Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 10:44 AM EST

PDB ID	:	2PCC
Title	:	CRYSTAL STRUCTURE OF A COMPLEX BETWEEN ELECTRON TRANSFER PARTNERS, CYTOCHROME C PEROXIDASE AND CYTOCHROME C
Authors	:	Pelletier, H.; Kraut, J.
Deposited on	:	1993-04-14
Resolution	:	2.30 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:

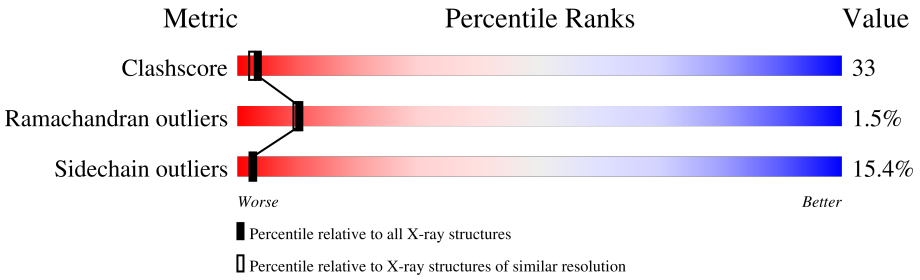
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 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%

Mol	Chain	Length	Quality of chain
1	A	296	44% 40% 12%
1	C	296	46% 38% 13%
2	B	108	39% 45% 15%
2	D	108	32% 46% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			
1	C	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			

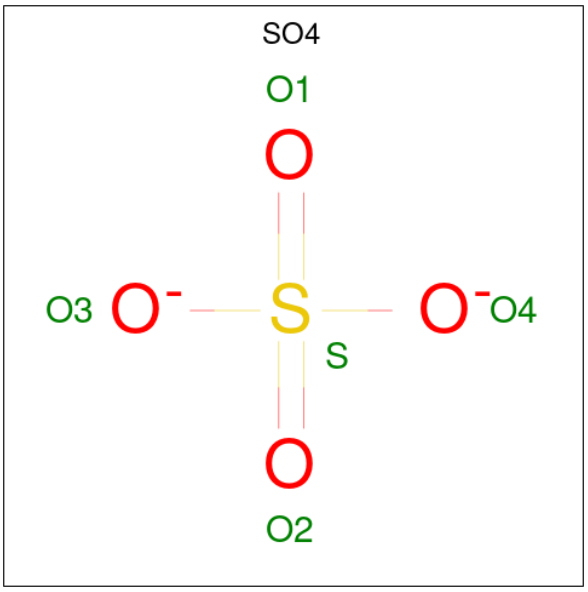
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	conflict	UNP P00431
A	152	GLY	ASP	conflict	UNP P00431
C	53	ILE	THR	conflict	UNP P00431
C	152	GLY	ASP	conflict	UNP P00431

- Molecule 2 is a protein called ISO-1-CYTOCHROME C.

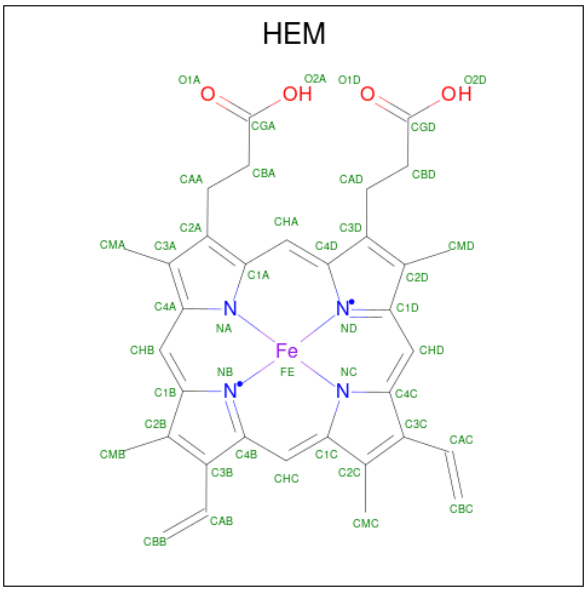
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			847	534	151	157	5			
2	D	108	Total	C	N	O	S	0	0	0
			847	534	151	157	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 2 1 1	0	0
3	C	1	Total O S 2 1 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 5 is water.

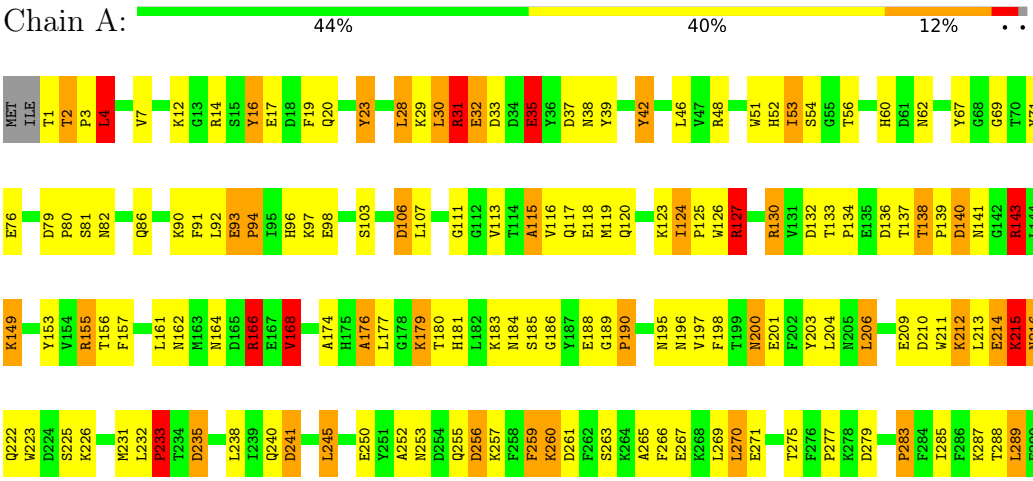
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	46	Total	O	0	0
			46	46		
5	C	212	Total	O	0	0
			212	212		
5	D	42	Total	O	0	0
			42	42		

3 Residue-property plots (i)

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

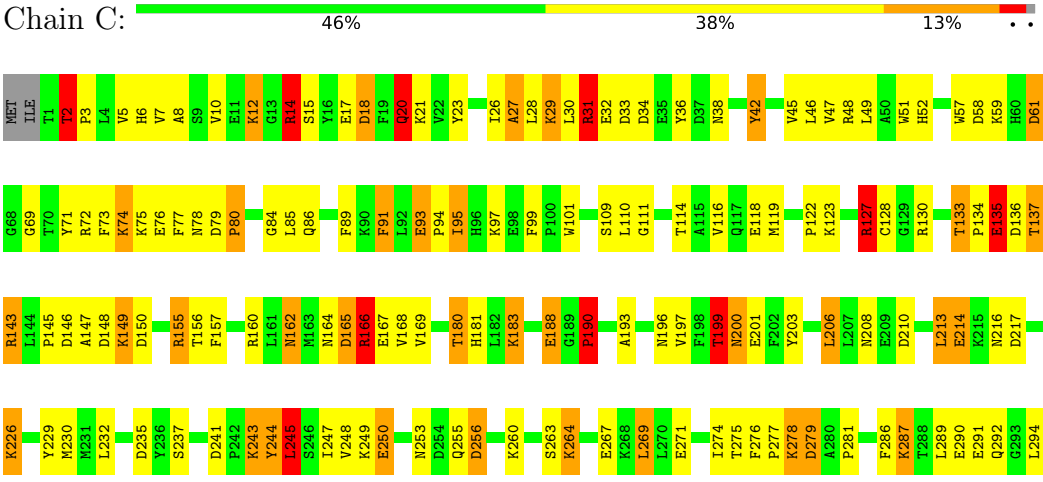
• Molecule 1: CYTOCHROME C PEROXIDASE

Chain A:



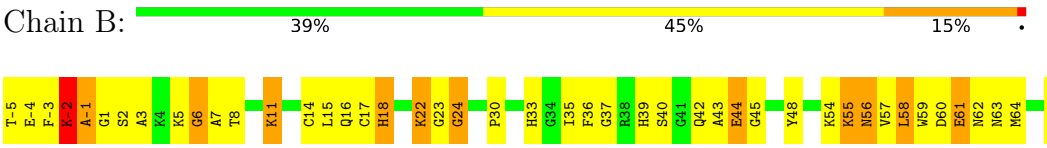
• Molecule 1: CYTOCHROME C PEROXIDASE

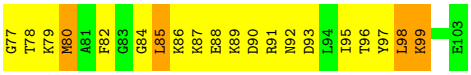
Chain C:



• Molecule 2: ISO-1-CYTOCHROME C

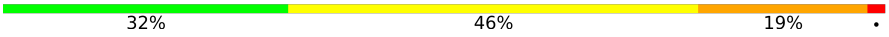
Chain B:

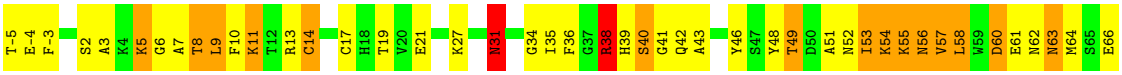


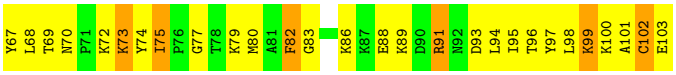


• Molecule 2: ISO-1-CYTOCHROME C

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.40Å 118.60Å 45.10Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 35.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 87.4 (35.89-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.10 (at 2.24Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.167 , (Not available) 0.284 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 127.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.095 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4

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	1.21	0/2438	2.08	74/3302 (2.2%)
1	C	1.18	2/2438 (0.1%)	2.09	97/3302 (2.9%)
2	B	0.93	0/865	1.71	4/1156 (0.3%)
2	D	0.93	0/865	1.73	11/1156 (1.0%)
All	All	1.13	2/6606 (0.0%)	2.00	186/8916 (2.1%)

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	A	0	4
1	C	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	SER	CA-CB	-5.76	1.44	1.52
1	C	181	HIS	CA-CB	5.43	1.65	1.53

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	23	TYR	CB-CG-CD2	15.44	130.26	121.00
1	A	155	ARG	NE-CZ-NH2	15.05	127.83	120.30
1	A	155	ARG	NE-CZ-NH1	-14.84	112.88	120.30
1	C	146	ASP	CB-CG-OD2	-14.44	105.31	118.30
1	A	130	ARG	NE-CZ-NH2	13.91	127.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	A	48	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	A	48	ARG	CD-NE-CZ	11.56	139.78	123.60
1	A	93	GLU	CA-CB-CG	11.44	138.56	113.40
1	C	18	ASP	CB-CG-OD1	-11.23	108.19	118.30
1	C	241	ASP	CB-CG-OD2	11.21	128.39	118.30
1	A	48	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	A	132	ASP	CB-CG-OD1	10.65	127.89	118.30
1	A	115	ALA	CB-CA-C	9.81	124.81	110.10
1	C	23	TYR	CB-CG-CD1	-9.64	115.22	121.00
1	A	106	ASP	CB-CG-OD1	9.48	126.84	118.30
1	C	150	ASP	CB-CG-OD1	9.44	126.79	118.30
1	C	14	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	A	98	GLU	CA-CB-CG	9.36	134.00	113.40
1	C	31	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	23	TYR	CB-CG-CD2	9.32	126.59	121.00
1	C	14	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	61	ASP	CB-CG-OD2	8.80	126.22	118.30
1	C	269	LEU	CA-CB-CG	8.75	135.42	115.30
1	A	166	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	A	261	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	A	143	ARG	CD-NE-CZ	-8.50	111.70	123.60
1	A	132	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	C	127	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	C	130	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	A	37	ASP	CB-CG-OD1	8.01	125.50	118.30
1	C	148	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	130	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	C	146	ASP	CB-CA-C	7.87	126.14	110.40
2	B	85	LEU	CA-CB-CG	7.83	133.31	115.30
2	B	18	HIS	CA-CB-CG	7.74	126.75	113.60
1	C	58	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	C	17	GLU	CB-CG-CD	7.69	134.97	114.20
1	A	30	LEU	CA-CB-CG	7.63	132.86	115.30
1	C	235	ASP	CB-CG-OD2	7.59	125.13	118.30
1	C	217	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	217	ASP	CB-CG-OD1	7.54	125.09	118.30
1	C	146	ASP	OD1-CG-OD2	7.50	137.54	123.30
1	C	48	ARG	CD-NE-CZ	7.46	134.05	123.60
1	A	23	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	C	2	THR	CA-CB-CG2	7.44	122.81	112.40
1	C	250	GLU	OE1-CD-OE2	7.42	132.21	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	14	CYS	N-CA-CB	-7.38	97.32	110.60
1	C	146	ASP	N-CA-CB	-7.34	97.39	110.60
1	C	168	VAL	CA-CB-CG1	7.29	121.83	110.90
1	C	67	TYR	CB-CG-CD2	7.27	125.36	121.00
1	C	244	TYR	CB-CG-CD1	7.25	125.35	121.00
1	C	214	GLU	CA-CB-CG	7.24	129.33	113.40
1	C	210	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	A	42	TYR	CB-CG-CD1	7.19	125.31	121.00
1	C	79	ASP	CB-CG-OD1	7.15	124.73	118.30
1	C	93	GLU	CA-CB-CG	7.12	129.07	113.40
1	A	28	LEU	O-C-N	7.06	134.00	122.70
1	C	165	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	216	ASN	CB-CA-C	7.04	124.48	110.40
1	C	225	SER	N-CA-CB	7.01	121.01	110.50
1	C	27	ALA	N-CA-CB	-6.96	100.36	110.10
1	C	181	HIS	CA-CB-CG	-6.93	101.82	113.60
1	A	289	LEU	CB-CA-C	6.84	123.20	110.20
1	C	165	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	256	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	33	ASP	CA-CB-CG	6.69	128.12	113.40
1	A	214	GLU	O-C-N	6.67	133.38	122.70
1	A	35	GLU	CA-CB-CG	6.62	127.97	113.40
1	C	28	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	17	GLU	CA-CB-CG	6.60	127.91	113.40
1	A	215	LYS	CB-CA-C	-6.59	97.22	110.40
1	A	106	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	34	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	150	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	217	ASP	O-C-N	6.52	133.13	122.70
1	A	166	ARG	CD-NE-CZ	-6.49	114.51	123.60
1	C	130	ARG	NH1-CZ-NH2	-6.41	112.34	119.40
1	C	67	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	C	263	SER	N-CA-CB	-6.34	100.99	110.50
1	A	118	GLU	CG-CD-OE2	6.34	130.97	118.30
1	C	119	MET	N-CA-CB	6.31	121.96	110.60
1	A	32	GLU	CG-CD-OE1	6.29	130.89	118.30
1	C	18	ASP	CB-CG-OD2	6.29	123.97	118.30
1	C	221	GLU	N-CA-CB	-6.29	99.29	110.60
1	C	193	ALA	CB-CA-C	6.28	119.53	110.10
1	C	201	GLU	OE1-CD-OE2	6.25	130.80	123.30
1	A	168	VAL	CA-CB-CG1	6.25	120.28	110.90
1	C	166	ARG	NE-CZ-NH2	-6.23	117.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	241	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	241	ASP	CB-CG-OD1	6.17	123.86	118.30
1	C	256	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	58	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	210	ASP	O-C-N	6.06	132.39	122.70
1	C	229	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	C	221	GLU	OE1-CD-OE2	6.03	130.54	123.30
1	C	199	THR	CA-CB-CG2	5.99	120.79	112.40
1	A	124	ILE	CB-CG1-CD1	5.96	130.58	113.90
1	C	221	GLU	CG-CD-OE1	-5.95	106.39	118.30
1	C	244	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	118	GLU	OE1-CD-OE2	-5.94	116.18	123.30
1	C	290	GLU	CA-CB-CG	5.91	126.40	113.40
1	A	203	TYR	CB-CG-CD1	5.91	124.54	121.00
2	B	44	GLU	CA-CB-CG	5.91	126.39	113.40
1	A	33	ASP	O-C-N	-5.89	113.28	122.70
2	D	103	GLU	CA-CB-CG	5.88	126.34	113.40
1	C	229	TYR	CB-CG-CD1	5.87	124.52	121.00
1	C	135	GLU	CG-CD-OE1	-5.86	106.59	118.30
1	A	146	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	143	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	222	GLN	CB-CG-CD	5.79	126.64	111.60
1	C	147	ALA	N-CA-CB	-5.78	102.00	110.10
1	A	31	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	4	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	29	LYS	CG-CD-CE	5.69	128.97	111.90
1	A	256	ASP	CB-CA-C	5.69	121.78	110.40
1	A	93	GLU	N-CA-CB	5.68	120.83	110.60
1	C	160	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	143	ARG	CG-CD-NE	-5.68	99.88	111.80
1	A	54	SER	CA-CB-OG	5.67	126.50	111.20
1	C	279	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	127	ARG	NE-CZ-NH1	-5.66	117.47	120.30
2	D	49	THR	N-CA-CB	5.66	121.05	110.30
1	A	209	GLU	C-N-CA	5.64	135.81	121.70
1	C	190	PRO	N-CA-CB	-5.64	96.40	102.60
1	A	168	VAL	N-CA-CB	5.63	123.89	111.50
1	C	206	LEU	CB-CA-C	5.63	120.89	110.20
1	C	23	TYR	CA-C-O	5.60	131.85	120.10
1	A	53	ILE	O-C-N	5.59	131.64	122.70
2	D	75	ILE	N-CA-CB	5.58	123.64	110.80
1	C	245	LEU	CA-CB-CG	5.55	128.07	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	33	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	C	203	TYR	CB-CG-CD1	5.53	124.32	121.00
1	A	179	LYS	CA-CB-CG	-5.52	101.25	113.40
1	C	118	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	C	147	ALA	CB-CA-C	-5.51	101.84	110.10
1	A	149	LYS	CA-CB-CG	-5.50	101.31	113.40
1	A	213	LEU	CB-CA-C	5.50	120.64	110.20
1	C	180	THR	CA-CB-CG2	5.49	120.08	112.40
2	D	88	GLU	CA-CB-CG	5.46	125.42	113.40
1	A	233	PRO	N-CA-CB	-5.46	96.60	102.60
2	D	9	LEU	N-CA-CB	-5.45	99.49	110.40
1	A	111	GLY	C-N-CA	-5.43	110.89	122.30
2	D	14	CYS	N-CA-C	5.43	125.65	111.00
1	C	42	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	C	95	ILE	CB-CG1-CD1	5.42	129.07	113.90
1	A	283	PRO	O-C-N	5.41	131.35	122.70
1	C	213	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	A	16	TYR	CB-CA-C	5.39	121.19	110.40
1	A	213	LEU	CB-CG-CD2	-5.39	101.83	111.00
2	D	58	LEU	CB-CA-C	5.38	120.42	110.20
1	C	277	PRO	C-N-CA	5.38	135.14	121.70
1	C	250	GLU	N-CA-CB	5.37	120.26	110.60
1	A	201	GLU	CG-CD-OE2	-5.34	107.62	118.30
1	A	214	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	A	185	SER	N-CA-CB	-5.28	102.58	110.50
1	A	206	LEU	CB-CA-C	5.27	120.22	110.20
1	A	215	LYS	O-C-N	5.27	131.14	122.70
1	C	17	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	C	137	THR	CA-CB-OG1	-5.25	97.97	109.00
1	A	238	LEU	CA-CB-CG	5.24	127.35	115.30
2	D	38	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	D	82	PHE	CA-C-N	5.20	126.60	116.20
1	A	259	PHE	CG-CD1-CE1	5.19	126.51	120.80
1	C	29	LYS	CA-CB-CG	-5.19	101.99	113.40
1	C	188	GLU	CB-CA-C	-5.17	100.06	110.40
1	A	92	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	269	LEU	CB-CG-CD2	5.14	119.74	111.00
1	C	232	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	116	VAL	CA-CB-CG2	5.14	118.60	110.90
1	C	167	GLU	CG-CD-OE1	-5.13	108.03	118.30
1	A	270	LEU	O-C-N	5.12	130.90	122.70
1	A	176	ALA	C-N-CA	5.10	134.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	31	ASN	N-CA-C	-5.10	97.22	111.00
1	A	31	ARG	O-C-N	-5.10	114.54	122.70
1	A	31	ARG	CD-NE-CZ	-5.09	116.47	123.60
1	C	214	GLU	O-C-N	5.08	130.83	122.70
1	C	20	GLN	O-C-N	-5.05	114.61	122.70
1	A	235	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	14	ARG	CD-NE-CZ	-5.05	116.54	123.60
1	A	115	ALA	N-CA-CB	-5.04	103.05	110.10
1	C	29	LYS	CD-CE-NZ	-5.04	100.12	111.70
1	C	36	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	C	130	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	B	92	ASN	CB-CA-C	5.01	120.42	110.40
1	C	250	GLU	CG-CD-OE2	-5.01	108.28	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	143	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	31	ARG	Sidechain
1	C	155	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	31	ARG	Sidechain

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	2371	0	2252	105	1
1	C	2371	0	2252	136	5
2	B	847	0	851	75	1
2	D	847	0	851	103	0
3	A	2	0	0	1	0
3	C	2	0	0	1	0
4	A	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	16	0
4	C	43	0	30	4	0
4	D	43	0	30	19	0
5	A	203	0	0	12	4
5	B	46	0	0	5	0
5	C	212	0	0	23	1
5	D	42	0	0	11	0
All	All	7115	0	6326	423	6

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 33.

All (423) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:CYS:SG	4:B:104:HEM:CAB	2.29	1.20
1:C:74:LYS:HE3	1:C:78:ASN:HD21	1.14	1.13
2:B:17:CYS:SG	4:B:104:HEM:CAC	2.39	1.10
2:B:8:THR:HA	2:B:11:LYS:HD2	1.34	1.08
2:D:17:CYS:SG	4:D:104:HEM:CAC	2.43	1.06
1:C:2:THR:HG22	1:C:3:PRO:HD3	1.37	1.04
2:B:14:CYS:HG	4:B:104:HEM:CAB	1.70	1.01
2:B:8:THR:HA	2:B:11:LYS:CD	1.91	1.00
2:B:87:LYS:HB2	2:B:90:ASP:OD2	1.61	0.99
2:D:3:ALA:HB2	2:D:96:THR:HG22	1.47	0.96
1:C:63:THR:HG22	1:C:143:ARG:HH12	1.29	0.96
1:A:20:GLN:HE22	1:A:287:LYS:H	1.15	0.95
1:C:74:LYS:HE3	1:C:78:ASN:ND2	1.82	0.93
2:B:17:CYS:HG	4:B:104:HEM:CAC	1.75	0.93
1:C:213:LEU:HD11	1:C:221:GLU:HG2	1.48	0.92
1:C:63:THR:HG22	1:C:143:ARG:NH1	1.84	0.92
2:D:91:ARG:HG3	2:D:91:ARG:HH11	1.35	0.91
2:B:14:CYS:SG	4:B:104:HEM:CBB	2.59	0.91
1:C:278:LYS:HD3	1:C:278:LYS:H	1.34	0.90
2:D:14:CYS:SG	4:D:104:HEM:CBB	2.60	0.90
1:C:84:GLY:H	1:C:86:GLN:HE22	1.14	0.90
2:D:14:CYS:SG	4:D:104:HEM:C3B	2.66	0.89
2:D:98:LEU:O	2:D:102:CYS:HB2	1.73	0.88
1:C:74:LYS:HG3	1:C:78:ASN:HD22	1.37	0.87
1:C:10:VAL:HG22	1:C:128:CYS:SG	2.15	0.86
1:C:2:THR:CG2	1:C:3:PRO:HD3	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:CYS:SG	4:D:104:HEM:CAB	2.65	0.85
1:C:213:LEU:CD1	1:C:221:GLU:HG2	2.07	0.84
2:B:22:LYS:HD2	2:B:33:HIS:CD2	2.12	0.84
2:D:17:CYS:HG	4:D:104:HEM:CAC	1.88	0.84
2:B:17:CYS:SG	4:B:104:HEM:C3C	2.71	0.83
1:A:146:ASP:HB2	5:A:439:HOH:O	1.77	0.83
1:A:2:THR:HG23	1:A:3:PRO:HD2	1.59	0.83
1:C:31:ARG:HD3	5:C:628:HOH:O	1.79	0.82
2:D:14:CYS:HB2	4:D:104:HEM:CBB	2.11	0.81
1:C:93:GLU:HB2	1:C:94:PRO:HD3	1.63	0.81
1:C:128:CYS:SG	5:C:848:HOH:O	2.38	0.81
2:D:100:LYS:HD3	2:D:101:ALA:N	1.95	0.80
1:A:147:ALA:O	1:A:233:PRO:HB2	1.82	0.80
2:D:17:CYS:SG	4:D:104:HEM:C3C	2.73	0.79
1:C:63:THR:HG21	1:C:143:ARG:HH22	1.47	0.79
2:D:73:LYS:HD2	5:D:774:HOH:O	1.81	0.79
1:A:31:ARG:HG3	5:A:384:HOH:O	1.82	0.79
1:C:52:HIS:NE2	3:C:300:SO4:O1	2.18	0.77
2:B:80:MET:HB2	4:B:104:HEM:C1D	2.20	0.77
1:A:200:ASN:H	1:A:200:ASN:HD22	1.33	0.77
1:A:69:GLY:O	1:A:72:ARG:HD3	1.86	0.75
1:C:3:PRO:HB2	5:C:732:HOH:O	1.86	0.75
1:C:133:THR:HG22	1:C:137:THR:OG1	1.86	0.75
1:C:133:THR:CG2	1:C:137:THR:OG1	2.35	0.75
1:C:216:ASN:HD22	1:C:222:GLN:HE21	1.32	0.74
2:D:7:ALA:O	2:D:11:LYS:HD3	1.87	0.74
2:B:55:LYS:HD3	2:B:57:VAL:HG13	1.68	0.74
1:C:84:GLY:N	1:C:86:GLN:HE22	1.83	0.73
1:A:17:GLU:CD	1:A:17:GLU:H	1.93	0.72
2:B:8:THR:HG22	2:B:11:LYS:HE3	1.69	0.72
2:D:60:ASP:N	2:D:63:ASN:HD21	1.88	0.72
2:B:17:CYS:SG	4:B:104:HEM:CBC	2.78	0.71
2:B:43:ALA:HB3	2:B:48:TYR:OH	1.91	0.71
2:D:38:ARG:HH11	2:D:38:ARG:HG3	1.55	0.71
2:B:14:CYS:SG	4:B:104:HEM:HAB	2.29	0.70
1:A:119:MET:O	1:A:120:GLN:HB2	1.91	0.70
1:C:14:ARG:HG3	1:C:14:ARG:HH11	1.55	0.70
2:B:87:LYS:O	2:B:90:ASP:HB2	1.92	0.69
1:C:74:LYS:CE	1:C:78:ASN:HD21	1.99	0.69
2:D:14:CYS:CB	4:D:104:HEM:CBB	2.69	0.69
2:D:36:PHE:CD2	2:D:99:LYS:HB3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:HIS:HB3	2:D:56:ASN:ND2	2.06	0.69
2:B:73:LYS:HD3	5:B:446:HOH:O	1.91	0.69
1:C:200:ASN:HB3	1:C:255:GLN:HG3	1.73	0.69
1:A:166:ARG:HH22	1:A:250:GLU:CD	1.96	0.69
2:D:38:ARG:HD3	2:D:42:GLN:HB2	1.73	0.69
1:C:200:ASN:HD22	1:C:200:ASN:H	1.41	0.68
2:D:17:CYS:SG	4:D:104:HEM:CBC	2.81	0.68
2:D:57:VAL:HG12	2:D:63:ASN:OD1	1.93	0.68
2:B:17:CYS:HG	4:B:104:HEM:CBC	2.06	0.68
1:C:63:THR:HG21	1:C:143:ARG:NH2	2.08	0.68
2:D:41:GLY:HA2	2:D:48:TYR:CE1	2.29	0.68
2:B:22:LYS:NZ	2:B:33:HIS:HD2	1.92	0.67
1:C:93:GLU:HB2	1:C:94:PRO:CD	2.24	0.67
2:D:94:LEU:O	2:D:97:TYR:HB3	1.95	0.67
1:A:16:TYR:O	1:A:19:PHE:N	2.28	0.67
1:C:74:LYS:HG3	1:C:78:ASN:ND2	2.10	0.67
2:D:74:TYR:HB2	5:D:744:HOH:O	1.94	0.67
1:C:133:THR:HG23	1:C:137:THR:HG21	1.78	0.66
4:C:296:HEM:HMC2	4:C:296:HEM:HBC2	1.75	0.66
2:B:14:CYS:HG	4:B:104:HEM:CBB	2.04	0.66
1:C:216:ASN:HD22	1:C:222:GLN:NE2	1.93	0.66
1:C:29:LYS:O	1:C:29:LYS:HG3	1.95	0.65
1:C:292:GLN:C	1:C:294:LEU:H	1.99	0.65
1:C:80:PRO:O	5:C:664:HOH:O	2.15	0.65
1:C:278:LYS:HD3	1:C:278:LYS:N	2.10	0.65
1:C:145:PRO:HD3	1:C:157:PHE:CZ	2.32	0.65
1:C:264:LYS:HB3	5:C:802:HOH:O	1.96	0.65
1:C:267:GLU:OE2	1:C:271:GLU:OE2	2.15	0.64
1:C:278:LYS:H	1:C:278:LYS:CD	1.96	0.64
1:A:245:LEU:O	1:A:245:LEU:HD22	1.97	0.64
1:C:7:VAL:HG22	5:C:623:HOH:O	1.97	0.63
1:C:59:LYS:NZ	5:C:757:HOH:O	2.31	0.63
2:B:8:THR:CG2	2:B:11:LYS:HE3	2.28	0.63
2:D:67:TYR:HA	5:D:744:HOH:O	1.99	0.63
2:B:1:GLY:O	2:B:96:THR:HG21	1.98	0.63
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.79	0.63
2:D:60:ASP:H	2:D:63:ASN:HD21	1.46	0.63
1:A:4:LEU:HD12	1:A:62:ASN:O	1.99	0.62
1:A:267:GLU:OE2	1:A:271:GLU:OE2	2.16	0.62
1:A:287:LYS:HA	1:A:291:GLU:OE1	1.99	0.62
1:A:127:ARG:HG2	1:A:283:PRO:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:OG1	1:A:291:GLU:HG3	2.00	0.62
1:C:200:ASN:HD22	1:C:200:ASN:N	1.95	0.62
1:A:2:THR:HG23	1:A:3:PRO:CD	2.30	0.62
1:A:23:TYR:CD1	1:A:23:TYR:C	2.73	0.62
1:A:292:GLN:O	1:A:294:LEU:HD12	2.00	0.61
2:D:53:ILE:HG13	5:D:782:HOH:O	2.00	0.61
1:C:29:LYS:HG2	1:C:91:PHE:CE2	2.36	0.61
1:C:287:LYS:HA	1:C:291:GLU:OE1	2.01	0.61
2:D:11:LYS:HD2	2:D:11:LYS:N	2.16	0.61
2:D:14:CYS:HG	4:D:104:HEM:CAB	2.11	0.61
2:D:19:THR:HA	5:D:641:HOH:O	2.00	0.61
1:A:186:GLY:O	1:A:216:ASN:ND2	2.34	0.60
1:C:20:GLN:HE22	1:C:287:LYS:H	1.50	0.60
1:C:42:TYR:O	1:C:46:LEU:HG	2.01	0.60
2:B:91:ARG:O	2:B:95:ILE:HG12	2.00	0.60
1:A:76:GLU:HB2	1:A:138:THR:CG2	2.30	0.60
2:B:6:GLY:HA3	2:B:93:ASP:O	2.01	0.60
2:D:91:ARG:HB3	5:D:779:HOH:O	2.00	0.60
2:D:9:LEU:O	2:D:13:ARG:HB2	2.01	0.59
1:A:86:GLN:O	1:A:90:LYS:HG2	2.02	0.59
2:B:8:THR:CB	2:B:11:LYS:HE3	2.31	0.59
1:C:71:TYR:O	1:C:77:PHE:HB2	2.01	0.59
2:D:51:ALA:HB1	2:D:75:ILE:CG2	2.32	0.59
1:A:113:VAL:O	1:A:117:GLN:HG3	2.02	0.59
2:B:44:GLU:HA	5:B:444:HOH:O	2.01	0.59
2:D:64:MET:HG2	2:D:95:ILE:CD1	2.33	0.59
2:D:54:LYS:HA	2:D:54:LYS:HE3	1.83	0.59
1:C:123:LYS:HE2	1:C:287:LYS:NZ	2.18	0.58
1:C:133:THR:HG23	1:C:137:THR:CG2	2.33	0.58
2:D:34:GLY:HA2	2:D:102:CYS:O	2.03	0.58
1:A:267:GLU:O	1:A:271:GLU:HG3	2.04	0.58
2:B:58:LEU:O	2:B:63:ASN:ND2	2.31	0.58
1:C:38:ASN:N	1:C:38:ASN:HD22	2.01	0.58
2:B:37:GLY:O	2:B:58:LEU:HD11	2.04	0.58
1:C:12:LYS:HE3	5:C:696:HOH:O	2.02	0.58
1:A:123:LYS:HE2	5:A:542:HOH:O	2.03	0.58
1:C:183:LYS:HD3	1:C:183:LYS:N	2.19	0.58
2:D:14:CYS:SG	4:D:104:HEM:HBB2	2.43	0.58
1:A:29:LYS:O	1:A:29:LYS:HG2	2.04	0.58
2:D:41:GLY:HA2	2:D:48:TYR:CZ	2.39	0.58
2:D:60:ASP:O	2:D:62:ASN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LYS:HB2	5:C:716:HOH:O	2.03	0.57
1:A:166:ARG:NH2	1:A:250:GLU:CD	2.57	0.57
1:C:190:PRO:O	1:C:190:PRO:HG2	2.03	0.57
1:A:156:THR:HG22	5:A:513:HOH:O	2.02	0.57
2:D:38:ARG:HH11	2:D:38:ARG:CG	2.17	0.57
1:A:103:SER:OG	1:A:106:ASP:HB2	2.05	0.57
2:B:87:LYS:CB	2:B:90:ASP:OD2	2.46	0.57
1:C:10:VAL:O	1:C:12:LYS:HE3	2.05	0.57
1:C:63:THR:CG2	1:C:143:ARG:HH22	2.16	0.57
1:C:26:ILE:HG22	1:C:114:THR:HG21	1.86	0.57
1:A:52:HIS:NE2	3:A:299:SO4:O1	2.38	0.57
2:B:8:THR:O	2:B:11:LYS:HD3	2.05	0.57
2:B:16:GLN:OE1	2:B:16:GLN:N	2.35	0.57
2:D:5:LYS:HA	2:D:8:THR:HG23	1.87	0.57
2:B:8:THR:HB	2:B:11:LYS:HE3	1.88	0.56
2:D:69:THR:O	2:D:86:LYS:HE2	2.05	0.56
1:C:29:LYS:O	1:C:29:LYS:CG	2.53	0.56
1:C:286:PHE:C	1:C:287:LYS:HE2	2.26	0.56
2:B:22:LYS:C	2:B:24:GLY:H	2.09	0.56
1:A:255:GLN:NE2	1:A:259:PHE:CZ	2.73	0.56
1:C:166:ARG:HH22	1:C:250:GLU:CD	2.09	0.56
1:C:51:TRP:CD1	1:C:52:HIS:HD2	2.24	0.56
2:D:3:ALA:HB1	2:D:97:TYR:HA	1.87	0.56
1:A:79:ASP:O	1:A:82:ASN:HB2	2.06	0.55
1:A:42:TYR:O	1:A:46:LEU:HG	2.05	0.55
1:A:96:HIS:CD2	1:A:107:LEU:HD22	2.41	0.55
1:C:256:ASP:O	1:C:260:LYS:HG2	2.05	0.55
2:B:5:LYS:O	2:B:7:ALA:N	2.40	0.55
2:B:89:LYS:HB3	2:B:93:ASP:OD2	2.05	0.55
4:C:296:HEM:HBC2	4:C:296:HEM:CMC	2.36	0.55
2:B:39:HIS:CD2	2:B:56:ASN:OD1	2.60	0.55
1:C:140:ASP:HB3	5:C:731:HOH:O	2.07	0.55
1:C:7:VAL:O	1:C:7:VAL:HG23	2.06	0.55
2:D:80:MET:HE1	4:D:104:HEM:NB	2.22	0.54
2:B:82:PHE:CE2	2:B:84:GLY:HA2	2.42	0.54
1:C:226:LYS:HE2	5:C:702:HOH:O	2.07	0.54
2:D:83:GLY:HA3	5:D:640:HOH:O	2.06	0.54
1:A:75:LYS:HE3	1:A:140:ASP:HA	1.89	0.54
2:B:55:LYS:HD3	2:B:57:VAL:CG1	2.36	0.54
1:A:155:ARG:NH1	1:A:241:ASP:OD2	2.33	0.54
1:C:49:LEU:HB2	1:C:85:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:HB3	5:C:749:HOH:O	2.07	0.54
2:D:46:TYR:C	2:D:46:TYR:CD1	2.80	0.54
2:D:60:ASP:H	2:D:63:ASN:ND2	2.04	0.54
1:A:166:ARG:NH2	1:A:250:GLU:OE2	2.41	0.54
1:A:145:PRO:HD3	1:A:157:PHE:CZ	2.44	0.53
1:A:60:HIS:HE1	5:A:341:HOH:O	1.91	0.53
1:C:133:THR:HG22	1:C:137:THR:HG1	1.72	0.53
1:C:61:ASP:N	1:C:61:ASP:OD1	2.30	0.53
2:D:39:HIS:CE1	2:D:58:LEU:HB2	2.43	0.53
2:B:22:LYS:HD2	2:B:33:HIS:NE2	2.23	0.53
1:C:20:GLN:HG3	1:C:20:GLN:O	2.07	0.53
1:C:133:THR:CG2	1:C:137:THR:HG21	2.39	0.53
1:A:93:GLU:N	1:A:94:PRO:CD	2.71	0.53
1:C:63:THR:CG2	1:C:143:ARG:NH2	2.72	0.52
1:A:164:ASN:O	1:A:168:VAL:HG13	2.09	0.52
1:A:216:ASN:HB2	5:A:420:HOH:O	2.10	0.52
2:D:2:SER:O	2:D:93:ASP:HB3	2.10	0.52
1:A:115:ALA:O	1:A:119:MET:HG3	2.09	0.52
2:B:7:ALA:HB2	2:B:97:TYR:CD2	2.44	0.52
2:B:8:THR:CA	2:B:11:LYS:CD	2.77	0.52
1:A:2:THR:CG2	1:A:3:PRO:HD2	2.36	0.52
2:D:7:ALA:HB2	2:D:97:TYR:CD1	2.44	0.52
1:A:86:GLN:OE1	1:A:86:GLN:N	2.34	0.52
1:C:183:LYS:H	1:C:183:LYS:CE	2.23	0.52
2:D:70:ASN:ND2	5:D:774:HOH:O	2.42	0.52
2:B:5:LYS:O	2:B:6:GLY:C	2.48	0.51
1:C:15:SER:O	1:C:18:ASP:HB2	2.10	0.51
1:A:161:LEU:O	1:A:162:ASN:HB3	2.10	0.51
1:A:188:GLU:H	1:A:222:GLN:HE22	1.58	0.51
1:C:281:PRO:HG2	5:C:848:HOH:O	2.09	0.51
1:A:141:ASN:N	1:A:141:ASN:HD22	2.07	0.51
1:A:200:ASN:H	1:A:200:ASN:ND2	2.05	0.51
1:A:30:LEU:HD12	1:A:42:TYR:HB2	1.92	0.51
1:A:81:SER:HB3	5:A:367:HOH:O	2.11	0.51
1:C:110:LEU:O	1:C:111:GLY:C	2.46	0.51
1:C:183:LYS:H	1:C:183:LYS:CD	2.23	0.51
2:B:18:HIS:CE1	2:B:30:PRO:HD2	2.45	0.51
2:D:10:PHE:O	2:D:14:CYS:HB3	2.11	0.51
2:B:8:THR:HA	2:B:11:LYS:HD3	1.87	0.51
2:D:19:THR:OG1	2:D:31:ASN:HB2	2.11	0.51
2:D:38:ARG:HD2	2:D:39:HIS:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:HIS:ND1	1:A:82:ASN:OD1	2.31	0.50
1:C:133:THR:CG2	1:C:137:THR:CB	2.89	0.50
2:D:49:THR:HG21	2:D:77:GLY:O	2.12	0.50
1:A:149:LYS:HD2	1:A:153:TYR:CD2	2.46	0.50
1:A:206:LEU:HD13	1:A:231:MET:SD	2.51	0.50
1:C:292:GLN:O	1:C:294:LEU:N	2.44	0.50
2:B:-2:LYS:O	2:B:-1:ALA:HB2	2.12	0.49
2:B:23:GLY:O	2:B:24:GLY:O	2.30	0.49
1:C:63:THR:HG22	1:C:143:ARG:CZ	2.42	0.49
2:D:55:LYS:HG3	2:D:57:VAL:HG22	1.95	0.49
1:A:180:THR:N	1:A:189:GLY:O	2.29	0.49
1:C:21:LYS:HB2	1:C:99:PHE:CE2	2.47	0.49
2:B:45:GLY:N	5:B:444:HOH:O	2.44	0.49
2:D:91:ARG:HG3	2:D:91:ARG:NH1	2.09	0.49
1:A:177:LEU:HD11	1:A:198:PHE:HD2	1.78	0.49
2:D:35:ILE:HG22	2:D:102:CYS:SG	2.53	0.49
1:A:60:HIS:CE1	5:A:341:HOH:O	2.65	0.49
1:A:183:LYS:HG2	5:A:375:HOH:O	2.12	0.49
1:C:45:VAL:HG22	1:C:45:VAL:O	2.12	0.48
1:A:38:ASN:O	1:A:39:TYR:HB2	2.13	0.48
1:A:166:ARG:HH12	1:A:257:LYS:HE2	1.78	0.48
1:A:204:LEU:HD21	1:A:252:ALA:O	2.12	0.48
1:C:180:THR:HG21	1:C:230:MET:HE1	1.95	0.48
1:A:250:GLU:O	1:A:253:ASN:HB2	2.13	0.48
2:B:3:ALA:HB2	2:B:96:THR:HG22	1.95	0.48
2:D:11:LYS:NZ	5:D:621:HOH:O	2.46	0.48
2:B:18:HIS:HE1	2:B:30:PRO:HD2	1.78	0.48
2:B:14:CYS:SG	4:B:104:HEM:C3B	3.02	0.48
4:B:104:HEM:HBC2	4:B:104:HEM:HMC2	1.95	0.48
1:C:183:LYS:N	1:C:183:LYS:CD	2.77	0.48
1:C:292:GLN:C	1:C:294:LEU:N	2.66	0.48
2:D:39:HIS:HB3	2:D:56:ASN:CG	2.33	0.48
2:B:55:LYS:O	2:B:56:ASN:C	2.52	0.48
2:B:42:GLN:O	2:B:43:ALA:C	2.50	0.48
1:C:190:PRO:O	1:C:190:PRO:CG	2.60	0.48
2:D:48:TYR:CE1	4:D:104:HEM:O2A	2.66	0.48
1:A:52:HIS:HE1	1:A:81:SER:O	1.97	0.47
1:A:156:THR:CG2	5:A:513:HOH:O	2.60	0.47
1:C:8:ALA:HB2	1:C:274:ILE:HG22	1.96	0.47
2:D:63:ASN:HD22	2:D:63:ASN:H	1.61	0.47
2:D:86:LYS:HA	2:D:86:LYS:HD3	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASN:N	1:C:38:ASN:ND2	2.63	0.47
2:D:34:GLY:N	2:D:102:CYS:O	2.46	0.47
1:C:8:ALA:HB3	1:C:276:PHE:HA	1.97	0.47
1:C:287:LYS:HA	1:C:287:LYS:NZ	2.30	0.47
1:C:72:ARG:NH2	1:C:133:THR:O	2.47	0.47
1:C:245:LEU:O	1:C:249:LYS:HG3	2.14	0.47
2:B:57:VAL:HA	5:B:474:HOH:O	2.13	0.47
1:C:155:ARG:HB2	1:C:244:TYR:OH	2.13	0.47
1:C:6:HIS:CD2	5:C:627:HOH:O	2.68	0.47
1:C:208:ASN:ND2	5:C:819:HOH:O	2.47	0.46
2:D:60:ASP:C	2:D:60:ASP:OD1	2.54	0.46
2:D:11:LYS:N	2:D:11:LYS:CD	2.77	0.46
2:D:34:GLY:CA	2:D:102:CYS:O	2.64	0.46
2:D:67:TYR:CD2	2:D:68:LEU:HD23	2.50	0.46
2:D:64:MET:O	2:D:68:LEU:HG	2.15	0.46
1:C:133:THR:CG2	1:C:137:THR:CG2	2.94	0.46
2:D:-3:PHE:HB3	2:D:62:ASN:OD1	2.15	0.46
2:D:52:ASN:OD1	2:D:52:ASN:O	2.33	0.46
2:D:36:PHE:CE1	2:D:64:MET:HE3	2.51	0.46
1:C:127:ARG:HA	5:C:674:HOH:O	2.16	0.46
2:B:55:LYS:O	2:B:56:ASN:O	2.34	0.46
1:C:93:GLU:N	1:C:94:PRO:HD2	2.31	0.46
2:D:17:CYS:HG	4:D:104:HEM:CBC	2.23	0.46
1:A:23:TYR:C	1:A:23:TYR:HD1	2.18	0.46
1:C:26:ILE:CG2	1:C:114:THR:HG21	2.46	0.46
1:C:183:LYS:HD3	1:C:183:LYS:H	1.80	0.46
2:D:5:LYS:O	2:D:9:LEU:HB2	2.17	0.46
2:D:60:ASP:C	2:D:62:ASN:H	2.19	0.46
1:A:4:LEU:CD1	1:A:62:ASN:O	2.63	0.45
2:B:23:GLY:O	2:B:24:GLY:C	2.55	0.45
2:B:86:LYS:N	5:B:507:HOH:O	2.50	0.45
2:D:80:MET:HE3	4:D:104:HEM:C4B	2.51	0.45
1:A:141:ASN:N	1:A:141:ASN:ND2	2.65	0.45
2:B:18:HIS:CD2	4:B:104:HEM:NB	2.85	0.45
1:C:226:LYS:HD3	1:C:226:LYS:HA	1.65	0.45
1:A:130:ARG:NH1	1:A:130:ARG:HG3	2.32	0.45
1:C:69:GLY:HA2	5:C:778:HOH:O	2.16	0.45
2:D:56:ASN:O	2:D:57:VAL:C	2.55	0.45
1:A:29:LYS:HD3	1:A:91:PHE:CE2	2.52	0.45
1:A:119:MET:O	1:A:120:GLN:CB	2.61	0.45
1:A:232:LEU:O	1:A:235:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LEU:O	2:B:16:GLN:C	2.54	0.45
2:D:93:ASP:N	2:D:93:ASP:OD1	2.44	0.45
1:A:7:VAL:HA	1:A:275:THR:O	2.17	0.45
1:A:211:TRP:CZ3	1:A:225:SER:HB3	2.52	0.45
1:A:294:LEU:HD11	1:C:294:LEU:CD1	2.47	0.45
1:A:86:GLN:H	1:A:86:GLN:CD	2.18	0.44
1:A:137:THR:O	1:A:139:PRO:HD3	2.17	0.44
2:D:14:CYS:HB2	4:D:104:HEM:HBB1	1.96	0.44
1:C:135:GLU:HG3	5:C:749:HOH:O	2.17	0.44
1:A:256:ASP:O	1:A:260:LYS:HD3	2.17	0.44
1:A:126:TRP:C	1:A:127:ARG:HG3	2.37	0.44
2:D:6:GLY:CA	2:D:94:LEU:HA	2.48	0.44
1:C:26:ILE:HA	1:C:95:ILE:HD13	1.99	0.44
1:A:155:ARG:HH11	1:A:155:ARG:HD2	1.33	0.44
1:C:264:LYS:HB2	1:C:264:LYS:HE3	1.45	0.44
2:D:100:LYS:HD3	2:D:101:ALA:CA	2.47	0.44
2:B:15:LEU:HD12	2:B:15:LEU:HA	1.82	0.44
1:C:200:ASN:H	1:C:200:ASN:ND2	2.11	0.44
2:B:40:SER:HA	2:B:59:TRP:HE1	1.83	0.44
1:C:30:LEU:HD23	1:C:42:TYR:HB2	1.99	0.44
1:C:84:GLY:CA	1:C:86:GLN:NE2	2.80	0.44
1:C:162:ASN:CG	5:C:723:HOH:O	2.56	0.44
2:D:13:ARG:NH1	2:D:82:PHE:CE1	2.85	0.44
2:D:19:THR:O	2:D:31:ASN:HA	2.18	0.44
2:D:60:ASP:O	2:D:63:ASN:ND2	2.51	0.44
2:D:93:ASP:O	2:D:94:LEU:C	2.56	0.43
1:A:93:GLU:N	1:A:94:PRO:HD2	2.32	0.43
2:B:43:ALA:CB	2:B:48:TYR:OH	2.62	0.43
2:D:42:GLN:C	2:D:43:ALA:O	2.56	0.43
1:A:265:ALA:O	1:A:266:PHE:C	2.56	0.43
1:C:206:LEU:HD12	1:C:206:LEU:HA	1.88	0.43
2:D:36:PHE:CE1	2:D:64:MET:CE	3.02	0.43
1:A:294:LEU:HD12	1:A:294:LEU:N	2.34	0.43
1:C:76:GLU:HB2	1:C:138:THR:CG2	2.48	0.43
1:C:133:THR:HA	1:C:134:PRO:HD3	1.81	0.43
1:A:28:LEU:O	1:A:31:ARG:HB3	2.17	0.43
1:A:116:VAL:HG11	1:A:124:ILE:HD12	2.00	0.43
1:A:214:GLU:O	1:A:221:GLU:HA	2.19	0.43
2:B:79:LYS:HE3	4:B:104:HEM:HMD1	2.01	0.43
1:C:74:LYS:CE	1:C:78:ASN:ND2	2.68	0.43
1:A:215:LYS:CB	1:A:215:LYS:NZ	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HA	1:A:220:ASN:O	2.18	0.43
1:C:8:ALA:HB2	1:C:274:ILE:CG2	2.49	0.43
1:C:14:ARG:HG2	1:C:101:TRP:CZ3	2.53	0.43
1:C:38:ASN:HD22	1:C:38:ASN:H	1.67	0.43
1:C:199:THR:HG23	5:C:652:HOH:O	2.18	0.43
4:C:296:HEM:HMB1	4:C:296:HEM:HBB2	2.00	0.43
2:D:46:TYR:C	2:D:46:TYR:HD1	2.21	0.43
2:D:96:THR:O	2:D:97:TYR:C	2.57	0.43
1:A:214:GLU:N	1:A:222:GLN:O	2.50	0.42
1:C:15:SER:HB2	5:C:738:HOH:O	2.19	0.42
1:C:127:ARG:HH11	1:C:127:ARG:HD2	1.68	0.42
1:C:165:ASP:O	1:C:169:VAL:HG23	2.19	0.42
1:A:181:HIS:HB2	1:A:184:ASN:HB2	2.01	0.42
2:B:35:ILE:HG23	2:B:36:PHE:N	2.34	0.42
2:D:48:TYR:HE1	4:D:104:HEM:O2A	2.02	0.42
1:C:6:HIS:HD2	5:C:627:HOH:O	2.02	0.42
2:B:22:LYS:HZ3	2:B:33:HIS:HD2	1.66	0.42
4:B:104:HEM:HBC2	4:B:104:HEM:CMC	2.49	0.42
2:D:67:TYR:CA	5:D:744:HOH:O	2.65	0.42
1:A:133:THR:HA	1:A:134:PRO:HD3	1.90	0.42
1:A:35:GLU:HG3	5:A:552:HOH:O	2.20	0.42
1:A:190:PRO:HG2	1:A:190:PRO:O	2.20	0.42
2:B:98:LEU:O	2:B:99:LYS:C	2.57	0.42
2:D:38:ARG:CD	2:D:42:GLN:HB2	2.44	0.42
5:C:838:HOH:O	2:D:13:ARG:CD	2.68	0.42
2:D:39:HIS:ND1	2:D:58:LEU:HB2	2.35	0.42
1:A:200:ASN:ND2	1:A:200:ASN:N	2.67	0.42
2:B:77:GLY:O	2:B:78:THR:C	2.58	0.42
2:D:39:HIS:O	2:D:40:SER:C	2.58	0.42
2:D:67:TYR:HB2	2:D:74:TYR:CD2	2.55	0.42
1:A:53:ILE:HG22	1:A:71:TYR:HB2	2.01	0.41
2:B:89:LYS:O	2:B:93:ASP:OD2	2.37	0.41
1:C:57:TRP:HE1	1:C:62:ASN:HD22	1.68	0.41
1:C:75:LYS:HE2	1:C:140:ASP:HA	2.02	0.41
2:B:22:LYS:HZ2	2:B:33:HIS:HD2	1.63	0.41
1:C:89:PHE:CD1	1:C:89:PHE:C	2.93	0.41
1:A:56:THR:O	1:A:143:ARG:HD2	2.21	0.41
1:C:243:LYS:HZ2	1:C:243:LYS:HG2	1.77	0.41
1:C:247:ILE:O	1:C:248:VAL:C	2.58	0.41
4:C:296:HEM:HBB2	4:C:296:HEM:CMB	2.50	0.41
2:D:21:GLU:H	2:D:21:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:LYS:HG2	4:D:104:HEM:HBD2	2.01	0.41
2:B:60:ASP:O	2:B:62:ASN:N	2.54	0.41
1:A:134:PRO:C	1:A:136:ASP:N	2.73	0.41
1:C:149:LYS:HA	1:C:149:LYS:HD2	1.78	0.41
1:A:212:LYS:O	1:A:223:TRP:HA	2.21	0.41
1:A:7:VAL:HG13	1:A:277:PRO:HD3	2.03	0.41
2:B:5:LYS:O	2:B:8:THR:N	2.53	0.41
1:C:164:ASN:C	1:C:164:ASN:OD1	2.60	0.41
1:A:79:ASP:OD1	1:A:80:PRO:HD2	2.20	0.41
1:C:74:LYS:O	1:C:78:ASN:N	2.50	0.41
1:C:133:THR:CG2	1:C:137:THR:HG1	2.26	0.41
1:C:162:ASN:HD22	1:C:162:ASN:HA	1.65	0.41
1:A:174:ALA:C	1:A:176:ALA:H	2.24	0.41
1:C:214:GLU:O	1:C:221:GLU:HA	2.20	0.41
2:B:64:MET:O	2:B:67:TYR:HB3	2.21	0.40
2:B:97:TYR:CD1	2:B:97:TYR:C	2.94	0.40
2:D:42:GLN:O	2:D:43:ALA:C	2.59	0.40
2:D:60:ASP:C	2:D:62:ASN:N	2.74	0.40
2:D:80:MET:HE3	4:D:104:HEM:CHC	2.51	0.40
1:A:35:GLU:CG	5:A:552:HOH:O	2.70	0.40
1:A:266:PHE:O	1:A:270:LEU:HG	2.21	0.40
1:A:294:LEU:HD21	1:C:294:LEU:HD22	2.04	0.40
2:B:22:LYS:HZ2	2:B:33:HIS:CD2	2.39	0.40
1:C:27:ALA:HB2	1:C:114:THR:CG2	2.52	0.40
1:C:73:PHE:CE2	1:C:135:GLU:HA	2.55	0.40
2:D:5:LYS:C	2:D:7:ALA:H	2.24	0.40
2:B:8:THR:CA	2:B:11:LYS:HD3	2.49	0.40
2:D:51:ALA:HA	5:D:649:HOH:O	2.20	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLU:OE2	5:A:549:HOH:O[1_656]	1.11	1.09
1:C:221:GLU:CD	5:A:549:HOH:O[1_656]	1.12	1.08
1:C:221:GLU:CG	5:A:549:HOH:O[1_656]	1.91	0.29
1:A:240:GLN:NE2	5:C:635:HOH:O[1_455]	2.15	0.05
2:B:54:LYS:CE	1:C:253:ASN:ND2[2_646]	2.15	0.05
1:C:221:GLU:OE1	5:A:549:HOH:O[1_656]	2.17	0.03

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	292/296 (99%)	264 (90%)	27 (9%)	1 (0%)	41	50
1	C	292/296 (99%)	272 (93%)	19 (6%)	1 (0%)	41	50
2	B	106/108 (98%)	91 (86%)	9 (8%)	6 (6%)	1	1
2	D	106/108 (98%)	89 (84%)	13 (12%)	4 (4%)	3	1
All	All	796/808 (98%)	716 (90%)	68 (8%)	12 (2%)	10	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	-2	LYS
2	B	-1	ALA
2	B	56	ASN
1	C	2	THR
2	D	61	GLU
2	B	6	GLY
2	B	24	GLY
2	B	61	GLU
2	D	56	ASN
1	A	67	TYR
2	D	40	SER
2	D	27	LYS

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	252/254 (99%)	221 (88%)	31 (12%)	4 5
1	C	252/254 (99%)	214 (85%)	38 (15%)	3 2
2	B	89/89 (100%)	73 (82%)	16 (18%)	1 1
2	D	89/89 (100%)	69 (78%)	20 (22%)	1 0
All	All	682/686 (99%)	577 (85%)	105 (15%)	2 2

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	THR
1	A	4	LEU
1	A	12	LYS
1	A	32	GLU
1	A	35	GLU
1	A	51	TRP
1	A	72	ARG
1	A	74	LYS
1	A	94	PRO
1	A	97	LYS
1	A	138	THR
1	A	140	ASP
1	A	168	VAL
1	A	179	LYS
1	A	190	PRO
1	A	195	ASN
1	A	196	ASN
1	A	197	VAL
1	A	200	ASN
1	A	210	ASP
1	A	212	LYS
1	A	215	LYS
1	A	226	LYS
1	A	233	PRO
1	A	245	LEU
1	A	260	LYS
1	A	263	SER
1	A	269	LEU
1	A	279	ASP
1	A	289	LEU
2	B	-5	THR
2	B	-4	GLU

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Mol	Chain	Res	Type
2	B	-3	PHE
2	B	-2	LYS
2	B	2	SER
2	B	11	LYS
2	B	22	LYS
2	B	55	LYS
2	B	58	LEU
2	B	61	GLU
2	B	73	LYS
2	B	80	MET
2	B	85	LEU
2	B	88	GLU
2	B	98	LEU
2	B	99	LYS
1	C	2	THR
1	C	5	VAL
1	C	12	LYS
1	C	14	ARG
1	C	20	GLN
1	C	32	GLU
1	C	47	VAL
1	C	63	THR
1	C	74	LYS
1	C	80	PRO
1	C	91	PHE
1	C	97	LYS
1	C	109	SER
1	C	122	PRO
1	C	127	ARG
1	C	133	THR
1	C	135	GLU
1	C	149	LYS
1	C	156	THR
1	C	162	ASN
1	C	183	LYS
1	C	188	GLU
1	C	190	PRO
1	C	196	ASN
1	C	197	VAL
1	C	199	THR
1	C	200	ASN
1	C	226	LYS

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Mol	Chain	Res	Type
1	C	237	SER
1	C	243	LYS
1	C	245	LEU
1	C	264	LYS
1	C	269	LEU
1	C	275	THR
1	C	278	LYS
1	C	279	ASP
1	C	287	LYS
1	C	289	LEU
2	D	-5	THR
2	D	-4	GLU
2	D	5	LYS
2	D	8	THR
2	D	11	LYS
2	D	31	ASN
2	D	38	ARG
2	D	53	ILE
2	D	54	LYS
2	D	55	LYS
2	D	57	VAL
2	D	60	ASP
2	D	63	ASN
2	D	66	GLU
2	D	72	LYS
2	D	73	LYS
2	D	89	LYS
2	D	91	ARG
2	D	99	LYS
2	D	102	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	38	ASN
1	A	60	HIS
1	A	96	HIS
1	A	141	ASN
1	A	200	ASN
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	292	GLN
2	B	33	HIS
2	B	39	HIS
2	B	52	ASN
1	C	20	GLN
1	C	24	ASN
1	C	38	ASN
1	C	62	ASN
1	C	78	ASN
1	C	86	GLN
1	C	141	ASN
1	C	162	ASN
1	C	196	ASN
1	C	200	ASN
1	C	208	ASN
1	C	222	GLN
1	C	292	GLN
2	D	26	HIS
2	D	52	ASN
2	D	63	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEM	B	104	2	41,50,50	1.70	6 (14%)	45,82,82	1.48	9 (20%)
4	HEM	A	296	3,1	41,50,50	1.81	13 (31%)	45,82,82	1.49	8 (17%)
4	HEM	D	104	2	41,50,50	1.43	5 (12%)	45,82,82	1.28	8 (17%)
4	HEM	C	296	3,1	41,50,50	1.41	7 (17%)	45,82,82	1.65	8 (17%)
3	SO4	C	300	4	0,1,4	-	-	-		
3	SO4	A	299	4	0,1,4	-	-	-		

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
4	HEM	C	296	3,1	-	2/12/54/54	-
4	HEM	D	104	2	-	0/12/54/54	-
4	HEM	B	104	2	-	1/12/54/54	-
4	HEM	A	296	3,1	-	3/12/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	104	HEM	C3C-C2C	-5.95	1.32	1.40
4	B	104	HEM	C3C-CAC	4.19	1.56	1.47
4	D	104	HEM	C3C-CAC	4.12	1.56	1.47
4	D	104	HEM	C3C-C2C	-3.92	1.34	1.40
4	A	296	HEM	C3C-C2C	-3.79	1.35	1.40
4	A	296	HEM	CAA-C2A	3.45	1.57	1.52
4	A	296	HEM	C3B-C2B	-3.42	1.30	1.37
4	B	104	HEM	CAA-C2A	3.41	1.57	1.52
4	C	296	HEM	C1A-NA	3.26	1.42	1.36
4	A	296	HEM	CAB-C3B	3.06	1.55	1.47
4	A	296	HEM	CMB-C2B	2.86	1.56	1.50
4	A	296	HEM	FE-NB	2.82	2.10	1.96
4	D	104	HEM	CAB-C3B	2.81	1.55	1.47
4	D	104	HEM	CAA-C2A	2.67	1.56	1.52
4	A	296	HEM	CMA-C3A	2.62	1.57	1.51
4	C	296	HEM	CAB-C3B	2.57	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	296	HEM	C3B-C2B	-2.56	1.32	1.37
4	C	296	HEM	C3C-C2C	-2.41	1.37	1.40
4	B	104	HEM	CMC-C2C	2.34	1.57	1.51
4	A	296	HEM	C3D-C2D	-2.32	1.31	1.36
4	A	296	HEM	C1B-NB	-2.32	1.36	1.40
4	D	104	HEM	CMD-C2D	2.22	1.55	1.50
4	C	296	HEM	CMB-C2B	2.20	1.55	1.50
4	C	296	HEM	CMA-C3A	2.19	1.56	1.51
4	A	296	HEM	C1A-NA	2.17	1.40	1.36
4	A	296	HEM	C4D-ND	-2.15	1.36	1.40
4	C	296	HEM	C4A-NA	2.15	1.40	1.36
4	A	296	HEM	CMD-C2D	2.05	1.55	1.50
4	A	296	HEM	FE-ND	2.03	2.06	1.96
4	B	104	HEM	CMD-C2D	2.02	1.55	1.50
4	B	104	HEM	CMA-C3A	2.02	1.55	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	296	HEM	CMA-C3A-C4A	-4.22	121.98	128.46
4	A	296	HEM	CMA-C3A-C4A	-4.04	122.25	128.46
4	B	104	HEM	O2D-CGD-O1D	3.86	132.91	123.30
4	C	296	HEM	CBA-CAA-C2A	3.48	118.55	112.62
4	C	296	HEM	C4C-CHD-C1D	3.47	127.13	122.56
4	B	104	HEM	CBA-CAA-C2A	-3.22	107.12	112.62
4	A	296	HEM	C4C-CHD-C1D	3.19	126.77	122.56
4	B	104	HEM	CMC-C2C-C3C	3.13	130.54	124.68
4	C	296	HEM	CHB-C1B-NB	-3.08	120.58	124.38
4	A	296	HEM	CMA-C3A-C2A	3.00	130.61	124.94
4	C	296	HEM	C2C-C3C-C4C	2.90	108.92	106.90
4	D	104	HEM	C4B-CHC-C1C	2.66	126.07	122.56
4	C	296	HEM	O1D-CGD-CBD	-2.63	114.62	123.08
4	D	104	HEM	C4C-CHD-C1D	2.59	125.98	122.56
4	C	296	HEM	CMA-C3A-C2A	2.50	129.65	124.94
4	D	104	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
4	D	104	HEM	O1D-CGD-CBD	-2.45	115.21	123.08
4	A	296	HEM	CMB-C2B-C1B	-2.43	121.33	125.04
4	B	104	HEM	O2A-CGA-O1A	2.43	129.35	123.30
4	A	296	HEM	CMD-C2D-C1D	-2.38	121.41	125.04
4	B	104	HEM	CBD-CAD-C3D	-2.28	106.28	112.63
4	A	296	HEM	O1D-CGD-CBD	-2.25	115.85	123.08
4	C	296	HEM	C4D-ND-C1D	2.25	107.39	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	104	HEM	CBA-CAA-C2A	-2.22	108.83	112.62
4	D	104	HEM	O2D-CGD-O1D	2.20	128.79	123.30
4	B	104	HEM	CHA-C4D-ND	2.20	127.10	124.38
4	D	104	HEM	CMC-C2C-C3C	2.14	128.68	124.68
4	A	296	HEM	CMD-C2D-C3D	2.11	131.85	126.12
4	B	104	HEM	CMA-C3A-C4A	-2.07	125.29	128.46
4	B	104	HEM	O1D-CGD-CBD	-2.05	116.50	123.08
4	B	104	HEM	CMB-C2B-C1B	-2.04	121.94	125.04
4	D	104	HEM	CHA-C4D-ND	2.02	126.88	124.38
4	A	296	HEM	CMC-C2C-C3C	2.01	128.44	124.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	296	HEM	CAA-CBA-CGA-O2A
4	A	296	HEM	CAA-CBA-CGA-O2A
4	A	296	HEM	CAA-CBA-CGA-O1A
4	B	104	HEM	CAA-CBA-CGA-O1A
4	A	296	HEM	CAD-CBD-CGD-O2D
4	C	296	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

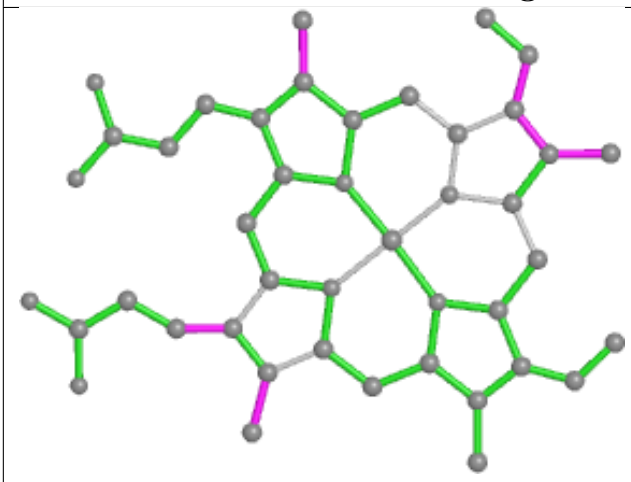
5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	104	HEM	16	0
4	D	104	HEM	19	0
4	C	296	HEM	4	0
3	C	300	SO4	1	0
3	A	299	SO4	1	0

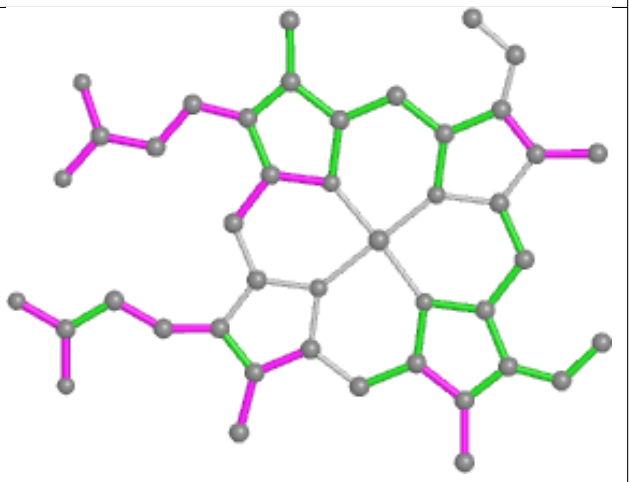
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

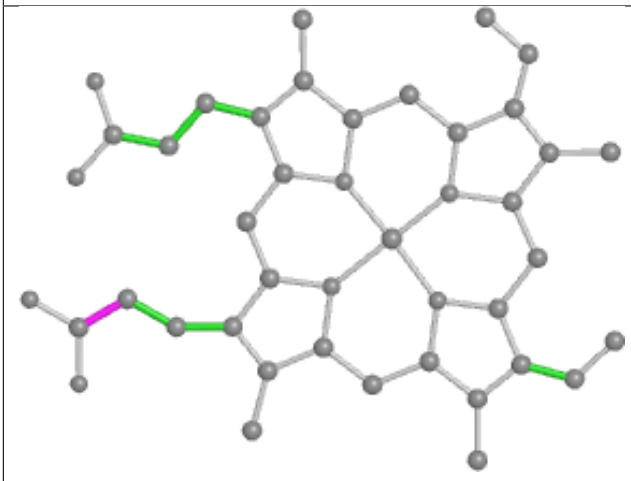
Ligand HEM B 104



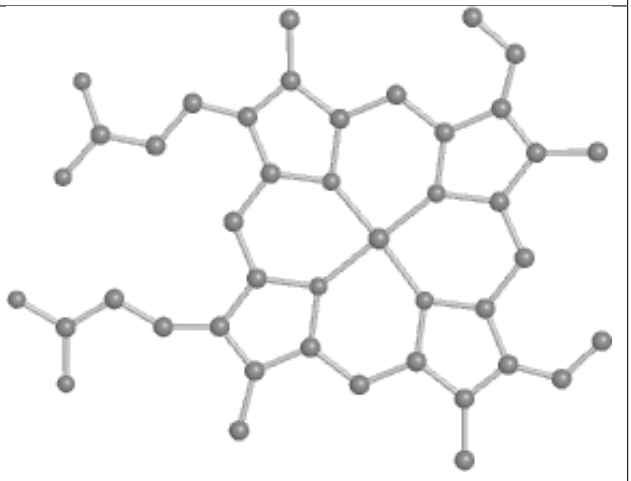
Bond lengths



Bond angles

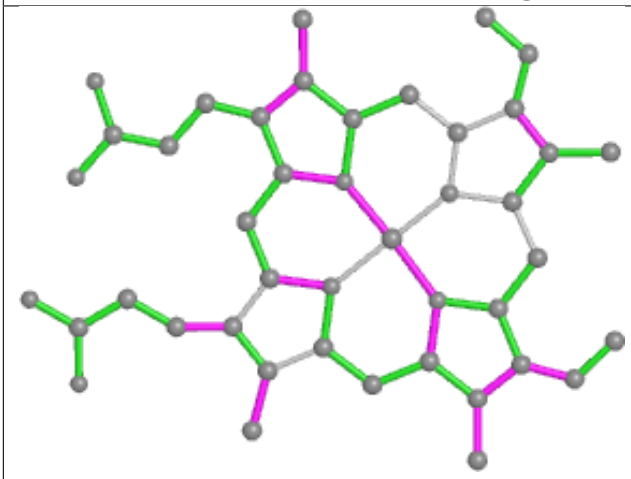


Torsions

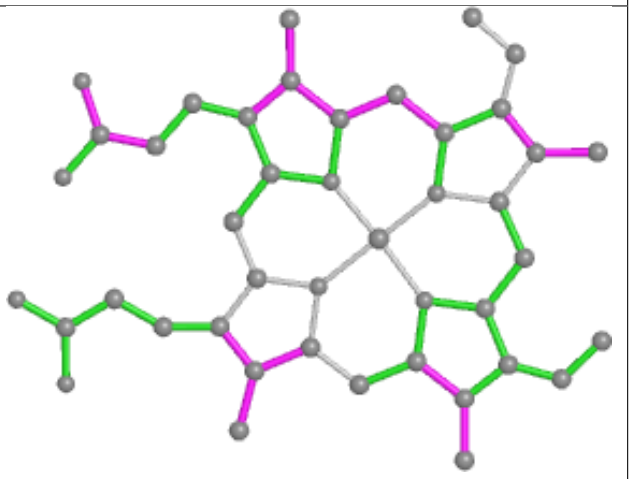


Rings

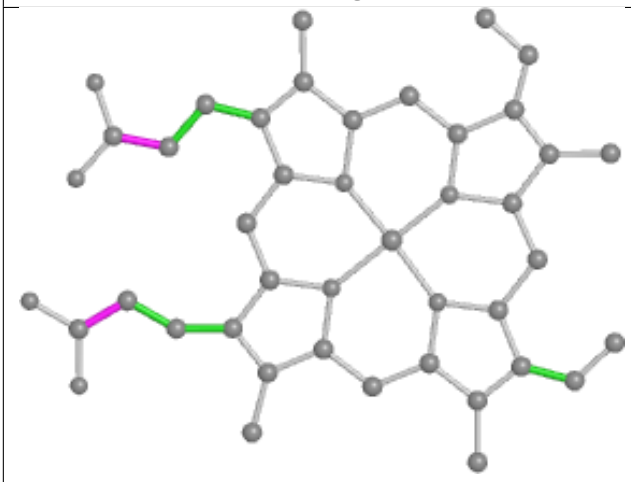
Ligand HEM A 296



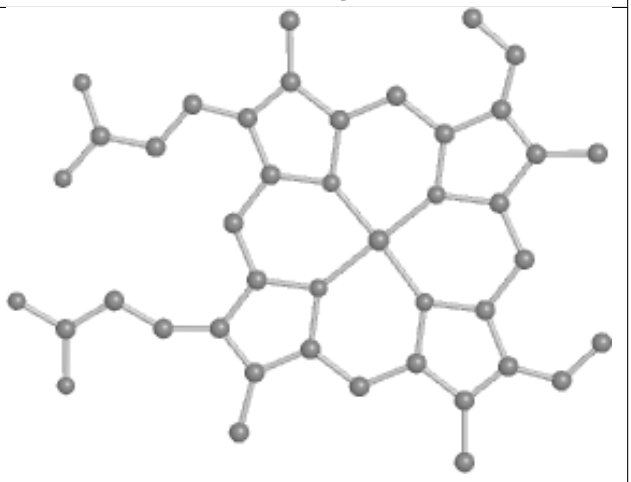
Bond lengths



Bond angles

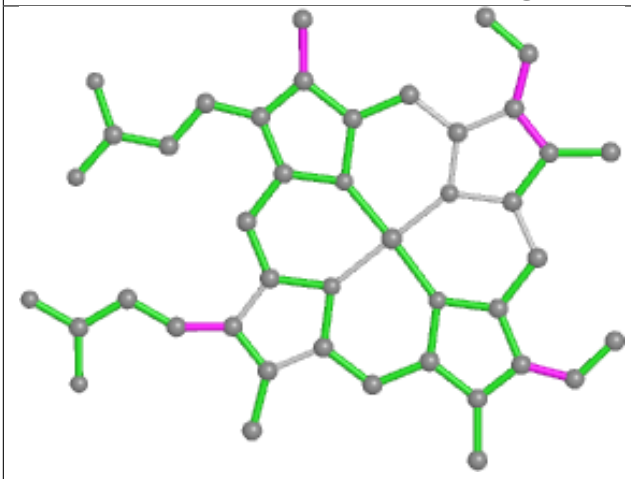


Torsions

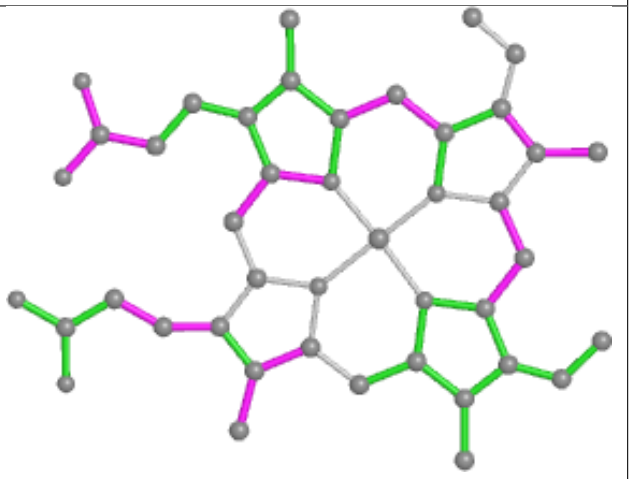


Rings

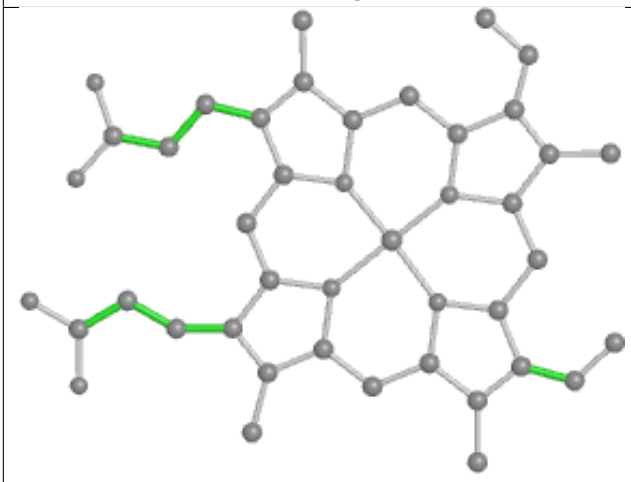
Ligand HEM D 104



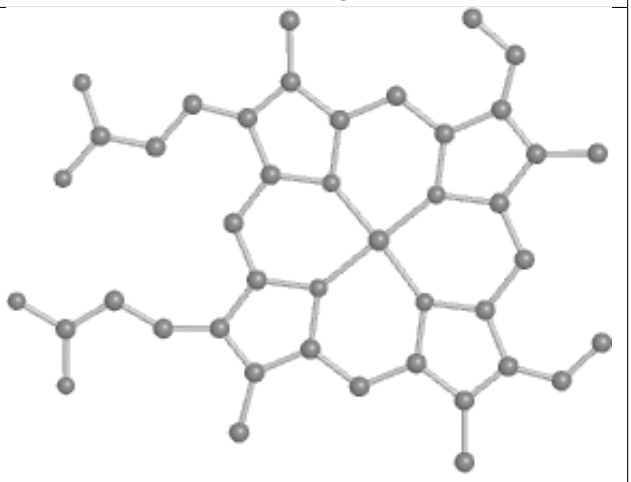
Bond lengths



Bond angles

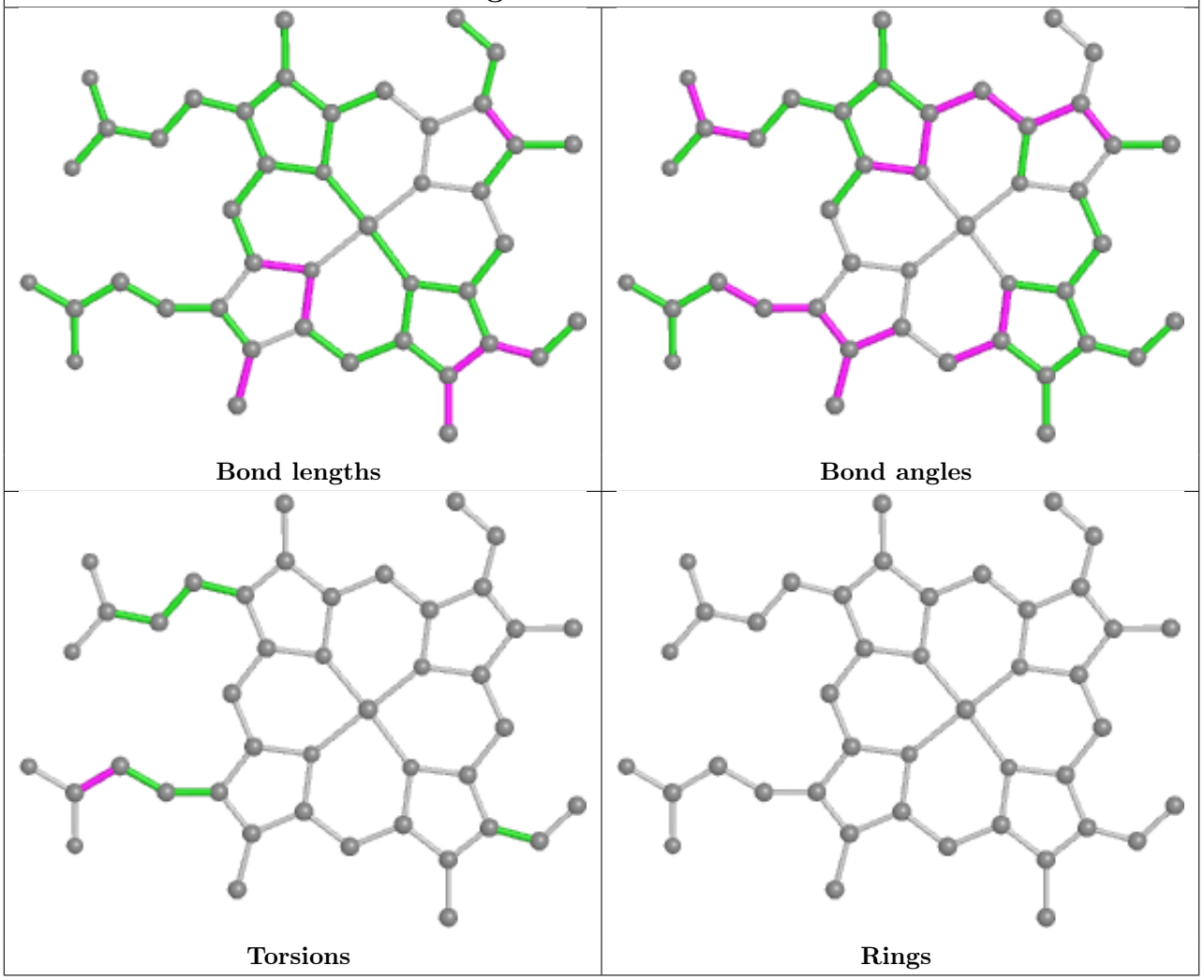


Torsions



Rings

Ligand HEM C 296



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

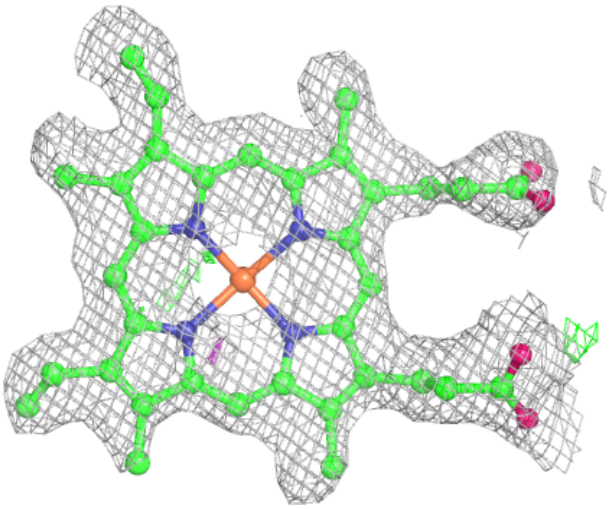
6.4 Ligands

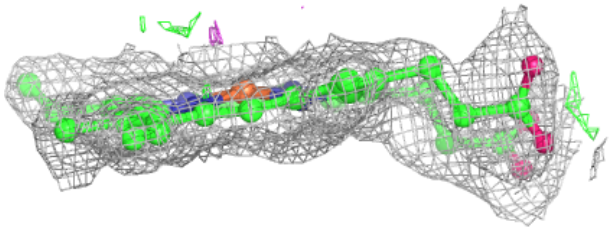
Unable to reproduce the depositors R factor - this section is therefore empty.

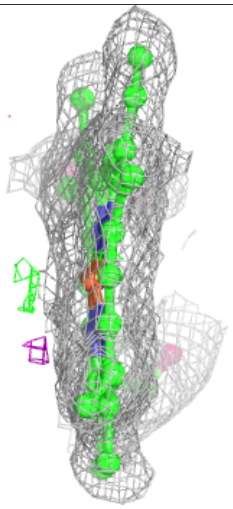
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 296:

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

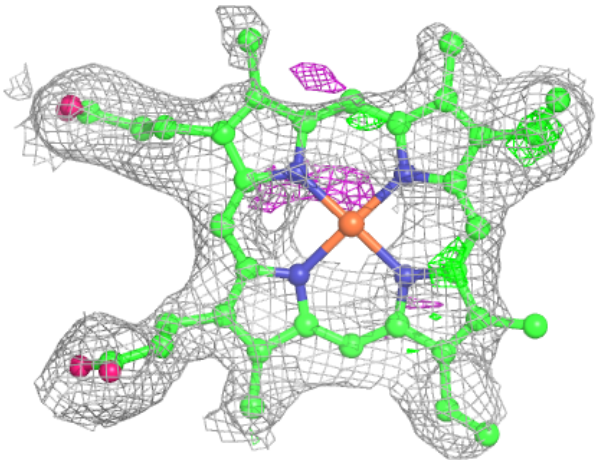


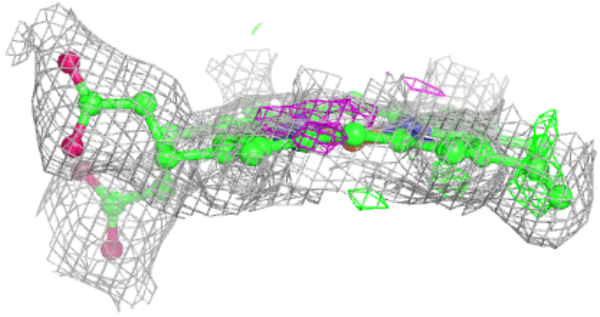


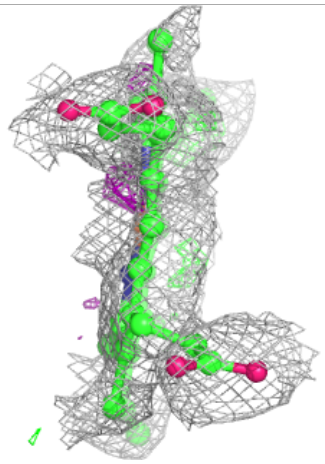


Electron density around HEM B 104:

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

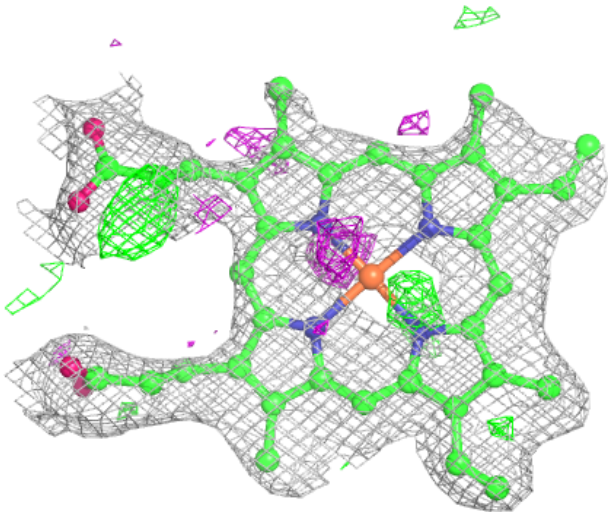


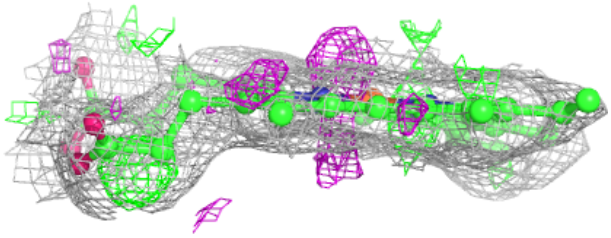


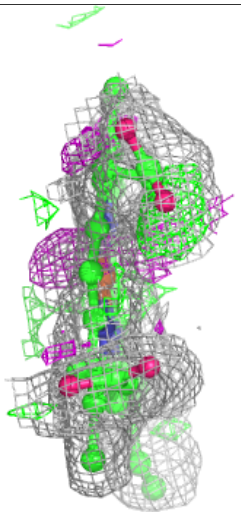


Electron density around HEM C 296:

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

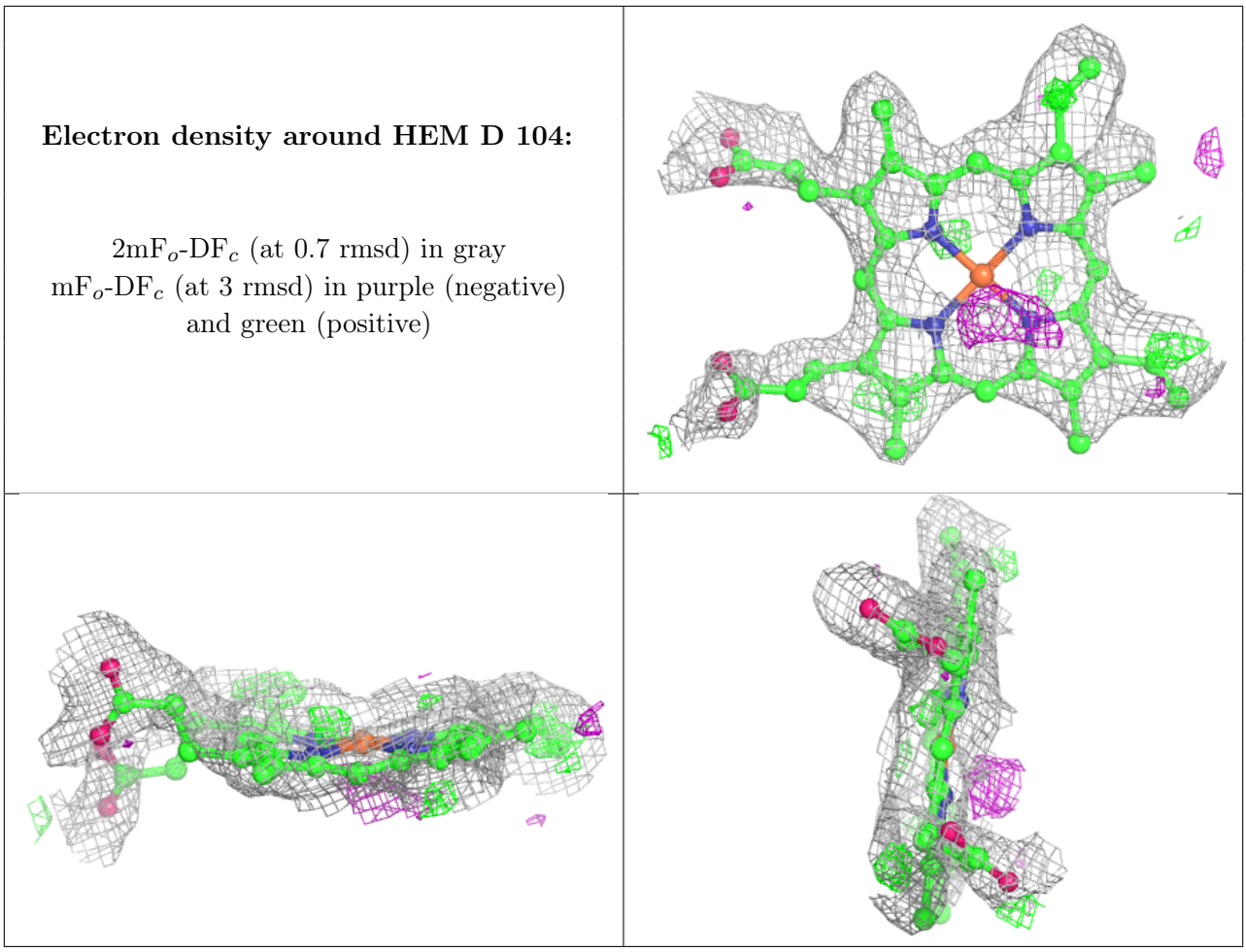






Electron density around HEM D 104:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.