Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 01:50 AM EDT

PDB ID	:	2QLS
Title	:	crystal structure of hemoglobin from dog (Canis familiaris) at 3.5 Angstrom resolution
Authors	:	Packianathan, C.; Sundaresan, S.; Palani, K.; Neeelagandan, K.; Ponnuswamy, M.N.
Deposited on	:	2007-07-13
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

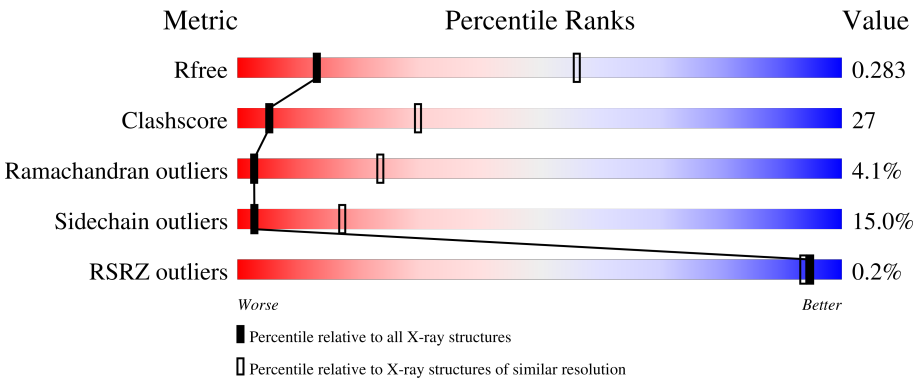
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	141	37% 35% 19% 9%
1	C	141	43% 38% 15% •
2	B	146	% 34% 38% 21% 8%
2	D	146	30% 49% 18% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4588 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.

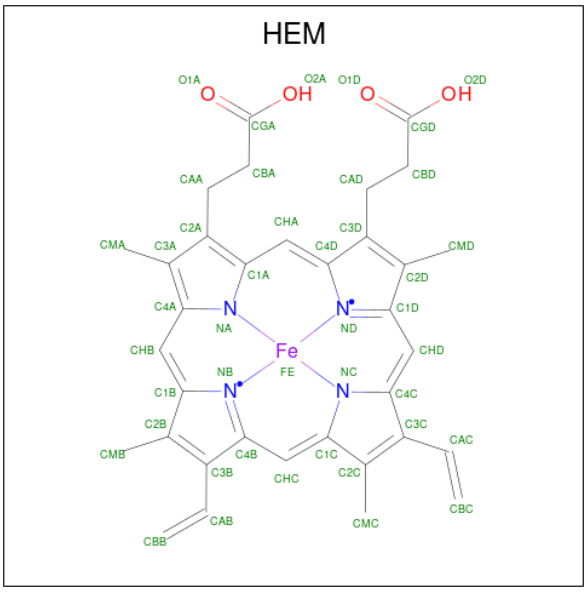
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1077	691	184	200	2	0	0	0
1	C	141	1077	691	184	200	2	0	0	0

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1131	727	196	205	3	0	0	0
2	D	146	1131	727	196	205	3	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



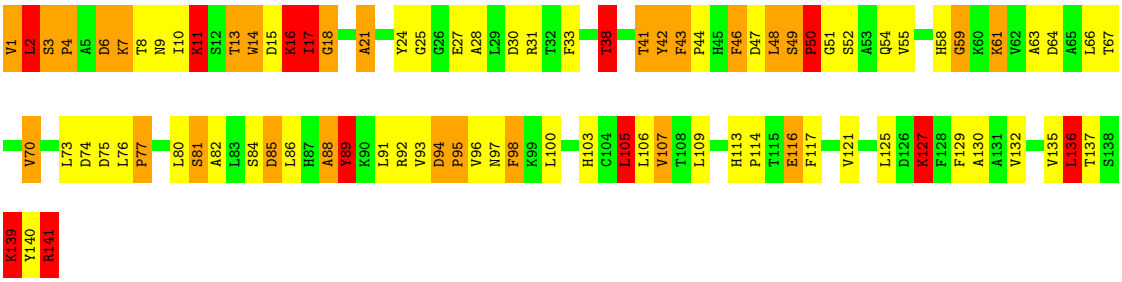
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0
3	C	1	43	34	1	4	4	0	0
3	D	1	43	34	1	4	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

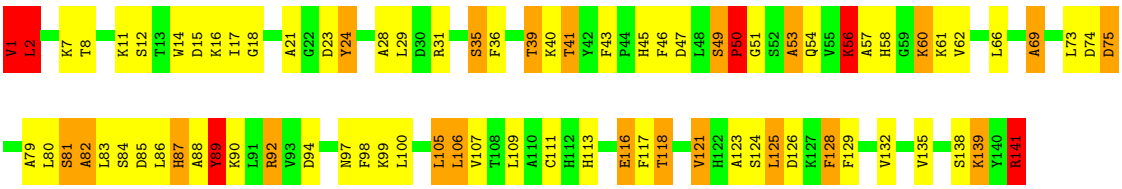
• Molecule 1: Hemoglobin subunit alpha

Chain A: 37% 35% 19% 9%



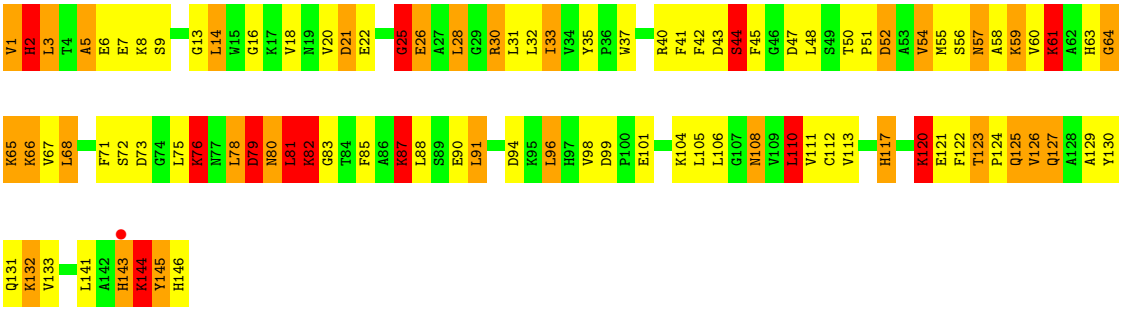
• Molecule 1: Hemoglobin subunit alpha

Chain C: 43% 38% 15% •



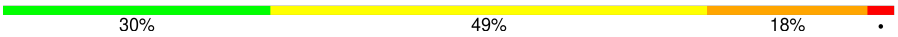
• Molecule 2: Hemoglobin subunit beta

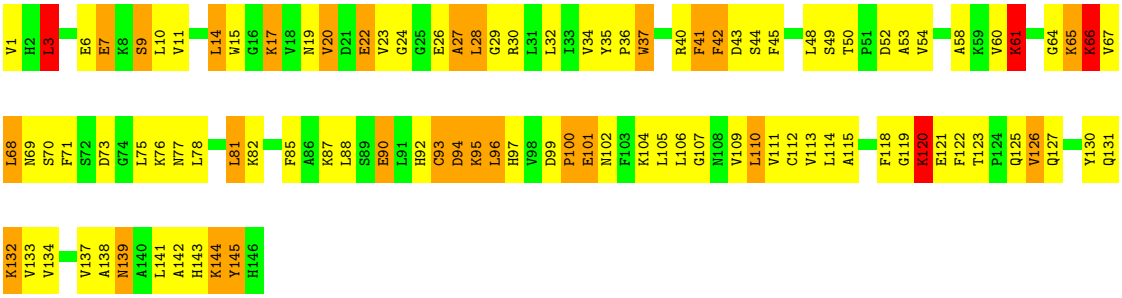
Chain B: % 34% 38% 21% 8%



• Molecule 2: Hemoglobin subunit beta

Chain D:


30%
49%
18%


V1 H2 L3 E6 E7 K8 S9 L10 V11 L14 W15 G16 K17 V18 N19 V20 D21 E22 V23 G24 G25 E26 A27 L28 G29 R30 L31 L32 I33 V34 Y35 P36 W37 R40 F41 F42 D43 S44 F45 L48 S49 T50 P51 D52 A53 V54 A58 K59 V60 K61 G64 K65 K66 V67
L68 N69 S70 F71 S72 D73 G74 L75 K76 N77 L78 L81 K82 F85 A86 K87 L88 S89 E90 L91 H92 C93 D94 K95 L96 H97 V98 D99 P100 E101 N102 F103 K104 L105 L106 G107 N108 V109 L110 V111 C112 V113 L114 A115 F118 G119 K120 E121 F122 T123 P124 Q125 V126 Q127 Y130 Q131
K132 V133 V134 V137 A138 N139 A140 L141 A142 H143 K144 Y145 H146

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.09Å 88.49Å 66.37Å 90.00° 105.72° 90.00°	Depositor
Resolution (Å)	27.87 – 3.50 27.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.87-3.50) 97.1 (27.87-3.50)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.293 0.192 , 0.283	Depositor DCC
R_{free} test set	345 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 75.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4588	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.56% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.84	88/1107 (7.9%)	2.17	41/1507 (2.7%)
1	C	2.60	72/1107 (6.5%)	2.11	41/1507 (2.7%)
2	B	2.73	79/1157 (6.8%)	2.07	44/1564 (2.8%)
2	D	2.87	91/1157 (7.9%)	2.11	38/1564 (2.4%)
All	All	2.76	330/4528 (7.3%)	2.12	164/6142 (2.7%)

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	C	0	1

All (330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	61	LYS	CE-NZ	18.87	1.96	1.49
1	A	3	SER	CB-OG	18.52	1.66	1.42
2	D	27	ALA	CA-CB	16.28	1.86	1.52
2	D	93	CYS	CB-SG	15.70	2.08	1.82
2	B	65	LYS	CE-NZ	15.49	1.87	1.49
2	D	132	LYS	CE-NZ	12.97	1.81	1.49
2	D	101	GLU	CD-OE2	12.41	1.39	1.25
2	D	41	PHE	CE1-CZ	11.69	1.59	1.37
2	B	66	LYS	CE-NZ	11.59	1.78	1.49
1	C	56	LYS	CD-CE	11.56	1.80	1.51
1	C	132	VAL	CB-CG2	-11.41	1.28	1.52
1	A	139	LYS	CE-NZ	11.19	1.77	1.49
1	A	24	TYR	CG-CD2	11.13	1.53	1.39
1	A	11	LYS	CE-NZ	10.88	1.76	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	66	LYS	CD-CE	10.74	1.78	1.51
2	D	101	GLU	CD-OE1	10.72	1.37	1.25
1	A	116	GLU	CD-OE2	10.63	1.37	1.25
1	A	63	ALA	CA-CB	-10.41	1.30	1.52
2	D	22	GLU	CB-CG	10.40	1.72	1.52
2	D	17	LYS	CD-CE	10.38	1.77	1.51
2	D	26	GLU	CD-OE1	10.37	1.37	1.25
2	B	145	TYR	CD1-CE1	10.28	1.54	1.39
1	A	11	LYS	CD-CE	10.27	1.76	1.51
2	B	113	VAL	CB-CG2	-10.15	1.31	1.52
2	B	26	GLU	CD-OE2	9.98	1.36	1.25
2	D	22	GLU	CD-OE1	9.96	1.36	1.25
1	A	70	VAL	CB-CG1	-9.95	1.31	1.52
1	A	27	GLU	CG-CD	9.91	1.66	1.51
2	D	120	LYS	CB-CG	9.85	1.79	1.52
1	A	141	ARG	CG-CD	9.76	1.76	1.51
2	B	6	GLU	CG-CD	9.74	1.66	1.51
1	C	141	ARG	NE-CZ	9.72	1.45	1.33
1	C	111	CYS	CB-SG	-9.70	1.65	1.82
2	D	118	PHE	CD1-CE1	9.68	1.58	1.39
2	B	130	TYR	CD2-CE2	9.65	1.53	1.39
2	D	115	ALA	CA-CB	-9.61	1.32	1.52
1	A	1	VAL	CB-CG2	9.48	1.72	1.52
2	D	118	PHE	CD2-CE2	9.46	1.58	1.39
1	A	135	VAL	CB-CG1	9.39	1.72	1.52
1	C	123	ALA	CA-CB	-9.36	1.32	1.52
2	B	121	GLU	CD-OE2	9.31	1.35	1.25
1	C	82	ALA	CA-CB	-9.27	1.32	1.52
2	B	66	LYS	CD-CE	9.22	1.74	1.51
1	C	89	TYR	CG-CD2	9.22	1.51	1.39
2	D	22	GLU	CG-CD	9.13	1.65	1.51
2	D	60	VAL	CB-CG1	-9.04	1.33	1.52
2	B	61	LYS	CD-CE	9.01	1.73	1.51
2	B	71	PHE	CB-CG	-8.98	1.36	1.51
1	A	42	TYR	CZ-OH	8.90	1.52	1.37
1	A	49	SER	CB-OG	8.89	1.53	1.42
1	A	50	PRO	CG-CD	8.88	1.79	1.50
1	C	60	LYS	CE-NZ	8.77	1.71	1.49
2	B	132	LYS	CE-NZ	8.75	1.71	1.49
2	D	45	PHE	CD1-CE1	-8.74	1.21	1.39
2	B	54	VAL	CB-CG1	-8.73	1.34	1.52
2	B	35	TYR	CE2-CZ	8.73	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	133	VAL	CB-CG2	-8.72	1.34	1.52
2	B	1	VAL	CB-CG2	8.70	1.71	1.52
1	A	121	VAL	CB-CG2	-8.67	1.34	1.52
1	A	98	PHE	CD1-CE1	8.66	1.56	1.39
1	A	16	LYS	CE-NZ	8.66	1.70	1.49
2	B	125	GLN	CG-CD	8.62	1.70	1.51
2	B	25	GLY	N-CA	8.43	1.58	1.46
2	D	120	LYS	CE-NZ	8.42	1.70	1.49
2	D	26	GLU	CD-OE2	8.41	1.34	1.25
2	B	59	LYS	CE-NZ	8.39	1.70	1.49
1	C	31	ARG	CZ-NH2	8.39	1.44	1.33
1	A	24	TYR	CE2-CZ	8.38	1.49	1.38
1	A	89	TYR	CE2-CZ	8.37	1.49	1.38
1	A	127	LYS	CE-NZ	8.35	1.70	1.49
2	D	138	ALA	CA-CB	-8.30	1.35	1.52
1	C	98	PHE	CE1-CZ	-8.29	1.21	1.37
1	A	4	PRO	N-CD	8.26	1.59	1.47
2	D	112	CYS	C-O	8.25	1.39	1.23
2	D	22	GLU	CD-OE2	8.24	1.34	1.25
1	A	88	ALA	C-O	-8.21	1.07	1.23
2	D	9	SER	CB-OG	8.10	1.52	1.42
1	A	6	ASP	CB-CG	8.01	1.68	1.51
2	B	85	PHE	CB-CG	-7.99	1.37	1.51
2	B	104	LYS	CD-CE	7.98	1.71	1.51
1	C	141	ARG	CD-NE	7.95	1.59	1.46
2	B	61	LYS	CG-CD	7.92	1.79	1.52
1	C	84	SER	CB-OG	7.89	1.52	1.42
1	C	35	SER	CB-OG	7.89	1.52	1.42
1	A	82	ALA	C-O	7.85	1.38	1.23
2	B	41	PHE	CE1-CZ	-7.83	1.22	1.37
1	A	3	SER	C-O	7.83	1.38	1.23
2	D	145	TYR	CG-CD1	7.82	1.49	1.39
1	C	11	LYS	CD-CE	7.80	1.70	1.51
2	B	76	LYS	CB-CG	7.76	1.73	1.52
2	B	71	PHE	CE1-CZ	7.75	1.52	1.37
1	A	116	GLU	CB-CG	7.75	1.66	1.52
2	D	121	GLU	CD-OE2	7.74	1.34	1.25
2	B	105	LEU	N-CA	-7.72	1.30	1.46
2	B	20	VAL	CB-CG2	7.71	1.69	1.52
1	A	98	PHE	CD2-CE2	7.70	1.54	1.39
2	D	35	TYR	CE1-CZ	-7.62	1.28	1.38
2	D	109	VAL	CB-CG1	-7.61	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	SER	CB-OG	7.60	1.52	1.42
1	C	89	TYR	CE2-CZ	7.58	1.48	1.38
1	A	4	PRO	CG-CD	7.58	1.75	1.50
1	A	2	LEU	C-O	7.55	1.37	1.23
2	D	6	GLU	CD-OE2	7.54	1.33	1.25
2	B	120	LYS	CE-NZ	7.52	1.67	1.49
2	D	66	LYS	CE-NZ	7.44	1.67	1.49
1	C	132	VAL	CB-CG1	-7.42	1.37	1.52
1	A	4	PRO	N-CA	7.41	1.59	1.47
2	B	76	LYS	CG-CD	7.40	1.77	1.52
1	C	36	PHE	CE2-CZ	-7.39	1.23	1.37
1	C	49	SER	CB-OG	-7.37	1.32	1.42
1	A	96	VAL	CB-CG1	-7.35	1.37	1.52
2	D	113	VAL	CB-CG1	-7.33	1.37	1.52
1	C	141	ARG	C-O	7.32	1.37	1.23
1	A	116	GLU	CG-CD	7.30	1.62	1.51
2	B	16	GLY	N-CA	7.28	1.56	1.46
2	D	15	TRP	CE2-CZ2	7.28	1.52	1.39
2	D	90	GLU	CD-OE1	7.27	1.33	1.25
2	D	137	VAL	CB-CG1	-7.24	1.37	1.52
1	C	53	ALA	CA-CB	7.19	1.67	1.52
1	A	130	ALA	CA-CB	7.16	1.67	1.52
1	C	14	TRP	CB-CG	-7.13	1.37	1.50
2	D	36	PRO	CA-CB	-7.11	1.39	1.53
2	B	6	GLU	CD-OE2	7.11	1.33	1.25
1	C	11	LYS	CE-NZ	7.10	1.66	1.49
2	D	20	VAL	CB-CG1	7.09	1.67	1.52
2	B	18	VAL	CB-CG2	-7.01	1.38	1.52
1	C	89	TYR	CE1-CZ	7.01	1.47	1.38
1	C	128	PHE	CD1-CE1	6.99	1.53	1.39
2	D	67	VAL	CB-CG1	-6.97	1.38	1.52
2	D	101	GLU	CG-CD	6.96	1.62	1.51
2	B	146	HIS	C-O	6.95	1.36	1.23
1	A	46	PHE	CD1-CE1	6.95	1.53	1.39
2	D	101	GLU	CB-CG	6.95	1.65	1.52
2	D	53	ALA	CA-CB	-6.92	1.38	1.52
2	D	54	VAL	CB-CG1	-6.88	1.38	1.52
2	D	111	VAL	CB-CG2	-6.88	1.38	1.52
1	C	40	LYS	CA-CB	-6.87	1.38	1.53
1	A	6	ASP	CG-OD1	6.80	1.41	1.25
1	C	14	TRP	CE3-CZ3	6.78	1.50	1.38
2	B	7	GLU	CD-OE2	6.76	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	7	GLU	CG-CD	6.74	1.62	1.51
2	D	145	TYR	CE2-CZ	6.73	1.47	1.38
2	D	15	TRP	CZ3-CH2	-6.73	1.29	1.40
2	B	120	LYS	CD-CE	6.71	1.68	1.51
2	B	76	LYS	CD-CE	6.64	1.67	1.51
2	B	6	GLU	CB-CG	6.62	1.64	1.52
1	C	43	PHE	CD1-CE1	6.61	1.52	1.39
2	D	125	GLN	CG-CD	6.61	1.66	1.51
1	C	15	ASP	CG-OD2	6.60	1.40	1.25
1	C	17	ILE	C-O	6.60	1.35	1.23
2	B	132	LYS	CD-CE	6.59	1.67	1.51
2	D	95	LYS	CA-C	-6.59	1.35	1.52
1	A	140	TYR	CD2-CE2	6.57	1.49	1.39
1	A	141	ARG	C-O	6.56	1.35	1.23
1	C	60	LYS	CB-CG	6.55	1.70	1.52
2	D	32	LEU	CG-CD2	-6.53	1.27	1.51
1	C	36	PHE	CE1-CZ	6.52	1.49	1.37
1	C	107	VAL	CB-CG1	-6.52	1.39	1.52
2	B	108	ASN	C-O	6.51	1.35	1.23
2	B	145	TYR	CD2-CE2	6.50	1.49	1.39
2	B	90	GLU	CB-CG	6.50	1.64	1.52
2	D	37	TRP	CZ3-CH2	-6.48	1.29	1.40
1	C	21	ALA	CA-CB	6.47	1.66	1.52
1	C	92	ARG	CB-CG	6.42	1.69	1.52
2	D	125	GLN	CD-NE2	6.42	1.49	1.32
1	A	141	ARG	CB-CG	6.41	1.69	1.52
1	C	116	GLU	CD-OE2	6.40	1.32	1.25
1	A	1	VAL	CB-CG1	6.37	1.66	1.52
2	B	13	GLY	N-CA	6.33	1.55	1.46
1	A	89	TYR	CZ-OH	6.32	1.48	1.37
2	D	133	VAL	CA-CB	-6.31	1.41	1.54
1	C	121	VAL	CB-CG1	-6.31	1.39	1.52
1	C	141	ARG	C-OXT	6.29	1.35	1.23
1	A	24	TYR	CG-CD1	6.29	1.47	1.39
2	D	104	LYS	CD-CE	6.27	1.67	1.51
1	A	74	ASP	CB-CG	6.26	1.64	1.51
1	C	56	LYS	CE-NZ	6.25	1.64	1.49
1	C	50	PRO	CB-CG	6.19	1.80	1.50
2	B	7	GLU	CG-CD	6.19	1.61	1.51
1	A	132	VAL	CA-CB	-6.18	1.41	1.54
1	C	43	PHE	CG-CD1	-6.17	1.29	1.38
2	D	45	PHE	CE1-CZ	6.14	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	35	TYR	CZ-OH	-6.13	1.27	1.37
2	B	37	TRP	CZ3-CH2	-6.12	1.30	1.40
1	A	43	PHE	CG-CD1	-6.11	1.29	1.38
1	C	24	TYR	CG-CD2	6.10	1.47	1.39
2	D	130	TYR	CZ-OH	6.10	1.48	1.37
2	D	30	ARG	N-CA	-6.08	1.34	1.46
2	D	15	TRP	CB-CG	-6.08	1.39	1.50
1	A	55	VAL	C-O	6.05	1.34	1.23
2	D	139	ASN	CG-ND2	6.05	1.48	1.32
1	C	84	SER	N-CA	-6.04	1.34	1.46
1	A	24	TYR	CE1-CZ	6.03	1.46	1.38
1	A	61	LYS	CE-NZ	6.02	1.64	1.49
2	D	109	VAL	CB-CG2	-6.02	1.40	1.52
2	D	67	VAL	CB-CG2	-6.01	1.40	1.52
1	A	42	TYR	CG-CD2	-5.98	1.31	1.39
1	A	116	GLU	CD-OE1	5.98	1.32	1.25
2	B	127	GLN	C-O	5.97	1.34	1.23
2	D	119	GLY	N-CA	5.96	1.54	1.46
1	A	140	TYR	CD1-CE1	5.96	1.48	1.39
2	D	71	PHE	CE2-CZ	5.96	1.48	1.37
1	C	141	ARG	CZ-NH1	5.95	1.40	1.33
1	A	97	ASN	CB-CG	5.92	1.64	1.51
1	C	46	PHE	C-O	5.92	1.34	1.23
2	D	34	VAL	CB-CG2	-5.92	1.40	1.52
1	C	1	VAL	CB-CG2	5.91	1.65	1.52
2	D	94	ASP	CG-OD1	5.91	1.39	1.25
2	D	100	PRO	CA-C	-5.89	1.41	1.52
2	B	28	LEU	CG-CD2	-5.89	1.30	1.51
1	A	7	LYS	N-CA	-5.89	1.34	1.46
1	A	24	TYR	CD2-CE2	5.88	1.48	1.39
2	B	37	TRP	CB-CG	-5.88	1.39	1.50
1	A	7	LYS	CG-CD	5.88	1.72	1.52
2	B	104	LYS	CG-CD	5.87	1.72	1.52
1	C	124	SER	CB-OG	5.84	1.49	1.42
1	A	140	TYR	CG-CD1	5.83	1.46	1.39
2	B	133	VAL	CB-CG1	-5.83	1.40	1.52
2	B	91	LEU	C-O	5.81	1.34	1.23
1	C	61	LYS	CD-CE	5.79	1.65	1.51
2	B	71	PHE	CA-CB	-5.79	1.41	1.53
2	D	54	VAL	CB-CG2	-5.78	1.40	1.52
2	B	108	ASN	CG-ND2	5.78	1.47	1.32
1	C	56	LYS	CB-CG	5.78	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLN	C-O	5.77	1.34	1.23
1	C	79	ALA	CA-CB	5.75	1.64	1.52
2	B	83	GLY	C-O	5.74	1.32	1.23
2	D	104	LYS	CE-NZ	5.74	1.63	1.49
2	D	6	GLU	CB-CG	5.73	1.63	1.52
2	B	55	MET	CB-CG	5.72	1.69	1.51
1	C	81	SER	N-CA	5.71	1.57	1.46
2	D	95	LYS	CD-CE	5.70	1.65	1.51
2	D	23	VAL	CB-CG1	-5.69	1.40	1.52
2	B	54	VAL	CB-CG2	-5.69	1.41	1.52
1	A	27	GLU	CD-OE1	5.68	1.31	1.25
2	B	44	SER	CA-CB	5.67	1.61	1.52
2	D	76	LYS	CD-CE	5.62	1.65	1.51
1	A	61	LYS	CD-CE	5.61	1.65	1.51
2	B	82	LYS	CD-CE	5.61	1.65	1.51
2	B	111	VAL	C-O	5.59	1.33	1.23
1	C	43	PHE	CE2-CZ	-5.59	1.26	1.37
2	D	14	LEU	CA-CB	-5.59	1.40	1.53
1	A	16	LYS	CG-CD	5.58	1.71	1.52
1	C	92	ARG	CG-CD	5.58	1.65	1.51
2	B	5	ALA	CA-CB	-5.56	1.40	1.52
2	D	49	SER	CB-OG	5.56	1.49	1.42
1	C	74	ASP	CG-OD2	5.54	1.38	1.25
1	A	94	ASP	CA-CB	-5.54	1.41	1.53
1	C	117	PHE	CE2-CZ	-5.54	1.26	1.37
1	C	90	LYS	CE-NZ	5.53	1.62	1.49
2	D	90	GLU	CD-OE2	5.53	1.31	1.25
1	A	51	GLY	N-CA	5.53	1.54	1.46
1	A	52	SER	C-O	5.53	1.33	1.23
2	D	37	TRP	CD2-CE2	-5.51	1.34	1.41
1	C	43	PHE	CD2-CE2	5.51	1.50	1.39
1	C	54	GLN	C-O	5.51	1.33	1.23
2	D	69	ASN	C-O	5.50	1.33	1.23
2	D	66	LYS	CG-CD	5.49	1.71	1.52
2	D	71	PHE	CA-CB	-5.49	1.41	1.53
2	D	122	PHE	N-CA	-5.48	1.35	1.46
1	C	56	LYS	CG-CD	5.48	1.71	1.52
2	B	43	ASP	C-O	5.47	1.33	1.23
2	B	40	ARG	CZ-NH2	5.46	1.40	1.33
2	D	77	ASN	CB-CG	5.46	1.63	1.51
1	A	31	ARG	CG-CD	5.45	1.65	1.51
2	B	45	PHE	CG-CD1	-5.44	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ASP	CA-C	-5.43	1.38	1.52
1	A	4	PRO	CA-CB	5.42	1.64	1.53
1	A	33	PHE	CB-CG	-5.41	1.42	1.51
2	B	20	VAL	C-O	5.40	1.33	1.23
1	A	85	ASP	CB-CG	5.40	1.63	1.51
1	C	89	TYR	CD2-CE2	5.38	1.47	1.39
2	B	79	ASP	CG-OD2	5.38	1.37	1.25
2	D	42	PHE	CE2-CZ	-5.38	1.27	1.37
2	B	98	VAL	CB-CG1	-5.37	1.41	1.52
2	D	87	LYS	CD-CE	5.37	1.64	1.51
2	B	37	TRP	CD2-CE2	-5.36	1.34	1.41
1	A	107	VAL	CA-CB	5.36	1.66	1.54
2	B	80	ASN	C-O	5.36	1.33	1.23
1	C	50	PRO	C-O	5.36	1.33	1.23
1	A	3	SER	C-N	5.33	1.44	1.34
2	B	44	SER	CB-OG	5.32	1.49	1.42
1	C	118	THR	CB-CG2	-5.31	1.34	1.52
1	C	1	VAL	N-CA	5.31	1.56	1.46
2	D	85	PHE	CE2-CZ	-5.31	1.27	1.37
2	B	45	PHE	CG-CD2	5.31	1.46	1.38
2	D	60	VAL	CB-CG2	-5.30	1.41	1.52
2	D	105	LEU	N-CA	-5.29	1.35	1.46
2	D	24	GLY	C-O	5.29	1.32	1.23
2	D	35	TYR	CE2-CZ	-5.29	1.31	1.38
1	A	7	LYS	CB-CG	5.29	1.66	1.52
2	B	124	PRO	CA-CB	-5.28	1.43	1.53
2	B	37	TRP	CG-CD1	-5.28	1.29	1.36
1	A	46	PHE	C-O	5.28	1.33	1.23
2	B	40	ARG	CZ-NH1	5.27	1.40	1.33
1	A	13	THR	N-CA	5.27	1.56	1.46
2	B	42	PHE	CE1-CZ	-5.25	1.27	1.37
2	D	126	VAL	CB-CG2	-5.23	1.41	1.52
2	B	144	LYS	CE-NZ	5.23	1.62	1.49
1	C	41	THR	CB-CG2	5.23	1.69	1.52
1	A	73	LEU	CG-CD1	5.21	1.71	1.51
1	A	139	LYS	CD-CE	5.21	1.64	1.51
2	B	61	LYS	CB-CG	5.20	1.66	1.52
1	A	106	LEU	N-CA	5.19	1.56	1.46
2	B	87	LYS	CD-CE	5.18	1.64	1.51
1	C	139	LYS	CD-CE	5.18	1.64	1.51
2	B	126	VAL	N-CA	5.17	1.56	1.46
1	A	137	THR	CB-CG2	-5.16	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	TYR	CG-CD1	5.16	1.45	1.39
1	C	60	LYS	CD-CE	5.16	1.64	1.51
1	A	141	ARG	CZ-NH2	5.15	1.39	1.33
1	A	4	PRO	C-O	5.13	1.33	1.23
1	A	8	THR	CB-CG2	5.12	1.69	1.52
1	A	67	THR	C-O	5.12	1.33	1.23
1	A	129	PHE	CE2-CZ	5.12	1.47	1.37
2	D	26	GLU	CA-CB	-5.12	1.42	1.53
1	A	25	GLY	C-O	-5.12	1.15	1.23
1	C	109	LEU	CG-CD2	-5.12	1.32	1.51
1	C	98	PHE	CG-CD2	-5.09	1.31	1.38
2	D	82	LYS	CE-NZ	5.09	1.61	1.49
1	A	14	TRP	CG-CD1	5.07	1.43	1.36
1	C	69	ALA	C-O	5.07	1.32	1.23
1	C	141	ARG	CG-CD	5.05	1.64	1.51
1	A	17	ILE	CA-CB	5.04	1.66	1.54
1	A	77	PRO	CB-CG	5.04	1.75	1.50
2	B	91	LEU	N-CA	5.03	1.56	1.46
1	A	85	ASP	C-O	-5.02	1.13	1.23
1	A	70	VAL	C-O	5.02	1.32	1.23
1	C	89	TYR	CD1-CE1	5.01	1.46	1.39
2	B	83	GLY	N-CA	5.01	1.53	1.46

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	ARG	NE-CZ-NH2	16.73	128.66	120.30
1	C	141	ARG	NE-CZ-NH1	15.57	128.08	120.30
2	D	73	ASP	CB-CG-OD2	14.67	131.50	118.30
2	D	94	ASP	CB-CG-OD2	-14.51	105.24	118.30
2	B	14	LEU	CB-CG-CD2	13.35	133.70	111.00
1	A	31	ARG	NE-CZ-NH1	-12.29	114.16	120.30
2	B	94	ASP	CB-CG-OD1	-12.17	107.35	118.30
1	A	64	ASP	CB-CG-OD1	-11.56	107.89	118.30
2	B	73	ASP	CB-CG-OD1	11.24	128.42	118.30
1	A	31	ARG	NE-CZ-NH2	11.24	125.92	120.30
1	A	64	ASP	CB-CG-OD2	11.22	128.40	118.30
1	A	92	ARG	NE-CZ-NH2	11.16	125.88	120.30
2	D	94	ASP	CB-CG-OD1	10.65	127.89	118.30
1	C	92	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	C	23	ASP	CB-CG-OD2	-10.47	108.88	118.30
1	A	94	ASP	CB-CG-OD1	10.29	127.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	LYS	CD-CE-NZ	-10.11	88.45	111.70
1	A	94	ASP	CB-CG-OD2	-10.02	109.28	118.30
1	A	47	ASP	CB-CG-OD1	-9.76	109.52	118.30
2	D	73	ASP	CB-CG-OD1	-9.74	109.54	118.30
1	A	47	ASP	CB-CG-OD2	9.73	127.06	118.30
2	D	32	LEU	CB-CG-CD2	-9.73	94.46	111.00
2	D	132	LYS	CD-CE-NZ	-9.69	89.41	111.70
2	B	106	LEU	CB-CG-CD2	-9.30	95.18	111.00
1	A	74	ASP	CB-CG-OD2	9.24	126.61	118.30
2	D	17	LYS	CD-CE-NZ	-9.16	90.63	111.70
1	C	109	LEU	CB-CG-CD2	-9.11	95.51	111.00
1	C	15	ASP	CB-CG-OD1	-9.04	110.16	118.30
1	A	30	ASP	CB-CG-OD2	8.96	126.36	118.30
1	C	31	ARG	NE-CZ-NH1	-8.92	115.84	120.30
2	D	99	ASP	CB-CG-OD1	-8.84	110.35	118.30
1	C	2	LEU	CB-CG-CD2	8.67	125.74	111.00
2	B	21	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	15	ASP	CB-CG-OD1	-8.33	110.81	118.30
1	A	105	LEU	CB-CG-CD2	-8.31	96.88	111.00
1	A	75	ASP	CB-CG-OD1	-8.30	110.83	118.30
1	A	136	LEU	CB-CG-CD2	-8.28	96.92	111.00
2	D	43	ASP	CB-CG-OD2	-8.14	110.97	118.30
2	D	88	LEU	CA-CB-CG	-8.10	96.67	115.30
1	C	80	LEU	CB-CG-CD2	8.05	124.69	111.00
1	A	30	ASP	CB-CG-OD1	-8.02	111.08	118.30
2	D	106	LEU	CB-CG-CD1	-7.92	97.53	111.00
1	C	83	LEU	CB-CG-CD1	-7.85	97.65	111.00
2	B	78	LEU	CA-CB-CG	-7.82	97.31	115.30
2	B	47	ASP	CB-CG-OD1	7.82	125.33	118.30
1	A	107	VAL	CG1-CB-CG2	-7.70	98.59	110.90
2	B	123	THR	CA-CB-CG2	-7.66	101.67	112.40
2	B	81	LEU	CB-CG-CD1	7.48	123.72	111.00
2	D	7	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	A	15	ASP	CB-CG-OD2	7.28	124.85	118.30
2	D	48	LEU	CB-CG-CD2	7.27	123.36	111.00
2	B	14	LEU	CB-CG-CD1	-7.09	98.94	111.00
1	A	6	ASP	CB-CG-OD1	7.08	124.67	118.30
2	B	33	ILE	CG1-CB-CG2	-7.07	95.84	111.40
1	A	74	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	C	126	ASP	CB-CG-OD1	7.03	124.63	118.30
1	C	94	ASP	CB-CG-OD1	6.96	124.56	118.30
2	D	36	PRO	N-CD-CG	-6.91	92.83	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	76	LYS	CD-CE-NZ	6.91	127.59	111.70
1	A	43	PHE	CG-CD2-CE2	6.90	128.39	120.80
1	A	24	TYR	CZ-CE2-CD2	-6.89	113.60	119.80
1	C	106	LEU	CB-CG-CD1	-6.87	99.31	111.00
1	C	92	ARG	NH1-CZ-NH2	-6.87	111.85	119.40
1	A	80	LEU	CB-CG-CD2	6.84	122.62	111.00
1	C	56	LYS	CD-CE-NZ	6.75	127.23	111.70
2	B	75	LEU	CB-CG-CD2	6.74	122.45	111.00
2	B	31	LEU	CB-CG-CD2	-6.69	99.62	111.00
1	C	141	ARG	CD-NE-CZ	6.68	132.95	123.60
1	A	6	ASP	CB-CG-OD2	-6.68	112.29	118.30
2	B	21	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	C	100	LEU	CB-CG-CD2	-6.62	99.74	111.00
1	A	100	LEU	CB-CG-CD1	6.62	122.25	111.00
2	D	32	LEU	CD1-CG-CD2	-6.58	90.76	110.50
1	A	3	SER	C-N-CD	6.57	142.20	128.40
2	B	30	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	D	14	LEU	CA-CB-CG	6.50	130.26	115.30
2	B	1	VAL	CB-CA-C	-6.47	99.10	111.40
2	B	120	LYS	CB-CA-C	-6.47	97.47	110.40
2	D	105	LEU	CB-CG-CD2	-6.38	100.16	111.00
2	B	35	TYR	CB-CG-CD1	-6.37	117.18	121.00
2	B	141	LEU	CB-CG-CD1	-6.36	100.19	111.00
1	C	1	VAL	CG1-CB-CG2	6.35	121.06	110.90
1	C	23	ASP	CB-CA-C	-6.35	97.69	110.40
2	B	144	LYS	CD-CE-NZ	-6.34	97.11	111.70
2	B	99	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	29	LEU	CB-CA-C	-6.31	98.21	110.20
2	B	52	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	B	28	LEU	CB-CG-CD1	6.13	121.42	111.00
1	C	89	TYR	N-CA-CB	-6.12	99.59	110.60
1	C	47	ASP	CB-CG-OD2	6.12	123.80	118.30
1	A	137	THR	CA-CB-CG2	-6.10	103.86	112.40
1	A	4	PRO	N-CD-CG	-6.09	94.06	103.20
1	A	81	SER	C-N-CA	-6.07	106.52	121.70
2	D	11	VAL	CA-CB-CG2	-6.06	101.81	110.90
2	D	60	VAL	CG1-CB-CG2	-6.04	101.24	110.90
2	B	2	HIS	N-CA-C	-6.02	94.73	111.00
2	D	43	ASP	OD1-CG-OD2	6.00	134.70	123.30
1	A	100	LEU	CB-CG-CD2	-6.00	100.81	111.00
2	B	105	LEU	CB-CG-CD1	5.97	121.15	111.00
2	D	145	TYR	CD1-CE1-CZ	-5.97	114.43	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	116	GLU	CA-CB-CG	5.94	126.46	113.40
2	B	28	LEU	CB-CA-C	-5.92	98.94	110.20
2	D	111	VAL	CA-CB-CG2	-5.90	102.05	110.90
1	A	92	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	C	84	SER	CB-CA-C	5.83	121.18	110.10
1	A	2	LEU	CB-CG-CD1	-5.80	101.13	111.00
1	C	100	LEU	CB-CG-CD1	5.80	120.87	111.00
2	B	28	LEU	CB-CG-CD2	5.75	120.78	111.00
2	B	110	LEU	CB-CA-C	-5.73	99.31	110.20
1	C	105	LEU	N-CA-CB	-5.72	98.96	110.40
2	D	88	LEU	CB-CG-CD2	5.71	120.71	111.00
2	B	35	TYR	CG-CD2-CE2	-5.71	116.74	121.30
2	B	35	TYR	CE1-CZ-OH	-5.71	104.70	120.10
2	D	11	VAL	CB-CA-C	-5.70	100.58	111.40
1	C	109	LEU	CD1-CG-CD2	-5.67	93.50	110.50
2	B	18	VAL	CB-CA-C	-5.66	100.65	111.40
1	A	11	LYS	O-C-N	5.65	131.75	122.70
2	D	81	LEU	CA-CB-CG	5.65	128.29	115.30
2	D	114	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	C	100	LEU	CB-CA-C	-5.63	99.50	110.20
1	A	2	LEU	CA-CB-CG	-5.59	102.44	115.30
2	B	64	GLY	N-CA-C	-5.56	99.21	113.10
2	D	45	PHE	CZ-CE2-CD2	-5.55	113.43	120.10
2	D	106	LEU	CA-CB-CG	5.55	128.07	115.30
2	B	125	GLN	N-CA-CB	5.55	120.59	110.60
1	C	141	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
2	D	93	CYS	CA-CB-SG	-5.47	104.16	114.00
2	B	101	GLU	N-CA-CB	-5.41	100.86	110.60
1	A	16	LYS	CB-CA-C	-5.40	99.60	110.40
2	D	144	LYS	CA-CB-CG	-5.38	101.56	113.40
2	D	52	ASP	CB-CG-OD2	5.36	123.13	118.30
1	C	39	THR	N-CA-C	5.34	125.43	111.00
2	B	121	GLU	CB-CG-CD	-5.33	99.81	114.20
2	D	130	TYR	CG-CD1-CE1	5.33	125.56	121.30
1	A	70	VAL	CA-CB-CG1	-5.33	102.91	110.90
1	A	50	PRO	N-CD-CG	-5.30	95.24	103.20
2	B	112	CYS	N-CA-CB	5.29	120.12	110.60
1	C	36	PHE	CG-CD2-CE2	5.29	126.62	120.80
1	C	16	LYS	CA-CB-CG	-5.28	101.79	113.40
1	A	38	THR	OG1-CB-CG2	-5.25	97.93	110.00
2	D	52	ASP	CB-CA-C	-5.25	99.90	110.40
2	D	3	LEU	CB-CG-CD2	-5.24	102.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	98	VAL	C-N-CA	-5.21	108.69	121.70
2	D	120	LYS	N-CA-C	5.18	124.99	111.00
2	B	35	TYR	CG-CD1-CE1	5.17	125.44	121.30
1	A	50	PRO	CB-CG-CD	-5.17	86.34	106.50
1	C	11	LYS	CA-CB-CG	-5.15	102.06	113.40
1	C	36	PHE	CG-CD1-CE1	-5.12	115.17	120.80
2	D	115	ALA	N-CA-CB	-5.11	102.94	110.10
1	C	75	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	C	21	ALA	N-CA-CB	5.09	117.22	110.10
2	B	56	SER	N-CA-CB	-5.09	102.87	110.50
1	C	87	HIS	CB-CA-C	5.09	120.57	110.40
1	C	15	ASP	OD1-CG-OD2	5.08	132.96	123.30
1	C	43	PHE	CG-CD2-CE2	5.08	126.39	120.80
2	B	1	VAL	CG1-CB-CG2	5.08	119.02	110.90
2	B	96	LEU	N-CA-C	5.07	124.70	111.00
1	C	128	PHE	CZ-CE2-CD2	5.07	126.18	120.10
2	B	52	ASP	OD1-CG-OD2	5.03	132.86	123.30
2	B	54	VAL	CB-CA-C	-5.03	101.84	111.40
2	D	27	ALA	CB-CA-C	5.03	117.64	110.10
1	A	64	ASP	CA-C-N	-5.01	106.17	117.20
1	C	23	ASP	OD1-CG-OD2	5.01	132.82	123.30
2	B	94	ASP	OD1-CG-OD2	5.00	132.81	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	51	GLY	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	1077	0	1069	83	0
1	C	1077	0	1069	37	1
2	B	1131	0	1135	56	1
2	D	1131	0	1135	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	0	30	5	0
3	B	43	0	30	6	0
3	C	43	0	30	4	0
3	D	43	0	30	5	0
All	All	4588	0	4528	242	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (242) 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:A:4:PRO:CD	1:A:4:PRO:CG	1.75	1.62
2:D:66:LYS:CE	2:D:66:LYS:CD	1.78	1.60
1:C:56:LYS:CD	1:C:56:LYS:CE	1.80	1.60
2:B:76:LYS:CD	2:B:76:LYS:CG	1.77	1.58
1:A:11:LYS:CE	1:A:11:LYS:CD	1.76	1.57
2:D:66:LYS:CE	2:D:66:LYS:NZ	1.67	1.56
2:B:120:LYS:CE	2:B:120:LYS:NZ	1.67	1.56
1:A:141:ARG:CD	1:A:141:ARG:CG	1.76	1.55
2:D:17:LYS:CE	2:D:17:LYS:CD	1.77	1.54
2:D:120:LYS:CG	2:D:120:LYS:CB	1.79	1.54
2:D:120:LYS:NZ	2:D:120:LYS:CE	1.70	1.54
1:C:60:LYS:NZ	1:C:60:LYS:CE	1.71	1.53
2:B:61:LYS:CD	2:B:61:LYS:CG	1.79	1.53
2:B:59:LYS:CE	2:B:59:LYS:NZ	1.70	1.52
2:D:27:ALA:CB	2:D:27:ALA:CA	1.86	1.52
2:B:132:LYS:NZ	2:B:132:LYS:CE	1.70	1.51
1:A:16:LYS:NZ	1:A:16:LYS:CE	1.70	1.51
1:A:127:LYS:NZ	1:A:127:LYS:CE	1.69	1.49
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.77	1.47
2:B:66:LYS:CE	2:B:66:LYS:NZ	1.78	1.46
1:A:77:PRO:CG	1:A:77:PRO:CB	1.75	1.44
1:A:50:PRO:CG	1:A:50:PRO:CD	1.80	1.43
1:A:11:LYS:CE	1:A:11:LYS:NZ	1.76	1.43
1:C:50:PRO:CB	1:C:50:PRO:CG	1.80	1.43
1:A:3:SER:OG	1:A:3:SER:CB	1.66	1.43
2:D:132:LYS:NZ	2:D:132:LYS:CE	1.81	1.41
2:D:93:CYS:CB	2:D:93:CYS:SG	2.08	1.40
2:B:65:LYS:CE	2:B:65:LYS:NZ	1.87	1.38
2:D:61:LYS:CE	2:D:61:LYS:NZ	1.96	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:93:CYS:SG	2:D:145:TYR:CE2	2.32	1.23
2:D:93:CYS:SG	2:D:145:TYR:CZ	2.35	1.19
1:A:1:VAL:HG12	1:C:141:ARG:O	1.46	1.15
1:A:141:ARG:O	1:C:1:VAL:HG23	1.55	1.06
1:A:58:HIS:O	1:A:61:LYS:N	1.98	0.96
1:A:1:VAL:HG13	1:A:2:LEU:H	1.28	0.96
2:B:63:HIS:O	2:B:66:LYS:N	1.99	0.95
2:D:120:LYS:HD2	2:D:120:LYS:HA	1.50	0.94
1:A:16:LYS:NZ	1:A:16:LYS:HG2	1.87	0.88
1:A:9:ASN:O	1:A:13:THR:HG23	1.74	0.87
1:A:139:LYS:NZ	1:A:139:LYS:CD	2.38	0.86
3:B:147:HEM:HMC1	3:B:147:HEM:HBC2	1.56	0.86
2:D:17:LYS:CD	2:D:17:LYS:NZ	2.38	0.85
2:D:120:LYS:CG	2:D:120:LYS:CA	2.57	0.82
2:D:132:LYS:NZ	2:D:132:LYS:CD	2.42	0.82
1:A:58:HIS:HA	1:A:61:LYS:HE3	1.63	0.78
2:D:93:CYS:SG	2:D:145:TYR:CD2	2.77	0.78
1:A:89:TYR:CD1	1:A:139:LYS:HD3	2.19	0.78
2:B:143:HIS:CD2	2:B:144:LYS:HE3	2.19	0.77
2:B:58:ALA:HA	2:B:61:LYS:HE2	1.66	0.77
1:C:1:VAL:O	1:C:2:LEU:HB2	1.86	0.75
1:A:46:PHE:HB3	1:A:48:LEU:HD13	1.68	0.74
2:B:87:LYS:HB2	2:B:87:LYS:NZ	2.02	0.73
2:B:63:HIS:ND1	2:B:67:VAL:HG23	2.05	0.71
3:B:147:HEM:HMD1	3:B:147:HEM:HBD1	1.73	0.71
3:B:147:HEM:HBC2	3:B:147:HEM:CMC	2.20	0.70
2:B:2:HIS:O	2:B:3:LEU:HB2	1.91	0.70
3:D:147:HEM:HBC2	3:D:147:HEM:HMC1	1.74	0.69
1:A:16:LYS:HG2	1:A:16:LYS:HZ3	1.58	0.68
2:B:1:VAL:O	2:B:1:VAL:CG2	2.40	0.68
2:D:120:LYS:HA	2:D:120:LYS:CD	2.24	0.68
1:A:141:ARG:CG	1:A:141:ARG:NE	2.56	0.68
1:A:11:LYS:CE	1:A:11:LYS:CG	2.73	0.67
2:D:41:PHE:CD1	3:D:147:HEM:HBC1	2.29	0.67
2:B:120:LYS:HA	2:B:120:LYS:HE3	1.77	0.66
2:D:100:PRO:HG3	2:D:145:TYR:CD2	2.30	0.66
1:A:17:ILE:HD11	1:A:21:ALA:HB2	1.75	0.66
1:A:10:ILE:HD13	1:A:125:LEU:HD12	1.78	0.66
1:A:139:LYS:O	1:A:139:LYS:HG3	1.96	0.65
1:A:89:TYR:CE1	1:A:139:LYS:HE2	2.32	0.65
1:A:127:LYS:NZ	1:A:127:LYS:CD	2.58	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG22	1:C:97:ASN:ND2	2.12	0.64
1:A:16:LYS:NZ	1:A:16:LYS:CG	2.59	0.64
1:A:58:HIS:HD2	1:A:61:LYS:HE3	1.62	0.64
2:D:17:LYS:CE	2:D:17:LYS:CG	2.76	0.63
2:B:59:LYS:NZ	2:B:59:LYS:CD	2.60	0.63
2:B:63:HIS:O	2:B:64:GLY:C	2.37	0.63
1:A:66:LEU:O	1:A:70:VAL:HG23	1.99	0.62
2:B:87:LYS:HB2	2:B:87:LYS:HZ3	1.63	0.62
2:D:65:LYS:O	2:D:68:LEU:N	2.30	0.62
2:D:37:TRP:HE1	2:D:102:ASN:HD21	1.45	0.61
1:A:1:VAL:CG1	1:A:2:LEU:H	2.05	0.61
1:A:11:LYS:CE	1:A:11:LYS:HB3	2.31	0.60
2:D:93:CYS:SG	2:D:145:TYR:CE1	2.90	0.60
2:D:93:CYS:SG	2:D:93:CYS:CA	2.88	0.60
1:A:38:THR:O	1:A:41:THR:HB	2.02	0.60
1:A:11:LYS:HB3	1:A:11:LYS:HE3	1.84	0.59
1:A:6:ASP:O	1:A:10:ILE:HG12	2.04	0.58
3:B:147:HEM:HBD1	3:B:147:HEM:CMD	2.33	0.58
1:A:113:HIS:N	1:A:114:PRO:CD	2.66	0.58
1:A:14:TRP:HA	1:A:17:ILE:HG23	1.84	0.58
1:C:8:THR:O	1:C:12:SER:HB3	2.03	0.57
2:B:127:GLN:O	2:B:131:GLN:HG2	2.04	0.57
2:D:100:PRO:HG3	2:D:145:TYR:CE2	2.38	0.57
1:C:39:THR:HG22	1:C:97:ASN:HD21	1.68	0.57
2:D:66:LYS:CE	2:D:66:LYS:CG	2.82	0.57
2:D:120:LYS:CA	2:D:120:LYS:CD	2.83	0.57
2:D:107:GLY:HA3	2:D:134:VAL:HG13	1.87	0.56
1:A:43:PHE:N	1:A:44:PRO:CD	2.68	0.56
2:B:33:ILE:HD13	2:B:51:PRO:HB3	1.86	0.56
1:C:60:LYS:NZ	1:C:60:LYS:CD	2.65	0.56
1:A:3:SER:OG	1:A:3:SER:CA	2.50	0.56
1:A:58:HIS:CD2	1:A:61:LYS:HE3	2.40	0.56
1:A:13:THR:O	1:A:17:ILE:CG2	2.54	0.56
2:D:142:ALA:O	2:D:145:TYR:HB2	2.06	0.55
1:A:43:PHE:N	1:A:44:PRO:HD3	2.21	0.55
3:A:142:HEM:CMC	3:A:142:HEM:HBC2	2.36	0.54
1:A:3:SER:CB	1:A:3:SER:HG	2.09	0.53
2:D:3:LEU:HA	2:D:7:GLU:OE2	2.07	0.53
2:B:50:THR:O	2:B:54:VAL:HG23	2.08	0.53
1:C:28:ALA:CB	1:C:105:LEU:HD13	2.38	0.53
1:C:53:ALA:HA	1:C:56:LYS:HE2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:HIS:O	1:A:59:GLY:C	2.46	0.53
1:A:76:LEU:N	1:A:77:PRO:CD	2.71	0.53
1:A:58:HIS:HD2	1:A:61:LYS:CE	2.21	0.53
3:D:147:HEM:HBC2	3:D:147:HEM:CMC	2.39	0.53
1:C:45:HIS:ND1	1:C:45:HIS:N	2.53	0.52
3:B:147:HEM:CMD	3:B:147:HEM:CBD	2.87	0.52
1:A:3:SER:O	1:A:6:ASP:HB2	2.08	0.52
1:A:141:ARG:O	1:C:1:VAL:CG2	2.43	0.52
1:A:1:VAL:HG13	1:A:2:LEU:N	2.12	0.52
1:C:57:ALA:HA	1:C:60:LYS:HD2	1.91	0.52
1:C:81:SER:O	1:C:82:ALA:C	2.48	0.51
2:B:123:THR:OG1	2:B:126:VAL:HG23	2.11	0.51
1:C:35:SER:HB3	2:D:131:GLN:HG3	1.92	0.51
1:A:1:VAL:O	1:A:2:LEU:HB2	2.09	0.51
1:C:56:LYS:HE2	1:C:56:LYS:HB2	1.92	0.51
1:A:89:TYR:CE1	1:A:139:LYS:CE	2.93	0.50
2:D:96:LEU:O	2:D:97:HIS:HB2	2.11	0.50
2:B:1:VAL:O	2:B:1:VAL:HG22	2.11	0.50
3:C:142:HEM:HMB2	3:C:142:HEM:HBB2	1.93	0.50
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.42	0.50
1:A:89:TYR:CZ	1:A:139:LYS:HE2	2.46	0.50
1:A:17:ILE:HD13	1:A:18:GLY:N	2.27	0.50
1:C:66:LEU:O	1:C:69:ALA:HB3	2.12	0.49
2:D:92:HIS:HA	2:D:96:LEU:HD12	1.93	0.49
2:B:57:ASN:OD1	2:B:57:ASN:C	2.51	0.49
2:B:122:PHE:CE2	2:B:127:GLN:HB2	2.47	0.49
2:D:90:GLU:O	2:D:94:ASP:HB2	2.13	0.49
1:A:13:THR:O	1:A:17:ILE:HG23	2.13	0.49
2:D:107:GLY:HA3	2:D:134:VAL:CG1	2.43	0.49
3:A:142:HEM:HBD1	3:A:142:HEM:HMD2	1.95	0.49
2:D:110:LEU:O	2:D:110:LEU:HD22	2.12	0.49
1:A:11:LYS:CE	1:A:11:LYS:CB	2.91	0.48
1:C:135:VAL:O	1:C:138:SER:OG	2.28	0.48
1:A:13:THR:O	1:A:17:ILE:HG22	2.13	0.48
3:A:142:HEM:HMB1	3:A:142:HEM:HBB2	1.94	0.48
2:D:110:LEU:HD22	2:D:110:LEU:C	2.34	0.48
1:A:98:PHE:HE1	1:A:136:LEU:HD12	1.78	0.48
2:B:76:LYS:CD	2:B:76:LYS:CB	2.87	0.48
1:A:141:ARG:HB3	1:A:141:ARG:NH1	2.29	0.47
1:A:89:TYR:CZ	1:A:139:LYS:CE	2.98	0.47
2:B:25:GLY:N	2:B:64:GLY:HA3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:HE3	2:B:65:LYS:HB3	1.56	0.47
2:B:108:ASN:HD21	2:B:131:GLN:HE22	1.62	0.47
3:D:147:HEM:HHC	3:D:147:HEM:HBB2	1.97	0.47
2:D:64:GLY:O	2:D:65:LYS:C	2.50	0.47
2:B:143:HIS:C	2:B:145:TYR:H	2.18	0.46
1:C:85:ASP:O	1:C:89:TYR:HB2	2.14	0.46
1:A:11:LYS:CD	1:A:11:LYS:NZ	2.77	0.46
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.72	0.46
2:B:63:HIS:O	2:B:65:LYS:N	2.48	0.46
1:A:42:TYR:C	1:A:44:PRO:HD3	2.35	0.46
1:A:89:TYR:CZ	1:A:139:LYS:NZ	2.83	0.46
1:A:7:LYS:O	1:A:11:LYS:HG3	2.16	0.46
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.98	0.46
2:B:88:LEU:HD23	2:B:88:LEU:HA	1.56	0.46
2:D:28:LEU:O	2:D:29:GLY:C	2.55	0.45
2:B:26:GLU:OE2	2:B:117:HIS:HE1	1.99	0.45
2:D:28:LEU:HA	2:D:28:LEU:HD23	1.51	0.45
1:C:89:TYR:CD1	1:C:139:LYS:CD	2.99	0.45
2:D:95:LYS:HA	2:D:95:LYS:HD3	1.67	0.45
1:A:16:LYS:NZ	1:A:16:LYS:CD	2.71	0.45
2:B:132:LYS:NZ	2:B:132:LYS:CD	2.75	0.45
1:C:49:SER:HA	1:C:50:PRO:HD2	1.71	0.45
1:C:99:LYS:HZ2	1:C:99:LYS:HG2	1.46	0.45
2:D:58:ALA:HA	2:D:61:LYS:NZ	2.31	0.45
2:D:120:LYS:NZ	2:D:120:LYS:CD	2.71	0.45
2:B:14:LEU:HD12	2:B:126:VAL:HG11	1.99	0.45
2:B:87:LYS:NZ	2:B:87:LYS:CB	2.76	0.45
3:C:142:HEM:HHC	3:C:142:HEM:HAB	1.57	0.45
2:B:110:LEU:O	2:B:110:LEU:HD22	2.16	0.44
1:C:89:TYR:CD1	1:C:139:LYS:NZ	2.82	0.44
3:A:142:HEM:CMC	3:A:142:HEM:CBC	2.95	0.44
3:A:142:HEM:CBC	3:A:142:HEM:HMC1	2.47	0.44
2:D:27:ALA:CB	2:D:27:ALA:N	2.71	0.44
1:A:1:VAL:CG1	1:A:2:LEU:N	2.78	0.44
2:B:63:HIS:CE1	2:B:67:VAL:HG23	2.51	0.44
1:A:46:PHE:CB	1:A:48:LEU:HD13	2.43	0.44
2:D:78:LEU:HD23	2:D:78:LEU:HA	1.79	0.44
1:A:17:ILE:HD13	1:A:17:ILE:C	2.38	0.44
2:B:66:LYS:HE3	2:B:66:LYS:HB3	1.39	0.43
2:B:63:HIS:ND1	2:B:67:VAL:CG2	2.80	0.43
1:C:7:LYS:HB3	1:C:73:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:GLN:O	2:D:131:GLN:HG2	2.18	0.43
2:B:26:GLU:O	2:B:30:ARG:HB2	2.18	0.43
1:C:128:PHE:O	1:C:129:PHE:C	2.57	0.43
2:B:143:HIS:CD2	2:B:144:LYS:CE	2.97	0.43
2:B:1:VAL:O	2:B:1:VAL:HG23	2.16	0.43
2:B:2:HIS:HB2	2:B:3:LEU:H	1.69	0.43
2:B:82:LYS:N	2:B:82:LYS:HD2	2.34	0.43
1:A:103:HIS:O	1:A:107:VAL:HG23	2.19	0.43
1:C:97:ASN:HB3	3:C:142:HEM:HMC1	2.01	0.42
1:C:118:THR:OG1	1:C:121:VAL:HG23	2.19	0.42
1:A:6:ASP:O	1:A:9:ASN:N	2.53	0.42
1:A:58:HIS:HA	1:A:61:LYS:CE	2.42	0.42
1:A:76:LEU:N	1:A:77:PRO:HD3	2.34	0.42
2:B:32:LEU:H	2:B:32:LEU:HG	1.73	0.42
1:A:88:ALA:CB	1:A:139:LYS:HB3	2.49	0.42
3:B:147:HEM:HMC1	3:B:147:HEM:CBC	2.40	0.42
1:C:87:HIS:HE1	3:C:142:HEM:NA	2.08	0.42
2:D:19:ASN:ND2	2:D:22:GLU:HB2	2.35	0.42
1:C:24:TYR:OH	1:C:113:HIS:HE1	2.01	0.42
2:D:100:PRO:O	2:D:102:ASN:N	2.53	0.42
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.85	0.42
2:B:57:ASN:OD1	2:B:60:VAL:HG23	2.20	0.42
2:B:63:HIS:CE1	2:B:67:VAL:CG2	3.03	0.42
2:B:96:LEU:HA	2:B:96:LEU:HD23	1.86	0.42
1:C:56:LYS:HE2	1:C:56:LYS:CB	2.49	0.42
2:D:28:LEU:C	2:D:28:LEU:CD2	2.86	0.42
1:A:1:VAL:O	1:A:2:LEU:CB	2.68	0.42
1:A:6:ASP:O	1:A:7:LYS:C	2.57	0.42
2:D:143:HIS:C	2:D:145:TYR:H	2.23	0.41
1:C:89:TYR:CD1	1:C:139:LYS:HD3	2.55	0.41
2:B:33:ILE:HD13	2:B:33:ILE:HG21	1.72	0.41
2:D:1:VAL:HG23	2:D:3:LEU:CD1	2.50	0.41
2:D:120:LYS:HD2	2:D:120:LYS:CA	2.31	0.41
1:A:91:LEU:HB2	1:A:93:VAL:HG23	2.02	0.41
1:C:88:ALA:CB	1:C:139:LYS:HB3	2.51	0.41
2:B:63:HIS:C	2:B:65:LYS:N	2.73	0.41
1:C:106:LEU:HD21	1:C:125:LEU:HB3	2.03	0.41
1:A:89:TYR:CE2	1:A:139:LYS:NZ	2.76	0.41
2:B:68:LEU:HD22	2:B:68:LEU:HA	1.90	0.41
2:B:79:ASP:HB3	2:B:80:ASN:H	1.48	0.41
2:B:129:ALA:O	2:B:132:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:HIS:O	1:C:62:VAL:HG23	2.21	0.41
2:D:123:THR:OG1	2:D:126:VAL:HG23	2.21	0.41
1:A:141:ARG:NH1	1:A:141:ARG:CB	2.84	0.41
1:C:56:LYS:CE	1:C:56:LYS:CB	2.98	0.41
3:D:147:HEM:HMC1	3:D:147:HEM:CBC	2.48	0.40
1:A:77:PRO:O	1:A:81:SER:HB3	2.22	0.40
2:B:81:LEU:N	2:B:82:LYS:HD2	2.36	0.40
2:D:132:LYS:CD	2:D:132:LYS:HZ3	2.29	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ASP:OD1	1:C:75:ASP:OD1[2_645]	2.00	0.20

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	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3	26
1	C	139/141 (99%)	124 (89%)	12 (9%)	3 (2%)	6	37
2	B	144/146 (99%)	121 (84%)	13 (9%)	10 (7%)	1	12
2	D	144/146 (99%)	121 (84%)	18 (12%)	5 (4%)	3	27
All	All	566/574 (99%)	483 (85%)	60 (11%)	23 (4%)	3	23

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	78	LEU
2	B	144	LYS

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Mol	Chain	Res	Type
1	C	50	PRO
1	A	2	LEU
1	A	18	GLY
1	A	59	GLY
1	A	136	LEU
2	B	3	LEU
2	B	5	ALA
2	B	25	GLY
2	B	82	LYS
2	B	125	GLN
1	C	18	GLY
2	D	44	SER
2	D	101	GLU
2	D	144	LYS
1	A	21	ALA
2	B	79	ASP
2	B	44	SER
2	D	3	LEU
2	D	139	ASN
2	B	143	HIS
1	C	2	LEU

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	116/116 (100%)	96 (83%)	20 (17%)	2 11
1	C	116/116 (100%)	106 (91%)	10 (9%)	10 38
2	B	121/121 (100%)	99 (82%)	22 (18%)	1 9
2	D	121/121 (100%)	102 (84%)	19 (16%)	2 15
All	All	474/474 (100%)	403 (85%)	71 (15%)	3 17

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	11	LYS
1	A	16	LYS
1	A	17	ILE
1	A	38	THR
1	A	41	THR
1	A	48	LEU
1	A	49	SER
1	A	50	PRO
1	A	84	SER
1	A	85	ASP
1	A	86	LEU
1	A	89	TYR
1	A	95	PRO
1	A	105	LEU
1	A	116	GLU
1	A	117	PHE
1	A	127	LYS
1	A	139	LYS
1	A	141	ARG
2	B	2	HIS
2	B	8	LYS
2	B	9	SER
2	B	22	GLU
2	B	28	LEU
2	B	44	SER
2	B	48	LEU
2	B	52	ASP
2	B	57	ASN
2	B	61	LYS
2	B	68	LEU
2	B	72	SER
2	B	76	LYS
2	B	79	ASP
2	B	81	LEU
2	B	82	LYS
2	B	87	LYS
2	B	91	LEU
2	B	110	LEU
2	B	117	HIS
2	B	120	LYS
2	B	144	LYS
1	C	1	VAL

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Mol	Chain	Res	Type
1	C	41	THR
1	C	50	PRO
1	C	56	LYS
1	C	86	LEU
1	C	89	TYR
1	C	92	ARG
1	C	116	GLU
1	C	125	LEU
1	C	141	ARG
2	D	9	SER
2	D	10	LEU
2	D	14	LEU
2	D	20	VAL
2	D	28	LEU
2	D	40	ARG
2	D	42	PHE
2	D	50	THR
2	D	61	LYS
2	D	65	LYS
2	D	66	LYS
2	D	68	LEU
2	D	70	SER
2	D	75	LEU
2	D	81	LEU
2	D	96	LEU
2	D	110	LEU
2	D	120	LYS
2	D	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	58	HIS
1	A	103	HIS
2	B	102	ASN
2	B	108	ASN
2	B	117	HIS
2	B	143	HIS
1	C	9	ASN
1	C	34	GLN
1	C	97	ASN

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Mol	Chain	Res	Type
1	C	103	HIS
1	C	113	HIS
2	D	77	ASN
2	D	102	ASN
2	D	108	ASN
2	D	131	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	D	147	2	42,50,50	2.70	16 (38%)	46,82,82	2.60	22 (47%)
3	HEM	A	142	1	42,50,50	2.77	16 (38%)	46,82,82	2.78	21 (45%)
3	HEM	C	142	1	42,50,50	2.08	18 (42%)	46,82,82	4.75	30 (65%)
3	HEM	B	147	2	42,50,50	2.53	18 (42%)	46,82,82	3.68	21 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	147	2	-	7/12/54/54	-
3	HEM	A	142	1	-	6/12/54/54	-
3	HEM	C	142	1	-	7/12/54/54	-
3	HEM	B	147	2	-	4/12/54/54	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	147	HEM	C3C-C2C	-12.11	1.24	1.40
3	A	142	HEM	C3C-C2C	-9.47	1.27	1.40
3	A	142	HEM	O1A-CGA	7.04	1.45	1.22
3	B	147	HEM	C3C-C2C	-7.02	1.30	1.40
3	B	147	HEM	C4D-C3D	-5.37	1.35	1.45
3	B	147	HEM	O1D-CGD	4.97	1.38	1.22
3	A	142	HEM	CBA-CGA	4.90	1.61	1.50
3	B	147	HEM	CBD-CGD	4.61	1.61	1.50
3	C	142	HEM	CBD-CAD	4.34	1.67	1.51
3	A	142	HEM	CBD-CAD	4.30	1.66	1.51
3	B	147	HEM	C4A-NA	4.24	1.45	1.36
3	A	142	HEM	C3D-C2D	4.09	1.45	1.36
3	D	147	HEM	C3D-C2D	4.07	1.45	1.36
3	D	147	HEM	C3B-C2B	-3.98	1.29	1.37
3	B	147	HEM	CMB-C2B	3.93	1.58	1.50
3	A	142	HEM	CAA-C2A	-3.76	1.42	1.52
3	C	142	HEM	C3C-CAC	3.73	1.56	1.47
3	C	142	HEM	C3D-C2D	3.57	1.44	1.36
3	D	147	HEM	C4A-NA	3.36	1.43	1.36
3	D	147	HEM	C4D-C3D	3.31	1.50	1.45
3	A	142	HEM	CBD-CGD	3.28	1.58	1.50
3	D	147	HEM	CMB-C2B	-3.20	1.44	1.50
3	A	142	HEM	O2A-CGA	3.18	1.41	1.30
3	C	142	HEM	O1A-CGA	3.15	1.32	1.22
3	C	142	HEM	CHD-C1D	-3.11	1.32	1.40
3	B	147	HEM	C3D-C2D	3.10	1.43	1.36
3	D	147	HEM	C3C-CAC	-3.09	1.40	1.47
3	C	142	HEM	C4B-NB	3.07	1.44	1.38
3	B	147	HEM	C3C-CAC	-3.02	1.40	1.47
3	C	142	HEM	CMB-C2B	-2.97	1.44	1.50
3	A	142	HEM	C2C-C1C	-2.96	1.35	1.42
3	B	147	HEM	C4B-NB	-2.96	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	C2A-C3A	-2.95	1.28	1.37
3	B	147	HEM	CBD-CAD	2.95	1.62	1.51
3	A	142	HEM	C4A-CHB	-2.94	1.32	1.41
3	C	142	HEM	C3C-C2C	-2.94	1.36	1.40
3	A	142	HEM	C4D-C3D	-2.93	1.40	1.45
3	D	147	HEM	O1A-CGA	2.88	1.31	1.22
3	C	142	HEM	CBD-CGD	2.75	1.56	1.50
3	C	142	HEM	CBC-CAC	2.73	1.46	1.29
3	D	147	HEM	CAD-C3D	2.72	1.58	1.51
3	B	147	HEM	CHC-C4B	-2.68	1.33	1.40
3	C	142	HEM	C1D-C2D	2.68	1.50	1.44
3	C	142	HEM	C1A-NA	2.68	1.41	1.36
3	D	147	HEM	CHA-C4D	2.65	1.41	1.34
3	C	142	HEM	C2A-C3A	-2.61	1.29	1.37
3	C	142	HEM	C1B-C2B	-2.60	1.39	1.44
3	D	147	HEM	C2A-C3A	-2.54	1.30	1.37
3	B	147	HEM	C2C-C1C	2.47	1.48	1.42
3	A	142	HEM	CHB-C1B	2.47	1.40	1.34
3	C	142	HEM	CMC-C2C	2.46	1.57	1.51
3	B	147	HEM	CBA-CGA	2.42	1.56	1.50
3	B	147	HEM	C3C-C4C	2.40	1.44	1.41
3	A	142	HEM	C4D-ND	-2.39	1.36	1.40
3	B	147	HEM	C1D-C2D	-2.35	1.39	1.44
3	B	147	HEM	CHD-C1D	-2.35	1.34	1.40
3	C	142	HEM	O1D-CGD	2.33	1.29	1.22
3	B	147	HEM	C1A-NA	2.32	1.41	1.36
3	D	147	HEM	C1B-NB	2.31	1.44	1.40
3	A	142	HEM	C1A-CHA	-2.28	1.34	1.41
3	A	142	HEM	CHC-C4B	-2.24	1.34	1.40
3	D	147	HEM	CMA-C3A	2.23	1.56	1.51
3	D	147	HEM	CBA-CGA	2.23	1.55	1.50
3	C	142	HEM	C3B-C4B	-2.21	1.40	1.44
3	D	147	HEM	C1B-C2B	-2.19	1.40	1.44
3	D	147	HEM	C1D-C2D	2.14	1.48	1.44
3	C	142	HEM	O2A-CGA	-2.08	1.23	1.30
3	B	147	HEM	CAA-C2A	2.06	1.57	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	147	HEM	C2C-C3C-C4C	14.01	116.68	106.90
3	C	142	HEM	C4A-C3A-C2A	12.72	115.85	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	142	HEM	CHC-C4B-NB	12.02	137.36	124.44
3	B	147	HEM	C3B-C2B-C1B	-11.93	97.45	106.41
3	C	142	HEM	C3B-C4B-NB	-11.47	101.23	109.47
3	C	142	HEM	CBA-CAA-C2A	9.85	129.11	112.54
3	C	142	HEM	CMD-C2D-C1D	8.94	139.01	125.03
3	C	142	HEM	C4B-CHC-C1C	-7.42	112.77	122.56
3	C	142	HEM	C4B-C3B-C2B	7.40	114.08	107.28
3	A	142	HEM	CHB-C1B-NB	6.88	132.90	124.37
3	A	142	HEM	C2C-C3C-C4C	6.53	111.46	106.90
3	C	142	HEM	O1D-CGD-CBD	-6.27	103.20	123.09
3	B	147	HEM	C2B-C1B-NB	6.26	117.04	109.84
3	A	142	HEM	CHC-C4B-NB	6.16	131.06	124.44
3	B	147	HEM	C4B-C3B-C2B	5.91	112.71	107.28
3	C	142	HEM	CHD-C1D-ND	-5.87	118.12	124.44
3	C	142	HEM	C1D-C2D-C3D	-5.54	101.16	106.98
3	D	147	HEM	C2C-C3C-C4C	5.47	110.72	106.90
3	D	147	HEM	C4C-CHD-C1D	5.34	129.61	122.56
3	B	147	HEM	CHA-C4D-C3D	-5.01	115.99	125.23
3	D	147	HEM	C3D-C4D-ND	4.92	115.56	110.17
3	D	147	HEM	CHD-C1D-ND	-4.90	119.16	124.44
3	D	147	HEM	CBD-CAD-C3D	-4.89	99.02	112.53
3	C	142	HEM	C2C-C3C-C4C	4.80	110.25	106.90
3	D	147	HEM	CBA-CAA-C2A	4.71	120.45	112.54
3	A	142	HEM	O2D-CGD-CBD	4.67	128.76	114.00
3	B	147	HEM	CHA-C4D-ND	4.65	130.14	124.37
3	C	142	HEM	C2D-C1D-ND	4.41	115.00	109.90
3	A	142	HEM	CMD-C2D-C1D	4.33	131.80	125.03
3	A	142	HEM	C4B-CHC-C1C	-4.30	116.88	122.56
3	A	142	HEM	CAA-CBA-CGA	-4.28	102.31	113.83
3	C	142	HEM	C1B-NB-C4B	4.12	110.08	105.21
3	A	142	HEM	C4C-CHD-C1D	4.10	127.97	122.56
3	D	147	HEM	C2D-C1D-ND	4.05	114.59	109.90
3	A	142	HEM	CHD-C1D-ND	-3.77	120.38	124.44
3	C	142	HEM	C4C-CHD-C1D	3.77	127.53	122.56
3	D	147	HEM	CHA-C4D-ND	-3.76	119.72	124.37
3	B	147	HEM	CBA-CAA-C2A	3.76	118.86	112.54
3	A	142	HEM	CBD-CAD-C3D	-3.76	102.15	112.53
3	D	147	HEM	C4B-C3B-C2B	3.75	110.73	107.28
3	D	147	HEM	CMD-C2D-C1D	3.74	130.87	125.03
3	A	142	HEM	O2D-CGD-O1D	-3.68	113.86	123.33
3	B	147	HEM	C1B-NB-C4B	-3.60	100.94	105.21
3	C	142	HEM	CAB-C3B-C4B	-3.60	108.48	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	147	HEM	C3C-C4C-NC	-3.54	104.26	110.94
3	C	142	HEM	O2D-CGD-O1D	3.47	132.25	123.33
3	B	147	HEM	CMD-C2D-C1D	3.45	130.43	125.03
3	A	142	HEM	C1D-C2D-C3D	-3.44	103.37	106.98
3	B	147	HEM	CBD-CAD-C3D	-3.43	103.05	112.53
3	B	147	HEM	C3D-C4D-ND	3.37	113.87	110.17
3	C	142	HEM	O2D-CGD-CBD	3.34	124.54	114.00
3	B	147	HEM	C3B-C4B-NB	3.23	111.79	109.47
3	C	142	HEM	C2B-C1B-NB	-3.20	106.17	109.84
3	A	142	HEM	CMB-C2B-C1B	-3.19	120.05	125.03
3	D	147	HEM	O1D-CGD-CBD	-3.13	113.17	123.09
3	D	147	HEM	CAA-C2A-C3A	-3.11	118.32	127.25
3	B	147	HEM	CMB-C2B-C3B	3.08	135.88	128.43
3	C	142	HEM	CMA-C3A-C2A	-2.97	119.35	124.94
3	D	147	HEM	CAD-C3D-C4D	2.93	129.80	124.70
3	D	147	HEM	C4D-ND-C1D	-2.87	101.81	105.21
3	B	147	HEM	CMC-C2C-C3C	2.86	130.40	124.68
3	D	147	HEM	C4D-C3D-C2D	-2.80	102.81	106.89
3	A	142	HEM	CHB-C1B-C2B	-2.80	119.02	126.94
3	C	142	HEM	CAB-C3B-C2B	2.74	137.33	128.43
3	C	142	HEM	CAD-C3D-C2D	-2.70	122.81	127.87
3	C	142	HEM	CAA-CBA-CGA	-2.68	106.60	113.83
3	B	147	HEM	C4B-CHC-C1C	2.67	126.08	122.56
3	A	142	HEM	CHD-C1D-C2D	2.64	129.20	125.03
3	C	142	HEM	CMA-C3A-C4A	-2.57	124.68	128.46
3	D	147	HEM	C1B-NB-C4B	-2.55	102.19	105.21
3	A	142	HEM	C3B-C2B-C1B	2.52	108.30	106.41
3	D	147	HEM	O2A-CGA-O1A	2.51	129.79	123.33
3	A	142	HEM	C4B-C3B-C2B	2.50	109.58	107.28
3	C	142	HEM	C3B-C2B-C1B	2.46	108.26	106.41
3	D	147	HEM	C4A-C3A-C2A	2.38	108.66	107.00
3	A	142	HEM	CHC-C4B-C3B	-2.34	120.98	124.57
3	C	142	HEM	CMD-C2D-C3D	-2.33	119.83	126.15
3	B	147	HEM	CHB-C1B-C2B	-2.33	120.35	126.94
3	A	142	HEM	C3B-C4B-NB	-2.28	107.83	109.47
3	A	142	HEM	CAD-C3D-C4D	-2.21	120.85	124.70
3	C	142	HEM	CAD-C3D-C4D	2.20	128.53	124.70
3	B	147	HEM	CMA-C3A-C4A	-2.18	125.26	128.46
3	C	142	HEM	C3D-C4D-ND	2.18	112.56	110.17
3	D	147	HEM	O1A-CGA-CBA	-2.18	116.19	123.09
3	C	142	HEM	O2A-CGA-CBA	-2.15	107.22	114.00
3	B	147	HEM	C4A-C3A-C2A	2.15	108.49	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	142	HEM	CMB-C2B-C1B	-2.13	121.70	125.03
3	D	147	HEM	O2D-CGD-CBD	2.13	120.72	114.00
3	B	147	HEM	CAD-C3D-C2D	2.11	131.82	127.87
3	D	147	HEM	CAB-C3B-C2B	-2.10	121.60	128.43
3	C	142	HEM	CHC-C4B-C3B	-2.09	121.38	124.57
3	A	142	HEM	C4D-ND-C1D	2.08	107.67	105.21
3	B	147	HEM	CAB-C3B-C4B	-2.07	115.24	124.39
3	D	147	HEM	CHB-C1B-NB	2.06	126.93	124.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C2D-C3D-CAD-CBD
3	C	142	HEM	C3A-C2A-CAA-CBA
3	D	147	HEM	C3A-C2A-CAA-CBA
3	D	147	HEM	C2A-CAA-CBA-CGA
3	B	147	HEM	C4D-C3D-CAD-CBD
3	A	142	HEM	C2D-C3D-CAD-CBD
3	C	142	HEM	C1A-C2A-CAA-CBA
3	C	142	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	C3D-CAD-CBD-CGD
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	C1A-C2A-CAA-CBA
3	A	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAA-CBA-CGA-O2A
3	D	147	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	C2A-CAA-CBA-CGA

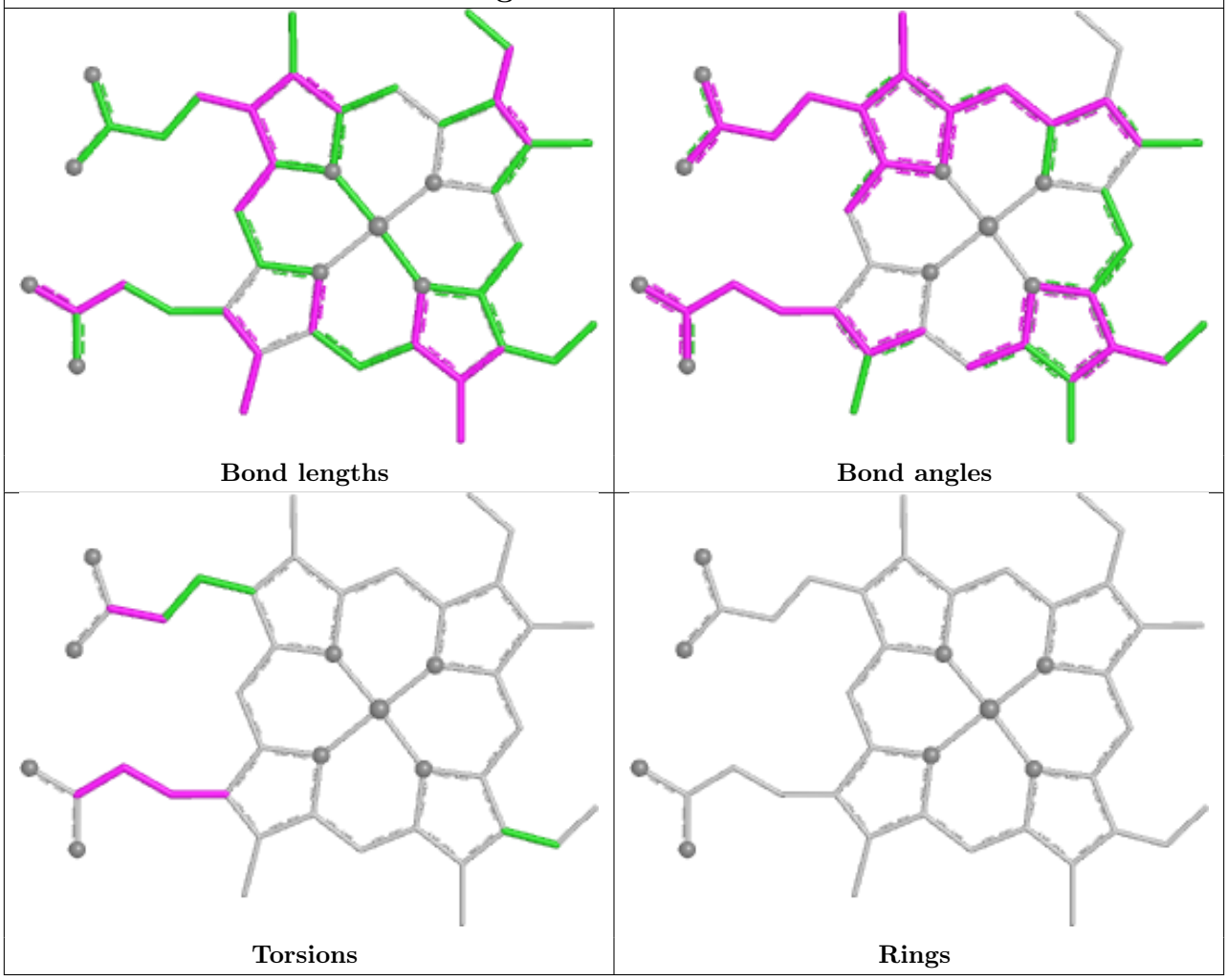
There are no ring outliers.

4 monomers are involved in 20 short contacts:

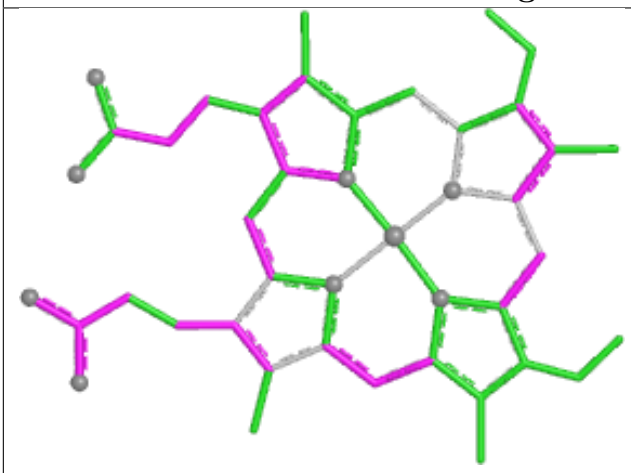
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	147	HEM	5	0
3	A	142	HEM	5	0
3	C	142	HEM	4	0
3	B	147	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

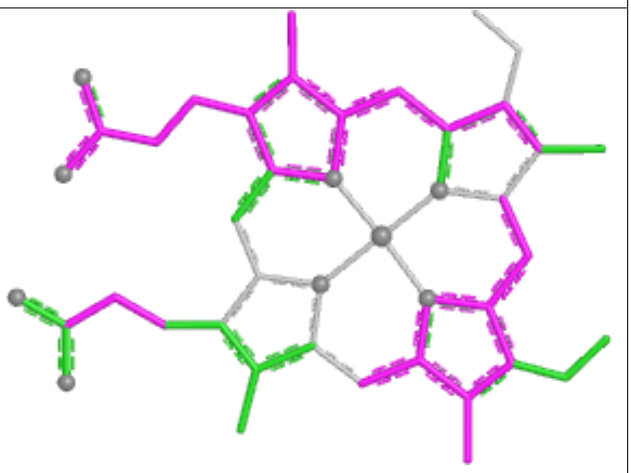
Ligand HEM D 147



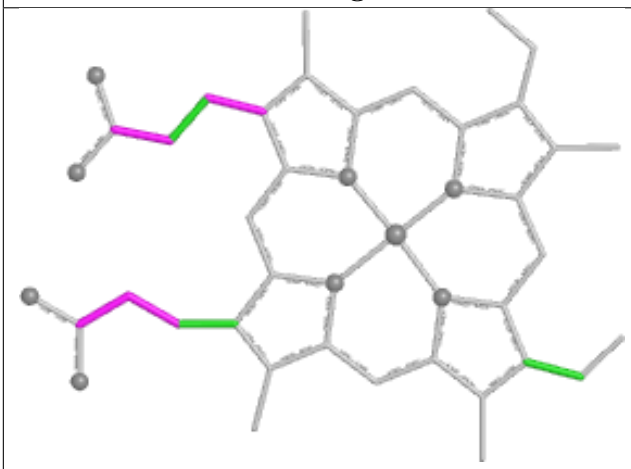
Ligand HEM A 142



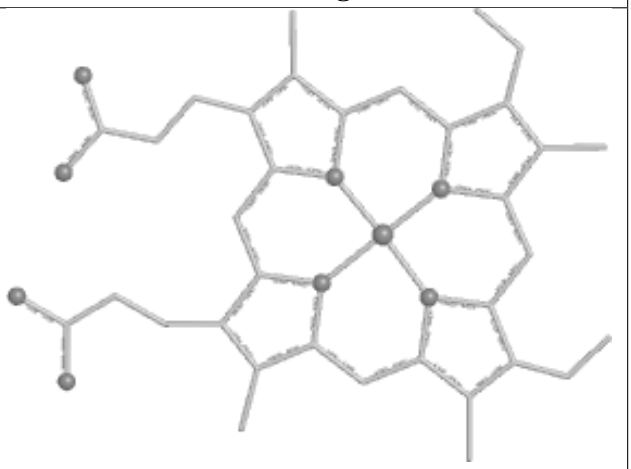
Bond lengths



Bond angles

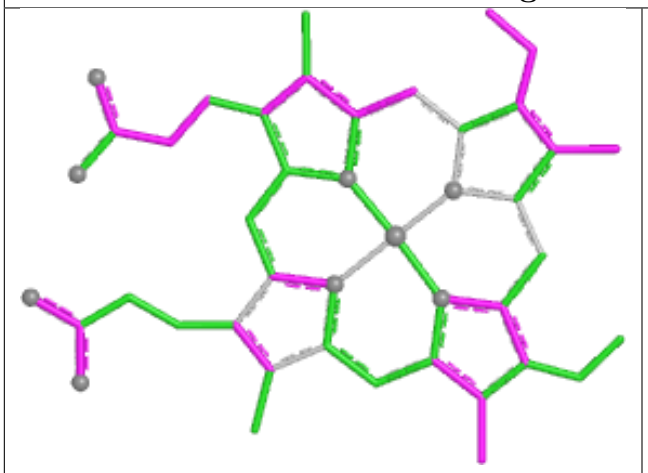


Torsions

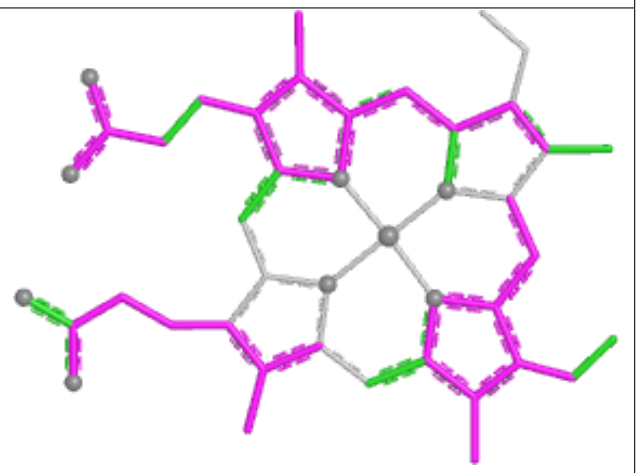


Rings

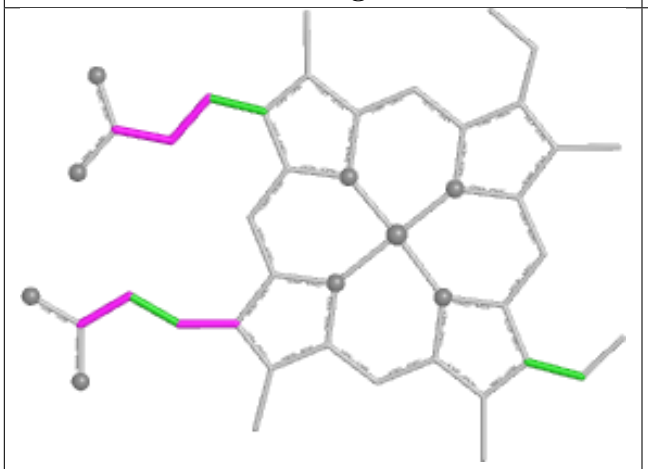
Ligand HEM C 142



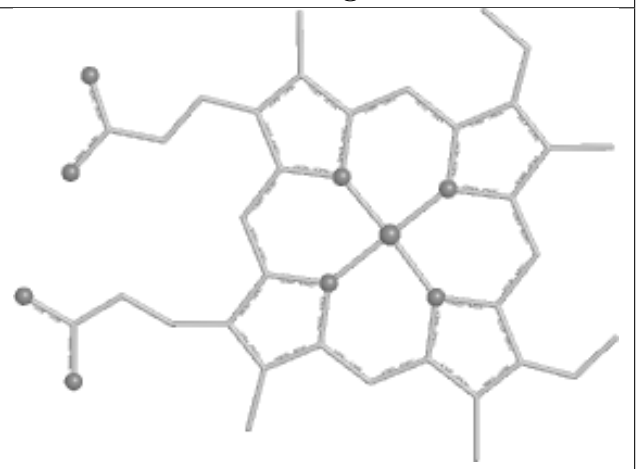
Bond lengths



Bond angles

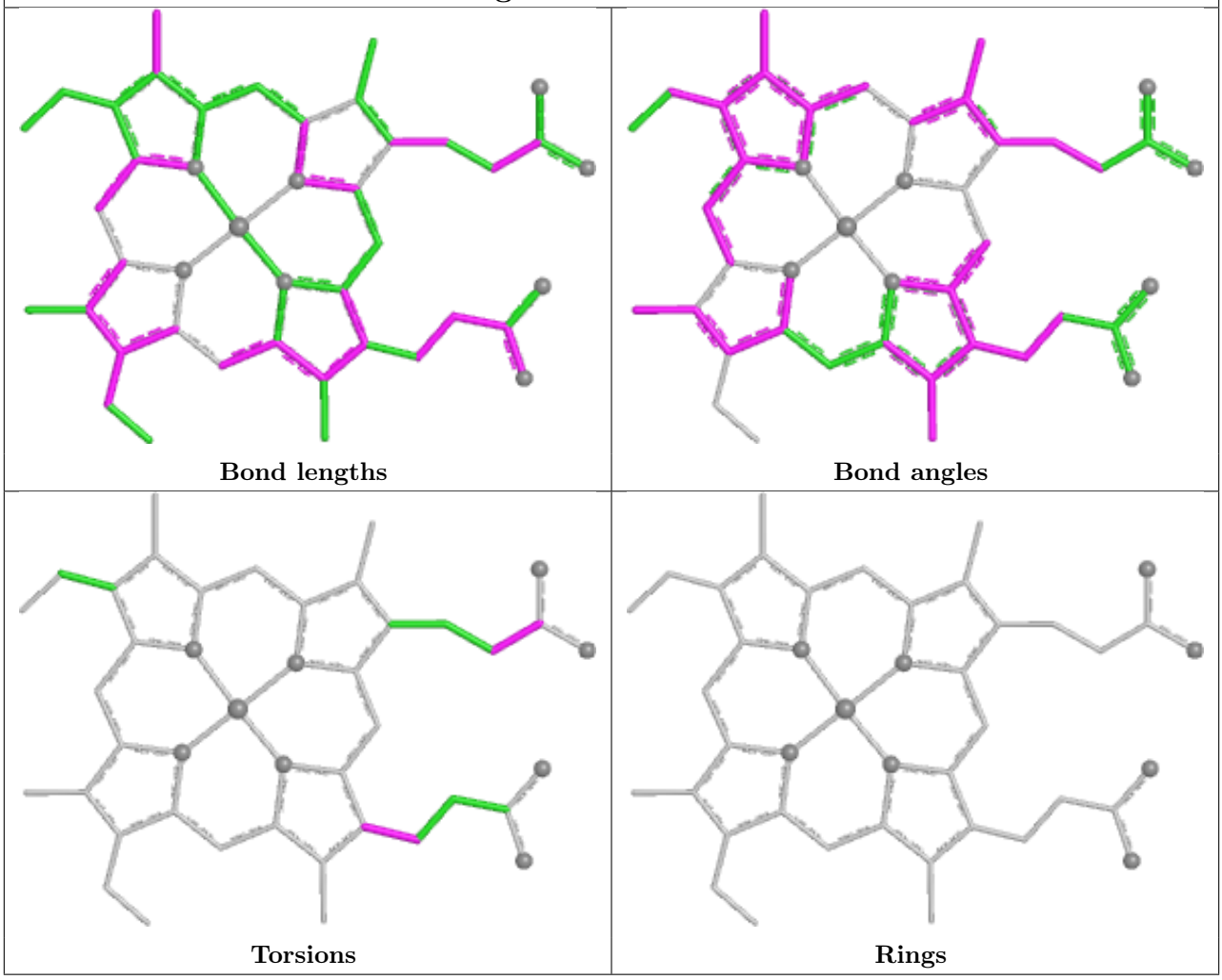


Torsions



Rings

Ligand HEM B 147



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	141/141 (100%)	-0.72	0 100 100	2, 19, 42, 56	0
1	C	141/141 (100%)	-0.75	0 100 100	3, 16, 40, 59	0
2	B	146/146 (100%)	-0.55	1 (0%) 87 83	2, 30, 53, 62	0
2	D	146/146 (100%)	-0.66	0 100 100	2, 21, 47, 71	0
All	All	574/574 (100%)	-0.67	1 (0%) 95 93	2, 21, 49, 71	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	143	HIS	2.3

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	HEM	B	147	43/43	0.96	0.17	3,21,51,68	0

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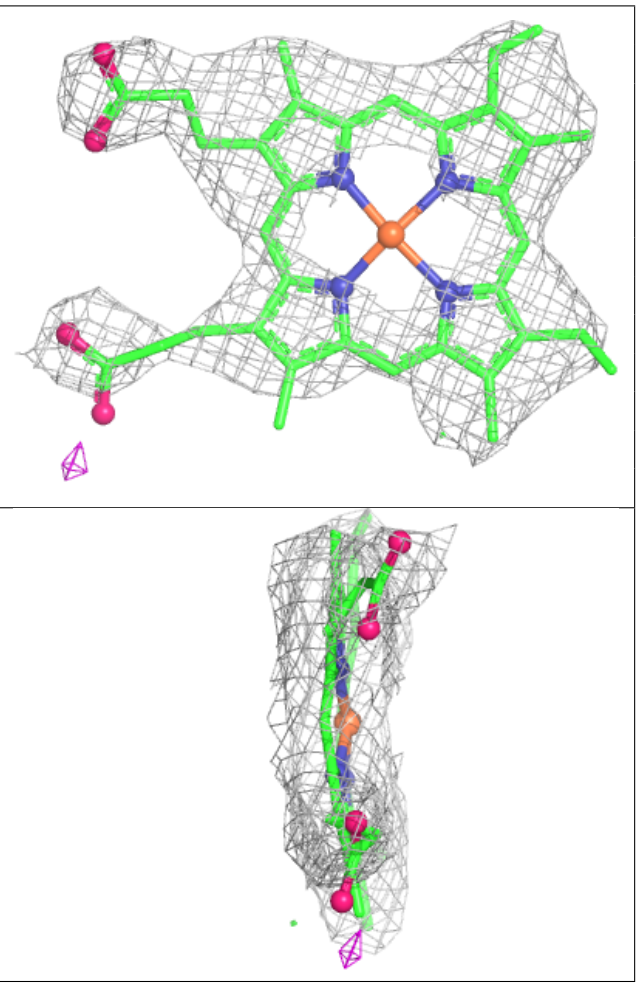
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	A	142	43/43	0.97	0.14	2,10,34,57	0
3	HEM	C	142	43/43	0.97	0.15	2,14,30,31	0
3	HEM	D	147	43/43	0.97	0.15	5,20,46,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

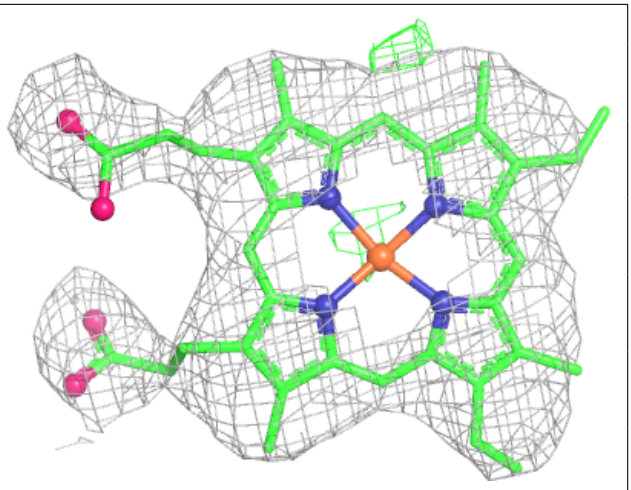
Electron density around HEM B 147:

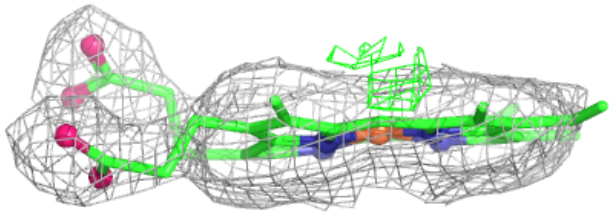
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

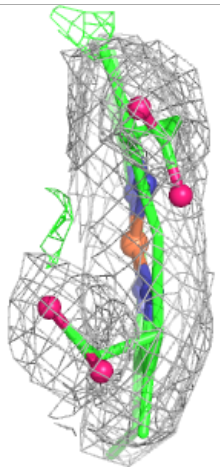


Electron density around HEM A 142:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

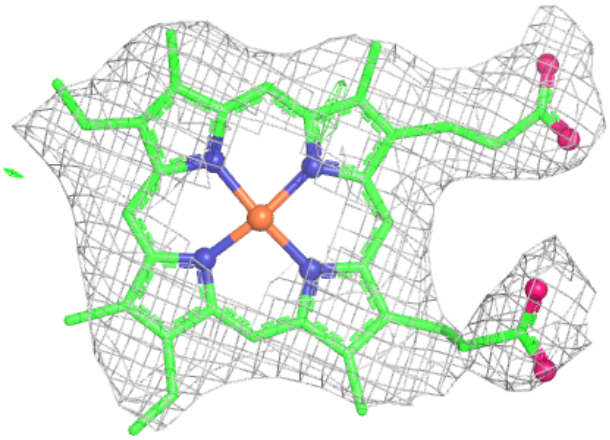


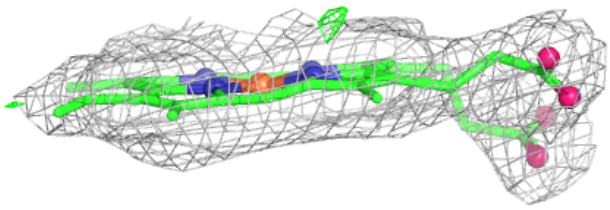


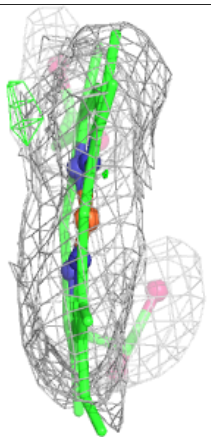


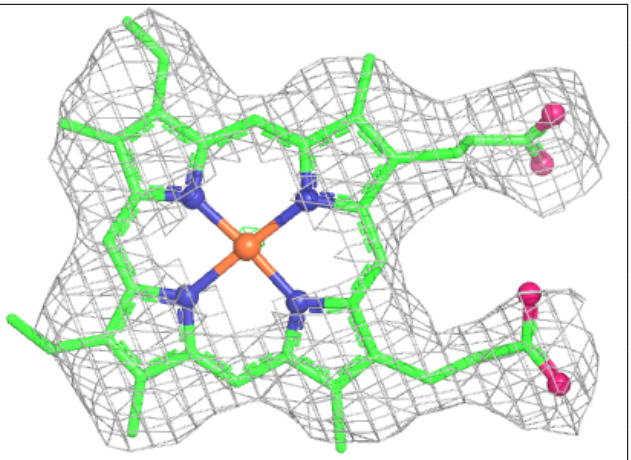
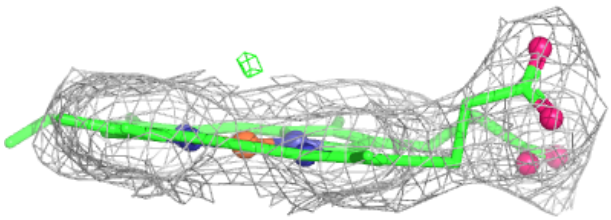
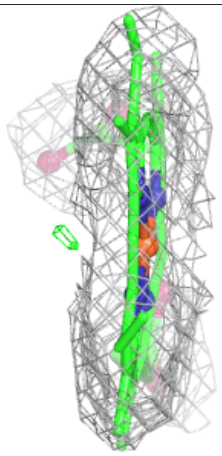
Electron density around HEM C 142:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM D 147: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.