Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:44 AM GMT

PDB ID	:	2NOX
Title	:	Crystal structure of tryptophan 2,3-dioxygenase from Ralstonia metallidurans
Authors	:	Zhang, Y.; Kang, S.A.; Mukherjee, T.; Bale, S.; Crane, B.R.; Begley, T.P.; Ealick, S.E.
Deposited on	:	2006-10-26
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

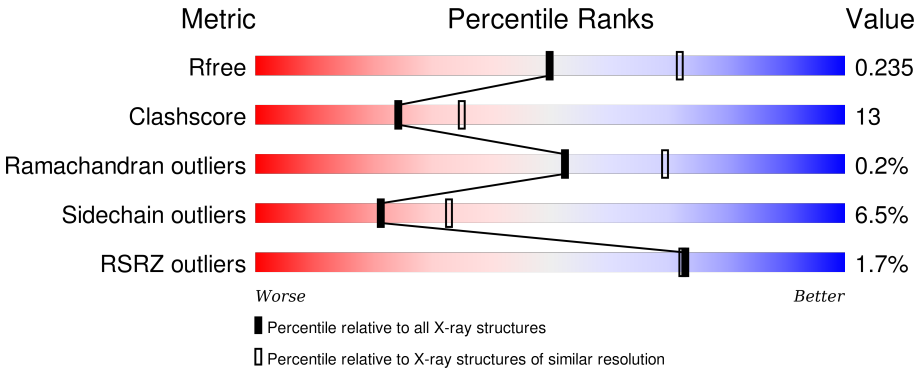
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	281	70% 21% • 7%
1	B	281	71% 21% • • 5%
1	C	281	70% 18% • 9%
1	D	281	70% 19% • 8%
1	E	281	71% 18% • 9%

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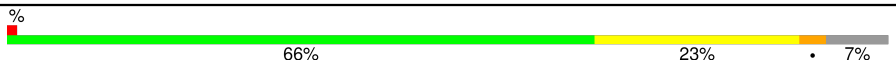
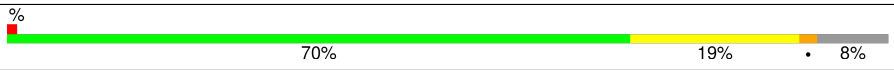
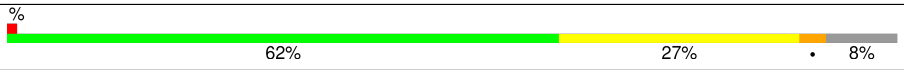
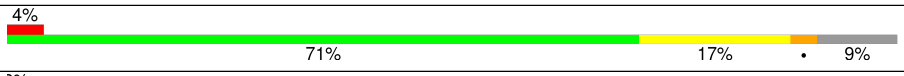
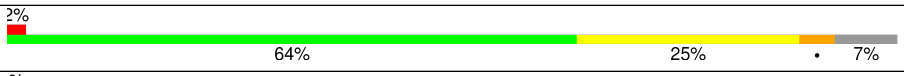
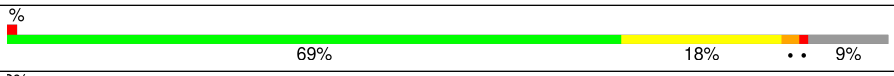
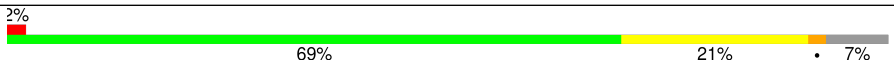
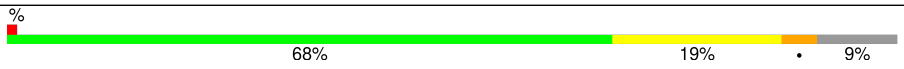
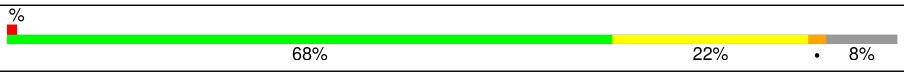
Mol	Chain	Length	Quality of chain
1	F	281	
1	G	281	
1	H	281	
1	I	281	
1	J	281	
1	K	281	
1	L	281	
1	M	281	
1	N	281	
1	O	281	
1	P	281	

2 Entry composition

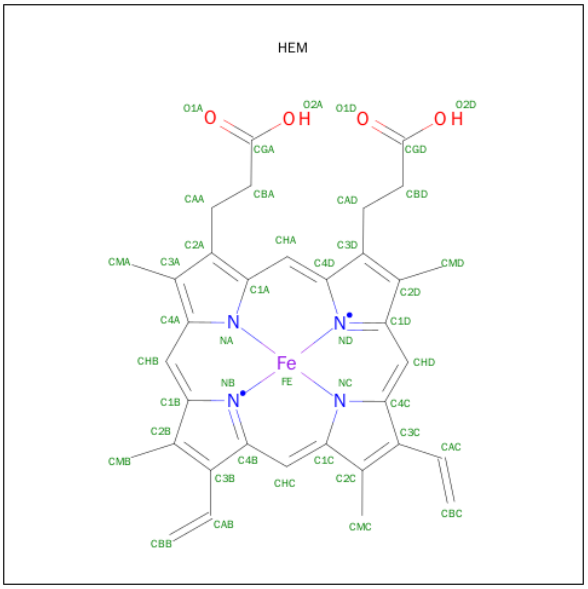
There are 3 unique types of molecules in this entry. The entry contains 36423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			2160	1375	382	390	13			
1	B	266	Total	C	N	O	S	0	0	0
			2192	1400	384	395	13			
1	C	255	Total	C	N	O	S	0	0	0
			2106	1344	368	382	12			
1	D	259	Total	C	N	O	S	0	0	0
			2133	1360	376	385	12			
1	E	256	Total	C	N	O	S	0	0	0
			2126	1356	376	382	12			
1	F	260	Total	C	N	O	S	0	0	0
			2152	1371	380	388	13			
1	G	259	Total	C	N	O	S	0	0	0
			2137	1362	376	387	12			
1	H	259	Total	C	N	O	S	0	2	0
			2147	1368	380	387	12			
1	I	259	Total	C	N	O	S	0	0	0
			2133	1360	376	385	12			
1	J	257	Total	C	N	O	S	0	0	0
			2126	1356	374	384	12			
1	K	255	Total	C	N	O	S	0	1	0
			2119	1352	372	383	12			
1	L	260	Total	C	N	O	S	0	0	0
			2141	1364	377	388	12			
1	M	255	Total	C	N	O	S	0	1	0
			2111	1349	370	380	12			
1	N	260	Total	C	N	O	S	0	1	0
			2150	1370	379	389	12			
1	O	257	Total	C	N	O	S	0	0	0
			2126	1356	374	384	12			
1	P	259	Total	C	N	O	S	0	0	0
			2133	1360	376	385	12			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	126	Total	O	0	0
			126	126		
3	C	107	Total	O	0	0
			107	107		
3	D	158	Total	O	0	0
			158	158		
3	E	107	Total	O	0	0
			107	107		
3	F	72	Total	O	0	0
			72	72		
3	G	56	Total	O	0	0
			56	56		
3	H	114	Total	O	0	0
			114	114		
3	I	85	Total	O	0	0
			85	85		
3	J	82	Total	O	0	0
			82	82		
3	K	74	Total	O	0	0
			74	74		
3	L	81	Total	O	0	0
			81	81		
3	M	116	Total	O	0	0
			116	116		
3	N	66	Total	O	0	0
			66	66		
3	O	61	Total	O	0	0
			61	61		

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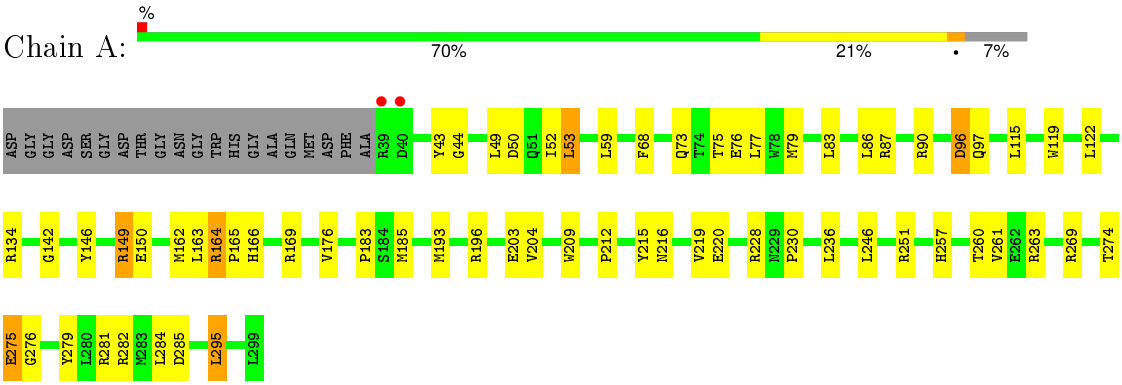
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	108	Total	O	0	0
			108	108		

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.

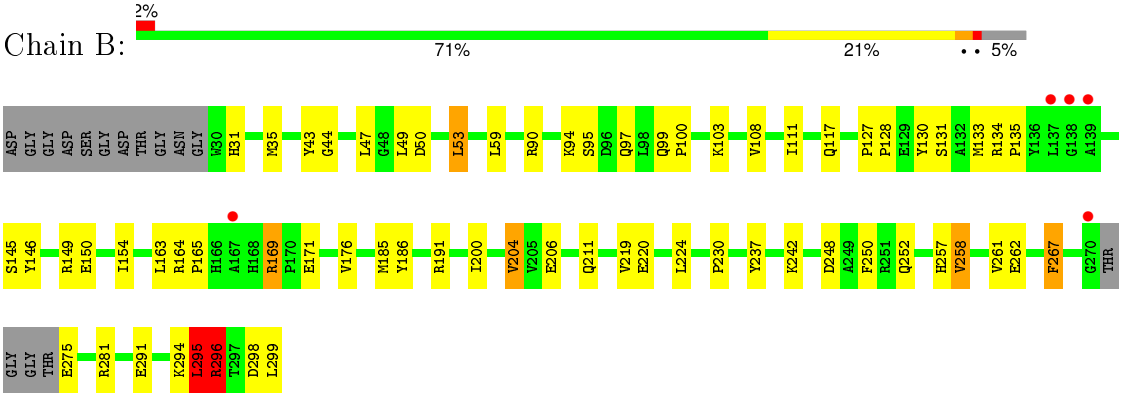
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



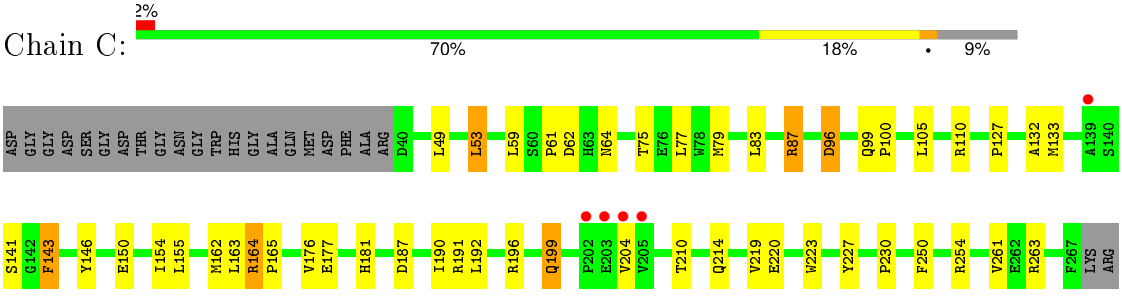
- Molecule 1: Tryptophan 2,3-dioxygenase

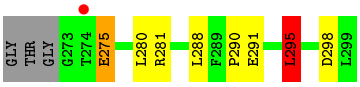
Chain B:



- Molecule 1: Tryptophan 2,3-dioxygenase

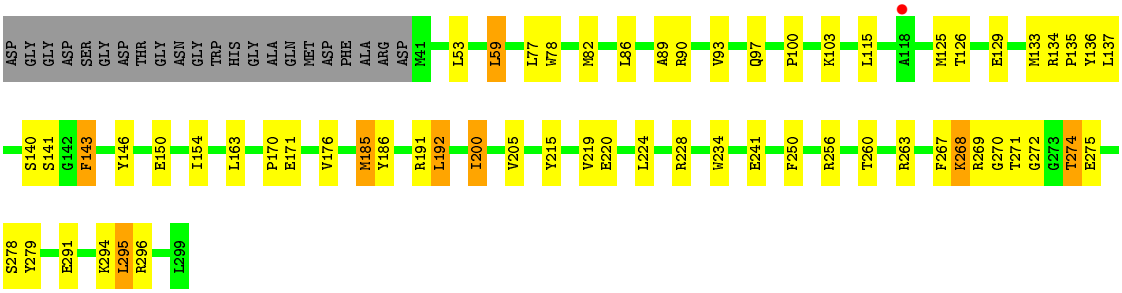
Chain C:





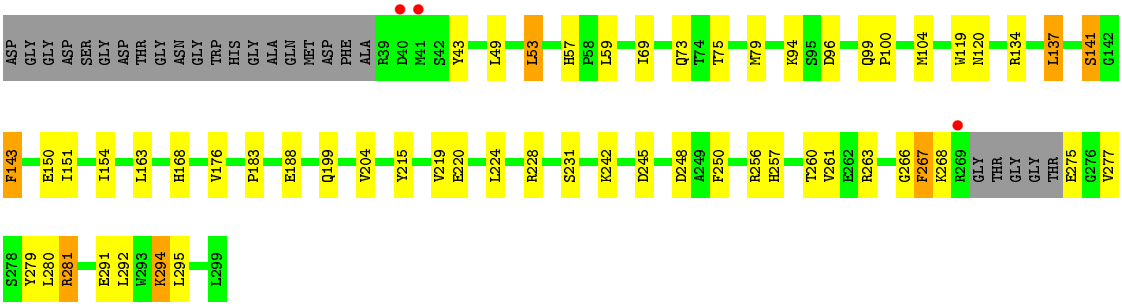
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:



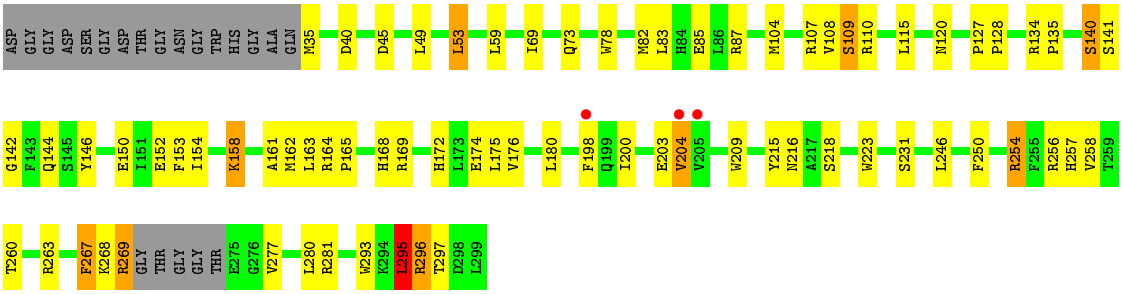
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain E:



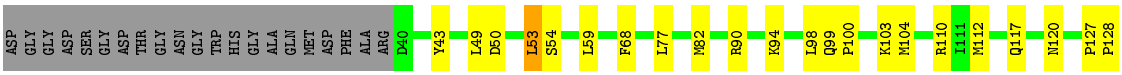
• Molecule 1: Tryptophan 2,3-dioxygenase

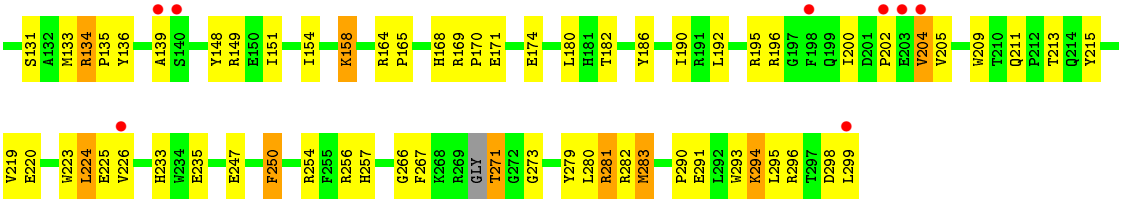
Chain F:



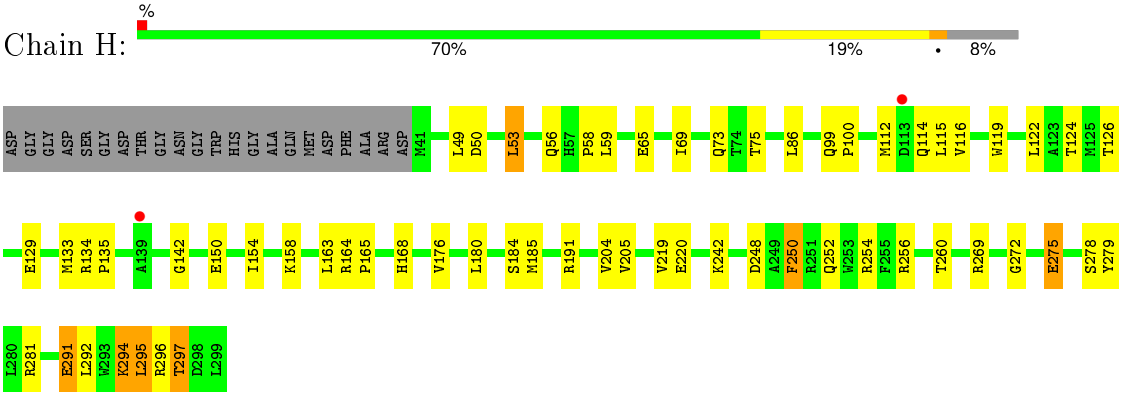
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain G:

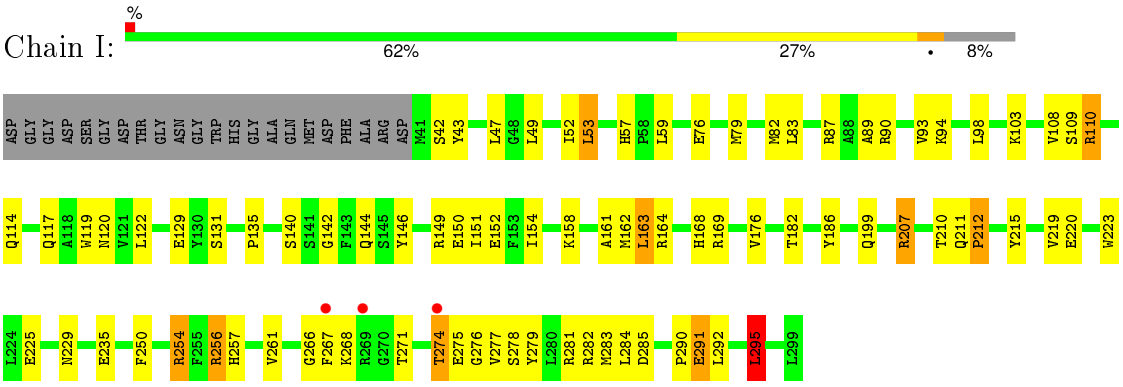




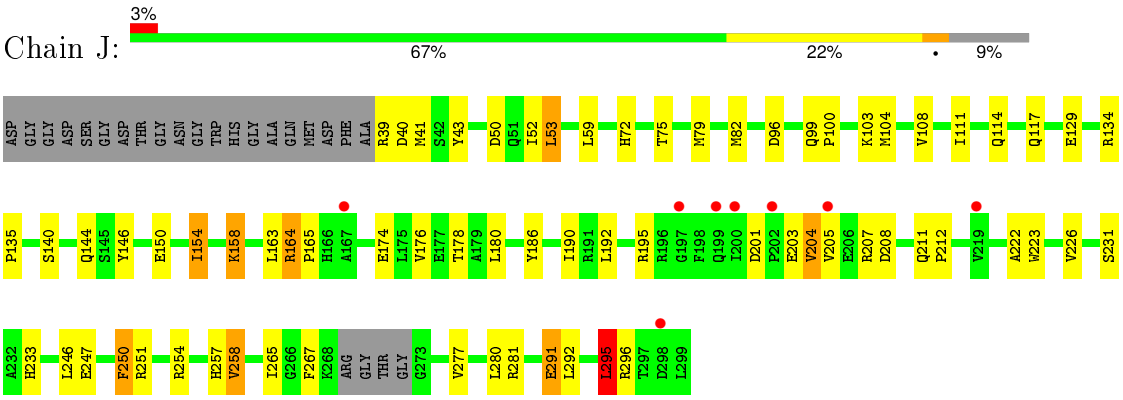
• Molecule 1: Tryptophan 2,3-dioxygenase



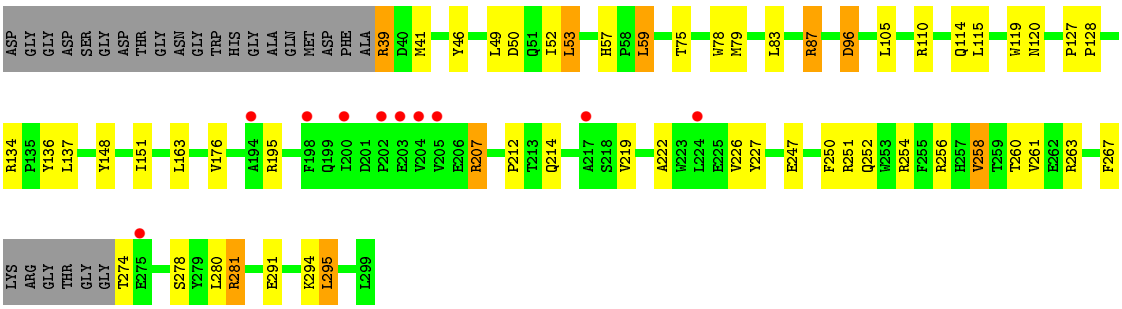
• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase

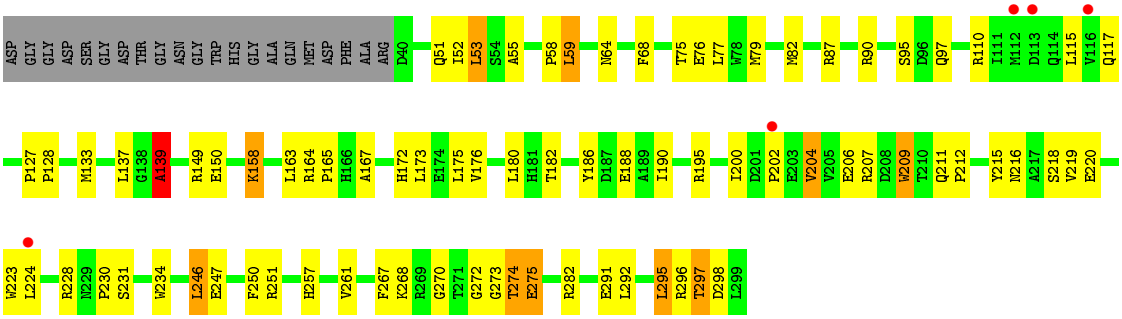


• Molecule 1: Tryptophan 2,3-dioxygenase



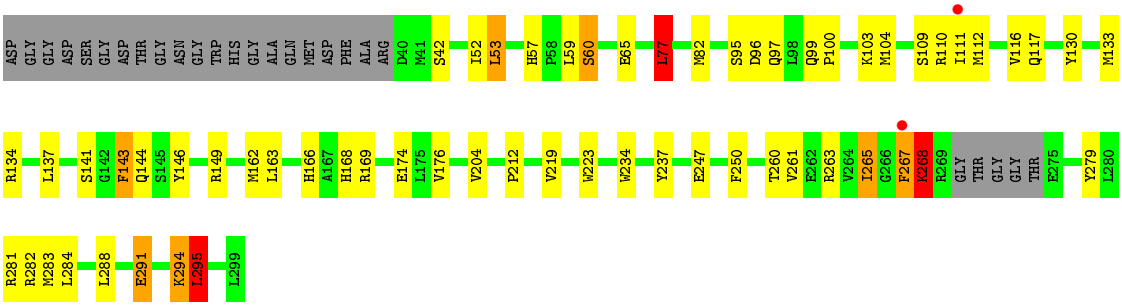
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain L:



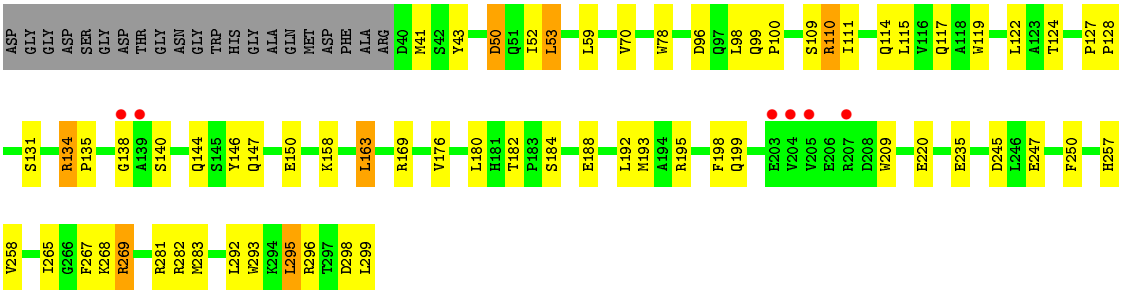
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain M:



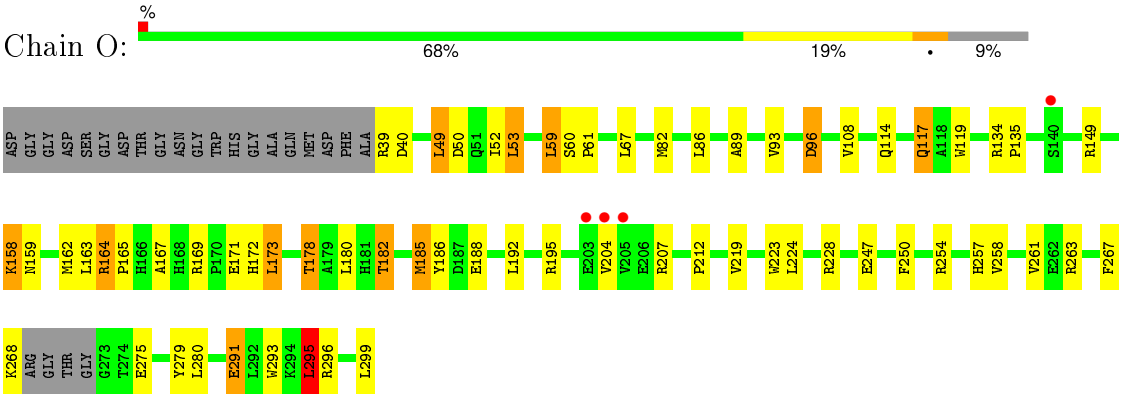
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain N:



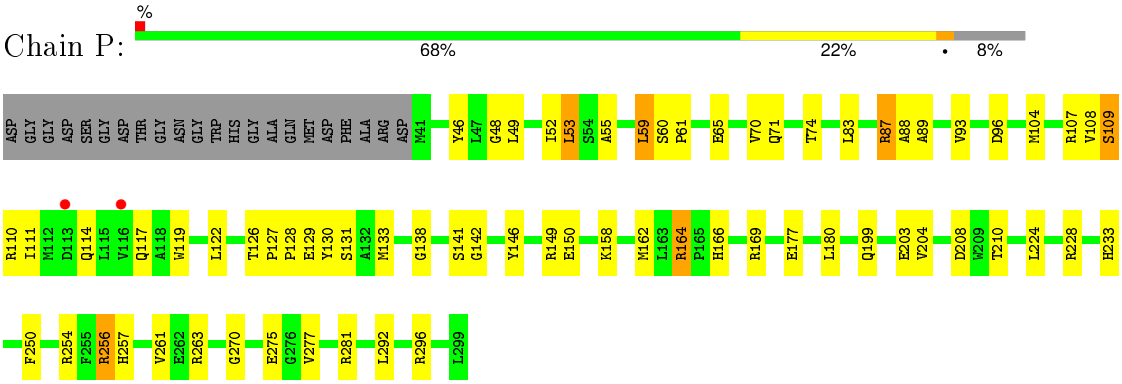
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain O:



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.54Å 132.12Å 139.95Å 66.97° 85.06° 89.89°	Depositor
Resolution (Å)	50.12 – 2.40 50.09 – 2.22	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.12-2.40) 77.0 (50.09-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.270 0.163 , 0.235	Depositor DCC
R_{free} test set	9133 reflections (5.65%)	DCC
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 224640 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36423	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: HEM

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	0.68	0/2217	0.80	3/3004 (0.1%)
1	B	0.64	0/2252	0.78	5/3053 (0.2%)
1	C	0.65	0/2162	0.76	2/2932 (0.1%)
1	D	0.68	0/2190	0.80	1/2969 (0.0%)
1	E	0.61	0/2182	0.68	1/2956 (0.0%)
1	F	0.58	0/2208	0.71	1/2991 (0.0%)
1	G	0.57	0/2193	0.66	0/2972
1	H	0.60	0/2207	0.73	1/2992 (0.0%)
1	I	0.57	0/2190	0.69	1/2969 (0.0%)
1	J	0.54	0/2182	0.69	1/2957 (0.0%)
1	K	0.51	0/2178	0.68	0/2953
1	L	0.54	0/2198	0.68	0/2980
1	M	0.64	0/2167	0.75	2/2938 (0.1%)
1	N	0.54	0/2207	0.67	0/2991
1	O	0.57	0/2182	0.68	1/2957 (0.0%)
1	P	0.61	0/2190	0.73	2/2969 (0.1%)
All	All	0.60	0/35105	0.72	21/47583 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	295	LEU	CA-CB-CG	9.07	136.17	115.30
1	M	295	LEU	CA-CB-CG	8.72	135.36	115.30
1	B	296	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	H	295	LEU	CA-CB-CG	7.93	133.53	115.30
1	B	296	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	I	295	LEU	CA-CB-CG	7.15	131.74	115.30
1	A	295	LEU	CA-CB-CG	7.13	131.69	115.30
1	F	295	LEU	CA-CB-CG	7.05	131.51	115.30
1	P	256	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	295	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	295	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	90	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	258	VAL	CB-CA-C	-6.02	99.97	111.40
1	P	263	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	O	295	LEU	CA-CB-CG	5.55	128.08	115.30
1	M	77	LEU	CA-CB-CG	5.51	127.98	115.30
1	J	295	LEU	CA-CB-CG	5.30	127.49	115.30
1	B	149	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	87	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	E	245	ASP	CB-CA-C	-5.12	100.17	110.40
1	A	263	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	139	ALA	Peptide

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	2160	0	2108	65	0
1	B	2192	0	2117	50	0
1	C	2106	0	2047	51	0
1	D	2133	0	2083	49	0
1	E	2126	0	2076	51	0
1	F	2152	0	2096	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2137	0	2083	75	0
1	H	2147	0	2101	34	0
1	I	2133	0	2083	87	0
1	J	2126	0	2073	56	0
1	K	2119	0	2065	53	0
1	L	2141	0	2087	78	0
1	M	2111	0	2051	46	0
1	N	2150	0	2099	60	0
1	O	2126	0	2073	58	0
1	P	2133	0	2083	62	0
2	A	43	0	30	6	0
2	B	43	0	30	0	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
2	E	43	0	30	7	0
2	F	43	0	30	3	0
2	G	43	0	30	3	0
2	H	43	0	30	2	0
2	I	43	0	30	9	0
2	J	43	0	30	1	0
2	K	43	0	30	4	0
2	L	43	0	30	5	0
2	M	43	0	30	2	0
2	N	43	0	30	1	0
2	O	43	0	30	4	0
2	P	43	0	30	7	0
3	A	130	0	0	10	0
3	B	126	0	0	6	0
3	C	107	0	0	7	0
3	D	158	0	0	4	0
3	E	107	0	0	4	0
3	F	72	0	0	6	0
3	G	56	0	0	8	0
3	H	114	0	0	3	0
3	I	85	0	0	8	0
3	J	82	0	0	6	0
3	K	74	0	0	7	0
3	L	81	0	0	10	0
3	M	116	0	0	5	0
3	N	66	0	0	1	0
3	O	61	0	0	4	0
3	P	108	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	36423	0	33805	893	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 13.

All (893) 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:N:109:SER:HB3	1:N:110:ARG:NH1	1.56	1.17
1:G:283:MET:HA	1:G:283:MET:HE2	1.18	1.15
1:P:65:GLU:HG3	1:P:133:MET:CE	1.77	1.15
1:G:82:MET:HE2	1:G:112:MET:HG2	1.31	1.11
1:C:219:VAL:HG12	1:C:291:GLU:HG3	1.31	1.09
1:E:281:ARG:HG2	1:E:281:ARG:HH11	1.05	1.09
1:C:199:GLN:HG3	1:C:199:GLN:O	1.52	1.07
1:P:65:GLU:HG3	1:P:133:MET:HE3	1.06	1.06
1:P:88:ALA:HB3	1:P:104:MET:CE	1.88	1.04
1:I:207:ARG:HH11	1:I:207:ARG:HG3	1.19	1.01
1:N:109:SER:CB	1:N:110:ARG:NH1	2.25	0.99
1:N:109:SER:HB3	1:N:110:ARG:HH12	1.16	0.97
1:A:274:THR:HG22	1:A:276:GLY:H	1.30	0.96
1:I:164:ARG:HD2	3:I:583:HOH:O	1.63	0.96
1:G:283:MET:HA	1:G:283:MET:CE	1.96	0.94
1:I:274:THR:HG22	1:I:276:GLY:H	1.29	0.94
1:G:82:MET:CE	1:G:112:MET:HG2	1.96	0.94
1:B:219:VAL:HG12	1:B:291:GLU:HG3	1.52	0.92
1:P:88:ALA:CB	1:P:104:MET:CE	2.47	0.92
1:J:96:ASP:HB2	3:J:534:HOH:O	1.68	0.92
1:C:219:VAL:CG1	1:C:291:GLU:HG3	1.99	0.91
1:K:278:SER:HB2	3:K:513:HOH:O	1.70	0.91
1:F:109:SER:HB2	3:F:543:HOH:O	1.68	0.91
1:C:181:HIS:HE1	3:C:584:HOH:O	1.52	0.91
1:K:57:HIS:HD2	3:K:570:HOH:O	1.52	0.90
1:O:169:ARG:HD2	1:O:171:GLU:OE2	1.70	0.90
1:M:60:SER:HB3	1:M:65:GLU:OE1	1.72	0.90
1:P:88:ALA:HB3	1:P:104:MET:HE1	1.51	0.90
1:K:83:LEU:O	1:K:87:ARG:HG3	1.72	0.89
1:E:281:ARG:HG2	1:E:281:ARG:NH1	1.82	0.88
1:N:269:ARG:HB3	1:N:269:ARG:NH1	1.88	0.88
1:G:82:MET:HE2	1:G:112:MET:CG	2.05	0.87
1:G:158:LYS:HG3	1:G:180:LEU:HD12	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:219:VAL:HG12	1:I:291:GLU:HG3	1.55	0.86
1:I:274:THR:CG2	1:I:276:GLY:H	1.89	0.86
1:L:87:ARG:NH2	1:L:150:GLU:OE2	2.10	0.85
1:C:96:ASP:HB2	3:C:549:HOH:O	1.75	0.85
1:D:219:VAL:HG12	1:D:291:GLU:HG3	1.59	0.84
1:L:275:GLU:HB2	2:L:500:HEM:O1A	1.75	0.84
1:I:207:ARG:HH11	1:I:207:ARG:CG	1.88	0.84
1:I:274:THR:HB	2:I:500:HEM:O1A	1.77	0.84
1:N:138:GLY:C	1:N:140:SER:H	1.79	0.84
1:P:164:ARG:HG3	1:P:164:ARG:HH11	1.43	0.84
1:N:122:LEU:HD21	2:N:500:HEM:HAB	1.60	0.83
1:J:163:LEU:HD22	1:J:176:VAL:HG12	1.60	0.83
1:K:295:LEU:C	1:K:295:LEU:HD23	2.00	0.82
1:P:88:ALA:CB	1:P:104:MET:HE3	2.08	0.82
1:P:65:GLU:CG	1:P:133:MET:HE3	2.02	0.82
1:O:254:ARG:O	1:O:258:VAL:HG23	1.79	0.81
1:C:177:GLU:HG2	3:C:520:HOH:O	1.80	0.81
1:O:158:LYS:HG3	1:O:180:LEU:HD12	1.62	0.81
1:C:163:LEU:HD22	1:C:176:VAL:HG12	1.61	0.80
1:N:299:LEU:HG	1:N:299:LEU:OXT	1.80	0.80
1:G:134:ARG:HG3	1:G:135:PRO:HD3	1.62	0.80
1:L:51:GLN:HG3	3:L:530:HOH:O	1.82	0.79
1:O:89:ALA:HB3	1:O:185:MET:CE	2.12	0.79
1:C:110:ARG:HD3	3:C:582:HOH:O	1.82	0.79
1:E:79:MET:HE2	1:E:151:ILE:HD12	1.64	0.79
1:F:127:PRO:HG3	1:G:296:ARG:CD	2.13	0.79
1:P:88:ALA:HB1	1:P:104:MET:HE3	1.63	0.78
1:G:50:ASP:HB2	3:G:524:HOH:O	1.83	0.78
1:K:207:ARG:HG3	1:K:207:ARG:HH11	1.49	0.78
1:F:127:PRO:HG3	1:G:296:ARG:NE	1.99	0.77
1:J:52:ILE:HG22	1:J:53:LEU:HD13	1.67	0.77
1:G:139:ALA:HA	3:G:545:HOH:O	1.85	0.76
1:L:295:LEU:HD23	1:L:296:ARG:N	2.01	0.76
1:J:150:GLU:O	1:J:154:ILE:HG12	1.86	0.76
1:B:171:GLU:HG2	3:B:553:HOH:O	1.85	0.76
1:L:206:GLU:HG2	3:L:544:HOH:O	1.86	0.76
1:B:150:GLU:O	1:B:154:ILE:HG13	1.86	0.76
2:E:500:HEM:HBB2	2:E:500:HEM:HMB2	1.67	0.76
1:P:88:ALA:CB	1:P:104:MET:HE1	2.11	0.75
2:I:500:HEM:HMB2	2:I:500:HEM:HBB2	1.69	0.75
1:I:82:MET:HG3	1:I:108:VAL:HG13	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:MET:CE	1:E:151:ILE:HD12	2.16	0.75
1:D:146:TYR:O	1:D:150:GLU:HG3	1.85	0.74
1:M:219:VAL:HG12	1:M:291:GLU:HG3	1.68	0.74
1:L:295:LEU:C	1:L:295:LEU:HD23	2.07	0.74
1:P:166:HIS:HD2	3:P:579:HOH:O	1.71	0.74
1:I:122:LEU:HD21	2:I:500:HEM:HAB	1.70	0.74
2:P:500:HEM:HBB2	2:P:500:HEM:HMB2	1.68	0.73
1:H:150:GLU:O	1:H:154:ILE:HG13	1.87	0.73
1:M:53:LEU:HD21	1:N:147:GLN:NE2	2.03	0.73
1:I:219:VAL:CG1	1:I:291:GLU:HG3	2.17	0.73
1:I:274:THR:HG22	1:I:276:GLY:N	2.04	0.73
1:O:149:ARG:NH1	3:O:529:HOH:O	2.21	0.72
1:A:274:THR:HG21	1:A:279:TYR:CG	2.24	0.72
1:J:158:LYS:HG3	1:J:180:LEU:HD12	1.69	0.72
1:K:96:ASP:OD2	1:K:195:ARG:NH2	2.22	0.72
1:A:96:ASP:OD1	1:A:196:ARG:NH2	2.17	0.72
1:L:257:HIS:O	1:L:261:VAL:HG23	1.89	0.72
1:A:86:LEU:HD22	1:A:185:MET:HE1	1.71	0.72
1:K:295:LEU:O	1:K:295:LEU:HD23	1.89	0.71
3:A:507:HOH:O	1:D:256:ARG:HD2	1.90	0.71
1:A:274:THR:HB	2:A:500:HEM:O1A	1.91	0.71
1:E:267:PHE:HE2	1:E:281:ARG:HE	1.36	0.71
1:I:211:GLN:O	1:I:212:PRO:O	2.08	0.71
1:J:277:VAL:O	1:J:281:ARG:HG3	1.91	0.71
2:I:500:HEM:CMB	2:I:500:HEM:HBB2	2.21	0.71
1:D:192:LEU:O	1:D:192:LEU:HD12	1.92	0.70
1:F:267:PHE:HD2	1:F:268:LYS:H	1.37	0.70
1:G:134:ARG:HG3	1:G:135:PRO:CD	2.20	0.70
1:J:258:VAL:HG13	1:J:280:LEU:HB3	1.74	0.70
1:E:150:GLU:O	1:E:154:ILE:HG13	1.91	0.70
1:G:219:VAL:HG12	1:G:291:GLU:HG3	1.74	0.70
3:M:510:HOH:O	1:P:256:ARG:HD2	1.92	0.70
1:G:82:MET:HE1	1:G:112:MET:SD	2.31	0.70
1:P:149:ARG:HD2	1:P:162:MET:HB3	1.73	0.70
1:P:52:ILE:HG22	1:P:53:LEU:HD13	1.73	0.69
1:C:164:ARG:HG3	1:C:164:ARG:HH11	1.56	0.69
1:J:192:LEU:HD12	1:J:195:ARG:NH2	2.06	0.69
1:B:95:SER:OG	1:B:97:GLN:HG3	1.92	0.69
1:G:117:GLN:HG2	1:H:114:GLN:OE1	1.92	0.69
2:E:500:HEM:HBB2	2:E:500:HEM:CMB	2.22	0.69
1:M:42:SER:HB2	1:N:144:GLN:OE1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:PHE:O	1:J:254:ARG:HG3	1.92	0.69
1:G:169:ARG:HH21	1:G:171:GLU:HG3	1.57	0.69
1:C:290:PRO:HG3	3:C:580:HOH:O	1.91	0.69
1:N:269:ARG:HB3	1:N:269:ARG:HH11	1.56	0.69
1:N:295:LEU:HD23	1:N:295:LEU:C	2.13	0.69
1:G:219:VAL:CG1	1:G:291:GLU:HG3	2.23	0.69
2:H:500:HEM:HBB2	2:H:500:HEM:HMB2	1.75	0.69
1:A:274:THR:CG2	1:A:279:TYR:CB	2.71	0.68
1:N:138:GLY:C	1:N:140:SER:N	2.43	0.68
1:D:89:ALA:HB3	1:D:185:MET:CE	2.22	0.68
1:L:224:LEU:O	1:L:228:ARG:HG3	1.93	0.68
1:D:275:GLU:HB2	2:D:500:HEM:O1A	1.94	0.68
1:K:219:VAL:HG12	1:K:291:GLU:HG3	1.76	0.68
1:J:146:TYR:O	1:J:150:GLU:HG3	1.94	0.67
1:C:181:HIS:CE1	3:C:584:HOH:O	2.33	0.67
1:L:275:GLU:HB2	2:L:500:HEM:CGA	2.24	0.67
1:I:120:ASN:OD1	1:I:256:ARG:NH2	2.20	0.67
1:B:275:GLU:HG3	3:B:615:HOH:O	1.93	0.67
1:A:274:THR:HG21	1:A:279:TYR:CD2	2.30	0.67
1:J:163:LEU:CD2	1:J:176:VAL:HG12	2.25	0.67
1:P:65:GLU:CG	1:P:133:MET:CE	2.65	0.67
1:A:274:THR:HG21	1:A:279:TYR:CB	2.25	0.67
1:B:219:VAL:CG1	1:B:291:GLU:HG3	2.23	0.67
1:F:82:MET:HG3	1:F:108:VAL:HG13	1.77	0.67
1:B:134:ARG:N	1:B:135:PRO:HD2	2.11	0.66
1:L:58:PRO:HD2	3:L:581:HOH:O	1.94	0.66
1:D:133:MET:HE2	1:D:137:LEU:HD11	1.77	0.66
1:N:295:LEU:CD2	1:N:295:LEU:C	2.64	0.66
1:M:267:PHE:CE1	1:M:281:ARG:NH1	2.64	0.66
1:G:82:MET:CE	1:G:112:MET:CG	2.69	0.66
1:E:75:THR:O	1:E:79:MET:HG3	1.94	0.66
1:F:168:HIS:CD2	1:F:169:ARG:HG2	2.31	0.66
1:I:199:GLN:HG3	3:I:552:HOH:O	1.96	0.66
1:K:79:MET:CE	1:K:151:ILE:HD12	2.25	0.66
1:A:282:ARG:HH21	1:B:31:HIS:CD2	2.14	0.66
1:A:52:ILE:HG22	1:A:53:LEU:HD13	1.78	0.66
1:A:274:THR:CG2	1:A:275:GLU:N	2.58	0.66
1:K:79:MET:HE3	1:K:151:ILE:HD12	1.77	0.65
1:I:163:LEU:HD22	1:I:176:VAL:HG12	1.78	0.65
1:P:52:ILE:HG22	1:P:53:LEU:CD1	2.26	0.65
1:P:250:PHE:CE1	1:P:254:ARG:NH2	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:VAL:HG12	1:M:291:GLU:CG	2.27	0.65
1:F:49:LEU:O	1:F:53:LEU:HB2	1.96	0.65
1:A:274:THR:HG22	1:A:275:GLU:N	2.10	0.65
1:P:199:GLN:HG3	3:P:571:HOH:O	1.97	0.65
1:B:220:GLU:HG2	1:B:224:LEU:HD12	1.78	0.64
1:G:82:MET:CE	1:G:112:MET:SD	2.85	0.64
1:G:90:ARG:O	1:G:94:LYS:HG2	1.95	0.64
1:F:257:HIS:HE1	2:F:500:HEM:C4D	2.15	0.64
1:K:87:ARG:HD2	3:K:569:HOH:O	1.96	0.64
1:H:250:PHE:O	1:H:254:ARG:HG3	1.97	0.64
1:K:295:LEU:CD2	1:K:295:LEU:C	2.65	0.64
1:L:247:GLU:O	1:L:251:ARG:HG3	1.97	0.64
1:M:267:PHE:HE1	1:M:281:ARG:NH1	1.96	0.64
1:O:82:MET:HG3	1:O:108:VAL:HG13	1.79	0.64
1:E:295:LEU:HD12	1:E:295:LEU:C	2.17	0.64
1:E:134:ARG:HA	1:E:137:LEU:HD22	1.77	0.64
1:N:109:SER:CB	1:N:110:ARG:HH11	2.09	0.64
1:I:186:TYR:OH	1:I:291:GLU:HG2	1.97	0.64
1:B:164:ARG:HB3	1:B:165:PRO:HD3	1.80	0.64
1:A:68:PHE:HE1	2:A:500:HEM:HAB	1.63	0.64
1:J:295:LEU:C	1:J:295:LEU:HD23	2.18	0.64
1:D:126:THR:OG1	1:D:129:GLU:HG3	1.98	0.63
1:K:52:ILE:HD11	1:L:55:ALA:HB3	1.80	0.63
1:N:138:GLY:HA3	1:N:140:SER:OG	1.97	0.63
1:J:231:SER:HB2	3:J:540:HOH:O	1.97	0.63
1:M:166:HIS:HD2	3:M:582:HOH:O	1.81	0.63
2:L:500:HEM:HBC2	2:L:500:HEM:HHD	1.79	0.63
1:H:272:GLY:HA3	1:I:57:HIS:CD2	2.33	0.63
1:K:207:ARG:CG	1:K:207:ARG:HH11	2.11	0.63
1:A:146:TYR:HE2	3:A:597:HOH:O	1.80	0.63
1:P:166:HIS:HE1	3:P:558:HOH:O	1.81	0.63
1:O:178:THR:O	1:O:182:THR:OG1	2.17	0.62
1:O:219:VAL:HG12	1:O:291:GLU:HG3	1.81	0.62
1:L:273:GLY:HA3	1:N:41:MET:HE1	1.81	0.62
1:G:100:PRO:O	1:G:104:MET:HG3	1.98	0.62
1:A:68:PHE:CE1	2:A:500:HEM:HAB	2.33	0.62
1:G:281:ARG:NH2	3:G:520:HOH:O	2.33	0.62
1:L:200:ILE:HA	1:L:218:SER:OG	1.98	0.62
1:L:207:ARG:HG2	1:L:209:TRP:CZ3	2.35	0.62
1:B:248:ASP:O	1:B:252:GLN:HG3	1.99	0.62
1:O:257:HIS:O	1:O:261:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:HIS:HA	1:F:35:MET:HA	1.82	0.62
1:F:87:ARG:HD2	3:F:562:HOH:O	1.99	0.62
1:L:82:MET:HE1	1:L:115:LEU:HD12	1.82	0.62
1:C:295:LEU:HD23	1:C:295:LEU:O	2.00	0.62
1:B:49:LEU:O	1:B:53:LEU:HB2	2.00	0.62
1:E:99:GLN:HB2	1:E:100:PRO:HD3	1.82	0.61
1:P:292:LEU:O	1:P:296:ARG:NH1	2.32	0.61
1:M:149:ARG:CZ	1:M:162:MET:CE	2.78	0.61
1:M:141:SER:OG	1:M:143:PHE:HB2	2.00	0.61
1:C:164:ARG:CG	1:C:164:ARG:HH11	2.14	0.61
1:M:219:VAL:CG1	1:M:291:GLU:HG3	2.29	0.61
1:L:219:VAL:HG12	1:L:291:GLU:HG3	1.81	0.61
1:N:109:SER:CB	1:N:110:ARG:HH12	1.95	0.61
1:F:164:ARG:N	1:F:165:PRO:HD2	2.16	0.61
1:L:220:GLU:OE2	1:L:298:ASP:OD2	2.18	0.61
1:A:163:LEU:HD22	1:A:176:VAL:HG12	1.81	0.61
1:C:295:LEU:C	1:C:295:LEU:HD23	2.21	0.60
1:J:75:THR:O	1:J:79:MET:HG3	2.01	0.60
1:H:158:LYS:HG3	1:H:180:LEU:HD12	1.83	0.60
1:P:49:LEU:O	1:P:53:LEU:HB2	2.01	0.60
1:J:39:ARG:HA	3:J:541:HOH:O	2.01	0.60
1:J:186:TYR:OH	1:J:291:GLU:HG2	2.01	0.60
1:F:150:GLU:O	1:F:154:ILE:HG13	2.01	0.60
1:M:149:ARG:CZ	1:M:162:MET:HE3	2.31	0.60
1:H:134:ARG:HG2	1:H:135:PRO:HD3	1.83	0.60
2:K:500:HEM:HHD	2:K:500:HEM:HBC2	1.83	0.60
1:O:119:TRP:CH2	1:O:257:HIS:HD2	2.20	0.60
1:C:146:TYR:O	1:C:150:GLU:HG3	2.01	0.60
1:C:275:GLU:N	1:C:275:GLU:OE2	2.35	0.60
1:N:269:ARG:CB	1:N:269:ARG:HH11	2.15	0.60
1:F:83:LEU:O	1:F:87:ARG:HG3	2.02	0.60
1:E:219:VAL:CG1	1:E:291:GLU:HG3	2.32	0.60
1:K:163:LEU:HD22	1:K:176:VAL:HG12	1.84	0.60
1:L:90:ARG:HB3	3:L:534:HOH:O	2.01	0.60
1:K:258:VAL:HG13	1:K:280:LEU:CB	2.32	0.60
1:J:222:ALA:O	1:J:226:VAL:HG23	2.02	0.60
1:B:146:TYR:O	1:B:150:GLU:HG3	2.01	0.60
1:D:274:THR:HG21	3:E:550:HOH:O	2.01	0.60
1:C:150:GLU:O	1:C:154:ILE:HG13	2.02	0.60
1:O:114:GLN:OE1	1:P:117:GLN:HG2	2.02	0.60
1:P:122:LEU:HD21	2:P:500:HEM:HAB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:MET:HE1	1:K:148:TYR:HD1	1.67	0.59
1:L:270:GLY:HA3	1:N:50:ASP:HB2	1.84	0.59
1:P:126:THR:OG1	1:P:129:GLU:HG3	2.01	0.59
1:C:77:LEU:HD12	1:D:77:LEU:HD12	1.84	0.59
1:F:127:PRO:HG3	1:G:296:ARG:HD2	1.84	0.59
2:P:500:HEM:HBB2	2:P:500:HEM:CMB	2.31	0.59
1:P:89:ALA:O	1:P:93:VAL:HG23	2.03	0.59
1:N:109:SER:HB2	1:N:110:ARG:HH11	1.67	0.59
1:A:261:VAL:HG22	2:A:500:HEM:C1B	2.37	0.59
1:G:120:ASN:OD1	1:G:256:ARG:NH2	2.26	0.59
1:G:151:ILE:O	1:G:154:ILE:HG22	2.02	0.59
1:L:186:TYR:O	1:L:190:ILE:HG13	2.02	0.59
1:I:89:ALA:O	1:I:93:VAL:HG23	2.03	0.59
1:D:219:VAL:CG1	1:D:291:GLU:HG3	2.29	0.59
1:C:141:SER:OG	1:C:143:PHE:HB2	2.02	0.59
1:K:75:THR:O	1:K:79:MET:HG3	2.03	0.58
1:D:89:ALA:HB3	1:D:185:MET:HE1	1.85	0.58
1:J:295:LEU:HD23	1:J:295:LEU:O	2.03	0.58
1:O:49:LEU:O	1:O:53:LEU:HB2	2.01	0.58
1:E:183:PRO:HG2	3:E:502:HOH:O	2.03	0.58
1:B:99:GLN:HB2	1:B:100:PRO:HD3	1.84	0.58
2:O:500:HEM:HBB2	2:O:500:HEM:CMB	2.34	0.58
1:E:100:PRO:O	1:E:104:MET:HG3	2.04	0.58
1:K:214:GLN:HG2	3:K:553:HOH:O	2.04	0.58
1:K:119:TRP:CD1	1:K:256:ARG:HG2	2.39	0.58
1:J:190:ILE:HG21	1:J:204:VAL:CG1	2.34	0.58
1:L:163:LEU:HD23	1:L:176:VAL:HG12	1.85	0.58
1:C:49:LEU:O	1:C:53:LEU:HB2	2.03	0.58
1:A:282:ARG:HH21	1:B:31:HIS:HD2	1.52	0.58
1:D:141:SER:OG	1:D:143:PHE:HB2	2.04	0.58
1:O:295:LEU:HD23	1:O:295:LEU:C	2.24	0.58
1:P:166:HIS:CE1	3:P:558:HOH:O	2.55	0.58
1:I:52:ILE:HG22	1:I:53:LEU:HD13	1.85	0.58
1:L:274:THR:HG22	1:L:275:GLU:OE2	2.04	0.57
1:A:212:PRO:HB2	3:A:586:HOH:O	2.04	0.57
1:N:163:LEU:HD22	1:N:176:VAL:HG12	1.85	0.57
1:E:79:MET:CE	1:E:151:ILE:CD1	2.82	0.57
1:D:103:LYS:HG2	3:D:520:HOH:O	2.04	0.57
1:E:143:PHE:HE2	1:E:279:TYR:HH	1.53	0.57
1:G:283:MET:CE	1:G:283:MET:CA	2.77	0.57
1:G:99:GLN:HB2	1:G:100:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:TYR:HB3	1:J:144:GLN:HB2	1.86	0.57
1:I:109:SER:HB3	1:I:110:ARG:HH21	1.68	0.57
1:N:158[A]:LYS:NZ	1:N:209:TRP:O	2.37	0.57
1:K:222:ALA:O	1:K:226:VAL:HG23	2.04	0.57
1:L:167:ALA:HA	1:L:173:LEU:HD22	1.86	0.57
1:O:224:LEU:O	1:O:228:ARG:HG3	2.05	0.57
1:B:296:ARG:HD3	1:C:127:PRO:HG3	1.86	0.57
1:L:95:SER:HB3	1:L:97:GLN:HG3	1.86	0.57
1:N:292:LEU:HA	1:N:295:LEU:HD13	1.87	0.57
1:J:258:VAL:HG13	1:J:280:LEU:CB	2.35	0.57
1:P:250:PHE:CD1	1:P:254:ARG:NH2	2.72	0.57
1:E:219:VAL:HG12	1:E:291:GLU:HG3	1.87	0.57
1:K:258:VAL:HG13	1:K:280:LEU:HB3	1.87	0.57
1:K:50:ASP:HB2	3:K:563:HOH:O	2.05	0.57
1:D:192:LEU:C	1:D:192:LEU:HD12	2.26	0.57
1:F:146:TYR:O	1:F:150:GLU:HG3	2.05	0.57
1:H:248:ASP:O	1:H:252:GLN:HG3	2.05	0.57
1:A:216:ASN:OD1	1:A:219:VAL:HG23	2.04	0.57
1:O:188:GLU:OE2	3:O:516:HOH:O	2.17	0.56
1:I:82:MET:CG	1:I:108:VAL:HG13	2.35	0.56
1:L:282:ARG:HD2	1:N:41:MET:HE3	1.85	0.56
1:L:268:LYS:HG3	3:L:573:HOH:O	2.05	0.56
1:I:140:SER:O	1:I:271:THR:OG1	2.22	0.56
1:O:279:TYR:HD2	1:O:280:LEU:HD23	1.70	0.56
1:O:52:ILE:HD11	1:P:55:ALA:HB3	1.87	0.56
1:O:50:ASP:OD1	1:P:169:ARG:NH2	2.38	0.56
1:G:127:PRO:HB2	1:G:128:PRO:HD3	1.87	0.56
1:J:267:PHE:CE1	1:J:281:ARG:HD2	2.41	0.56
1:D:90:ARG:HB2	1:D:185:MET:HG3	1.87	0.56
1:P:146:TYR:O	1:P:150:GLU:HG3	2.05	0.56
1:J:207:ARG:HG3	1:J:208:ASP:N	2.21	0.56
1:B:163:LEU:HD23	1:B:176:VAL:HG12	1.88	0.56
1:G:186:TYR:OH	1:G:291:GLU:HG2	2.06	0.55
1:J:201:ASP:HB3	1:J:203:GLU:HG2	1.88	0.55
1:I:207:ARG:CG	1:I:207:ARG:NH1	2.57	0.55
2:O:500:HEM:HBB2	2:O:500:HEM:HMB2	1.88	0.55
1:F:216:ASN:OD1	1:F:218:SER:HB3	2.05	0.55
1:I:207:ARG:HG3	1:I:207:ARG:NH1	2.01	0.55
1:H:191:ARG:HG2	1:H:205:VAL:HG13	1.88	0.55
1:G:68:PHE:CB	1:G:133:MET:HE1	2.36	0.55
1:F:267:PHE:HD2	1:F:268:LYS:N	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:ALA:HB3	1:O:185:MET:HE2	1.86	0.55
1:J:192:LEU:HD12	1:J:195:ARG:HH21	1.71	0.55
2:L:500:HEM:CBC	2:L:500:HEM:HHD	2.36	0.55
1:I:168:HIS:CE1	1:I:169:ARG:HG2	2.41	0.55
2:G:500:HEM:HHD	2:G:500:HEM:HBC2	1.89	0.55
1:I:279:TYR:CE1	1:I:283:MET:CE	2.90	0.55
1:O:167:ALA:HA	1:O:173:LEU:HD22	1.89	0.55
1:H:49:LEU:O	1:H:53:LEU:HB2	2.07	0.55
1:N:109:SER:HB2	1:N:110:ARG:NH1	2.17	0.55
1:E:79:MET:HE3	1:E:151:ILE:CD1	2.37	0.55
1:I:290:PRO:HG3	3:I:577:HOH:O	2.06	0.55
1:A:146:TYR:HD2	3:A:595:HOH:O	1.90	0.54
1:C:192:LEU:O	1:C:196:ARG:HG3	2.06	0.54
1:E:256:ARG:HD2	3:H:502:HOH:O	2.06	0.54
1:N:293:TRP:CZ3	1:O:263:ARG:HB3	2.42	0.54
1:M:282:ARG:NH2	3:M:536:HOH:O	2.40	0.54
1:D:200:ILE:HG22	1:D:205:VAL:HG23	1.88	0.54
1:I:149:ARG:CZ	1:I:162:MET:CE	2.85	0.54
1:I:266:GLY:HA3	1:L:297:THR:HG22	1.90	0.54
1:I:149:ARG:CZ	1:I:162:MET:HE3	2.37	0.54
1:A:274:THR:CG2	1:A:279:TYR:HB2	2.38	0.54
1:L:219:VAL:CG1	1:L:291:GLU:HG3	2.38	0.54
1:I:211:GLN:C	1:I:212:PRO:O	2.44	0.54
1:L:295:LEU:CD2	1:L:296:ARG:N	2.70	0.54
1:G:59:LEU:HD23	1:G:136:TYR:O	2.07	0.54
1:G:223:TRP:HB3	1:G:295:LEU:HD12	1.90	0.54
1:K:261:VAL:HG22	2:K:500:HEM:C2B	2.43	0.54
1:M:247:GLU:HG3	1:M:288:LEU:HD12	1.90	0.54
1:I:250:PHE:O	1:I:254:ARG:CD	2.56	0.54
1:N:131:SER:HB2	1:O:299:LEU:HD23	1.90	0.54
1:F:172:HIS:O	1:F:176:VAL:HG23	2.08	0.53
1:G:254:ARG:NH1	3:G:537:HOH:O	2.41	0.53
1:H:126:THR:OG1	1:H:129:GLU:HG3	2.07	0.53
1:A:275:GLU:HB2	3:A:572:HOH:O	2.06	0.53
1:I:254:ARG:HB2	3:I:521:HOH:O	2.07	0.53
1:N:192:LEU:HD13	1:N:195:ARG:NH2	2.23	0.53
1:I:122:LEU:HD21	2:I:500:HEM:CAB	2.35	0.53
1:B:262:GLU:OE1	1:B:281:ARG:NH2	2.40	0.53
1:M:267:PHE:HE1	1:M:281:ARG:HH11	1.54	0.53
1:C:275:GLU:OE2	1:C:275:GLU:CA	2.57	0.53
1:K:114:GLN:OE1	1:L:117:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:C	1:C:295:LEU:CD2	2.77	0.53
1:L:291:GLU:O	1:L:295:LEU:HB3	2.09	0.53
1:O:159:ASN:OD1	1:O:162:MET:HG2	2.09	0.53
1:G:148:TYR:CE1	1:G:250:PHE:HZ	2.26	0.53
1:A:119:TRP:CH2	1:A:257:HIS:HD2	2.27	0.53
1:M:99:GLN:HB2	1:M:100:PRO:HD3	1.91	0.53
1:G:279:TYR:O	1:G:282:ARG:HB2	2.08	0.53
1:O:223:TRP:HB3	1:O:295:LEU:HD12	1.91	0.53
1:E:266:GLY:HA3	1:H:297:THR:HG22	1.90	0.53
1:D:272:GLY:HA3	3:D:589:HOH:O	2.08	0.53
1:P:83:LEU:HD21	1:P:150:GLU:HB2	1.92	0.52
1:F:110:ARG:CD	3:F:534:HOH:O	2.56	0.52
1:D:150:GLU:O	1:D:154:ILE:HG13	2.09	0.52
1:K:127:PRO:N	1:K:128:PRO:HD2	2.24	0.52
1:O:186:TYR:OH	1:O:291:GLU:HG2	2.10	0.52
1:K:39:ARG:HH11	1:K:39:ARG:HA	1.73	0.52
1:L:195:ARG:NH1	3:L:548:HOH:O	2.42	0.52
1:I:76:GLU:HA	1:I:79:MET:HE2	1.90	0.52
1:C:75:THR:O	1:C:79:MET:HG3	2.09	0.52
1:F:158:LYS:HG3	1:F:180:LEU:HD12	1.91	0.52
1:P:164:ARG:NH1	1:P:164:ARG:HG3	2.19	0.52
1:I:267:PHE:H	1:L:297:THR:CG2	2.23	0.52
1:L:273:GLY:HA3	1:N:41:MET:CE	2.39	0.52
1:L:75:THR:HG23	1:L:115:LEU:HD22	1.91	0.52
1:N:146:TYR:O	1:N:150:GLU:HG3	2.09	0.52
1:E:163:LEU:HD23	1:E:176:VAL:HG12	1.92	0.52
1:J:163:LEU:HD22	1:J:176:VAL:CG1	2.35	0.52
1:F:127:PRO:N	1:F:128:PRO:HD2	2.25	0.52
2:H:500:HEM:CMB	2:H:500:HEM:HBB2	2.39	0.52
1:B:296:ARG:HD3	1:C:127:PRO:CG	2.40	0.52
1:I:114:GLN:OE1	1:J:117:GLN:HG2	2.10	0.52
1:I:163:LEU:CD2	1:I:176:VAL:HG12	2.40	0.52
1:F:254:ARG:HD2	3:F:506:HOH:O	2.10	0.52
1:H:99:GLN:HB2	1:H:100:PRO:HD3	1.91	0.52
1:L:64:ASN:HA	3:L:529:HOH:O	2.09	0.52
1:O:169:ARG:HH21	1:O:172:HIS:CE1	2.28	0.51
1:L:295:LEU:CD2	1:L:295:LEU:C	2.77	0.51
1:N:292:LEU:O	1:N:296:ARG:NH1	2.41	0.51
1:K:261:VAL:HG22	2:K:500:HEM:C1B	2.44	0.51
1:N:269:ARG:HB3	1:N:269:ARG:CZ	2.40	0.51
1:P:65:GLU:HA	1:P:133:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:MET:HG3	1:J:111:ILE:HG21	1.92	0.51
1:I:90:ARG:O	1:I:94:LYS:HG3	2.10	0.51
1:H:275:GLU:HG2	3:H:595:HOH:O	2.10	0.51
1:E:267:PHE:CE2	1:E:281:ARG:NE	2.77	0.51
1:E:261:VAL:HG22	2:E:500:HEM:C1B	2.45	0.51
1:I:275:GLU:HB3	1:I:278:SER:OG	2.10	0.51
1:A:146:TYR:O	1:A:150:GLU:HG3	2.11	0.51
1:M:281:ARG:O	1:M:284:LEU:HB2	2.10	0.51
1:M:261:VAL:HG22	2:M:500:HEM:C1B	2.46	0.51
1:C:99:GLN:HB2	1:C:100:PRO:HD3	1.92	0.51
1:H:168:HIS:H	1:H:168:HIS:CD2	2.29	0.51
1:I:223:TRP:CD2	1:I:292:LEU:HD21	2.46	0.51
1:M:168:HIS:CE1	1:M:169:ARG:HG2	2.47	0.51
1:E:215:TYR:CE1	1:E:294:LYS:HD3	2.46	0.51
1:N:99:GLN:HB2	1:N:100:PRO:HD3	1.92	0.51
1:G:226:VAL:HG13	1:G:233:HIS:HB2	1.93	0.51
1:G:158:LYS:CG	1:G:180:LEU:HD12	2.36	0.50
1:O:89:ALA:CB	1:O:185:MET:HE2	2.40	0.50
1:F:152:GLU:OE2	1:F:254:ARG:NH1	2.41	0.50
1:N:119:TRP:CH2	1:N:257:HIS:HD2	2.29	0.50
1:P:119:TRP:CH2	1:P:257:HIS:CD2	3.00	0.50
1:L:188:GLU:HA	1:L:188:GLU:OE2	2.12	0.50
1:N:295:LEU:HD23	1:N:295:LEU:O	2.10	0.50
1:O:163:LEU:HD22	1:O:173:LEU:CD1	2.41	0.50
1:D:269:ARG:NH1	1:F:45:ASP:OD1	2.45	0.50
1:F:258:VAL:HG21	1:F:281:ARG:HG2	1.93	0.50
1:C:164:ARG:HB2	1:C:164:ARG:CZ	2.41	0.50
1:F:200:ILE:HG22	1:F:204:VAL:HG23	1.92	0.50
1:I:279:TYR:CE1	1:I:283:MET:HE3	2.45	0.50
1:I:49:LEU:HB3	1:I:53:LEU:HD22	1.94	0.50
1:G:257:HIS:HE1	2:G:500:HEM:C4D	2.29	0.50
1:H:65:GLU:HG3	1:H:133:MET:CE	2.41	0.50
1:M:261:VAL:HG22	2:M:500:HEM:C2B	2.47	0.50
1:G:131:SER:HA	1:G:134:ARG:HG2	1.93	0.50
1:I:250:PHE:O	1:I:254:ARG:HD2	2.11	0.50
1:F:163:LEU:CD2	1:F:176:VAL:HG12	2.41	0.50
1:O:247:GLU:OE1	1:O:293:TRP:NE1	2.40	0.50
1:P:149:ARG:HD2	1:P:162:MET:CB	2.42	0.50
1:P:119:TRP:CH2	1:P:257:HIS:HD2	2.30	0.50
1:G:134:ARG:N	1:G:135:PRO:HD2	2.27	0.50
1:N:247:GLU:CD	1:N:293:TRP:HE1	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:119:TRP:CH2	1:N:257:HIS:CD2	3.00	0.49
1:D:274:THR:HG22	1:D:275:GLU:OE2	2.13	0.49
1:B:267:PHE:CE1	1:B:281:ARG:CD	2.95	0.49
1:F:174:GLU:HG2	1:F:175:LEU:N	2.27	0.49
1:F:161:ALA:O	1:F:164:ARG:HG2	2.12	0.49
1:F:158:LYS:HG2	1:F:209:TRP:O	2.12	0.49
1:A:165:PRO:HA	1:B:35:MET:O	2.13	0.49
1:A:282:ARG:HG2	3:A:623:HOH:O	2.12	0.49
1:D:163:LEU:HD23	1:D:176:VAL:HG12	1.95	0.49
1:G:202:PRO:HD2	3:G:540:HOH:O	2.13	0.49
1:K:120:ASN:OD1	1:K:256:ARG:NH1	2.31	0.49
1:E:143:PHE:HE2	1:E:279:TYR:CZ	2.31	0.49
1:G:247:GLU:OE1	1:G:293:TRP:NE1	2.45	0.49
1:G:68:PHE:HB3	1:G:133:MET:HE1	1.94	0.49
1:F:153:PHE:O	1:F:158:LYS:HE3	2.13	0.49
1:K:134:ARG:HA	1:K:137:LEU:HG	1.95	0.49
1:A:269:ARG:NH1	1:A:275:GLU:OE2	2.46	0.49
1:O:158:LYS:O	1:O:212:PRO:HG3	2.12	0.49
1:A:76:GLU:HA	1:A:79:MET:HE2	1.94	0.49
1:K:247:GLU:O	1:K:251:ARG:HG3	2.12	0.49
1:E:119:TRP:CH2	1:E:257:HIS:CD2	3.01	0.49
2:I:500:HEM:HBC2	2:I:500:HEM:HHD	1.95	0.48
1:L:272:GLY:HA3	1:M:57:HIS:CD2	2.48	0.48
1:K:49:LEU:O	1:K:53:LEU:HB2	2.13	0.48
1:C:83:LEU:O	1:C:87:ARG:HG3	2.13	0.48
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.38	0.48
1:C:223:TRP:HB3	1:C:295:LEU:HD12	1.95	0.48
1:N:158[A]:LYS:HD2	1:N:180:LEU:HD12	1.94	0.48
1:O:171:GLU:CD	1:O:171:GLU:H	2.16	0.48
1:B:99:GLN:HB3	1:D:234:TRP:NE1	2.28	0.48
1:P:158:LYS:HD2	1:P:180:LEU:HD12	1.94	0.48
1:B:257:HIS:O	1:B:261:VAL:HG23	2.13	0.48
1:L:202:PRO:HD2	3:L:547:HOH:O	2.13	0.48
1:E:267:PHE:CZ	1:E:281:ARG:HD2	2.47	0.48
1:L:190:ILE:HG21	1:L:204:VAL:HG13	1.95	0.48
1:M:219:VAL:CG1	1:M:291:GLU:CG	2.89	0.48
1:A:282:ARG:NH2	1:B:31:HIS:HD2	2.11	0.48
1:C:227:TYR:O	1:C:230:PRO:HD3	2.14	0.48
1:O:39:ARG:O	1:P:138:GLY:HA3	2.13	0.48
1:P:88:ALA:HB1	1:P:104:MET:CE	2.29	0.48
1:K:57:HIS:CD2	3:K:570:HOH:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:ALA:HB3	1:O:185:MET:HE1	1.92	0.48
2:E:500:HEM:CBB	2:E:500:HEM:HMB2	2.41	0.48
1:J:39:ARG:NH1	3:J:556:HOH:O	2.46	0.48
1:L:76:GLU:HA	1:L:79:MET:HE2	1.96	0.48
1:G:54:SER:HA	3:G:551:HOH:O	2.14	0.48
1:N:188:GLU:OE2	1:N:188:GLU:HA	2.14	0.48
1:G:223:TRP:HB3	1:G:295:LEU:CD1	2.44	0.48
1:E:295:LEU:HD12	1:E:295:LEU:O	2.12	0.48
1:I:49:LEU:O	1:I:53:LEU:HB2	2.13	0.48
1:O:195:ARG:NH2	3:O:516:HOH:O	2.47	0.48
1:O:117:GLN:HB3	1:P:114:GLN:OE1	2.13	0.48
1:E:69:ILE:O	1:E:73:GLN:HG3	2.14	0.48
1:E:261:VAL:HG22	2:E:500:HEM:C2B	2.49	0.48
1:C:220:GLU:OE2	1:C:298:ASP:OD2	2.32	0.48
1:H:122:LEU:HD23	1:H:260:THR:HG21	1.96	0.48
1:O:86:LEU:O	1:O:185:MET:HE3	2.14	0.48
1:I:120:ASN:CG	1:I:256:ARG:HH22	2.14	0.48
2:I:500:HEM:CBB	2:I:500:HEM:HMB2	2.40	0.47
1:L:68:PHE:HB2	1:L:133:MET:HE1	1.96	0.47
1:I:142:GLY:HA3	2:I:500:HEM:C1D	2.48	0.47
1:O:223:TRP:HB3	1:O:295:LEU:CD1	2.44	0.47
1:C:62:ASP:OD1	1:C:64:ASN:HB2	2.14	0.47
1:I:117:GLN:HB2	3:I:547:HOH:O	2.13	0.47
1:L:246:LEU:HD13	3:L:579:HOH:O	2.14	0.47
1:L:158:LYS:NZ	1:L:182:THR:O	2.33	0.47
1:P:48:GLY:HA2	3:P:568:HOH:O	2.14	0.47
1:D:171:GLU:HG2	3:D:600:HOH:O	2.14	0.47
1:E:281:ARG:NH1	1:E:281:ARG:CG	2.62	0.47
1:O:275:GLU:HA	1:O:279:TYR:HB2	1.96	0.47
1:I:279:TYR:CE1	1:I:283:MET:HE2	2.48	0.47
1:M:96:ASP:HB3	3:M:594:HOH:O	2.13	0.47
1:L:158:LYS:HG3	1:L:180:LEU:HD12	1.96	0.47
1:I:267:PHE:H	1:L:297:THR:HG22	1.80	0.47
1:K:39:ARG:O	1:L:139:ALA:HB2	2.14	0.47
1:P:224:LEU:O	1:P:228:ARG:HG3	2.15	0.47
1:F:215:TYR:CD2	1:F:215:TYR:C	2.87	0.47
1:B:186:TYR:OH	1:B:291:GLU:HG2	2.15	0.47
1:C:164:ARG:NH1	1:C:164:ARG:CG	2.76	0.47
1:N:293:TRP:O	1:N:296:ARG:HB2	2.14	0.47
1:M:149:ARG:CZ	1:M:162:MET:HE2	2.44	0.47
1:K:258:VAL:HG13	1:K:280:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HD3	3:B:580:HOH:O	2.14	0.47
1:D:134:ARG:HB3	1:D:135:PRO:HD3	1.97	0.47
1:L:127:PRO:HB2	1:L:128:PRO:CD	2.45	0.47
1:P:70:VAL:O	1:P:74:THR:HG23	2.15	0.47
1:D:78:TRP:HB2	1:D:115:LEU:HD21	1.96	0.47
1:A:274:THR:CG2	1:A:279:TYR:HB3	2.44	0.47
1:J:203:GLU:HB3	3:J:544:HOH:O	2.15	0.47
1:I:149:ARG:NH2	1:I:162:MET:HE2	2.30	0.47
1:J:292:LEU:O	1:J:296:ARG:NH1	2.46	0.47
1:O:96:ASP:HB2	3:O:507:HOH:O	2.14	0.47
1:G:170:PRO:O	1:G:174:GLU:HB2	2.15	0.47
1:G:103:LYS:NZ	3:G:534:HOH:O	2.40	0.47
1:D:215:TYR:OH	1:D:220:GLU:OE1	2.21	0.47
1:N:52:ILE:HG22	1:N:53:LEU:HD13	1.96	0.47
1:O:67:LEU:O	1:O:67:LEU:HD12	2.14	0.47
1:O:119:TRP:CH2	1:O:257:HIS:CD2	3.01	0.47
1:M:260:THR:O	1:M:263:ARG:HB2	2.15	0.47
1:N:182:THR:HG22	3:N:532:HOH:O	2.15	0.47
1:L:274:THR:HB	1:M:57:HIS:HB3	1.97	0.46
1:C:164:ARG:NH1	1:C:164:ARG:HB2	2.30	0.46
1:D:133:MET:CE	1:D:137:LEU:HD11	2.42	0.46
1:O:134:ARG:N	1:O:135:PRO:HD2	2.30	0.46
1:G:220:GLU:OE2	1:G:298:ASP:OD2	2.32	0.46
1:A:86:LEU:CD2	1:A:185:MET:HE1	2.43	0.46
1:B:295:LEU:C	1:B:295:LEU:CD2	2.84	0.46
1:H:112:MET:O	1:H:116:VAL:HG23	2.16	0.46
1:F:267:PHE:CZ	1:F:281:ARG:HD2	2.51	0.46
2:D:500:HEM:HHD	2:D:500:HEM:HBC2	1.96	0.46
1:O:134:ARG:HB3	1:O:135:PRO:CD	2.45	0.46
1:M:212:PRO:HB3	3:M:588:HOH:O	2.15	0.46
1:G:49:LEU:O	1:G:53:LEU:HB2	2.15	0.46
1:P:277:VAL:O	1:P:281:ARG:HG3	2.15	0.46
1:B:130:TYR:CE1	1:B:134:ARG:HG3	2.50	0.46
1:E:141:SER:HA	3:E:554:HOH:O	2.15	0.46
1:E:280:LEU:HD11	2:E:500:HEM:C2A	2.51	0.46
1:L:82:MET:HE1	1:L:115:LEU:CD1	2.45	0.46
1:F:296:ARG:HD3	1:G:127:PRO:HG3	1.98	0.46
1:F:200:ILE:HA	1:F:218:SER:OG	2.14	0.46
1:I:149:ARG:HD3	1:I:149:ARG:HA	1.72	0.46
1:L:52:ILE:HG22	1:L:53:LEU:HD13	1.98	0.46
1:D:241:GLU:OE2	1:D:296:ARG:NH2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:40:ASP:O	1:O:40:ASP:CG	2.53	0.46
1:P:59:LEU:HA	1:P:59:LEU:HD12	1.68	0.46
1:I:168:HIS:CD2	3:I:551:HOH:O	2.69	0.46
1:E:120:ASN:OD1	1:E:256:ARG:NH2	2.35	0.46
1:M:100:PRO:O	1:M:104:MET:HG3	2.15	0.46
1:G:294:LYS:NZ	1:G:294:LYS:HB3	2.29	0.46
1:J:207:ARG:CG	1:J:208:ASP:N	2.77	0.46
1:A:183:PRO:HG3	1:A:209:TRP:CE2	2.51	0.46
1:A:274:THR:HG21	1:A:279:TYR:HB3	1.96	0.46
1:J:295:LEU:CD2	1:J:295:LEU:C	2.84	0.46
1:F:164:ARG:HB2	1:F:165:PRO:HD3	1.96	0.46
1:I:42:SER:HB2	1:J:144:GLN:OE1	2.16	0.46
1:B:103:LYS:HG2	3:B:533:HOH:O	2.16	0.46
1:I:129:GLU:OE2	1:J:103:LYS:NZ	2.37	0.46
1:D:93:VAL:HG13	1:D:192:LEU:HD23	1.97	0.46
2:K:500:HEM:HBB2	2:K:500:HEM:CMB	2.46	0.46
2:O:500:HEM:HHD	2:O:500:HEM:HBC2	1.97	0.46
1:I:149:ARG:NH2	1:I:162:MET:CE	2.79	0.46
1:J:104:MET:O	1:J:108:VAL:HG23	2.15	0.46
1:J:134:ARG:N	1:J:135:PRO:CD	2.78	0.46
1:L:223:TRP:HB3	1:L:295:LEU:HD12	1.97	0.45
1:B:127:PRO:N	1:B:128:PRO:HD2	2.30	0.45
1:I:215:TYR:OH	1:I:220:GLU:OE1	2.22	0.45
1:G:192:LEU:HD13	1:G:195:ARG:NH2	2.31	0.45
1:N:193:MET:O	1:N:198:PHE:HD1	1.98	0.45
1:L:186:TYR:OH	1:L:291:GLU:HG2	2.17	0.45
1:E:261:VAL:HG12	1:E:277:VAL:CG2	2.46	0.45
1:K:41:MET:O	1:L:139:ALA:HB3	2.16	0.45
1:A:149:ARG:HD3	1:A:149:ARG:HA	1.59	0.45
1:G:190:ILE:HG21	1:G:204:VAL:HG13	1.98	0.45
1:J:247:GLU:O	1:J:251:ARG:HG3	2.16	0.45
1:B:191:ARG:NH2	1:B:206:GLU:OE2	2.49	0.45
1:F:127:PRO:CD	1:F:128:PRO:HD2	2.46	0.45
1:B:267:PHE:HE1	1:B:281:ARG:CD	2.29	0.45
1:L:158:LYS:CG	1:L:180:LEU:HD12	2.47	0.45
1:A:43:TYR:CE1	1:B:145:SER:HB2	2.51	0.45
1:I:161:ALA:O	1:I:164:ARG:HG3	2.16	0.45
1:O:169:ARG:CD	1:O:171:GLU:OE2	2.55	0.45
1:J:257:HIS:HE1	2:J:500:HEM:C4D	2.34	0.45
1:F:277:VAL:O	1:F:281:ARG:HG3	2.16	0.45
1:P:83:LEU:O	1:P:87:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:192:LEU:HD12	1:N:192:LEU:O	2.16	0.45
1:G:148:TYR:CE1	1:G:250:PHE:CZ	3.04	0.45
1:F:198:PHE:HA	3:F:552:HOH:O	2.17	0.45
1:F:142:GLY:C	1:F:144:GLN:H	2.20	0.45
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.87	0.45
1:E:119:TRP:CH2	1:E:257:HIS:HD2	2.35	0.45
1:H:163:LEU:HD22	1:H:176:VAL:HG12	1.98	0.45
1:C:261:VAL:HG22	2:C:500:HEM:C1B	2.52	0.45
1:G:149:ARG:HA	1:G:149:ARG:HD3	1.70	0.45
1:L:292:LEU:HA	1:L:292:LEU:HD23	1.68	0.45
1:A:274:THR:CG2	1:A:275:GLU:H	2.30	0.45
1:K:79:MET:CE	1:K:148:TYR:HA	2.47	0.45
1:J:201:ASP:O	1:J:205:VAL:HG23	2.17	0.45
1:G:209:TRP:C	1:G:211:GLN:H	2.19	0.45
1:J:211:GLN:NE2	1:J:212:PRO:HD2	2.32	0.45
1:G:77:LEU:HA	1:G:77:LEU:HD23	1.58	0.45
1:E:260:THR:HA	1:E:263:ARG:HG2	1.99	0.45
1:B:186:TYR:HH	1:B:291:GLU:HG2	1.82	0.45
1:P:164:ARG:CG	1:P:164:ARG:HH11	2.20	0.45
1:F:78:TRP:HB2	1:F:115:LEU:HD21	1.99	0.45
1:B:90:ARG:HB2	1:B:185:MET:HE2	1.99	0.45
1:E:248:ASP:C	1:E:248:ASP:OD1	2.56	0.45
1:D:260:THR:HA	1:D:263:ARG:HG2	1.99	0.45
1:M:234:TRP:O	1:M:237:TYR:HB3	2.17	0.45
1:P:142:GLY:HA3	2:P:500:HEM:C2D	2.52	0.45
1:M:52:ILE:HG22	1:M:53:LEU:HD13	1.98	0.45
1:F:104:MET:O	1:F:108:VAL:HG23	2.17	0.45
1:I:250:PHE:O	1:I:254:ARG:HD3	2.16	0.45
1:D:59:LEU:HB3	1:D:136:TYR:HB3	1.98	0.45
1:L:295:LEU:HD22	1:L:296:ARG:HD2	1.99	0.44
1:B:230:PRO:HB3	1:B:237:TYR:CD2	2.53	0.44
1:A:122:LEU:HD21	2:A:500:HEM:CBB	2.48	0.44
1:P:261:VAL:HG22	2:P:500:HEM:C1B	2.52	0.44
1:J:226:VAL:HG13	1:J:233:HIS:HB2	1.98	0.44
1:G:98:LEU:HD12	1:G:235:GLU:OE1	2.18	0.44
1:O:60:SER:CB	1:O:61:PRO:CD	2.95	0.44
1:O:149:ARG:HD2	1:O:162:MET:HB3	1.99	0.44
1:B:296:ARG:HG2	1:B:296:ARG:H	1.68	0.44
1:M:279:TYR:O	1:M:283:MET:HG2	2.17	0.44
1:N:268:LYS:HB3	1:N:268:LYS:HE2	1.80	0.44
1:L:110:ARG:HA	1:L:110:ARG:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:ILE:CG2	1:F:204:VAL:HG23	2.47	0.44
1:N:134:ARG:HB3	1:N:135:PRO:HD3	1.99	0.44
1:F:120:ASN:OD1	1:F:256:ARG:NH2	2.40	0.44
1:C:199:GLN:O	1:C:199:GLN:CG	2.42	0.44
1:A:274:THR:HG23	1:A:279:TYR:HB2	1.97	0.44
1:A:146:TYR:HB3	1:A:166:HIS:CE1	2.52	0.44
1:L:82:MET:CE	1:L:115:LEU:CD1	2.95	0.44
1:I:87:ARG:HD2	3:I:584:HOH:O	2.16	0.44
1:M:82:MET:HG3	1:M:111:ILE:HG21	1.99	0.44
1:O:280:LEU:HD21	2:O:500:HEM:HAA2	2.00	0.44
1:K:39:ARG:HH11	1:K:39:ARG:CA	2.31	0.44
1:P:107:ARG:O	1:P:111:ILE:HG13	2.16	0.44
1:E:49:LEU:O	1:E:53:LEU:HB2	2.18	0.44
1:M:223:TRP:HB3	1:M:295:LEU:HD12	1.99	0.44
1:F:85:GLU:OE2	1:F:107:ARG:NH1	2.43	0.44
1:O:223:TRP:CB	1:O:295:LEU:HD12	2.48	0.44
1:F:293:TRP:O	1:F:296:ARG:HG2	2.18	0.44
1:N:220:GLU:OE2	1:N:298:ASP:OD2	2.36	0.44
1:H:56:GLN:O	1:H:58:PRO:HD3	2.17	0.44
1:P:122:LEU:HD21	2:P:500:HEM:CAB	2.48	0.44
1:D:270:GLY:HA2	1:F:45:ASP:HA	1.99	0.44
1:O:117:GLN:HB3	1:O:117:GLN:HE21	1.71	0.44
1:D:134:ARG:N	1:D:135:PRO:HD2	2.32	0.44
1:M:163:LEU:CD2	1:M:176:VAL:HG12	2.48	0.44
1:N:78:TRP:HB2	1:N:115:LEU:HD21	2.00	0.44
1:F:134:ARG:N	1:F:135:PRO:CD	2.81	0.44
1:I:274:THR:HG23	1:I:275:GLU:N	2.32	0.43
1:I:163:LEU:HD22	1:I:176:VAL:CG1	2.46	0.43
1:I:268:LYS:HD2	1:L:297:THR:HA	1.99	0.43
1:M:168:HIS:ND1	1:M:169:ARG:HG2	2.33	0.43
1:A:149:ARG:NE	1:A:162:MET:HE2	2.34	0.43
1:C:190:ILE:HG21	1:C:204:VAL:HG13	2.00	0.43
1:D:186:TYR:OH	1:D:291:GLU:HG2	2.18	0.43
1:O:279:TYR:CD2	1:O:280:LEU:HD23	2.53	0.43
1:L:164:ARG:N	1:L:165:PRO:CD	2.81	0.43
1:I:131:SER:O	1:I:135:PRO:HD3	2.18	0.43
1:I:47:LEU:HD13	1:J:72:HIS:HB3	2.00	0.43
2:I:500:HEM:CMB	2:I:500:HEM:CBB	2.95	0.43
1:E:224:LEU:HD22	1:E:228:ARG:CZ	2.48	0.43
1:P:71:GLN:HG2	2:P:500:HEM:CMC	2.48	0.43
1:O:167:ALA:HA	1:O:173:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164[B]:ARG:HB3	1:H:165:PRO:HD3	1.99	0.43
1:D:97:GLN:O	1:D:100:PRO:HD2	2.18	0.43
1:H:75:THR:HG23	1:H:115:LEU:HD22	2.00	0.43
1:M:144:GLN:HB2	1:N:43:TYR:HB3	1.99	0.43
1:L:216:ASN:OD1	1:L:218:SER:HB3	2.18	0.43
1:L:127:PRO:HB2	1:L:128:PRO:HD3	2.01	0.43
1:A:142:GLY:HA2	1:B:43:TYR:CE2	2.54	0.43
1:B:44:GLY:O	1:P:270:GLY:HA2	2.18	0.43
1:I:281:ARG:O	1:I:284:LEU:HB2	2.19	0.43
1:I:211:GLN:O	1:I:212:PRO:C	2.56	0.43
1:K:79:MET:HE2	1:K:148:TYR:HA	2.01	0.43
1:I:292:LEU:O	1:I:295:LEU:HD13	2.19	0.43
1:D:224:LEU:O	1:D:228:ARG:HG3	2.19	0.43
1:G:205:VAL:O	1:G:205:VAL:HG12	2.18	0.43
1:O:169:ARG:HH21	1:O:172:HIS:HE1	1.65	0.43
1:D:143:PHE:HE2	1:D:279:TYR:CZ	2.37	0.43
2:G:500:HEM:HHD	2:G:500:HEM:CBC	2.49	0.43
1:I:266:GLY:O	1:I:277:VAL:HG21	2.19	0.43
1:M:163:LEU:HD22	1:M:176:VAL:HG12	2.01	0.43
1:N:258:VAL:HG21	1:N:281:ARG:HG3	2.01	0.43
1:H:219:VAL:HB	1:H:291:GLU:HG3	1.99	0.43
1:A:203:GLU:HG2	3:A:573:HOH:O	2.18	0.43
1:F:269:ARG:HE	1:F:269:ARG:HB2	1.61	0.43
1:K:79:MET:HE2	1:K:151:ILE:HD12	2.00	0.43
1:E:141:SER:OG	1:E:143:PHE:HB2	2.18	0.43
1:I:168:HIS:HD2	3:I:551:HOH:O	2.01	0.43
1:A:119:TRP:CH2	1:A:257:HIS:CD2	3.05	0.43
1:I:151:ILE:O	1:I:154:ILE:HG22	2.18	0.43
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.88	0.43
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.69	0.43
1:K:105:LEU:HA	1:K:105:LEU:HD23	1.90	0.43
1:A:122:LEU:HD23	1:A:260:THR:HG21	2.00	0.43
1:C:288:LEU:C	1:C:290:PRO:HD3	2.39	0.43
1:A:282:ARG:O	1:A:285:ASP:HB2	2.19	0.43
1:A:164:ARG:C	1:A:166:HIS:H	2.22	0.43
1:P:130:TYR:O	1:P:133:MET:HG2	2.18	0.43
1:A:134:ARG:NH2	1:A:269:ARG:O	2.51	0.43
1:D:272:GLY:HA3	1:E:57:HIS:CD2	2.54	0.43
1:D:134:ARG:HB3	1:D:135:PRO:CD	2.49	0.43
1:I:257:HIS:O	1:I:261:VAL:HG23	2.18	0.43
2:L:500:HEM:CHD	2:L:500:HEM:HBC2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:LEU:HD11	2:E:500:HEM:C3A	2.54	0.42
1:A:49:LEU:O	1:A:53:LEU:HB2	2.19	0.42
1:A:164:ARG:C	1:A:166:HIS:N	2.72	0.42
1:I:149:ARG:CZ	1:I:162:MET:HE2	2.48	0.42
1:G:192:LEU:HD13	1:G:195:ARG:HH21	1.84	0.42
1:F:141:SER:O	1:F:144:GLN:HB2	2.18	0.42
1:J:41:MET:HA	3:J:538:HOH:O	2.18	0.42
1:D:89:ALA:CB	1:D:185:MET:HE2	2.49	0.42
1:E:43:TYR:HA	1:F:140:SER:HB2	2.00	0.42
1:P:109:SER:HB3	1:P:110:ARG:NH2	2.34	0.42
1:A:50:ASP:OD1	1:B:169:ARG:NH2	2.52	0.42
1:G:280:LEU:HD23	1:G:280:LEU:HA	1.85	0.42
1:A:83:LEU:O	1:A:87:ARG:HG3	2.19	0.42
1:M:95:SER:O	1:M:97:GLN:HG3	2.19	0.42
1:K:227:TYR:CD2	1:K:295:LEU:HD11	2.54	0.42
1:B:94:LYS:NZ	3:B:526:HOH:O	2.46	0.42
1:G:164:ARG:N	1:G:165:PRO:HD2	2.34	0.42
1:I:146:TYR:O	1:I:150:GLU:HG3	2.18	0.42
1:F:83:LEU:HD23	1:F:83:LEU:HA	1.72	0.42
1:E:215:TYR:OH	1:E:220:GLU:OE1	2.28	0.42
1:G:110:ARG:HH11	1:G:110:ARG:HG2	1.84	0.42
1:F:162:MET:HE2	3:F:501:HOH:O	2.19	0.42
1:P:127:PRO:HB2	1:P:128:PRO:HD3	2.01	0.42
1:H:292:LEU:O	1:H:296:ARG:NH1	2.51	0.42
1:F:164:ARG:N	1:F:165:PRO:CD	2.83	0.42
1:C:162:MET:O	1:C:165:PRO:HD2	2.20	0.42
3:A:588:HOH:O	1:M:294:LYS:HE2	2.20	0.42
1:G:224:LEU:HD21	1:G:299:LEU:HA	2.01	0.42
1:K:278:SER:CB	3:K:513:HOH:O	2.48	0.42
1:K:252:GLN:O	1:K:256:ARG:HB2	2.18	0.42
1:H:275:GLU:N	1:H:279:TYR:HB2	2.34	0.42
1:G:103:LYS:NZ	1:H:124:THR:O	2.43	0.42
1:D:59:LEU:HD23	1:D:136:TYR:O	2.18	0.42
1:C:132:ALA:HB1	3:C:587:HOH:O	2.18	0.42
1:I:144:GLN:HB2	1:J:43:TYR:HB3	2.02	0.42
1:K:78:TRP:HB2	1:K:115:LEU:HD21	2.00	0.42
1:F:297:THR:HG23	1:G:266:GLY:HA3	2.00	0.42
1:G:168:HIS:CD2	1:G:168:HIS:H	2.38	0.42
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.63	0.42
1:N:269:ARG:CB	1:N:269:ARG:NH1	2.69	0.42
1:G:290:PRO:HD2	1:G:291:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:163:LEU:HD22	1:N:176:VAL:CG1	2.48	0.42
1:G:200:ILE:HG22	1:G:204:VAL:HG12	2.01	0.42
1:A:251:ARG:HG2	3:A:525:HOH:O	2.19	0.42
1:I:98:LEU:HD12	1:I:235:GLU:HB3	2.02	0.42
1:K:59:LEU:HD23	1:K:136:TYR:O	2.20	0.42
1:A:68:PHE:HE1	2:A:500:HEM:CAB	2.31	0.42
1:O:89:ALA:CB	1:O:185:MET:CE	2.89	0.42
1:N:111:ILE:O	1:N:114:GLN:HB2	2.20	0.42
1:J:164:ARG:HG2	1:J:165:PRO:HD3	2.02	0.42
1:B:220:GLU:OE2	1:B:298:ASP:OD2	2.38	0.42
1:I:110:ARG:HH12	1:K:110:ARG:CZ	2.33	0.42
1:I:149:ARG:NH1	1:I:152:GLU:OE2	2.52	0.42
1:F:69:ILE:O	1:F:73:GLN:HG3	2.20	0.42
1:I:158:LYS:NZ	1:I:182:THR:O	2.29	0.42
1:M:65:GLU:HG3	1:M:133:MET:HE1	2.02	0.41
1:D:186:TYR:HH	1:D:291:GLU:HG2	1.84	0.41
3:A:507:HOH:O	1:D:256:ARG:CD	2.60	0.41
1:P:162:MET:HA	1:P:162:MET:HE3	2.01	0.41
1:A:75:THR:O	1:A:79:MET:HG3	2.20	0.41
1:D:170:PRO:HB2	3:D:600:HOH:O	2.20	0.41
1:G:215:TYR:OH	1:G:220:GLU:OE1	2.23	0.41
1:B:90:ARG:HD2	3:B:556:HOH:O	2.19	0.41
1:I:103:LYS:NZ	1:J:129:GLU:OE2	2.52	0.41
1:J:99:GLN:HB2	1:J:100:PRO:HD3	2.02	0.41
1:J:99:GLN:HB3	1:L:234:TRP:NE1	2.35	0.41
1:K:267:PHE:HE1	1:K:281:ARG:HE	1.66	0.41
1:I:282:ARG:O	1:I:285:ASP:HB2	2.20	0.41
1:M:146:TYR:HB3	1:M:166:HIS:CD2	2.54	0.41
1:I:292:LEU:HA	1:I:295:LEU:CD1	2.50	0.41
1:I:292:LEU:HA	1:I:295:LEU:HD12	2.02	0.41
1:G:192:LEU:O	1:G:196:ARG:HG3	2.20	0.41
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.90	0.41
1:D:274:THR:HB	1:E:57:HIS:HB3	2.01	0.41
1:K:219:VAL:CG1	1:K:291:GLU:HG3	2.49	0.41
1:H:269:ARG:HH22	1:J:39:ARG:HH21	1.68	0.41
1:H:220:GLU:HB2	1:H:291:GLU:HB2	2.03	0.41
1:F:223:TRP:HB3	1:F:295:LEU:HD12	2.02	0.41
1:L:82:MET:HE2	1:L:82:MET:HB2	1.74	0.41
1:O:60:SER:HB2	1:O:61:PRO:HD2	2.01	0.41
1:C:163:LEU:CD2	1:C:176:VAL:HG12	2.42	0.41
1:L:295:LEU:CD2	1:L:296:ARG:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:HA2	1:A:49:LEU:HD12	2.02	0.41
1:N:158[B]:LYS:HE3	1:N:184:SER:HB3	2.02	0.41
1:K:46:TYR:CE1	1:L:59:LEU:HD22	2.55	0.41
1:H:69:ILE:O	1:H:73:GLN:HG3	2.21	0.41
1:J:192:LEU:O	1:J:192:LEU:HG	2.20	0.41
1:N:127:PRO:N	1:N:128:PRO:HD2	2.35	0.41
1:P:104:MET:O	1:P:108:VAL:HG23	2.21	0.41
1:J:154:ILE:HG12	1:J:154:ILE:H	1.77	0.41
1:G:219:VAL:HG11	1:G:291:GLU:HG3	2.00	0.41
1:F:164:ARG:HB2	1:F:165:PRO:CD	2.51	0.41
1:L:215:TYR:HE1	1:L:220:GLU:OE1	2.04	0.41
1:L:158:LYS:HD3	3:L:516:HOH:O	2.20	0.41
1:M:112:MET:O	1:M:116:VAL:HG23	2.21	0.41
1:C:105:LEU:HA	1:C:105:LEU:HD23	1.76	0.41
1:F:257:HIS:CE1	2:F:500:HEM:C4D	3.01	0.41
1:N:98:LEU:HD12	1:N:235:GLU:OE1	2.20	0.41
1:P:60:SER:HB2	1:P:61:PRO:HD2	2.03	0.41
1:A:73:GLN:NE2	1:B:47:LEU:O	2.43	0.41
1:H:294:LYS:HE2	3:H:604:HOH:O	2.21	0.41
1:L:149:ARG:HD3	1:L:149:ARG:HA	1.69	0.41
1:K:260:THR:HA	1:K:263:ARG:HG2	2.03	0.41
1:M:103:LYS:NZ	1:N:124:THR:O	2.54	0.41
1:A:185:MET:HB2	1:A:185:MET:HE2	1.93	0.41
1:B:295:LEU:C	1:B:295:LEU:HD22	2.41	0.41
1:F:280:LEU:HD21	2:F:500:HEM:CHA	2.51	0.41
1:E:292:LEU:HA	1:E:295:LEU:HD23	2.03	0.41
1:E:168:HIS:H	1:E:168:HIS:CD2	2.39	0.41
1:H:134:ARG:N	1:H:135:PRO:HD2	2.36	0.41
1:L:53:LEU:HD12	1:L:53:LEU:HA	1.90	0.41
1:C:261:VAL:HG22	2:C:500:HEM:C2B	2.55	0.41
1:I:119:TRP:CH2	1:I:257:HIS:CD2	3.09	0.41
1:D:268:LYS:HG3	1:D:271:THR:HG21	2.02	0.41
1:E:188:GLU:OE2	1:E:188:GLU:HA	2.21	0.41
1:I:83:LEU:HD23	1:I:83:LEU:HA	1.77	0.41
1:H:119:TRP:CD1	1:H:256:ARG:HB3	2.56	0.41
1:C:133:MET:HB2	1:C:133:MET:HE2	1.79	0.41
1:M:268:LYS:H	1:M:268:LYS:HG2	1.55	0.41
1:A:215:TYR:OH	1:A:220:GLU:OE1	2.28	0.41
1:G:295:LEU:HD22	1:G:296:ARG:HH11	1.84	0.41
1:F:152:GLU:CD	1:F:254:ARG:HH12	2.24	0.41
1:H:86:LEU:O	1:H:185:MET:CE	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:208:ASP:OD1	1:P:210:THR:HB	2.21	0.41
1:B:200:ILE:HG22	1:B:204:VAL:HG12	2.03	0.41
1:D:86:LEU:O	1:D:185:MET:HE3	2.21	0.40
1:L:228:ARG:C	1:L:230:PRO:HD3	2.42	0.40
1:B:134:ARG:N	1:B:135:PRO:CD	2.83	0.40
1:I:110:ARG:HE	1:I:110:ARG:N	2.19	0.40
1:J:111:ILE:O	1:J:114:GLN:HB2	2.21	0.40
1:B:108:VAL:HA	1:B:111:ILE:HD12	2.03	0.40
1:C:187:ASP:O	1:C:191:ARG:HG3	2.21	0.40
1:O:93:VAL:O	1:O:192:LEU:HD13	2.21	0.40
1:J:186:TYR:OH	1:J:291:GLU:CG	2.69	0.40
1:J:186:TYR:O	1:J:190:ILE:HG13	2.20	0.40
1:M:130:TYR:CE1	1:M:265:ILE:HG22	2.56	0.40
1:N:169:ARG:HB3	1:N:169:ARG:HE	1.77	0.40
1:P:65:GLU:CG	1:P:133:MET:HE1	2.49	0.40
1:C:291:GLU:O	1:C:295:LEU:HB3	2.22	0.40
1:E:261:VAL:HG12	1:E:277:VAL:HG22	2.03	0.40
1:K:79:MET:HE1	1:K:148:TYR:CD1	2.52	0.40
1:J:223:TRP:HB3	1:J:295:LEU:HD12	2.04	0.40
1:B:296:ARG:HD2	1:C:263:ARG:O	2.22	0.40
1:L:133:MET:HG3	1:L:137:LEU:HD11	2.02	0.40
1:H:220:GLU:HB2	1:H:291:GLU:CB	2.51	0.40
1:A:228:ARG:C	1:A:230:PRO:HD3	2.42	0.40
1:O:164:ARG:N	1:O:165:PRO:CD	2.85	0.40
1:L:211:GLN:HG3	1:L:212:PRO:CD	2.51	0.40
1:B:224:LEU:HG	1:B:295:LEU:HB2	2.04	0.40
1:F:142:GLY:C	1:F:144:GLN:N	2.74	0.40
1:G:43:TYR:CE2	1:H:142:GLY:HA2	2.56	0.40
1:L:77:LEU:HD23	1:L:77:LEU:HA	1.87	0.40
1:M:77:LEU:HD23	1:N:70:VAL:HG22	2.03	0.40
1:K:207:ARG:NH1	1:K:207:ARG:CG	2.78	0.40
1:F:267:PHE:CD2	1:F:268:LYS:N	2.86	0.40
1:B:299:LEU:HD22	1:C:127:PRO:HB2	2.02	0.40
1:D:191:ARG:HG2	1:D:205:VAL:HG13	2.03	0.40
1:L:172:HIS:HA	1:L:175:LEU:HD12	2.02	0.40
1:F:260:THR:HA	1:F:263:ARG:HG2	2.04	0.40
1:G:271:THR:HG23	3:G:554:HOH:O	2.22	0.40
1:N:282:ARG:HG3	1:N:283:MET:CE	2.51	0.40
1:E:242:LYS:HD2	3:E:563:HOH:O	2.21	0.40
1:O:59:LEU:HD22	1:P:46:TYR:HD1	1.86	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	260/281 (92%)	254 (98%)	6 (2%)	0	100	100
1	B	262/281 (93%)	254 (97%)	8 (3%)	0	100	100
1	C	251/281 (89%)	244 (97%)	7 (3%)	0	100	100
1	D	257/281 (92%)	248 (96%)	8 (3%)	1 (0%)	39	56
1	E	252/281 (90%)	241 (96%)	9 (4%)	2 (1%)	24	35
1	F	256/281 (91%)	249 (97%)	6 (2%)	1 (0%)	39	56
1	G	255/281 (91%)	242 (95%)	12 (5%)	1 (0%)	39	56
1	H	259/281 (92%)	254 (98%)	5 (2%)	0	100	100
1	I	257/281 (92%)	249 (97%)	7 (3%)	1 (0%)	39	56
1	J	253/281 (90%)	244 (96%)	9 (4%)	0	100	100
1	K	252/281 (90%)	246 (98%)	5 (2%)	1 (0%)	39	56
1	L	258/281 (92%)	250 (97%)	6 (2%)	2 (1%)	24	35
1	M	252/281 (90%)	244 (97%)	7 (3%)	1 (0%)	39	56
1	N	259/281 (92%)	250 (96%)	9 (4%)	0	100	100
1	O	253/281 (90%)	238 (94%)	15 (6%)	0	100	100
1	P	257/281 (92%)	249 (97%)	8 (3%)	0	100	100
All	All	4093/4496 (91%)	3956 (97%)	127 (3%)	10 (0%)	52	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	SER
1	E	268	LYS
1	I	212	PRO
1	M	268	LYS
1	E	141	SER
1	L	139	ALA

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Mol	Chain	Res	Type
1	F	140	SER
1	L	209	TRP
1	K	212	PRO
1	G	273	GLY

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	229/240 (95%)	217 (95%)	12 (5%)	29	45
1	B	230/240 (96%)	214 (93%)	16 (7%)	19	29
1	C	224/240 (93%)	210 (94%)	14 (6%)	22	35
1	D	226/240 (94%)	211 (93%)	15 (7%)	21	32
1	E	226/240 (94%)	212 (94%)	14 (6%)	23	35
1	F	228/240 (95%)	213 (93%)	15 (7%)	21	32
1	G	227/240 (95%)	213 (94%)	14 (6%)	23	35
1	H	228/240 (95%)	214 (94%)	14 (6%)	23	36
1	I	226/240 (94%)	213 (94%)	13 (6%)	25	39
1	J	226/240 (94%)	209 (92%)	17 (8%)	17	26
1	K	226/240 (94%)	213 (94%)	13 (6%)	25	39
1	L	227/240 (95%)	215 (95%)	12 (5%)	28	44
1	M	223/240 (93%)	204 (92%)	19 (8%)	13	20
1	N	228/240 (95%)	213 (93%)	15 (7%)	21	32
1	O	226/240 (94%)	207 (92%)	19 (8%)	14	20
1	P	226/240 (94%)	213 (94%)	13 (6%)	25	39
All	All	3626/3840 (94%)	3391 (94%)	235 (6%)	21	33

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	59	LEU
1	A	96	ASP
1	A	97	GLN
1	A	149	ARG
1	A	164	ARG
1	A	193	MET
1	A	204	VAL
1	A	246	LEU
1	A	275	GLU
1	A	281	ARG
1	A	295	LEU
1	B	50	ASP
1	B	53	LEU
1	B	59	LEU
1	B	117	GLN
1	B	131	SER
1	B	133	MET
1	B	169	ARG
1	B	204	VAL
1	B	211	GLN
1	B	242	LYS
1	B	250	PHE
1	B	258	VAL
1	B	267	PHE
1	B	294	LYS
1	B	295	LEU
1	B	296	ARG
1	C	53	LEU
1	C	59	LEU
1	C	61	PRO
1	C	96	ASP
1	C	143	PHE
1	C	164	ARG
1	C	199	GLN
1	C	210	THR
1	C	214	GLN
1	C	250	PHE
1	C	254	ARG
1	C	275	GLU
1	C	281	ARG
1	C	295	LEU
1	D	53	LEU

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Mol	Chain	Res	Type
1	D	59	LEU
1	D	82	MET
1	D	125	MET
1	D	143	PHE
1	D	185	MET
1	D	192	LEU
1	D	200	ILE
1	D	250	PHE
1	D	267	PHE
1	D	268	LYS
1	D	274	THR
1	D	278	SER
1	D	294	LYS
1	D	295	LEU
1	E	53	LEU
1	E	59	LEU
1	E	94	LYS
1	E	96	ASP
1	E	137	LEU
1	E	143	PHE
1	E	199	GLN
1	E	204	VAL
1	E	231	SER
1	E	250	PHE
1	E	267	PHE
1	E	275	GLU
1	E	281	ARG
1	E	294	LYS
1	F	40	ASP
1	F	53	LEU
1	F	59	LEU
1	F	109	SER
1	F	158	LYS
1	F	203	GLU
1	F	204	VAL
1	F	231	SER
1	F	246	LEU
1	F	250	PHE
1	F	254	ARG
1	F	267	PHE
1	F	269	ARG
1	F	295	LEU

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Mol	Chain	Res	Type
1	F	296	ARG
1	G	53	LEU
1	G	134	ARG
1	G	158	LYS
1	G	182	THR
1	G	204	VAL
1	G	213	THR
1	G	224	LEU
1	G	225	GLU
1	G	250	PHE
1	G	267	PHE
1	G	271	THR
1	G	281	ARG
1	G	283	MET
1	G	294	LYS
1	H	50	ASP
1	H	53	LEU
1	H	59	LEU
1	H	184	SER
1	H	204	VAL
1	H	242	LYS
1	H	250	PHE
1	H	275	GLU
1	H	278	SER
1	H	281	ARG
1	H	291	GLU
1	H	294	LYS
1	H	295	LEU
1	H	297	THR
1	I	53	LEU
1	I	59	LEU
1	I	110	ARG
1	I	163	LEU
1	I	207	ARG
1	I	210	THR
1	I	225	GLU
1	I	229	ASN
1	I	254	ARG
1	I	256	ARG
1	I	274	THR
1	I	291	GLU
1	I	295	LEU

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Mol	Chain	Res	Type
1	J	40	ASP
1	J	50	ASP
1	J	53	LEU
1	J	59	LEU
1	J	140	SER
1	J	154	ILE
1	J	158	LYS
1	J	164	ARG
1	J	174	GLU
1	J	178	THR
1	J	204	VAL
1	J	246	LEU
1	J	250	PHE
1	J	258	VAL
1	J	265	ILE
1	J	291	GLU
1	J	295	LEU
1	K	39	ARG
1	K	53	LEU
1	K	59	LEU
1	K	87	ARG
1	K	96	ASP
1	K	207	ARG
1	K	250	PHE
1	K	254	ARG
1	K	258	VAL
1	K	274	THR
1	K	281	ARG
1	K	294	LYS
1	K	295	LEU
1	L	53	LEU
1	L	59	LEU
1	L	158	LYS
1	L	204	VAL
1	L	231	SER
1	L	246	LEU
1	L	250	PHE
1	L	267	PHE
1	L	274	THR
1	L	275	GLU
1	L	295	LEU
1	L	297	THR

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Mol	Chain	Res	Type
1	M	53	LEU
1	M	59	LEU
1	M	60	SER
1	M	77	LEU
1	M	109	SER
1	M	110	ARG
1	M	117	GLN
1	M	134	ARG
1	M	137	LEU
1	M	143	PHE
1	M	174	GLU
1	M	204	VAL
1	M	250	PHE
1	M	265	ILE
1	M	267	PHE
1	M	268	LYS
1	M	291	GLU
1	M	294	LYS
1	M	295	LEU
1	N	50	ASP
1	N	53	LEU
1	N	59	LEU
1	N	96	ASP
1	N	110	ARG
1	N	117	GLN
1	N	134	ARG
1	N	163	LEU
1	N	199	GLN
1	N	245	ASP
1	N	250	PHE
1	N	265	ILE
1	N	267	PHE
1	N	269	ARG
1	N	295	LEU
1	O	49	LEU
1	O	53	LEU
1	O	59	LEU
1	O	96	ASP
1	O	117	GLN
1	O	158	LYS
1	O	164	ARG
1	O	173	LEU

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Mol	Chain	Res	Type
1	O	178	THR
1	O	182	THR
1	O	185	MET
1	O	204	VAL
1	O	207	ARG
1	O	250	PHE
1	O	267	PHE
1	O	268	LYS
1	O	291	GLU
1	O	295	LEU
1	O	296	ARG
1	P	53	LEU
1	P	59	LEU
1	P	87	ARG
1	P	96	ASP
1	P	109	SER
1	P	131	SER
1	P	141	SER
1	P	164	ARG
1	P	177	GLU
1	P	203	GLU
1	P	204	VAL
1	P	233	HIS
1	P	275	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	252	GLN
1	B	31	HIS
1	B	34	GLN
1	C	214	GLN
1	C	252	GLN
1	D	252	GLN
1	E	172	HIS
1	E	211	GLN
1	E	252	GLN
1	G	166	HIS
1	G	181	HIS
1	J	51	GLN
1	J	211	GLN

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Mol	Chain	Res	Type
1	K	144	GLN
1	K	252	GLN
1	L	51	GLN
1	L	114	GLN
1	M	252	GLN
1	N	181	HIS
1	O	172	HIS
1	O	181	HIS
1	P	233	HIS

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

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	500	1,3	30,50,50	2.49	11 (36%)	24,82,82	2.63	10 (41%)
2	HEM	B	500	1	30,50,50	2.63	7 (23%)	24,82,82	2.42	9 (37%)
2	HEM	C	500	1	30,50,50	2.16	10 (33%)	24,82,82	2.33	9 (37%)
2	HEM	D	500	1,3	30,50,50	2.34	10 (33%)	24,82,82	2.40	9 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	E	500	1,3	30,50,50	2.52	8 (26%)	24,82,82	2.51	8 (33%)
2	HEM	F	500	1	30,50,50	2.28	9 (30%)	24,82,82	2.50	11 (45%)
2	HEM	G	500	1	30,50,50	2.36	11 (36%)	24,82,82	2.37	11 (45%)
2	HEM	H	500	1	30,50,50	2.31	8 (26%)	24,82,82	2.61	12 (50%)
2	HEM	I	500	1	30,50,50	2.25	7 (23%)	24,82,82	2.54	12 (50%)
2	HEM	J	500	1	30,50,50	2.12	9 (30%)	24,82,82	2.33	11 (45%)
2	HEM	K	500	1	30,50,50	2.24	6 (20%)	24,82,82	2.37	10 (41%)
2	HEM	L	500	1	30,50,50	2.41	9 (30%)	24,82,82	2.66	11 (45%)
2	HEM	M	500	1	30,50,50	2.39	11 (36%)	24,82,82	2.67	11 (45%)
2	HEM	N	500	1	30,50,50	2.22	10 (33%)	24,82,82	2.40	11 (45%)
2	HEM	O	500	1	30,50,50	2.33	9 (30%)	24,82,82	2.46	11 (45%)
2	HEM	P	500	1,3	30,50,50	2.44	8 (26%)	24,82,82	2.36	10 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1,3	-	0/10/54/54	0/0/8/8
2	HEM	B	500	1	-	0/10/54/54	0/0/8/8
2	HEM	C	500	1	-	0/10/54/54	0/0/8/8
2	HEM	D	500	1,3	-	0/10/54/54	0/0/8/8
2	HEM	E	500	1,3	-	0/10/54/54	0/0/8/8
2	HEM	F	500	1	-	0/10/54/54	0/0/8/8
2	HEM	G	500	1	-	0/10/54/54	0/0/8/8
2	HEM	H	500	1	-	0/10/54/54	0/0/8/8
2	HEM	I	500	1	-	0/10/54/54	0/0/8/8
2	HEM	J	500	1	-	0/10/54/54	0/0/8/8
2	HEM	K	500	1	-	0/10/54/54	0/0/8/8
2	HEM	L	500	1	-	0/10/54/54	0/0/8/8
2	HEM	M	500	1	-	0/10/54/54	0/0/8/8
2	HEM	N	500	1	-	0/10/54/54	0/0/8/8
2	HEM	O	500	1	-	0/10/54/54	0/0/8/8
2	HEM	P	500	1,3	-	0/10/54/54	0/0/8/8

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-8.73	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	HEM	C3B-C4B	-8.48	1.44	1.51
2	P	500	HEM	C3B-C4B	-8.17	1.44	1.51
2	F	500	HEM	C3B-C4B	-7.91	1.44	1.51
2	L	500	HEM	C3B-C4B	-7.81	1.44	1.51
2	K	500	HEM	C3B-C4B	-7.76	1.44	1.51
2	M	500	HEM	C3B-C4B	-7.66	1.45	1.51
2	H	500	HEM	C3B-C4B	-7.43	1.45	1.51
2	I	500	HEM	C3B-C4B	-7.42	1.45	1.51
2	O	500	HEM	C3B-C4B	-7.42	1.45	1.51
2	J	500	HEM	C3B-C4B	-6.68	1.45	1.51
2	E	500	HEM	C3D-C4D	-6.67	1.43	1.51
2	N	500	HEM	C3B-C4B	-6.65	1.45	1.51
2	G	500	HEM	C3B-C4B	-6.57	1.46	1.51
2	A	500	HEM	C3B-C4B	-6.52	1.46	1.51
2	C	500	HEM	C3B-C4B	-6.35	1.46	1.51
2	L	500	HEM	C3D-C4D	-6.22	1.43	1.51
2	A	500	HEM	C3D-C4D	-6.09	1.43	1.51
2	D	500	HEM	C3B-C4B	-5.92	1.46	1.51
2	F	500	HEM	C3D-C4D	-5.80	1.44	1.51
2	P	500	HEM	C3D-C4D	-5.61	1.44	1.51
2	K	500	HEM	C3D-C4D	-5.31	1.44	1.51
2	B	500	HEM	C3D-C4D	-5.15	1.45	1.51
2	C	500	HEM	C3D-C4D	-5.14	1.45	1.51
2	N	500	HEM	C3D-C4D	-5.06	1.45	1.51
2	M	500	HEM	C3D-C4D	-4.97	1.45	1.51
2	O	500	HEM	C3D-C4D	-4.77	1.45	1.51
2	I	500	HEM	C3D-C4D	-4.76	1.45	1.51
2	B	500	HEM	C2C-C1C	-4.56	1.43	1.52
2	H	500	HEM	C3D-C4D	-4.55	1.45	1.51
2	H	500	HEM	C2C-C1C	-4.44	1.44	1.52
2	J	500	HEM	C2C-C1C	-4.38	1.44	1.52
2	D	500	HEM	C3D-C4D	-4.38	1.46	1.51
2	G	500	HEM	C3D-C4D	-4.38	1.46	1.51
2	M	500	HEM	C2C-C1C	-4.29	1.44	1.52
2	D	500	HEM	C2C-C1C	-4.24	1.44	1.52
2	G	500	HEM	C2C-C1C	-4.19	1.44	1.52
2	L	500	HEM	C2C-C1C	-4.19	1.44	1.52
2	A	500	HEM	C2C-C1C	-4.14	1.44	1.52
2	I	500	HEM	C2C-C1C	-4.13	1.44	1.52
2	C	500	HEM	C2C-C1C	-4.05	1.44	1.52
2	O	500	HEM	C2C-C1C	-3.82	1.45	1.52
2	F	500	HEM	C2C-C1C	-3.80	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	500	HEM	C2C-C1C	-3.70	1.45	1.52
2	J	500	HEM	C3D-C4D	-3.66	1.46	1.51
2	E	500	HEM	C2C-C1C	-3.62	1.45	1.52
2	P	500	HEM	C2C-C1C	-3.55	1.45	1.52
2	N	500	HEM	C2C-C1C	-3.31	1.46	1.52
2	N	500	HEM	C2B-C1B	-2.30	1.44	1.51
2	C	500	HEM	C2D-C1D	-2.23	1.44	1.51
2	A	500	HEM	C2D-C1D	-2.23	1.44	1.51
2	D	500	HEM	C2D-C1D	-2.19	1.44	1.51
2	O	500	HEM	C2D-C1D	-2.15	1.44	1.51
2	O	500	HEM	C2B-C1B	-2.13	1.44	1.51
2	J	500	HEM	C2D-C1D	-2.12	1.44	1.51
2	N	500	HEM	C2D-C1D	-2.09	1.45	1.51
2	L	500	HEM	C2D-C1D	-2.07	1.45	1.51
2	F	500	HEM	C2D-C1D	-2.03	1.45	1.51
2	E	500	HEM	C2D-C1D	-2.03	1.45	1.51
2	K	500	HEM	C2D-C1D	-2.02	1.45	1.51
2	I	500	HEM	C2D-C1D	-2.02	1.45	1.51
2	M	500	HEM	C2B-C1B	-2.00	1.45	1.51
2	L	500	HEM	FE-ND	2.01	2.08	1.97
2	M	500	HEM	FE-NB	2.04	2.08	1.97
2	F	500	HEM	C3B-CAB	2.05	1.55	1.51
2	F	500	HEM	C1C-NC	2.05	1.38	1.36
2	I	500	HEM	CAA-C2A	2.06	1.55	1.52
2	E	500	HEM	FE-ND	2.08	2.08	1.97
2	A	500	HEM	C3B-CAB	2.09	1.55	1.51
2	M	500	HEM	C3C-CAC	2.10	1.55	1.51
2	I	500	HEM	C3C-CAC	2.10	1.55	1.51
2	C	500	HEM	C3C-CAC	2.12	1.55	1.51
2	M	500	HEM	C3B-CAB	2.13	1.55	1.51
2	F	500	HEM	FE-NC	2.15	2.04	1.95
2	M	500	HEM	CMA-C3A	2.15	1.56	1.51
2	J	500	HEM	FE-ND	2.15	2.08	1.97
2	P	500	HEM	C1C-NC	2.16	1.38	1.36
2	O	500	HEM	C3C-CAC	2.17	1.55	1.51
2	F	500	HEM	C4C-NC	2.18	1.38	1.36
2	C	500	HEM	C4C-NC	2.18	1.38	1.36
2	A	500	HEM	FE-ND	2.19	2.09	1.97
2	H	500	HEM	CAA-C2A	2.21	1.55	1.52
2	L	500	HEM	CAA-C2A	2.23	1.55	1.52
2	B	500	HEM	CAA-C2A	2.25	1.55	1.52
2	P	500	HEM	C3C-CAC	2.25	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	500	HEM	C3B-CAB	2.27	1.55	1.51
2	H	500	HEM	C1C-NC	2.32	1.38	1.36
2	G	500	HEM	C3C-CAC	2.33	1.55	1.51
2	E	500	HEM	C3C-CAC	2.35	1.55	1.51
2	C	500	HEM	CAA-C2A	2.36	1.56	1.52
2	N	500	HEM	C1C-NC	2.36	1.38	1.36
2	C	500	HEM	C3B-CAB	2.36	1.55	1.51
2	F	500	HEM	FE-NB	2.39	2.10	1.97
2	J	500	HEM	C3B-CAB	2.39	1.55	1.51
2	G	500	HEM	C3B-CAB	2.39	1.55	1.51
2	B	500	HEM	C4C-NC	2.40	1.39	1.36
2	N	500	HEM	C3C-CAC	2.40	1.55	1.51
2	G	500	HEM	CAA-C2A	2.40	1.56	1.52
2	E	500	HEM	CAA-C2A	2.47	1.56	1.52
2	K	500	HEM	CAA-C2A	2.47	1.56	1.52
2	O	500	HEM	C4C-NC	2.49	1.39	1.36
2	J	500	HEM	C4C-NC	2.50	1.39	1.36
2	A	500	HEM	C3C-CAC	2.53	1.56	1.51
2	D	500	HEM	C3B-CAB	2.54	1.56	1.51
2	J	500	HEM	C1C-NC	2.59	1.39	1.36
2	L	500	HEM	C3B-CAB	2.61	1.56	1.51
2	M	500	HEM	C4C-NC	2.62	1.39	1.36
2	C	500	HEM	FE-ND	2.65	2.11	1.97
2	N	500	HEM	FE-NB	2.69	2.11	1.97
2	A	500	HEM	C4C-NC	2.72	1.39	1.36
2	L	500	HEM	C1C-NC	2.74	1.39	1.36
2	P	500	HEM	FE-ND	2.88	2.12	1.97
2	L	500	HEM	C4C-NC	2.91	1.39	1.36
2	P	500	HEM	CAA-C2A	2.91	1.57	1.52
2	G	500	HEM	FE-NB	2.94	2.13	1.97
2	D	500	HEM	FE-NC	2.95	2.07	1.95
2	H	500	HEM	C4C-NC	2.96	1.39	1.36
2	M	500	HEM	C1C-NC	3.00	1.39	1.36
2	C	500	HEM	FE-NC	3.03	2.07	1.95
2	H	500	HEM	FE-NC	3.04	2.07	1.95
2	G	500	HEM	C4C-NC	3.19	1.39	1.36
2	D	500	HEM	FE-ND	3.27	2.14	1.97
2	G	500	HEM	FE-NC	3.36	2.09	1.95
2	G	500	HEM	C1C-NC	3.45	1.40	1.36
2	K	500	HEM	FE-NC	3.46	2.09	1.95
2	G	500	HEM	FE-ND	3.52	2.16	1.97
2	D	500	HEM	C4C-NC	3.57	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	FE-ND	3.65	2.16	1.97
2	J	500	HEM	FE-NC	3.65	2.10	1.95
2	A	500	HEM	C1C-NC	3.66	1.40	1.36
2	D	500	HEM	C1C-NC	3.71	1.40	1.36
2	A	500	HEM	FE-NC	3.73	2.10	1.95
2	A	500	HEM	FE-NB	3.75	2.17	1.97
2	O	500	HEM	FE-NC	3.80	2.10	1.95
2	D	500	HEM	FE-NB	3.82	2.17	1.97
2	N	500	HEM	FE-NC	3.88	2.11	1.95
2	H	500	HEM	FE-ND	3.92	2.18	1.97
2	O	500	HEM	FE-ND	4.01	2.18	1.97
2	M	500	HEM	FE-ND	4.05	2.18	1.97
2	P	500	HEM	C4C-NC	4.13	1.41	1.36
2	E	500	HEM	C4C-NC	4.18	1.41	1.36
2	I	500	HEM	C4C-NC	4.18	1.41	1.36
2	B	500	HEM	FE-NC	5.38	2.17	1.95

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CBD-CAD-C3D	-4.57	100.24	113.55
2	B	500	HEM	C3C-CAC-CBC	-4.34	117.79	124.46
2	M	500	HEM	CBD-CAD-C3D	-4.30	101.05	113.55
2	H	500	HEM	CMA-C3A-C4A	-4.26	121.32	128.36
2	H	500	HEM	CBD-CAD-C3D	-4.22	101.28	113.55
2	A	500	HEM	CAA-CBA-CGA	-4.03	105.36	112.75
2	L	500	HEM	CAA-CBA-CGA	-3.94	105.52	112.75
2	P	500	HEM	CBD-CAD-C3D	-3.87	102.30	113.55
2	F	500	HEM	CAA-CBA-CGA	-3.78	105.82	112.75
2	H	500	HEM	CAA-C2A-C1A	-3.71	122.98	127.01
2	L	500	HEM	C3C-CAC-CBC	-3.67	118.83	124.46
2	I	500	HEM	CMA-C3A-C4A	-3.61	122.38	128.36
2	J	500	HEM	CMA-C3A-C4A	-3.61	122.39	128.36
2	K	500	HEM	C3B-CAB-CBB	-3.52	119.06	124.46
2	C	500	HEM	CBD-CAD-C3D	-3.50	103.38	113.55
2	F	500	HEM	C3C-CAC-CBC	-3.45	119.16	124.46
2	F	500	HEM	CBD-CAD-C3D	-3.41	103.64	113.55
2	O	500	HEM	CBD-CAD-C3D	-3.35	103.81	113.55
2	E	500	HEM	C3B-CAB-CBB	-3.31	119.38	124.46
2	E	500	HEM	CMA-C3A-C4A	-3.30	122.91	128.36
2	L	500	HEM	CMA-C3A-C4A	-3.22	123.03	128.36
2	M	500	HEM	CAA-C2A-C1A	-3.19	123.55	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	CBD-CAD-C3D	-3.18	104.30	113.55
2	N	500	HEM	CMA-C3A-C4A	-3.09	123.25	128.36
2	I	500	HEM	C3B-CAB-CBB	-3.02	119.83	124.46
2	L	500	HEM	CAA-C2A-C1A	-3.00	123.75	127.01
2	D	500	HEM	C3C-CAC-CBC	-2.99	119.88	124.46
2	K	500	HEM	CMA-C3A-C4A	-2.97	123.45	128.36
2	J	500	HEM	C3B-CAB-CBB	-2.96	119.91	124.46
2	I	500	HEM	CAA-C2A-C1A	-2.92	123.84	127.01
2	L	500	HEM	CBD-CAD-C3D	-2.89	105.15	113.55
2	O	500	HEM	C3B-CAB-CBB	-2.85	120.09	124.46
2	P	500	HEM	CMA-C3A-C4A	-2.83	123.68	128.36
2	J	500	HEM	C3C-CAC-CBC	-2.83	120.12	124.46
2	G	500	HEM	C3B-CAB-CBB	-2.65	120.39	124.46
2	M	500	HEM	CMA-C3A-C4A	-2.56	124.14	128.36
2	M	500	HEM	C3B-CAB-CBB	-2.55	120.54	124.46
2	E	500	HEM	CBD-CAD-C3D	-2.42	106.51	113.55
2	P	500	HEM	C3B-CAB-CBB	-2.40	120.78	124.46
2	O	500	HEM	CBA-CAA-C2A	-2.39	108.24	112.53
2	D	500	HEM	CBD-CAD-C3D	-2.37	106.64	113.55
2	A	500	HEM	C3B-C4B-NB	-2.34	107.16	111.63
2	H	500	HEM	CAA-CBA-CGA	-2.22	108.67	112.75
2	N	500	HEM	CBA-CAA-C2A	-2.22	108.55	112.53
2	G	500	HEM	C3C-CAC-CBC	-2.15	121.16	124.46
2	K	500	HEM	C3C-CAC-CBC	-2.13	121.19	124.46
2	I	500	HEM	CBA-CAA-C2A	-2.12	108.74	112.53
2	C	500	HEM	C3B-CAB-CBB	-2.11	121.22	124.46
2	O	500	HEM	C3B-C4B-NB	-2.11	107.60	111.63
2	F	500	HEM	CAA-C2A-C1A	-2.10	124.73	127.01
2	G	500	HEM	CBD-CAD-C3D	-2.10	107.45	113.55
2	F	500	HEM	CMA-C3A-C4A	-2.09	124.90	128.36
2	P	500	HEM	C3C-CAC-CBC	-2.06	121.30	124.46
2	H	500	HEM	C3C-CAC-CBC	-2.05	121.31	124.46
2	J	500	HEM	CBD-CAD-C3D	-2.04	107.62	113.55
2	A	500	HEM	C3C-CAC-CBC	-2.04	121.33	124.46
2	G	500	HEM	C3B-C4B-NB	-2.03	107.74	111.63
2	N	500	HEM	C3B-C4B-NB	-2.03	107.75	111.63
2	B	500	HEM	C3B-CAB-CBB	-2.02	121.35	124.46
2	K	500	HEM	CAA-CBA-CGA	-2.02	109.04	112.75
2	M	500	HEM	CAA-CBA-CGA	-2.01	109.07	112.75
2	C	500	HEM	CAA-C2A-C1A	-2.00	124.84	127.01
2	K	500	HEM	C2D-C3D-C4D	2.01	104.91	101.50
2	J	500	HEM	C2D-C3D-C4D	2.02	104.92	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	500	HEM	C3B-C4B-CHC	2.02	126.01	123.16
2	D	500	HEM	C2D-C3D-C4D	2.06	104.99	101.50
2	P	500	HEM	C2D-C3D-C4D	2.07	105.02	101.50
2	B	500	HEM	C2D-C3D-C4D	2.08	105.02	101.50
2	F	500	HEM	C2D-C3D-C4D	2.10	105.06	101.50
2	J	500	HEM	CMA-C3A-C2A	2.11	129.64	125.24
2	H	500	HEM	C2D-C3D-C4D	2.13	105.11	101.50
2	H	500	HEM	CMA-C3A-C2A	2.17	129.78	125.24
2	C	500	HEM	C2D-C3D-C4D	2.25	105.32	101.50
2	M	500	HEM	C3B-C4B-CHC	2.30	126.40	123.16
2	I	500	HEM	C2D-C3D-C4D	2.30	105.40	101.50
2	N	500	HEM	C2D-C3D-C4D	2.30	105.40	101.50
2	O	500	HEM	C2C-C1C-CHC	2.32	127.21	123.68
2	O	500	HEM	C2D-C3D-C4D	2.36	105.49	101.50
2	I	500	HEM	CMA-C3A-C2A	2.39	130.23	125.24
2	N	500	HEM	C2C-C1C-CHC	2.47	127.44	123.68
2	N	500	HEM	C3B-C4B-CHC	2.56	126.77	123.16
2	G	500	HEM	C2D-C3D-C4D	2.68	106.05	101.50
2	H	500	HEM	CMD-C2D-C3D	2.74	126.47	114.35
2	B	500	HEM	CMD-C2D-C3D	2.80	126.72	114.35
2	P	500	HEM	CMD-C2D-C3D	2.80	126.75	114.35
2	L	500	HEM	C2D-C3D-C4D	2.81	106.26	101.50
2	I	500	HEM	CMD-C2D-C3D	2.81	126.79	114.35
2	G	500	HEM	CMD-C2D-C3D	2.83	126.87	114.35
2	N	500	HEM	CMD-C2D-C3D	2.90	127.20	114.35
2	G	500	HEM	C3B-C4B-CHC	2.91	127.25	123.16
2	L	500	HEM	CMD-C2D-C3D	2.93	127.30	114.35
2	A	500	HEM	CMD-C2D-C3D	2.96	127.43	114.35
2	K	500	HEM	CMD-C2D-C3D	2.98	127.52	114.35
2	F	500	HEM	CMD-C2D-C3D	2.98	127.55	114.35
2	J	500	HEM	CMD-C2D-C3D	3.08	127.96	114.35
2	C	500	HEM	CMD-C2D-C3D	3.09	128.02	114.35
2	O	500	HEM	CMD-C2D-C3D	3.13	128.20	114.35
2	A	500	HEM	C3B-C4B-CHC	3.14	127.58	123.16
2	D	500	HEM	C3B-C4B-CHC	3.15	127.60	123.16
2	L	500	HEM	CAD-C3D-C4D	3.16	123.62	112.47
2	E	500	HEM	CAD-C3D-C4D	3.18	123.69	112.47
2	J	500	HEM	CMB-C2B-C3B	3.23	124.60	116.53
2	C	500	HEM	CMB-C2B-C3B	3.31	124.80	116.53
2	M	500	HEM	CMD-C2D-C3D	3.45	129.62	114.35
2	J	500	HEM	CMC-C2C-C3C	3.62	125.56	116.53
2	D	500	HEM	CMD-C2D-C3D	3.66	130.54	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	500	HEM	CMC-C2C-C3C	3.66	125.67	116.53
2	F	500	HEM	CMC-C2C-C3C	3.72	125.83	116.53
2	F	500	HEM	CAD-C3D-C4D	3.73	125.63	112.47
2	E	500	HEM	CMD-C2D-C3D	3.77	131.01	114.35
2	E	500	HEM	CMB-C2B-C3B	3.81	126.05	116.53
2	A	500	HEM	CMB-C2B-C3B	3.82	126.08	116.53
2	B	500	HEM	CAD-C3D-C4D	3.83	125.98	112.47
2	B	500	HEM	CMB-C2B-C3B	3.84	126.12	116.53
2	D	500	HEM	CMB-C2B-C3B	3.85	126.14	116.53
2	D	500	HEM	CAD-C3D-C4D	3.85	126.05	112.47
2	L	500	HEM	CMB-C2B-C3B	3.85	126.15	116.53
2	F	500	HEM	CMB-C2B-C3B	3.89	126.25	116.53
2	G	500	HEM	CMB-C2B-C3B	3.91	126.30	116.53
2	N	500	HEM	CMC-C2C-C3C	3.91	126.30	116.53
2	K	500	HEM	CMC-C2C-C3C	3.97	126.43	116.53
2	A	500	HEM	CAD-C3D-C4D	3.97	126.46	112.47
2	D	500	HEM	CMC-C2C-C3C	3.98	126.47	116.53
2	C	500	HEM	CAD-C3D-C4D	4.00	126.59	112.47
2	M	500	HEM	CAD-C3D-C4D	4.02	126.64	112.47
2	C	500	HEM	CMC-C2C-C3C	4.04	126.61	116.53
2	K	500	HEM	CMB-C2B-C3B	4.05	126.64	116.53
2	O	500	HEM	CMC-C2C-C3C	4.06	126.66	116.53
2	H	500	HEM	CMB-C2B-C3B	4.09	126.74	116.53
2	I	500	HEM	CAD-C3D-C2D	4.14	125.12	113.22
2	P	500	HEM	CMB-C2B-C3B	4.17	126.93	116.53
2	G	500	HEM	CMC-C2C-C3C	4.19	126.98	116.53
2	K	500	HEM	CAD-C3D-C4D	4.28	127.57	112.47
2	O	500	HEM	CAD-C3D-C4D	4.28	127.58	112.47
2	G	500	HEM	CAD-C3D-C4D	4.30	127.63	112.47
2	N	500	HEM	CMB-C2B-C3B	4.30	127.27	116.53
2	P	500	HEM	CAD-C3D-C4D	4.37	127.89	112.47
2	O	500	HEM	CMB-C2B-C3B	4.42	127.55	116.53
2	N	500	HEM	CAD-C3D-C4D	4.42	128.06	112.47
2	I	500	HEM	CMB-C2B-C3B	4.44	127.61	116.53
2	M	500	HEM	CMB-C2B-C3B	4.45	127.63	116.53
2	H	500	HEM	CMC-C2C-C3C	4.45	127.64	116.53
2	H	500	HEM	CAD-C3D-C4D	4.48	128.26	112.47
2	G	500	HEM	CAD-C3D-C2D	4.55	126.31	113.22
2	J	500	HEM	CAD-C3D-C4D	4.57	128.58	112.47
2	J	500	HEM	CAD-C3D-C2D	4.62	126.51	113.22
2	N	500	HEM	CAD-C3D-C2D	4.63	126.54	113.22
2	H	500	HEM	CAD-C3D-C2D	4.65	126.59	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	CMC-C2C-C3C	4.69	128.23	116.53
2	O	500	HEM	CAD-C3D-C2D	4.76	126.91	113.22
2	A	500	HEM	CMC-C2C-C3C	4.81	128.54	116.53
2	I	500	HEM	CAD-C3D-C4D	4.82	129.47	112.47
2	P	500	HEM	CAD-C3D-C2D	4.82	127.08	113.22
2	E	500	HEM	CMC-C2C-C3C	4.87	128.68	116.53
2	I	500	HEM	CMC-C2C-C3C	4.94	128.86	116.53
2	K	500	HEM	CAD-C3D-C2D	4.98	127.52	113.22
2	L	500	HEM	CMC-C2C-C3C	5.14	129.36	116.53
2	C	500	HEM	CAD-C3D-C2D	5.16	128.06	113.22
2	M	500	HEM	CMC-C2C-C3C	5.19	129.49	116.53
2	A	500	HEM	CAD-C3D-C2D	5.47	128.94	113.22
2	D	500	HEM	CAD-C3D-C2D	5.47	128.96	113.22
2	B	500	HEM	CAD-C3D-C2D	5.48	128.97	113.22
2	M	500	HEM	CAD-C3D-C2D	5.50	129.04	113.22
2	F	500	HEM	CAD-C3D-C2D	5.60	129.31	113.22
2	L	500	HEM	CAD-C3D-C2D	5.88	130.12	113.22
2	E	500	HEM	CAD-C3D-C2D	6.38	131.56	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	6	0
2	C	500	HEM	2	0
2	D	500	HEM	2	0
2	E	500	HEM	7	0
2	F	500	HEM	3	0
2	G	500	HEM	3	0
2	H	500	HEM	2	0
2	I	500	HEM	9	0
2	J	500	HEM	1	0
2	K	500	HEM	4	0
2	L	500	HEM	5	0
2	M	500	HEM	2	0
2	N	500	HEM	1	0
2	O	500	HEM	4	0
2	P	500	HEM	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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	261/281 (92%)	-0.37	2 (0%)	87 87	27, 41, 65, 121	0
1	B	266/281 (94%)	-0.29	5 (1%)	70 69	30, 43, 70, 102	0
1	C	255/281 (90%)	-0.27	6 (2%)	62 61	29, 43, 70, 101	0
1	D	259/281 (92%)	-0.41	1 (0%)	93 93	27, 40, 64, 92	0
1	E	256/281 (91%)	-0.45	3 (1%)	81 81	26, 42, 70, 120	0
1	F	260/281 (92%)	-0.29	3 (1%)	81 81	29, 44, 80, 106	0
1	G	259/281 (92%)	-0.16	8 (3%)	52 52	29, 45, 76, 106	0
1	H	259/281 (92%)	-0.42	2 (0%)	87 87	27, 41, 63, 92	0
1	I	259/281 (92%)	-0.32	3 (1%)	81 81	29, 44, 68, 83	0
1	J	257/281 (91%)	-0.04	8 (3%)	52 52	28, 43, 71, 109	0
1	K	255/281 (90%)	0.01	10 (3%)	43 44	28, 41, 66, 99	0
1	L	260/281 (92%)	-0.29	5 (1%)	70 69	28, 43, 66, 91	0
1	M	255/281 (90%)	-0.42	2 (0%)	87 87	27, 42, 70, 97	0
1	N	260/281 (92%)	-0.12	6 (2%)	64 63	29, 44, 74, 105	0
1	O	257/281 (91%)	-0.19	4 (1%)	74 74	28, 44, 74, 116	0
1	P	259/281 (92%)	-0.42	2 (0%)	87 87	27, 43, 65, 93	0
All	All	4137/4496 (92%)	-0.28	70 (1%)	73 72	26, 43, 70, 121	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ALA	5.4
1	B	270	GLY	4.5
1	N	139	ALA	4.3
1	G	139	ALA	4.0
1	J	200	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	39	ARG	3.8
1	K	275	GLU	3.7
1	F	205	VAL	3.5
1	J	202	PRO	3.4
1	I	274	THR	3.3
1	N	205	VAL	3.2
1	K	205	VAL	3.2
1	C	274	THR	3.0
1	E	269	ARG	3.0
1	J	199	GLN	3.0
1	A	40	ASP	3.0
1	B	167	ALA	3.0
1	O	204	VAL	2.9
1	I	267	PHE	2.9
1	H	139	ALA	2.9
1	G	202	PRO	2.9
1	G	299	LEU	2.9
1	C	205	VAL	2.9
1	K	204	VAL	2.8
1	J	167	ALA	2.8
1	K	224	LEU	2.7
1	K	194	ALA	2.7
1	C	139	ALA	2.6
1	N	204	VAL	2.6
1	G	204	VAL	2.6
1	E	40	ASP	2.6
1	L	116	VAL	2.5
1	K	202	PRO	2.5
1	N	207	ARG	2.5
1	B	137	LEU	2.5
1	I	269	ARG	2.4
1	L	202	PRO	2.4
1	C	204	VAL	2.4
1	O	140	SER	2.4
1	K	200	ILE	2.4
1	G	198	PHE	2.4
1	J	205	VAL	2.4
1	G	140	SER	2.4
1	N	203	GLU	2.4
1	J	197	GLY	2.3
1	G	203	GLU	2.3
1	J	219	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	41	MET	2.3
1	C	203	GLU	2.3
1	L	113	ASP	2.3
1	L	224	LEU	2.3
1	J	298	ASP	2.3
1	F	198	PHE	2.2
1	K	198	PHE	2.2
1	D	118	ALA	2.2
1	L	112	MET	2.1
1	P	116	VAL	2.1
1	M	267	PHE	2.1
1	H	113	ASP	2.1
1	C	202	PRO	2.1
1	M	111	ILE	2.1
1	N	138	GLY	2.1
1	G	226	VAL	2.0
1	O	205	VAL	2.0
1	P	113	ASP	2.0
1	K	217	ALA	2.0
1	B	138	GLY	2.0
1	F	204	VAL	2.0
1	K	203	GLU	2.0
1	O	203	GLU	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
2	HEM	F	500	43/43	0.98	0.12	0.03	39,47,58,74	0
2	HEM	O	500	43/43	0.97	0.10	-0.62	48,58,68,80	0
2	HEM	N	500	43/43	0.98	0.10	-0.63	37,56,65,74	0
2	HEM	I	500	43/43	0.97	0.10	-0.71	24,37,57,60	0
2	HEM	B	500	43/43	0.98	0.10	-0.73	32,43,56,62	0
2	HEM	K	500	43/43	0.98	0.10	-0.75	28,43,61,71	0
2	HEM	G	500	43/43	0.98	0.10	-0.78	43,52,63,70	0
2	HEM	L	500	43/43	0.98	0.10	-0.82	20,34,53,63	0
2	HEM	M	500	43/43	0.98	0.10	-0.83	25,37,48,52	0
2	HEM	J	500	43/43	0.98	0.10	-0.90	27,42,57,67	0
2	HEM	E	500	43/43	0.98	0.09	-1.06	21,32,48,58	0
2	HEM	A	500	43/43	0.98	0.09	-1.15	18,28,39,57	0
2	HEM	P	500	43/43	0.99	0.08	-1.18	20,31,42,54	0
2	HEM	C	500	43/43	0.98	0.09	-1.24	28,42,62,68	0
2	HEM	D	500	43/43	0.98	0.10	-1.30	18,29,37,44	0
2	HEM	H	500	43/43	0.98	0.09	-1.44	16,29,37,43	0

6.5 Other polymers (i)

There are no such residues in this entry.