Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:32 AM JST

PDB ID	:	7WCA
Title	:	CATPO mutant - E484A
Authors	:	Yuzugullu Karakus, Y.; Balci Unver, S.; Zengin Karatas, M.; Goc, G.; Pearson, A.R.; Yorke, B.
Deposited on	:	2021-12-18
Resolution	:	1.78 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 ⓘ 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 ⓘ) were used in the production of this report:

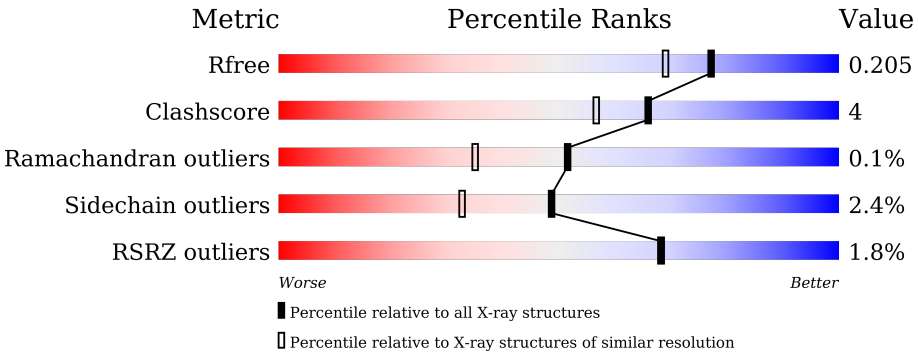
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	720	2% 85% 8% • 6%
1	B	720	3% 86% 7% • 6%
1	C	720	% 84% 8% • 6%
1	D	720	% 87% 6% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23643 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
1	A	678	Total	C	N	O	S	0	3	0
			5299	3345	929	1014	11			
1	B	679	Total	C	N	O	S	0	4	0
			5318	3355	936	1016	11			
1	C	677	Total	C	N	O	S	0	5	0
			5314	3352	934	1017	11			
1	D	677	Total	C	N	O	S	0	4	0
			5300	3346	931	1012	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP M4GGR7
A	-20	GLY	-	expression tag	UNP M4GGR7
A	-19	SER	-	expression tag	UNP M4GGR7
A	-18	SER	-	expression tag	UNP M4GGR7
A	-17	HIS	-	expression tag	UNP M4GGR7
A	-16	HIS	-	expression tag	UNP M4GGR7
A	-15	HIS	-	expression tag	UNP M4GGR7
A	-14	HIS	-	expression tag	UNP M4GGR7
A	-13	HIS	-	expression tag	UNP M4GGR7
A	-12	HIS	-	expression tag	UNP M4GGR7
A	-11	SER	-	expression tag	UNP M4GGR7
A	-10	SER	-	expression tag	UNP M4GGR7
A	-9	GLY	-	expression tag	UNP M4GGR7
A	-8	GLU	-	expression tag	UNP M4GGR7
A	-7	ASN	-	expression tag	UNP M4GGR7
A	-6	LEU	-	expression tag	UNP M4GGR7
A	-5	TYR	-	expression tag	UNP M4GGR7
A	-4	PHE	-	expression tag	UNP M4GGR7
A	-3	GLN	-	expression tag	UNP M4GGR7
A	-2	GLY	-	expression tag	UNP M4GGR7
A	-1	HIS	-	expression tag	UNP M4GGR7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	engineered mutation	UNP M4GGR7
B	-21	MET	-	initiating methionine	UNP M4GGR7
B	-20	GLY	-	expression tag	UNP M4GGR7
B	-19	SER	-	expression tag	UNP M4GGR7
B	-18	SER	-	expression tag	UNP M4GGR7
B	-17	HIS	-	expression tag	UNP M4GGR7
B	-16	HIS	-	expression tag	UNP M4GGR7
B	-15	HIS	-	expression tag	UNP M4GGR7
B	-14	HIS	-	expression tag	UNP M4GGR7
B	-13	HIS	-	expression tag	UNP M4GGR7
B	-12	HIS	-	expression tag	UNP M4GGR7
B	-11	SER	-	expression tag	UNP M4GGR7
B	-10	SER	-	expression tag	UNP M4GGR7
B	-9	GLY	-	expression tag	UNP M4GGR7
B	-8	GLU	-	expression tag	UNP M4GGR7
B	-7	ASN	-	expression tag	UNP M4GGR7
B	-6	LEU	-	expression tag	UNP M4GGR7
B	-5	TYR	-	expression tag	UNP M4GGR7
B	-4	PHE	-	expression tag	UNP M4GGR7
B	-3	GLN	-	expression tag	UNP M4GGR7
B	-2	GLY	-	expression tag	UNP M4GGR7
B	-1	HIS	-	expression tag	UNP M4GGR7
B	484	ALA	GLU	engineered mutation	UNP M4GGR7
C	-21	MET	-	initiating methionine	UNP M4GGR7
C	-20	GLY	-	expression tag	UNP M4GGR7
C	-19	SER	-	expression tag	UNP M4GGR7
C	-18	SER	-	expression tag	UNP M4GGR7
C	-17	HIS	-	expression tag	UNP M4GGR7
C	-16	HIS	-	expression tag	UNP M4GGR7
C	-15	HIS	-	expression tag	UNP M4GGR7
C	-14	HIS	-	expression tag	UNP M4GGR7
C	-13	HIS	-	expression tag	UNP M4GGR7
C	-12	HIS	-	expression tag	UNP M4GGR7
C	-11	SER	-	expression tag	UNP M4GGR7
C	-10	SER	-	expression tag	UNP M4GGR7
C	-9	GLY	-	expression tag	UNP M4GGR7
C	-8	GLU	-	expression tag	UNP M4GGR7
C	-7	ASN	-	expression tag	UNP M4GGR7
C	-6	LEU	-	expression tag	UNP M4GGR7
C	-5	TYR	-	expression tag	UNP M4GGR7
C	-4	PHE	-	expression tag	UNP M4GGR7
C	-3	GLN	-	expression tag	UNP M4GGR7

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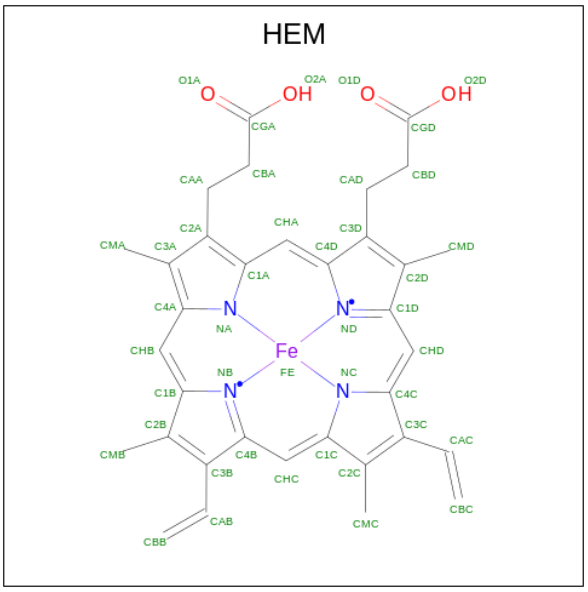
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP M4GGR7
C	-1	HIS	-	expression tag	UNP M4GGR7
C	484	ALA	GLU	engineered mutation	UNP M4GGR7
D	-21	MET	-	initiating methionine	UNP M4GGR7
D	-20	GLY	-	expression tag	UNP M4GGR7
D	-19	SER	-	expression tag	UNP M4GGR7
D	-18	SER	-	expression tag	UNP M4GGR7
D	-17	HIS	-	expression tag	UNP M4GGR7
D	-16	HIS	-	expression tag	UNP M4GGR7
D	-15	HIS	-	expression tag	UNP M4GGR7
D	-14	HIS	-	expression tag	UNP M4GGR7
D	-13	HIS	-	expression tag	UNP M4GGR7
D	-12	HIS	-	expression tag	UNP M4GGR7
D	-11	SER	-	expression tag	UNP M4GGR7
D	-10	SER	-	expression tag	UNP M4GGR7
D	-9	GLY	-	expression tag	UNP M4GGR7
D	-8	GLU	-	expression tag	UNP M4GGR7
D	-7	ASN	-	expression tag	UNP M4GGR7
D	-6	LEU	-	expression tag	UNP M4GGR7
D	-5	TYR	-	expression tag	UNP M4GGR7
D	-4	PHE	-	expression tag	UNP M4GGR7
D	-3	GLN	-	expression tag	UNP M4GGR7
D	-2	GLY	-	expression tag	UNP M4GGR7
D	-1	HIS	-	expression tag	UNP M4GGR7
D	484	ALA	GLU	engineered mutation	UNP M4GGR7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

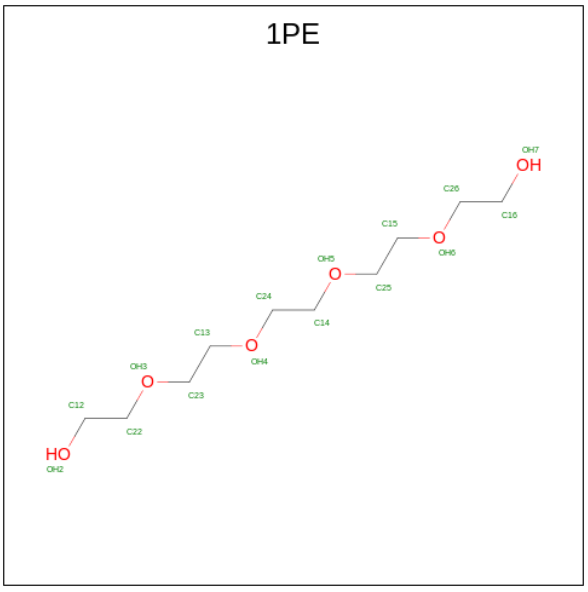
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Ca 4 4	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 10 6	0	0
4	A	1	Total C O 16 10 6	0	0
4	A	1	Total C O 16 10 6	0	0
4	A	1	Total C O 16 10 6	0	0
4	A	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0
4	B	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0
4	C	1	Total C O 16 10 6	0	0
4	D	1	Total C O 16 10 6	0	0
4	D	1	Total C O 16 10 6	0	0
4	D	1	Total C O 16 10 6	0	0
4	D	1	Total C O 16 10 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 16 10 6	0	0
4	D	1	Total C O 16 10 6	0	0

- Molecule 5 is water.

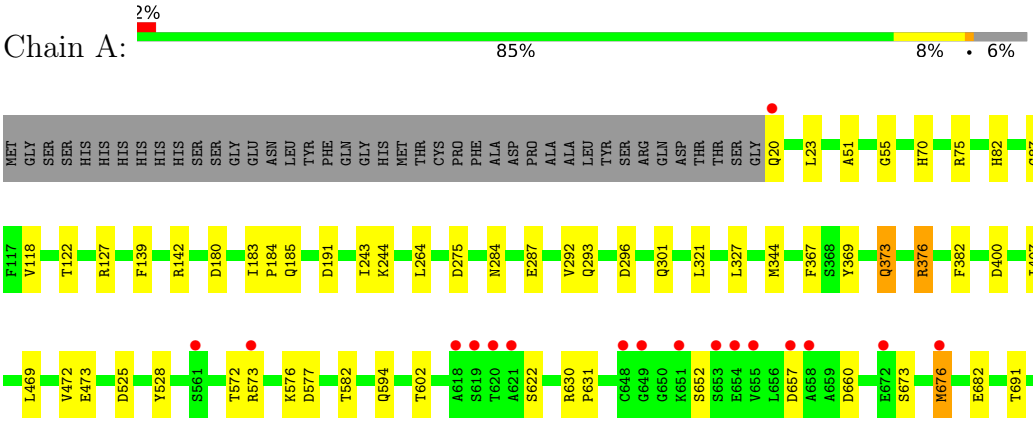
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	450	Total O 450 450	0	0
5	B	462	Total O 462 462	0	0
5	C	471	Total O 471 471	0	0
5	D	463	Total O 463 463	0	0

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.

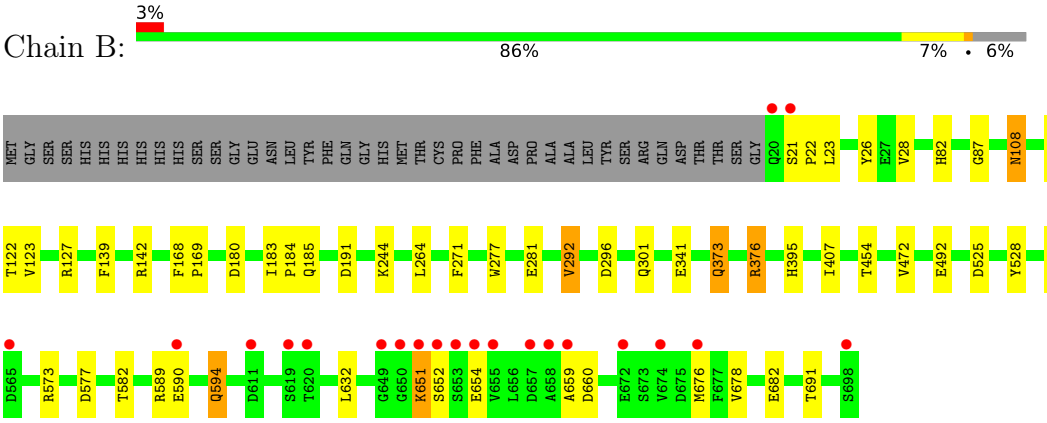
• Molecule 1: Catalase

Chain A:



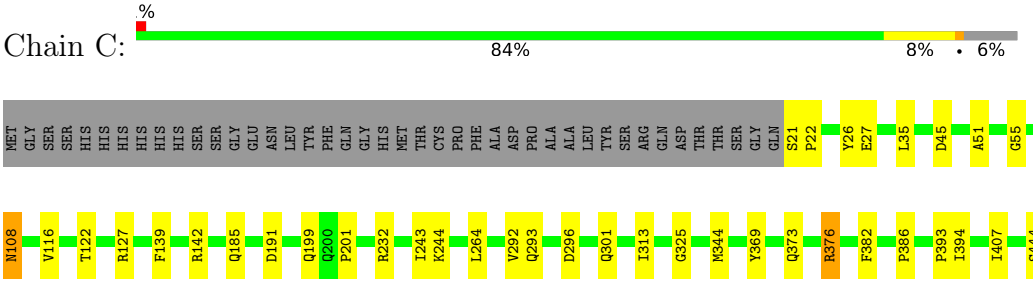
• Molecule 1: Catalase

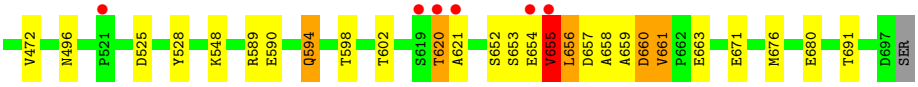
Chain B:



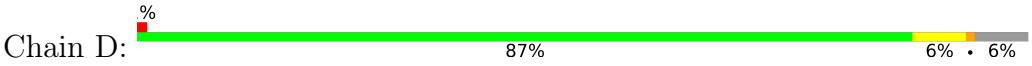
• Molecule 1: Catalase

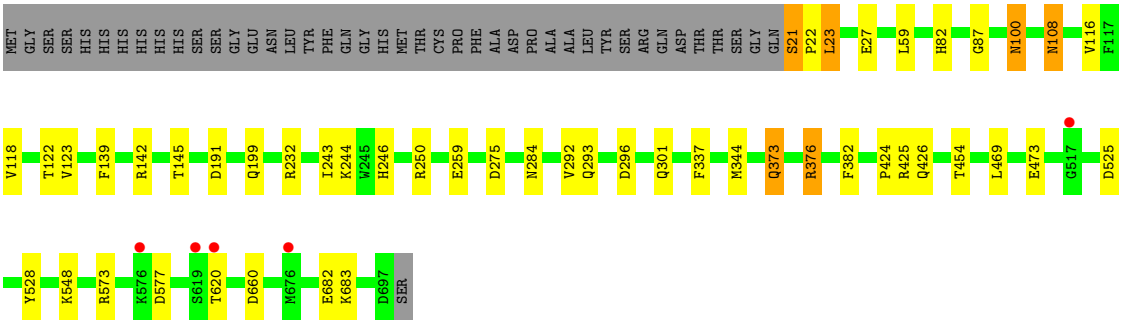
Chain C:





• Molecule 1: Catalase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.79Å 120.20Å 184.08Å 90.00° 101.72° 90.00°	Depositor
Resolution (Å)	46.43 – 1.78 46.38 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.43-1.78) 98.8 (46.38-1.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.162 , 0.202 0.171 , 0.205	Depositor DCC
R_{free} test set	12365 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23643	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9061e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, CA, 1PE

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	0.70	0/5437	0.85	4/7393 (0.1%)
1	B	0.70	0/5459	0.83	2/7420 (0.0%)
1	C	0.71	0/5449	0.87	3/7409 (0.0%)
1	D	0.71	0/5441	0.86	3/7398 (0.0%)
All	All	0.71	0/21786	0.85	12/29620 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	376	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	697	ASP	CA-C-O	-6.89	105.63	120.10
1	A	425	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	C	232	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	376	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	376	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	75	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	232	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	376	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	232	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	376	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	259	GLU	CB-CA-C	-5.05	100.29	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	292	VAL	Peptide
1	C	653	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5299	0	5082	36	0
1	B	5318	0	5109	39	0
1	C	5314	0	5092	58	0
1	D	5300	0	5091	38	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	2	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
4	A	80	0	110	3	0
4	B	96	0	132	5	0
4	C	112	0	154	17	0
4	D	96	0	132	5	0
5	A	450	0	0	4	0
5	B	462	0	0	5	0
5	C	471	0	0	8	0
5	D	463	0	0	5	0
All	All	23643	0	21022	171	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 4.

All (171) 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:C:659:ALA:C	1:C:660[A]:ASP:OD1	1.70	1.27
1:B:127[B]:ARG:NH2	5:B:801:HOH:O	1.59	1.26
1:C:127[A]:ARG:NH2	5:C:801:HOH:O	1.59	1.23
1:C:660[A]:ASP:OD1	1:C:660[A]:ASP:N	1.79	1.13
1:B:127[B]:ARG:O	5:B:802:HOH:O	1.67	1.10
1:C:676:MET:HG3	5:C:1244:HOH:O	1.50	1.09
1:C:313:ILE:H	1:C:461:GLN:HE22	1.24	0.82
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.48	0.78
1:D:373:GLN:HE21	1:D:373:GLN:HA	1.51	0.74
1:D:301:GLN:NE2	1:D:454:THR:HG21	2.06	0.69
4:C:710:1PE:H151	4:C:710:1PE:H241	1.75	0.68
1:C:373:GLN:HE21	1:C:373:GLN:HA	1.56	0.68
1:C:376:ARG:NH1	3:C:703:HEM:O1D	2.27	0.68
1:C:393:PRO:HB3	4:C:708:1PE:H261	1.77	0.66
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.60	0.66
1:B:531:ASN:ND2	4:B:707:1PE:H132	2.11	0.66
1:C:199:GLN:HE22	4:C:710:1PE:H151	1.61	0.66
4:C:707:1PE:H142	1:D:199:GLN:OE1	1.96	0.66
1:C:655:VAL:O	1:C:659:ALA:HB2	1.96	0.65
1:B:531:ASN:HD22	4:B:707:1PE:C13	2.10	0.65
1:C:658:ALA:O	1:C:660[A]:ASP:N	2.30	0.64
4:C:707:1PE:C26	1:D:199:GLN:HE22	2.13	0.62
1:B:531:ASN:ND2	4:B:707:1PE:C13	2.63	0.61
1:A:20:GLN:HB3	1:A:23:LEU:HD12	1.82	0.60
4:C:707:1PE:H261	1:D:199:GLN:HE22	1.67	0.60
1:B:185:GLN:HG3	5:B:1171:HOH:O	2.01	0.59
1:B:651:LYS:O	1:B:654:GLU:HB3	2.04	0.58
1:C:655:VAL:HA	1:C:658:ALA:HB3	1.86	0.57
1:C:264:LEU:HD13	1:C:602:THR:HB	1.86	0.57
1:D:469:LEU:HB3	1:D:473:GLU:HB3	1.87	0.57
1:B:127[B]:ARG:NH1	5:B:804:HOH:O	2.36	0.57
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.20	0.57
1:A:127[B]:ARG:NH1	5:A:803:HOH:O	2.37	0.57
1:D:82:HIS:CE1	1:D:123:VAL:HG22	2.41	0.56
1:D:301:GLN:HE21	1:D:454:THR:HG21	1.70	0.56
1:B:573:ARG:HG3	1:B:678:VAL:HG11	1.88	0.56
1:B:531:ASN:HD22	4:B:707:1PE:H131	1.71	0.56
1:C:21:SER:N	1:C:22:PRO:HD2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:GLN:NE2	1:C:454:THR:HG21	2.21	0.56
1:D:284:ASN:HD21	4:D:708:1PE:H232	1.70	0.55
4:A:708:1PE:H122	1:B:180:ASP:HB3	1.87	0.55
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.41	0.55
1:D:250:ARG:NH1	5:D:802:HOH:O	2.21	0.55
1:D:246:HIS:HD2	5:D:1146:HOH:O	1.89	0.54
1:C:373:GLN:HA	1:C:373:GLN:NE2	2.23	0.54
1:D:22:PRO:HD2	5:D:829:HOH:O	2.07	0.54
1:D:244:LYS:O	1:D:292:VAL:HA	2.08	0.54
1:C:185:GLN:HG3	5:C:1162:HOH:O	2.08	0.54
1:D:548:LYS:HZ3	4:D:708:1PE:H231	1.72	0.54
1:B:244:LYS:O	1:B:292:VAL:HA	2.08	0.53
1:B:582:THR:HG21	1:B:594:GLN:HE21	1.73	0.53
1:D:373:GLN:HA	1:D:373:GLN:NE2	2.20	0.53
1:B:472:VAL:HG11	1:B:691:THR:HB	1.91	0.53
1:C:657:ASP:O	1:C:661:VAL:N	2.40	0.52
1:D:525:ASP:HA	1:D:528:TYR:CD2	2.44	0.52
1:C:116:VAL:HA	1:C:142:ARG:O	2.10	0.52
1:C:472:VAL:HG11	1:C:691:THR:HB	1.91	0.52
4:C:705:1PE:H261	5:C:974:HOH:O	2.09	0.52
1:D:100:ASN:H	1:D:100:ASN:HD22	1.58	0.51
1:A:572:THR:HG22	5:A:1207:HOH:O	2.11	0.51
1:C:127[A]:ARG:CZ	5:C:801:HOH:O	2.26	0.51
1:A:577:ASP:OD2	1:A:682:GLU:OE2	2.29	0.51
4:C:707:1PE:C14	1:D:199:GLN:OE1	2.59	0.50
1:C:658:ALA:C	1:C:660[A]:ASP:H	2.15	0.50
1:A:573:ARG:HD2	1:A:576:LYS:HE3	1.94	0.50
5:A:1166:HOH:O	1:D:424:PRO:HG3	2.12	0.50
1:B:301:GLN:NE2	1:B:454:THR:HG21	2.26	0.50
1:A:369:TYR:O	1:A:373:GLN:HG2	2.11	0.49
1:D:577:ASP:OD2	1:D:682:GLU:OE2	2.30	0.49
1:C:676:MET:CE	1:C:680:GLU:OE2	2.60	0.49
1:C:21:SER:N	1:C:22:PRO:CD	2.76	0.49
1:C:656:LEU:HB2	5:C:1090:HOH:O	2.13	0.48
1:D:108:ASN:HD22	1:D:108:ASN:C	2.15	0.48
1:C:51:ALA:O	1:C:55:GLY:HA3	2.13	0.48
1:C:108:ASN:C	1:C:108:ASN:HD22	2.16	0.48
1:C:496:ASN:CG	4:C:710:1PE:H152	2.34	0.48
1:B:632:LEU:HD11	1:B:659:ALA:HA	1.96	0.48
1:C:243:ILE:HA	1:C:293:GLN:O	2.14	0.48
1:D:376:ARG:NH1	3:D:703:HEM:O2D	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:THR:HG21	1:A:594:GLN:HE21	1.79	0.47
1:B:82:HIS:HA	1:B:122:THR:O	2.14	0.47
1:C:199:GLN:HE22	4:C:710:1PE:C15	2.25	0.47
1:A:344:MET:HG2	1:A:373:GLN:NE2	2.29	0.47
1:C:658:ALA:C	1:C:660[A]:ASP:N	2.67	0.47
1:D:284:ASN:ND2	4:D:708:1PE:H232	2.29	0.47
1:B:127[B]:ARG:CZ	5:B:801:HOH:O	2.34	0.46
1:A:264:LEU:HD13	1:A:602:THR:HB	1.97	0.46
1:B:277:TRP:CZ3	1:B:281:GLU:HG3	2.51	0.46
1:C:654:GLU:C	1:C:656:LEU:N	2.67	0.46
1:D:21:SER:N	1:D:22:PRO:HD2	2.29	0.46
1:B:301:GLN:HE21	1:B:454:THR:HG21	1.80	0.46
1:C:82:HIS:HA	1:C:122:THR:O	2.15	0.46
1:C:676:MET:HE1	1:C:680:GLU:OE2	2.15	0.46
1:D:243:ILE:HA	1:D:293:GLN:O	2.15	0.46
1:B:341:GLU:O	1:B:376:ARG:NH2	2.49	0.46
1:A:407:ILE:HD12	1:D:23:LEU:HB3	1.98	0.46
1:C:127[A]:ARG:NH1	5:C:816:HOH:O	2.49	0.46
1:A:108:ASN:C	1:A:108:ASN:HD22	2.20	0.45
1:A:244:LYS:O	1:A:292:VAL:HA	2.17	0.45
1:A:301:GLN:NE2	1:A:454:THR:HG21	2.32	0.45
1:C:301:GLN:HE21	1:C:454:THR:HG21	1.80	0.45
1:C:369:TYR:O	1:C:373:GLN:HG2	2.16	0.45
1:A:284:ASN:ND2	4:A:706:1PE:OH4	2.49	0.45
1:B:277:TRP:CH2	1:B:281:GLU:HG3	2.52	0.45
1:C:313:ILE:N	1:C:461:GLN:HE22	2.04	0.45
1:A:243:ILE:HA	1:A:293:GLN:O	2.17	0.45
1:D:373:GLN:NE2	1:D:373:GLN:CA	2.80	0.45
1:D:426:GLN:HG2	5:D:1064:HOH:O	2.16	0.45
1:C:671:GLU:OE2	1:C:680:GLU:OE2	2.34	0.45
4:C:708:1PE:H161	5:C:810:HOH:O	2.16	0.45
1:B:116:VAL:HA	1:B:142:ARG:O	2.17	0.45
1:C:199:GLN:HE22	4:C:710:1PE:H261	1.80	0.45
1:C:652:SER:O	1:C:656:LEU:HB3	2.18	0.44
1:B:23:LEU:HD23	1:C:407:ILE:CD1	2.47	0.44
1:A:472:VAL:HG11	1:A:691:THR:HB	2.00	0.44
1:B:108:ASN:C	1:B:108:ASN:HD22	2.21	0.44
1:C:201:PRO:HG3	4:C:710:1PE:C12	2.48	0.44
4:A:708:1PE:C12	1:B:180:ASP:HB3	2.46	0.43
1:A:673:SER:HB3	1:A:676:MET:HB2	2.01	0.43
1:D:344:MET:SD	1:D:382:PHE:HB2	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLY:HA2	1:A:118:VAL:O	2.19	0.43
1:C:658:ALA:O	1:C:660[B]:ASP:N	2.51	0.43
1:D:87:GLY:HA2	1:D:118:VAL:O	2.19	0.43
1:A:344:MET:SD	1:A:382:PHE:HB2	2.58	0.43
1:C:95:TYR:CG	1:C:325:GLY:HA2	2.54	0.43
1:C:344:MET:SD	1:C:382:PHE:HB2	2.58	0.43
1:A:51:ALA:O	1:A:55:GLY:HA3	2.19	0.43
1:A:376:ARG:HD2	3:A:705:HEM:O1D	2.19	0.43
4:D:705:1PE:H231	5:D:803:HOH:O	2.19	0.43
1:C:548:LYS:NZ	4:C:704:1PE:H262	2.34	0.42
1:B:577:ASP:OD2	1:B:682:GLU:OE2	2.37	0.42
1:C:663:GLU:O	1:C:663:GLU:HG2	2.18	0.42
1:A:180:ASP:OD2	4:B:706:1PE:H231	2.19	0.42
1:C:394:ILE:O	4:C:708:1PE:H151	2.19	0.42
3:B:703:HEM:HMC1	3:B:703:HEM:HBC2	2.02	0.42
1:D:82:HIS:HA	1:D:122:THR:O	2.20	0.42
1:C:244:LYS:O	1:C:292:VAL:HA	2.20	0.42
1:A:82:HIS:HA	1:A:122:THR:O	2.20	0.42
1:C:393:PRO:HB3	4:C:708:1PE:C26	2.48	0.42
1:D:21:SER:N	1:D:22:PRO:CD	2.83	0.42
1:A:293:GLN:HG3	1:A:321:LEU:HD23	2.01	0.42
1:A:582:THR:HG21	1:A:594:GLN:NE2	2.35	0.41
1:A:116:VAL:HA	1:A:142:ARG:O	2.20	0.41
1:A:407:ILE:O	1:D:27:GLU:HA	2.20	0.41
1:B:82:HIS:CE1	1:B:123:VAL:HG22	2.55	0.41
1:C:26:TYR:CD1	1:C:386:PRO:HG3	2.55	0.41
1:A:400:ASP:HA	1:D:337:PHE:CD2	2.55	0.41
1:A:630:ARG:HB3	1:A:631:PRO:HD3	2.03	0.41
1:A:185:GLN:HG3	5:A:1112:HOH:O	2.20	0.41
3:B:703:HEM:HBC2	3:B:703:HEM:CMC	2.51	0.41
1:D:548:LYS:NZ	4:D:708:1PE:H231	2.34	0.41
1:B:28:VAL:HG13	4:C:708:1PE:H151	2.02	0.41
1:B:183:ILE:HA	1:B:184:PRO:HA	1.80	0.41
1:B:407:ILE:O	1:C:27:GLU:HA	2.20	0.41
1:C:35:LEU:HD21	1:C:45:ASP:HB3	2.03	0.41
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.55	0.41
1:A:367:PHE:HB2	1:D:59:LEU:HD11	2.02	0.41
1:B:264:LEU:HD21	1:B:271:PHE:CD2	2.56	0.41
1:B:395:HIS:O	1:C:35:LEU:HA	2.21	0.41
1:C:656:LEU:C	1:C:656:LEU:CD1	2.89	0.41
3:D:703:HEM:HBC2	3:D:703:HEM:HMC1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PRO:O	1:B:26:TYR:HD2	2.04	0.40
1:D:344:MET:HG2	1:D:373:GLN:NE2	2.36	0.40
1:B:168:PHE:N	1:B:169:PRO:CD	2.85	0.40
1:D:116:VAL:HA	1:D:142:ARG:O	2.21	0.40
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.55	0.40
1:A:287:GLU:HA	1:A:327:LEU:O	2.21	0.40
1:A:469:LEU:HB3	1:A:473:GLU:HB3	2.04	0.40
1:B:87:GLY:HA2	1:B:118:VAL:O	2.21	0.40
1:A:183:ILE:HA	1:A:184:PRO:HA	1.89	0.40
1:C:594:GLN:HG2	1:C:598:THR:OG1	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	679/720 (94%)	659 (97%)	19 (3%)	1 (0%)	51 35
1	B	681/720 (95%)	656 (96%)	25 (4%)	0	100 100
1	C	680/720 (94%)	654 (96%)	23 (3%)	3 (0%)	34 19
1	D	679/720 (94%)	663 (98%)	16 (2%)	0	100 100
All	All	2719/2880 (94%)	2632 (97%)	83 (3%)	4 (0%)	51 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	621	ALA
1	A	622	SER
1	C	620	THR
1	C	655	VAL

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	563/596 (94%)	552 (98%)	11 (2%)	55	40
1	B	565/596 (95%)	550 (97%)	15 (3%)	44	28
1	C	564/596 (95%)	549 (97%)	15 (3%)	44	28
1	D	563/596 (94%)	548 (97%)	15 (3%)	44	28
All	All	2255/2384 (95%)	2199 (98%)	56 (2%)	49	31

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	108	ASN
1	A	139	PHE
1	A	191	ASP
1	A	275	ASP
1	A	296	ASP
1	A	373	GLN
1	A	652	SER
1	A	657	ASP
1	A	660	ASP
1	A	676	MET
1	B	21	SER
1	B	108	ASN
1	B	139	PHE
1	B	191	ASP
1	B	296	ASP
1	B	373	GLN
1	B	492	GLU
1	B	562	SER
1	B	589	ARG
1	B	590	GLU
1	B	594	GLN
1	B	651	LYS
1	B	652	SER

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Mol	Chain	Res	Type
1	B	660	ASP
1	B	676	MET
1	C	108	ASN
1	C	139	PHE
1	C	191	ASP
1	C	296	ASP
1	C	444	SER
1	C	589[A]	ARG
1	C	589[B]	ARG
1	C	590	GLU
1	C	594	GLN
1	C	620	THR
1	C	655	VAL
1	C	656	LEU
1	C	660[A]	ASP
1	C	660[B]	ASP
1	C	661	VAL
1	D	21	SER
1	D	23	LEU
1	D	100	ASN
1	D	108	ASN
1	D	139	PHE
1	D	145	THR
1	D	191	ASP
1	D	275	ASP
1	D	296	ASP
1	D	373	GLN
1	D	425	ARG
1	D	573	ARG
1	D	620	THR
1	D	660	ASP
1	D	683	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	274	GLN
1	A	284	ASN
1	A	301	GLN
1	A	373	GLN
1	A	594	GLN

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Mol	Chain	Res	Type
1	B	20	GLN
1	B	108	ASN
1	B	301	GLN
1	B	373	GLN
1	B	531	ASN
1	B	594	GLN
1	C	108	ASN
1	C	167	GLN
1	C	199	GLN
1	C	301	GLN
1	C	373	GLN
1	C	461	GLN
1	D	100	ASN
1	D	108	ASN
1	D	199	GLN
1	D	246	HIS
1	D	284	ASN
1	D	301	GLN
1	D	373	GLN
1	D	569	GLN
1	D	594	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 10 are monoatomic - leaving 28 for Mogul analysis.

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	1PE	B	707	-	15,15,15	0.34	0	14,14,14	0.20	0
4	1PE	C	706	-	15,15,15	0.32	0	14,14,14	0.16	0
4	1PE	A	708	-	15,15,15	0.27	0	14,14,14	0.21	0
3	HEM	C	703	1	41,50,50	1.32	5 (12%)	45,82,82	2.02	17 (37%)
4	1PE	B	709	-	15,15,15	0.35	0	14,14,14	0.22	0
4	1PE	D	705	-	15,15,15	0.25	0	14,14,14	0.19	0
4	1PE	C	710	-	15,15,15	0.37	0	14,14,14	0.28	0
3	HEM	D	703	1	41,50,50	1.44	6 (14%)	45,82,82	2.11	12 (26%)
4	1PE	A	706	-	15,15,15	0.38	0	14,14,14	0.41	0
4	1PE	C	704	-	15,15,15	0.23	0	14,14,14	0.31	0
4	1PE	D	709	-	15,15,15	0.25	0	14,14,14	0.18	0
3	HEM	B	703	1	41,50,50	1.44	5 (12%)	45,82,82	1.91	9 (20%)
4	1PE	B	706	-	15,15,15	0.24	0	14,14,14	0.22	0
4	1PE	B	705	-	15,15,15	0.37	0	14,14,14	0.24	0
4	1PE	C	709	-	15,15,15	0.23	0	14,14,14	0.19	0
4	1PE	A	709	-	15,15,15	0.26	0	14,14,14	0.13	0
4	1PE	C	705	-	15,15,15	0.25	0	14,14,14	0.32	0
3	HEM	A	705	1	41,50,50	1.53	8 (19%)	45,82,82	1.96	12 (26%)
4	1PE	B	704	-	15,15,15	0.23	0	14,14,14	0.10	0
4	1PE	B	708	-	15,15,15	0.25	0	14,14,14	0.17	0
4	1PE	A	710	-	15,15,15	0.19	0	14,14,14	0.16	0
4	1PE	D	707	-	15,15,15	0.41	0	14,14,14	0.21	0
4	1PE	D	706	-	15,15,15	0.40	0	14,14,14	0.29	0
4	1PE	C	707	-	15,15,15	0.37	0	14,14,14	0.32	0
4	1PE	C	708	-	15,15,15	0.34	0	14,14,14	0.36	0
4	1PE	D	704	-	15,15,15	0.30	0	14,14,14	0.10	0
4	1PE	D	708	-	15,15,15	0.29	0	14,14,14	0.29	0
4	1PE	A	707	-	15,15,15	0.20	0	14,14,14	0.21	0

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	1PE	B	707	-	-	9/13/13/13	-
4	1PE	C	706	-	-	5/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	A	708	-	-	4/13/13/13	-
3	HEM	C	703	1	-	3/12/54/54	-
4	1PE	B	709	-	-	10/13/13/13	-
4	1PE	D	705	-	-	4/13/13/13	-
4	1PE	C	710	-	-	8/13/13/13	-
3	HEM	D	703	1	-	2/12/54/54	-
4	1PE	A	706	-	-	10/13/13/13	-
4	1PE	C	704	-	-	9/13/13/13	-
4	1PE	D	709	-	-	9/13/13/13	-
3	HEM	B	703	1	-	2/12/54/54	-
4	1PE	B	706	-	-	8/13/13/13	-
4	1PE	B	705	-	-	6/13/13/13	-
4	1PE	C	709	-	-	6/13/13/13	-
4	1PE	A	709	-	-	6/13/13/13	-
4	1PE	C	705	-	-	8/13/13/13	-
3	HEM	A	705	1	-	2/12/54/54	-
4	1PE	B	704	-	-	2/13/13/13	-
4	1PE	B	708	-	-	5/13/13/13	-
4	1PE	A	710	-	-	6/13/13/13	-
4	1PE	D	707	-	-	8/13/13/13	-
4	1PE	D	706	-	-	5/13/13/13	-
4	1PE	C	707	-	-	8/13/13/13	-
4	1PE	C	708	-	-	9/13/13/13	-
4	1PE	D	704	-	-	7/13/13/13	-
4	1PE	D	708	-	-	5/13/13/13	-
4	1PE	A	707	-	-	7/13/13/13	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	HEM	C1B-NB	-4.41	1.32	1.40
3	C	703	HEM	C1B-NB	-4.35	1.32	1.40
3	D	703	HEM	C1B-NB	-4.30	1.32	1.40
3	A	705	HEM	C1B-NB	-3.53	1.34	1.40
3	A	705	HEM	C4B-NB	-3.03	1.32	1.38
3	B	703	HEM	FE-NB	2.90	2.11	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	HEM	FE-NB	2.90	2.11	1.96
3	D	703	HEM	C4D-ND	-2.87	1.35	1.40
3	D	703	HEM	C4B-NB	-2.83	1.33	1.38
3	A	705	HEM	O1D-CGD	2.74	1.31	1.22
3	C	703	HEM	FE-NB	2.65	2.10	1.96
3	B	703	HEM	O1D-CGD	2.60	1.30	1.22
3	B	703	HEM	C3C-C2C	-2.59	1.36	1.40
3	A	705	HEM	FE-NB	2.51	2.09	1.96
3	C	703	HEM	CHB-C1B	2.50	1.41	1.35
3	A	705	HEM	C1D-ND	-2.35	1.34	1.38
3	D	703	HEM	O1D-CGD	2.32	1.29	1.22
3	A	705	HEM	CAA-C2A	2.29	1.55	1.52
3	C	703	HEM	C4D-C3D	2.27	1.48	1.45
3	A	705	HEM	C3C-C2C	-2.20	1.37	1.40
3	C	703	HEM	CBD-CAD	2.16	1.58	1.52
3	D	703	HEM	C4D-C3D	2.15	1.48	1.45
3	B	703	HEM	CHA-C4D	2.15	1.40	1.35
3	A	705	HEM	C1B-C2B	-2.14	1.40	1.44

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	703	HEM	CBD-CAD-C3D	-6.24	95.28	112.63
3	A	705	HEM	C1B-NB-C4B	5.91	111.18	105.07
3	C	703	HEM	CBD-CAD-C3D	-5.85	96.37	112.63
3	D	703	HEM	C1B-NB-C4B	5.78	111.05	105.07
3	B	703	HEM	CBD-CAD-C3D	-5.76	96.63	112.63
3	A	705	HEM	CBD-CAD-C3D	-5.69	96.81	112.63
3	D	703	HEM	CHC-C4B-NB	5.37	130.27	124.43
3	B	703	HEM	CHC-C4B-NB	4.94	129.80	124.43
3	B	703	HEM	C1B-NB-C4B	4.17	109.38	105.07
3	A	705	HEM	CHC-C4B-NB	4.04	128.82	124.43
3	C	703	HEM	CHC-C4B-NB	4.02	128.79	124.43
3	B	703	HEM	CHA-C4D-ND	3.68	128.92	124.38
3	A	705	HEM	CHA-C4D-ND	3.53	128.74	124.38
3	D	703	HEM	CHA-C4D-ND	3.53	128.74	124.38
3	C	703	HEM	C1B-NB-C4B	3.40	108.59	105.07
3	B	703	HEM	CMD-C2D-C1D	3.34	130.13	125.04
3	A	705	HEM	CMD-C2D-C1D	3.20	129.91	125.04
3	C	703	HEM	CAD-CBD-CGD	-2.99	107.16	113.60
3	C	703	HEM	CMA-C3A-C4A	-2.85	124.08	128.46
3	C	703	HEM	O2A-CGA-O1A	-2.70	116.58	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	703	HEM	CHA-C4D-C3D	-2.69	120.27	125.33
3	C	703	HEM	C4B-C3B-C2B	-2.69	104.98	107.11
3	A	705	HEM	CHA-C4D-C3D	-2.66	120.33	125.33
3	C	703	HEM	O2D-CGD-O1D	-2.63	116.76	123.30
3	C	703	HEM	O2A-CGA-CBA	2.60	122.39	114.03
3	D	703	HEM	CAD-CBD-CGD	-2.59	108.02	113.60
3	B	703	HEM	CHD-C1D-ND	2.58	127.23	124.43
3	C	703	HEM	C2D-C1D-ND	2.55	112.94	109.88
3	D	703	HEM	CMC-C2C-C3C	2.50	129.35	124.68
3	A	705	HEM	CHD-C1D-C2D	-2.48	121.10	124.98
3	D	703	HEM	CAA-CBA-CGA	-2.45	106.89	113.76
3	C	703	HEM	C4B-CHC-C1C	2.45	125.79	122.56
3	D	703	HEM	C1D-C2D-C3D	-2.42	104.41	106.96
3	D	703	HEM	O2D-CGD-O1D	-2.40	117.31	123.30
3	B	703	HEM	CAD-CBD-CGD	-2.38	108.48	113.60
3	C	703	HEM	O2D-CGD-CBD	2.34	121.54	114.03
3	C	703	HEM	CMC-C2C-C3C	2.33	129.05	124.68
3	C	703	HEM	CAA-CBA-CGA	-2.33	107.22	113.76
3	A	705	HEM	CHD-C1D-ND	2.27	126.90	124.43
3	A	705	HEM	CMC-C2C-C3C	2.27	128.92	124.68
3	C	703	HEM	CHA-C4D-ND	2.27	127.18	124.38
3	A	705	HEM	CAA-CBA-CGA	-2.22	107.53	113.76
3	B	703	HEM	CAA-CBA-CGA	-2.10	107.86	113.76
3	D	703	HEM	CHA-C4D-C3D	-2.08	121.42	125.33
3	D	703	HEM	O2D-CGD-CBD	2.06	120.66	114.03
3	D	703	HEM	CHD-C1D-C2D	-2.05	121.78	124.98
3	A	705	HEM	CHB-C1B-NB	2.03	126.89	124.38
3	B	703	HEM	CHA-C4D-C3D	-2.03	121.52	125.33
3	A	705	HEM	C4B-CHC-C1C	2.02	125.23	122.56
3	C	703	HEM	C3D-C4D-ND	2.01	112.40	110.17

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	706	1PE	C15-C25-OH5-C14
4	B	708	1PE	C24-C14-OH5-C25
4	B	705	1PE	OH5-C14-C24-OH4
4	C	704	1PE	OH6-C15-C25-OH5
4	C	708	1PE	OH6-C15-C25-OH5
4	C	710	1PE	OH6-C15-C25-OH5
4	A	706	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
4	B	705	1PE	OH4-C13-C23-OH3
4	B	706	1PE	OH6-C15-C25-OH5
4	C	704	1PE	OH4-C13-C23-OH3
4	C	705	1PE	OH6-C15-C25-OH5
4	A	706	1PE	C16-C26-OH6-C15
4	B	705	1PE	OH6-C15-C25-OH5
4	A	709	1PE	OH5-C14-C24-OH4
4	A	709	1PE	OH4-C13-C23-OH3
4	B	704	1PE	OH6-C15-C25-OH5
4	D	704	1PE	OH6-C15-C25-OH5
4	D	709	1PE	OH4-C13-C23-OH3
4	B	707	1PE	OH4-C13-C23-OH3
4	B	707	1PE	OH6-C15-C25-OH5
4	C	705	1PE	OH4-C13-C23-OH3
4	C	709	1PE	OH6-C15-C25-OH5
4	D	709	1PE	OH6-C15-C25-OH5
4	C	710	1PE	OH4-C13-C23-OH3
4	B	709	1PE	C24-C14-OH5-C25
4	A	706	1PE	OH2-C12-C22-OH3
4	A	707	1PE	OH7-C16-C26-OH6
4	C	704	1PE	OH2-C12-C22-OH3
4	C	705	1PE	OH2-C12-C22-OH3
4	D	707	1PE	OH7-C16-C26-OH6
4	D	709	1PE	OH7-C16-C26-OH6
4	B	709	1PE	OH6-C15-C25-OH5
4	C	709	1PE	OH5-C14-C24-OH4
4	D	708	1PE	OH4-C13-C23-OH3
4	D	704	1PE	OH4-C13-C23-OH3
4	A	710	1PE	OH6-C15-C25-OH5
4	B	707	1PE	OH7-C16-C26-OH6
4	C	706	1PE	OH2-C12-C22-OH3
4	C	707	1PE	OH2-C12-C22-OH3
4	C	709	1PE	OH7-C16-C26-OH6
4	D	705	1PE	OH7-C16-C26-OH6
4	B	709	1PE	OH5-C14-C24-OH4
4	C	710	1PE	C23-C13-OH4-C24
4	C	708	1PE	OH5-C14-C24-OH4
4	B	708	1PE	OH5-C14-C24-OH4
4	B	708	1PE	OH2-C12-C22-OH3
4	B	709	1PE	OH7-C16-C26-OH6
4	C	707	1PE	OH6-C15-C25-OH5
4	D	704	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
4	C	708	1PE	C12-C22-OH3-C23
4	C	710	1PE	C14-C24-OH4-C13
4	B	706	1PE	OH2-C12-C22-OH3
4	C	710	1PE	OH7-C16-C26-OH6
4	C	708	1PE	OH4-C13-C23-OH3
4	D	707	1PE	OH6-C15-C25-OH5
4	B	707	1PE	OH5-C14-C24-OH4
4	D	708	1PE	OH6-C15-C25-OH5
4	C	704	1PE	OH5-C14-C24-OH4
4	D	707	1PE	OH2-C12-C22-OH3
4	B	706	1PE	C16-C26-OH6-C15
4	A	708	1PE	OH7-C16-C26-OH6
4	A	710	1PE	OH7-C16-C26-OH6
4	B	706	1PE	OH7-C16-C26-OH6
4	B	709	1PE	OH2-C12-C22-OH3
4	C	708	1PE	OH7-C16-C26-OH6
4	C	709	1PE	OH2-C12-C22-OH3
4	D	709	1PE	OH2-C12-C22-OH3
4	A	707	1PE	OH5-C14-C24-OH4
4	D	704	1PE	C25-C15-OH6-C26
4	D	706	1PE	OH7-C16-C26-OH6
4	A	706	1PE	C25-C15-OH6-C26
4	C	710	1PE	OH5-C14-C24-OH4
4	D	707	1PE	OH4-C13-C23-OH3
4	A	706	1PE	OH7-C16-C26-OH6
4	D	708	1PE	C13-C23-OH3-C22
4	B	704	1PE	C16-C26-OH6-C15
4	D	709	1PE	C16-C26-OH6-C15
4	C	705	1PE	C12-C22-OH3-C23
4	B	709	1PE	C14-C24-OH4-C13
4	D	709	1PE	C13-C23-OH3-C22
4	C	707	1PE	C25-C15-OH6-C26
4	A	707	1PE	C14-C24-OH4-C13
4	A	709	1PE	C24-C14-OH5-C25
4	A	707	1PE	C13-C23-OH3-C22
4	A	709	1PE	C13-C23-OH3-C22
4	A	707	1PE	OH2-C12-C22-OH3
4	A	706	1PE	C12-C22-OH3-C23
4	B	707	1PE	C25-C15-OH6-C26
4	B	709	1PE	C25-C15-OH6-C26
4	C	707	1PE	C16-C26-OH6-C15
4	D	704	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
4	C	708	1PE	C14-C24-OH4-C13
4	B	706	1PE	C12-C22-OH3-C23
4	C	707	1PE	C23-C13-OH4-C24
4	C	705	1PE	OH7-C16-C26-OH6
4	C	708	1PE	OH2-C12-C22-OH3
4	D	706	1PE	OH4-C13-C23-OH3
4	B	706	1PE	OH5-C14-C24-OH4
4	C	706	1PE	C12-C22-OH3-C23
4	D	707	1PE	C13-C23-OH3-C22
4	A	710	1PE	C13-C23-OH3-C22
4	D	706	1PE	C16-C26-OH6-C15
4	A	706	1PE	C23-C13-OH4-C24
4	C	707	1PE	OH5-C14-C24-OH4
4	B	707	1PE	C13-C23-OH3-C22
4	C	710	1PE	OH2-C12-C22-OH3
4	D	709	1PE	C15-C25-OH5-C14
4	A	709	1PE	C23-C13-OH4-C24
4	D	708	1PE	C24-C14-OH5-C25
4	B	709	1PE	C12-C22-OH3-C23
4	C	704	1PE	C13-C23-OH3-C22
4	B	707	1PE	OH2-C12-C22-OH3
4	C	704	1PE	OH7-C16-C26-OH6
4	D	705	1PE	OH2-C12-C22-OH3
4	C	706	1PE	C16-C26-OH6-C15
4	C	708	1PE	C13-C23-OH3-C22
4	A	708	1PE	C13-C23-OH3-C22
4	A	707	1PE	OH4-C13-C23-OH3
4	C	705	1PE	C13-C23-OH3-C22
4	D	708	1PE	C16-C26-OH6-C15
4	A	708	1PE	C16-C26-OH6-C15
4	B	706	1PE	C13-C23-OH3-C22
4	D	707	1PE	C25-C15-OH6-C26
3	B	703	HEM	CAA-CBA-CGA-O1A
4	B	705	1PE	C13-C23-OH3-C22
4	B	707	1PE	C24-C14-OH5-C25
4	C	705	1PE	C23-C13-OH4-C24
4	C	704	1PE	C12-C22-OH3-C23
3	B	703	HEM	CAA-CBA-CGA-O2A
3	C	703	HEM	CAA-CBA-CGA-O2A
4	B	707	1PE	C15-C25-OH5-C14
4	C	705	1PE	C16-C26-OH6-C15
3	A	705	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	705	HEM	CAA-CBA-CGA-O2A
4	C	709	1PE	C24-C14-OH5-C25
4	D	709	1PE	C25-C15-OH6-C26
3	C	703	HEM	CAA-CBA-CGA-O1A
4	C	710	1PE	C16-C26-OH6-C15
4	C	707	1PE	C13-C23-OH3-C22
4	A	708	1PE	C15-C25-OH5-C14
4	C	704	1PE	C16-C26-OH6-C15
3	D	703	HEM	CAA-CBA-CGA-O2A
4	B	709	1PE	OH4-C13-C23-OH3
4	D	707	1PE	C12-C22-OH3-C23
4	D	709	1PE	C14-C24-OH4-C13
4	B	705	1PE	C25-C15-OH6-C26
3	D	703	HEM	CAA-CBA-CGA-O1A
4	C	709	1PE	C25-C15-OH6-C26
4	A	706	1PE	OH5-C14-C24-OH4
4	B	706	1PE	C23-C13-OH4-C24
4	D	705	1PE	C16-C26-OH6-C15
4	C	708	1PE	C24-C14-OH5-C25
4	A	706	1PE	OH6-C15-C25-OH5
4	D	706	1PE	C24-C14-OH5-C25
4	D	704	1PE	C24-C14-OH5-C25
4	C	704	1PE	C14-C24-OH4-C13
4	A	710	1PE	C23-C13-OH4-C24
4	B	708	1PE	C13-C23-OH3-C22
4	A	709	1PE	C16-C26-OH6-C15
4	D	707	1PE	C15-C25-OH5-C14
3	C	703	HEM	CAD-CBD-CGD-O2D
4	B	708	1PE	C15-C25-OH5-C14
4	B	709	1PE	C15-C25-OH5-C14
4	D	704	1PE	OH7-C16-C26-OH6
4	A	710	1PE	C25-C15-OH6-C26
4	C	706	1PE	C25-C15-OH6-C26
4	B	705	1PE	C23-C13-OH4-C24
4	C	707	1PE	OH4-C13-C23-OH3
4	A	710	1PE	C15-C25-OH5-C14
4	D	706	1PE	OH5-C14-C24-OH4
4	D	705	1PE	C15-C25-OH5-C14
4	A	707	1PE	C15-C25-OH5-C14
4	C	706	1PE	C13-C23-OH3-C22

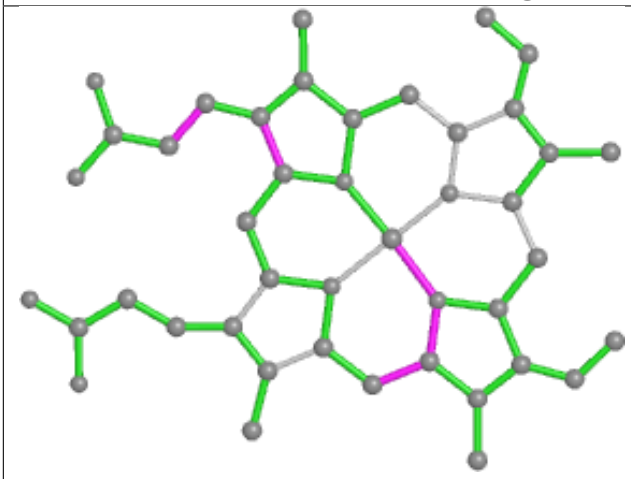
There are no ring outliers.

15 monomers are involved in 36 short contacts:

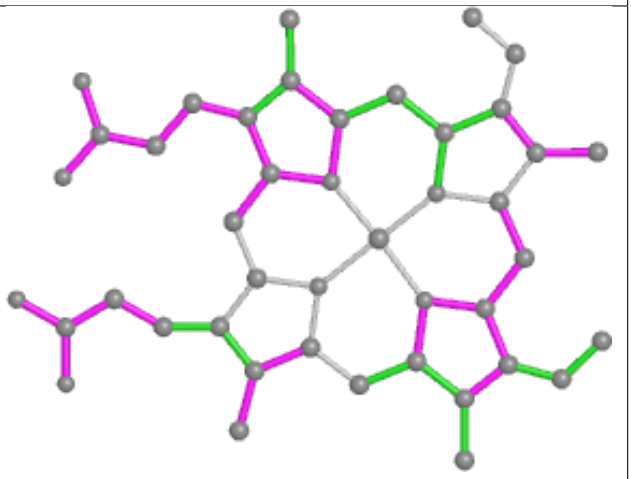
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	707	1PE	4	0
4	A	708	1PE	2	0
3	C	703	HEM	1	0
4	D	705	1PE	1	0
4	C	710	1PE	6	0
3	D	703	HEM	2	0
4	A	706	1PE	1	0
4	C	704	1PE	1	0
3	B	703	HEM	2	0
4	B	706	1PE	1	0
4	C	705	1PE	1	0
3	A	705	HEM	1	0
4	C	707	1PE	4	0
4	C	708	1PE	5	0
4	D	708	1PE	4	0

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.

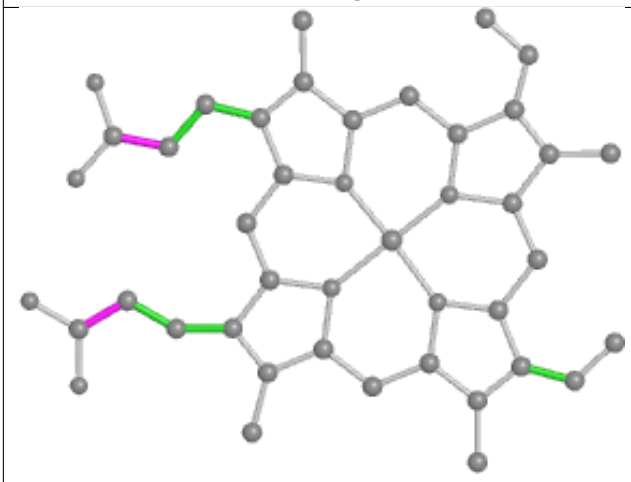
Ligand HEM C 703



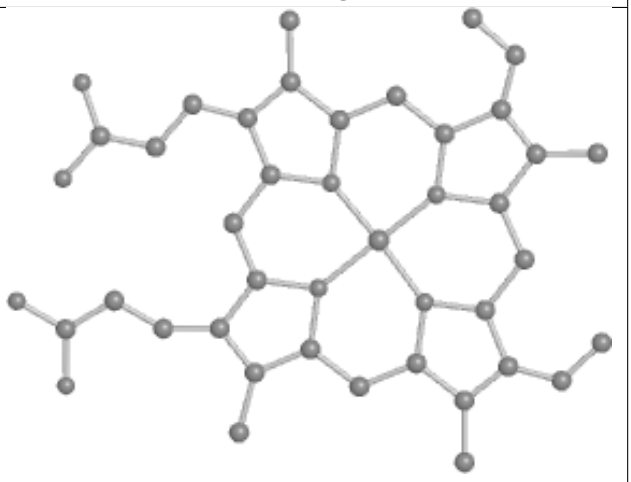
Bond lengths



Bond angles

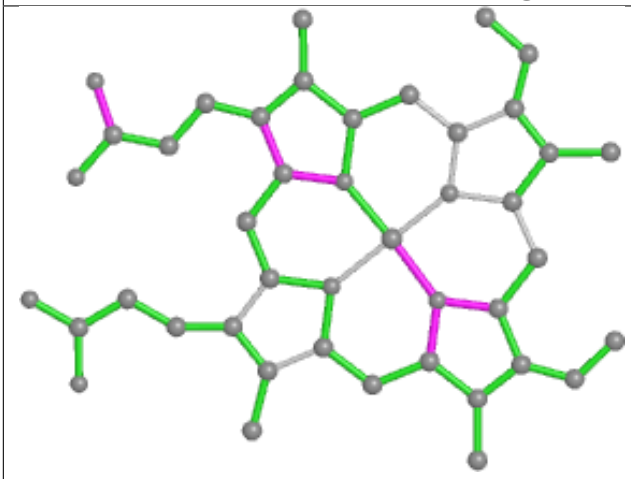


Torsions

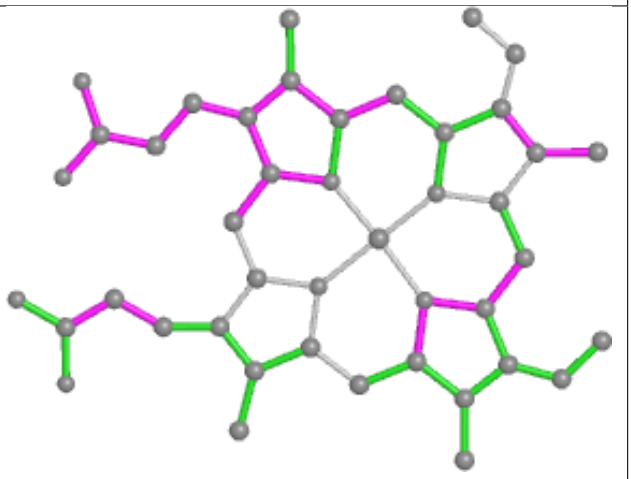


Rings

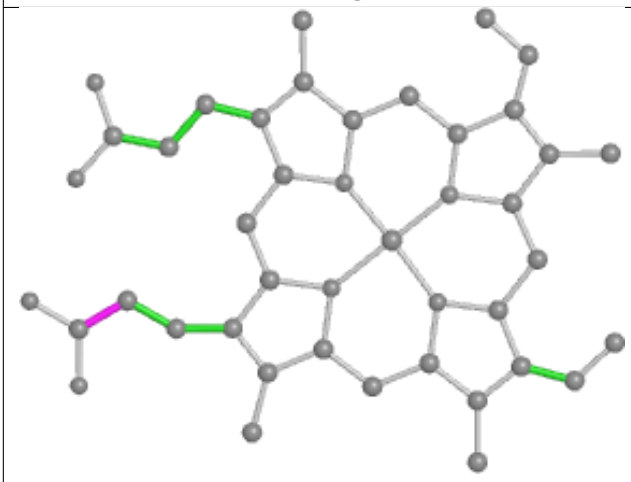
Ligand HEM D 703



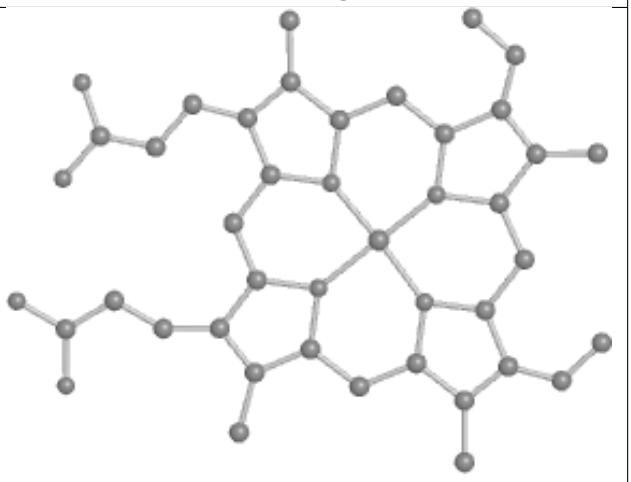
Bond lengths



Bond angles

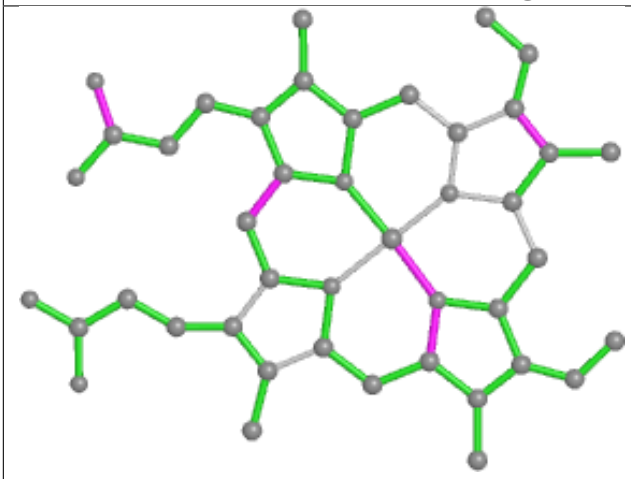


Torsions

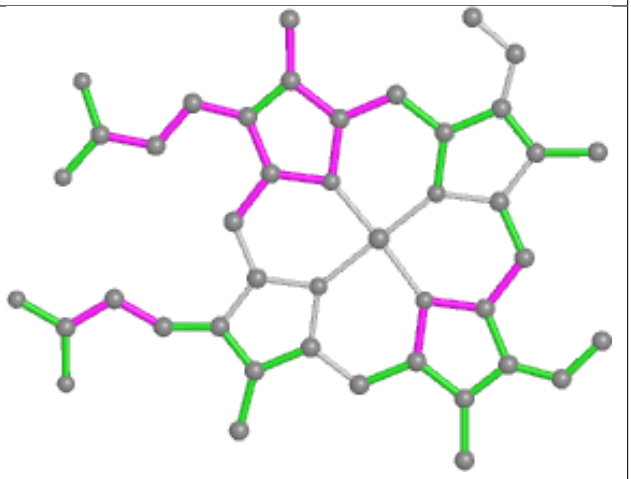


Rings

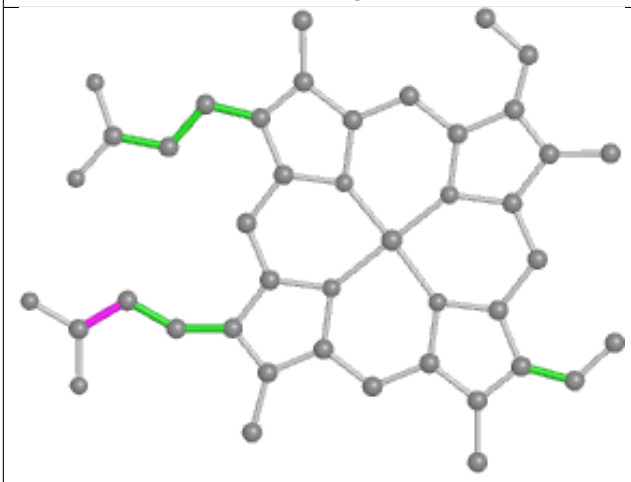
Ligand HEM B 703



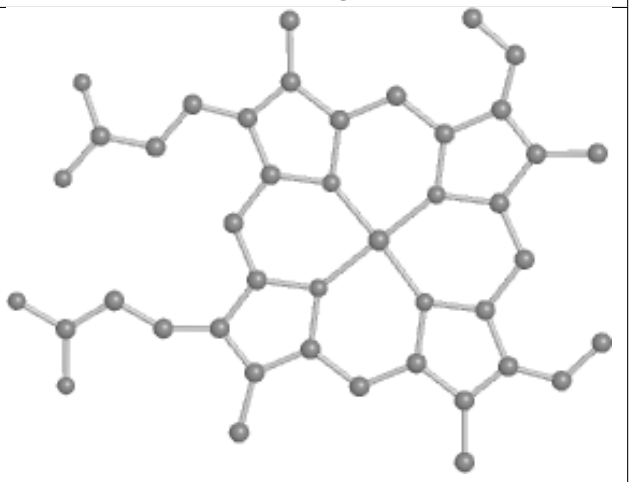
Bond lengths



Bond angles

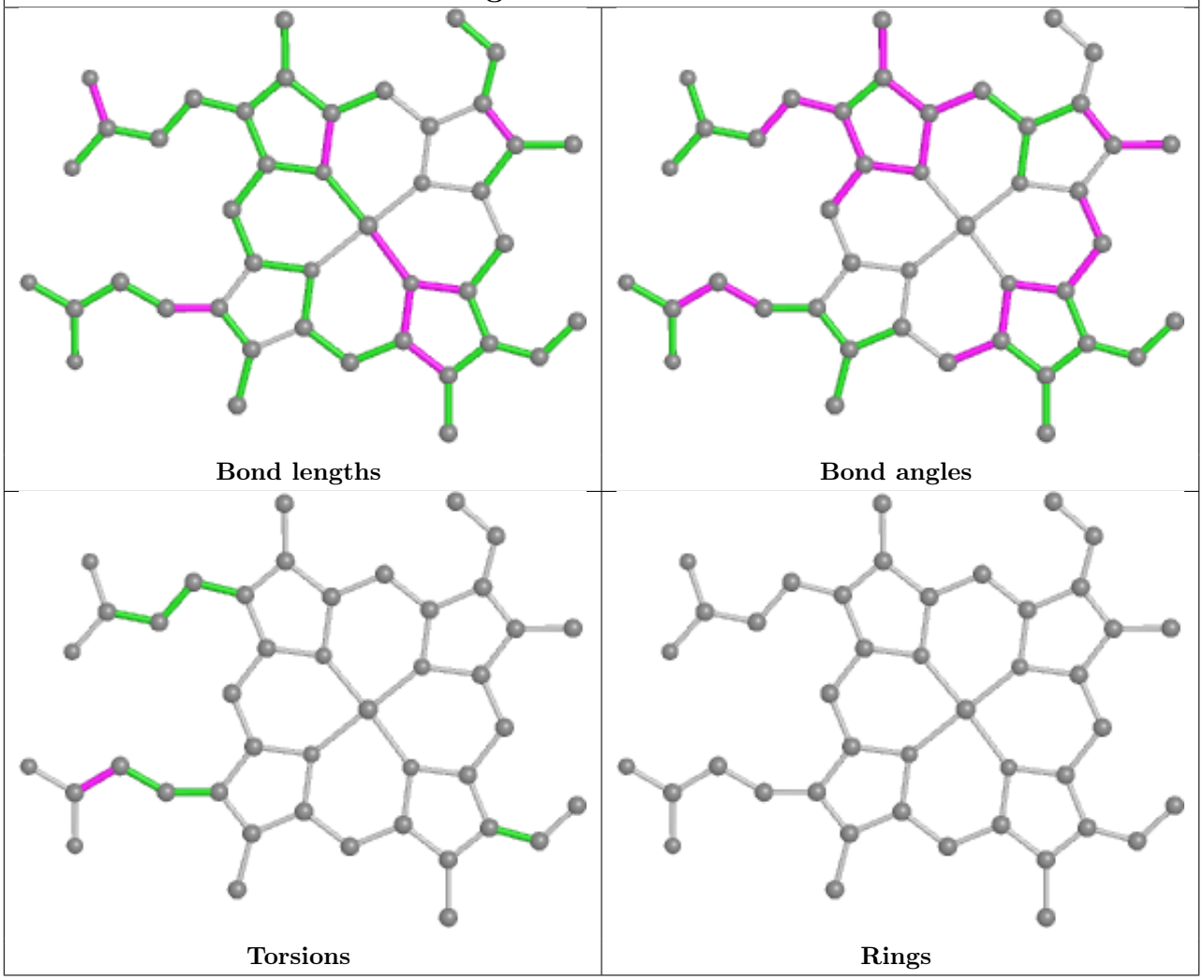


Torsions



Rings

Ligand HEM A 705



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	678/720 (94%)	-0.28	17 (2%)	57	56	12, 20, 43, 85	0
1	B	679/720 (94%)	-0.25	21 (3%)	49	47	11, 20, 44, 74	0
1	C	677/720 (94%)	-0.31	6 (0%)	84	84	12, 19, 33, 84	0
1	D	677/720 (94%)	-0.32	5 (0%)	87	88	12, 20, 33, 52	0
All	All	2711/2880 (94%)	-0.29	49 (1%)	68	68	11, 20, 38, 85	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	655	VAL	15.4
1	C	620	THR	7.4
1	C	621	ALA	6.9
1	A	20	GLN	6.8
1	A	620	THR	5.8
1	A	655	VAL	5.5
1	A	653	SER	5.0
1	C	654	GLU	4.9
1	B	653	SER	4.7
1	A	619	SER	4.7
1	A	621	ALA	4.6
1	B	652	SER	4.6
1	A	649	GLY	4.3
1	A	618	ALA	4.1
1	B	20	GLN	4.0
1	D	620	THR	3.7
1	D	619	SER	3.6
1	B	651	LYS	3.6
1	C	619	SER	3.5
1	B	659	ALA	3.4
1	B	655	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	651	LYS	3.2
1	B	657	ASP	3.2
1	B	650	GLY	3.1
1	A	654	GLU	3.0
1	A	657	ASP	2.9
1	B	654	GLU	2.9
1	D	576	LYS	2.8
1	B	620	THR	2.7
1	B	698	SER	2.7
1	D	517	GLY	2.7
1	B	590	GLU	2.6
1	B	649	GLY	2.6
1	A	676	MET	2.6
1	B	611	ASP	2.5
1	B	658	ALA	2.5
1	B	676	MET	2.4
1	B	565	ASP	2.4
1	A	648	CYS	2.3
1	B	674	VAL	2.3
1	C	521	PRO	2.3
1	D	676	MET	2.3
1	B	672	GLU	2.2
1	A	573	ARG	2.1
1	B	619	SER	2.1
1	A	658	ALA	2.1
1	A	561	SER	2.0
1	B	21	SER	2.0
1	A	672	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

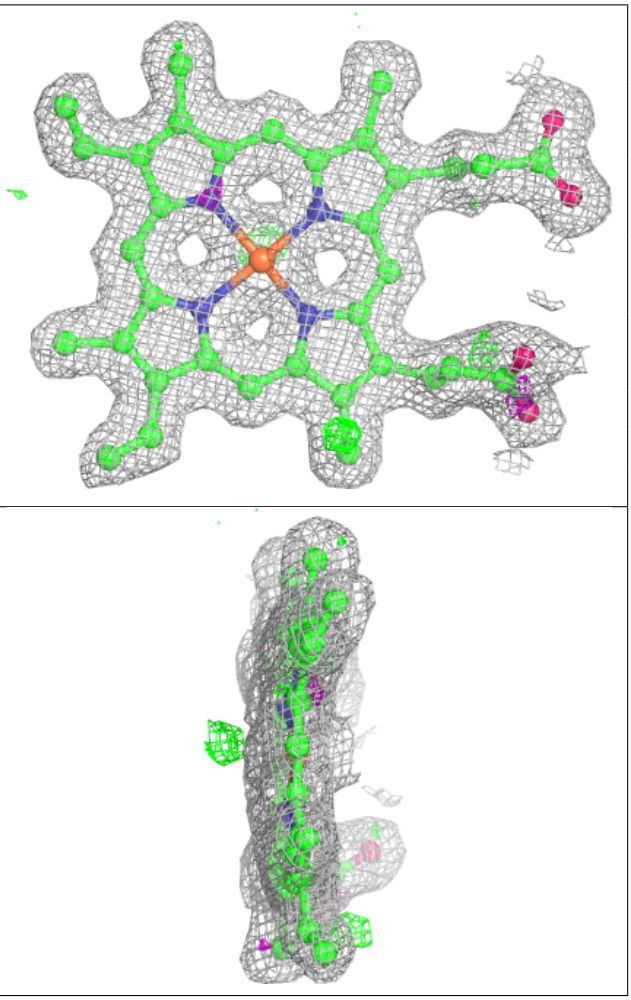
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1PE	B	709	16/16	0.50	0.31	65,75,88,88	0
4	1PE	D	704	16/16	0.62	0.40	62,80,94,94	0
4	1PE	B	708	16/16	0.64	0.23	70,74,85,85	0
4	1PE	C	709	16/16	0.65	0.26	50,76,84,85	0
4	1PE	C	707	16/16	0.65	0.37	57,76,79,81	0
4	1PE	A	706	16/16	0.68	0.35	48,68,86,89	0
4	1PE	C	706	16/16	0.69	0.28	59,66,78,78	0
4	1PE	A	709	16/16	0.70	0.20	48,68,74,74	0
4	1PE	B	705	16/16	0.71	0.16	49,62,67,70	0
4	1PE	D	709	16/16	0.73	0.33	50,79,101,103	0
4	1PE	A	708	16/16	0.74	0.27	51,56,62,63	0
4	1PE	D	707	16/16	0.75	0.22	47,67,89,99	0
4	1PE	B	707	16/16	0.75	0.19	49,57,69,75	0
4	1PE	C	705	16/16	0.78	0.24	43,52,75,75	0
4	1PE	D	705	16/16	0.78	0.30	59,67,83,89	0
4	1PE	C	708	16/16	0.78	0.26	38,51,62,65	0
4	1PE	B	706	16/16	0.78	0.27	51,56,75,77	0
4	1PE	C	710	16/16	0.79	0.27	44,57,68,69	0
4	1PE	D	708	16/16	0.79	0.24	41,57,65,66	0
4	1PE	D	706	16/16	0.79	0.29	35,53,88,91	0
4	1PE	A	710	16/16	0.80	0.24	48,62,74,76	0
4	1PE	A	707	16/16	0.82	0.20	47,61,78,79	0
4	1PE	C	704	16/16	0.87	0.17	46,51,60,61	0
4	1PE	B	704	16/16	0.90	0.14	28,38,66,70	0
2	CA	A	701	1/1	0.98	0.05	40,40,40,40	0
2	CA	D	702	1/1	0.98	0.03	28,28,28,28	0
3	HEM	A	705	43/43	0.98	0.09	12,14,20,29	0
3	HEM	B	703	43/43	0.98	0.10	11,14,18,26	0
3	HEM	C	703	43/43	0.98	0.09	11,14,16,22	0
3	HEM	D	703	43/43	0.98	0.09	13,14,17,24	0
2	CA	C	702	1/1	0.99	0.03	29,29,29,29	0
2	CA	A	702	1/1	0.99	0.02	23,23,23,23	0
2	CA	A	703	1/1	0.99	0.05	32,32,32,32	0
2	CA	A	704	1/1	0.99	0.11	34,34,34,34	0
2	CA	B	701	1/1	0.99	0.03	23,23,23,23	0
2	CA	B	702	1/1	0.99	0.03	30,30,30,30	0
2	CA	D	701	1/1	1.00	0.03	23,23,23,23	0
2	CA	C	701	1/1	1.00	0.04	25,25,25,25	0

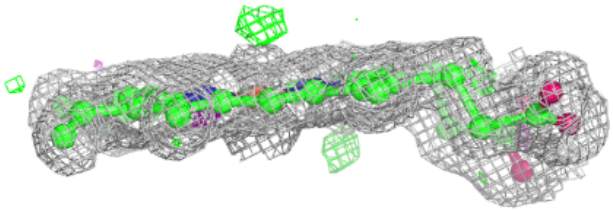
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 A 705:

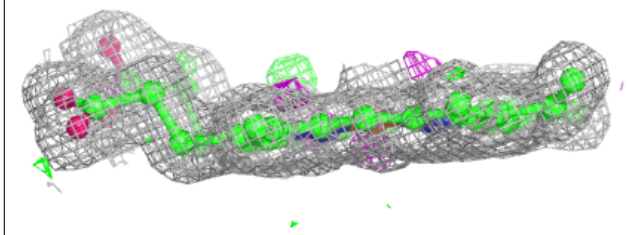
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

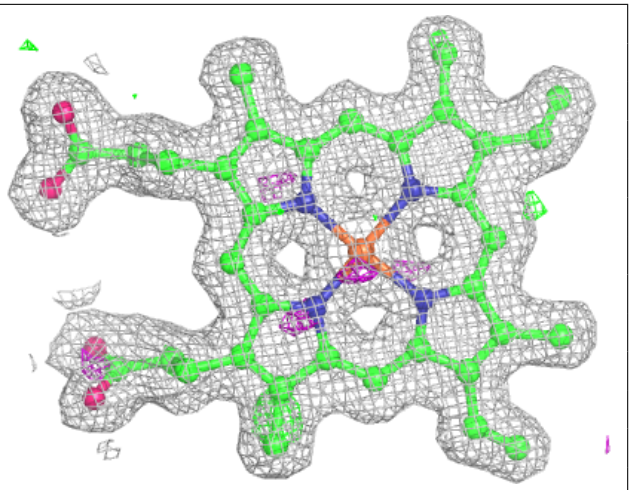


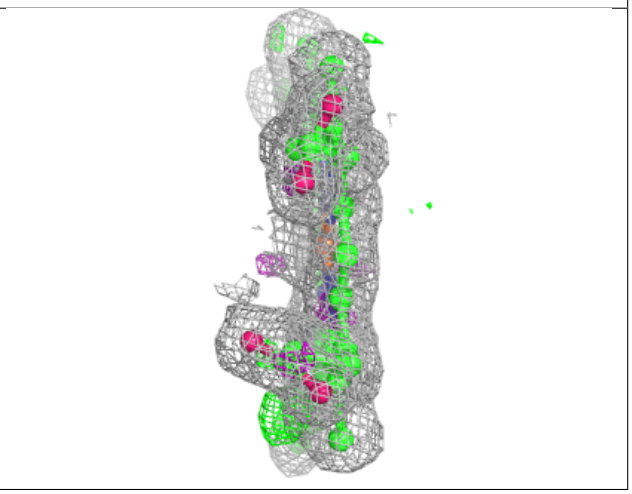


Electron density around HEM B 703:

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

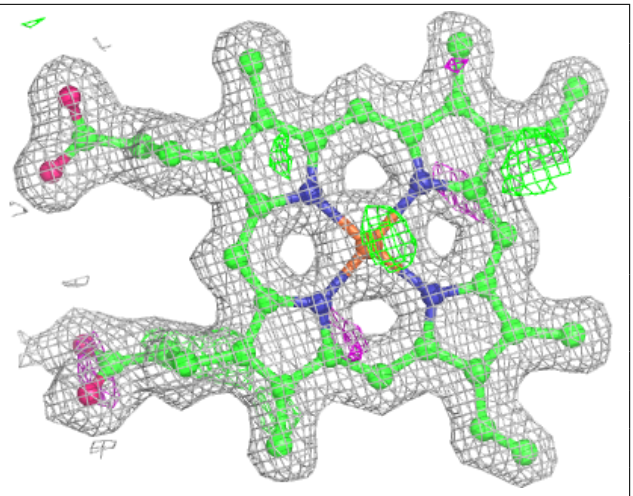


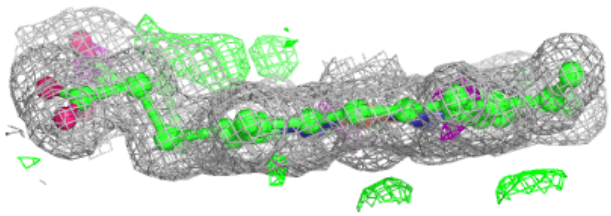


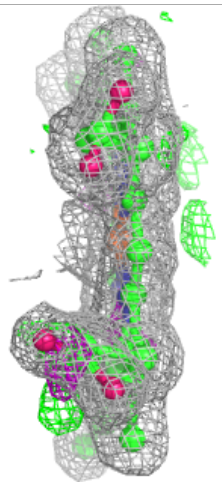


Electron density around HEM C 703:

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

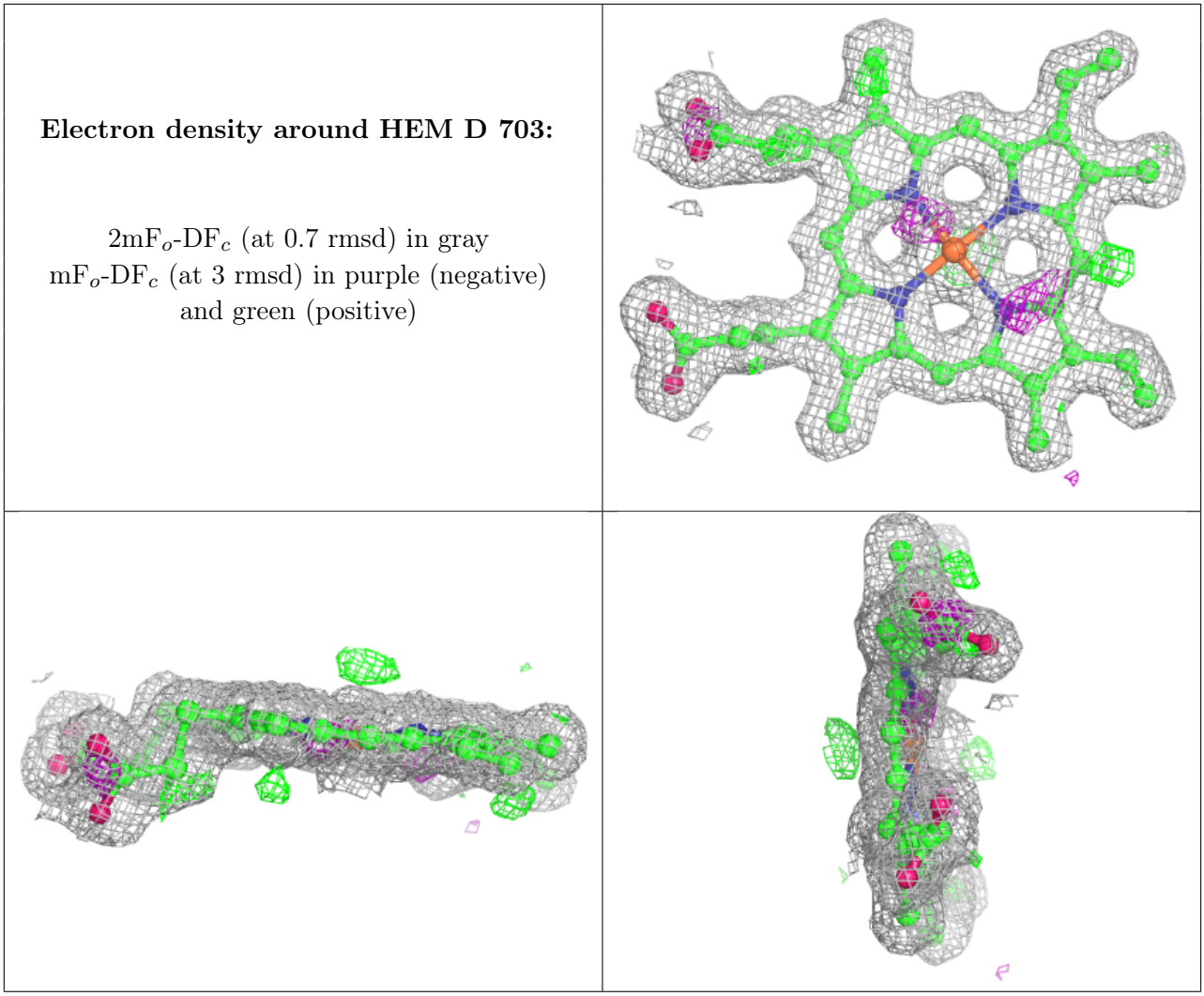






Electron density around HEM D 703:

$2mF_o$-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

There are no such residues in this entry.