Full wwPDB X-ray Structure Validation Report (i)

Feb 3, 2024 – 04:33 PM EST

PDB ID	:	1M7S
Title	:	Crystal Structure Analysis of Catalase CatF of Pseudomonas syringae
Authors	:	Carpena, X.; Soriano, M.; Klotz, M.G.; Duckworth, H.W.; Donald, L.J.; Melik-Adamyan, W.; Fita, I.; Loewen, P.C.
Deposited on	:	2002-07-22
Resolution	:	1.80 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:

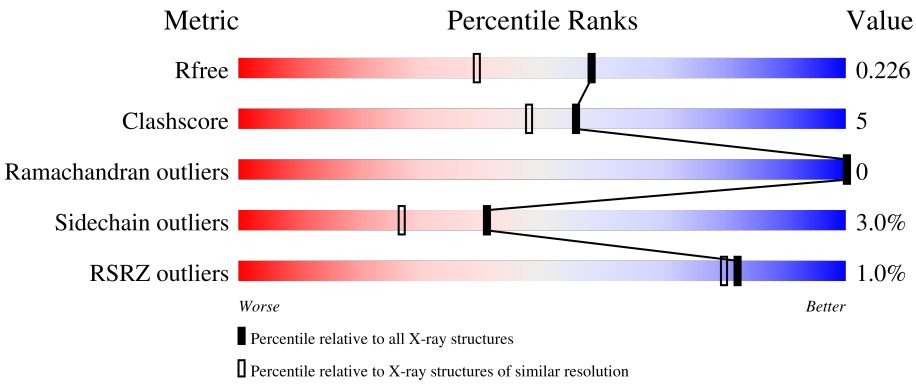
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	484	.% 84% 14% •
1	B	484	.% 82% 15% •
1	C	484	2% 84% 13% •
1	D	484	.% 87% 12% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17561 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 Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	484	3820	2406	671	737	6	0	3	0
1	B	483	3810	2401	670	733	6	0	3	0
1	C	483	3810	2401	670	733	6	0	3	0
1	D	484	3820	2406	671	737	6	0	3	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	ASN	ILE	SEE REMARK 999	UNP P46206
A	445	TYR	PHE	SEE REMARK 999	UNP P46206
A	459	LYS	ARG	SEE REMARK 999	UNP P46206
A	468	LEU	HIS	SEE REMARK 999	UNP P46206
A	478	TYR	VAL	SEE REMARK 999	UNP P46206
A	484	PRO	ARG	SEE REMARK 999	UNP P46206
A	485	ASN	HIS	SEE REMARK 999	UNP P46206
B	369	ASN	ILE	SEE REMARK 999	UNP P46206
B	445	TYR	PHE	SEE REMARK 999	UNP P46206
B	459	LYS	ARG	SEE REMARK 999	UNP P46206
B	468	LEU	HIS	SEE REMARK 999	UNP P46206
B	478	TYR	VAL	SEE REMARK 999	UNP P46206
B	484	PRO	ARG	SEE REMARK 999	UNP P46206
B	485	ASN	HIS	SEE REMARK 999	UNP P46206
C	369	ASN	ILE	SEE REMARK 999	UNP P46206
C	445	TYR	PHE	SEE REMARK 999	UNP P46206
C	459	LYS	ARG	SEE REMARK 999	UNP P46206
C	468	LEU	HIS	SEE REMARK 999	UNP P46206
C	478	TYR	VAL	SEE REMARK 999	UNP P46206
C	484	PRO	ARG	SEE REMARK 999	UNP P46206
C	485	ASN	HIS	SEE REMARK 999	UNP P46206

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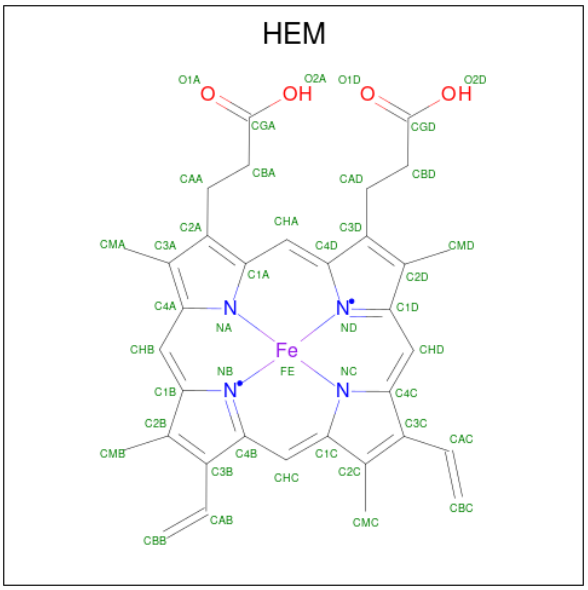
Chain	Residue	Modelled	Actual	Comment	Reference
D	369	ASN	ILE	SEE REMARK 999	UNP P46206
D	445	TYR	PHE	SEE REMARK 999	UNP P46206
D	459	LYS	ARG	SEE REMARK 999	UNP P46206
D	468	LEU	HIS	SEE REMARK 999	UNP P46206
D	478	TYR	VAL	SEE REMARK 999	UNP P46206
D	484	PRO	ARG	SEE REMARK 999	UNP P46206
D	485	ASN	HIS	SEE REMARK 999	UNP P46206

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	602	602	602	0	0

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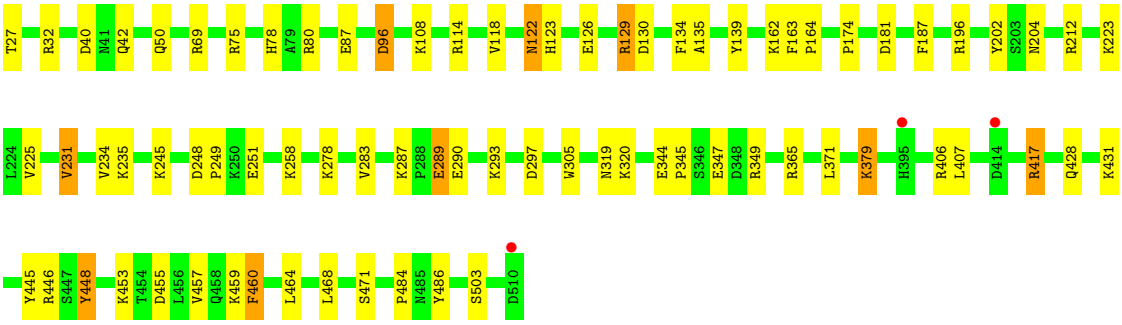
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	475	475	475	0	0
			Total	O		
3	C	438	438	438	0	0
			Total	O		
3	D	614	614	614	0	0

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.

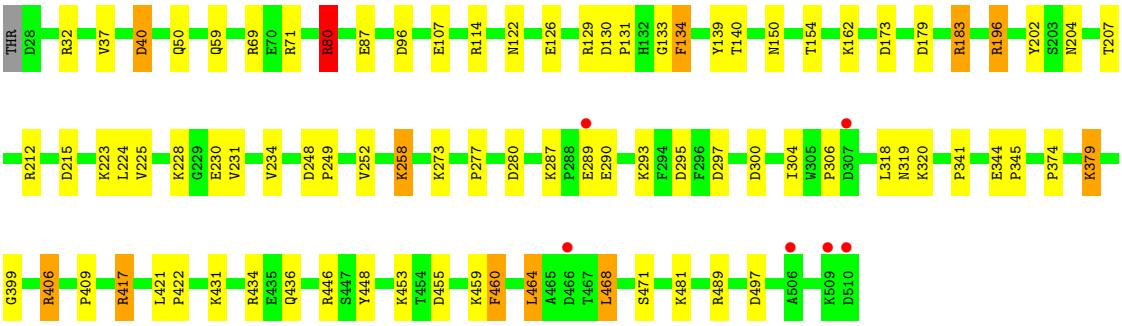
- Molecule 1: Catalase

Chain A:



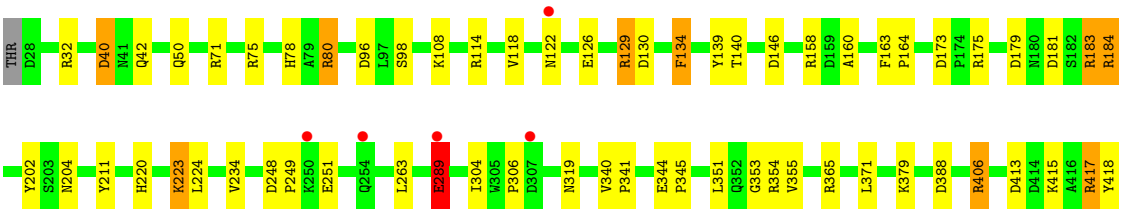
- Molecule 1: Catalase

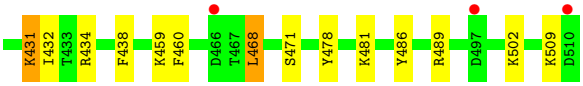
Chain B:



- Molecule 1: Catalase

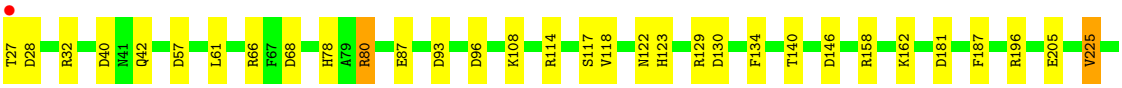
Chain C:

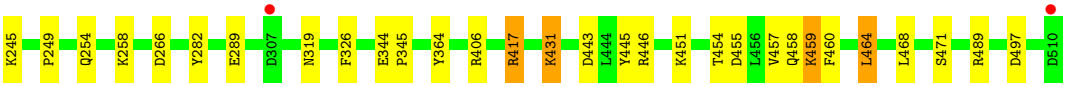




- Molecule 1: Catalase

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	60.63Å 153.87Å 109.19Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	21.90 – 1.80 21.89 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (21.90-1.80) 97.8 (21.89-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.240 0.174 , 0.226	Depositor DCC
R_{free} test set	8773 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	12.9	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17561	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.71	0/3915	1.47	38/5305 (0.7%)
1	B	0.64	0/3905	1.42	32/5291 (0.6%)
1	C	0.62	0/3905	1.38	37/5291 (0.7%)
1	D	0.73	0/3915	1.50	34/5305 (0.6%)
All	All	0.68	0/15640	1.44	141/21192 (0.7%)

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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	446	ARG	NE-CZ-NH2	-29.59	105.50	120.30
1	D	417	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	C	32	ARG	CD-NE-CZ	13.89	143.04	123.60
1	A	129	ARG	NE-CZ-NH1	13.79	127.20	120.30
1	B	183	ARG	NE-CZ-NH2	-13.73	113.44	120.30
1	D	446	ARG	NE-CZ-NH1	13.57	127.08	120.30
1	B	417	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	C	183	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	D	66	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	114	ARG	NE-CZ-NH1	12.40	126.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	B	32	ARG	NE-CZ-NH1	-11.21	114.69	120.30
1	C	129	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	C	32	ARG	NE-CZ-NH1	-10.50	115.05	120.30
1	A	129	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	C	489	ARG	NE-CZ-NH2	10.39	125.49	120.30
1	A	196	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	379	LYS	CA-CB-CG	10.23	135.91	113.40
1	C	71	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	C	417	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	417	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	D	114	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	B	71	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	A	365	ARG	NE-CZ-NH2	9.85	125.23	120.30
1	A	75	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	417	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	486	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	D	196	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	B	417	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	B	69	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	B	32	ARG	CD-NE-CZ	8.58	135.61	123.60
1	B	87	GLU	OE1-CD-OE2	-8.41	113.21	123.30
1	D	443	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	196	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	80	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	B	69	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	B	406	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	297	ASP	CB-CG-OD2	7.87	125.38	118.30
1	D	80	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	A	75	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	446	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	C	129	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	280	ASP	CB-CG-OD1	7.62	125.15	118.30
1	C	434	ARG	CD-NE-CZ	7.61	134.26	123.60
1	D	196	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	C	40	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	446	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	460	PHE	CB-CG-CD2	7.51	126.06	120.80
1	C	184	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	B	32	ARG	NH1-CZ-NH2	7.42	127.56	119.40
1	B	40	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	134	PHE	CB-CG-CD2	7.39	125.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	ASP	CB-CG-OD1	7.30	124.87	118.30
1	D	446	ARG	NH1-CZ-NH2	7.28	127.41	119.40
1	A	212	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	B	489	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	D	497	ASP	CB-CG-OD2	7.14	124.73	118.30
1	C	183	ARG	NH1-CZ-NH2	7.08	127.18	119.40
1	D	80	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	B	80	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	B	212	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	349	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	C	134	PHE	CB-CG-CD2	6.80	125.56	120.80
1	D	32	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	A	69	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	417	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	71	ARG	CD-NE-CZ	6.66	132.93	123.60
1	C	96	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	289	GLU	CA-CB-CG	6.60	127.91	113.40
1	B	300	ASP	CB-CG-OD2	6.58	124.22	118.30
1	D	181	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	445	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	D	68	ASP	CB-CG-OD1	6.38	124.05	118.30
1	D	417	ARG	CG-CD-NE	-6.35	98.46	111.80
1	C	175	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	183	ARG	NH1-CZ-NH2	6.28	126.31	119.40
1	A	196	ARG	CD-NE-CZ	6.24	132.34	123.60
1	B	173	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	418	TYR	CB-CG-CD2	6.22	124.73	121.00
1	D	93	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	446	ARG	CD-NE-CZ	6.11	132.16	123.60
1	B	107	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	A	460	PHE	CB-CG-CD1	-6.03	116.58	120.80
1	C	365	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	C	478	TYR	CB-CG-CD2	5.99	124.59	121.00
1	C	365	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	96	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	66	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
1	D	282	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	C	114	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	126	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	B	446	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	289	GLU	CG-CD-OE1	5.76	129.83	118.30
1	C	406	ARG	NE-CZ-NH1	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	158	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	B	434	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	75	ARG	CD-NE-CZ	5.68	131.55	123.60
1	C	96	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	297	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	B	114	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	146	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	446	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	69	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	486	TYR	CB-CG-CD1	5.56	124.34	121.00
1	C	486	TYR	CB-CG-CD1	5.55	124.33	121.00
1	C	388	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	158	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	497	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	87	GLU	CB-CG-CD	5.48	129.00	114.20
1	B	196	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	354	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	231	VAL	N-CA-CB	-5.38	99.66	111.50
1	B	215	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	146	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	32	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	289	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	A	187	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	A	126	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	A	347	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	A	445	TYR	CB-CG-CD1	5.27	124.16	121.00
1	B	126	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	D	129	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	179	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	32	ARG	CD-NE-CZ	5.24	130.94	123.60
1	D	326	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	D	187	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	A	187	PHE	CB-CG-CD1	5.21	124.45	120.80
1	D	364	TYR	CB-CG-CD2	5.19	124.11	121.00
1	B	179	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	225	VAL	CB-CA-C	5.16	121.20	111.40
1	C	173	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	464	LEU	CB-CG-CD2	5.14	119.74	111.00
1	C	223	LYS	CA-CB-CG	5.13	124.69	113.40
1	B	32	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	445	TYR	CB-CG-CD2	5.10	124.06	121.00
1	C	417	ARG	CD-NE-CZ	-5.08	116.48	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	134	PHE	CB-CG-CD1	-5.08	117.25	120.80
1	D	266	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	D	32	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	A	448	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	D	205	GLU	OE1-CD-OE2	-5.03	117.26	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123[A]	HIS	Mainchain
1	D	123[B]	HIS	Mainchain

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	3820	0	3732	45	0
1	B	3810	0	3723	52	0
1	C	3810	0	3723	41	0
1	D	3820	0	3732	30	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	602	0	0	12	0
3	B	475	0	0	12	0
3	C	438	0	0	9	0
3	D	614	0	0	8	0
All	All	17561	0	15030	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (156) 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:129:ARG:NH2	1:A:459:LYS:HD2	1.74	1.00
1:A:249:PRO:HG3	1:A:459:LYS:HD3	1.48	0.94
1:A:407:LEU:HD21	1:B:468:LEU:HD22	1.48	0.94
1:C:249:PRO:HG3	1:C:459:LYS:HD3	1.53	0.91
1:C:129:ARG:NH2	1:C:459:LYS:HD2	1.89	0.87
1:A:204:ASN:OD1	1:A:459:LYS:NZ	2.10	0.85
1:A:129:ARG:HH22	1:A:459:LYS:HD2	1.40	0.84
1:B:249:PRO:HG3	1:B:459:LYS:HD2	1.61	0.83
1:D:468:LEU:HD23	3:D:1279:HOH:O	1.79	0.83
1:B:248:ASP:HB2	1:B:249:PRO:HD2	1.64	0.80
1:C:202:TYR:O	1:C:459:LYS:HE3	1.82	0.79
1:A:468:LEU:HD23	3:A:1283:HOH:O	1.82	0.78
1:C:468:LEU:HD11	1:D:406:ARG:HD2	1.65	0.77
1:A:468:LEU:HD13	3:A:2289:HOH:O	1.85	0.75
1:D:468:LEU:HD21	1:D:471:SER:OG	1.87	0.75
1:A:87:GLU:OE2	1:A:108:LYS:HG2	1.88	0.73
1:D:245:LYS:HE3	3:D:2730:HOH:O	1.87	0.73
1:C:129:ARG:HH22	1:C:459:LYS:HD2	1.53	0.72
1:B:468:LEU:HD23	3:B:1872:HOH:O	1.89	0.72
1:A:468:LEU:HD21	1:A:471:SER:OG	1.91	0.71
1:D:468:LEU:HD13	3:D:2543:HOH:O	1.92	0.70
1:A:406:ARG:HD2	1:B:468:LEU:HD11	1.73	0.69
1:A:468:LEU:HD11	1:B:406:ARG:HD2	1.73	0.69
1:A:468:LEU:CD1	1:A:471:SER:H	2.06	0.67
1:B:204:ASN:OD1	1:B:459:LYS:NZ	2.28	0.66
1:D:468:LEU:HD11	1:D:471:SER:H	1.60	0.65
1:C:406:ARG:HD2	1:D:468:LEU:HD11	1.79	0.65
1:C:468:LEU:HD23	3:C:2178:HOH:O	1.95	0.65
1:A:468:LEU:HD11	1:A:471:SER:H	1.62	0.63
1:B:468:LEU:HD21	1:B:471:SER:OG	1.99	0.63
1:B:129:ARG:NH2	1:B:459:LYS:HE3	2.14	0.63
1:B:249:PRO:HG3	1:B:459:LYS:CD	2.29	0.63
1:B:154:THR:HG21	1:B:196:ARG:HD3	1.81	0.62
1:C:468:LEU:HD21	1:C:471:SER:OG	1.99	0.61
1:D:468:LEU:CD1	1:D:471:SER:H	2.13	0.61
1:A:278:LYS:HE3	3:A:2622:HOH:O	2.02	0.60
1:A:249:PRO:CG	1:A:459:LYS:HD3	2.28	0.60
1:B:320:LYS:HD2	3:B:2814:HOH:O	2.00	0.59
1:C:163:PHE:HB3	1:C:164:PRO:HD3	1.83	0.59
1:B:59:GLN:HB3	3:B:2644:HOH:O	2.03	0.59
1:C:224:LEU:HD12	1:C:234:VAL:HG21	1.85	0.59
1:C:431:LYS:HD2	1:C:432:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG21	3:C:2240:HOH:O	2.03	0.58
1:C:204:ASN:OD1	1:C:459:LYS:NZ	2.23	0.57
1:B:290:GLU:HA	1:B:293:LYS:HD2	1.86	0.57
1:D:78:HIS:CE1	1:D:118:VAL:HG22	2.40	0.57
1:B:409:PRO:O	1:D:27:THR:HG21	2.05	0.57
1:A:344:GLU:HB3	1:A:345:PRO:HD2	1.86	0.57
1:C:78:HIS:CE1	1:C:118:VAL:HG22	2.41	0.56
1:B:481:LYS:NZ	3:B:2435:HOH:O	2.36	0.56
1:A:135:ALA:N	3:A:3059:HOH:O	2.39	0.56
1:B:224:LEU:HD12	1:B:234:VAL:HG21	1.87	0.55
1:A:289:GLU:H	1:A:289:GLU:CD	2.10	0.55
1:B:80:ARG:HD3	1:B:122[B]:ASN:O	2.06	0.55
1:B:139:TYR:HB3	1:B:379:LYS:HG3	1.88	0.55
1:C:98:SER:HB2	1:C:224:LEU:HB3	1.88	0.54
1:B:40:ASP:OD2	1:D:417:ARG:NH2	2.40	0.54
1:B:202:TYR:O	1:B:459:LYS:HE2	2.07	0.54
1:A:202:TYR:O	1:A:459:LYS:HE2	2.09	0.53
1:B:287:LYS:HB2	1:B:290:GLU:HG3	1.90	0.53
1:B:277:PRO:HD2	1:B:318:LEU:O	2.09	0.53
1:C:413:ASP:OD1	1:C:415:LYS:HG2	2.07	0.53
1:B:417:ARG:NH2	1:D:40:ASP:OD2	2.41	0.53
1:D:80:ARG:HD3	1:D:122[A]:ASN:O	2.08	0.53
1:C:248:ASP:HB2	1:C:249:PRO:HD2	1.90	0.53
1:C:344:GLU:HB3	1:C:345:PRO:HD2	1.91	0.52
1:A:78:HIS:CE1	1:A:118:VAL:HG22	2.45	0.52
1:B:133:GLY:HA2	1:B:150:ASN:OD1	2.10	0.52
1:A:287:LYS:HB2	1:A:290:GLU:HG3	1.91	0.52
1:A:448:TYR:O	1:A:453:LYS:NZ	2.43	0.52
1:B:129:ARG:HH22	1:B:459:LYS:HE3	1.73	0.52
1:B:223:LYS:HG2	1:B:231:VAL:HG13	1.91	0.52
1:C:468:LEU:HG	1:C:468:LEU:O	2.08	0.51
1:A:455:ASP:HB3	1:A:459:LYS:NZ	2.25	0.51
1:D:454:THR:HG22	3:D:2503:HOH:O	2.11	0.51
1:A:202:TYR:O	1:A:459:LYS:CE	2.58	0.51
1:A:162:LYS:HD3	1:D:42:GLN:HA	1.93	0.51
1:C:289:GLU:HG3	3:C:2320:HOH:O	2.10	0.51
1:B:162:LYS:HD3	1:C:42:GLN:HA	1.92	0.50
1:D:254:GLN:HG2	3:D:2793:HOH:O	2.12	0.50
1:A:139:TYR:HB3	1:A:379:LYS:HG2	1.92	0.50
3:B:2232:HOH:O	1:D:27:THR:HG22	2.12	0.50
1:C:355:VAL:HB	3:C:2917:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:TYR:CE1	1:C:263:LEU:HD13	2.47	0.49
2:A:600:HEM:HMA2	3:A:3059:HOH:O	2.12	0.49
1:B:468:LEU:CD1	1:B:471:SER:H	2.24	0.49
1:D:455:ASP:O	1:D:459:LYS:HG2	2.12	0.49
1:C:139:TYR:HB3	1:C:379:LYS:HG2	1.95	0.49
1:B:304:ILE:O	1:B:306:PRO:HD3	2.13	0.49
1:D:122[B]:ASN:HB2	3:D:1685:HOH:O	2.12	0.49
1:D:458:GLN:HB3	1:D:459:LYS:HE2	1.95	0.49
1:A:42:GLN:HA	1:D:162:LYS:HD3	1.94	0.48
1:B:183:ARG:HD3	3:B:1133:HOH:O	2.12	0.48
1:B:448:TYR:O	1:B:453:LYS:NZ	2.46	0.48
1:C:122[B]:ASN:H	1:C:122[B]:ASN:HD22	1.59	0.48
1:C:160:ALA:CB	1:C:353:GLY:HA3	2.43	0.48
1:A:122[A]:ASN:HB3	3:A:3126:HOH:O	2.11	0.48
1:C:509:LYS:HD3	3:C:2510:HOH:O	2.14	0.47
1:C:438:PHE:CD1	1:C:481:LYS:HG2	2.50	0.47
1:D:57:ASP:O	1:D:61:LEU:HD23	2.15	0.47
1:C:80:ARG:HD3	1:C:122[A]:ASN:O	2.15	0.47
1:D:457:VAL:HG11	1:D:489:ARG:HB3	1.96	0.46
1:A:417:ARG:NH2	1:C:40:ASP:OD2	2.49	0.46
1:A:455:ASP:HB3	1:A:459:LYS:HZ1	1.81	0.46
1:C:248:ASP:OD2	1:C:251:GLU:HG3	2.15	0.46
1:B:421:LEU:HA	1:B:422:PRO:HD3	1.84	0.46
1:B:207:THR:HG21	1:B:252:VAL:HG21	1.97	0.46
1:B:50:GLN:HG2	3:B:2549:HOH:O	2.16	0.46
1:D:78:HIS:HA	1:D:117:SER:O	2.16	0.46
1:B:122[A]:ASN:HB2	3:B:3127:HOH:O	2.17	0.45
1:C:502:LYS:HE2	3:C:2647:HOH:O	2.15	0.45
1:D:249:PRO:HG2	1:D:459:LYS:HE3	1.99	0.45
1:D:27:THR:HG22	1:D:28:ASP:N	2.32	0.45
1:C:181:ASP:O	1:C:184:ARG:HG2	2.16	0.45
1:C:371:LEU:HD22	3:C:2054:HOH:O	2.16	0.45
1:B:130:ASP:HB3	1:B:131:PRO:O	2.17	0.45
1:A:174:PRO:HG2	1:B:399:GLY:HA2	1.98	0.45
1:A:248:ASP:OD2	1:A:251:GLU:HG3	2.17	0.45
1:C:481:LYS:NZ	3:C:2272:HOH:O	2.28	0.45
1:B:37:VAL:HG22	3:D:1053:HOH:O	2.18	0.44
1:A:223:LYS:HG3	1:A:231:VAL:HG13	1.97	0.44
1:A:234:VAL:HG13	1:A:283:VAL:HB	1.99	0.44
1:A:371:LEU:HD13	3:A:2998:HOH:O	2.17	0.44
1:B:468:LEU:HD11	1:B:471:SER:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LYS:HA	1:B:273:LYS:HD3	1.73	0.43
1:C:183:ARG:HD3	3:C:1011:HOH:O	2.18	0.43
1:B:139:TYR:HB3	1:B:379:LYS:CG	2.47	0.43
1:B:460:PHE:O	1:B:464:LEU:HB2	2.18	0.43
1:D:344:GLU:HB3	1:D:345:PRO:HD2	1.99	0.43
3:B:2393:HOH:O	1:D:27:THR:HG21	2.17	0.43
1:A:50:GLN:HG2	3:A:2821:HOH:O	2.19	0.43
1:A:163:PHE:HB3	1:A:164:PRO:HD3	2.01	0.43
1:B:455:ASP:O	1:B:459:LYS:HD3	2.18	0.43
1:D:87:GLU:OE2	1:D:108:LYS:HG2	2.18	0.43
1:C:223:LYS:HG3	1:C:344:GLU:HB2	2.00	0.42
1:B:228:LYS:NZ	1:B:230:GLU:OE2	2.52	0.42
1:C:340:VAL:HB	1:C:341:PRO:HD2	2.00	0.42
1:D:431:LYS:HB2	1:D:431:LYS:NZ	2.34	0.42
1:A:503:SER:HB2	3:A:3043:HOH:O	2.18	0.42
1:C:220:HIS:CD2	1:C:351:LEU:HD13	2.55	0.42
1:A:484:PRO:HG3	3:A:2988:HOH:O	2.19	0.42
3:B:2127:HOH:O	1:C:50:GLN:HG3	2.19	0.42
1:A:40:ASP:OD2	1:C:417:ARG:NH2	2.54	0.41
1:B:223:LYS:CG	1:B:231:VAL:HG13	2.51	0.41
1:C:304:ILE:O	1:C:306:PRO:HD3	2.20	0.41
1:A:235:LYS:HE3	1:A:305:TRP:NE1	2.35	0.41
1:B:344:GLU:HB3	1:B:345:PRO:HD2	2.02	0.41
1:A:245:LYS:HE3	1:A:245:LYS:HB2	1.82	0.41
1:B:295:ASP:OD2	1:B:436:GLN:NE2	2.53	0.41
1:A:379:LYS:NZ	3:A:2669:HOH:O	2.53	0.41
1:A:468:LEU:HD11	1:A:471:SER:N	2.34	0.40
1:B:431:LYS:HG2	3:B:2023:HOH:O	2.21	0.40
1:B:224:LEU:CD1	1:B:234:VAL:HG21	2.51	0.40
1:B:341:PRO:HG3	3:D:2185:HOH:O	2.21	0.40
2:A:600:HEM:CMA	3:A:3059:HOH:O	2.68	0.40
1:B:258:LYS:HB2	3:B:2093:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/484 (100%)	472 (97%)	13 (3%)	0	100	100
1	B	484/484 (100%)	468 (97%)	16 (3%)	0	100	100
1	C	484/484 (100%)	476 (98%)	8 (2%)	0	100	100
1	D	485/484 (100%)	473 (98%)	12 (2%)	0	100	100
All	All	1938/1936 (100%)	1889 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	414/414 (100%)	399 (96%)	15 (4%)	35	20
1	B	412/414 (100%)	399 (97%)	13 (3%)	39	25
1	C	412/414 (100%)	402 (98%)	10 (2%)	49	36
1	D	414/414 (100%)	401 (97%)	13 (3%)	40	25
All	All	1652/1656 (100%)	1601 (97%)	51 (3%)	41	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
1	A	122[A]	ASN
1	A	122[B]	ASN
1	A	130	ASP
1	A	134	PHE
1	A	225	VAL
1	A	258	LYS
1	A	293	LYS

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Mol	Chain	Res	Type
1	A	319	ASN
1	A	320	LYS
1	A	428	GLN
1	A	431	LYS
1	A	457	VAL
1	A	460	PHE
1	A	464	LEU
1	B	80	ARG
1	B	96	ASP
1	B	134	PHE
1	B	140	THR
1	B	225	VAL
1	B	258	LYS
1	B	289	GLU
1	B	319	ASN
1	B	374	PRO
1	B	379	LYS
1	B	460	PHE
1	B	464	LEU
1	B	468	LEU
1	C	80	ARG
1	C	108	LYS
1	C	130	ASP
1	C	134	PHE
1	C	140	THR
1	C	289	GLU
1	C	319	ASN
1	C	431	LYS
1	C	460	PHE
1	C	468	LEU
1	D	96	ASP
1	D	130	ASP
1	D	134	PHE
1	D	140	THR
1	D	225	VAL
1	D	258	LYS
1	D	289	GLU
1	D	319	ASN
1	D	431	LYS
1	D	451	LYS
1	D	459	LYS
1	D	460	PHE

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Mol	Chain	Res	Type
1	D	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	ASN
1	B	319	ASN
1	C	319	ASN
1	D	319	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)

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	$\#\|Z\| > 2$
2	HEM	C	600	3,1	41,50,50	1.42	4 (9%)	45,82,82	1.51	9 (20%)
2	HEM	A	600	3,1	41,50,50	1.50	5 (12%)	45,82,82	1.47	8 (17%)
2	HEM	D	600	3,1	41,50,50	1.40	4 (9%)	45,82,82	1.07	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	600	3,1	41,50,50	1.56	5 (12%)	45,82,82	1.33	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	600	3,1	-	2/12/54/54	-
2	HEM	A	600	3,1	-	4/12/54/54	-
2	HEM	D	600	3,1	-	3/12/54/54	-
2	HEM	B	600	3,1	-	2/12/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3C-C2C	-4.30	1.34	1.40
2	B	600	HEM	C3C-C2C	-3.98	1.34	1.40
2	C	600	HEM	C3C-C2C	-3.85	1.35	1.40
2	A	600	HEM	C3C-CAC	3.30	1.54	1.47
2	D	600	HEM	C3C-C2C	-3.27	1.35	1.40
2	C	600	HEM	C3C-CAC	3.27	1.54	1.47
2	B	600	HEM	C3C-CAC	3.09	1.54	1.47
2	D	600	HEM	C3C-CAC	2.63	1.53	1.47
2	B	600	HEM	CAB-C3B	2.60	1.54	1.47
2	C	600	HEM	CAB-C3B	2.57	1.54	1.47
2	A	600	HEM	CHA-C4D	2.51	1.41	1.35
2	B	600	HEM	C4D-ND	-2.51	1.36	1.40
2	D	600	HEM	CAB-C3B	2.40	1.54	1.47
2	D	600	HEM	CAA-C2A	2.34	1.55	1.52
2	A	600	HEM	CBA-CGA	2.19	1.55	1.50
2	A	600	HEM	CAB-C3B	2.16	1.53	1.47
2	C	600	HEM	CAD-C3D	2.11	1.56	1.51
2	B	600	HEM	C4A-NA	2.10	1.40	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	600	HEM	CMA-C3A-C4A	-4.45	121.63	128.46
2	A	600	HEM	O2A-CGA-O1A	4.40	134.26	123.30
2	A	600	HEM	CMA-C3A-C4A	-3.23	123.50	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	O1A-CGA-CBA	-3.18	112.86	123.08
2	C	600	HEM	CMA-C3A-C2A	3.17	130.91	124.94
2	B	600	HEM	C4D-ND-C1D	3.10	108.28	105.07
2	C	600	HEM	CMC-C2C-C3C	3.01	130.32	124.68
2	C	600	HEM	C4D-ND-C1D	2.84	108.01	105.07
2	A	600	HEM	CHD-C1D-ND	2.77	127.44	124.43
2	A	600	HEM	O2D-CGD-CBD	2.75	122.85	114.03
2	C	600	HEM	CHD-C1D-ND	2.64	127.30	124.43
2	C	600	HEM	C1B-NB-C4B	2.60	107.76	105.07
2	B	600	HEM	O1A-CGA-CBA	-2.52	114.99	123.08
2	B	600	HEM	C4C-CHD-C1D	2.38	125.70	122.56
2	D	600	HEM	C4C-CHD-C1D	2.31	125.61	122.56
2	A	600	HEM	O1D-CGD-CBD	-2.27	115.79	123.08
2	B	600	HEM	CHD-C1D-ND	2.26	126.89	124.43
2	C	600	HEM	CBA-CAA-C2A	2.22	116.42	112.62
2	D	600	HEM	O1D-CGD-CBD	-2.19	116.05	123.08
2	B	600	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
2	C	600	HEM	O1A-CGA-CBA	-2.18	116.09	123.08
2	A	600	HEM	CMA-C3A-C2A	2.17	129.04	124.94
2	B	600	HEM	C1B-NB-C4B	2.16	107.30	105.07
2	A	600	HEM	C4D-ND-C1D	2.07	107.21	105.07
2	C	600	HEM	CAD-CBD-CGD	2.01	117.94	113.60

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAA-CBA-CGA-O1A
2	C	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O2A
2	D	600	HEM	CAA-CBA-CGA-O1A
2	B	600	HEM	CAA-CBA-CGA-O2A
2	C	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAD-CBD-CGD-O2D
2	A	600	HEM	CAD-CBD-CGD-O1D
2	D	600	HEM	CAD-CBD-CGD-O2D

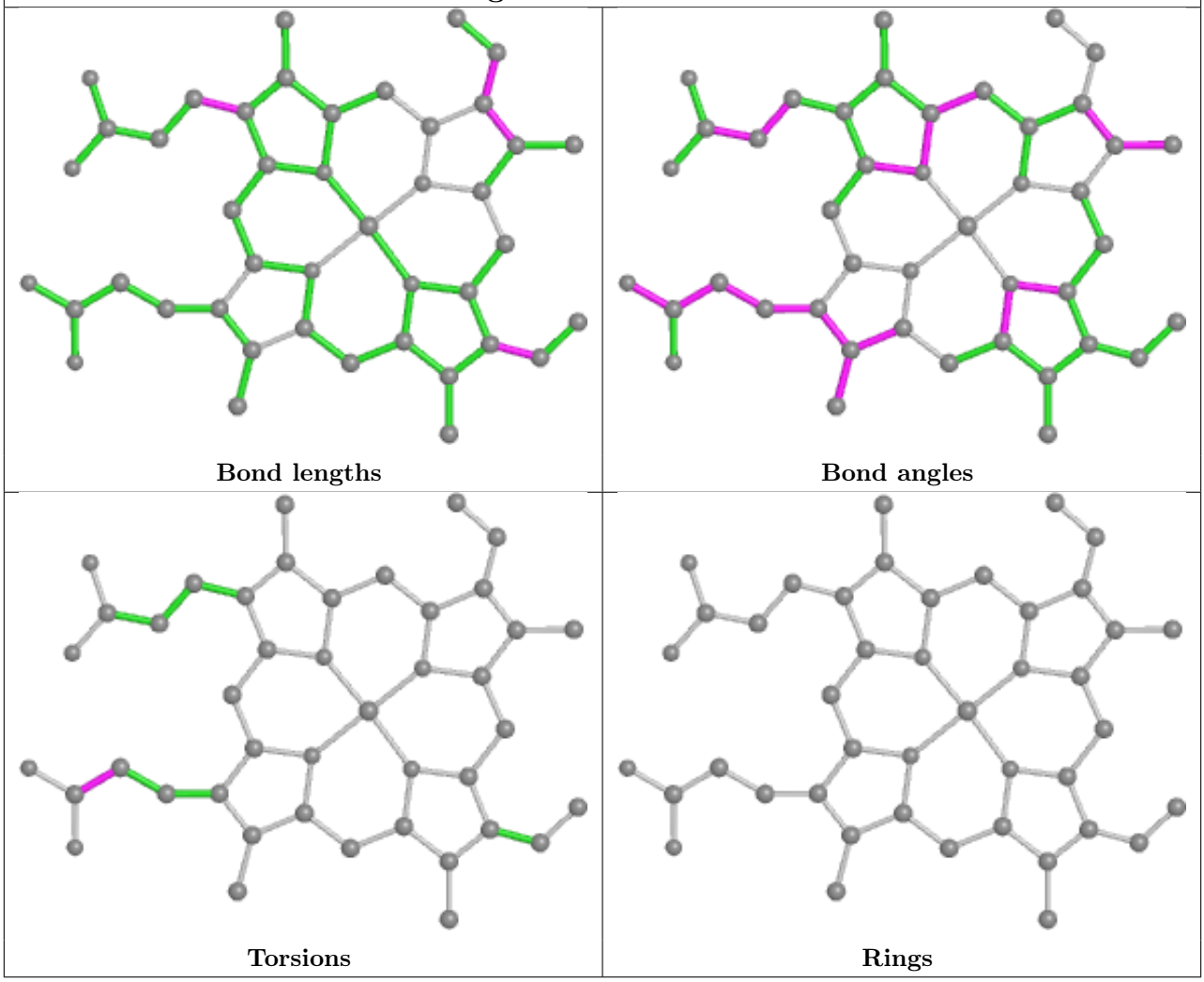
There are no ring outliers.

1 monomer is involved in 2 short contacts:

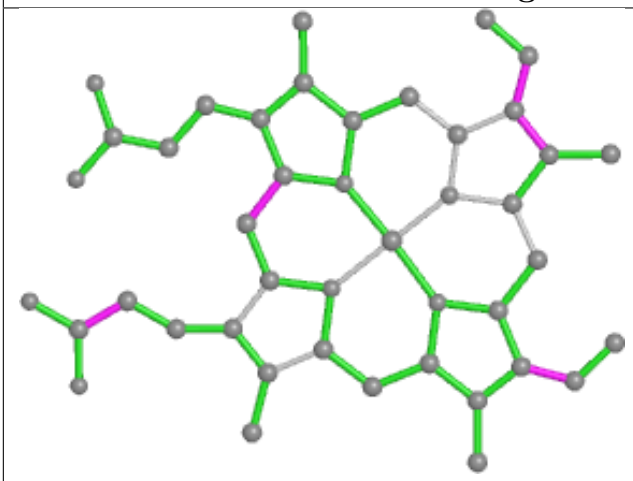
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0

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.

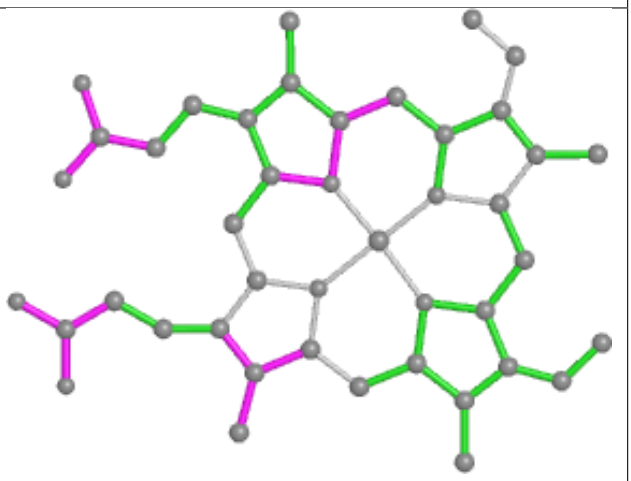
Ligand HEM C 600



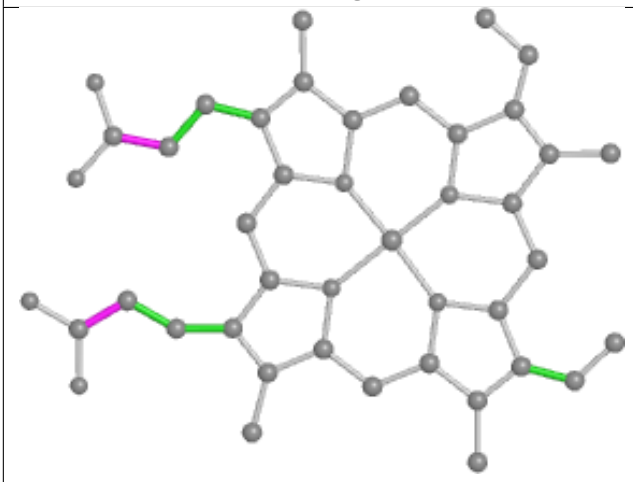
Ligand HEM A 600



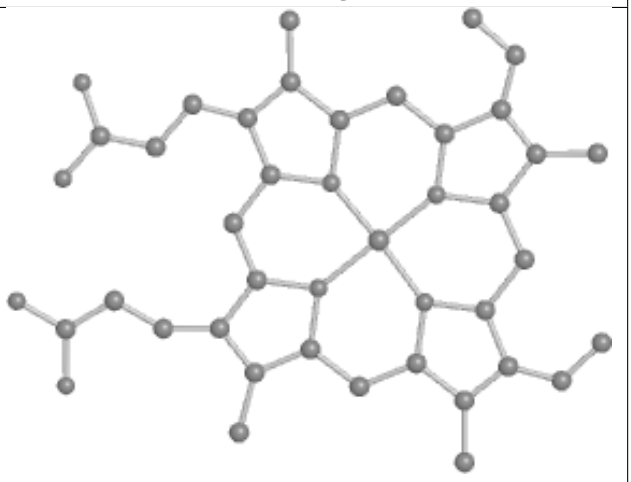
Bond lengths



Bond angles

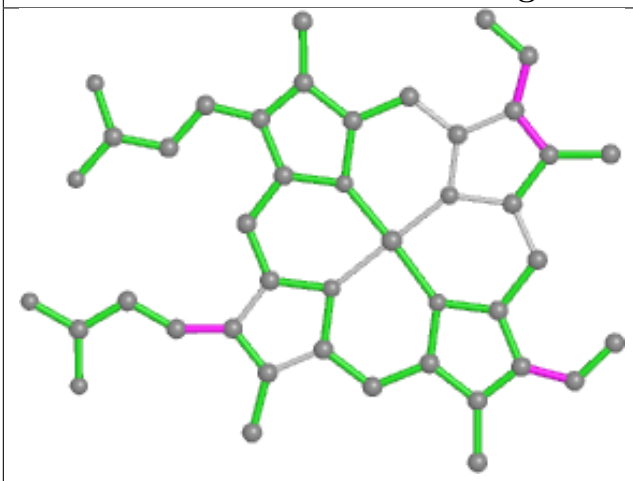


Torsions

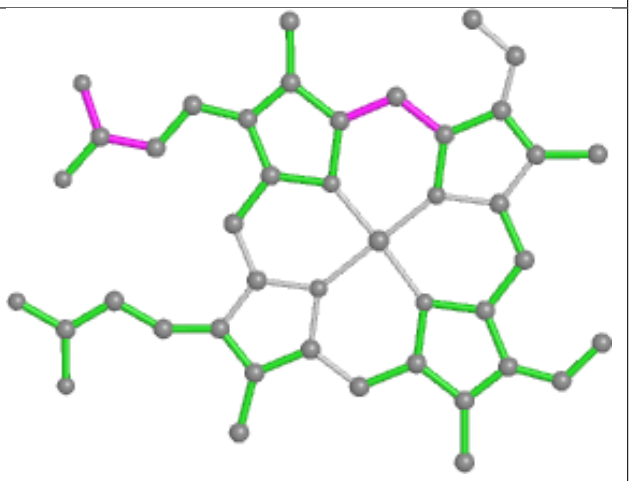


Rings

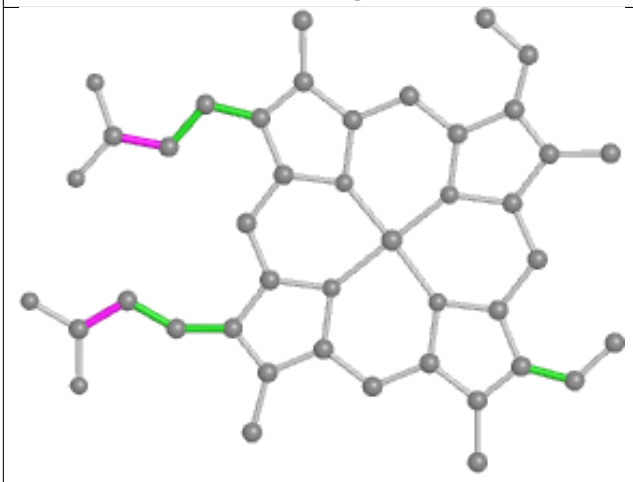
Ligand HEM D 600



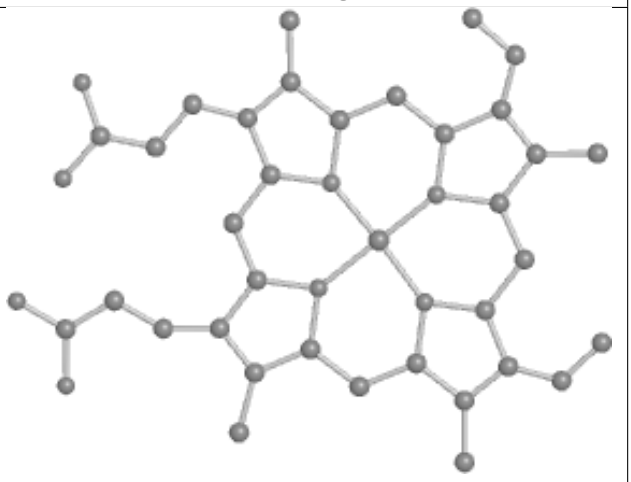
Bond lengths



Bond angles

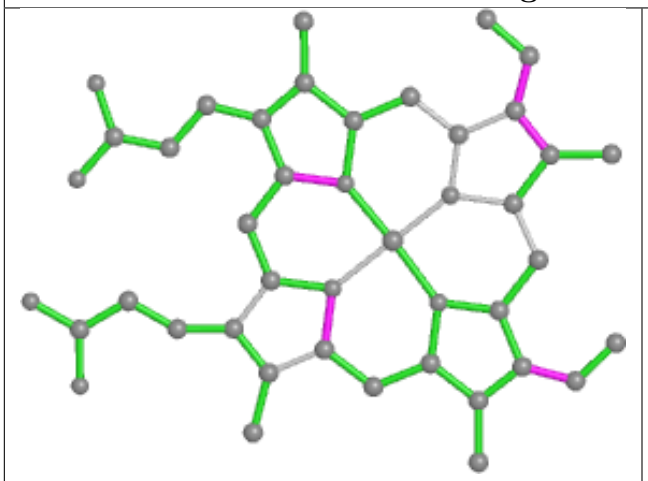


Torsions

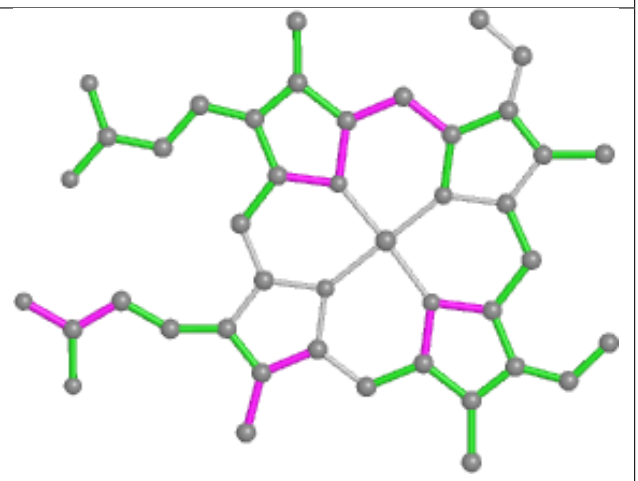


Rings

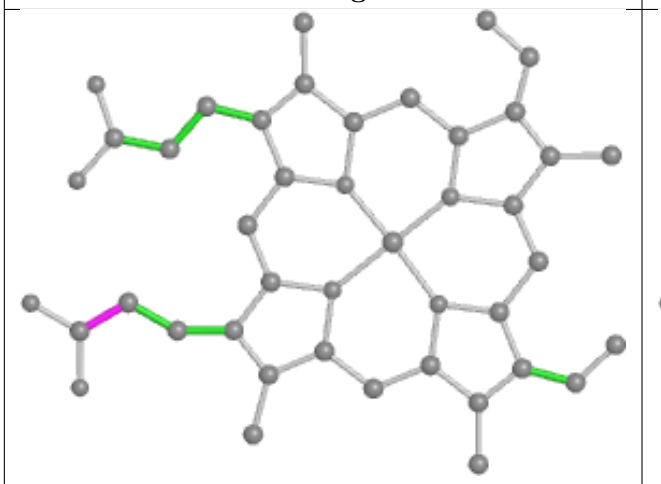
Ligand HEM B 600



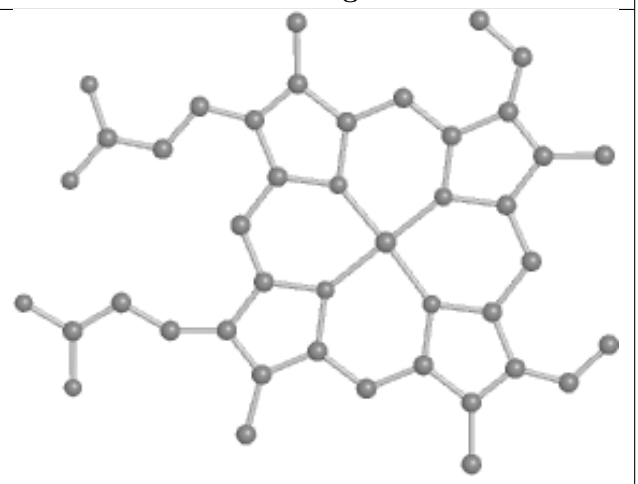
Bond lengths



Bond angles



Torsions



Rings

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	484/484 (100%)	-0.52	3 (0%)	89	87	5, 12, 24, 39	0
1	B	483/484 (99%)	-0.07	6 (1%)	79	76	5, 20, 34, 51	0
1	C	483/484 (99%)	-0.16	8 (1%)	70	66	8, 20, 33, 47	0
1	D	484/484 (100%)	-0.56	3 (0%)	89	87	4, 11, 23, 43	0
All	All	1934/1936 (99%)	-0.33	20 (1%)	82	80	4, 15, 31, 51	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	ASP	3.9
1	A	510	ASP	3.7
1	C	510	ASP	3.4
1	D	510	ASP	3.2
1	D	307	ASP	3.1
1	B	466	ASP	3.0
1	B	506	ALA	3.0
1	C	466	ASP	2.9
1	B	307	ASP	2.9
1	C	289	GLU	2.7
1	B	289	GLU	2.5
1	C	497	ASP	2.5
1	D	27	THR	2.3
1	B	509	LYS	2.3
1	A	395	HIS	2.1
1	C	254	GLN	2.1
1	C	250	LYS	2.1
1	C	307	ASP	2.0
1	C	122[A]	ASN	2.0
1	A	414	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

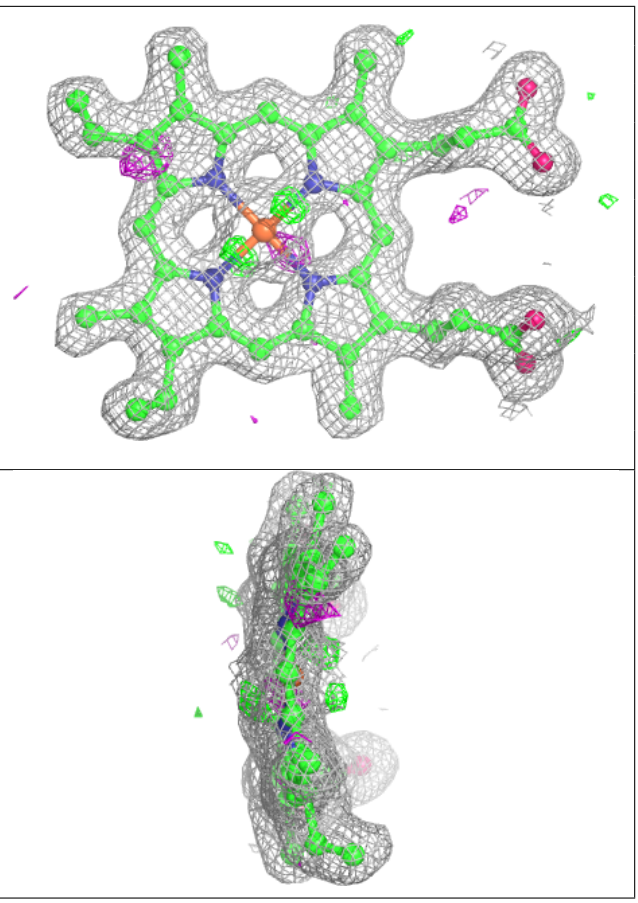
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	600	43/43	0.97	0.08	9,14,17,19	0
2	HEM	C	600	43/43	0.97	0.07	8,14,18,20	0
2	HEM	A	600	43/43	0.98	0.07	4,7,12,14	0
2	HEM	D	600	43/43	0.98	0.07	3,7,12,15	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.

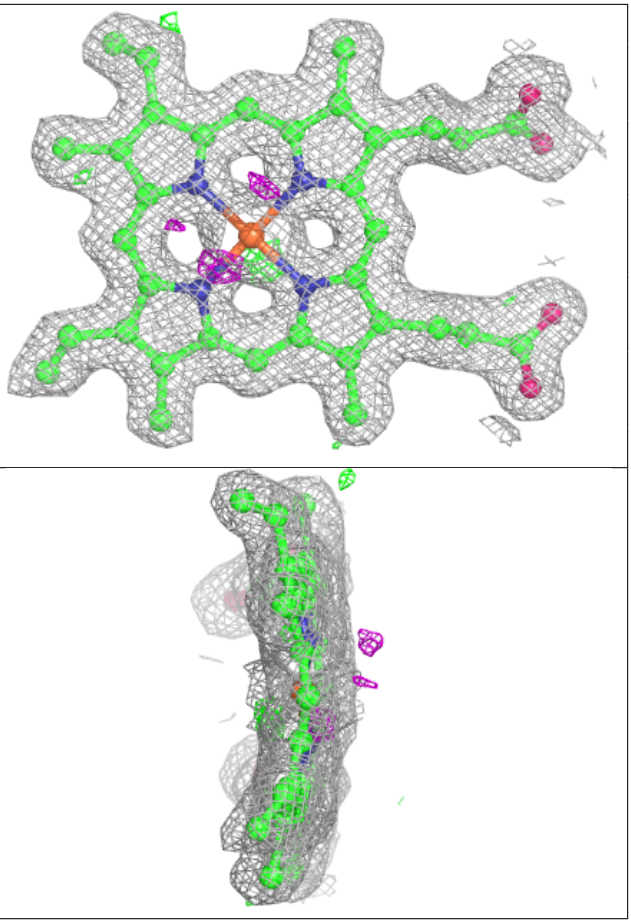
Electron density around HEM B 600:

$2mF_o$-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 600:

$2mF_o$-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 600:

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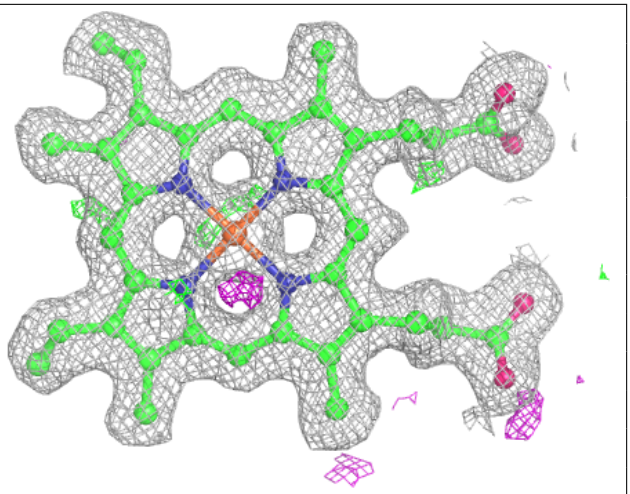
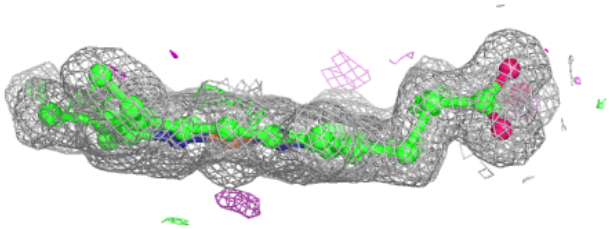
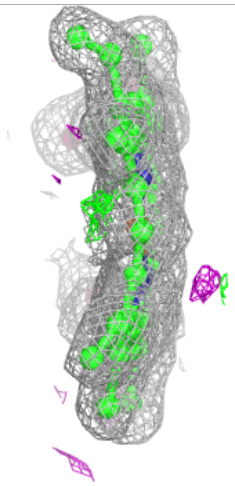
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM D 600:

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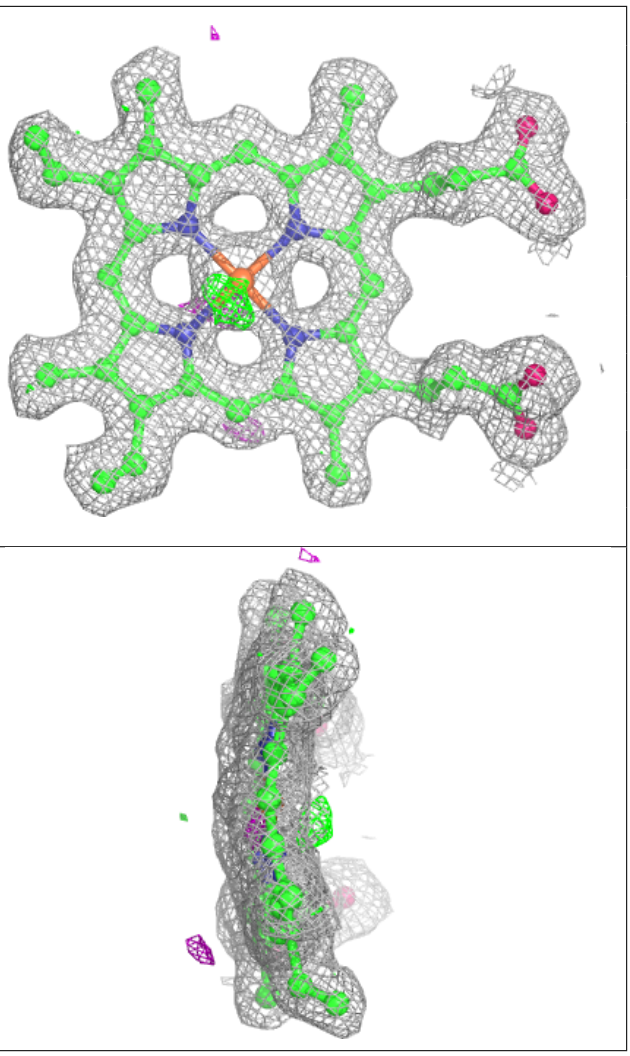
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.