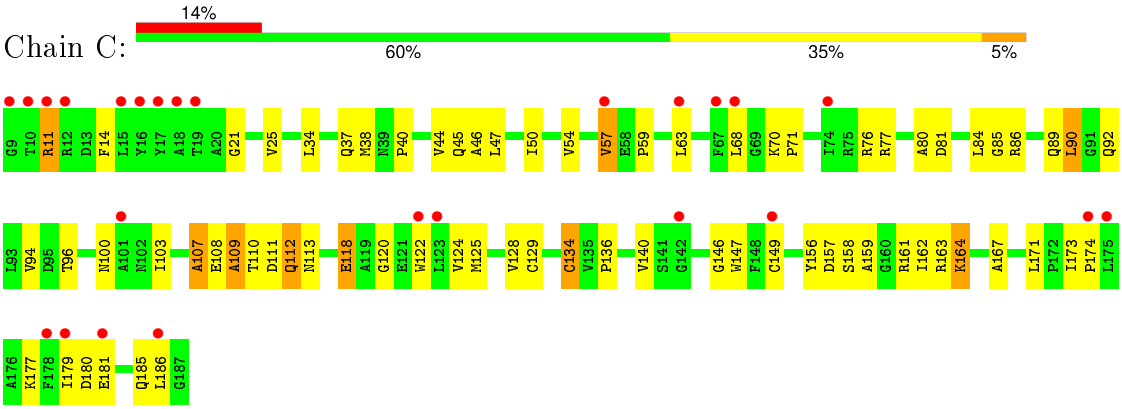
• Molecule 2: Cytochrome c1

Chain K:



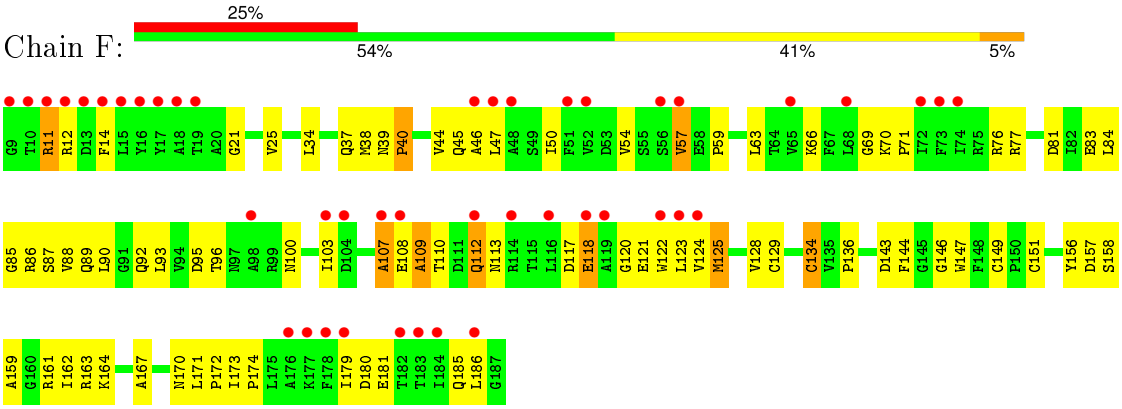
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C:



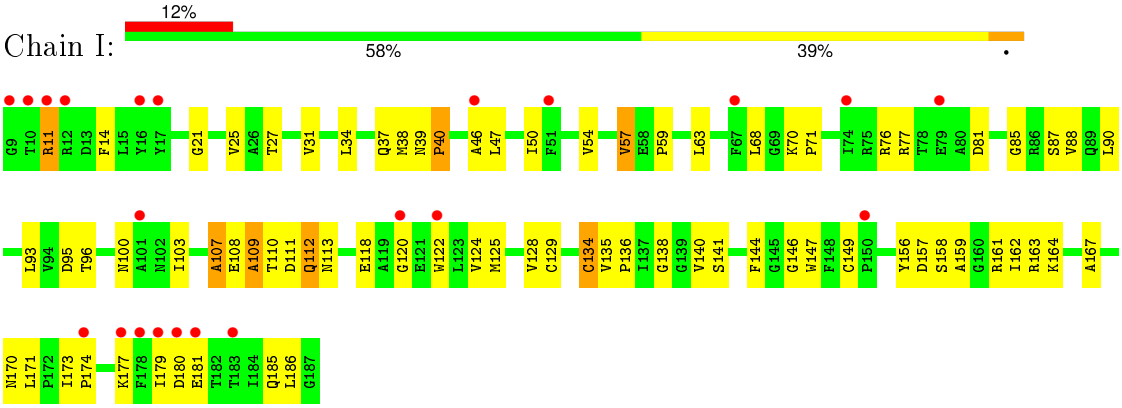
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain F:



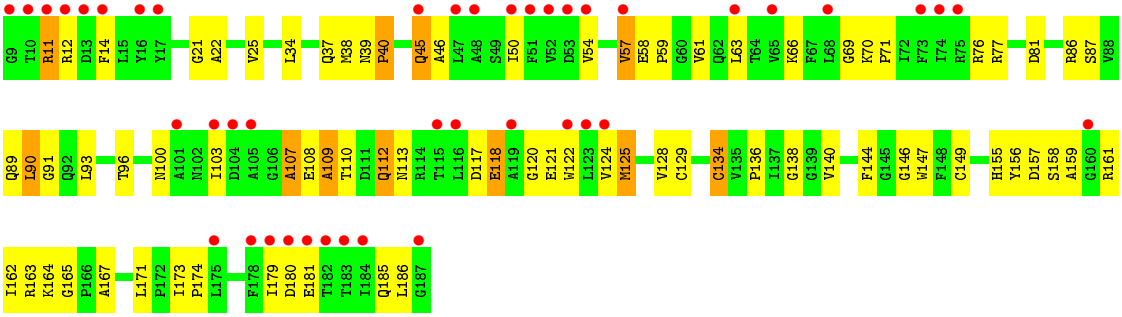
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain I:



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain L:


G9 T10 R11 R12 D13 F14 L15 Y16 Y17 G21 A22 V25 L34 Q37 N38 N39 P40 Q45 A46 L47 A48 S49 I50 F51 V52 D53 V54 V57 E58 P59 G60 V61 Q62 L63 T64 V65 K66 F67 L68 G69 K70 P71 I72 F73 I74 R75 R76 R77 D81 R86 S87 V88
Q89 L90 G91 Q92 L93 T96 N100 A101 N102 I103 D104 A105 G106 A107 E108 A109 T110 D111 Q112 N113 R114 T115 L116 D117 E118 A119 G120 E121 W122 L123 V124 M125 V128 C129 C134 V135 P136 I137 G138 G139 V140 F144 G145 G146 W147 F148 C149 H155 Y156 D157 S158 A159 G160 R161
I162 R163 K164 G165 P166 A167 L171 P172 I173 P174 L175 F178 I179 D180 E181 T182 T183 I184 Q185 L186 G187

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.06Å 146.52Å 141.00Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	17.98 – 2.60 47.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.98-2.60) 97.7 (47.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.277 0.257 , 0.267	Depositor DCC
R_{free} test set	3028 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.9	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 276080 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28227	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.77 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3332e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SR, BGL, ANJ, LOP, FES, HEM, SMA

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	0.36	0/3565	0.64	0/4891
1	D	0.35	0/3565	0.63	0/4891
1	G	0.35	0/3565	0.64	0/4891
1	J	0.36	0/3565	0.65	0/4891
2	B	0.32	0/2010	0.64	1/2733 (0.0%)
2	E	0.31	0/2010	0.64	1/2733 (0.0%)
2	H	0.32	0/2010	0.65	1/2733 (0.0%)
2	K	0.31	0/2010	0.65	1/2733 (0.0%)
3	C	0.32	0/1371	0.69	0/1868
3	F	0.31	0/1371	0.68	1/1868 (0.1%)
3	I	0.32	0/1371	0.70	0/1868
3	L	0.31	0/1371	0.67	0/1868
All	All	0.34	0/27784	0.65	5/37968 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	137	GLY	N-CA-C	5.84	127.71	113.10
2	K	137	GLY	N-CA-C	5.55	126.98	113.10
2	E	137	GLY	N-CA-C	5.54	126.94	113.10
2	B	137	GLY	N-CA-C	5.51	126.87	113.10
3	F	47	LEU	CA-CB-CG	5.03	126.87	115.30

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	3435	0	3420	134	0
1	D	3435	0	3420	144	0
1	G	3435	0	3420	131	0
1	J	3435	0	3420	119	0
2	B	1953	0	1848	87	0
2	E	1953	0	1848	115	0
2	H	1953	0	1848	113	0
2	K	1953	0	1848	91	0
3	C	1341	0	1307	52	0
3	F	1341	0	1307	71	0
3	I	1341	0	1307	64	0
3	L	1341	0	1307	70	0
4	A	20	0	28	3	0
4	E	20	0	28	2	0
4	G	20	0	28	1	0
4	J	20	0	28	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	A	86	0	60	9	0
6	B	43	0	30	5	0
6	D	86	0	60	10	0
6	E	43	0	30	5	0
6	G	86	0	60	7	0
6	H	43	0	30	4	0
6	J	86	0	60	5	0
6	K	43	0	30	1	0
7	C	4	0	0	0	0
7	F	4	0	0	0	0
7	I	4	0	0	0	0
7	L	4	0	0	0	0
8	A	37	0	42	2	0
8	D	37	0	42	3	0
8	G	37	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	37	0	42	3	0
9	A	45	0	67	2	0
9	D	45	0	67	4	0
9	G	45	0	67	5	0
9	J	45	0	67	5	0
10	A	39	0	39	9	0
10	D	39	0	39	12	0
10	G	39	0	39	6	0
10	J	39	0	39	10	0
11	A	36	0	0	2	0
11	B	7	0	0	3	0
11	C	13	0	0	0	0
11	D	41	0	0	4	0
11	E	3	0	0	0	0
11	F	13	0	0	2	0
11	G	41	0	0	3	0
11	H	4	0	0	0	0
11	I	14	0	0	0	0
11	J	23	0	0	1	0
11	K	3	0	0	1	0
11	L	11	0	0	1	0
All	All	28227	0	27364	1123	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 20.

All (1123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ILE:HD11	10:D:504:ANJ:H14	1.39	1.05
1:J:213:ILE:HD11	10:J:505:ANJ:H14	1.40	1.04
1:A:317:ILE:O	1:A:321:ILE:HG22	1.60	1.02
1:A:213:ILE:HD11	10:A:504:ANJ:H14	1.39	1.01
1:J:317:ILE:O	1:J:321:ILE:HG22	1.62	1.00
1:D:4:ILE:HD12	1:D:4:ILE:H	1.22	0.99
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.08	0.99
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.11	0.98
3:C:47:LEU:HG	3:C:68:LEU:HD21	1.44	0.97
1:G:213:ILE:HD11	10:G:505:ANJ:H14	1.47	0.95
2:B:144:LYS:O	2:B:147:GLU:HG2	1.68	0.93
1:D:142:THR:HG21	6:D:502:HEM:HBB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:THR:HG22	2:H:79:GLU:HB2	1.51	0.91
1:G:142:THR:HG21	6:G:502:HEM:HBB2	1.54	0.90
2:H:144:LYS:O	2:H:147:GLU:HG2	1.72	0.89
6:A:502:HEM:HMC1	6:A:502:HEM:HBC2	1.55	0.89
1:J:8:HIS:H	1:J:8:HIS:CD2	1.89	0.87
2:E:42:MET:HE1	2:E:218:ALA:HB1	1.58	0.85
1:D:213:ILE:CD1	10:D:504:ANJ:H14	2.05	0.85
1:A:4:ILE:HD12	1:A:4:ILE:H	1.41	0.84
1:A:142:THR:HG21	6:A:502:HEM:HBB2	1.58	0.83
1:J:213:ILE:CD1	10:J:505:ANJ:H14	2.09	0.83
2:K:42:MET:HE1	2:K:218:ALA:HB1	1.60	0.83
3:C:179:ILE:HD11	3:C:185:GLN:HE21	1.44	0.83
1:G:213:ILE:CD1	10:G:505:ANJ:H14	2.08	0.83
1:G:236:GLU:HA	1:G:239:LYS:HG3	1.60	0.82
3:F:179:ILE:HD11	3:F:185:GLN:HE21	1.44	0.82
2:H:42:MET:HE1	2:H:218:ALA:HB1	1.60	0.82
2:B:42:MET:HE1	2:B:218:ALA:HB1	1.62	0.82
3:I:179:ILE:HD11	3:I:185:GLN:HE21	1.44	0.82
1:J:8:HIS:HD2	1:J:8:HIS:H	1.25	0.81
1:J:29:ALA:HA	10:J:505:ANJ:H233	1.63	0.81
1:A:213:ILE:CD1	10:A:504:ANJ:H14	2.11	0.81
1:A:195:PHE:HE2	1:D:195:PHE:CE2	1.97	0.81
3:L:112:GLN:H	3:L:112:GLN:NE2	1.79	0.81
3:L:179:ILE:HD11	3:L:185:GLN:HE21	1.44	0.80
2:H:74:ASP:HB2	2:H:81:ARG:HD3	1.64	0.80
2:E:236:PHE:HE2	3:F:25:VAL:HG12	1.47	0.80
1:J:142:THR:HG21	6:J:502:HEM:HBB2	1.61	0.80
2:H:86:THR:HG22	3:I:46:ALA:HB1	1.61	0.80
3:F:112:GLN:H	3:F:112:GLN:NE2	1.78	0.80
1:A:195:PHE:CE2	1:D:195:PHE:HE2	1.98	0.80
3:C:107:ALA:HB1	3:C:113:ASN:ND2	1.97	0.79
2:K:49:SER:HA	2:K:52:GLU:HG3	1.65	0.79
2:K:137:GLY:HA2	2:K:158:ARG:NH1	1.98	0.79
1:D:29:ALA:HB1	10:D:504:ANJ:H231	1.66	0.78
3:I:112:GLN:H	3:I:112:GLN:NE2	1.81	0.78
1:J:321:ILE:O	1:J:321:ILE:HG12	1.82	0.78
3:I:107:ALA:HB1	3:I:113:ASN:ND2	1.98	0.78
1:G:5:PRO:HB2	1:G:234:LYS:HA	1.62	0.78
3:L:89:GLN:HA	3:L:89:GLN:HE21	1.49	0.78
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.66	0.78
1:A:321:ILE:O	1:A:321:ILE:HG12	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:GLN:H	3:C:112:GLN:NE2	1.82	0.77
2:K:138:PHE:CD2	2:K:187:PRO:HG3	2.19	0.77
2:H:86:THR:CG2	3:I:46:ALA:HB1	2.15	0.76
1:G:281:ILE:HA	11:G:535:HOH:O	1.86	0.75
1:G:52:ALA:HB2	10:G:505:ANJ:H163	1.68	0.75
1:D:383:GLN:HE22	2:E:115:GLY:HA3	1.50	0.75
1:A:46:ILE:HG22	10:A:504:ANJ:H1	1.70	0.74
1:G:184:PRO:O	3:L:70:LYS:HE3	1.88	0.74
2:H:138:PHE:CD2	2:H:187:PRO:HG3	2.23	0.73
2:K:51:SER:OG	2:K:63:VAL:HG21	1.88	0.73
3:L:100:ASN:HB3	3:L:103:ILE:HG12	1.70	0.73
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.53	0.73
1:G:38:PRO:HG2	1:G:41:LEU:HD21	1.71	0.73
2:B:51:SER:OG	2:B:63:VAL:HG21	1.89	0.73
1:A:13:THR:HB	1:A:16:GLU:HB2	1.71	0.73
2:E:149:HIS:CE1	2:E:168:THR:HG21	2.23	0.72
2:E:128:PRO:HG2	2:E:129:GLU:OE1	1.90	0.72
10:D:504:ANJ:C12	10:D:504:ANJ:O6	2.38	0.72
10:J:505:ANJ:O6	10:J:505:ANJ:C12	2.37	0.72
1:D:13:THR:HB	1:D:16:GLU:HB2	1.71	0.72
1:D:103:LEU:HD13	9:D:503:LOP:H202	1.72	0.72
3:F:100:ASN:HB3	3:F:103:ILE:HG12	1.71	0.72
2:E:108:ALA:HA	2:E:125:ILE:HG22	1.71	0.72
1:A:383:GLN:HE22	2:B:115:GLY:HA3	1.54	0.72
3:C:100:ASN:HB3	3:C:103:ILE:HG12	1.71	0.72
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.02	0.72
2:E:49:SER:HA	2:E:52:GLU:HG3	1.72	0.72
1:G:13:THR:HB	1:G:16:GLU:HB2	1.71	0.71
1:A:13:THR:HG22	1:A:14:GLY:N	2.05	0.71
2:E:108:ALA:HA	2:E:125:ILE:O	1.89	0.71
3:I:100:ASN:HB3	3:I:103:ILE:HG12	1.70	0.71
1:D:332:GLY:HA3	11:D:539:HOH:O	1.90	0.71
1:J:39:ARG:HG2	1:J:242:VAL:HG13	1.73	0.71
1:D:39:ARG:HG2	1:D:242:VAL:HG13	1.72	0.71
1:J:13:THR:HG22	1:J:14:GLY:N	2.06	0.71
1:G:195:PHE:HE2	1:J:195:PHE:CE2	2.03	0.71
1:G:383:GLN:HE22	2:H:115:GLY:HA3	1.54	0.71
3:L:89:GLN:HA	3:L:89:GLN:NE2	2.06	0.71
1:D:13:THR:HG22	1:D:14:GLY:N	2.05	0.71
2:H:236:PHE:HE2	3:I:25:VAL:HG12	1.56	0.70
1:J:113:PHE:HB3	9:J:504:LOP:H272	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HB2	10:A:504:ANJ:C16	2.20	0.70
1:D:13:THR:HG22	1:D:14:GLY:H	1.56	0.70
2:H:77:THR:C	2:H:79:GLU:H	1.94	0.70
1:G:9:TYR:HB2	1:G:30:TYR:CD2	2.27	0.70
1:A:281:ILE:HA	11:A:527:HOH:O	1.91	0.70
1:G:13:THR:HG22	1:G:14:GLY:N	2.06	0.70
3:C:71:PRO:HB3	1:D:286:LEU:HD22	1.74	0.70
1:J:13:THR:HG22	1:J:14:GLY:H	1.57	0.70
1:A:13:THR:HG22	1:A:14:GLY:H	1.57	0.70
1:G:39:ARG:HG2	1:G:242:VAL:HG13	1.73	0.70
1:D:330:PHE:CE2	1:D:334:LEU:HD11	2.27	0.70
2:K:72:VAL:HG12	2:K:73:THR:H	1.57	0.70
3:L:179:ILE:HD11	3:L:185:GLN:NE2	2.07	0.69
1:G:309:THR:HG22	3:L:165:GLY:C	2.11	0.69
1:A:39:ARG:HG2	1:A:242:VAL:HG13	1.72	0.69
1:A:193:ARG:HH11	3:F:38:MET:HE2	1.57	0.69
1:J:13:THR:HB	1:J:16:GLU:HB2	1.72	0.69
1:J:128:THR:HG21	6:J:501:HEM:HBD1	1.73	0.69
10:A:504:ANJ:C12	10:A:504:ANJ:O6	2.40	0.69
10:G:505:ANJ:O6	10:G:505:ANJ:C12	2.41	0.69
1:D:105:PHE:HA	1:D:108:VAL:HG23	1.74	0.69
2:H:146:ALA:HA	2:H:149:HIS:HD2	1.56	0.69
2:E:167:ASP:HA	2:E:170:LYS:HE3	1.73	0.69
3:I:179:ILE:HD11	3:I:185:GLN:NE2	2.07	0.69
2:K:72:VAL:HG12	2:K:73:THR:N	2.08	0.69
1:A:330:PHE:CE2	1:A:334:LEU:HD11	2.28	0.69
1:J:9:TYR:HB2	1:J:30:TYR:CD2	2.27	0.69
2:K:59:PRO:HD2	2:K:62:GLN:NE2	2.09	0.68
1:D:10:GLU:HG2	1:D:12:ARG:NH2	2.07	0.68
3:C:179:ILE:HD11	3:C:185:GLN:NE2	2.07	0.68
3:F:179:ILE:HD11	3:F:185:GLN:NE2	2.07	0.68
3:L:66:LYS:HE2	3:L:69:GLY:HA2	1.74	0.68
1:G:105:PHE:HA	1:G:108:VAL:HG22	1.76	0.68
2:H:59:PRO:HD2	2:H:62:GLN:NE2	2.09	0.68
1:A:52:ALA:HB2	10:A:504:ANJ:H163	1.76	0.68
3:C:107:ALA:HB1	3:C:113:ASN:HD21	1.57	0.68
1:J:330:PHE:CE2	1:J:334:LEU:HD11	2.28	0.68
3:L:107:ALA:HB1	3:L:113:ASN:ND2	2.09	0.68
2:E:236:PHE:CE2	3:F:25:VAL:HG12	2.29	0.67
1:D:33:ILE:HD11	10:D:504:ANJ:H212	1.76	0.67
1:A:123:ALA:O	1:A:355:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:ASP:HB3	2:H:77:THR:HB	1.75	0.67
3:I:107:ALA:HB1	3:I:113:ASN:HD21	1.58	0.67
1:G:286:LEU:HD22	3:L:71:PRO:HB3	1.76	0.67
1:D:144:PHE:CD1	1:D:162:ILE:HD12	2.30	0.67
1:G:63:ILE:N	6:G:502:HEM:HBC2	2.10	0.67
6:D:502:HEM:HBC2	6:D:502:HEM:HHD	1.75	0.67
2:B:108:ALA:HA	2:B:125:ILE:HG22	1.77	0.67
2:B:59:PRO:HD2	2:B:62:GLN:NE2	2.09	0.67
1:A:184:PRO:O	3:F:70:LYS:HE3	1.94	0.67
2:H:51:SER:OG	2:H:63:VAL:HG21	1.94	0.67
1:G:13:THR:HG22	1:G:14:GLY:H	1.57	0.66
1:J:103:LEU:HD13	9:J:504:LOP:H202	1.77	0.66
1:D:240:ASP:HB3	1:D:424:ILE:HD12	1.78	0.66
2:H:232:THR:HG22	2:H:236:PHE:HE1	1.59	0.66
2:K:77:THR:C	2:K:79:GLU:H	1.99	0.66
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.28	0.66
2:E:250:ARG:HD3	3:F:12:ARG:HB2	1.77	0.66
1:G:351:THR:OG1	1:G:412:GLY:HA3	1.96	0.66
3:F:123:LEU:HD21	3:F:125:MET:HE1	1.77	0.66
2:H:108:ALA:HA	2:H:125:ILE:HG22	1.78	0.66
1:J:30:TYR:CE1	1:J:34:MET:HG3	2.31	0.66
1:D:125:ARG:NE	1:D:222:ASN:HB2	2.10	0.66
3:C:80:ALA:O	3:C:84:LEU:HD13	1.96	0.66
1:D:30:TYR:CE1	1:D:34:MET:HG3	2.30	0.66
2:E:59:PRO:HD2	2:E:62:GLN:NE2	2.08	0.66
3:L:40:PRO:HB2	3:L:45:GLN:HE21	1.61	0.66
1:D:319:ASN:OD1	1:D:324:GLY:HA2	1.96	0.66
2:B:140:GLU:H	2:B:140:GLU:CD	2.00	0.66
1:J:62:GLY:O	6:J:502:HEM:HBC2	1.96	0.65
1:A:105:PHE:HA	1:A:108:VAL:HG22	1.77	0.65
1:G:113:PHE:HB3	9:G:504:LOP:H271	1.77	0.65
1:G:330:PHE:CE2	1:G:334:LEU:HD11	2.30	0.65
2:H:184:ALA:HB3	6:H:301:HEM:HBD1	1.79	0.65
3:I:71:PRO:HB3	1:J:286:LEU:HD22	1.78	0.65
1:J:403:TYR:CE2	1:J:408:LEU:HD11	2.31	0.65
2:K:86:THR:HG22	3:L:46:ALA:HB1	1.77	0.65
2:B:29:LEU:HD22	2:B:50:LEU:HD22	1.79	0.65
2:E:144:LYS:HD2	2:E:147:GLU:OE2	1.96	0.65
1:G:319:ASN:OD1	1:G:324:GLY:HA2	1.96	0.65
1:G:30:TYR:CE1	1:G:34:MET:HG3	2.32	0.65
1:A:30:TYR:CE1	1:A:34:MET:HG3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.30	0.65
1:A:239:LYS:HE2	1:A:425:GLU:OE2	1.96	0.64
2:H:128:PRO:HG2	2:H:129:GLU:OE1	1.97	0.64
1:A:236:GLU:HA	1:A:239:LYS:HD3	1.79	0.64
2:K:29:LEU:HD22	2:K:50:LEU:HD22	1.80	0.64
1:G:103:LEU:HD13	9:G:504:LOP:H202	1.80	0.64
2:K:147:GLU:OE1	2:K:147:GLU:HA	1.98	0.64
2:B:77:THR:C	2:B:79:GLU:H	2.00	0.64
2:E:144:LYS:O	2:E:147:GLU:HG2	1.98	0.64
4:A:431:BGL:H5	2:B:15:GLY:H	1.62	0.64
2:B:108:ALA:HA	2:B:125:ILE:O	1.97	0.64
3:L:89:GLN:CA	3:L:89:GLN:HE21	2.09	0.64
3:L:89:GLN:C	3:L:91:GLY:H	2.01	0.64
2:K:149:HIS:CE1	2:K:168:THR:HG21	2.32	0.64
1:G:52:ALA:HB2	10:G:505:ANJ:C16	2.28	0.63
2:E:230:GLY:O	2:E:234:VAL:HG23	1.99	0.63
2:K:77:THR:HG22	2:K:79:GLU:HB2	1.79	0.63
3:I:90:LEU:HD11	3:I:108:GLU:HB3	1.80	0.63
3:L:90:LEU:O	3:L:90:LEU:HG	1.98	0.63
2:E:42:MET:CE	2:E:218:ALA:HB1	2.28	0.63
2:B:42:MET:CE	2:B:218:ALA:HB1	2.28	0.63
1:J:62:GLY:C	6:J:502:HEM:HBC2	2.19	0.63
3:F:118:GLU:CD	3:F:118:GLU:N	2.51	0.63
2:E:138:PHE:CE2	2:E:187:PRO:HA	2.33	0.63
2:E:139:PRO:HG3	2:E:158:ARG:NE	2.14	0.63
2:K:74:ASP:HB2	2:K:81:ARG:HD3	1.80	0.63
2:B:77:THR:HG22	2:B:79:GLU:HB2	1.79	0.63
3:L:136:PRO:HB2	3:L:147:TRP:HB3	1.81	0.63
2:K:42:MET:CE	2:K:218:ALA:HB1	2.28	0.63
2:B:138:PHE:CD1	2:B:187:PRO:HG3	2.33	0.63
2:H:113:PRO:HD3	2:H:119:SER:HB2	1.81	0.62
2:E:29:LEU:HD22	2:E:50:LEU:HD22	1.80	0.62
2:H:77:THR:CG2	2:H:79:GLU:HB2	2.28	0.62
3:I:136:PRO:HB2	3:I:147:TRP:HB3	1.81	0.62
3:F:136:PRO:HB2	3:F:147:TRP:HB3	1.81	0.62
2:E:137:GLY:O	2:E:139:PRO:HD3	1.99	0.62
1:J:84:MET:HE2	11:K:303:HOH:O	1.99	0.62
2:B:113:PRO:HD3	2:B:119:SER:HB2	1.81	0.62
2:H:29:LEU:HD22	2:H:50:LEU:HD22	1.79	0.62
2:K:230:GLY:O	2:K:234:VAL:HG23	2.00	0.62
2:H:27:ARG:HD2	2:H:196:TYR:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:MET:CE	2:H:218:ALA:HB1	2.28	0.62
3:F:125:MET:SD	3:F:171:LEU:HD12	2.40	0.62
2:E:77:THR:C	2:E:79:GLU:H	2.03	0.62
3:F:107:ALA:HB1	3:F:113:ASN:ND2	2.15	0.62
2:E:29:LEU:HD12	2:E:29:LEU:O	2.00	0.61
1:J:52:ALA:HB2	10:J:505:ANJ:C16	2.30	0.61
3:C:136:PRO:HB2	3:C:147:TRP:HB3	1.81	0.61
2:E:113:PRO:HD3	2:E:119:SER:HB2	1.81	0.61
2:B:184:ALA:HB3	6:B:301:HEM:CBD	2.30	0.61
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.35	0.61
1:J:64:VAL:HG11	1:J:93:LEU:HD13	1.82	0.61
1:A:41:LEU:HD23	1:A:224:PRO:HD3	1.82	0.61
1:J:318:ALA:HA	1:J:321:ILE:CG2	2.30	0.61
1:J:319:ASN:OD1	1:J:324:GLY:HA2	2.00	0.61
1:G:132:GLY:HA3	6:G:501:HEM:HBC2	1.83	0.61
1:J:46:ILE:HG22	10:J:505:ANJ:H1	1.83	0.61
1:D:13:THR:O	1:D:17:LYS:HG3	2.00	0.61
1:D:64:VAL:O	1:D:67:MET:HB2	2.00	0.61
2:B:230:GLY:O	2:B:234:VAL:HG23	2.00	0.61
2:K:29:LEU:O	2:K:29:LEU:HD12	2.00	0.61
1:J:362:MET:CE	1:J:415:GLU:HA	2.31	0.61
2:B:29:LEU:O	2:B:29:LEU:HD12	2.01	0.61
1:J:64:VAL:O	1:J:67:MET:HB2	2.01	0.60
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.81	0.60
1:A:319:ASN:OD1	1:A:324:GLY:HA2	2.00	0.60
2:H:230:GLY:O	2:H:234:VAL:HG23	2.02	0.60
2:K:113:PRO:HD3	2:K:119:SER:HB2	1.81	0.60
2:H:183:ILE:HG23	2:H:185:MET:H	1.65	0.60
2:H:4:GLY:O	2:H:111:HIS:HD2	1.83	0.60
1:D:32:THR:HG23	1:D:217:HIS:HE1	1.65	0.60
1:A:318:ALA:HA	1:A:321:ILE:CG2	2.31	0.60
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.15	0.60
2:K:160:PHE:CD2	2:K:183:ILE:HB	2.37	0.60
1:G:64:VAL:O	1:G:67:MET:HB2	2.01	0.60
1:D:4:ILE:CD1	1:D:4:ILE:H	1.97	0.60
1:G:262:VAL:HG13	4:G:431:BGL:H8'1	1.84	0.60
1:D:64:VAL:HG11	1:D:93:LEU:HD13	1.83	0.60
3:L:90:LEU:HD21	3:L:108:GLU:CD	2.21	0.60
1:D:236:GLU:HA	1:D:239:LYS:HG3	1.83	0.60
2:H:29:LEU:O	2:H:29:LEU:HD12	2.01	0.60
2:E:184:ALA:HB3	6:E:301:HEM:HBD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:140:VAL:O	3:L:140:VAL:HG12	2.02	0.60
2:K:250:ARG:HD3	3:L:12:ARG:HB2	1.84	0.60
3:C:90:LEU:HD11	3:C:108:GLU:HB3	1.83	0.60
2:H:86:THR:HG22	3:I:46:ALA:CB	2.32	0.59
2:K:250:ARG:HH12	3:L:11:ARG:CD	2.14	0.59
1:A:64:VAL:O	1:A:67:MET:HB2	2.02	0.59
1:A:4:ILE:HD12	1:A:4:ILE:N	2.15	0.59
1:G:64:VAL:HG11	1:G:93:LEU:HD13	1.83	0.59
1:D:52:ALA:HB2	10:D:504:ANJ:C16	2.33	0.59
8:J:503:SMA:H39	8:J:503:SMA:H33	1.84	0.59
2:E:66:TYR:CE1	2:E:69:GLN:NE2	2.71	0.59
10:A:504:ANJ:O6	10:A:504:ANJ:O4	2.21	0.58
1:G:54:CYS:SG	1:G:103:LEU:HG	2.43	0.58
2:E:42:MET:HE1	2:E:218:ALA:CB	2.32	0.58
2:K:74:ASP:HB3	2:K:77:THR:HB	1.85	0.58
1:D:236:GLU:HA	1:D:239:LYS:CD	2.33	0.58
1:G:193:ARG:HH11	3:L:38:MET:HE2	1.69	0.58
1:A:286:LEU:HD22	3:F:71:PRO:HB3	1.85	0.58
1:D:269:PHE:HB3	4:E:257:BGL:H1'2	1.85	0.58
1:J:38:PRO:HG2	1:J:41:LEU:HD21	1.85	0.58
10:G:505:ANJ:O4	10:G:505:ANJ:O6	2.22	0.58
3:F:86:ARG:HG2	3:F:112:GLN:OE1	2.03	0.58
1:G:39:ARG:HH12	2:H:255:VAL:HG12	1.69	0.58
1:D:144:PHE:HE2	8:D:2:SMA:H43	1.69	0.58
1:D:9:TYR:HB2	1:D:30:TYR:CD2	2.38	0.58
1:D:273:TYR:HE1	2:E:120:GLN:HB2	1.67	0.58
1:J:362:MET:HE3	1:J:415:GLU:HG3	1.86	0.58
2:K:250:ARG:HH12	3:L:11:ARG:HD3	1.69	0.58
1:J:54:CYS:SG	1:J:103:LEU:HG	2.44	0.58
1:A:54:CYS:SG	1:A:103:LEU:HG	2.43	0.58
1:G:62:GLY:C	6:G:502:HEM:HBC2	2.24	0.57
1:D:9:TYR:HE1	1:D:11:PRO:HG3	1.70	0.57
2:K:66:TYR:O	2:K:69:GLN:HG2	2.04	0.57
1:J:9:TYR:HB2	1:J:30:TYR:CG	2.39	0.57
1:A:105:PHE:HA	1:A:108:VAL:CG2	2.34	0.57
2:K:149:HIS:ND1	2:K:168:THR:HG21	2.19	0.57
10:D:504:ANJ:O4	10:D:504:ANJ:O6	2.21	0.57
1:D:125:ARG:CZ	1:D:222:ASN:HB2	2.35	0.57
2:H:96:ASN:O	6:H:301:HEM:HAD1	2.04	0.57
1:G:405:LEU:O	1:G:409:PRO:HG2	2.04	0.57
1:D:38:PRO:HG2	1:D:41:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:505:ANJ:O4	10:J:505:ANJ:O6	2.21	0.57
2:B:140:GLU:N	2:B:140:GLU:CD	2.58	0.57
3:L:124:VAL:O	3:L:173:ILE:HG23	2.05	0.57
2:K:205:HIS:C	2:K:205:HIS:ND1	2.59	0.57
3:L:89:GLN:O	3:L:91:GLY:N	2.37	0.56
2:E:149:HIS:CD2	2:E:168:THR:HG21	2.40	0.56
1:D:54:CYS:SG	1:D:103:LEU:HG	2.45	0.56
2:H:205:HIS:C	2:H:205:HIS:ND1	2.59	0.56
1:A:33:ILE:HG22	1:A:33:ILE:O	2.05	0.56
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.86	0.56
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.87	0.56
3:I:124:VAL:O	3:I:173:ILE:HG23	2.05	0.56
1:G:33:ILE:HG22	1:G:33:ILE:O	2.05	0.56
1:D:52:ALA:HB2	10:D:504:ANJ:H163	1.87	0.56
1:G:13:THR:O	1:G:17:LYS:HG3	2.04	0.56
2:E:77:THR:HG22	2:E:79:GLU:HB2	1.87	0.56
3:I:77:ARG:HB3	3:I:81:ASP:HB2	1.88	0.56
2:B:77:THR:CG2	2:B:79:GLU:HB2	2.36	0.56
1:G:125:ARG:NE	1:G:222:ASN:HB2	2.20	0.56
2:E:27:ARG:HD2	2:E:196:TYR:CZ	2.41	0.56
1:D:33:ILE:HG22	1:D:33:ILE:O	2.06	0.56
1:A:295:GLU:OE2	8:A:1:SMA:H10	2.06	0.56
1:J:33:ILE:HG22	1:J:33:ILE:O	2.06	0.56
2:E:205:HIS:C	2:E:205:HIS:ND1	2.58	0.56
1:D:359:TYR:CD2	1:D:420:PRO:HB3	2.41	0.56
1:D:391:TRP:O	1:D:395:ILE:HG13	2.06	0.56
3:F:89:GLN:HB2	3:F:92:GLN:OE1	2.05	0.55
3:I:85:GLY:HA3	3:I:111:ASP:OD2	2.06	0.55
3:L:125:MET:SD	3:L:171:LEU:HD12	2.45	0.55
2:H:232:THR:HG22	2:H:236:PHE:CE1	2.41	0.55
2:B:128:PRO:HG2	2:B:129:GLU:OE1	2.06	0.55
3:C:77:ARG:HB3	3:C:81:ASP:HB2	1.87	0.55
1:D:294:PRO:HG2	1:D:302:TYR:CG	2.41	0.55
3:L:86:ARG:HG2	3:L:112:GLN:OE1	2.06	0.55
3:C:124:VAL:O	3:C:173:ILE:HG23	2.06	0.55
3:C:90:LEU:HD21	3:C:108:GLU:OE2	2.06	0.55
2:B:205:HIS:C	2:B:205:HIS:ND1	2.59	0.55
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.87	0.55
1:G:239:LYS:HE2	1:G:425:GLU:OE2	2.06	0.55
3:L:77:ARG:HB3	3:L:81:ASP:HB2	1.88	0.55
3:F:85:GLY:O	3:F:88:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:GLY:O	1:D:162:ILE:HG13	2.06	0.55
1:D:236:GLU:HA	1:D:239:LYS:CG	2.37	0.55
1:J:294:PRO:HG2	1:J:302:TYR:CG	2.42	0.55
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.40	0.55
2:H:74:ASP:HB2	2:H:81:ARG:CD	2.35	0.55
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.40	0.55
3:C:70:LYS:HE3	1:D:184:PRO:O	2.06	0.55
2:H:250:ARG:HH12	3:I:11:ARG:HD3	1.70	0.55
1:A:418:VAL:HG12	1:A:419:ALA:N	2.22	0.55
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.70	0.55
2:E:227:LYS:HE2	4:E:257:BGL:O1	2.06	0.55
3:F:124:VAL:O	3:F:173:ILE:HG23	2.06	0.55
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.87	0.55
2:B:160:PHE:CD2	2:B:183:ILE:HB	2.41	0.54
2:B:184:ALA:HB3	6:B:301:HEM:HBD1	1.88	0.54
1:J:161:VAL:HG11	8:J:503:SMA:O5	2.07	0.54
2:K:194:VAL:HB	2:K:207:MET:CE	2.37	0.54
3:F:90:LEU:HD12	3:F:93:LEU:HD12	1.89	0.54
1:G:39:ARG:NH1	2:H:255:VAL:HG12	2.21	0.54
1:A:269:PHE:HB3	4:A:431:BGL:H1'2	1.87	0.54
2:H:184:ALA:HB3	6:H:301:HEM:CBD	2.37	0.54
1:J:391:TRP:O	1:J:395:ILE:HG13	2.07	0.54
1:A:72:HIS:HE1	1:A:74:ASP:OD2	1.91	0.54
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.20	0.54
1:A:121:TYR:CE1	1:A:122:LYS:HG3	2.42	0.54
3:F:144:PHE:N	3:F:144:PHE:CD1	2.76	0.54
2:E:147:GLU:HA	2:E:147:GLU:OE1	2.06	0.54
1:A:118:TYR:OH	9:A:503:LOP:H32	2.07	0.54
3:C:37:GLN:NE2	3:C:38:MET:HG3	2.23	0.54
1:J:234:LYS:O	1:J:238:GLN:HG3	2.08	0.54
1:A:294:PRO:HG2	1:A:302:TYR:CG	2.43	0.54
3:F:77:ARG:HB3	3:F:81:ASP:HB2	1.88	0.54
2:H:81:ARG:CZ	2:H:84:LYS:HE2	2.38	0.54
1:D:46:ILE:HG22	10:D:504:ANJ:H1	1.90	0.54
2:E:149:HIS:CG	2:E:168:THR:HG21	2.43	0.54
1:D:39:ARG:HD3	1:D:428:PHE:CD2	2.43	0.54
3:F:110:THR:OG1	3:F:113:ASN:HB2	2.08	0.54
3:F:21:GLY:O	3:F:25:VAL:HG23	2.08	0.54
2:E:51:SER:OG	2:E:63:VAL:HG21	2.08	0.54
3:C:21:GLY:O	3:C:25:VAL:HG23	2.08	0.54
2:H:77:THR:C	2:H:79:GLU:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:ARG:HH11	2:H:81:ARG:HG3	1.73	0.53
1:D:161:VAL:HG11	8:D:2:SMA:O5	2.08	0.53
1:A:113:PHE:HB3	9:A:503:LOP:H272	1.91	0.53
2:E:194:VAL:HB	2:E:207:MET:CE	2.38	0.53
2:K:192:ASP:HA	2:K:202:ALA:HB3	1.91	0.53
2:B:192:ASP:HA	2:B:202:ALA:HB3	1.91	0.53
1:D:263:PHE:HD1	9:D:503:LOP:H221	1.73	0.53
2:E:165:VAL:HG13	2:E:182:TRP:CZ3	2.43	0.53
2:E:66:TYR:CD1	2:E:69:GLN:NE2	2.77	0.53
3:I:37:GLN:NE2	3:I:38:MET:HG3	2.23	0.53
3:L:37:GLN:NE2	3:L:38:MET:HG3	2.22	0.53
1:G:294:PRO:HG2	1:G:302:TYR:CG	2.44	0.53
2:E:104:ALA:O	2:E:127:GLY:HA3	2.09	0.53
3:I:21:GLY:O	3:I:25:VAL:HG23	2.09	0.53
3:F:37:GLN:NE2	3:F:38:MET:HG3	2.24	0.53
1:A:391:TRP:O	1:A:395:ILE:HG13	2.08	0.53
3:I:70:LYS:NZ	3:I:70:LYS:HB2	2.23	0.53
6:J:501:HEM:CMA	10:J:505:ANJ:O7	2.57	0.53
1:J:358:ARG:HH21	9:J:504:LOP:H21	1.73	0.53
3:L:110:THR:OG1	3:L:113:ASN:HB2	2.08	0.53
1:D:130:ILE:HD11	1:D:348:TRP:HH2	1.73	0.53
2:E:194:VAL:HB	2:E:207:MET:HE3	1.91	0.53
1:G:359:TYR:CZ	1:G:421:PRO:HD3	2.44	0.53
2:E:86:THR:HG22	3:F:46:ALA:HB1	1.90	0.53
1:G:391:TRP:O	1:G:395:ILE:HG13	2.09	0.53
1:D:103:LEU:HB2	9:D:503:LOP:H222	1.90	0.53
2:B:238:THR:O	2:B:242:VAL:HG23	2.09	0.53
2:E:155:TYR:CZ	2:E:186:PRO:HB3	2.44	0.53
1:J:362:MET:HE1	1:J:415:GLU:HA	1.91	0.53
2:H:194:VAL:HB	2:H:207:MET:CE	2.38	0.53
2:H:250:ARG:HH12	3:I:11:ARG:CD	2.22	0.52
3:C:85:GLY:HA3	3:C:111:ASP:OD2	2.09	0.52
2:H:66:TYR:O	2:H:69:GLN:HG2	2.09	0.52
2:K:155:TYR:CZ	2:K:186:PRO:HB3	2.44	0.52
3:L:107:ALA:HB1	3:L:113:ASN:HD21	1.75	0.52
2:B:127:GLY:O	2:B:131:ILE:HG13	2.09	0.52
1:G:256:LEU:O	1:G:260:LEU:HG	2.08	0.52
2:E:238:THR:O	2:E:242:VAL:HG23	2.09	0.52
2:H:127:GLY:O	2:H:131:ILE:HG13	2.09	0.52
2:E:192:ASP:HA	2:E:202:ALA:HB3	1.91	0.52
2:H:155:TYR:CZ	2:H:186:PRO:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:138:GLY:O	3:I:141:SER:OG	2.24	0.52
2:H:68:THR:HG23	2:H:82:GLU:OE2	2.10	0.52
2:B:194:VAL:HB	2:B:207:MET:CE	2.39	0.52
1:A:403:TYR:CE2	1:A:408:LEU:HD11	2.44	0.52
1:D:75:LEU:O	1:D:79:SER:HB3	2.09	0.52
2:K:238:THR:O	2:K:242:VAL:HG23	2.09	0.52
1:G:212:HIS:O	1:G:215:ALA:HB3	2.10	0.52
1:A:256:LEU:O	1:A:260:LEU:HG	2.09	0.52
3:I:34:LEU:O	3:I:37:GLN:HG3	2.10	0.52
2:H:238:THR:O	2:H:242:VAL:HG23	2.09	0.52
1:J:269:PHE:HB3	4:J:431:BGL:H1'2	1.92	0.52
2:K:59:PRO:HD2	2:K:62:GLN:HE21	1.75	0.52
3:F:66:LYS:HE3	3:F:69:GLY:HA2	1.92	0.52
3:L:21:GLY:O	3:L:25:VAL:HG23	2.09	0.52
2:E:143:PRO:HG3	2:E:178:THR:HG21	1.92	0.52
3:L:34:LEU:O	3:L:37:GLN:HG3	2.10	0.51
1:G:4:ILE:H	1:G:4:ILE:HD12	1.75	0.51
3:F:172:PRO:HG3	11:F:213:HOH:O	2.10	0.51
3:F:34:LEU:O	3:F:37:GLN:HG3	2.10	0.51
3:C:34:LEU:O	3:C:37:GLN:HG3	2.10	0.51
2:H:192:ASP:HA	2:H:202:ALA:HB3	1.91	0.51
1:J:52:ALA:HB2	10:J:505:ANJ:H163	1.92	0.51
8:D:2:SMA:H33	8:D:2:SMA:H39	1.93	0.51
1:G:249:ILE:O	1:G:253:VAL:HG23	2.10	0.51
1:D:83:ILE:O	1:D:90:GLY:HA3	2.11	0.51
3:C:163:ARG:O	3:C:164:LYS:HB2	2.08	0.51
2:K:127:GLY:O	2:K:131:ILE:HG13	2.10	0.51
1:A:59:ILE:O	1:A:63:ILE:HG13	2.11	0.51
2:E:127:GLY:O	2:E:131:ILE:HG13	2.10	0.51
1:G:263:PHE:HD1	9:G:504:LOP:H221	1.75	0.51
1:J:249:ILE:O	1:J:253:VAL:HG23	2.11	0.51
1:G:42:ASN:OD1	1:G:44:MET:HB2	2.11	0.51
2:K:144:LYS:O	2:K:147:GLU:HG2	2.10	0.51
2:B:96:ASN:O	6:B:301:HEM:HAD1	2.11	0.51
1:J:256:LEU:O	1:J:260:LEU:HG	2.10	0.51
2:B:53:PRO:HA	2:B:57:GLU:CD	2.31	0.51
1:G:59:ILE:O	1:G:63:ILE:HG13	2.11	0.51
1:J:42:ASN:OD1	1:J:44:MET:HB2	2.11	0.51
1:A:39:ARG:NH1	2:B:255:VAL:CG1	2.73	0.51
2:E:165:VAL:HG13	2:E:182:TRP:HZ3	1.76	0.51
1:G:44:MET:HE3	9:G:504:LOP:H92	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:75:LEU:O	1:J:79:SER:HB3	2.11	0.51
1:D:256:LEU:O	1:D:260:LEU:HG	2.10	0.51
1:D:128:THR:HG21	6:D:501:HEM:HBD1	1.93	0.51
2:H:66:TYR:CE1	2:H:69:GLN:NE2	2.79	0.51
1:A:249:ILE:O	1:A:253:VAL:HG23	2.11	0.51
1:A:351:THR:OG1	1:A:412:GLY:HA3	2.11	0.51
2:H:43:LYS:HE3	2:H:91:HIS:CE1	2.46	0.51
3:C:47:LEU:HG	3:C:68:LEU:CD2	2.29	0.51
2:B:77:THR:C	2:B:79:GLU:N	2.63	0.51
3:C:90:LEU:HD21	3:C:108:GLU:CD	2.31	0.51
3:F:44:VAL:O	3:F:46:ALA:N	2.44	0.51
1:A:200:LEU:HD22	1:D:63:ILE:HD13	1.92	0.51
1:G:403:TYR:O	1:G:408:LEU:HG	2.11	0.51
3:C:125:MET:SD	3:C:171:LEU:HD12	2.50	0.51
1:A:428:PHE:CZ	2:B:256:LYS:HB2	2.45	0.51
1:A:39:ARG:NH1	2:B:255:VAL:HG12	2.26	0.51
1:A:408:LEU:HB2	1:A:409:PRO:HD3	1.92	0.51
3:F:87:SER:O	3:F:87:SER:OG	2.28	0.51
1:D:45:TRP:CZ3	1:D:224:PRO:HG3	2.46	0.50
2:K:73:THR:O	2:K:73:THR:HG22	2.11	0.50
2:B:59:PRO:HD2	2:B:62:GLN:HE21	1.76	0.50
1:D:182:GLY:HA3	1:D:193:ARG:NH2	2.26	0.50
1:D:42:ASN:OD1	1:D:44:MET:HB2	2.11	0.50
1:A:407:ILE:HG22	1:A:411:LEU:HD12	1.93	0.50
2:B:224:MET:HB2	11:B:307:HOH:O	2.09	0.50
1:D:281:ILE:HD11	2:E:107:ARG:HH12	1.75	0.50
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.11	0.50
2:B:155:TYR:CZ	2:B:186:PRO:HB3	2.45	0.50
3:I:125:MET:SD	3:I:171:LEU:HD12	2.51	0.50
1:D:249:ILE:O	1:D:253:VAL:HG23	2.11	0.50
1:G:13:THR:CG2	1:G:14:GLY:N	2.75	0.50
1:J:92:MET:CE	2:K:226:ARG:HG3	2.41	0.50
1:J:292:ILE:O	1:J:293:VAL:HG23	2.12	0.50
1:D:212:HIS:O	1:D:215:ALA:HB3	2.11	0.50
2:H:42:MET:HE1	2:H:218:ALA:CB	2.36	0.50
1:A:366:TYR:CD2	1:A:411:LEU:HD11	2.47	0.50
2:K:42:MET:HE1	2:K:218:ALA:CB	2.36	0.50
1:A:182:GLY:HA3	1:A:193:ARG:NH2	2.27	0.50
2:H:165:VAL:HG12	2:H:169:CYS:HB2	1.93	0.50
2:H:30:GLN:HG2	2:H:34:GLU:OE2	2.12	0.50
1:D:73:VAL:HG12	1:D:151:TRP:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:42:MET:HE2	2:K:101:SER:HA	1.94	0.50
1:J:39:ARG:HH12	2:K:255:VAL:HG12	1.77	0.50
1:A:39:ARG:HH12	2:B:255:VAL:HG12	1.76	0.50
3:L:90:LEU:CG	3:L:90:LEU:O	2.59	0.50
2:E:250:ARG:CD	3:F:12:ARG:HG3	2.42	0.50
2:E:74:ASP:HB3	2:E:77:THR:HB	1.94	0.50
2:K:183:ILE:HG12	2:K:185:MET:H	1.76	0.50
3:L:89:GLN:C	3:L:91:GLY:N	2.65	0.50
1:D:13:THR:CG2	1:D:14:GLY:N	2.74	0.50
1:J:83:ILE:O	1:J:90:GLY:HA3	2.12	0.50
1:D:418:VAL:CG1	1:D:419:ALA:N	2.75	0.50
1:J:158:GLY:O	1:J:162:ILE:HG13	2.12	0.50
1:J:359:TYR:CD2	1:J:420:PRO:HB3	2.47	0.50
1:A:102:SER:O	1:A:106:ILE:HG13	2.11	0.50
1:J:182:GLY:HA3	1:J:193:ARG:NH2	2.26	0.50
1:G:44:MET:CE	9:G:504:LOP:H92	2.42	0.50
1:D:53:PHE:CE2	1:D:260:LEU:HD21	2.47	0.50
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.12	0.50
2:H:67:ALA:O	2:H:83:GLY:HA3	2.10	0.50
1:J:212:HIS:O	1:J:215:ALA:HB3	2.12	0.49
1:J:53:PHE:CE2	1:J:260:LEU:HD21	2.47	0.49
1:A:234:LYS:O	1:A:238:GLN:HG3	2.12	0.49
2:K:30:GLN:HG2	2:K:34:GLU:OE2	2.12	0.49
1:G:75:LEU:O	1:G:79:SER:HB3	2.12	0.49
2:E:143:PRO:HG3	2:E:178:THR:CG2	2.41	0.49
1:G:4:ILE:N	1:G:4:ILE:HD12	2.27	0.49
1:A:346:VAL:CG1	1:A:347:PRO:HD3	2.42	0.49
1:A:114:ARG:HD2	1:A:114:ARG:C	2.33	0.49
2:K:138:PHE:HD2	2:K:187:PRO:HG3	1.73	0.49
1:A:75:LEU:O	1:A:79:SER:HB3	2.12	0.49
1:A:212:HIS:O	1:A:215:ALA:HB3	2.11	0.49
2:H:26:GLN:HG3	2:H:58:LEU:HD21	1.95	0.49
1:D:342:VAL:HG13	1:D:404:PHE:CB	2.43	0.49
2:H:112:GLY:O	2:H:119:SER:HB3	2.13	0.49
1:D:239:LYS:HE2	1:D:425:GLU:OE2	2.12	0.49
1:D:59:ILE:O	1:D:63:ILE:HG13	2.13	0.49
1:A:128:THR:HG21	6:A:501:HEM:HBD1	1.93	0.49
2:B:165:VAL:HG12	2:B:169:CYS:HB2	1.95	0.49
2:B:30:GLN:HG2	2:B:34:GLU:OE2	2.12	0.49
2:B:26:GLN:HG3	2:B:58:LEU:HD21	1.94	0.49
1:A:313:TRP:HA	1:A:316:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:ILE:O	1:G:90:GLY:HA3	2.13	0.49
2:E:26:GLN:HG3	2:E:58:LEU:HD21	1.95	0.49
2:H:94:LEU:HD22	6:H:301:HEM:HAC	1.95	0.49
2:H:27:ARG:HD2	2:H:196:TYR:CE2	2.48	0.49
2:B:183:ILE:HG13	6:B:301:HEM:O2D	2.13	0.49
1:G:182:GLY:HA3	1:G:193:ARG:NH2	2.27	0.49
1:G:53:PHE:CE2	1:G:260:LEU:HD21	2.47	0.49
1:A:42:ASN:OD1	1:A:44:MET:HB2	2.12	0.49
2:K:26:GLN:HG3	2:K:58:LEU:HD21	1.95	0.49
2:E:42:MET:HE2	2:E:101:SER:HA	1.95	0.49
1:G:144:PHE:CD1	1:G:162:ILE:HD12	2.47	0.49
1:A:127:VAL:N	11:A:515:HOH:O	2.43	0.49
1:A:58:GLN:CB	6:A:502:HEM:HAB	2.42	0.49
2:E:149:HIS:NE2	2:E:168:THR:HG21	2.27	0.49
1:J:9:TYR:N	1:J:30:TYR:CE2	2.81	0.49
1:J:92:MET:HE3	2:K:226:ARG:HG3	1.95	0.49
3:C:89:GLN:O	3:C:92:GLN:N	2.23	0.49
1:A:6:HIS:C	1:A:6:HIS:CD2	2.84	0.49
3:I:71:PRO:HG3	3:I:135:VAL:CG2	2.43	0.49
1:A:112:ILE:HG12	6:A:501:HEM:HAC	1.94	0.49
3:L:162:ILE:HD13	3:L:167:ALA:HB3	1.95	0.49
1:D:114:ARG:HD2	1:D:114:ARG:C	2.34	0.49
1:J:39:ARG:NH1	2:K:255:VAL:HG12	2.27	0.48
1:D:292:ILE:O	1:D:293:VAL:HG23	2.12	0.48
3:I:96:THR:O	3:I:109:ALA:N	2.37	0.48
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.26	0.48
2:K:72:VAL:CG1	2:K:73:THR:H	2.26	0.48
2:E:59:PRO:HD2	2:E:62:GLN:HE21	1.75	0.48
1:J:122:LYS:NZ	1:J:352:SER:O	2.46	0.48
1:J:13:THR:CG2	1:J:14:GLY:H	2.25	0.48
2:K:112:GLY:O	2:K:119:SER:HB3	2.14	0.48
2:B:116:THR:HG22	2:B:118:ILE:HG13	1.95	0.48
2:B:42:MET:HE2	2:B:101:SER:HA	1.94	0.48
1:J:383:GLN:HE22	2:K:115:GLY:HA3	1.78	0.48
1:J:342:VAL:HG13	1:J:404:PHE:CB	2.43	0.48
1:G:114:ARG:HD2	1:G:114:ARG:C	2.33	0.48
1:D:376:ILE:O	1:D:380:VAL:HG22	2.14	0.48
1:A:342:VAL:HG13	1:A:404:PHE:CB	2.44	0.48
1:G:292:ILE:O	1:G:293:VAL:HG23	2.14	0.48
1:A:292:ILE:O	1:A:293:VAL:HG23	2.14	0.48
1:J:114:ARG:HD2	1:J:114:ARG:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:O	1:A:46:ILE:HG13	2.14	0.48
6:D:502:HEM:HHD	6:D:502:HEM:CBC	2.42	0.48
2:E:77:THR:C	2:E:79:GLU:N	2.67	0.48
2:E:143:PRO:HD3	2:E:156:TYR:CD2	2.48	0.48
2:H:59:PRO:HD2	2:H:62:GLN:HE21	1.76	0.48
2:E:112:GLY:O	2:E:119:SER:HB3	2.14	0.48
1:J:194:PHE:CE1	8:J:503:SMA:H28	2.49	0.48
1:A:346:VAL:HG12	1:A:347:PRO:HD3	1.96	0.48
1:J:121:TYR:HB3	1:J:129:TRP:CE3	2.49	0.48
3:F:156:TYR:HA	3:F:161:ARG:O	2.14	0.48
1:G:121:TYR:HB3	1:G:129:TRP:CE3	2.49	0.48
1:G:295:GLU:OE1	1:G:295:GLU:N	2.47	0.48
1:J:13:THR:CG2	1:J:14:GLY:N	2.75	0.48
2:B:194:VAL:HB	2:B:207:MET:HE3	1.95	0.48
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.48	0.48
3:C:96:THR:O	3:C:109:ALA:N	2.36	0.48
2:H:199:GLY:O	2:H:200:HIS:O	2.32	0.48
3:C:86:ARG:HG2	3:C:112:GLN:OE1	2.14	0.48
1:G:92:MET:CE	2:H:226:ARG:HG3	2.44	0.48
2:B:112:GLY:O	2:B:119:SER:HB3	2.13	0.48
2:H:223:LEU:CD2	2:H:227:LYS:HD2	2.43	0.48
1:J:105:PHE:HA	1:J:108:VAL:CG2	2.44	0.48
2:E:116:THR:HG22	2:E:118:ILE:HG13	1.96	0.48
1:G:45:TRP:CZ3	1:G:224:PRO:HG3	2.49	0.48
1:A:13:THR:CG2	1:A:14:GLY:N	2.74	0.47
1:G:13:THR:CG2	1:G:14:GLY:H	2.25	0.47
2:K:194:VAL:HB	2:K:207:MET:HE3	1.95	0.47
1:G:346:VAL:CG1	1:G:347:PRO:HD3	2.43	0.47
1:G:272:ASN:ND2	2:H:105:LYS:HD2	2.28	0.47
1:A:83:ILE:O	1:A:90:GLY:HA3	2.14	0.47
1:D:51:LEU:HD13	6:D:501:HEM:C3B	2.48	0.47
2:B:42:MET:HE1	2:B:218:ALA:CB	2.39	0.47
1:A:13:THR:CG2	1:A:14:GLY:H	2.25	0.47
2:H:119:SER:O	2:H:123:ASN:HB2	2.15	0.47
1:A:45:TRP:CZ3	1:A:224:PRO:HG3	2.48	0.47
1:G:209:VAL:CG2	6:G:501:HEM:HBB2	2.44	0.47
3:F:143:ASP:HB2	3:F:144:PHE:CE1	2.49	0.47
2:H:116:THR:HG22	2:H:118:ILE:HG13	1.95	0.47
1:J:376:ILE:O	1:J:380:VAL:HG22	2.14	0.47
1:J:45:TRP:CZ3	1:J:224:PRO:HG3	2.49	0.47
1:J:8:HIS:N	1:J:8:HIS:CD2	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:SER:O	2:B:123:ASN:HB2	2.14	0.47
2:E:67:ALA:O	2:E:83:GLY:HA3	2.15	0.47
3:C:162:ILE:HD13	3:C:167:ALA:HB3	1.96	0.47
2:K:138:PHE:CE1	2:K:157:ASN:ND2	2.82	0.47
1:A:422:ALA:HB3	1:A:426:GLU:OE1	2.13	0.47
2:K:199:GLY:O	2:K:200:HIS:O	2.32	0.47
1:J:346:VAL:CG1	1:J:347:PRO:HD3	2.45	0.47
2:H:199:GLY:O	2:H:200:HIS:C	2.53	0.47
1:G:418:VAL:HG12	1:G:419:ALA:N	2.30	0.47
3:I:162:ILE:HD13	3:I:167:ALA:HB3	1.96	0.47
6:D:501:HEM:CMA	10:D:504:ANJ:O7	2.62	0.47
1:A:46:ILE:C	1:A:46:ILE:HD12	2.35	0.47
3:C:177:LYS:HE2	3:C:185:GLN:NE2	2.28	0.47
1:J:44:MET:CE	9:J:504:LOP:H92	2.45	0.47
1:G:8:HIS:CD2	1:G:8:HIS:N	2.80	0.47
2:K:72:VAL:CG1	2:K:73:THR:N	2.77	0.47
2:K:77:THR:C	2:K:79:GLU:N	2.67	0.47
2:B:77:THR:HG22	2:B:79:GLU:CB	2.44	0.47
2:E:136:THR:O	2:E:138:PHE:N	2.43	0.47
2:E:119:SER:O	2:E:123:ASN:HB2	2.15	0.47
1:G:112:ILE:HG12	6:G:501:HEM:HAC	1.97	0.47
1:A:67:MET:HG2	1:D:193:ARG:HA	1.96	0.47
2:K:113:PRO:O	2:K:114:MET:HB2	2.14	0.47
2:H:160:PHE:CE2	2:H:183:ILE:HG13	2.49	0.47
3:F:92:GLN:HG2	11:F:207:HOH:O	2.14	0.47
3:C:44:VAL:C	3:C:46:ALA:H	2.18	0.47
2:B:6:VAL:HG11	2:B:130:TYR:HA	1.97	0.47
2:E:199:GLY:O	2:E:200:HIS:O	2.32	0.47
2:K:116:THR:HG22	2:K:118:ILE:HG13	1.95	0.47
3:I:156:TYR:HA	3:I:161:ARG:O	2.14	0.47
1:D:91:PHE:HE2	1:D:92:MET:CE	2.26	0.47
1:G:376:ILE:O	1:G:380:VAL:HG22	2.14	0.47
2:H:113:PRO:O	2:H:114:MET:HB2	2.15	0.47
1:G:406:VAL:O	1:G:409:PRO:HD2	2.15	0.47
1:D:91:PHE:CE2	1:D:92:MET:HE2	2.49	0.47
2:E:48:ARG:HB3	2:E:85:PRO:O	2.15	0.47
1:J:39:ARG:NH1	2:K:255:VAL:CG1	2.78	0.47
1:J:91:PHE:CE2	1:J:92:MET:HE2	2.49	0.47
1:D:121:TYR:HB3	1:D:129:TRP:CE3	2.49	0.47
2:K:67:ALA:O	2:K:83:GLY:HA3	2.15	0.47
3:F:128:VAL:O	3:F:129:CYS:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:TRP:CD1	1:D:313:TRP:N	2.82	0.47
1:D:202:PRO:HG2	6:D:502:HEM:HMC3	1.97	0.46
3:C:179:ILE:O	3:C:180:ASP:HB3	2.15	0.46
1:D:39:ARG:HD3	1:D:428:PHE:HD2	1.80	0.46
1:D:91:PHE:CE2	1:D:92:MET:CE	2.98	0.46
3:L:163:ARG:O	3:L:164:LYS:HB2	2.15	0.46
1:J:59:ILE:O	1:J:63:ILE:HG13	2.15	0.46
3:L:156:TYR:HA	3:L:161:ARG:O	2.15	0.46
3:I:164:LYS:HG3	11:J:524:HOH:O	2.14	0.46
1:D:346:VAL:CG1	1:D:347:PRO:HD3	2.45	0.46
2:H:81:ARG:HG3	2:H:81:ARG:NH1	2.30	0.46
3:F:179:ILE:O	3:F:180:ASP:HB3	2.16	0.46
3:L:110:THR:O	3:L:113:ASN:N	2.47	0.46
2:E:77:THR:CG2	2:E:79:GLU:HB2	2.45	0.46
2:E:120:GLN:C	2:E:122:PHE:N	2.69	0.46
3:F:54:VAL:HG13	3:F:57:VAL:HG21	1.97	0.46
3:C:156:TYR:HA	3:C:161:ARG:O	2.15	0.46
2:E:154:PHE:HB3	2:E:182:TRP:HB3	1.98	0.46
2:H:165:VAL:HG21	2:H:176:LYS:CD	2.46	0.46
3:I:118:GLU:C	3:I:120:GLY:N	2.69	0.46
3:L:50:ILE:HD11	3:L:186:LEU:HD12	1.98	0.46
2:K:6:VAL:HG11	2:K:130:TYR:HA	1.98	0.46
1:G:122:LYS:NZ	1:G:354:VAL:O	2.45	0.46
1:D:405:LEU:O	1:D:409:PRO:HG2	2.15	0.46
2:B:66:TYR:CE1	2:B:69:GLN:NE2	2.83	0.46
2:B:43:LYS:HD2	2:B:44:PHE:CE2	2.50	0.46
2:H:42:MET:HE2	2:H:101:SER:HA	1.96	0.46
1:D:13:THR:CG2	1:D:14:GLY:H	2.25	0.46
3:I:54:VAL:HG13	3:I:57:VAL:HG21	1.97	0.46
3:I:128:VAL:O	3:I:129:CYS:C	2.54	0.46
1:J:236:GLU:O	1:J:239:LYS:HB2	2.15	0.46
3:L:118:GLU:C	3:L:120:GLY:H	2.18	0.46
2:B:199:GLY:O	2:B:200:HIS:O	2.33	0.46
2:E:81:ARG:HG3	2:E:81:ARG:HH11	1.80	0.46
1:G:342:VAL:HG13	1:G:404:PHE:CB	2.45	0.46
2:E:250:ARG:HH22	3:F:11:ARG:HD3	1.80	0.46
2:B:120:GLN:C	2:B:122:PHE:N	2.69	0.46
3:F:162:ILE:HD13	3:F:167:ALA:HB3	1.96	0.46
1:A:376:ILE:O	1:A:380:VAL:HG22	2.16	0.46
1:A:122:LYS:O	1:A:123:ALA:C	2.52	0.46
2:E:77:THR:HG22	2:E:79:GLU:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:ASP:C	3:C:159:ALA:H	2.19	0.46
1:A:121:TYR:HB3	1:A:129:TRP:CE3	2.50	0.46
3:I:11:ARG:CB	3:I:11:ARG:HH11	2.29	0.46
1:G:346:VAL:HG12	1:G:347:PRO:HD3	1.97	0.46
3:L:157:ASP:HB2	11:L:210:HOH:O	2.15	0.46
1:D:346:VAL:HG12	1:D:347:PRO:HD3	1.98	0.46
3:L:118:GLU:C	3:L:120:GLY:N	2.68	0.46
1:G:360:ARG:O	1:G:364:LYS:HG3	2.15	0.46
2:H:6:VAL:HG11	2:H:130:TYR:HA	1.97	0.46
1:J:46:ILE:HD12	1:J:46:ILE:C	2.36	0.46
1:D:9:TYR:CE1	1:D:11:PRO:HG3	2.50	0.46
1:D:273:TYR:CE2	2:E:121:LEU:HD13	2.51	0.46
3:F:96:THR:O	3:F:109:ALA:N	2.36	0.46
1:A:245:TRP:CE3	1:A:246:PRO:HA	2.51	0.46
1:D:213:ILE:HD12	10:D:504:ANJ:O9	2.16	0.46
2:H:149:HIS:CD2	2:H:168:THR:OG1	2.69	0.46
3:L:179:ILE:O	3:L:180:ASP:HB3	2.16	0.46
2:K:119:SER:O	2:K:123:ASN:HB2	2.15	0.46
3:L:11:ARG:HH11	3:L:11:ARG:CB	2.29	0.46
2:K:199:GLY:O	2:K:200:HIS:C	2.54	0.46
1:G:156:PHE:CE1	1:G:186:VAL:HG12	2.51	0.46
1:G:46:ILE:HD12	1:G:46:ILE:C	2.37	0.46
2:E:231:PHE:HD1	2:E:231:PHE:O	1.98	0.46
3:C:11:ARG:CB	3:C:11:ARG:HH11	2.28	0.46
2:E:138:PHE:CD2	2:E:187:PRO:HA	2.51	0.46
2:E:184:ALA:HB3	6:E:301:HEM:CBD	2.44	0.46
3:C:94:VAL:HG23	3:C:162:ILE:O	2.15	0.46
1:G:245:TRP:CE3	1:G:246:PRO:HA	2.51	0.46
3:F:112:GLN:CD	3:F:112:GLN:H	2.20	0.45
1:D:291:HIS:O	1:D:293:VAL:HG23	2.17	0.45
3:L:155:HIS:CD2	3:L:164:LYS:HD3	2.51	0.45
3:C:146:GLY:HA3	3:C:156:TYR:O	2.15	0.45
3:F:50:ILE:HD11	3:F:186:LEU:HD12	1.98	0.45
2:H:86:THR:HG21	3:I:46:ALA:HB1	1.98	0.45
2:K:149:HIS:N	2:K:149:HIS:CD2	2.85	0.45
3:I:157:ASP:C	3:I:159:ALA:H	2.19	0.45
3:F:163:ARG:O	3:F:164:LYS:HB2	2.16	0.45
1:D:102:SER:O	1:D:106:ILE:HG13	2.17	0.45
2:K:165:VAL:HG12	2:K:169:CYS:HB2	1.98	0.45
1:J:156:PHE:O	1:J:159:ALA:HB3	2.16	0.45
3:L:144:PHE:N	3:L:144:PHE:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:CG2	10:A:504:ANJ:H1	2.44	0.45
3:F:107:ALA:HB1	3:F:113:ASN:HD21	1.81	0.45
2:B:226:ARG:NH2	11:B:308:HOH:O	2.49	0.45
2:E:6:VAL:HG11	2:E:130:TYR:HA	1.98	0.45
3:C:54:VAL:HG13	3:C:57:VAL:HG21	1.97	0.45
1:D:144:PHE:CE1	1:D:162:ILE:HD12	2.51	0.45
3:F:11:ARG:CB	3:F:11:ARG:HH11	2.29	0.45
1:A:265:ALA:HB1	4:A:431:BGL:H5'2	1.98	0.45
2:H:155:TYR:N	2:H:155:TYR:CD1	2.85	0.45
3:I:93:LEU:HD12	3:I:109:ALA:HB3	1.98	0.45
1:A:291:HIS:O	1:A:293:VAL:HG23	2.16	0.45
3:F:157:ASP:C	3:F:159:ALA:H	2.20	0.45
2:B:67:ALA:O	2:B:83:GLY:HA3	2.17	0.45
2:B:48:ARG:HB3	2:B:85:PRO:O	2.16	0.45
2:H:48:ARG:HB3	2:H:85:PRO:O	2.16	0.45
2:H:194:VAL:HB	2:H:207:MET:HE3	1.98	0.45
2:K:48:ARG:HB3	2:K:85:PRO:O	2.16	0.45
1:D:351:THR:OG1	1:D:412:GLY:HA3	2.16	0.45
1:D:245:TRP:CE3	1:D:246:PRO:HA	2.51	0.45
1:D:46:ILE:HD12	1:D:46:ILE:C	2.37	0.45
2:H:236:PHE:CE2	3:I:25:VAL:HG12	2.45	0.45
3:F:118:GLU:C	3:F:120:GLY:N	2.70	0.45
3:L:128:VAL:O	3:L:129:CYS:C	2.53	0.45
3:I:144:PHE:CD1	3:I:144:PHE:N	2.85	0.45
2:K:86:THR:HG22	3:L:46:ALA:CB	2.46	0.45
3:F:83:GLU:O	3:F:84:LEU:C	2.55	0.45
3:F:146:GLY:HA3	3:F:156:TYR:O	2.16	0.45
3:L:96:THR:O	3:L:109:ALA:N	2.37	0.45
2:E:149:HIS:ND1	2:E:168:THR:HG21	2.31	0.45
2:E:74:ASP:CB	2:E:77:THR:HB	2.47	0.45
3:F:108:GLU:O	3:F:110:THR:N	2.44	0.45
3:F:44:VAL:C	3:F:46:ALA:H	2.20	0.45
2:B:143:PRO:HD3	2:B:156:TYR:CD2	2.52	0.45
2:H:49:SER:HA	2:H:52:GLU:OE1	2.17	0.45
1:G:291:HIS:O	1:G:293:VAL:HG23	2.17	0.45
2:B:199:GLY:O	2:B:200:HIS:C	2.55	0.45
2:K:120:GLN:C	2:K:122:PHE:N	2.69	0.45
3:C:50:ILE:HD11	3:C:186:LEU:HD12	1.98	0.45
3:I:50:ILE:HD11	3:I:186:LEU:HD12	1.97	0.45
1:A:4:ILE:CD1	1:A:4:ILE:H	2.16	0.45
1:G:406:VAL:C	1:G:409:PRO:HD2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD13	1:D:200:LEU:HD22	1.97	0.45
1:G:156:PHE:O	1:G:159:ALA:HB3	2.17	0.45
1:D:321:ILE:O	1:D:321:ILE:HG22	2.17	0.45
2:E:175:VAL:HG12	2:E:176:LYS:N	2.32	0.44
1:D:9:TYR:HB2	1:D:30:TYR:CG	2.52	0.44
2:E:77:THR:HG22	2:E:79:GLU:CG	2.47	0.44
2:H:170:LYS:HA	2:H:176:LYS:HA	1.99	0.44
3:L:157:ASP:C	3:L:159:ALA:H	2.19	0.44
1:A:156:PHE:CE1	1:A:186:VAL:HG12	2.52	0.44
2:E:250:ARG:HH12	3:F:11:ARG:CD	2.30	0.44
2:K:86:THR:CG2	3:L:46:ALA:HB1	2.45	0.44
2:B:155:TYR:N	2:B:155:TYR:CD1	2.85	0.44
1:J:346:VAL:HG12	1:J:347:PRO:HD3	1.99	0.44
1:D:292:ILE:O	1:D:293:VAL:CG2	2.65	0.44
3:C:128:VAL:O	3:C:129:CYS:C	2.54	0.44
2:B:27:ARG:HD2	2:B:196:TYR:CZ	2.52	0.44
3:L:54:VAL:HG13	3:L:57:VAL:HG21	1.98	0.44
2:H:120:GLN:C	2:H:122:PHE:H	2.20	0.44
3:I:71:PRO:HG3	3:I:135:VAL:HG21	1.99	0.44
1:J:156:PHE:CE1	1:J:186:VAL:HG12	2.53	0.44
3:I:179:ILE:O	3:I:180:ASP:HB3	2.16	0.44
3:C:112:GLN:H	3:C:112:GLN:HE21	1.61	0.44
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.48	0.44
2:H:8:ASP:OD1	2:H:110:PHE:HZ	2.01	0.44
1:A:236:GLU:HA	1:A:239:LYS:CD	2.47	0.44
1:A:39:ARG:HG2	1:A:242:VAL:CG1	2.45	0.44
2:K:59:PRO:CD	2:K:62:GLN:NE2	2.80	0.44
2:E:155:TYR:N	2:E:155:TYR:CD1	2.86	0.44
1:J:245:TRP:CE3	1:J:246:PRO:HA	2.51	0.44
1:J:292:ILE:O	1:J:293:VAL:CG2	2.66	0.44
1:D:376:ILE:O	1:D:380:VAL:CG2	2.66	0.44
1:A:156:PHE:O	1:A:159:ALA:HB3	2.18	0.44
1:J:201:LEU:HA	1:J:201:LEU:HD23	1.76	0.44
1:D:51:LEU:HB3	6:D:501:HEM:HMB1	2.00	0.44
1:J:405:LEU:O	1:J:409:PRO:HG2	2.18	0.44
2:H:154:PHE:C	2:H:155:TYR:CD1	2.92	0.44
1:J:262:VAL:O	1:J:266:ILE:HG12	2.18	0.44
1:G:312:VAL:O	1:G:316:GLN:HG3	2.18	0.44
2:H:73:THR:HG23	2:H:78:GLY:O	2.18	0.44
3:I:112:GLN:NE2	3:I:112:GLN:N	2.60	0.43
1:A:418:VAL:CG1	1:A:419:ALA:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:PHE:C	2:B:155:TYR:CD1	2.91	0.43
3:L:109:ALA:O	3:L:161:ARG:NH1	2.44	0.43
2:B:120:GLN:C	2:B:122:PHE:H	2.21	0.43
3:L:117:ASP:OD2	3:L:121:GLU:HB3	2.17	0.43
1:A:387:PHE:CZ	1:A:388:PRO:HB3	2.53	0.43
1:D:112:ILE:HG12	6:D:501:HEM:HAC	2.00	0.43
1:A:41:LEU:HD22	1:A:45:TRP:CD1	2.53	0.43
1:G:209:VAL:HG22	6:G:501:HEM:HBB2	2.00	0.43
1:D:406:VAL:O	1:D:409:PRO:HD2	2.18	0.43
3:C:134:CYS:HB2	3:C:149:CYS:SG	2.59	0.43
1:A:52:ALA:HB2	10:A:504:ANJ:H161	1.98	0.43
1:G:418:VAL:CG1	1:G:419:ALA:N	2.81	0.43
1:G:377:LEU:HA	1:G:380:VAL:HG23	2.01	0.43
2:B:48:ARG:HG3	2:B:48:ARG:HH11	1.82	0.43
3:L:134:CYS:HB2	3:L:149:CYS:SG	2.58	0.43
2:H:76:GLU:O	2:H:77:THR:C	2.55	0.43
3:I:177:LYS:HE3	3:I:179:ILE:CD1	2.49	0.43
1:J:13:THR:O	1:J:17:LYS:HG3	2.18	0.43
2:E:170:LYS:HA	2:E:175:VAL:O	2.17	0.43
1:A:9:TYR:HB2	1:A:30:TYR:CD2	2.52	0.43
2:K:155:TYR:CD1	2:K:155:TYR:N	2.86	0.43
3:C:44:VAL:O	3:C:46:ALA:N	2.52	0.43
3:L:146:GLY:HA3	3:L:156:TYR:O	2.17	0.43
2:K:120:GLN:C	2:K:122:PHE:H	2.20	0.43
2:E:154:PHE:C	2:E:155:TYR:CD1	2.92	0.43
3:F:118:GLU:C	3:F:120:GLY:H	2.20	0.43
2:H:165:VAL:HG21	2:H:176:LYS:HD3	1.99	0.43
3:F:157:ASP:OD2	3:F:161:ARG:HB2	2.19	0.43
2:B:86:THR:HG22	3:C:46:ALA:HB1	2.00	0.43
3:I:118:GLU:N	3:I:118:GLU:CD	2.71	0.43
2:H:120:GLN:C	2:H:122:PHE:N	2.69	0.43
3:F:134:CYS:HB2	3:F:149:CYS:SG	2.59	0.43
2:K:71:THR:HG22	2:K:71:THR:O	2.18	0.43
1:A:193:ARG:HA	1:D:67:MET:HG2	2.00	0.43
3:L:138:GLY:HA2	3:L:147:TRP:CD1	2.54	0.43
1:A:37:THR:HG22	1:A:41:LEU:HD11	1.99	0.43
1:A:153:GLN:HA	1:A:153:GLN:OE1	2.19	0.43
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.54	0.43
2:E:73:THR:HA	2:E:79:GLU:O	2.18	0.43
2:B:194:VAL:O	2:B:194:VAL:HG12	2.19	0.43
1:A:403:TYR:O	1:A:408:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:197:ALA:C	2:E:199:GLY:H	2.22	0.43
3:I:157:ASP:OD2	3:I:161:ARG:HB2	2.19	0.43
3:C:157:ASP:OD2	3:C:161:ARG:HB2	2.19	0.43
3:I:118:GLU:C	3:I:120:GLY:H	2.20	0.43
2:B:81:ARG:NH1	2:B:84:LYS:HG3	2.34	0.43
1:D:201:LEU:HD23	1:D:201:LEU:HA	1.76	0.43
1:A:39:ARG:HD3	1:A:428:PHE:CD2	2.54	0.43
2:E:250:ARG:HD2	3:F:12:ARG:HG3	2.00	0.43
1:G:262:VAL:O	1:G:266:ILE:HG12	2.19	0.43
2:K:154:PHE:C	2:K:155:TYR:CD1	2.92	0.43
1:J:376:ILE:O	1:J:380:VAL:CG2	2.66	0.43
2:E:48:ARG:HH11	2:E:48:ARG:HG3	1.84	0.43
3:L:157:ASP:OD2	3:L:161:ARG:HB2	2.19	0.43
2:B:66:TYR:O	2:B:69:GLN:HG2	2.18	0.43
3:F:117:ASP:OD2	3:F:121:GLU:HB2	2.18	0.43
3:C:59:PRO:HA	3:C:76:ARG:HB3	2.00	0.43
2:E:120:GLN:C	2:E:122:PHE:H	2.20	0.43
1:G:118:TYR:CD1	1:G:224:PRO:HA	2.54	0.43
2:K:197:ALA:C	2:K:199:GLY:H	2.22	0.43
2:E:199:GLY:O	2:E:200:HIS:C	2.57	0.43
2:K:94:LEU:HD22	6:K:301:HEM:HAC	1.99	0.43
1:D:66:ALA:HB2	6:D:502:HEM:CBC	2.48	0.43
1:J:39:ARG:HG2	1:J:242:VAL:CG1	2.47	0.43
1:J:44:MET:HE3	9:J:504:LOP:H92	2.01	0.43
2:E:150:GLU:HG2	2:E:182:TRP:HE1	1.83	0.43
2:E:36:CYS:N	6:E:301:HEM:HAB	2.33	0.43
1:J:92:MET:HE2	1:J:92:MET:CA	2.49	0.43
3:I:162:ILE:CD1	3:I:167:ALA:HB3	2.49	0.43
3:I:163:ARG:O	3:I:164:LYS:HB2	2.17	0.43
2:H:6:VAL:HG21	2:H:109:GLY:HA3	2.00	0.43
3:L:54:VAL:HG11	3:L:122:TRP:CZ3	2.54	0.43
2:H:81:ARG:NH1	2:H:82:GLU:O	2.52	0.42
3:F:110:THR:O	3:F:113:ASN:N	2.51	0.42
2:E:185:MET:HB2	6:E:301:HEM:C1D	2.53	0.42
3:F:54:VAL:HG12	3:F:54:VAL:O	2.19	0.42
3:I:54:VAL:HG11	3:I:122:TRP:CZ3	2.54	0.42
2:K:240:LEU:HD13	3:L:22:ALA:HB3	2.01	0.42
1:D:156:PHE:O	1:D:159:ALA:HB3	2.18	0.42
1:J:153:GLN:OE1	1:J:153:GLN:HA	2.19	0.42
2:H:146:ALA:O	2:H:147:GLU:C	2.57	0.42
2:E:49:SER:HA	2:E:52:GLU:CG	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:TYR:HB3	2:H:252:TRP:CZ2	2.55	0.42
3:C:38:MET:HE2	1:D:193:ARG:HH11	1.84	0.42
2:E:94:LEU:HD22	6:E:301:HEM:HAC	2.01	0.42
1:G:292:ILE:O	1:G:293:VAL:CG2	2.67	0.42
3:I:54:VAL:O	3:I:54:VAL:HG12	2.20	0.42
2:B:197:ALA:C	2:B:199:GLY:H	2.23	0.42
1:D:262:VAL:O	1:D:266:ILE:HG12	2.19	0.42
3:C:118:GLU:C	3:C:120:GLY:H	2.21	0.42
1:G:296:TRP:HA	1:G:299:LEU:HG	2.01	0.42
2:B:56:PRO:HD2	11:B:304:HOH:O	2.18	0.42
2:B:146:ALA:O	2:B:147:GLU:C	2.57	0.42
2:E:146:ALA:O	2:E:147:GLU:C	2.58	0.42
1:J:291:HIS:O	1:J:293:VAL:HG23	2.18	0.42
1:D:117:TYR:HB2	1:D:367:PHE:CZ	2.55	0.42
1:G:5:PRO:HB2	1:G:234:LYS:CA	2.41	0.42
1:D:39:ARG:HH12	2:E:255:VAL:CG1	2.33	0.42
1:D:93:LEU:HA	1:D:93:LEU:HD23	1.88	0.42
3:L:108:GLU:O	3:L:110:THR:N	2.44	0.42
1:J:92:MET:HA	1:J:92:MET:HE2	2.01	0.42
3:L:162:ILE:CD1	3:L:167:ALA:HB3	2.49	0.42
1:G:43:TRP:O	1:G:46:ILE:HG13	2.19	0.42
3:I:59:PRO:HA	3:I:76:ARG:HB3	2.01	0.42
1:G:214:TRP:CH2	1:J:25:ILE:HA	2.54	0.42
1:G:161:VAL:HG11	8:G:503:SMA:O5	2.19	0.42
1:A:262:VAL:O	1:A:266:ILE:HG12	2.19	0.42
2:E:72:VAL:O	2:E:80:ASP:HA	2.19	0.42
3:L:59:PRO:HA	3:L:76:ARG:HB3	2.00	0.42
2:B:114:MET:HG2	2:B:114:MET:O	2.18	0.42
1:G:273:TYR:CE2	2:H:121:LEU:HD13	2.54	0.42
1:A:425:GLU:O	1:A:429:ASN:ND2	2.53	0.42
2:E:139:PRO:HG3	2:E:158:ARG:CZ	2.48	0.42
2:H:13:PHE:O	2:H:227:LYS:NZ	2.53	0.42
1:D:122:LYS:O	1:D:123:ALA:C	2.58	0.42
3:I:140:VAL:O	3:I:140:VAL:HG12	2.20	0.42
2:E:232:THR:HG22	2:E:236:PHE:HE1	1.84	0.42
2:E:165:VAL:HG21	2:E:176:LYS:HD3	2.01	0.42
1:A:120:SER:HB3	6:A:501:HEM:HAD2	2.02	0.42
1:A:292:ILE:O	1:A:293:VAL:CG2	2.68	0.42
2:H:197:ALA:C	2:H:199:GLY:H	2.23	0.42
3:C:162:ILE:CD1	3:C:167:ALA:HB3	2.49	0.42
3:C:118:GLU:C	3:C:120:GLY:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ILE:HG22	1:D:5:PRO:CD	2.50	0.42
1:A:199:TYR:CZ	6:A:502:HEM:HBC1	2.55	0.42
2:B:59:PRO:CD	2:B:62:GLN:NE2	2.81	0.42
3:F:123:LEU:HG	3:F:125:MET:HE2	2.02	0.42
3:F:95:ASP:OD2	3:F:170:ASN:ND2	2.52	0.42
3:L:54:VAL:HG12	3:L:54:VAL:O	2.19	0.42
1:G:153:GLN:HA	1:G:153:GLN:OE1	2.19	0.42
1:G:6:HIS:C	1:G:6:HIS:ND1	2.72	0.42
1:A:317:ILE:C	1:A:321:ILE:HG22	2.36	0.42
2:E:182:TRP:N	2:E:182:TRP:CE3	2.88	0.42
1:D:27:ALA:O	1:D:30:TYR:HB3	2.20	0.42
3:F:57:VAL:HG22	3:F:63:LEU:HD13	2.02	0.42
2:K:27:ARG:HD2	2:K:196:TYR:CZ	2.54	0.42
1:G:276:HIS:HA	1:G:277:PRO:HD3	1.91	0.42
1:A:296:TRP:HA	1:A:299:LEU:HG	2.00	0.42
1:G:37:THR:CG2	1:G:41:LEU:HD11	2.49	0.42
1:D:118:TYR:CD1	1:D:224:PRO:HA	2.55	0.42
1:G:4:ILE:CG2	1:G:237:ALA:HB1	2.50	0.42
1:A:132:GLY:HA3	6:A:501:HEM:HBC2	2.01	0.42
1:J:377:LEU:HA	1:J:380:VAL:HG23	2.02	0.42
3:I:146:GLY:HA3	3:I:156:TYR:O	2.20	0.42
3:C:54:VAL:HG11	3:C:122:TRP:CZ3	2.54	0.42
2:B:106:ALA:O	2:B:107:ARG:HD3	2.19	0.42
1:G:10:GLU:HA	1:G:11:PRO:HD3	1.91	0.42
3:F:59:PRO:HA	3:F:76:ARG:HB3	2.01	0.42
1:D:416:LYS:HA	1:D:417:PRO:HD2	1.85	0.42
1:D:234:LYS:O	1:D:238:GLN:HG3	2.19	0.42
1:D:276:HIS:HA	1:D:277:PRO:HD3	1.92	0.42
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.55	0.42
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.55	0.42
1:A:130:ILE:HD11	1:A:348:TRP:CH2	2.43	0.42
1:D:39:ARG:HG2	1:D:242:VAL:CG1	2.46	0.42
1:G:8:HIS:O	1:G:30:TYR:CE2	2.72	0.42
2:H:59:PRO:CD	2:H:62:GLN:NE2	2.81	0.42
1:J:408:LEU:HB2	1:J:409:PRO:HD3	2.01	0.42
1:J:362:MET:HE3	1:J:415:GLU:HA	2.00	0.42
2:E:20:PHE:CB	2:E:25:LEU:HD11	2.49	0.42
2:H:154:PHE:HB3	2:H:182:TRP:HB3	2.01	0.42
2:H:170:LYS:HA	2:H:175:VAL:O	2.19	0.42
3:F:54:VAL:HG11	3:F:122:TRP:CZ3	2.54	0.42
1:A:193:ARG:NH1	3:F:38:MET:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:THR:O	2:B:79:GLU:N	2.53	0.41
2:H:20:PHE:CB	2:H:25:LEU:HD11	2.50	0.41
1:J:118:TYR:CD1	1:J:224:PRO:HA	2.54	0.41
1:G:11:PRO:HG2	1:G:20:HIS:CG	2.55	0.41
2:K:167:ASP:HA	2:K:170:LYS:HE3	2.02	0.41
1:A:92:MET:HE2	1:A:92:MET:HA	2.02	0.41
1:A:150:PRO:HG3	6:A:502:HEM:O2D	2.19	0.41
3:C:110:THR:OG1	3:C:113:ASN:HB2	2.20	0.41
1:D:39:ARG:NH1	2:E:255:VAL:HG12	2.35	0.41
1:J:93:LEU:HA	1:J:93:LEU:HD23	1.87	0.41
2:K:20:PHE:CB	2:K:25:LEU:HD11	2.49	0.41
1:G:376:ILE:O	1:G:380:VAL:CG2	2.68	0.41
1:G:200:LEU:HD22	1:J:63:ILE:HD13	2.02	0.41
2:E:231:PHE:HE1	2:E:235:MET:CE	2.33	0.41
3:I:47:LEU:HG	3:I:68:LEU:HD21	2.02	0.41
1:G:321:ILE:HG22	1:G:321:ILE:O	2.18	0.41
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.55	0.41
1:J:317:ILE:C	1:J:321:ILE:HG22	2.36	0.41
1:D:3:GLY:N	1:D:4:ILE:HD12	2.35	0.41
1:D:4:ILE:HG22	1:D:5:PRO:HD2	2.02	0.41
2:H:77:THR:O	2:H:79:GLU:N	2.50	0.41
2:K:252:TRP:O	2:K:255:VAL:HG23	2.20	0.41
1:A:122:LYS:NZ	1:A:352:SER:O	2.53	0.41
2:E:59:PRO:CD	2:E:62:GLN:NE2	2.80	0.41
1:A:239:LYS:HE2	1:A:425:GLU:CD	2.40	0.41
1:A:118:TYR:CD1	1:A:224:PRO:HA	2.55	0.41
3:L:93:LEU:HD13	3:L:109:ALA:HB3	2.01	0.41
1:G:122:LYS:HE2	1:G:350:ASP:CG	2.41	0.41
1:A:410:ILE:HG22	1:A:414:ILE:HD12	2.01	0.41
1:J:117:TYR:HB2	1:J:367:PHE:CZ	2.55	0.41
2:K:146:ALA:O	2:K:147:GLU:C	2.58	0.41
1:D:236:GLU:HA	1:D:239:LYS:HD3	2.02	0.41
2:B:43:LYS:HD2	2:B:44:PHE:CZ	2.56	0.41
1:A:376:ILE:O	1:A:380:VAL:CG2	2.69	0.41
3:I:134:CYS:HB2	3:I:149:CYS:SG	2.60	0.41
1:D:153:GLN:OE1	1:D:153:GLN:HA	2.19	0.41
8:A:1:SMA:H4	3:F:151:CYS:HB3	2.02	0.41
3:F:162:ILE:CD1	3:F:167:ALA:HB3	2.50	0.41
1:A:11:PRO:O	1:A:17:LYS:NZ	2.54	0.41
1:J:73:VAL:HG12	1:J:151:TRP:CE2	2.56	0.41
2:B:231:PHE:CD1	2:B:231:PHE:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:PHE:CD1	1:D:323:PHE:N	2.88	0.41
1:D:366:TYR:HD2	1:D:411:LEU:HD11	1.85	0.41
1:A:405:LEU:O	1:A:409:PRO:HG2	2.21	0.41
3:C:54:VAL:O	3:C:54:VAL:HG12	2.19	0.41
2:H:48:ARG:HH11	2:H:48:ARG:HG3	1.85	0.41
1:D:156:PHE:CE1	1:D:186:VAL:HG12	2.54	0.41
2:H:42:MET:CE	2:H:218:ALA:CB	2.97	0.41
1:A:233:SER:OG	1:A:236:GLU:HG2	2.21	0.41
1:D:296:TRP:HA	1:D:299:LEU:HG	2.02	0.41
1:G:117:TYR:HB2	1:G:367:PHE:CZ	2.56	0.41
2:K:126:GLY:HA2	2:K:129:GLU:OE1	2.21	0.41
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.84	0.41
2:B:184:ALA:HB3	6:B:301:HEM:HBD2	2.01	0.41
3:I:57:VAL:HG22	3:I:63:LEU:HD13	2.02	0.41
1:J:236:GLU:HA	1:J:239:LYS:HG3	2.03	0.41
3:C:57:VAL:HG22	3:C:63:LEU:HD13	2.03	0.41
2:B:139:PRO:HG3	2:B:156:TYR:HD2	1.86	0.41
3:I:95:ASP:OD2	3:I:170:ASN:ND2	2.54	0.41
3:I:110:THR:OG1	3:I:113:ASN:HB2	2.20	0.41
2:B:252:TRP:O	2:B:255:VAL:HG23	2.21	0.41
2:E:20:PHE:CZ	2:E:217:TRP:HA	2.56	0.41
1:G:359:TYR:CD2	1:G:420:PRO:HB3	2.56	0.41
2:H:194:VAL:HB	2:H:207:MET:HE2	2.03	0.41
1:G:403:TYR:CE2	1:G:408:LEU:HD11	2.55	0.41
3:F:83:GLU:OE2	3:F:87:SER:HB3	2.21	0.41
2:K:26:GLN:NE2	2:K:56:PRO:O	2.54	0.41
1:G:291:HIS:HE1	2:H:2:GLY:N	2.19	0.41
1:D:406:VAL:C	1:D:409:PRO:HD2	2.41	0.41
1:D:321:ILE:O	1:D:321:ILE:CG2	2.69	0.41
1:G:323:PHE:CD1	1:G:323:PHE:N	2.89	0.41
1:D:41:LEU:CD1	10:D:504:ANJ:H3	2.51	0.41
2:E:109:GLY:N	2:E:125:ILE:O	2.52	0.41
2:H:252:TRP:O	2:H:255:VAL:HG23	2.21	0.41
1:A:27:ALA:O	1:A:30:TYR:HB3	2.21	0.41
1:D:233:SER:OG	1:D:236:GLU:HG2	2.20	0.41
2:K:175:VAL:HG12	2:K:176:LYS:N	2.36	0.41
2:E:232:THR:HG22	2:E:236:PHE:CE1	2.55	0.40
1:G:27:ALA:O	1:G:30:TYR:HB3	2.21	0.40
1:J:80:VAL:O	1:J:84:MET:HG2	2.21	0.40
2:H:183:ILE:HG23	2:H:185:MET:N	2.32	0.40
1:G:125:ARG:HD2	11:G:517:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:177:LYS:HE3	3:I:179:ILE:HD11	2.03	0.40
2:E:252:TRP:O	2:E:255:VAL:HG23	2.21	0.40
1:G:39:ARG:HG2	1:G:242:VAL:CG1	2.46	0.40
1:J:233:SER:OG	1:J:236:GLU:HG2	2.21	0.40
2:K:48:ARG:HG3	2:K:48:ARG:HH11	1.85	0.40
2:B:81:ARG:NH1	2:B:82:GLU:O	2.53	0.40
1:D:366:TYR:CD2	1:D:411:LEU:HD11	2.55	0.40
1:D:306:ARG:HG3	11:D:540:HOH:O	2.20	0.40
1:A:117:TYR:HB2	1:A:367:PHE:CZ	2.56	0.40
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.76	0.40
3:I:112:GLN:H	3:I:112:GLN:HE21	1.61	0.40
2:E:127:GLY:N	2:E:128:PRO:HD2	2.36	0.40
1:D:118:TYR:OH	9:D:503:LOP:H32	2.21	0.40
1:J:247:TYR:HB3	2:K:252:TRP:CZ2	2.55	0.40
1:G:309:THR:HG22	3:L:165:GLY:CA	2.50	0.40
2:K:59:PRO:CD	2:K:62:GLN:HE21	2.35	0.40
3:I:135:VAL:HA	3:I:136:PRO:HD2	1.92	0.40
2:B:77:THR:HG22	2:B:79:GLU:CG	2.51	0.40
1:G:272:ASN:HD21	2:H:105:LYS:HD2	1.85	0.40
1:D:80:VAL:O	1:D:84:MET:HG2	2.21	0.40
1:J:276:HIS:HA	1:J:277:PRO:HD3	1.92	0.40
3:I:39:ASN:O	3:I:40:PRO:C	2.59	0.40
1:J:56:VAL:HG23	10:J:505:ANJ:H281	2.03	0.40
2:H:235:MET:O	2:H:236:PHE:C	2.60	0.40
2:B:109:GLY:N	2:B:125:ILE:O	2.49	0.40
1:G:92:MET:HE2	1:G:92:MET:HA	2.03	0.40
2:H:129:GLU:N	2:H:129:GLU:OE1	2.48	0.40
2:H:194:VAL:O	2:H:194:VAL:HG12	2.21	0.40
1:G:116:LEU:HA	1:G:121:TYR:HE2	1.87	0.40
2:E:231:PHE:HE1	2:E:235:MET:SD	2.44	0.40
1:J:418:VAL:HG12	1:J:419:ALA:N	2.36	0.40
3:I:27:THR:O	3:I:31:VAL:HG23	2.22	0.40
1:D:270:MET:C	11:D:532:HOH:O	2.60	0.40
3:I:110:THR:O	3:I:113:ASN:N	2.55	0.40
3:L:39:ASN:O	3:L:40:PRO:C	2.60	0.40
2:K:20:PHE:CZ	2:K:217:TRP:HA	2.56	0.40
1:J:245:TRP:HE3	1:J:249:ILE:HG13	1.86	0.40
3:F:162:ILE:HG22	3:F:170:ASN:OD1	2.22	0.40
1:A:377:LEU:HA	1:A:380:VAL:HG23	2.03	0.40
3:L:57:VAL:HG22	3:L:63:LEU:HD13	2.02	0.40
1:G:306:ARG:NH1	11:G:542:HOH:O	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:GLU:HA	2:B:142:PRO:HD3	1.84	0.40
1:D:68:HIS:ND1	11:D:507:HOH:O	2.37	0.40
3:F:39:ASN:O	3:F:40:PRO:C	2.59	0.40
3:L:58:GLU:O	3:L:61:VAL:HB	2.22	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	A	426/428 (100%)	398 (93%)	24 (6%)	4 (1%)	21 42
1	D	426/428 (100%)	402 (94%)	21 (5%)	3 (1%)	26 51
1	G	426/428 (100%)	400 (94%)	22 (5%)	4 (1%)	21 42
1	J	426/428 (100%)	397 (93%)	26 (6%)	3 (1%)	26 51
2	B	254/256 (99%)	227 (89%)	21 (8%)	6 (2%)	7 13
2	E	254/256 (99%)	229 (90%)	18 (7%)	7 (3%)	6 10
2	H	254/256 (99%)	225 (89%)	21 (8%)	8 (3%)	5 8
2	K	254/256 (99%)	229 (90%)	18 (7%)	7 (3%)	6 10
3	C	177/179 (99%)	143 (81%)	23 (13%)	11 (6%)	2 2
3	F	177/179 (99%)	144 (81%)	25 (14%)	8 (4%)	3 4
3	I	177/179 (99%)	144 (81%)	26 (15%)	7 (4%)	4 4
3	L	177/179 (99%)	142 (80%)	26 (15%)	9 (5%)	2 3
All	All	3428/3452 (99%)	3080 (90%)	271 (8%)	77 (2%)	8 15

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	137	GLY
2	B	147	GLU
2	B	200	HIS
3	C	109	ALA
2	E	137	GLY
2	E	147	GLU
2	E	200	HIS
3	F	109	ALA
1	G	8	HIS
2	H	137	GLY
2	H	147	GLU
2	H	200	HIS
3	I	109	ALA
2	K	137	GLY
2	K	147	GLU
2	K	200	HIS
3	L	90	LEU
3	L	109	ALA
3	C	57	VAL
3	C	158	SER
3	C	181	GLU
2	E	37	ALA
3	F	45	GLN
3	F	57	VAL
3	F	158	SER
3	F	181	GLU
2	H	37	ALA
3	I	57	VAL
3	I	158	SER
3	I	181	GLU
2	K	37	ALA
2	K	72	VAL
3	L	57	VAL
3	L	158	SER
3	L	181	GLU
1	A	13	THR
2	B	37	ALA
2	B	198	ASP
3	C	45	GLN
3	C	90	LEU
3	C	134	CYS
1	D	13	THR
2	E	74	ASP

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Mol	Chain	Res	Type
2	E	198	ASP
3	F	134	CYS
1	G	13	THR
2	H	188	PRO
2	H	198	ASP
1	J	13	THR
2	K	198	ASP
3	L	134	CYS
2	B	188	PRO
3	C	107	ALA
3	F	107	ALA
1	G	73	VAL
2	H	75	GLU
3	I	134	CYS
3	L	45	GLN
3	L	107	ALA
1	A	73	VAL
1	A	98	ALA
3	C	164	LYS
1	D	98	ALA
1	G	98	ALA
3	I	107	ALA
1	D	73	VAL
2	E	188	PRO
2	H	43	LYS
1	J	98	ALA
2	K	188	PRO
1	A	123	ALA
3	I	40	PRO
3	L	40	PRO
3	C	40	PRO
3	C	140	VAL
3	F	40	PRO
1	J	73	VAL

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	353/353 (100%)	336 (95%)	17 (5%)	31	58
1	D	353/353 (100%)	337 (96%)	16 (4%)	34	62
1	G	353/353 (100%)	334 (95%)	19 (5%)	27	52
1	J	353/353 (100%)	336 (95%)	17 (5%)	31	58
2	B	203/203 (100%)	198 (98%)	5 (2%)	55	81
2	E	203/203 (100%)	197 (97%)	6 (3%)	48	76
2	H	203/203 (100%)	195 (96%)	8 (4%)	39	68
2	K	203/203 (100%)	196 (97%)	7 (3%)	44	72
3	C	138/138 (100%)	133 (96%)	5 (4%)	42	71
3	F	138/138 (100%)	132 (96%)	6 (4%)	35	64
3	I	138/138 (100%)	132 (96%)	6 (4%)	35	64
3	L	138/138 (100%)	131 (95%)	7 (5%)	29	55
All	All	2776/2776 (100%)	2657 (96%)	119 (4%)	35	64

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	7	ASP
1	A	8	HIS
1	A	79	SER
1	A	92	MET
1	A	94	ARG
1	A	104	PHE
1	A	108	VAL
1	A	192	ASN
1	A	199	TYR
1	A	231	ARG
1	A	246	PRO
1	A	321	ILE
1	A	342	VAL
1	A	380	VAL
1	A	385	THR
1	A	388	PRO
2	B	26	GLN
2	B	80	ASP
2	B	140	GLU
2	B	194	VAL
2	B	205	HIS

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Mol	Chain	Res	Type
3	C	11	ARG
3	C	14	PHE
3	C	112	GLN
3	C	118	GLU
3	C	174	PRO
1	D	4	ILE
1	D	8	HIS
1	D	10	GLU
1	D	79	SER
1	D	94	ARG
1	D	104	PHE
1	D	108	VAL
1	D	175	SER
1	D	192	ASN
1	D	199	TYR
1	D	231	ARG
1	D	246	PRO
1	D	342	VAL
1	D	380	VAL
1	D	385	THR
1	D	388	PRO
2	E	26	GLN
2	E	167	ASP
2	E	188	PRO
2	E	194	VAL
2	E	205	HIS
2	E	231	PHE
3	F	11	ARG
3	F	14	PHE
3	F	112	GLN
3	F	118	GLU
3	F	125	MET
3	F	174	PRO
1	G	7	ASP
1	G	8	HIS
1	G	79	SER
1	G	92	MET
1	G	94	ARG
1	G	104	PHE
1	G	108	VAL
1	G	192	ASN
1	G	199	TYR

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Mol	Chain	Res	Type
1	G	231	ARG
1	G	246	PRO
1	G	252	ASP
1	G	287	SER
1	G	309	THR
1	G	342	VAL
1	G	380	VAL
1	G	385	THR
1	G	388	PRO
1	G	417	PRO
2	H	26	GLN
2	H	80	ASP
2	H	84	LYS
2	H	149	HIS
2	H	167	ASP
2	H	194	VAL
2	H	205	HIS
2	H	231	PHE
3	I	11	ARG
3	I	14	PHE
3	I	87	SER
3	I	88	VAL
3	I	112	GLN
3	I	174	PRO
1	J	8	HIS
1	J	74	ASP
1	J	79	SER
1	J	92	MET
1	J	94	ARG
1	J	104	PHE
1	J	108	VAL
1	J	162	ILE
1	J	192	ASN
1	J	199	TYR
1	J	231	ARG
1	J	246	PRO
1	J	321	ILE
1	J	342	VAL
1	J	380	VAL
1	J	385	THR
1	J	388	PRO
2	K	26	GLN

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Mol	Chain	Res	Type
2	K	73	THR
2	K	76	GLU
2	K	158	ARG
2	K	167	ASP
2	K	194	VAL
2	K	205	HIS
3	L	11	ARG
3	L	14	PHE
3	L	87	SER
3	L	112	GLN
3	L	118	GLU
3	L	125	MET
3	L	174	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	8	HIS
1	A	217	HIS
1	A	238	GLN
1	A	383	GLN
1	A	429	ASN
2	B	22	GLN
2	B	26	GLN
2	B	62	GLN
2	B	69	GLN
2	B	111	HIS
2	B	228	GLN
3	C	36	ASN
3	C	39	ASN
3	C	112	GLN
3	C	113	ASN
3	C	185	GLN
1	D	217	HIS
1	D	291	HIS
1	D	383	GLN
2	E	22	GLN
2	E	26	GLN
2	E	62	GLN
2	E	69	GLN
2	E	111	HIS

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Mol	Chain	Res	Type
2	E	149	HIS
2	E	228	GLN
3	F	36	ASN
3	F	39	ASN
3	F	89	GLN
3	F	112	GLN
3	F	113	ASN
3	F	185	GLN
1	G	8	HIS
1	G	217	HIS
1	G	272	ASN
1	G	291	HIS
1	G	383	GLN
1	G	429	ASN
2	H	22	GLN
2	H	26	GLN
2	H	62	GLN
2	H	69	GLN
2	H	111	HIS
2	H	149	HIS
2	H	228	GLN
3	I	36	ASN
3	I	39	ASN
3	I	89	GLN
3	I	112	GLN
3	I	113	ASN
3	I	185	GLN
1	J	8	HIS
1	J	217	HIS
1	J	383	GLN
1	J	429	ASN
2	K	22	GLN
2	K	26	GLN
2	K	62	GLN
2	K	69	GLN
2	K	111	HIS
2	K	149	HIS
2	K	228	GLN
3	L	36	ASN
3	L	39	ASN
3	L	45	GLN
3	L	89	GLN

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Mol	Chain	Res	Type
3	L	112	GLN
3	L	113	ASN
3	L	185	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 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
8	SMA	A	1	-	35,38,38	2.16	6 (17%)	40,52,52	2.00	6 (15%)
4	BGL	A	431	-	19,20,20	0.82	0	23,25,25	0.76	0
6	HEM	A	501	1	30,50,50	2.79	11 (36%)	24,82,82	3.22	8 (33%)
6	HEM	A	502	1	30,50,50	2.94	12 (40%)	24,82,82	3.21	8 (33%)
9	LOP	A	503	-	43,44,44	0.59	0	44,49,49	1.34	8 (18%)
10	ANJ	A	504	-	40,40,40	1.78	8 (20%)	34,54,54	2.09	8 (23%)
6	HEM	B	301	2	30,50,50	2.99	11 (36%)	24,82,82	3.27	8 (33%)
7	FES	C	200	3	0,4,4	0.00	-	0,4,4	0.00	-
8	SMA	D	2	-	35,38,38	2.08	5 (14%)	40,52,52	1.71	7 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	HEM	D	501	1	30,50,50	2.94	11 (36%)	24,82,82	3.25	8 (33%)
6	HEM	D	502	1	30,50,50	2.95	12 (40%)	24,82,82	3.07	9 (37%)
9	LOP	D	503	-	43,44,44	0.57	0	44,49,49	1.30	8 (18%)
10	ANJ	D	504	-	40,40,40	1.79	10 (25%)	34,54,54	2.14	8 (23%)
4	BGL	E	257	-	19,20,20	0.76	1 (5%)	23,25,25	1.12	2 (8%)
6	HEM	E	301	2	30,50,50	2.99	11 (36%)	24,82,82	3.27	8 (33%)
7	FES	F	200	3	0,4,4	0.00	-	0,4,4	0.00	-
4	BGL	G	431	-	19,20,20	0.70	0	23,25,25	1.08	2 (8%)
6	HEM	G	501	1	30,50,50	2.83	12 (40%)	24,82,82	3.26	8 (33%)
6	HEM	G	502	1	30,50,50	2.91	12 (40%)	24,82,82	3.33	8 (33%)
8	SMA	G	503	-	35,38,38	2.21	7 (20%)	40,52,52	1.76	6 (15%)
9	LOP	G	504	-	43,44,44	0.62	0	44,49,49	1.32	4 (9%)
10	ANJ	G	505	-	40,40,40	1.77	9 (22%)	34,54,54	2.06	7 (20%)
6	HEM	H	301	2	30,50,50	2.95	12 (40%)	24,82,82	3.29	8 (33%)
7	FES	I	200	3	0,4,4	0.00	-	0,4,4	0.00	-
4	BGL	J	431	-	19,20,20	0.72	0	23,25,25	0.82	0
6	HEM	J	501	1	30,50,50	2.89	11 (36%)	24,82,82	3.22	8 (33%)
6	HEM	J	502	1	30,50,50	2.92	12 (40%)	24,82,82	3.15	9 (37%)
8	SMA	J	503	-	35,38,38	2.00	6 (17%)	40,52,52	1.71	6 (15%)
9	LOP	J	504	-	43,44,44	0.56	0	44,49,49	1.42	10 (22%)
10	ANJ	J	505	-	40,40,40	1.80	11 (27%)	34,54,54	1.93	8 (23%)
6	HEM	K	301	2	30,50,50	2.86	11 (36%)	24,82,82	3.26	8 (33%)
7	FES	L	200	3	0,4,4	0.00	-	0,4,4	0.00	-

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
8	SMA	A	1	-	-	0/33/34/34	0/2/2/2
4	BGL	A	431	-	-	0/11/31/31	0/1/1/1
6	HEM	A	501	1	-	0/10/54/54	0/0/8/8
6	HEM	A	502	1	-	0/10/54/54	0/0/8/8
9	LOP	A	503	-	-	0/48/48/48	0/0/0/0
10	ANJ	A	504	-	-	0/38/55/55	0/1/2/2
6	HEM	B	301	2	-	0/10/54/54	0/0/8/8
7	FES	C	200	3	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SMA	D	2	-	-	0/33/34/34	0/2/2/2
6	HEM	D	501	1	-	0/10/54/54	0/0/8/8
6	HEM	D	502	1	-	0/10/54/54	0/0/8/8
9	LOP	D	503	-	-	0/48/48/48	0/0/0/0
10	ANJ	D	504	-	-	0/38/55/55	0/1/2/2
4	BGL	E	257	-	-	0/11/31/31	0/1/1/1
6	HEM	E	301	2	-	0/10/54/54	0/0/8/8
7	FES	F	200	3	-	0/0/4/4	0/1/1/1
4	BGL	G	431	-	-	0/11/31/31	0/1/1/1
6	HEM	G	501	1	-	0/10/54/54	0/0/8/8
6	HEM	G	502	1	-	0/10/54/54	0/0/8/8
8	SMA	G	503	-	-	0/33/34/34	0/2/2/2
9	LOP	G	504	-	-	0/48/48/48	0/0/0/0
10	ANJ	G	505	-	-	0/38/55/55	0/1/2/2
6	HEM	H	301	2	-	0/10/54/54	0/0/8/8
7	FES	I	200	3	-	0/0/4/4	0/1/1/1
4	BGL	J	431	-	-	0/11/31/31	0/1/1/1
6	HEM	J	501	1	-	0/10/54/54	0/0/8/8
6	HEM	J	502	1	-	0/10/54/54	0/0/8/8
8	SMA	J	503	-	-	0/33/34/34	0/2/2/2
9	LOP	J	504	-	-	0/48/48/48	0/0/0/0
10	ANJ	J	505	-	-	0/38/55/55	0/1/2/2
6	HEM	K	301	2	-	0/10/54/54	0/0/8/8
7	FES	L	200	3	-	0/0/4/4	0/1/1/1

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	502	HEM	C3B-C4B	-7.68	1.45	1.51
6	B	301	HEM	C3B-C4B	-7.59	1.45	1.51
6	E	301	HEM	C3B-C4B	-7.41	1.45	1.51
6	A	502	HEM	C3B-C4B	-7.24	1.45	1.51
6	J	502	HEM	C3B-C4B	-7.09	1.45	1.51
6	D	501	HEM	C3B-C4B	-6.95	1.45	1.51
6	G	502	HEM	C3B-C4B	-6.92	1.45	1.51
6	K	301	HEM	C3B-C4B	-6.80	1.45	1.51
6	D	502	HEM	C2D-C3D	-6.64	1.34	1.54
6	D	501	HEM	C2D-C3D	-6.56	1.34	1.54
6	H	301	HEM	C3C-CAC	-6.56	1.39	1.51
6	G	501	HEM	C3B-C4B	-6.51	1.46	1.51
6	J	502	HEM	C2D-C3D	-6.48	1.35	1.54
6	A	502	HEM	C2D-C3D	-6.48	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	301	HEM	C3B-C4B	-6.43	1.46	1.51
6	E	301	HEM	C3B-CAB	-6.40	1.39	1.51
6	J	501	HEM	C2D-C3D	-6.38	1.35	1.54
6	B	301	HEM	C2D-C3D	-6.32	1.35	1.54
6	H	301	HEM	C2D-C3D	-6.27	1.35	1.54
6	A	501	HEM	C2D-C3D	-6.22	1.35	1.54
6	K	301	HEM	C2D-C3D	-6.19	1.35	1.54
6	B	301	HEM	C3C-CAC	-6.16	1.39	1.51
6	G	502	HEM	C3C-CAC	-6.14	1.39	1.51
6	G	502	HEM	C2D-C3D	-6.07	1.36	1.54
6	D	501	HEM	C3C-CAC	-6.07	1.39	1.51
6	A	501	HEM	C3C-CAC	-6.06	1.40	1.51
6	E	301	HEM	C2D-C3D	-6.03	1.36	1.54
6	G	501	HEM	C3C-CAC	-5.99	1.40	1.51
6	J	501	HEM	C3B-C4B	-5.96	1.46	1.51
6	D	502	HEM	C3B-CAB	-5.95	1.40	1.51
6	G	501	HEM	C2D-C3D	-5.92	1.36	1.54
6	G	502	HEM	C3B-CAB	-5.79	1.40	1.51
6	K	301	HEM	C3C-CAC	-5.76	1.40	1.51
6	E	301	HEM	C3C-CAC	-5.62	1.40	1.51
6	K	301	HEM	C3B-CAB	-5.62	1.40	1.51
6	H	301	HEM	C3B-CAB	-5.61	1.40	1.51
6	A	502	HEM	C3B-CAB	-5.60	1.40	1.51
6	A	502	HEM	C3D-C4D	-5.55	1.44	1.51
6	J	501	HEM	C3D-C4D	-5.54	1.44	1.51
6	J	501	HEM	C3B-CAB	-5.50	1.41	1.51
6	J	502	HEM	C3B-CAB	-5.47	1.41	1.51
6	J	502	HEM	C3C-CAC	-5.44	1.41	1.51
6	A	501	HEM	C3B-C4B	-5.44	1.47	1.51
6	D	501	HEM	C3B-CAB	-5.43	1.41	1.51
6	J	502	HEM	C3D-C4D	-5.40	1.44	1.51
6	H	301	HEM	C3D-C4D	-5.39	1.44	1.51
6	B	301	HEM	C3B-CAB	-5.35	1.41	1.51
6	G	502	HEM	C3D-C4D	-5.33	1.44	1.51
6	J	501	HEM	C3C-CAC	-5.32	1.41	1.51
6	G	501	HEM	C3B-CAB	-5.30	1.41	1.51
6	E	301	HEM	C3D-C4D	-5.28	1.44	1.51
6	B	301	HEM	C3D-C4D	-5.21	1.44	1.51
6	A	502	HEM	C3C-CAC	-5.11	1.41	1.51
6	D	501	HEM	C3D-C4D	-5.08	1.45	1.51
6	D	502	HEM	C3D-C4D	-4.99	1.45	1.51
6	G	501	HEM	C3D-C4D	-4.94	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	501	HEM	C3D-C4D	-4.86	1.45	1.51
6	A	501	HEM	C3B-CAB	-4.74	1.42	1.51
6	A	502	HEM	C2C-C1C	-4.55	1.43	1.52
6	K	301	HEM	C3D-C4D	-4.43	1.45	1.51
6	D	502	HEM	C3C-CAC	-4.19	1.43	1.51
6	K	301	HEM	C2C-C1C	-4.12	1.44	1.52
6	D	502	HEM	C2C-C1C	-4.08	1.44	1.52
6	G	501	HEM	C2C-C1C	-4.08	1.44	1.52
6	E	301	HEM	C2C-C1C	-4.07	1.44	1.52
6	B	301	HEM	C2C-C1C	-4.05	1.44	1.52
6	H	301	HEM	C2C-C1C	-4.04	1.44	1.52
6	J	502	HEM	C2C-C1C	-4.03	1.44	1.52
6	G	502	HEM	C2C-C1C	-3.91	1.45	1.52
6	J	501	HEM	C2C-C1C	-3.86	1.45	1.52
6	A	501	HEM	C2C-C1C	-3.84	1.45	1.52
6	D	501	HEM	C2C-C1C	-3.70	1.45	1.52
6	D	502	HEM	C2D-C1D	-2.48	1.43	1.51
6	E	301	HEM	C2B-C1B	-2.39	1.44	1.51
6	J	501	HEM	C2B-C1B	-2.38	1.44	1.51
6	J	502	HEM	C2B-C1B	-2.32	1.44	1.51
6	K	301	HEM	C2B-C1B	-2.27	1.44	1.51
6	B	301	HEM	C2D-C1D	-2.20	1.44	1.51
6	A	501	HEM	C2B-C1B	-2.14	1.44	1.51
6	A	502	HEM	C2B-C1B	-2.12	1.44	1.51
6	D	502	HEM	C2B-C1B	-2.12	1.44	1.51
6	G	502	HEM	C2D-C1D	-2.11	1.45	1.51
6	J	502	HEM	C2D-C1D	-2.09	1.45	1.51
6	D	501	HEM	C2B-C1B	-2.09	1.45	1.51
6	H	301	HEM	C2B-C1B	-2.08	1.45	1.51
6	A	502	HEM	C2D-C1D	-2.07	1.45	1.51
8	J	503	SMA	C7-C8	-2.06	1.37	1.40
6	G	501	HEM	C2B-C1B	-2.05	1.45	1.51
6	H	301	HEM	C2D-C1D	-2.04	1.45	1.51
6	G	502	HEM	C2B-C1B	-2.01	1.45	1.51
8	G	503	SMA	O12-C12	2.01	1.48	1.42
8	J	503	SMA	O1-C8A	2.06	1.40	1.36
10	J	505	ANJ	C13-C14	2.08	1.57	1.53
6	A	502	HEM	C4C-NC	2.09	1.38	1.36
10	D	504	ANJ	C13-C12	2.09	1.55	1.51
4	E	257	BGL	O5-C1	2.10	1.47	1.43
10	J	505	ANJ	C13-C12	2.15	1.55	1.51
10	J	505	ANJ	C1-N1	2.17	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	503	SMA	C9-C2	2.19	1.53	1.50
10	J	505	ANJ	C26-C25	2.22	1.60	1.52
6	G	501	HEM	CHD-C4C	2.23	1.41	1.36
8	D	2	SMA	O1-C8A	2.23	1.40	1.36
10	D	504	ANJ	C26-C25	2.24	1.60	1.52
6	K	301	HEM	C1C-NC	2.26	1.38	1.36
6	E	301	HEM	C4C-NC	2.35	1.38	1.36
6	A	502	HEM	C1C-NC	2.36	1.38	1.36
6	J	502	HEM	C4C-NC	2.36	1.38	1.36
10	G	505	ANJ	C26-C25	2.37	1.61	1.52
6	G	501	HEM	C1C-NC	2.37	1.38	1.36
8	A	1	SMA	O1-C8A	2.38	1.40	1.36
6	G	501	HEM	C4C-NC	2.39	1.38	1.36
6	K	301	HEM	C4C-NC	2.39	1.38	1.36
6	B	301	HEM	C4C-NC	2.40	1.39	1.36
6	H	301	HEM	C4C-NC	2.42	1.39	1.36
6	B	301	HEM	C1C-NC	2.43	1.39	1.36
6	E	301	HEM	C1C-NC	2.44	1.39	1.36
10	D	504	ANJ	C1-N1	2.47	1.37	1.34
6	D	502	HEM	C1C-NC	2.49	1.39	1.36
6	G	502	HEM	C1C-NC	2.50	1.39	1.36
6	J	502	HEM	C1C-NC	2.50	1.39	1.36
8	G	503	SMA	O1-C8A	2.51	1.41	1.36
8	A	1	SMA	C9-C2	2.53	1.54	1.50
10	G	505	ANJ	O8-C14	2.53	1.48	1.44
10	G	505	ANJ	C1-N1	2.55	1.37	1.34
6	D	501	HEM	C4C-NC	2.57	1.39	1.36
6	H	301	HEM	C1C-NC	2.65	1.39	1.36
10	D	504	ANJ	C4-C3	2.73	1.44	1.38
10	G	505	ANJ	C4-C3	2.73	1.44	1.38
8	A	1	SMA	O8-C8	2.73	1.45	1.35
6	G	502	HEM	C4C-NC	2.74	1.39	1.36
10	A	504	ANJ	C26-C25	2.75	1.62	1.52
6	A	501	HEM	C4C-NC	2.75	1.39	1.36
6	J	501	HEM	C4C-NC	2.83	1.39	1.36
8	G	503	SMA	O8-C8	2.89	1.46	1.35
10	A	504	ANJ	C2-N1	2.93	1.46	1.41
10	A	504	ANJ	C4-C3	2.98	1.45	1.38
6	D	501	HEM	C1C-NC	2.98	1.39	1.36
10	D	504	ANJ	C2-N1	2.99	1.46	1.41
10	J	505	ANJ	C4-C3	3.02	1.45	1.38
10	G	505	ANJ	O4-C10	3.03	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	503	SMA	O8-C8	3.03	1.46	1.35
6	D	502	HEM	C4C-NC	3.03	1.39	1.36
6	A	501	HEM	C1C-NC	3.08	1.39	1.36
8	D	2	SMA	O8-C8	3.09	1.46	1.35
10	A	504	ANJ	O8-C14	3.10	1.49	1.44
10	J	505	ANJ	C2-N1	3.13	1.46	1.41
6	J	501	HEM	C1C-NC	3.18	1.39	1.36
10	D	504	ANJ	O4-C12	3.31	1.42	1.34
10	J	505	ANJ	O4-C12	3.33	1.42	1.34
10	D	504	ANJ	O4-C10	3.38	1.52	1.46
10	J	505	ANJ	C5-C6	3.39	1.45	1.39
10	G	505	ANJ	C2-N1	3.43	1.47	1.41
10	A	504	ANJ	O4-C10	3.52	1.52	1.46
10	A	504	ANJ	C5-C6	3.54	1.45	1.39
6	G	502	HEM	CBC-CAC	3.58	1.50	1.29
10	J	505	ANJ	O4-C10	3.58	1.52	1.46
10	D	504	ANJ	O8-C14	3.60	1.50	1.44
10	D	504	ANJ	C5-C6	3.62	1.46	1.39
10	G	505	ANJ	C5-C6	3.64	1.46	1.39
10	G	505	ANJ	O4-C12	3.67	1.43	1.34
10	J	505	ANJ	O8-C14	3.71	1.50	1.44
10	A	504	ANJ	O4-C12	3.75	1.43	1.34
6	J	502	HEM	CBC-CAC	3.83	1.51	1.29
6	A	502	HEM	CBC-CAC	3.89	1.51	1.29
6	G	501	HEM	CBC-CAC	3.98	1.52	1.29
6	D	501	HEM	CBC-CAC	3.99	1.52	1.29
6	A	501	HEM	CBC-CAC	4.00	1.52	1.29
6	G	502	HEM	CBB-CAB	4.02	1.52	1.29
8	J	503	SMA	O1-C2	4.02	1.40	1.35
6	J	501	HEM	CBB-CAB	4.03	1.52	1.29
6	G	501	HEM	CBB-CAB	4.05	1.52	1.29
6	H	301	HEM	CBB-CAB	4.05	1.52	1.29
6	D	502	HEM	CBB-CAB	4.07	1.52	1.29
6	D	502	HEM	CBC-CAC	4.08	1.52	1.29
6	K	301	HEM	CBC-CAC	4.10	1.53	1.29
10	D	504	ANJ	C10-C9	4.12	1.61	1.53
10	J	505	ANJ	C10-C9	4.13	1.61	1.53
6	J	502	HEM	CBB-CAB	4.13	1.53	1.29
6	A	502	HEM	CBB-CAB	4.13	1.53	1.29
6	D	501	HEM	CBB-CAB	4.13	1.53	1.29
6	H	301	HEM	CBC-CAC	4.13	1.53	1.29
6	J	501	HEM	CBC-CAC	4.13	1.53	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	301	HEM	CBC-CAC	4.14	1.53	1.29
8	D	2	SMA	O1-C2	4.14	1.40	1.35
6	K	301	HEM	CBB-CAB	4.15	1.53	1.29
6	B	301	HEM	CBC-CAC	4.15	1.53	1.29
6	E	301	HEM	CBB-CAB	4.17	1.53	1.29
6	B	301	HEM	CBB-CAB	4.17	1.53	1.29
6	A	501	HEM	CBB-CAB	4.30	1.54	1.29
10	G	505	ANJ	C10-C9	4.33	1.62	1.53
10	A	504	ANJ	C10-C9	4.36	1.62	1.53
8	G	503	SMA	O1-C2	5.04	1.41	1.35
8	A	1	SMA	O1-C2	5.09	1.41	1.35
8	J	503	SMA	O5-C5	5.96	1.48	1.36
8	D	2	SMA	O5-C5	6.40	1.48	1.36
8	A	1	SMA	O5-C5	6.50	1.49	1.36
8	G	503	SMA	O5-C5	6.53	1.49	1.36
8	J	503	SMA	O7-C7	6.92	1.48	1.37
8	D	2	SMA	O7-C7	7.04	1.48	1.37
8	A	1	SMA	O7-C7	7.15	1.48	1.37
8	G	503	SMA	O7-C7	7.39	1.49	1.37

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	502	HEM	C3B-CAB-CBB	-9.34	110.13	124.46
6	D	501	HEM	C3C-CAC-CBC	-9.34	110.14	124.46
6	A	501	HEM	C3C-CAC-CBC	-9.32	110.16	124.46
6	G	501	HEM	C3C-CAC-CBC	-9.32	110.16	124.46
6	G	502	HEM	C3C-CAC-CBC	-9.17	110.40	124.46
6	A	502	HEM	C3B-CAB-CBB	-9.11	110.48	124.46
6	H	301	HEM	C3B-CAB-CBB	-9.03	110.60	124.46
6	D	502	HEM	C3B-CAB-CBB	-9.03	110.60	124.46
6	B	301	HEM	C3B-CAB-CBB	-8.91	110.79	124.46
6	E	301	HEM	C3B-CAB-CBB	-8.88	110.83	124.46
6	B	301	HEM	C3C-CAC-CBC	-8.87	110.85	124.46
6	J	502	HEM	C3B-CAB-CBB	-8.85	110.89	124.46
6	K	301	HEM	C3B-CAB-CBB	-8.84	110.89	124.46
6	J	501	HEM	C3C-CAC-CBC	-8.84	110.90	124.46
6	H	301	HEM	C3C-CAC-CBC	-8.80	110.96	124.46
6	E	301	HEM	C3C-CAC-CBC	-8.79	110.97	124.46
6	K	301	HEM	C3C-CAC-CBC	-8.74	111.04	124.46
6	D	501	HEM	C3B-CAB-CBB	-8.61	111.25	124.46
6	J	501	HEM	C3B-CAB-CBB	-8.56	111.33	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	501	HEM	C3B-CAB-CBB	-8.30	111.72	124.46
10	G	505	ANJ	O6-C17-C9	-8.14	101.65	110.32
10	A	504	ANJ	O6-C17-C9	-8.09	101.70	110.32
6	A	501	HEM	C3B-CAB-CBB	-8.03	112.14	124.46
6	A	502	HEM	C3C-CAC-CBC	-7.89	112.35	124.46
6	J	502	HEM	C3C-CAC-CBC	-7.86	112.40	124.46
10	D	504	ANJ	O6-C17-C9	-7.56	102.27	110.32
10	J	505	ANJ	O6-C17-C9	-7.35	102.49	110.32
6	D	502	HEM	C3C-CAC-CBC	-7.13	113.51	124.46
8	A	1	SMA	C9-C10-C11	-5.43	108.35	114.75
10	D	504	ANJ	C19-C18-C13	-5.01	104.68	114.38
8	J	503	SMA	C9-C10-C11	-4.54	109.40	114.75
8	G	503	SMA	C9-C10-C11	-4.52	109.43	114.75
8	D	2	SMA	C9-C10-C11	-4.31	109.68	114.75
8	J	503	SMA	C5M-O5-C5	-4.04	111.86	117.77
9	G	504	LOP	C19-C18-C17	-3.75	95.16	114.53
8	G	503	SMA	C16-C17-C18	-3.68	116.49	124.66
9	J	504	LOP	C19-C18-C17	-3.61	95.90	114.53
8	G	503	SMA	C5M-O5-C5	-3.59	112.51	117.77
8	A	1	SMA	O7-C7-C6	-3.50	118.24	124.21
8	D	2	SMA	C5M-O5-C5	-3.40	112.79	117.77
10	D	504	ANJ	C5-C6-C7	-3.32	115.15	118.70
9	D	503	LOP	C19-C18-C17	-3.26	97.69	114.53
8	A	1	SMA	C5M-O5-C5	-3.23	113.04	117.77
10	J	505	ANJ	C5-C6-C7	-3.16	115.33	118.70
10	A	504	ANJ	C5-C6-C7	-3.12	115.37	118.70
9	A	503	LOP	C19-C18-C17	-3.08	98.65	114.53
10	J	505	ANJ	O6-C15-C14	-3.00	95.90	108.20
4	G	431	BGL	C1'-O2-C2	-2.96	106.28	114.40
4	E	257	BGL	C1'-O2-C2	-2.94	106.33	114.40
10	G	505	ANJ	C5-C6-C7	-2.93	115.57	118.70
10	G	505	ANJ	O6-C15-C14	-2.91	96.25	108.20
9	J	504	LOP	C21-C20-C19	-2.88	99.64	114.53
10	A	504	ANJ	O6-C15-C14	-2.86	96.47	108.20
10	D	504	ANJ	O6-C15-C14	-2.83	96.56	108.20
10	G	505	ANJ	O3-C8-N2	-2.82	117.34	122.44
9	G	504	LOP	C17-C16-C15	-2.82	97.63	112.45
8	D	2	SMA	C7M-O7-C7	-2.81	113.28	117.54
9	J	504	LOP	C17-C16-C15	-2.78	97.86	112.45
10	D	504	ANJ	O3-C8-N2	-2.78	117.42	122.44
8	D	2	SMA	C16-C17-C18	-2.73	118.59	124.66
9	D	503	LOP	C29-C28-C27	-2.73	100.45	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	504	ANJ	O3-C8-N2	-2.68	117.61	122.44
8	J	503	SMA	C7M-O7-C7	-2.66	113.50	117.54
9	J	504	LOP	C9-C8-C7	-2.65	103.58	113.29
9	G	504	LOP	C21-C20-C19	-2.64	100.88	114.53
9	D	503	LOP	C9-C8-C7	-2.63	103.64	113.29
9	D	503	LOP	C21-C20-C19	-2.55	101.37	114.53
9	A	503	LOP	C17-C16-C15	-2.54	99.11	112.45
9	A	503	LOP	C27-C26-C25	-2.46	104.28	113.29
9	D	503	LOP	C17-C16-C15	-2.45	99.57	112.45
8	A	1	SMA	C7M-O7-C7	-2.39	113.91	117.54
9	A	503	LOP	C21-C20-C19	-2.39	102.19	114.53
9	A	503	LOP	C9-C8-C7	-2.32	104.78	113.29
10	J	505	ANJ	O3-C8-N2	-2.30	118.29	122.44
6	D	502	HEM	CBA-CAA-C2A	-2.28	108.44	112.53
10	J	505	ANJ	C20-C19-C18	-2.24	105.70	113.66
9	D	503	LOP	C31-C30-C29	-2.23	103.00	114.53
8	G	503	SMA	C7M-O7-C7	-2.22	114.18	117.54
9	A	503	LOP	C29-C28-C27	-2.17	103.32	114.53
10	A	504	ANJ	C20-C19-C18	-2.17	105.96	113.66
9	J	504	LOP	C29-C28-C27	-2.13	103.51	114.53
4	E	257	BGL	C3'-C2'-C1'	-2.11	104.03	113.47
6	J	502	HEM	CBA-CAA-C2A	-2.09	108.78	112.53
9	J	504	LOP	C31-C30-C29	-2.08	103.80	114.53
8	J	503	SMA	O5-C5-C6	-2.05	120.37	123.60
9	J	504	LOP	C27-C26-C25	-2.04	105.81	113.29
8	D	2	SMA	C14-C15-C16	-2.04	120.93	125.66
9	D	503	LOP	C27-C26-C25	-2.00	105.94	113.29
4	G	431	BGL	C3'-C2'-C1'	-2.00	104.52	113.47
9	J	504	LOP	C18-C17-C16	2.03	121.78	113.86
10	J	505	ANJ	O1-C1-N1	2.10	128.44	125.84
10	J	505	ANJ	C6-C8-N2	2.12	120.84	116.88
9	D	503	LOP	O6-C24-C25	2.18	118.55	111.90
10	G	505	ANJ	O1-C1-N1	2.22	128.59	125.84
10	D	504	ANJ	O1-C1-N1	2.28	128.66	125.84
10	A	504	ANJ	O1-C1-N1	2.32	128.71	125.84
9	A	503	LOP	O5-C6-C7	2.37	116.68	111.53
9	J	504	LOP	O5-C6-C7	2.39	116.73	111.53
8	A	1	SMA	O5-C5-C4A	2.50	119.83	115.89
10	D	504	ANJ	C6-C8-N2	2.55	121.64	116.88
9	J	504	LOP	O6-C24-C25	2.57	119.74	111.90
6	D	501	HEM	CMD-C2D-C3D	2.58	125.78	114.35
6	J	501	HEM	CMD-C2D-C3D	2.59	125.80	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	501	HEM	CMD-C2D-C3D	2.71	126.34	114.35
6	A	502	HEM	CMD-C2D-C3D	2.73	126.43	114.35
6	D	502	HEM	CMD-C2D-C3D	2.78	126.64	114.35
10	A	504	ANJ	C6-C8-N2	2.78	122.08	116.88
6	J	502	HEM	CMD-C2D-C3D	2.79	126.70	114.35
6	G	501	HEM	CMD-C2D-C3D	2.80	126.72	114.35
6	G	501	HEM	C2D-C3D-C4D	2.80	106.25	101.50
6	E	301	HEM	CMD-C2D-C3D	2.80	126.75	114.35
6	G	502	HEM	CMD-C2D-C3D	2.81	126.79	114.35
6	B	301	HEM	CMD-C2D-C3D	2.82	126.82	114.35
6	K	301	HEM	CMD-C2D-C3D	2.82	126.84	114.35
6	H	301	HEM	CMD-C2D-C3D	2.84	126.92	114.35
6	E	301	HEM	C2D-C3D-C4D	2.86	106.36	101.50
6	K	301	HEM	C2D-C3D-C4D	2.88	106.38	101.50
6	B	301	HEM	C2D-C3D-C4D	2.89	106.41	101.50
9	G	504	LOP	O5-C6-C7	2.91	117.86	111.53
6	A	501	HEM	C2D-C3D-C4D	2.92	106.44	101.50
6	G	502	HEM	C2D-C3D-C4D	2.93	106.46	101.50
6	H	301	HEM	C2D-C3D-C4D	2.94	106.49	101.50
6	D	501	HEM	C2D-C3D-C4D	2.96	106.52	101.50
6	A	502	HEM	C2D-C3D-C4D	2.98	106.56	101.50
9	A	503	LOP	O6-C24-C25	3.00	121.03	111.90
6	J	501	HEM	C2D-C3D-C4D	3.01	106.59	101.50
6	J	502	HEM	C2D-C3D-C4D	3.04	106.66	101.50
6	D	502	HEM	C2D-C3D-C4D	3.05	106.67	101.50
10	G	505	ANJ	C6-C8-N2	3.05	122.58	116.88
8	G	503	SMA	O5-C5-C4A	3.12	120.81	115.89
8	J	503	SMA	O5-C5-C4A	3.20	120.95	115.89
8	D	2	SMA	O5-C5-C4A	3.29	121.09	115.89
6	D	502	HEM	CMC-C2C-C3C	3.80	126.01	116.53
6	G	501	HEM	CAD-C3D-C4D	3.84	126.03	112.47
6	E	301	HEM	CAD-C3D-C4D	3.87	126.12	112.47
6	H	301	HEM	CAD-C3D-C4D	3.89	126.19	112.47
6	D	502	HEM	CMB-C2B-C3B	3.92	126.31	116.53
6	D	501	HEM	CMC-C2C-C3C	3.93	126.35	116.53
6	A	501	HEM	CMC-C2C-C3C	3.94	126.36	116.53
10	J	505	ANJ	O6-C17-O7	3.95	129.52	124.19
6	B	301	HEM	CAD-C3D-C4D	4.02	126.64	112.47
10	D	504	ANJ	O6-C17-O7	4.04	129.64	124.19
6	G	502	HEM	CAD-C3D-C4D	4.06	126.81	112.47
6	J	502	HEM	CAD-C3D-C4D	4.07	126.83	112.47
6	G	502	HEM	CMC-C2C-C3C	4.07	126.70	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	502	HEM	CMC-C2C-C3C	4.08	126.71	116.53
6	A	502	HEM	CMB-C2B-C3B	4.11	126.79	116.53
6	G	501	HEM	CMC-C2C-C3C	4.15	126.89	116.53
6	K	301	HEM	CAD-C3D-C4D	4.15	127.12	112.47
6	A	501	HEM	CAD-C3D-C4D	4.16	127.16	112.47
6	J	501	HEM	CMC-C2C-C3C	4.17	126.94	116.53
6	B	301	HEM	CMB-C2B-C3B	4.18	126.96	116.53
6	A	502	HEM	CAD-C3D-C4D	4.18	127.23	112.47
6	J	501	HEM	CAD-C3D-C4D	4.22	127.36	112.47
6	G	502	HEM	CMB-C2B-C3B	4.22	127.07	116.53
6	D	502	HEM	CAD-C3D-C2D	4.23	125.38	113.22
6	J	502	HEM	CMB-C2B-C3B	4.26	127.17	116.53
10	A	504	ANJ	O6-C17-O7	4.30	130.00	124.19
6	D	501	HEM	CAD-C3D-C2D	4.30	125.59	113.22
6	H	301	HEM	CMC-C2C-C3C	4.32	127.30	116.53
10	G	505	ANJ	O6-C17-O7	4.33	130.03	124.19
6	E	301	HEM	CMB-C2B-C3B	4.34	127.35	116.53
8	D	2	SMA	O7-C7-C8	4.36	118.85	114.47
6	E	301	HEM	CMC-C2C-C3C	4.36	127.42	116.53
6	D	501	HEM	CAD-C3D-C4D	4.37	127.88	112.47
6	H	301	HEM	CMB-C2B-C3B	4.39	127.48	116.53
6	D	502	HEM	CAD-C3D-C4D	4.39	127.95	112.47
6	K	301	HEM	CMC-C2C-C3C	4.41	127.53	116.53
6	D	501	HEM	CMB-C2B-C3B	4.44	127.61	116.53
6	B	301	HEM	CMC-C2C-C3C	4.45	127.64	116.53
6	J	501	HEM	CAD-C3D-C2D	4.46	126.04	113.22
6	A	502	HEM	CAD-C3D-C2D	4.50	126.16	113.22
6	G	501	HEM	CMB-C2B-C3B	4.51	127.80	116.53
6	K	301	HEM	CMB-C2B-C3B	4.52	127.81	116.53
8	J	503	SMA	O7-C7-C8	4.53	119.03	114.47
6	A	501	HEM	CAD-C3D-C2D	4.56	126.34	113.22
6	J	502	HEM	CAD-C3D-C2D	4.60	126.46	113.22
6	K	301	HEM	CAD-C3D-C2D	4.61	126.47	113.22
8	G	503	SMA	O7-C7-C8	4.62	119.11	114.47
6	J	501	HEM	CMB-C2B-C3B	4.64	128.11	116.53
6	G	502	HEM	CAD-C3D-C2D	4.70	126.72	113.22
6	A	501	HEM	CMB-C2B-C3B	4.73	128.34	116.53
6	B	301	HEM	CAD-C3D-C2D	4.74	126.85	113.22
6	H	301	HEM	CAD-C3D-C2D	4.85	127.15	113.22
6	A	502	HEM	CMC-C2C-C3C	4.97	128.93	116.53
6	E	301	HEM	CAD-C3D-C2D	4.98	127.52	113.22
6	G	501	HEM	CAD-C3D-C2D	4.98	127.54	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1	SMA	O7-C7-C8	7.55	122.06	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 113 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1	SMA	2	0
4	A	431	BGL	3	0
6	A	501	HEM	4	0
6	A	502	HEM	5	0
9	A	503	LOP	2	0
10	A	504	ANJ	9	0
6	B	301	HEM	5	0
8	D	2	SMA	3	0
6	D	501	HEM	5	0
6	D	502	HEM	5	0
9	D	503	LOP	4	0
10	D	504	ANJ	12	0
4	E	257	BGL	2	0
6	E	301	HEM	5	0
4	G	431	BGL	1	0
6	G	501	HEM	4	0
6	G	502	HEM	3	0
8	G	503	SMA	1	0
9	G	504	LOP	5	0
10	G	505	ANJ	6	0
6	H	301	HEM	4	0
4	J	431	BGL	1	0
6	J	501	HEM	2	0
6	J	502	HEM	3	0
8	J	503	SMA	3	0
9	J	504	LOP	5	0
10	J	505	ANJ	10	0
6	K	301	HEM	1	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, 95^{th} 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	A	428/428 (100%)	0.70	27 (6%)	23	17	42, 63, 104, 129	0
1	D	428/428 (100%)	0.60	28 (6%)	22	16	43, 62, 100, 128	0
1	G	428/428 (100%)	0.61	19 (4%)	38	30	43, 64, 104, 128	0
1	J	428/428 (100%)	0.53	18 (4%)	40	32	43, 62, 100, 126	0
2	B	256/256 (100%)	0.96	40 (15%)	3	1	55, 89, 125, 149	0
2	E	256/256 (100%)	1.31	62 (24%)	1	0	65, 93, 128, 148	0
2	H	256/256 (100%)	0.92	39 (15%)	3	1	57, 90, 126, 151	0
2	K	256/256 (100%)	1.05	51 (19%)	1	1	62, 91, 127, 150	0
3	C	179/179 (100%)	1.03	25 (13%)	4	2	49, 82, 123, 155	0
3	F	179/179 (100%)	1.24	44 (24%)	1	0	49, 84, 124, 155	0
3	I	179/179 (100%)	0.97	22 (12%)	5	3	50, 83, 125, 156	0
3	L	179/179 (100%)	1.23	43 (24%)	1	0	52, 85, 124, 156	0
All	All	3452/3452 (100%)	0.85	418 (12%)	6	3	42, 75, 122, 156	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	GLY	12.9
2	K	4	GLY	12.4
2	B	2	GLY	11.5
3	I	9	GLY	11.4
2	K	3	GLY	11.3
2	K	1	ALA	11.1
3	F	10	THR	11.0
3	C	9	GLY	10.9
2	E	4	GLY	10.2
3	F	11	ARG	10.1
3	F	12	ARG	9.8

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Mol	Chain	Res	Type	RSRZ
3	C	12	ARG	9.8
3	L	12	ARG	9.7
3	I	10	THR	9.0
2	E	1	ALA	8.8
2	B	1	ALA	8.5
2	H	2	GLY	8.3
2	K	110	PHE	8.2
3	L	10	THR	8.1
2	H	1	ALA	8.0
2	K	6	VAL	8.0
3	C	11	ARG	7.8
3	L	52	VAL	7.6
2	H	4	GLY	7.6
3	C	16	TYR	7.6
3	I	179	ILE	7.5
3	C	10	THR	7.5
3	C	179	ILE	7.4
2	K	122	PHE	6.9
2	K	5	HIS	6.8
3	L	11	ARG	6.7
2	E	150	GLU	6.7
2	E	143	PRO	6.6
2	H	3	GLY	6.5
1	J	9	TYR	6.4
3	F	184	ILE	6.4
2	E	5	HIS	6.3
2	E	187	PRO	6.2
3	L	179	ILE	6.0
2	E	9	VAL	5.9
3	F	14	PHE	5.8
3	F	9	GLY	5.8
3	L	184	ILE	5.8
3	L	123	LEU	5.7
1	D	9	TYR	5.7
2	E	144	LYS	5.7
2	K	124	GLY	5.6
2	E	7	GLU	5.5
3	L	178	PHE	5.5
3	L	9	GLY	5.3
1	G	12	ARG	5.2
3	L	116	LEU	5.2
3	I	46	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	13	THR	5.2
3	I	178	PHE	5.1
1	A	414	ILE	5.1
3	C	15	LEU	5.0
1	A	12	ARG	5.0
2	E	3	GLY	5.0
2	E	124	GLY	5.0
3	F	13	ASP	5.0
2	H	5	HIS	4.9
1	D	8	HIS	4.9
1	A	13	THR	4.9
2	K	7	GLU	4.8
2	E	149	HIS	4.8
2	E	142	PRO	4.8
2	H	251	LEU	4.7
3	F	179	ILE	4.7
2	B	5	HIS	4.7
3	L	182	THR	4.6
1	J	11	PRO	4.6
1	A	15	ILE	4.6
3	I	181	GLU	4.6
3	F	116	LEU	4.6
1	D	15	ILE	4.5
2	B	122	PHE	4.5
2	K	143	PRO	4.4
3	F	47	LEU	4.4
3	L	48	ALA	4.4
2	B	250	ARG	4.4
2	H	147	GLU	4.4
1	D	11	PRO	4.3
1	J	10	GLU	4.3
2	B	110	PHE	4.3
2	K	132	TYR	4.3
2	E	145	CYS	4.3
2	E	147	GLU	4.3
1	D	12	ARG	4.2
3	L	183	THR	4.2
2	B	206	ALA	4.2
1	J	12	ARG	4.2
2	E	11	PHE	4.2
3	F	17	TYR	4.2
3	F	51	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
3	L	17	TYR	4.2
3	I	183	THR	4.1
3	I	11	ARG	4.1
1	G	362	MET	4.1
2	E	208	ALA	4.1
2	B	182	TRP	4.0
3	F	124	VAL	4.0
3	F	18	ALA	4.0
2	E	193	LEU	4.0
2	K	204	VAL	4.0
2	K	109	GLY	4.0
3	L	181	GLU	4.0
3	L	14	PHE	4.0
2	H	72	VAL	3.9
3	L	187	GLY	3.9
2	E	111	HIS	3.9
3	F	103	ILE	3.9
3	F	123	LEU	3.9
3	I	12	ARG	3.9
1	G	17	LYS	3.9
3	C	181	GLU	3.9
3	L	124	VAL	3.9
1	G	414	ILE	3.8
1	G	416	LYS	3.8
2	E	155	TYR	3.8
1	D	10	GLU	3.8
1	A	11	PRO	3.8
2	H	82	GLU	3.8
3	L	68	LEU	3.8
3	L	103	ILE	3.7
2	E	96	ASN	3.7
2	E	58	LEU	3.7
2	E	182	TRP	3.7
3	L	13	ASP	3.7
2	B	116	THR	3.7
2	E	10	PRO	3.7
1	J	16	GLU	3.7
3	C	122	TRP	3.7
2	B	252	TRP	3.7
1	G	250	ILE	3.7
1	G	11	PRO	3.7
1	A	18	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	232	THR	3.6
2	B	256	LYS	3.6
3	F	52	VAL	3.6
2	K	8	ASP	3.6
2	H	198	ASP	3.5
2	E	158	ARG	3.5
2	E	34	GLU	3.5
2	H	121	LEU	3.5
1	D	170	PRO	3.5
2	E	151	PRO	3.5
1	A	14	GLY	3.5
1	G	3	GLY	3.5
2	B	251	LEU	3.5
3	I	17	TYR	3.5
1	J	8	HIS	3.5
1	D	20	HIS	3.5
2	K	11	PHE	3.4
3	C	123	LEU	3.4
2	K	9	VAL	3.4
3	I	67	PHE	3.4
2	E	178	THR	3.4
3	F	182	THR	3.4
1	G	18	TRP	3.4
3	F	183	THR	3.4
3	L	47	LEU	3.4
1	A	8	HIS	3.4
2	H	83	GLY	3.4
1	A	357	GLY	3.4
2	K	196	TYR	3.3
1	D	323	PHE	3.3
1	A	416	LYS	3.3
1	A	413	ALA	3.3
3	C	18	ALA	3.3
2	B	121	LEU	3.3
2	E	189	LEU	3.3
2	K	2	GLY	3.3
2	E	6	VAL	3.3
1	D	235	ALA	3.3
1	D	14	GLY	3.2
2	K	114	MET	3.2
3	F	56	SER	3.2
2	B	4	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	122	TRP	3.2
2	B	243	LEU	3.2
2	E	94	LEU	3.2
2	B	114	MET	3.2
3	C	101	ALA	3.2
3	F	178	PHE	3.2
2	H	123	ASN	3.2
1	D	247	TYR	3.2
2	E	146	ALA	3.2
1	G	15	ILE	3.2
2	H	151	PRO	3.2
3	L	122	TRP	3.2
3	F	16	TYR	3.2
3	L	74	ILE	3.2
1	G	429	ASN	3.2
1	A	415	GLU	3.2
1	J	247	TYR	3.1
2	E	139	PRO	3.1
2	E	207	MET	3.1
3	L	63	LEU	3.1
1	A	16	GLU	3.1
2	H	182	TRP	3.1
2	K	208	ALA	3.1
2	E	255	VAL	3.1
2	K	256	LYS	3.0
3	C	178	PHE	3.0
1	D	362	MET	3.0
2	E	184	ALA	3.0
3	F	15	LEU	3.0
3	L	73	PHE	3.0
2	B	151	PRO	3.0
2	E	110	PHE	3.0
3	I	174	PRO	3.0
2	B	255	VAL	3.0
3	I	16	TYR	3.0
2	H	149	HIS	2.9
2	B	79	GLU	2.9
3	F	98	ALA	2.9
3	L	16	TYR	2.9
2	H	110	PHE	2.9
2	K	142	PRO	2.9
3	C	68	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	79	GLU	2.9
2	E	8	ASP	2.9
2	B	247	THR	2.9
1	A	324	GLY	2.8
1	D	234	LYS	2.8
3	I	120	GLY	2.8
2	E	246	LEU	2.8
2	K	58	LEU	2.8
2	H	122	PHE	2.8
2	H	165	VAL	2.8
2	E	196	TYR	2.8
2	K	123	ASN	2.8
2	E	191	ASP	2.8
3	L	104	ASP	2.8
1	J	20	HIS	2.8
3	C	63	LEU	2.8
3	C	175	LEU	2.8
3	F	114	ARG	2.8
1	G	430	ALA	2.7
2	K	147	GLU	2.7
2	E	141	GLU	2.7
1	A	320	PHE	2.7
3	C	57	VAL	2.7
2	H	67	ALA	2.7
2	K	10	PRO	2.7
2	K	155	TYR	2.7
1	A	428	PHE	2.7
3	F	48	ALA	2.7
2	E	205	HIS	2.7
2	K	200	HIS	2.7
1	A	174	HIS	2.7
2	E	153	GLY	2.7
3	L	57	VAL	2.7
1	G	13	THR	2.7
2	H	69	GLN	2.6
3	F	112	GLN	2.6
2	B	196	TYR	2.6
2	B	253	ALA	2.6
3	C	19	THR	2.6
3	I	177	LYS	2.6
3	F	68	LEU	2.6
1	G	14	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	250	ARG	2.6
3	I	101	ALA	2.6
2	E	135	LEU	2.6
3	F	186	LEU	2.6
2	B	72	VAL	2.6
2	E	154	PHE	2.6
3	C	174	PRO	2.6
2	H	145	CYS	2.6
3	C	67	PHE	2.6
3	I	79	GLU	2.6
2	H	189	LEU	2.6
1	J	184	PRO	2.6
1	A	411	LEU	2.6
1	A	196	SER	2.6
1	J	17	LYS	2.5
2	E	148	GLY	2.5
2	H	244	LEU	2.5
1	D	70	THR	2.5
3	I	122	TRP	2.5
1	A	325	ILE	2.5
2	E	125	ILE	2.5
1	J	13	THR	2.5
1	D	30	TYR	2.5
1	G	16	GLU	2.5
1	J	31	ASP	2.5
2	K	13	PHE	2.5
2	K	145	CYS	2.5
3	F	74	ILE	2.5
2	K	205	HIS	2.5
3	F	118	GLU	2.5
1	D	5	PRO	2.5
2	H	231	PHE	2.5
3	L	50	ILE	2.5
3	L	75	ARG	2.5
1	A	356	SER	2.5
2	K	153	GLY	2.5
3	L	105	ALA	2.4
2	H	150	GLU	2.4
2	H	200	HIS	2.4
2	E	190	MET	2.4
2	E	256	LYS	2.4
1	J	414	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	101	ALA	2.4
2	K	251	LEU	2.4
3	I	150	PRO	2.4
1	G	148	VAL	2.4
2	H	146	ALA	2.4
3	F	65	VAL	2.4
2	K	189	LEU	2.4
1	J	4	ILE	2.4
3	F	57	VAL	2.4
3	L	51	PHE	2.4
3	I	74	ILE	2.4
1	D	288	THR	2.4
3	L	53	ASP	2.4
2	H	144	LYS	2.4
1	D	202	PRO	2.4
1	D	83	ILE	2.4
2	E	12	SER	2.4
2	H	58	LEU	2.3
3	C	17	TYR	2.3
2	H	143	PRO	2.3
2	K	190	MET	2.3
3	F	177	LYS	2.3
2	K	249	LYS	2.3
2	B	23	HIS	2.3
2	B	197	ALA	2.3
3	C	74	ILE	2.3
2	H	158	ARG	2.3
3	C	142	GLY	2.3
2	H	208	ALA	2.3
1	A	359	TYR	2.3
2	B	140	GLU	2.3
1	J	15	ILE	2.3
2	B	117	GLY	2.3
2	K	178	THR	2.3
3	L	45	GLN	2.3
2	K	154	PHE	2.3
2	B	80	ASP	2.3
2	K	156	TYR	2.3
3	F	72	ILE	2.3
2	K	94	LEU	2.2
3	I	51	PHE	2.2
2	K	207	MET	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	180	ASP	2.2
1	D	236	GLU	2.2
3	C	149	CYS	2.2
1	G	172	ILE	2.2
2	E	250	ARG	2.2
3	F	19	THR	2.2
3	C	186	LEU	2.2
2	B	231	PHE	2.2
3	F	108	GLU	2.2
2	K	206	ALA	2.2
2	B	118	ILE	2.2
2	E	192	ASP	2.2
2	K	223	LEU	2.2
3	L	175	LEU	2.2
1	J	323	PHE	2.2
2	B	155	TYR	2.2
2	K	57	GLU	2.2
3	F	119	ALA	2.2
1	A	236	GLU	2.2
2	E	140	GLU	2.2
2	K	141	GLU	2.2
1	G	141	ALA	2.2
1	D	325	ILE	2.1
2	K	24	GLN	2.1
2	B	147	GLU	2.1
1	D	172	ILE	2.1
1	D	150	PRO	2.1
3	F	107	ALA	2.1
3	L	119	ALA	2.1
2	B	194	VAL	2.1
3	L	65	VAL	2.1
3	L	115	THR	2.1
1	A	226	GLY	2.1
2	B	109	GLY	2.1
2	K	125	ILE	2.1
1	A	283	ALA	2.1
3	I	180	ASP	2.1
2	E	175	VAL	2.1
3	L	160	GLY	2.1
2	B	123	ASN	2.1
1	J	6	HIS	2.1
2	H	205	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	172	ALA	2.1
2	B	3	GLY	2.1
2	K	78	GLY	2.1
2	B	82	GLU	2.1
1	D	331	PHE	2.1
2	B	208	ALA	2.1
1	A	227	VAL	2.1
3	F	104	ASP	2.1
3	F	46	ALA	2.1
2	E	21	ASP	2.0
2	K	149	HIS	2.0
1	D	79	SER	2.0
1	G	19	LEU	2.0
3	L	54	VAL	2.0
1	J	320	PHE	2.0
2	B	125	ILE	2.0
2	E	114	MET	2.0
2	E	131	ILE	2.0
2	E	224	MET	2.0
2	K	23	HIS	2.0
2	E	179	ALA	2.0
2	E	204	VAL	2.0
2	H	178	THR	2.0
3	F	73	PHE	2.0
1	D	33	ILE	2.0
2	B	200	HIS	2.0
3	F	176	ALA	2.0
2	K	250	ARG	2.0
2	H	247	THR	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, 95^{th} 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	BGL	G	431	20/20	0.79	0.37	1.90	97,99,102,102	0
9	LOP	J	504	45/45	0.84	0.28	1.81	81,84,95,97	0
9	LOP	D	503	45/45	0.88	0.24	1.32	75,88,94,94	0
4	BGL	E	257	20/20	0.84	0.36	1.20	101,101,102,102	0
10	ANJ	G	505	39/39	0.92	0.25	0.93	69,72,79,81	0
4	BGL	A	431	20/20	0.82	0.33	0.86	89,92,93,93	0
8	SMA	D	2	37/37	0.93	0.25	0.71	47,53,62,64	0
4	BGL	J	431	20/20	0.76	0.36	0.68	95,96,100,101	0
10	ANJ	A	504	39/39	0.93	0.24	0.65	70,74,77,78	0
8	SMA	J	503	37/37	0.92	0.24	0.58	45,50,56,56	0
6	HEM	B	301	43/43	0.96	0.22	0.58	61,65,67,69	0
9	LOP	A	503	45/45	0.86	0.23	0.51	79,99,105,107	0
9	LOP	G	504	45/45	0.84	0.23	0.44	70,87,96,98	0
6	HEM	G	501	43/43	0.97	0.23	0.28	55,59,63,65	0
8	SMA	A	1	37/37	0.94	0.23	0.22	46,55,58,58	0
7	FES	L	200	4/4	0.98	0.22	0.16	56,57,57,57	0
6	HEM	H	301	43/43	0.96	0.21	0.10	66,70,71,72	0
10	ANJ	D	504	39/39	0.92	0.21	0.07	49,66,79,82	0
6	HEM	G	502	43/43	0.96	0.24	0.02	47,52,54,54	0
10	ANJ	J	505	39/39	0.92	0.21	0.00	51,67,82,85	0
6	HEM	J	501	43/43	0.97	0.18	-0.05	55,56,57,58	0
6	HEM	K	301	43/43	0.95	0.21	-0.07	73,79,80,81	0
8	SMA	G	503	37/37	0.94	0.22	-0.09	51,58,60,62	0
7	FES	F	200	4/4	0.98	0.18	-0.13	55,55,55,55	0
7	FES	I	200	4/4	0.98	0.21	-0.25	53,53,54,54	0
6	HEM	J	502	43/43	0.97	0.22	-0.33	36,43,47,48	0
6	HEM	A	502	43/43	0.96	0.24	-0.36	43,47,51,52	0
6	HEM	A	501	43/43	0.96	0.19	-0.36	61,64,70,73	0
6	HEM	D	501	43/43	0.96	0.19	-0.42	60,61,62,64	0
6	HEM	E	301	43/43	0.96	0.21	-0.45	74,80,81,81	0
7	FES	C	200	4/4	0.97	0.19	-0.54	54,54,54,54	0
6	HEM	D	502	43/43	0.96	0.23	-0.72	34,42,45,46	0
5	SR	H	257	1/1	0.75	0.09	-1.80	117,117,117,117	0
5	SR	K	257	1/1	0.87	0.04	-1.99	144,144,144,144	0
5	SR	B	257	1/1	0.93	0.08	-2.78	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	SR	E	258	1/1	0.75	0.08	-2.87	126,126,126,126	0
5	SR	J	432	1/1	0.86	0.30	-	114,114,114,114	0
5	SR	G	432	1/1	0.87	0.26	-	135,135,135,135	0

6.5 Other polymers (i)

There are no such residues in this entry.