W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:05 am GMT

PDB ID	:	1UC3
Title	:	Crystal Structure of hemoglobin I from river lamprey
Authors	:	Seki, M.; Yao, M.; Yazawa, Y.; Tanaka, I.
Deposited on	:	2003-04-08
Resolution	:	2.30 Å(reported)

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

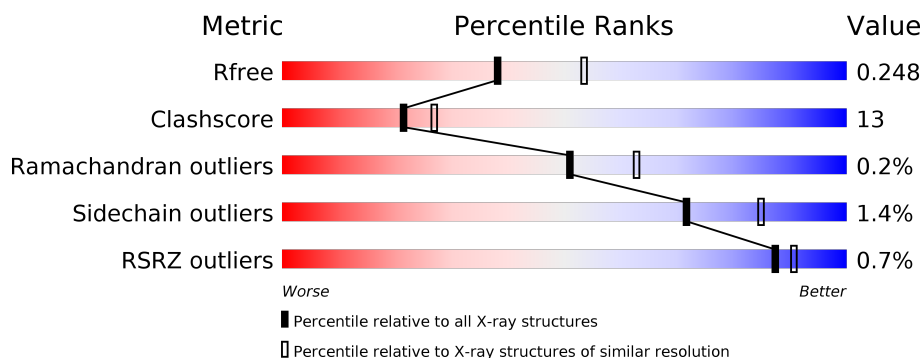|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		1.4%
RSRZ outliers		0.7%

Worse — Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	149	4% · 70% / 30%
1	B	149	66% / 34%
1	C	149	% · 74% / 26%
1	D	149	74% / 25% ·
1	E	149	81% / 19% ·
1	F	149	66% / 34%

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Mol	Chain	Length	Quality of chain
1	G	149	75% 25%
1	H	149	% 78% 22%
1	I	149	% 77% 20%
1	J	149	% 69% 30%
1	K	149	66% 34%
1	L	149	% 73% 26%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 15098 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 Globin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	B	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	C	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	D	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	E	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	F	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	G	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	H	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	I	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	J	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	K	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			
1	L	149	Total	C	N	O	S	0	0	0
			1143	729	190	217	7			

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

HEM

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		

- Molecule 3 is water.

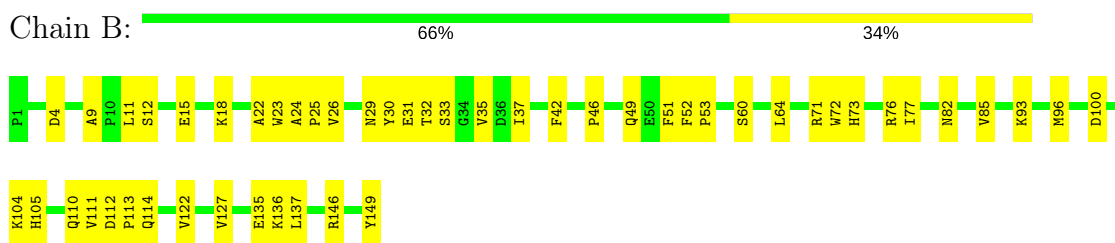| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total 27	O 27	0	0
3	B	51	Total 51	O 51	0	0
3	C	62	Total 62	O 62	0	0
3	D	91	Total 91	O 91	0	0
3	E	109	Total 109	O 109	0	0
3	F	59	Total 59	O 59	0	0
3	G	61	Total 61	O 61	0	0
3	H	75	Total 75	O 75	0	0
3	I	105	Total 105	O 105	0	0
3	J	97	Total 97	O 97	0	0
3	K	63	Total 63	O 63	0	0
3	L	66	Total 66	O 66	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.
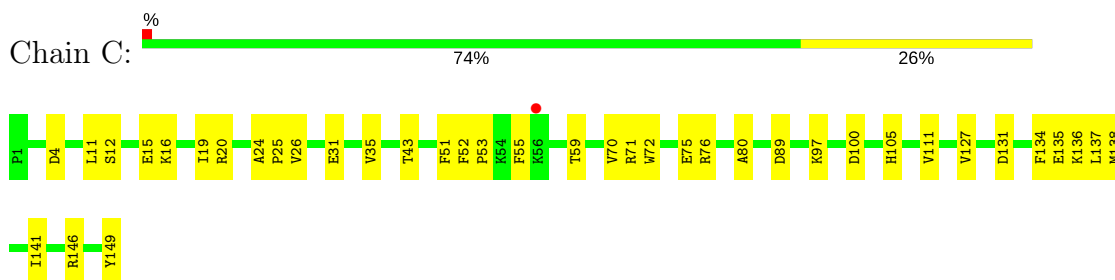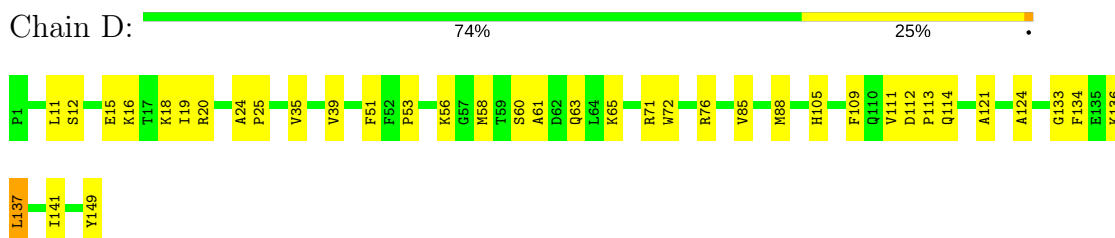
- Molecule 1: Globin

Chain A:

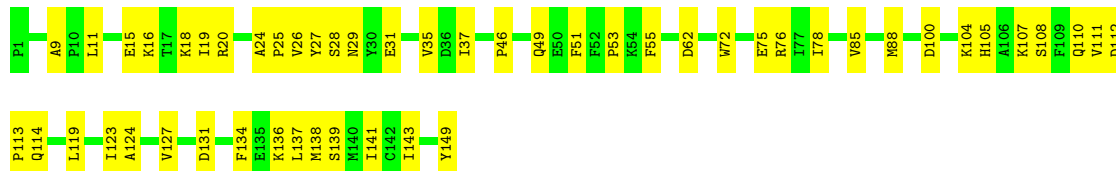- Molecule 1: Globin

Chain B:

- Molecule 1: Globin

Chain C:

- Molecule 1: Globin

Chain D:

• Molecule 1: Globin

Chain E:

81%   19%

P1 L11 S12 E15 A24 P25 V26 F51 F52 P53 K56 A68 R71 W72 H73 A74 E75 R76 I77 I78 T91 M94 K97 L98 L101 F116 V127 D131 E135 K136 L137 I143 Y149

• Molecule 1: Globin

Chain F:

66%   34%

P1 A9 P10 L11 E15 K16 T17 K18 I19 R20 A24 P25 V26 Y27 S28 N29 Y30 E31 V35 D36 I37 P46 Q49 E50 F51 F52 P53 K54 F55 D62 W72 E75 R76 I77 I78 V85 M88 D100 K104 H105 A106 K107 S108 F109 Q110 V111 D112

P113 Q114 L119 I123 A124 V127 D131 F134 E135 K136 L137 M138 S139 M140 I141 C142 I143 Y149

• Molecule 1: Globin

Chain G:

75%   25%

P1 V8 A9 P10 L11 S12 E15 K16 I19 R20 A24 P25 F51 F52 P53 K66 S67 V70 R71 W72 E75 R76 I77 I78 S95 M96 K97 L98 R99 K107 S108 P113 A120 A124 D131 A132 G133 F134 E135 K136 L137 M138 S139 I143

Y149

• Molecule 1: Globin

Chain H:

%
78%   22%

P1 V8 L11 S12 E15 K18 A22 W23 A24 P25 E31 F42 Q49 E50 F51 F52 P53 K54 F55 T59 S60 A61 D62 Q63 R71 W72 H73 R76 I77 T91 E92 S95 M96 R99 H105 E135 K136 L137 M140 Y149

• Molecule 1: Globin

Chain I:

%
77%   20%

P1 A9 I19 A24 P25 V26 Y27 S28 N29 Y30 S33 I37 F51 F55 S60 A61 D62 Q63 V70 R71 W72 R76 I77 I78 K93 M94 S95 M96 K97 L98 R99 H105 V111 D112 P113 I123 V127 K136 L137 Y149

• Molecule 1: Globin

Chain J:

%
69%   30%

P1 D4 S7 V8 L11 S12 E15 K18 A24 P25 S28 N29 Y30 E31 T32 S33 G34 V35 D36 I37 L38 V39 P46 Q49 E50 F51 F52 P53 K54 F55 K56 G57 M58 T59 S60 A61 D62 Q63 L64 K65 A68 D69 V70 R71 W72 R76 E92

L101 H105 V111 D112 P113 V122 G133 K136 L137 M138 S139 M140 R146 Y149

● Molecule 1: Globin

Chain K:

66%   34%

P1 V8 A9 P10 L11 S12 E15 K16 R20 A24 P25 N29 Y30 E31 T32 S33 G34 V35 D36 I37 K40 F41 F42 P46 A47 A48 Q49 E50 F51 F52 P53 K54 F55 M58 T59 S60 Q63 L64 R71 W72 R76 S95 R99 G103 A106

K107 D112 P113 Q114 Y115 F116 L119 I123 A124 F134 E135 K136 L137 M140 Y149

● Molecule 1: Globin

%

Chain L:

73%   26%   •

P1 S7 V8 A9 P10 L11 S12 K16 A22 W23 A24 P25 V26 Y30 E31 V35 V39 P46 Q49 E50 F51 F52 P53 M58 D62 Q63 W72 R76 I77 I78 M88 E92 K93 M94 H105 V111 D112 P113 F116 K117 V127

G133 K136 L137 C142 I143 L144 Y149

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.21Å 73.61Å 105.87Å 103.95° 91.52° 97.64°	Depositor
Resolution (Å)	10.00 – 2.30 102.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.30) 89.8 (102.56-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.29Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.197 , 0.258 0.193 , 0.248	Depositor DCC
R_{free} test set	7524 reflections (11.23%)	DCC
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15098	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.33	0/1166	0.50	0/1573
1	B	0.35	0/1166	0.55	0/1573
1	C	0.35	0/1166	0.56	0/1573
1	D	0.36	0/1166	0.56	0/1573
1	E	0.36	0/1166	0.59	0/1573
1	F	0.35	0/1166	0.59	0/1573
1	G	0.33	0/1166	0.57	0/1573
1	H	0.34	0/1166	0.58	0/1573
1	I	0.38	0/1166	0.59	0/1573
1	J	0.39	0/1166	0.57	0/1573
1	K	0.35	0/1166	0.56	0/1573
1	L	0.35	0/1166	0.58	0/1573
All	All	0.35	0/13992	0.57	0/18876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1143	0	1151	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1143	0	1151	40	0
1	C	1143	0	1151	33	0
1	D	1143	0	1151	29	0
1	E	1143	0	1151	25	0
1	F	1143	0	1151	34	0
1	G	1143	0	1151	30	0
1	H	1143	0	1151	25	0
1	I	1143	0	1151	30	0
1	J	1143	0	1151	40	0
1	K	1143	0	1151	37	0
1	L	1143	0	1151	27	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
2	E	43	0	30	3	0
2	F	43	0	30	1	0
2	G	43	0	30	2	0
2	H	43	0	30	2	0
2	I	43	0	30	1	0
2	J	43	0	30	1	0
2	K	43	0	30	0	0
2	L	43	0	30	2	0
3	A	27	0	0	2	0
3	B	51	0	0	3	0
3	C	62	0	0	3	0
3	D	91	0	0	5	0
3	E	109	0	0	3	0
3	F	59	0	0	2	0
3	G	61	0	0	4	0
3	H	75	0	0	4	0
3	I	105	0	0	2	0
3	J	97	0	0	6	0
3	K	63	0	0	1	0
3	L	66	0	0	4	0
All	All	15098	0	14172	383	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 (383) 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:I:95:SER:HB3	1:I:99:ARG:NH1	1.81	0.94
1:G:11:LEU:HD23	1:G:136:LYS:HD2	1.51	0.91
1:J:72:TRP:CE2	1:J:76:ARG:HD2	2.11	0.86
1:J:11:LEU:HD23	1:J:136:LYS:HD2	1.57	0.86
1:K:95:SER:HB3	1:K:99:ARG:NH1	1.92	0.83
1:C:105:HIS:HD2	1:C:111:VAL:HG21	1.45	0.81
1:A:72:TRP:CE2	1:A:76:ARG:HD2	2.17	0.79
1:I:93:LYS:HA	1:I:96:MET:HE2	1.63	0.79
1:J:113:PRO:HG3	1:J:149:TYR:CD2	2.18	0.79
1:L:72:TRP:CE2	1:L:76:ARG:HD2	2.19	0.78
1:E:56:LYS:HG3	1:I:24:ALA:HB3	1.65	0.78
1:L:30:TYR:HB2	1:L:78:ILE:HG21	1.64	0.78
1:B:11:LEU:HD23	1:B:136:LYS:HD2	1.66	0.76
1:J:7:SER:HB3	3:J:183:HOH:O	1.85	0.76
1:I:113:PRO:HG3	1:I:149:TYR:CD2	2.21	0.76
1:E:72:TRP:CE2	1:E:76:ARG:HD2	2.23	0.74
1:J:28:SER:HB2	3:J:196:HOH:O	1.87	0.74
1:I:72:TRP:CE2	1:I:76:ARG:HD2	2.23	0.73
1:A:11:LEU:HD23	1:A:136:LYS:HD2	1.70	0.73
1:D:112:ASP:OD1	1:D:114:GLN:HG2	1.89	0.72
1:J:113:PRO:HG3	1:J:149:TYR:CE2	2.24	0.72
1:F:113:PRO:HG3	1:F:149:TYR:CD2	2.25	0.72
1:K:11:LEU:HD23	1:K:136:LYS:HD2	1.73	0.71
1:B:112:ASP:OD1	1:B:114:GLN:HG3	1.91	0.71
1:C:11:LEU:HD23	1:C:136:LYS:HD2	1.73	0.70
1:H:72:TRP:CE2	1:H:76:ARG:HD2	2.26	0.70
1:E:68:ALA:HB2	1:F:28:SER:HA	1.73	0.70
1:A:137:LEU:HD22	1:A:138:MET:HE2	1.74	0.69
1:G:24:ALA:HB3	1:G:25:PRO:HD3	1.75	0.69
1:K:47:ALA:O	1:K:50:GLU:HG2	1.93	0.68
1:H:12:SER:OG	1:H:15:GLU:HG3	1.92	0.68
1:D:113:PRO:HG3	1:D:149:TYR:CE2	2.29	0.68
1:F:72:TRP:CE2	1:F:76:ARG:HD2	2.29	0.68
1:G:72:TRP:CE2	1:G:76:ARG:HD2	2.28	0.67
1:A:95:SER:O	1:A:99:ARG:HG3	1.94	0.67
1:D:72:TRP:CE2	1:D:76:ARG:HD2	2.30	0.67
1:G:9:ALA:O	1:G:136:LYS:HD3	1.94	0.67
1:K:72:TRP:CE2	1:K:76:ARG:HD2	2.30	0.67
1:D:113:PRO:HG3	1:D:149:TYR:CD2	2.29	0.66
1:E:101:LEU:HD21	2:E:150:HEM:HMA1	1.77	0.66
1:F:9:ALA:O	1:F:136:LYS:HD3	1.95	0.66
1:I:93:LYS:HA	1:I:96:MET:CE	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:ALA:HB3	1:H:25:PRO:HD3	1.78	0.65
1:L:105:HIS:HD2	1:L:111:VAL:HG21	1.62	0.65
1:B:4:ASP:HB2	1:B:146:ARG:HD3	1.77	0.65
1:K:95:SER:HB3	1:K:99:ARG:HH11	1.61	0.65
1:J:24:ALA:HB3	1:J:25:PRO:HD3	1.78	0.65
1:E:11:LEU:HD23	1:E:136:LYS:HD2	1.79	0.65
1:I:113:PRO:HG3	1:I:149:TYR:CE2	2.33	0.64
1:F:26:VAL:HG21	1:F:127:VAL:HG22	1.78	0.64
1:F:139:SER:O	1:F:143:ILE:HG13	1.98	0.64
1:L:51:PHE:C	1:L:53:PRO:HD3	2.18	0.64
1:A:24:ALA:HB3	1:A:25:PRO:HD3	1.79	0.64
1:F:85:VAL:O	1:F:88:MET:HG3	1.96	0.63
1:K:24:ALA:HB3	1:K:25:PRO:HD3	1.79	0.63
1:A:29:ASN:ND2	1:A:32:THR:HB	2.13	0.63
1:F:124:ALA:HB1	3:F:177:HOH:O	1.97	0.63
1:J:57:GLY:O	1:J:59:THR:HG23	1.99	0.63
1:C:105:HIS:CD2	1:C:111:VAL:HG21	2.31	0.63
1:D:24:ALA:HB3	1:D:25:PRO:HD3	1.81	0.62
1:F:11:LEU:HD23	1:F:136:LYS:HD2	1.81	0.62
1:G:67:SER:HB3	1:G:70:VAL:HG23	1.80	0.62
1:I:95:SER:HB3	1:I:99:ARG:HH12	1.63	0.62
1:D:11:LEU:HD23	1:D:136:LYS:HD2	1.82	0.61
1:A:9:ALA:O	1:A:136:LYS:HD3	2.00	0.61
1:I:62:ASP:HB3	3:I:196:HOH:O	2.00	0.61
1:G:66:LYS:HE3	3:G:204:HOH:O	2.00	0.61
1:L:72:TRP:O	1:L:76:ARG:HD3	2.00	0.61
1:B:93:LYS:HA	1:B:96:MET:HE3	1.83	0.61
1:E:24:ALA:HB3	1:E:25:PRO:HD3	1.83	0.61
1:D:72:TRP:O	1:D:76:ARG:HD3	2.01	0.61
1:E:26:VAL:HG21	1:E:127:VAL:HG22	1.81	0.61
1:H:72:TRP:O	1:H:76:ARG:HD3	2.00	0.61
1:B:24:ALA:HB3	1:B:25:PRO:HD3	1.81	0.60
1:D:35:VAL:O	1:D:39:VAL:HG23	2.01	0.60
1:J:133:GLY:HA3	3:J:202:HOH:O	2.01	0.60
1:F:113:PRO:HG3	1:F:149:TYR:CE2	2.36	0.60
1:H:71:ARG:NH2	3:H:155:HOH:O	2.34	0.60
1:J:46:PRO:HA	1:J:49:GLN:HG3	1.83	0.60
1:B:72:TRP:CE2	1:B:76:ARG:HD2	2.37	0.60
1:B:23:TRP:CD1	1:B:85:VAL:HG21	2.37	0.60
1:D:51:PHE:C	1:D:53:PRO:HD3	2.22	0.60
1:C:24:ALA:HB3	1:C:25:PRO:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:VAL:HG21	1:J:71:ARG:HG2	1.85	0.59
1:J:72:TRP:O	1:J:76:ARG:HD3	2.03	0.59
1:A:97:LYS:HD3	3:A:165:HOH:O	2.03	0.59
1:C:72:TRP:CE2	1:C:76:ARG:HD2	2.38	0.59
1:B:93:LYS:HA	1:B:96:MET:CE	2.32	0.59
1:A:137:LEU:HD22	1:A:138:MET:CE	2.33	0.58
1:L:12:SER:O	1:L:16:LYS:HG3	2.03	0.58
1:C:12:SER:OG	1:C:15:GLU:HG3	2.03	0.58
1:C:97:LYS:NZ	1:C:97:LYS:HB3	2.18	0.58
2:L:150:HEM:HMC1	2:L:150:HEM:HBC2	1.85	0.58
1:G:95:SER:O	1:G:99:ARG:HG3	2.03	0.58
3:E:153:HOH:O	1:G:107:LYS:HE3	2.03	0.58
1:I:97:LYS:HD3	3:I:179:HOH:O	2.02	0.58
1:F:110:GLN:HE21	1:H:8:VAL:HG23	1.68	0.57
1:F:15:GLU:O	1:F:19:ILE:HG13	2.04	0.57
1:D:12:SER:OG	1:D:15:GLU:HG3	2.04	0.57
1:D:61:ALA:O	1:D:65:LYS:HG3	2.04	0.57
1:J:92:GLU:HG2	3:J:222:HOH:O	2.04	0.57
1:E:71:ARG:HD2	1:F:31:GLU:OE1	2.04	0.57
1:L:24:ALA:HB3	1:L:25:PRO:HD3	1.87	0.57
2:E:150:HEM:HMC2	2:E:150:HEM:HBC2	1.86	0.57
1:L:7:SER:HB3	3:L:164:HOH:O	2.04	0.56
1:K:112:ASP:OD1	1:K:114:GLN:HG3	2.05	0.56
1:A:73:HIS:O	1:A:77:ILE:HG13	2.06	0.56
1:K:42:PHE:CE1	1:K:49:GLN:HA	2.40	0.56
1:A:80:ALA:HB2	2:A:150:HEM:HMA2	1.87	0.56
1:H:135:GLU:HG3	3:H:193:HOH:O	2.06	0.56
1:B:72:TRP:O	1:B:76:ARG:HD3	2.04	0.56
1:E:56:LYS:HE3	1:I:24:ALA:HB1	1.87	0.56
1:A:72:TRP:O	1:A:76:ARG:HD3	2.07	0.55
1:G:71:ARG:NH1	1:H:31:GLU:OE2	2.40	0.55
1:D:18:LYS:O	1:D:18:LYS:HD3	2.07	0.55
1:J:72:TRP:CD2	1:J:76:ARG:HD2	2.41	0.55
1:F:18:LYS:HD2	1:F:131:ASP:OD1	2.07	0.55
2:H:150:HEM:HMC2	2:H:150:HEM:HBC2	1.88	0.55
1:B:113:PRO:HD3	1:B:149:TYR:CE2	2.42	0.55
1:L:144:LEU:HD23	3:L:216:HOH:O	2.07	0.55
1:F:100:ASP:OD1	1:F:104:LYS:HE3	2.07	0.54
1:A:71:ARG:CB	1:A:71:ARG:HH11	2.20	0.54
1:J:101:LEU:HD21	2:J:150:HEM:HMA1	1.89	0.54
1:K:46:PRO:HA	1:K:49:GLN:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:TRP:O	1:C:76:ARG:HD3	2.07	0.54
1:K:60:SER:OG	1:K:63:GLN:HG3	2.08	0.54
1:A:123:ILE:O	1:A:127:VAL:HG23	2.07	0.54
1:D:51:PHE:CZ	1:D:112:ASP:HB2	2.42	0.54
1:I:24:ALA:HB3	1:I:25:PRO:HD3	1.88	0.54
1:I:55:PHE:CZ	1:I:70:VAL:HA	2.42	0.54
1:D:121:ALA:HB3	3:D:218:HOH:O	2.07	0.54
1:F:112:ASP:OD1	1:F:114:GLN:HG2	2.08	0.54
1:J:56:LYS:HE2	3:J:211:HOH:O	2.08	0.54
1:C:55:PHE:CZ	1:C:70:VAL:HA	2.43	0.54
1:C:43:THR:HG22	1:C:59:THR:O	2.09	0.53
1:E:73:HIS:O	1:E:77:ILE:HG13	2.09	0.53
1:C:72:TRP:CD2	1:C:76:ARG:HD2	2.43	0.53
1:J:137:LEU:HD13	1:J:138:MET:CE	2.38	0.53
1:K:36:ASP:O	1:K:40:LYS:HB2	2.09	0.53
1:G:16:LYS:O	1:G:20:ARG:HG3	2.08	0.53
1:G:72:TRP:O	1:G:76:ARG:HD3	2.07	0.53
1:H:11:LEU:HD23	1:H:136:LYS:HD2	1.90	0.53
1:A:75:GLU:O	1:A:78:ILE:HG22	2.09	0.53
1:D:133:GLY:HA3	3:D:207:HOH:O	2.09	0.53
1:F:24:ALA:HB3	1:F:25:PRO:HD3	1.91	0.53
1:L:88:MET:HA	1:L:94:MET:CE	2.39	0.52
1:J:30:TYR:HA	1:J:33:SER:HB2	1.91	0.52
1:D:16:LYS:O	1:D:20:ARG:HG3	2.09	0.52
1:E:91:THR:HG21	1:G:108:SER:O	2.09	0.52
1:I:27:TYR:O	1:I:28:SER:CB	2.56	0.52
1:H:60:SER:OG	1:H:63:GLN:HG3	2.09	0.52
1:A:12:SER:OG	1:A:15:GLU:HG3	2.10	0.52
1:B:42:PHE:CE1	1:B:49:GLN:HG2	2.45	0.52
1:I:30:TYR:HA	1:I:33:SER:HB2	1.92	0.52
1:J:37:ILE:HG23	1:J:122:VAL:HG12	1.91	0.52
1:B:29:ASN:ND2	1:B:32:THR:HB	2.24	0.52
1:K:71:ARG:NH1	1:L:31:GLU:OE2	2.42	0.52
1:B:100:ASP:OD2	1:B:104:LYS:HE3	2.09	0.52
1:H:95:SER:HB3	1:H:99:ARG:NH1	2.25	0.52
1:F:31:GLU:O	1:F:35:VAL:HG23	2.10	0.51
2:G:150:HEM:HMB1	2:G:150:HEM:HBB2	1.92	0.51
1:H:95:SER:HB3	1:H:99:ARG:HH11	1.74	0.51
1:D:51:PHE:O	1:D:53:PRO:HD3	2.10	0.51
1:F:27:TYR:C	1:F:29:ASN:H	2.14	0.51
1:H:73:HIS:CE1	1:H:77:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:LYS:HE3	3:H:166:HOH:O	2.11	0.51
1:B:29:ASN:OD1	1:B:32:THR:HB	2.11	0.51
1:C:131:ASP:O	1:C:135:GLU:HG3	2.11	0.51
1:B:37:ILE:HG23	1:B:122:VAL:HG12	1.92	0.51
1:F:16:LYS:O	1:F:20:ARG:HG3	2.10	0.51
1:C:138:MET:HE1	1:C:141:ILE:HD12	1.91	0.51
1:E:75:GLU:O	1:E:78:ILE:HG22	2.11	0.50
1:K:51:PHE:O	1:K:53:PRO:HD3	2.10	0.50
1:D:111:VAL:HG11	2:D:150:HEM:CHD	2.41	0.50
1:D:60:SER:OG	1:D:63:GLN:HG3	2.12	0.50
1:B:110:GLN:HG2	3:B:180:HOH:O	2.12	0.50
1:B:26:VAL:HG21	1:B:127:VAL:HG22	1.95	0.49
1:B:18:LYS:HD3	1:B:18:LYS:O	2.13	0.49
1:A:42:PHE:CE1	1:A:49:GLN:HG2	2.48	0.49
1:J:105:HIS:HD2	1:J:111:VAL:HG21	1.76	0.49
1:K:55:PHE:HA	1:K:58:MET:HE1	1.94	0.49
1:A:95:SER:HB3	1:A:99:ARG:NH1	2.28	0.49
1:B:12:SER:OG	1:B:15:GLU:HG3	2.13	0.49
1:L:88:MET:HA	1:L:94:MET:HE1	1.95	0.49
3:F:167:HOH:O	1:H:91:THR:HG21	2.12	0.49
1:K:116:PHE:HB2	3:K:155:HOH:O	2.12	0.49
1:C:111:VAL:HG23	1:C:149:TYR:HH	1.78	0.49
1:G:11:LEU:CD2	1:G:136:LYS:HD2	2.36	0.49
1:G:97:LYS:HE3	3:G:180:HOH:O	2.13	0.49
1:A:71:ARG:NH1	1:B:31:GLU:OE1	2.45	0.48
1:C:51:PHE:C	1:C:53:PRO:HD3	2.33	0.48
1:I:105:HIS:HD2	1:I:111:VAL:HG11	1.78	0.48
1:I:19:ILE:HD13	1:I:137:LEU:HD12	1.95	0.48
1:J:60:SER:HB3	1:J:63:GLN:HG3	1.95	0.48
1:G:131:ASP:O	1:G:135:GLU:HG3	2.13	0.48
1:H:51:PHE:C	1:H:53:PRO:HD3	2.33	0.48
1:D:105:HIS:HA	1:D:109:PHE:HB2	1.95	0.48
1:I:99:ARG:HH11	1:I:99:ARG:HG3	1.79	0.48
1:J:12:SER:OG	1:J:15:GLU:HG3	2.13	0.48
1:B:42:PHE:CZ	1:B:49:GLN:HG2	2.49	0.48
1:A:119:LEU:O	1:A:123:ILE:HG13	2.13	0.48
1:C:52:PHE:CZ	2:C:150:HEM:HAC	2.49	0.48
1:H:42:PHE:CE1	1:H:49:GLN:HA	2.49	0.48
1:K:95:SER:HB3	1:K:99:ARG:HH12	1.73	0.48
1:A:82:ASN:O	1:A:85:VAL:HG22	2.13	0.48
1:C:89:ASP:HB2	3:C:156:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:SER:HB3	1:G:70:VAL:CG2	2.42	0.48
1:E:97:LYS:HD3	3:E:155:HOH:O	2.14	0.48
1:H:18:LYS:HD3	1:H:18:LYS:O	2.14	0.48
2:I:150:HEM:HBC2	2:I:150:HEM:HMC2	1.95	0.48
1:C:71:ARG:O	1:C:75:GLU:HG3	2.13	0.48
1:L:113:PRO:HA	1:L:116:PHE:CE2	2.49	0.48
1:I:28:SER:HA	1:J:68:ALA:HB2	1.96	0.48
1:I:37:ILE:HG21	1:I:123:ILE:HG12	1.96	0.48
1:K:33:SER:O	1:K:37:ILE:HG13	2.14	0.47
1:L:46:PRO:HA	1:L:49:GLN:HG3	1.96	0.47
1:C:20:ARG:NH1	3:C:168:HOH:O	2.46	0.47
1:J:137:LEU:HD13	1:J:138:MET:HE2	1.95	0.47
1:E:143:ILE:HG22	1:G:107:LYS:HG2	1.96	0.47
1:F:51:PHE:CZ	1:F:112:ASP:HB2	2.49	0.47
1:L:26:VAL:HG21	1:L:127:VAL:HG22	1.97	0.47
1:F:105:HIS:HD2	1:F:111:VAL:HG21	1.79	0.47
1:G:19:ILE:HD11	1:G:133:GLY:O	2.14	0.47
1:H:22:ALA:O	1:H:25:PRO:HD2	2.14	0.47
1:J:55:PHE:O	1:J:56:LYS:C	2.53	0.47
1:K:29:ASN:ND2	1:K:32:THR:HB	2.29	0.47
1:B:51:PHE:C	1:B:53:PRO:HD3	2.35	0.47
1:F:75:GLU:O	1:F:78:ILE:HG22	2.14	0.47
1:B:82:ASN:O	1:B:85:VAL:HG22	2.15	0.47
1:C:97:LYS:HE3	3:C:184:HOH:O	2.14	0.47
1:L:72:TRP:CD2	1:L:76:ARG:HD2	2.49	0.47
1:B:29:ASN:CG	1:B:32:THR:HB	2.36	0.47
1:B:4:ASP:HB2	1:B:146:ARG:CD	2.42	0.47
1:I:72:TRP:O	1:I:76:ARG:HD3	2.14	0.47
1:C:111:VAL:HG23	1:C:149:TYR:OH	2.15	0.46
1:G:12:SER:OG	1:G:15:GLU:HG3	2.16	0.46
1:H:135:GLU:N	3:H:193:HOH:O	2.48	0.46
1:L:105:HIS:HB3	1:L:149:TYR:OH	2.16	0.46
1:C:15:GLU:O	1:C:19:ILE:HG13	2.15	0.46
1:E:143:ILE:CG2	1:G:107:LYS:HG2	2.46	0.46
1:B:72:TRP:CD2	1:B:76:ARG:HD2	2.51	0.46
1:J:8:VAL:HG21	1:J:140:MET:HG3	1.97	0.46
2:L:150:HEM:CMC	2:L:150:HEM:HBC2	2.46	0.46
1:A:38:LEU:HD13	1:A:77:ILE:HD12	1.98	0.46
1:K:58:MET:HE3	1:K:64:LEU:HD23	1.98	0.46
1:F:51:PHE:C	1:F:53:PRO:HD3	2.36	0.46
1:J:31:GLU:O	1:J:35:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:O	1:A:8:VAL:HG23	2.16	0.45
1:F:19:ILE:HG23	1:F:134:PHE:HD1	1.80	0.45
1:H:92:GLU:HG2	1:H:96:MET:CE	2.45	0.45
1:A:18:LYS:HD3	1:A:18:LYS:O	2.16	0.45
1:C:16:LYS:NZ	1:C:89:ASP:OD1	2.35	0.45
1:I:30:TYR:HB2	1:I:78:ILE:HG21	1.98	0.45
1:K:103:GLY:O	1:K:107:LYS:HG3	2.16	0.45
1:L:133:GLY:HA3	3:L:178:HOH:O	2.16	0.45
1:L:8:VAL:HG23	1:L:9:ALA:O	2.16	0.45
1:A:111:VAL:HB	2:A:150:HEM:CBC	2.46	0.45
1:A:136:LYS:O	1:A:140:MET:HG3	2.17	0.45
1:J:51:PHE:C	1:J:53:PRO:HD3	2.37	0.45
1:E:116:PHE:HB2	3:E:152:HOH:O	2.15	0.45
1:F:138:MET:HE2	1:F:141:ILE:HD12	1.99	0.45
1:G:113:PRO:HD3	1:G:149:TYR:CE2	2.52	0.45
1:J:4:ASP:HB2	1:J:146:ARG:HD3	1.99	0.45
1:B:35:VAL:HG21	1:B:71:ARG:HG2	1.99	0.45
1:C:80:ALA:HB2	2:C:150:HEM:HMA2	1.98	0.45
1:D:137:LEU:O	1:D:141:ILE:HG13	2.17	0.45
2:H:150:HEM:CMC	2:H:150:HEM:HBC2	2.46	0.44
1:J:55:PHE:CZ	1:J:70:VAL:HA	2.52	0.44
1:K:55:PHE:HA	1:K:58:MET:CE	2.47	0.44
1:J:60:SER:HB3	1:J:63:GLN:OE1	2.17	0.44
1:A:51:PHE:C	1:A:53:PRO:HD3	2.37	0.44
1:B:96:MET:HE3	1:B:96:MET:HB2	1.87	0.44
1:K:12:SER:OG	1:K:15:GLU:HG3	2.17	0.44
1:K:124:ALA:HA	1:K:134:PHE:CE2	2.52	0.44
1:K:29:ASN:HD21	1:K:32:THR:HB	1.82	0.44
1:H:8:VAL:HG21	1:H:140:MET:HG3	2.00	0.44
1:K:37:ILE:HG21	1:K:123:ILE:HG12	1.99	0.44
1:I:112:ASP:HA	1:I:113:PRO:HD3	1.84	0.44
1:I:9:ALA:O	1:I:136:LYS:HD3	2.16	0.44
1:F:72:TRP:O	1:F:76:ARG:HD3	2.17	0.44
1:G:139:SER:O	1:G:143:ILE:HG13	2.17	0.44
1:G:75:GLU:O	1:G:78:ILE:HG22	2.18	0.44
1:K:46:PRO:O	1:K:49:GLN:HG3	2.18	0.44
1:I:60:SER:OG	1:I:63:GLN:HG3	2.17	0.44
1:G:120:ALA:HB1	1:G:138:MET:HB3	1.99	0.43
1:E:72:TRP:CD2	1:E:76:ARG:HD2	2.53	0.43
1:E:94:MET:HG2	1:E:98:LEU:HD12	2.00	0.43
1:G:8:VAL:HG23	1:G:8:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:VAL:HG21	1:K:140:MET:HG3	2.00	0.43
1:B:73:HIS:O	1:B:77:ILE:HG13	2.18	0.43
2:E:150:HEM:CMC	2:E:150:HEM:HBC2	2.47	0.43
1:G:72:TRP:CD2	1:G:76:ARG:HD2	2.54	0.43
1:B:110:GLN:HG2	3:B:194:HOH:O	2.19	0.43
1:D:124:ALA:HA	1:D:134:PHE:CE2	2.53	0.43
1:E:131:ASP:O	1:E:135:GLU:HG3	2.19	0.43
1:A:95:SER:HB3	1:A:99:ARG:CZ	2.48	0.43
1:B:60:SER:O	1:B:64:LEU:HG	2.18	0.43
1:C:31:GLU:O	1:C:35:VAL:HG23	2.19	0.43
1:E:51:PHE:C	1:E:53:PRO:HD3	2.38	0.43
1:F:37:ILE:HG21	1:F:123:ILE:HG12	2.00	0.43
1:E:73:HIS:CD2	1:E:77:ILE:HD11	2.53	0.43
1:J:35:VAL:O	1:J:39:VAL:HG23	2.19	0.43
1:G:51:PHE:C	1:G:53:PRO:HD3	2.39	0.43
1:F:108:SER:OG	1:H:99:ARG:NH1	2.50	0.43
1:D:112:ASP:HA	1:D:113:PRO:HD3	1.84	0.42
1:E:12:SER:OG	1:E:15:GLU:HG3	2.19	0.42
1:L:58:MET:HA	1:L:63:GLN:OE1	2.18	0.42
1:D:72:TRP:HA	1:D:72:TRP:CE3	2.54	0.42
1:K:119:LEU:HD12	1:K:119:LEU:O	2.20	0.42
1:B:105:HIS:HB3	1:B:111:VAL:HG22	2.00	0.42
1:A:137:LEU:O	1:A:137:LEU:HD23	2.20	0.42
1:B:9:ALA:O	1:B:136:LYS:HD3	2.20	0.42
1:E:56:LYS:HE3	1:I:24:ALA:CB	2.48	0.42
1:G:124:ALA:HB1	3:G:202:HOH:O	2.19	0.42
1:A:40:LYS:HD2	3:A:168:HOH:O	2.19	0.42
1:F:46:PRO:HA	1:F:49:GLN:HG3	2.00	0.42
1:K:9:ALA:O	1:K:136:LYS:HD3	2.19	0.42
1:B:30:TYR:HA	1:B:33:SER:HB2	2.02	0.42
1:B:52:PHE:CZ	2:B:150:HEM:HAC	2.54	0.42
1:G:133:GLY:HA3	3:G:207:HOH:O	2.19	0.42
1:K:16:LYS:O	1:K:20:ARG:HG3	2.20	0.42
1:L:22:ALA:O	1:L:25:PRO:HD2	2.19	0.42
1:J:18:LYS:O	1:J:18:LYS:HD3	2.19	0.42
1:K:31:GLU:O	1:K:35:VAL:HG23	2.20	0.42
1:B:105:HIS:HD2	1:B:111:VAL:HG21	1.84	0.42
1:C:26:VAL:HG21	1:C:127:VAL:HG22	2.01	0.42
1:C:72:TRP:O	1:C:76:ARG:CD	2.68	0.42
1:A:134:PHE:O	1:A:138:MET:HG2	2.20	0.42
1:A:95:SER:HA	1:A:144:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:TRP:CD2	1:H:76:ARG:HD2	2.55	0.42
1:L:7:SER:HA	3:L:188:HOH:O	2.19	0.42
1:I:26:VAL:HG21	1:I:127:VAL:HG22	2.01	0.41
1:J:61:ALA:O	1:J:65:LYS:HG3	2.20	0.41
1:A:105:HIS:HD2	1:A:111:VAL:HG21	1.85	0.41
1:I:27:TYR:C	1:I:29:ASN:H	2.22	0.41
1:L:10:PRO:O	1:L:136:LYS:NZ	2.51	0.41
1:L:117:LYS:HA	1:L:142:CYS:SG	2.60	0.41
1:L:31:GLU:N	1:L:31:GLU:OE2	2.49	0.41
1:D:15:GLU:O	1:D:19:ILE:HG13	2.20	0.41
1:J:56:LYS:HA	3:J:227:HOH:O	2.21	0.41
1:L:35:VAL:O	1:L:39:VAL:HG23	2.19	0.41
1:I:105:HIS:CD2	1:I:111:VAL:HG11	2.56	0.41
1:J:35:VAL:CG2	1:J:71:ARG:HG2	2.49	0.41
1:A:105:HIS:HA	1:A:109:PHE:HB2	2.02	0.41
1:A:67:SER:O	1:A:71:ARG:HG3	2.20	0.41
1:B:29:ASN:O	1:B:29:ASN:CG	2.58	0.41
1:D:134:PHE:HB3	3:D:188:HOH:O	2.20	0.41
1:E:72:TRP:HA	1:E:72:TRP:CE3	2.56	0.41
1:H:105:HIS:HB3	1:H:149:TYR:OH	2.21	0.41
1:H:55:PHE:CD1	1:H:55:PHE:N	2.89	0.41
1:F:119:LEU:HD23	2:F:150:HEM:CHC	2.51	0.41
1:F:55:PHE:N	1:F:55:PHE:CD1	2.87	0.41
1:A:98:LEU:HB2	1:A:144:LEU:HD13	2.02	0.41
1:B:135:GLU:HG2	3:B:199:HOH:O	2.21	0.41
1:E:56:LYS:HA	1:E:56:LYS:HD2	1.85	0.41
1:F:11:LEU:CD2	1:F:136:LYS:HD2	2.48	0.41
1:J:137:LEU:O	1:J:137:LEU:HD22	2.20	0.41
1:B:22:ALA:O	1:B:25:PRO:HD2	2.20	0.41
1:G:72:TRP:O	1:G:76:ARG:CD	2.69	0.41
1:K:1:PRO:N	1:K:135:GLU:OE1	2.53	0.41
1:K:42:PHE:HE1	1:K:49:GLN:HA	1.84	0.41
1:C:137:LEU:HD12	1:C:138:MET:HE2	2.03	0.41
1:C:4:ASP:OD1	1:C:4:ASP:C	2.60	0.41
1:C:4:ASP:O	1:C:146:ARG:HD3	2.21	0.41
1:D:58:MET:HG2	3:D:184:HOH:O	2.21	0.41
1:D:71:ARG:NH2	3:D:223:HOH:O	2.53	0.41
1:J:60:SER:HB3	1:J:63:GLN:CG	2.51	0.41
1:K:119:LEU:O	1:K:123:ILE:HG13	2.21	0.41
1:K:51:PHE:C	1:K:53:PRO:HD3	2.42	0.41
1:B:105:HIS:HB3	1:B:111:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:HIS:HB3	1:C:149:TYR:OH	2.21	0.40
1:C:97:LYS:HB3	1:C:97:LYS:HZ3	1.84	0.40
1:K:106:ALA:HB2	1:K:149:TYR:CE1	2.56	0.40
1:K:106:ALA:HB2	1:K:149:TYR:CZ	2.56	0.40
1:A:67:SER:OG	1:A:70:VAL:HG23	2.21	0.40
1:L:52:PHE:N	1:L:53:PRO:HD3	2.36	0.40
1:A:77:ILE:O	1:A:81:VAL:HG23	2.21	0.40
1:C:127:VAL:HG11	1:C:134:PHE:CE1	2.57	0.40
1:D:85:VAL:O	1:D:88:MET:HG3	2.22	0.40
2:G:150:HEM:HBB2	2:G:150:HEM:CMB	2.51	0.40
1:I:51:PHE:CZ	1:I:112:ASP:HB2	2.57	0.40
1:J:60:SER:HB3	1:J:63:GLN:CD	2.41	0.40
1:J:55:PHE:CE2	1:J:70:VAL:HG22	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
1	B	147/149 (99%)	136 (92%)	10 (7%)	1 (1%)	25	30
1	C	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
1	D	147/149 (99%)	141 (96%)	5 (3%)	1 (1%)	25	30
1	E	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
1	F	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
1	G	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
1	H	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
1	I	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
1	J	147/149 (99%)	139 (95%)	7 (5%)	1 (1%)	25	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
1	L	147/149 (99%)	143 (97%)	4 (3%)	0	100	100
All	All	1764/1788 (99%)	1688 (96%)	73 (4%)	3 (0%)	51	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	56	LYS
1	J	56	LYS
1	B	46	PRO

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	122/122 (100%)	122 (100%)	0	100	100
1	B	122/122 (100%)	121 (99%)	1 (1%)	85	93
1	C	122/122 (100%)	121 (99%)	1 (1%)	85	93
1	D	122/122 (100%)	121 (99%)	1 (1%)	85	93
1	E	122/122 (100%)	120 (98%)	2 (2%)	68	82
1	F	122/122 (100%)	120 (98%)	2 (2%)	68	82
1	G	122/122 (100%)	121 (99%)	1 (1%)	85	93
1	H	122/122 (100%)	120 (98%)	2 (2%)	68	82
1	I	122/122 (100%)	118 (97%)	4 (3%)	43	59
1	J	122/122 (100%)	121 (99%)	1 (1%)	85	93
1	K	122/122 (100%)	121 (99%)	1 (1%)	85	93
1	L	122/122 (100%)	118 (97%)	4 (3%)	43	59
All	All	1464/1464 (100%)	1444 (99%)	20 (1%)	71	85

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	137	LEU
1	C	100	ASP
1	D	137	LEU
1	E	101	LEU
1	E	137	LEU
1	F	62	ASP
1	F	137	LEU
1	G	137	LEU
1	H	62	ASP
1	H	137	LEU
1	I	29	ASN
1	I	62	ASP
1	I	111	VAL
1	I	137	LEU
1	J	137	LEU
1	K	137	LEU
1	L	8	VAL
1	L	62	ASP
1	L	92	GLU
1	L	137	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	73	HIS
1	D	114	GLN
1	F	29	ASN
1	F	110	GLN
1	I	114	GLN
1	K	29	ASN
1	K	73	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 ⓘ

12 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	150	1	28,50,50	1.80	7 (25%)	17,82,82	1.12	1 (5%)
2	HEM	B	150	1	28,50,50	1.64	7 (25%)	17,82,82	1.80	5 (29%)
2	HEM	C	150	1	28,50,50	1.99	11 (39%)	17,82,82	1.55	3 (17%)
2	HEM	D	150	1	28,50,50	1.69	6 (21%)	17,82,82	1.25	3 (17%)
2	HEM	E	150	1	28,50,50	1.62	5 (17%)	17,82,82	1.53	3 (17%)
2	HEM	F	150	1	28,50,50	1.77	7 (25%)	17,82,82	1.09	0
2	HEM	G	150	1	28,50,50	1.75	6 (21%)	17,82,82	1.09	2 (11%)
2	HEM	H	150	1	28,50,50	1.64	7 (25%)	17,82,82	1.20	1 (5%)
2	HEM	I	150	1	28,50,50	1.68	8 (28%)	17,82,82	1.45	2 (11%)
2	HEM	J	150	1	28,50,50	1.92	8 (28%)	17,82,82	1.32	4 (23%)
2	HEM	K	150	1	28,50,50	1.66	7 (25%)	17,82,82	1.21	2 (11%)
2	HEM	L	150	1	28,50,50	1.76	6 (21%)	17,82,82	1.15	1 (5%)

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	150	1	-	0/6/54/54	0/0/8/8
2	HEM	B	150	1	-	0/6/54/54	0/0/8/8
2	HEM	C	150	1	-	0/6/54/54	0/0/8/8
2	HEM	D	150	1	-	0/6/54/54	0/0/8/8
2	HEM	E	150	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	F	150	1	-	0/6/54/54	0/0/8/8
2	HEM	G	150	1	-	0/6/54/54	0/0/8/8
2	HEM	H	150	1	-	0/6/54/54	0/0/8/8
2	HEM	I	150	1	-	0/6/54/54	0/0/8/8
2	HEM	J	150	1	-	0/6/54/54	0/0/8/8
2	HEM	K	150	1	-	0/6/54/54	0/0/8/8
2	HEM	L	150	1	-	0/6/54/54	0/0/8/8

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	150	HEM	C3B-CAB	-4.18	1.39	1.47
2	A	150	HEM	C3B-CAB	-4.16	1.39	1.47
2	C	150	HEM	C3B-CAB	-4.13	1.39	1.47
2	G	150	HEM	C3B-CAB	-4.09	1.39	1.47
2	E	150	HEM	C3B-CAB	-4.08	1.39	1.47
2	J	150	HEM	C3B-CAB	-4.00	1.39	1.47
2	F	150	HEM	C3C-CAC	-3.96	1.39	1.47
2	H	150	HEM	C3B-CAB	-3.95	1.40	1.47
2	L	150	HEM	C3B-C2B	-3.93	1.35	1.40
2	J	150	HEM	C3B-C2B	-3.93	1.35	1.40
2	G	150	HEM	C3C-CAC	-3.92	1.39	1.47
2	C	150	HEM	C3C-CAC	-3.91	1.39	1.47
2	K	150	HEM	C3B-CAB	-3.90	1.40	1.47
2	A	150	HEM	C3C-CAC	-3.81	1.40	1.47
2	E	150	HEM	C3C-CAC	-3.63	1.40	1.47
2	D	150	HEM	C3B-CAB	-3.62	1.40	1.47
2	L	150	HEM	C3B-CAB	-3.58	1.40	1.47
2	L	150	HEM	C3C-CAC	-3.58	1.40	1.47
2	I	150	HEM	C3C-CAC	-3.52	1.40	1.47
2	B	150	HEM	C3C-CAC	-3.52	1.40	1.47
2	D	150	HEM	C3C-CAC	-3.49	1.40	1.47
2	C	150	HEM	C3B-C2B	-3.49	1.35	1.40
2	B	150	HEM	C3B-CAB	-3.42	1.41	1.47
2	J	150	HEM	C3C-CAC	-3.27	1.41	1.47
2	D	150	HEM	C3C-C2C	-3.25	1.36	1.40
2	F	150	HEM	C3B-C2B	-3.22	1.36	1.40
2	H	150	HEM	C3C-CAC	-3.21	1.41	1.47
2	K	150	HEM	C3B-C2B	-3.21	1.36	1.40
2	I	150	HEM	C3B-C2B	-3.15	1.36	1.40
2	C	150	HEM	C3C-C2C	-3.13	1.36	1.40
2	B	150	HEM	C3C-C2C	-3.12	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	150	HEM	C3C-CAC	-3.04	1.41	1.47
2	I	150	HEM	C3B-CAB	-3.04	1.41	1.47
2	G	150	HEM	C3C-C2C	-2.98	1.36	1.40
2	A	150	HEM	C3B-C2B	-2.94	1.36	1.40
2	A	150	HEM	C3C-C2C	-2.89	1.36	1.40
2	B	150	HEM	C3B-C2B	-2.80	1.36	1.40
2	H	150	HEM	C3C-C2C	-2.69	1.36	1.40
2	G	150	HEM	C3B-C2B	-2.63	1.36	1.40
2	I	150	HEM	C3C-C2C	-2.57	1.37	1.40
2	L	150	HEM	C3C-C2C	-2.47	1.37	1.40
2	K	150	HEM	C3C-C2C	-2.39	1.37	1.40
2	F	150	HEM	C3C-C2C	-2.18	1.37	1.40
2	H	150	HEM	C3B-C2B	-2.11	1.37	1.40
2	C	150	HEM	C1C-NC	2.03	1.39	1.36
2	K	150	HEM	C4D-ND	2.05	1.39	1.36
2	D	150	HEM	C1D-ND	2.08	1.40	1.36
2	L	150	HEM	C1C-NC	2.11	1.39	1.36
2	C	150	HEM	C4A-NA	2.13	1.40	1.36
2	H	150	HEM	C4A-NA	2.16	1.40	1.36
2	I	150	HEM	C4A-NA	2.19	1.40	1.36
2	E	150	HEM	C4A-NA	2.19	1.40	1.36
2	I	150	HEM	C1D-ND	2.24	1.40	1.36
2	C	150	HEM	C4B-NB	2.27	1.41	1.36
2	H	150	HEM	C4C-NC	2.29	1.39	1.36
2	G	150	HEM	C4C-NC	2.30	1.39	1.36
2	B	150	HEM	C1D-ND	2.30	1.41	1.36
2	B	150	HEM	C4A-NA	2.30	1.41	1.36
2	B	150	HEM	C4C-NC	2.31	1.39	1.36
2	F	150	HEM	C1D-ND	2.34	1.41	1.36
2	A	150	HEM	C4D-ND	2.38	1.39	1.36
2	A	150	HEM	C1B-NB	2.41	1.39	1.36
2	J	150	HEM	C1A-NA	2.43	1.41	1.36
2	E	150	HEM	C1C-NC	2.44	1.39	1.36
2	I	150	HEM	C4C-NC	2.46	1.39	1.36
2	F	150	HEM	C1C-NC	2.51	1.39	1.36
2	C	150	HEM	C1D-ND	2.55	1.41	1.36
2	K	150	HEM	C1C-NC	2.58	1.39	1.36
2	C	150	HEM	C1B-NB	2.60	1.39	1.36
2	K	150	HEM	C4C-NC	2.75	1.40	1.36
2	J	150	HEM	C1C-NC	2.76	1.40	1.36
2	J	150	HEM	C1B-NB	2.77	1.40	1.36
2	C	150	HEM	C4D-ND	2.78	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	HEM	C4C-NC	2.86	1.40	1.36
2	H	150	HEM	C1B-NB	2.91	1.40	1.36
2	F	150	HEM	C4C-NC	2.95	1.40	1.36
2	L	150	HEM	C4D-ND	3.02	1.40	1.36
2	A	150	HEM	C1C-NC	3.05	1.40	1.36
2	J	150	HEM	C4C-NC	3.18	1.40	1.36
2	G	150	HEM	C1B-NB	3.23	1.40	1.36
2	C	150	HEM	C4C-NC	3.26	1.40	1.36
2	E	150	HEM	C4C-NC	3.30	1.40	1.36
2	D	150	HEM	C1B-NB	3.39	1.40	1.36
2	J	150	HEM	C4D-ND	3.59	1.41	1.36
2	I	150	HEM	C1B-NB	3.81	1.41	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	HEM	C4A-C3A-C2A	-3.99	104.22	107.00
2	B	150	HEM	C1D-C2D-C3D	-3.78	104.37	107.00
2	B	150	HEM	CBD-CAD-C3D	-3.42	105.94	112.47
2	I	150	HEM	C4C-C3C-C2C	-3.29	104.60	106.90
2	E	150	HEM	C4C-C3C-C2C	-3.09	104.74	106.90
2	A	150	HEM	CAA-C2A-C3A	-2.94	120.62	129.00
2	C	150	HEM	C1D-C2D-C3D	-2.69	105.13	107.00
2	E	150	HEM	C1D-C2D-C3D	-2.53	105.23	107.00
2	K	150	HEM	C4C-C3C-C2C	-2.49	105.16	106.90
2	H	150	HEM	CBD-CAD-C3D	-2.49	107.72	112.47
2	B	150	HEM	CAA-C2A-C3A	-2.42	122.09	129.00
2	J	150	HEM	CBD-CAD-C3D	-2.38	107.92	112.47
2	J	150	HEM	CAA-C2A-C3A	-2.35	122.29	129.00
2	D	150	HEM	C4C-C3C-C2C	-2.21	105.36	106.90
2	G	150	HEM	C4C-C3C-C2C	-2.08	105.45	106.90
2	G	150	HEM	CAA-C2A-C3A	-2.02	123.23	129.00
2	L	150	HEM	C4C-C3C-C2C	-2.01	105.50	106.90
2	J	150	HEM	C4C-C3C-C2C	-2.00	105.50	106.90
2	D	150	HEM	CMB-C2B-C3B	2.01	128.62	124.89
2	K	150	HEM	C3B-C4B-NB	2.12	111.96	109.21
2	J	150	HEM	CMC-C2C-C3C	2.22	129.01	124.89
2	D	150	HEM	C3B-C4B-NB	2.22	112.09	109.21
2	B	150	HEM	CMD-C2D-C3D	2.23	129.14	124.94
2	C	150	HEM	C3B-C4B-NB	2.30	112.19	109.21
2	E	150	HEM	C3B-C4B-NB	2.53	112.48	109.21
2	I	150	HEM	C3B-C4B-NB	2.68	112.67	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	150	HEM	C3B-C4B-NB	2.70	112.70	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	150	HEM	2	0
2	B	150	HEM	1	0
2	C	150	HEM	2	0
2	D	150	HEM	1	0
2	E	150	HEM	3	0
2	F	150	HEM	1	0
2	G	150	HEM	2	0
2	H	150	HEM	2	0
2	I	150	HEM	1	0
2	J	150	HEM	1	0
2	L	150	HEM	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	149/149 (100%)	0.48	6 (4%)	39	46	31, 47, 61, 65	0
1	B	149/149 (100%)	-0.06	0	100	100	15, 33, 61, 65	0
1	C	149/149 (100%)	-0.23	1 (0%)	87	90	17, 28, 44, 56	0
1	D	149/149 (100%)	-0.35	0	100	100	17, 26, 40, 43	0
1	E	149/149 (100%)	-0.41	0	100	100	14, 24, 38, 48	0
1	F	149/149 (100%)	-0.25	0	100	100	20, 29, 38, 43	0
1	G	149/149 (100%)	-0.25	0	100	100	17, 29, 45, 48	0
1	H	149/149 (100%)	-0.38	1 (0%)	87	90	16, 25, 42, 56	0
1	I	149/149 (100%)	-0.42	1 (0%)	87	90	11, 20, 37, 47	0
1	J	149/149 (100%)	-0.28	2 (1%)	77	81	16, 25, 41, 57	0
1	K	149/149 (100%)	-0.25	0	100	100	16, 27, 46, 54	0
1	L	149/149 (100%)	-0.24	1 (0%)	87	90	18, 29, 44, 53	0
All	All	1788/1788 (100%)	-0.22	12 (0%)	87	90	11, 28, 49, 65	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	PRO	4.5
1	H	59	THR	3.1
1	J	56	LYS	2.9
1	L	7	SER	2.9
1	A	2	ILE	2.5
1	J	57	GLY	2.4
1	A	57	GLY	2.4
1	A	114	GLN	2.4
1	A	23	TRP	2.3
1	C	56	LYS	2.2
1	I	28	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	THR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	HEM	G	150	43/43	0.97	0.12	-0.06	18,21,26,29	0
2	HEM	E	150	43/43	0.98	0.12	-0.14	11,17,20,24	0
2	HEM	J	150	43/43	0.97	0.12	-0.16	14,20,23,24	0
2	HEM	H	150	43/43	0.97	0.11	-0.17	13,22,30,35	0
2	HEM	F	150	43/43	0.97	0.12	-0.18	17,20,25,28	0
2	HEM	A	150	43/43	0.94	0.15	-0.20	29,34,39,41	0
2	HEM	L	150	43/43	0.98	0.12	-0.30	15,24,26,28	0
2	HEM	D	150	43/43	0.98	0.11	-0.42	9,17,21,26	0
2	HEM	I	150	43/43	0.97	0.10	-0.63	10,15,19,20	0
2	HEM	B	150	43/43	0.97	0.12	-0.66	21,25,30,34	0
2	HEM	K	150	43/43	0.98	0.11	-0.78	13,22,26,34	0
2	HEM	C	150	43/43	0.97	0.11	-0.81	11,20,23,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.