Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 09:04 PM EDT

PDB ID	:	4K9W
Title	:	Complex of human CYP3A4 with a desoxyritonavir analog
Authors	:	Sevrioukova, I.F.; Poulos, T.L.
Deposited on	:	2013-04-21
Resolution	:	2.40 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:

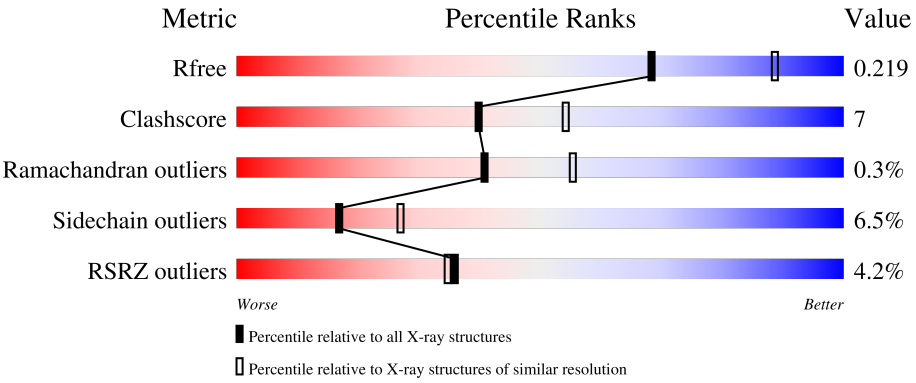
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	2% 76% 15% · 6%
1	B	487	3% 76% 16% · 6%
1	C	487	5% 76% 16% · 6%
1	D	487	5% 74% 19% · 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total 3687	C 2400	N 605	O 658	S 24	0	0	0
1	B	457	Total 3682	C 2397	N 603	O 658	S 24	0	1	0
1	C	458	Total 3688	C 2400	N 606	O 658	S 24	0	0	0
1	D	458	Total 3688	C 2400	N 606	O 658	S 24	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	UNP P08684
A	?	-	TRP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	SER	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	VAL	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	504	HIS	-	expression tag	UNP P08684

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Chain	Residue	Modelled	Actual	Comment	Reference
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	GLU	deletion	UNP P08684
B	?	-	THR	deletion	UNP P08684
B	?	-	TRP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	VAL	deletion	UNP P08684
B	?	-	SER	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	VAL	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	504	HIS	-	expression tag	UNP P08684
B	505	HIS	-	expression tag	UNP P08684
B	506	HIS	-	expression tag	UNP P08684
B	507	HIS	-	expression tag	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	ILE	deletion	UNP P08684
C	?	-	PRO	deletion	UNP P08684
C	?	-	ASP	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	ALA	deletion	UNP P08684
C	?	-	MET	deletion	UNP P08684
C	?	-	GLU	deletion	UNP P08684
C	?	-	THR	deletion	UNP P08684
C	?	-	TRP	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	ALA	deletion	UNP P08684
C	?	-	VAL	deletion	UNP P08684

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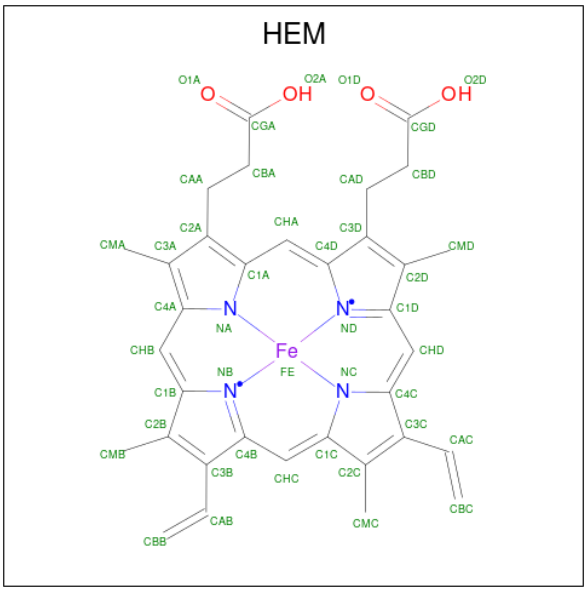
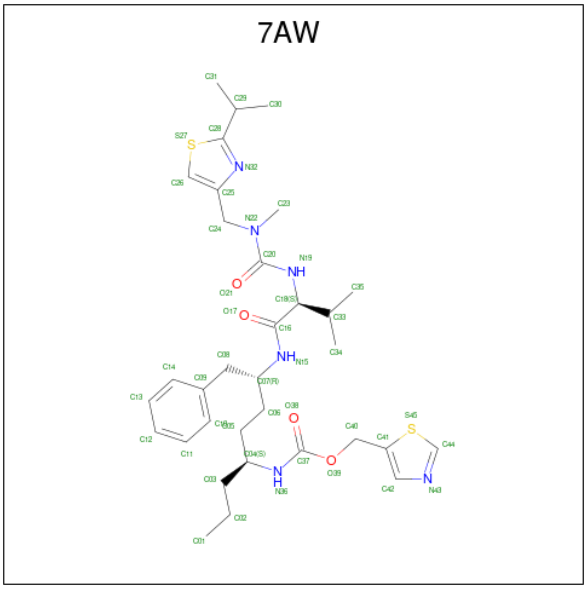
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	VAL	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	?	-	LEU	deletion	UNP P08684
C	504	HIS	-	expression tag	UNP P08684
C	505	HIS	-	expression tag	UNP P08684
C	506	HIS	-	expression tag	UNP P08684
C	507	HIS	-	expression tag	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	ILE	deletion	UNP P08684
D	?	-	PRO	deletion	UNP P08684
D	?	-	ASP	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	ALA	deletion	UNP P08684
D	?	-	MET	deletion	UNP P08684
D	?	-	GLU	deletion	UNP P08684
D	?	-	THR	deletion	UNP P08684
D	?	-	TRP	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	ALA	deletion	UNP P08684
D	?	-	VAL	deletion	UNP P08684
D	?	-	SER	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	VAL	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	?	-	LEU	deletion	UNP P08684
D	504	HIS	-	expression tag	UNP P08684
D	505	HIS	-	expression tag	UNP P08684
D	506	HIS	-	expression tag	UNP P08684
D	507	HIS	-	expression tag	UNP P08684

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is N 2 -(methyl{[2-(propan-2-yl)-1,3-thiazol-4-yl]methyl}carbamoyl)-N-[(2 R,5S)-1-phenyl-5-{[(1,3-thiazol-5-ylmethoxy)carbonyl]amino}octan-2-yl]-L-valinamide (three-letter code: 7AW) (formula: $C_{33}H_{48}N_6O_4S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			45	33	6	4	2		
3	B	1	Total	C	N	O	S	0	0
			45	33	6	4	2		
3	C	1	Total	C	N	O	S	0	0
			45	33	6	4	2		
3	D	1	Total	C	N	O	S	0	0
			45	33	6	4	2		

- Molecule 4 is water.

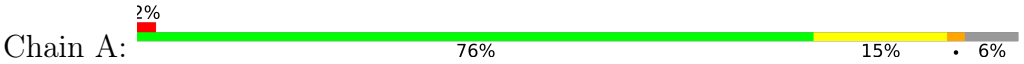
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	7	Total	O	0	0
			7	7		
4	C	7	Total	O	0	0
			7	7		
4	D	4	Total	O	0	0
			4	4		

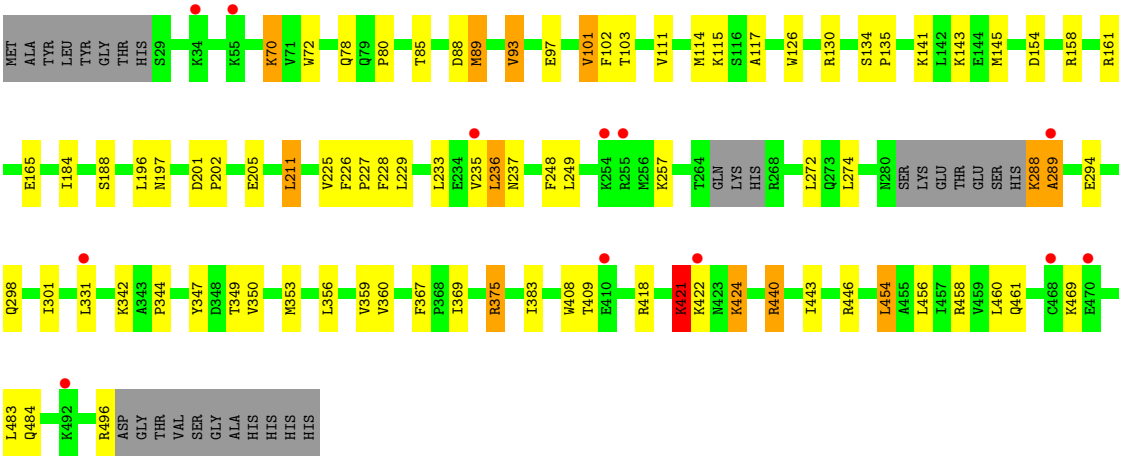
3 Residue-property plots (i)

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: Cytochrome P450 3A4

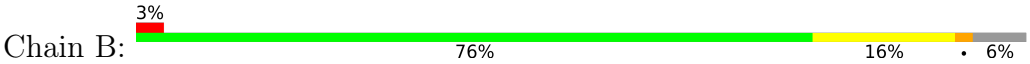
Chain A:

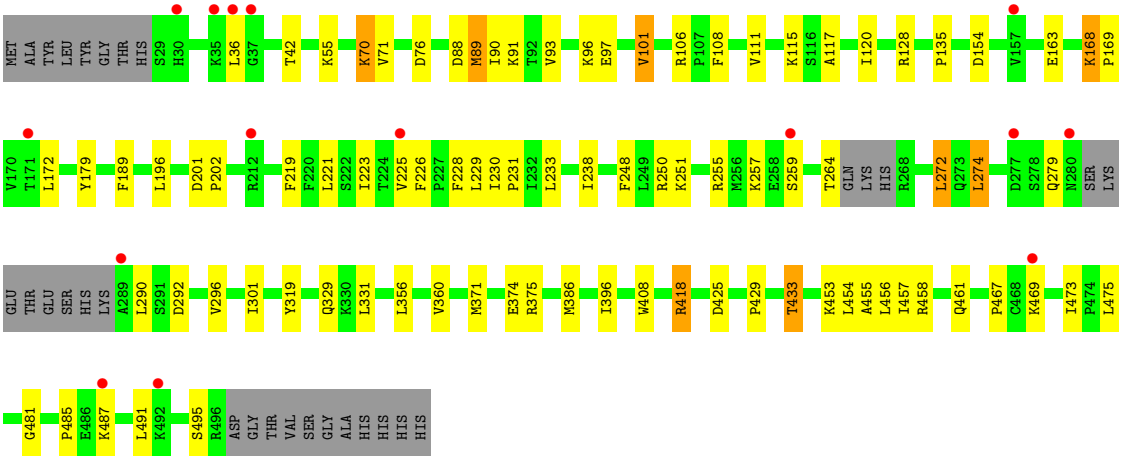




• Molecule 1: Cytochrome P450 3A4

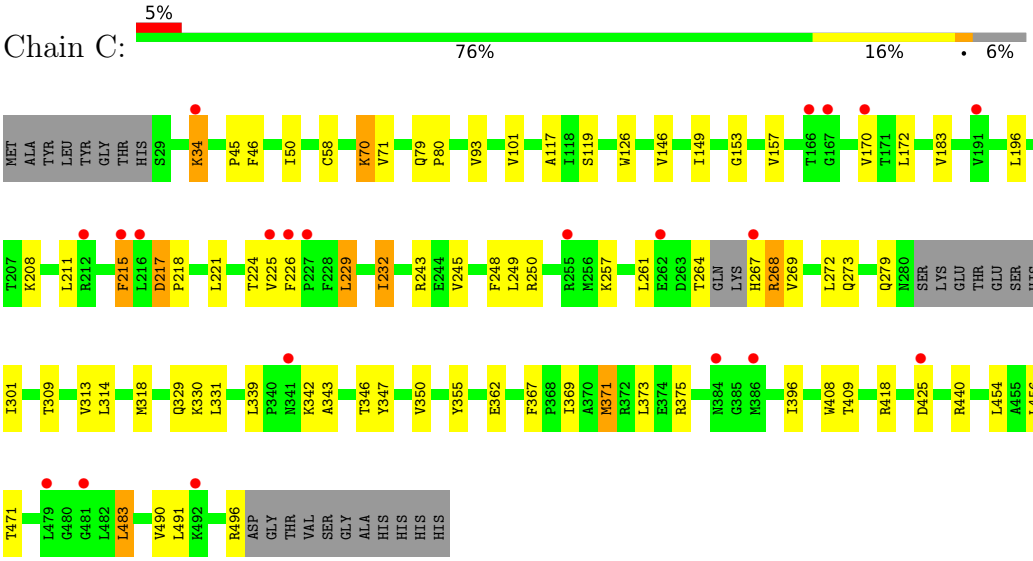
Chain B:





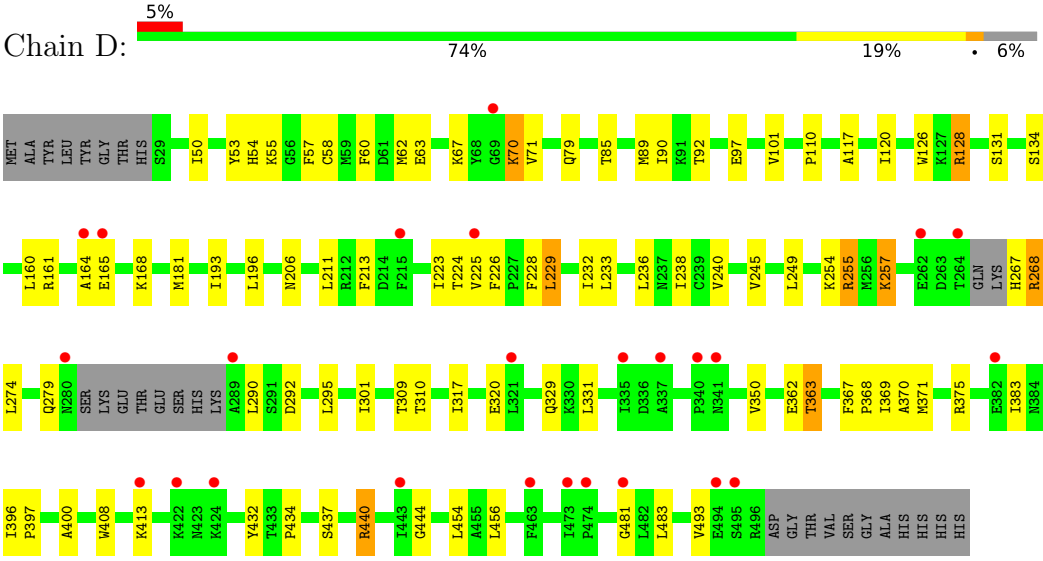
• Molecule 1: Cytochrome P450 3A4

Chain C:



• Molecule 1: Cytochrome P450 3A4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	94.02Å 94.02Å 199.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.01 – 2.40 47.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.01-2.40) 98.7 (47.01-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.198 0.182 , 0.219	Depositor DCC
R_{free} test set	3792 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.048 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
Reported twinning fraction	0.650 for H, K, L 0.350 for K, H, -L	Depositor
Outliers	0 of 76002 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15119	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 7AW

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	0.47	2/3775 (0.1%)	0.62	2/5105 (0.0%)
1	B	0.46	1/3773 (0.0%)	0.61	0/5104
1	C	0.48	1/3777 (0.0%)	0.62	0/5109
1	D	0.49	1/3777 (0.0%)	0.62	0/5109
All	All	0.47	5/15102 (0.0%)	0.62	2/20427 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	408	TRP	CD2-CE2	5.56	1.48	1.41
1	B	408	TRP	CD2-CE2	5.44	1.47	1.41
1	D	408	TRP	CD2-CE2	5.30	1.47	1.41
1	A	408	TRP	CD2-CE2	5.26	1.47	1.41
1	A	72	TRP	CD2-CE2	5.20	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	440	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	A	375	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3687	0	3777	61	0
1	B	3682	0	3771	40	0
1	C	3688	0	3771	43	0
1	D	3688	0	3771	62	0
2	A	43	0	30	8	0
2	B	43	0	30	4	0
2	C	43	0	30	8	0
2	D	43	0	30	11	0
3	A	45	0	48	8	0
3	B	45	0	48	5	0
3	C	45	0	48	4	0
3	D	45	0	48	4	0
4	A	4	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	1	0
4	D	4	0	0	0	0
All	All	15119	0	15402	223	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 7.

All (223) 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:288:LYS:CB	1:A:289:ALA:HB2	1.19	1.62
1:A:288:LYS:CB	1:A:289:ALA:CB	2.06	1.32
1:A:288:LYS:HB2	1:A:289:ALA:HB2	1.10	1.08
1:A:288:LYS:HB3	1:A:289:ALA:CB	1.77	1.00
1:A:288:LYS:N	1:A:289:ALA:HB3	1.80	0.96
1:A:288:LYS:HB3	1:A:289:ALA:HB2	0.98	0.94
1:A:288:LYS:CA	1:A:289:ALA:CB	2.46	0.92
1:A:288:LYS:HB2	1:A:289:ALA:CB	1.86	0.89
1:A:369:ILE:HG12	2:A:601:HEM:CMB	2.08	0.83
1:B:221:LEU:O	1:B:225:VAL:HG22	1.78	0.82
2:C:601:HEM:C1D	3:C:602:7AW:H4	2.15	0.81
1:A:369:ILE:HG12	2:A:601:HEM:HMB1	1.63	0.81
1:A:367:PHE:HB3	1:A:483:LEU:HD21	1.63	0.81
1:A:288:LYS:CA	1:A:289:ALA:HB2	2.09	0.80
1:D:110:PRO:HD2	1:D:240:VAL:HG13	1.64	0.80
2:A:601:HEM:ND	3:A:602:7AW:H4	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LEU:O	1:C:225:VAL:HG23	1.87	0.75
1:C:215:PHE:CZ	1:C:224:THR:HG21	2.24	0.73
1:A:134:SER:HA	1:A:443:ILE:HD11	1.69	0.73
1:C:58:CYS:SG	1:C:371:MET:HG2	2.30	0.71
2:B:601:HEM:C1D	3:B:602:7AW:H4	2.26	0.70
1:D:267:HIS:O	1:D:268:ARG:HB2	1.91	0.70
1:D:350:VAL:HG21	1:D:454:LEU:CD1	2.22	0.69
1:A:226:PHE:HB3	1:A:228:PHE:CE2	2.28	0.69
1:B:457:ILE:O	1:B:461:GLN:HG2	1.94	0.68
1:A:288:LYS:HB3	1:A:289:ALA:CA	2.23	0.67
1:A:369:ILE:CG1	2:A:601:HEM:HMB1	2.25	0.67
1:C:264:THR:O	1:C:267:HIS:NE2	2.23	0.67
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.79	0.64
1:C:330:LYS:HD3	1:C:355:TYR:CZ	2.32	0.64
1:A:211:LEU:HD12	3:A:602:7AW:H10	1.78	0.64
1:D:90:ILE:HG23	1:D:396:ILE:HD13	1.80	0.64
1:D:375:ARG:NH2	2:D:601:HEM:O1A	2.30	0.64
2:C:601:HEM:ND	3:C:602:7AW:C42	2.61	0.64
1:B:97:GLU:HB3	1:B:101:VAL:HG13	1.79	0.63
1:A:331:LEU:HD12	1:A:359:VAL:HG21	1.80	0.63
1:A:422:LYS:HD2	1:C:34:LYS:HA	1.82	0.62
2:C:601:HEM:ND	3:C:602:7AW:H4	2.15	0.62
1:D:350:VAL:HG21	1:D:454:LEU:HD12	1.81	0.62
1:C:215:PHE:HZ	1:C:224:THR:HG21	1.63	0.62
1:C:172:LEU:HD11	1:C:491:LEU:HD12	1.81	0.62
1:A:446:ARG:HH11	1:B:425:ASP:HB2	1.64	0.61
1:A:288:LYS:CA	1:A:289:ALA:HB3	2.22	0.61
1:A:409:THR:O	1:A:418:ARG:NH2	2.32	0.61
1:D:269:VAL:HG13	1:D:273:GLN:HB3	1.81	0.61
1:B:485:PRO:HB2	1:B:487:LYS:O	2.01	0.61
1:A:70:LYS:HA	1:A:85:THR:OG1	2.00	0.61
1:A:97:GLU:HB3	1:A:101:VAL:HG13	1.84	0.60
1:D:110:PRO:O	1:D:240:VAL:HG22	2.01	0.60
2:A:601:HEM:C1D	3:A:602:7AW:H4	2.37	0.59
1:A:294:GLU:O	1:A:298:GLN:HG2	2.03	0.59
1:A:421:LYS:HA	1:A:424:LYS:HD3	1.84	0.59
1:A:383:ILE:O	1:A:383:ILE:HG13	2.03	0.59
2:B:601:HEM:ND	3:B:602:7AW:H4	2.18	0.58
1:D:368:PRO:O	1:D:483:LEU:HD13	2.03	0.58
1:B:429:PRO:O	1:B:433:THR:HG23	2.03	0.58
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:N	1:A:289:ALA:CB	2.55	0.58
1:D:126:TRP:CZ2	1:D:440:ARG:HG2	2.39	0.58
1:C:46:PHE:HD2	1:C:226:PHE:CZ	2.22	0.58
1:D:58:CYS:SG	1:D:371:MET:CE	2.92	0.57
1:D:236:LEU:HB2	1:D:238:ILE:HG12	1.87	0.57
1:A:184:ILE:O	1:A:188:SER:HB2	2.06	0.56
1:D:53:TYR:CD2	1:D:57:PHE:HB3	2.40	0.56
1:C:126:TRP:CZ2	1:C:440:ARG:HG2	2.42	0.55
1:B:108:PHE:CE2	1:B:120:ILE:HG12	2.42	0.55
1:A:117:ALA:HB1	1:A:301:ILE:CG1	2.38	0.54
1:D:161:ARG:O	1:D:165:GLU:HG2	2.07	0.54
1:C:369:ILE:HG12	2:C:601:HEM:CMB	2.37	0.54
2:B:601:HEM:ND	3:B:602:7AW:C42	2.71	0.54
1:D:309:THR:HG22	2:D:601:HEM:HAB	1.89	0.54
1:B:108:PHE:HE2	1:B:120:ILE:HG12	1.73	0.54
1:B:356:LEU:O	1:B:360:VAL:HG23	2.07	0.54
1:A:461:GLN:HA	1:A:496:ARG:HH21	1.73	0.53
1:A:226:PHE:HB3	1:A:228:PHE:HE2	1.73	0.53
1:C:225:VAL:HG12	1:C:226:PHE:CG	2.43	0.53
1:D:317:ILE:HA	1:D:363:THR:HG21	1.91	0.52
1:B:225:VAL:HG23	1:B:226:PHE:CD1	2.44	0.52
1:B:356:LEU:HD21	1:B:453:LYS:HB3	1.92	0.52
1:D:160:LEU:HD22	1:D:493:VAL:HG21	1.92	0.52
2:D:601:HEM:C1D	3:D:602:7AW:H4	2.45	0.52
3:A:602:7AW:H5	3:A:602:7AW:H18	1.75	0.51
1:D:135:PRO:HB2	1:D:274:LEU:HD21	1.92	0.51
1:C:375:ARG:NH2	2:C:601:HEM:O1A	2.39	0.51
2:C:601:HEM:NB	3:C:602:7AW:H3	2.25	0.51
1:D:375:ARG:HH22	2:D:601:HEM:CGA	2.23	0.51
2:D:601:HEM:ND	3:D:602:7AW:H4	2.25	0.51
1:D:53:TYR:CE2	1:D:57:PHE:HB3	2.46	0.50
1:D:257:LYS:NZ	1:D:292:ASP:OD2	2.44	0.50
2:A:601:HEM:ND	3:A:602:7AW:C42	2.69	0.50
1:C:267:HIS:O	1:C:268:ARG:HB3	2.11	0.50
1:C:269:VAL:HG13	1:C:273:GLN:CG	2.41	0.50
1:B:375:ARG:NH2	2:B:601:HEM:O1A	2.45	0.50
1:C:202:PRO:HB2	1:C:248:PHE:CZ	2.47	0.50
1:A:143:LYS:HE3	1:A:347:TYR:CD1	2.47	0.50
1:D:58:CYS:SG	1:D:371:MET:HE2	2.52	0.50
1:C:269:VAL:HG13	1:C:273:GLN:HG3	1.94	0.49
2:A:601:HEM:C4D	3:A:602:7AW:H4	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ILE:HG12	2:C:601:HEM:HMB1	1.94	0.49
1:D:371:MET:CE	1:D:483:LEU:HD12	2.43	0.49
1:D:367:PHE:HB3	1:D:483:LEU:HD21	1.93	0.49
1:C:117:ALA:HB1	1:C:301:ILE:CG1	2.43	0.48
1:D:255:ARG:HH11	1:D:255:ARG:HB2	1.78	0.48
1:C:153:GLY:O	1:C:157:VAL:HG22	2.14	0.48
1:D:213:PHE:CD2	1:D:481:GLY:HA3	2.49	0.48
1:B:251:LYS:HG2	1:B:255:ARG:HH21	1.79	0.48
1:C:206:ASN:HB3	1:C:245:VAL:HG13	1.96	0.48
1:A:111:VAL:O	1:A:114:MET:HB2	2.14	0.48
1:A:235:VAL:C	1:A:237:ASN:H	2.17	0.47
1:C:146:VAL:HG21	1:C:347:TYR:HB2	1.96	0.47
1:D:223:ILE:HG13	1:D:224:THR:N	2.29	0.47
1:A:89:MET:O	1:A:93:VAL:HG13	2.15	0.47
1:B:257:LYS:NZ	1:B:292:ASP:OD2	2.47	0.47
1:D:350:VAL:HG21	1:D:454:LEU:HD11	1.95	0.47
1:D:362:GLU:OE2	1:D:362:GLU:HA	2.14	0.47
1:C:172:LEU:HD11	1:C:491:LEU:CD1	2.43	0.47
1:D:229:LEU:HD12	1:D:232:ILE:HD12	1.96	0.47
1:D:54:HIS:CE1	1:D:55:LYS:HG2	2.49	0.47
1:D:320:GLU:OE2	1:D:320:GLU:HA	2.15	0.46
1:B:106:ARG:NH2	1:B:374:GLU:OE1	2.26	0.46
1:D:58:CYS:SG	1:D:371:MET:HE1	2.55	0.46
1:B:202:PRO:HB2	1:B:248:PHE:CZ	2.50	0.46
1:D:117:ALA:HB3	1:D:120:ILE:HD12	1.96	0.46
1:D:233:LEU:HB3	1:D:238:ILE:HB	1.98	0.46
1:A:134:SER:N	1:A:135:PRO:CD	2.77	0.46
1:A:356:LEU:O	1:A:360:VAL:HG23	2.15	0.46
1:B:71:VAL:HG21	1:B:386:MET:HE1	1.97	0.46
1:B:189:PHE:HD2	1:B:272:LEU:HG	1.80	0.46
1:A:134:SER:CA	1:A:443:ILE:HD11	2.40	0.46
1:A:141:LYS:O	1:A:145:MET:HG3	2.16	0.46
1:B:76:ASP:OD2	1:B:106:ARG:NH1	2.47	0.46
1:C:243:ARG:NH1	4:C:707:HOH:O	2.48	0.46
1:B:250:ARG:HG3	1:B:296:VAL:HG11	1.98	0.45
1:A:331:LEU:HD22	1:A:460:LEU:HD13	1.98	0.45
1:B:154:ASP:OD2	1:B:458:ARG:NH2	2.48	0.45
1:D:432:TYR:CZ	1:D:434:PRO:HG3	2.52	0.45
1:C:79:GLN:NE2	1:C:80:PRO:HD2	2.32	0.45
1:C:170:VAL:O	1:C:490:VAL:HA	2.17	0.45
1:C:346:THR:O	1:C:350:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:LEU:HB3	1:C:343:ALA:HB3	1.99	0.45
1:D:70:LYS:HA	1:D:85:THR:OG1	2.17	0.45
1:A:331:LEU:HD21	1:A:356:LEU:HD13	1.98	0.45
1:A:349:THR:O	1:A:353:MET:HG3	2.17	0.45
1:B:233:LEU:HB3	1:B:238:ILE:HB	1.99	0.45
1:A:350:VAL:HG21	1:A:454:LEU:HD13	1.99	0.44
3:D:602:7AW:C26	3:D:602:7AW:H34	2.47	0.44
1:A:135:PRO:O	1:A:141:LYS:NZ	2.49	0.44
1:B:467:PRO:HB3	1:B:473:ILE:HD11	2.00	0.44
1:C:373:LEU:HB2	1:C:396:ILE:HB	2.00	0.44
1:D:397:PRO:HB2	1:D:400:ALA:HB3	1.99	0.44
1:A:126:TRP:CZ2	1:A:440:ARG:HG2	2.52	0.44
1:D:79:GLN:NE2	1:D:393:VAL:HG23	2.32	0.44
1:A:154:ASP:OD2	1:A:458:ARG:NH2	2.51	0.44
1:C:471:THR:OG1	1:C:490:VAL:O	2.24	0.44
1:A:201:ASP:HA	1:A:202:PRO:HD2	1.87	0.44
1:B:89:MET:HE2	1:B:89:MET:HB2	1.90	0.43
3:B:602:7AW:N36	3:B:602:7AW:H18	2.33	0.43
1:D:369:ILE:HG13	1:D:370:ALA:H	1.83	0.43
1:A:369:ILE:HD11	2:A:601:HEM:CHB	2.49	0.43
3:B:602:7AW:H37	3:B:602:7AW:H20	2.00	0.43
1:C:309:THR:O	1:C:313:VAL:HG23	2.18	0.43
1:A:78:GLN:O	1:A:80:PRO:HD3	2.19	0.43
1:B:91:LYS:HE3	1:B:96:LYS:HE3	2.00	0.43
1:B:230:ILE:HB	1:B:231:PRO:HD3	2.00	0.43
1:A:202:PRO:HB2	1:A:248:PHE:CZ	2.54	0.43
1:B:163:GLU:H	1:B:163:GLU:HG2	1.70	0.43
1:C:70:LYS:HE2	1:C:70:LYS:HB2	1.90	0.43
1:D:63:GLU:O	1:D:67:LYS:HB2	2.18	0.43
1:D:369:ILE:HG12	2:D:601:HEM:CMB	2.49	0.43
1:A:158:ARG:NH2	1:A:197:ASN:OD1	2.50	0.43
1:C:217:ASP:HA	1:C:218:PRO:HD3	1.90	0.43
1:A:301:ILE:HD12	3:A:602:7AW:O38	2.19	0.42
1:D:92:THR:HG22	1:D:97:GLU:HG3	2.01	0.42
1:B:279:GLN:HG2	1:B:290:LEU:O	2.18	0.42
2:D:601:HEM:ND	3:D:602:7AW:C42	2.81	0.42
1:B:319:TYR:CZ	1:B:475:LEU:HB2	2.54	0.42
1:D:117:ALA:HB1	1:D:301:ILE:HG13	2.01	0.42
1:D:57:PHE:HA	1:D:60:PHE:HB3	2.02	0.42
1:B:168:LYS:HA	1:B:169:PRO:HD2	1.88	0.42
1:B:90:ILE:HG12	1:B:396:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PRO:HB2	1:B:274:LEU:HD21	2.00	0.42
1:D:257:LYS:HE3	1:D:295:LEU:HD13	2.02	0.42
1:C:314:LEU:O	1:C:318:MET:HG2	2.20	0.42
1:D:90:ILE:HG23	1:D:396:ILE:CD1	2.49	0.42
1:D:279:GLN:HG2	1:D:290:LEU:O	2.20	0.42
1:A:461:GLN:HA	1:A:496:ARG:NH2	2.34	0.42
1:B:117:ALA:HB1	1:B:301:ILE:HG13	2.02	0.42
1:B:179:TYR:CZ	1:B:455:ALA:HB2	2.55	0.42
1:C:369:ILE:CG1	2:C:601:HEM:HMB1	2.50	0.42
1:D:89:MET:HG3	1:D:383:ILE:HD12	2.02	0.42
1:D:164:ALA:HB2	1:D:493:VAL:HG12	2.02	0.41
1:D:224:THR:HG22	1:D:224:THR:O	2.20	0.41
1:D:309:THR:CG2	2:D:601:HEM:HAB	2.50	0.41
3:A:602:7AW:O38	3:A:602:7AW:H8	2.21	0.41
1:B:219:PHE:O	1:B:223:ILE:HG12	2.20	0.41
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.85	0.41
1:C:149:ILE:HG12	1:C:183:VAL:HG13	2.02	0.41
1:D:128:ARG:H	1:D:128:ARG:HG2	1.65	0.41
1:D:146:VAL:HB	1:D:147:PRO:HD3	2.01	0.41
1:A:130:ARG:O	1:A:134:SER:HB3	2.20	0.41
1:D:226:PHE:HB3	1:D:228:PHE:CE2	2.55	0.41
1:A:225:VAL:O	1:A:227:PRO:HD3	2.21	0.41
1:C:225:VAL:HG12	1:C:226:PHE:CD1	2.56	0.41
1:D:206:ASN:HB3	1:D:245:VAL:HG13	2.03	0.41
1:B:226:PHE:HB3	1:B:228:PHE:CZ	2.56	0.41
1:D:444:GLY:HA3	2:D:601:HEM:C3C	2.55	0.41
1:A:102:PHE:O	1:A:375:ARG:HD3	2.21	0.41
1:B:70:LYS:HE2	1:B:70:LYS:HB2	1.95	0.41
1:C:45:PRO:O	1:C:46:PHE:HB2	2.21	0.41
1:D:413:LYS:HA	1:D:413:LYS:HD3	1.79	0.41
1:A:161:ARG:O	1:A:165:GLU:HG2	2.21	0.41
1:C:362:GLU:HA	1:C:362:GLU:OE2	2.21	0.41
1:D:181:MET:HG3	1:D:193:ILE:HD11	2.03	0.41
1:D:223:ILE:C	1:D:225:VAL:H	2.23	0.41
1:A:233:LEU:HA	1:A:236:LEU:HD12	2.04	0.40
1:C:279:GLN:HG2	1:C:290:LEU:O	2.21	0.40
1:C:330:LYS:HD3	1:C:355:TYR:CE2	2.56	0.40
1:D:309:THR:HG22	2:D:601:HEM:CAB	2.49	0.40
1:D:309:THR:HG21	2:D:601:HEM:C3B	2.56	0.40
1:C:367:PHE:HB3	1:C:483:LEU:HD21	2.03	0.40
1:C:229:LEU:HD12	1:C:232:ILE:HD11	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PRO:HB2	1:B:248:PHE:CE2	2.56	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	452/487 (93%)	431 (95%)	18 (4%)	3 (1%)	22	32
1	B	452/487 (93%)	435 (96%)	16 (4%)	1 (0%)	47	62
1	C	452/487 (93%)	429 (95%)	22 (5%)	1 (0%)	47	62
1	D	452/487 (93%)	428 (95%)	23 (5%)	1 (0%)	47	62
All	All	1808/1948 (93%)	1723 (95%)	79 (4%)	6 (0%)	41	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	ALA
1	A	236	LEU
1	A	421	LYS
1	C	268	ARG
1	D	268	ARG
1	B	481	GLY

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	419/443 (95%)	395 (94%)	24 (6%)	20	33
1	B	419/443 (95%)	391 (93%)	28 (7%)	16	26
1	C	419/443 (95%)	386 (92%)	33 (8%)	12	19
1	D	419/443 (95%)	395 (94%)	24 (6%)	20	33
All	All	1676/1772 (95%)	1567 (94%)	109 (6%)	17	27

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	88	ASP
1	A	89	MET
1	A	93	VAL
1	A	101	VAL
1	A	103	THR
1	A	115	LYS
1	A	196	LEU
1	A	205	GLU
1	A	211	LEU
1	A	229	LEU
1	A	249	LEU
1	A	257	LYS
1	A	272	LEU
1	A	274	LEU
1	A	288	LYS
1	A	342	LYS
1	A	344	PRO
1	A	421	LYS
1	A	424	LYS
1	A	454	LEU
1	A	456	LEU
1	A	469	LYS
1	A	484	GLN
1	B	36	LEU
1	B	42	THR
1	B	55	LYS
1	B	70	LYS
1	B	88	ASP
1	B	89	MET
1	B	93	VAL

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Mol	Chain	Res	Type
1	B	101	VAL
1	B	111	VAL
1	B	115	LYS
1	B	128	ARG
1	B	168	LYS
1	B	196	LEU
1	B	201	ASP
1	B	229	LEU
1	B	259	SER
1	B	264	THR
1	B	272	LEU
1	B	274	LEU
1	B	329	GLN
1	B	331	LEU
1	B	371	MET
1	B	418	ARG
1	B	433	THR
1	B	454	LEU
1	B	456	LEU
1	B	469	LYS
1	B	495	SER
1	C	34	LYS
1	C	50	ILE
1	C	70	LYS
1	C	71	VAL
1	C	93	VAL
1	C	101	VAL
1	C	119	SER
1	C	196	LEU
1	C	205	GLU
1	C	208	LYS
1	C	211	LEU
1	C	215	PHE
1	C	217	ASP
1	C	229	LEU
1	C	232	ILE
1	C	249	LEU
1	C	250	ARG
1	C	257	LYS
1	C	261	LEU
1	C	272	LEU
1	C	329	GLN

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Mol	Chain	Res	Type
1	C	331	LEU
1	C	342	LYS
1	C	371	MET
1	C	409	THR
1	C	418	ARG
1	C	425	ASP
1	C	454	LEU
1	C	456	LEU
1	C	468	CYS
1	C	469	LYS
1	C	483	LEU
1	C	496	ARG
1	D	50	ILE
1	D	62	MET
1	D	70	LYS
1	D	71	VAL
1	D	101	VAL
1	D	128	ARG
1	D	131	SER
1	D	134	SER
1	D	168	LYS
1	D	196	LEU
1	D	211	LEU
1	D	229	LEU
1	D	249	LEU
1	D	254	LYS
1	D	255	ARG
1	D	257	LYS
1	D	272	LEU
1	D	310	THR
1	D	329	GLN
1	D	331	LEU
1	D	363	THR
1	D	437	SER
1	D	440	ARG
1	D	456	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	B	352	GLN

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Mol	Chain	Res	Type
1	B	451	ASN
1	B	461	GLN
1	B	472	GLN
1	C	237	ASN
1	C	247	ASN
1	C	352	GLN
1	C	384	ASN
1	C	451	ASN
1	C	472	GLN
1	D	198	ASN
1	D	332	GLN
1	D	384	ASN
1	D	451	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)

8 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	601	3,1	41,50,50	2.50	18 (43%)	45,82,82	2.98	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	7AW	C	602	2	42,47,47	0.98	1 (2%)	44,62,62	1.85	10 (22%)
3	7AW	A	602	2	42,47,47	1.05	2 (4%)	44,62,62	1.81	9 (20%)
2	HEM	B	601	3,1	41,50,50	2.44	14 (34%)	45,82,82	3.08	21 (46%)
2	HEM	A	601	3,1	41,50,50	2.44	16 (39%)	45,82,82	2.94	19 (42%)
3	7AW	D	602	2	42,47,47	0.92	2 (4%)	44,62,62	1.92	10 (22%)
3	7AW	B	602	2	42,47,47	0.96	1 (2%)	44,62,62	1.78	5 (11%)
2	HEM	D	601	3,1	41,50,50	2.42	15 (36%)	45,82,82	3.13	19 (42%)

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	601	3,1	-	3/12/54/54	-
3	7AW	C	602	2	-	22/45/49/49	0/3/3/3
3	7AW	A	602	2	-	22/45/49/49	0/3/3/3
2	HEM	B	601	3,1	-	2/12/54/54	-
2	HEM	A	601	3,1	-	1/12/54/54	-
3	7AW	D	602	2	-	20/45/49/49	0/3/3/3
3	7AW	B	602	2	-	18/45/49/49	0/3/3/3
2	HEM	D	601	3,1	-	4/12/54/54	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C1A-NA	5.70	1.47	1.36
2	D	601	HEM	C1A-NA	5.52	1.47	1.36
2	C	601	HEM	C4A-NA	5.28	1.47	1.36
3	A	602	7AW	O39-C37	5.26	1.45	1.35
2	A	601	HEM	C4A-NA	5.16	1.46	1.36
3	B	602	7AW	O39-C37	5.16	1.45	1.35
3	C	602	7AW	O39-C37	5.06	1.44	1.35
2	B	601	HEM	C3C-C2C	4.99	1.47	1.40
2	B	601	HEM	C4A-NA	4.95	1.46	1.36
2	B	601	HEM	C1A-NA	4.91	1.46	1.36
2	A	601	HEM	C3D-C2D	4.85	1.47	1.36
2	A	601	HEM	C1A-NA	4.85	1.46	1.36
2	D	601	HEM	C3C-C2C	4.83	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	7AW	O39-C37	4.78	1.44	1.35
2	B	601	HEM	C3B-C2B	4.77	1.46	1.37
2	A	601	HEM	C3C-C2C	4.70	1.46	1.40
2	C	601	HEM	C3D-C2D	4.70	1.46	1.36
2	D	601	HEM	C4A-NA	4.69	1.45	1.36
2	B	601	HEM	C3D-C2D	4.68	1.46	1.36
2	C	601	HEM	CHA-C4D	4.52	1.46	1.35
2	D	601	HEM	CHA-C4D	4.45	1.46	1.35
2	D	601	HEM	C3D-C2D	4.42	1.46	1.36
2	C	601	HEM	C3B-C2B	4.32	1.46	1.37
2	B	601	HEM	CHA-C4D	4.31	1.46	1.35
2	D	601	HEM	C3B-C2B	4.26	1.45	1.37
2	C	601	HEM	C3C-C2C	4.21	1.46	1.40
2	A	601	HEM	C3B-C2B	4.09	1.45	1.37
2	A	601	HEM	CHA-C4D	3.98	1.45	1.35
2	C	601	HEM	CHB-C1B	3.94	1.45	1.35
2	A	601	HEM	CHB-C1B	3.70	1.44	1.35
2	B	601	HEM	CHB-C1B	3.70	1.44	1.35
2	C	601	HEM	FE-NB	3.66	2.15	1.96
2	D	601	HEM	FE-NB	3.62	2.14	1.96
2	A	601	HEM	C4D-ND	-3.60	1.34	1.40
2	A	601	HEM	C2A-C3A	3.58	1.48	1.37
2	D	601	HEM	CHB-C1B	3.57	1.44	1.35
2	D	601	HEM	C4D-ND	-3.53	1.34	1.40
2	C	601	HEM	C4D-ND	-3.50	1.34	1.40
2	B	601	HEM	FE-ND	3.31	2.13	1.96
2	A	601	HEM	FE-NB	3.23	2.12	1.96
2	B	601	HEM	FE-NB	3.21	2.12	1.96
2	C	601	HEM	FE-ND	3.21	2.12	1.96
2	B	601	HEM	C2A-C3A	3.18	1.47	1.37
2	B	601	HEM	C1B-NB	-3.11	1.34	1.40
2	D	601	HEM	C2A-C3A	3.06	1.46	1.37
2	C	601	HEM	C2A-C3A	2.94	1.46	1.37
2	A	601	HEM	C2C-C1C	2.91	1.49	1.42
2	B	601	HEM	C4D-ND	-2.83	1.35	1.40
2	A	601	HEM	FE-ND	2.76	2.10	1.96
2	D	601	HEM	C1B-NB	-2.68	1.35	1.40
2	D	601	HEM	C2C-C1C	2.62	1.48	1.42
2	D	601	HEM	FE-ND	2.55	2.09	1.96
2	C	601	HEM	C2C-C1C	2.55	1.48	1.42
2	C	601	HEM	C4A-CHB	2.50	1.47	1.41
2	A	601	HEM	C1B-C2B	2.48	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C4D-C3D	2.46	1.49	1.45
2	B	601	HEM	C2C-C1C	2.37	1.47	1.42
2	D	601	HEM	C3B-C4B	2.33	1.49	1.44
2	D	601	HEM	C1B-C2B	2.30	1.49	1.44
2	C	601	HEM	C1B-C2B	2.28	1.49	1.44
2	A	601	HEM	C1B-NB	-2.22	1.36	1.40
2	C	601	HEM	C1B-NB	-2.20	1.36	1.40
2	C	601	HEM	C1A-CHA	2.17	1.47	1.41
2	A	601	HEM	C1D-C2D	2.16	1.48	1.44
3	A	602	7AW	C26-S27	2.13	1.74	1.70
3	D	602	7AW	C26-S27	2.09	1.73	1.70
2	C	601	HEM	O2A-CGA	-2.06	1.23	1.30
2	A	601	HEM	CHD-C1D	2.01	1.46	1.41
2	B	601	HEM	C1B-C2B	2.00	1.48	1.44

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	HEM	C3B-C2B-C1B	-9.70	99.29	106.49
2	D	601	HEM	C3B-C2B-C1B	-8.97	99.83	106.49
2	D	601	HEM	C2B-C1B-NB	8.82	120.29	109.84
2	A	601	HEM	C3B-C2B-C1B	-8.80	99.95	106.49
2	B	601	HEM	C3B-C2B-C1B	-8.45	100.22	106.49
2	B	601	HEM	C2B-C1B-NB	7.99	119.31	109.84
2	A	601	HEM	C2B-C1B-NB	7.50	118.72	109.84
2	C	601	HEM	C2B-C1B-NB	7.28	118.46	109.84
2	C	601	HEM	C2D-C1D-ND	6.39	117.54	109.88
2	B	601	HEM	C2D-C1D-ND	6.39	117.54	109.88
2	D	601	HEM	C2D-C1D-ND	6.22	117.34	109.88
3	D	602	7AW	C42-N43-C44	6.10	115.30	105.78
3	B	602	7AW	C42-N43-C44	6.05	115.23	105.78
2	B	601	HEM	C3D-C4D-ND	6.04	116.89	110.17
2	A	601	HEM	C3D-C4D-ND	6.02	116.87	110.17
3	A	602	7AW	C42-N43-C44	5.94	115.05	105.78
2	D	601	HEM	C1D-C2D-C3D	-5.90	100.75	106.96
2	C	601	HEM	C1D-C2D-C3D	-5.51	101.16	106.96
2	A	601	HEM	C2D-C1D-ND	5.51	116.48	109.88
2	D	601	HEM	C1B-NB-C4B	-5.50	99.39	105.07
2	B	601	HEM	C1D-C2D-C3D	-5.15	101.54	106.96
2	C	601	HEM	C3D-C4D-ND	4.88	115.60	110.17
2	A	601	HEM	C1D-C2D-C3D	-4.87	101.83	106.96
3	D	602	7AW	C24-C25-C26	-4.87	122.29	129.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	7AW	C24-C25-C26	-4.79	122.42	129.62
3	C	602	7AW	C42-N43-C44	4.78	113.24	105.78
3	D	602	7AW	C29-C28-N32	4.77	134.16	125.08
2	D	601	HEM	C3D-C4D-ND	4.73	115.43	110.17
3	A	602	7AW	C04-N36-C37	4.64	129.45	122.30
3	C	602	7AW	C29-C28-N32	4.55	133.74	125.08
3	B	602	7AW	O39-C37-N36	4.54	119.73	110.50
2	A	601	HEM	C1B-NB-C4B	-4.54	100.39	105.07
3	B	602	7AW	C24-C25-C26	-4.50	122.84	129.62
2	B	601	HEM	C1B-NB-C4B	-4.47	100.46	105.07
2	D	601	HEM	CBD-CAD-C3D	-4.24	100.83	112.63
2	C	601	HEM	CHD-C1D-C2D	-4.17	118.46	124.98
3	A	602	7AW	C24-C25-C26	-4.15	123.38	129.62
3	B	602	7AW	C29-C28-N32	4.13	132.94	125.08
3	B	602	7AW	O39-C37-O38	-4.09	116.39	124.25
2	C	601	HEM	C1B-NB-C4B	-4.07	100.87	105.07
2	B	601	HEM	C4A-C3A-C2A	-4.06	104.17	107.00
2	C	601	HEM	CBD-CAD-C3D	-4.06	101.35	112.63
2	B	601	HEM	C4B-C3B-C2B	-4.03	103.91	107.11
2	B	601	HEM	C4D-ND-C1D	-4.03	100.91	105.07
2	C	601	HEM	CMB-C2B-C1B	3.97	131.09	125.04
3	D	602	7AW	O39-C37-O38	-3.94	116.69	124.25
2	D	601	HEM	C4A-C3A-C2A	-3.92	104.27	107.00
3	C	602	7AW	C04-N36-C37	3.78	128.12	122.30
3	C	602	7AW	O39-C37-O38	-3.69	117.16	124.25
3	A	602	7AW	C29-C28-N32	3.64	132.00	125.08
2	B	601	HEM	CBD-CAD-C3D	-3.50	102.90	112.63
2	C	601	HEM	CHC-C4B-C3B	-3.49	119.23	124.57
2	A	601	HEM	C4A-C3A-C2A	-3.49	104.57	107.00
2	D	601	HEM	CHD-C1D-C2D	-3.46	119.58	124.98
2	A	601	HEM	CBD-CAD-C3D	-3.43	103.09	112.63
2	D	601	HEM	C4B-C3B-C2B	-3.41	104.41	107.11
3	C	602	7AW	O39-C37-N36	3.39	117.40	110.50
3	A	602	7AW	C09-C08-C07	-3.38	106.10	113.78
2	B	601	HEM	CHD-C1D-C2D	-3.37	119.72	124.98
2	A	601	HEM	CMB-C2B-C1B	3.30	130.07	125.04
2	A	601	HEM	CHC-C4B-C3B	-3.24	119.61	124.57
2	A	601	HEM	C4B-C3B-C2B	-3.16	104.60	107.11
2	D	601	HEM	CHB-C1B-C2B	-3.16	117.97	126.72
3	D	602	7AW	O39-C37-N36	3.16	116.92	110.50
2	C	601	HEM	C4D-ND-C1D	-3.09	101.88	105.07
3	D	602	7AW	C04-N36-C37	3.08	127.05	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	HEM	CMD-C2D-C1D	3.01	129.62	125.04
3	A	602	7AW	O39-C37-O38	-2.99	118.52	124.25
3	D	602	7AW	C03-C04-N36	2.98	114.74	110.54
2	A	601	HEM	CMD-C2D-C1D	2.97	129.56	125.04
2	A	601	HEM	C4D-ND-C1D	-2.96	102.02	105.07
2	B	601	HEM	CHB-C1B-C2B	-2.91	118.67	126.72
3	A	602	7AW	O39-C37-N36	2.90	116.39	110.50
2	A	601	HEM	C4D-C3D-C2D	-2.89	102.69	106.90
2	D	601	HEM	C4D-ND-C1D	-2.89	102.09	105.07
2	B	601	HEM	CBA-CAA-C2A	-2.88	107.70	112.62
2	A	601	HEM	CHD-C1D-C2D	-2.87	120.50	124.98
2	C	601	HEM	CHB-C1B-NB	-2.84	120.87	124.38
2	B	601	HEM	CAD-C3D-C4D	2.79	129.54	124.66
3	A	602	7AW	C03-C04-N36	2.78	114.45	110.54
2	B	601	HEM	CMD-C2D-C1D	2.68	129.12	125.04
2	B	601	HEM	C4D-C3D-C2D	-2.68	103.00	106.90
2	D	601	HEM	CMB-C2B-C1B	2.67	129.10	125.04
2	B	601	HEM	CMC-C2C-C3C	2.66	129.65	124.68
3	C	602	7AW	C05-C04-N36	2.66	114.28	110.54
3	C	602	7AW	C06-C07-N15	2.64	114.25	110.54
2	D	601	HEM	CMC-C2C-C3C	2.59	129.53	124.68
2	A	601	HEM	CHB-C1B-NB	-2.56	121.22	124.38
2	D	601	HEM	CAA-CBA-CGA	-2.51	106.72	113.76
2	A	601	HEM	CHA-C4D-C3D	-2.48	120.67	125.33
2	A	601	HEM	CHB-C1B-C2B	-2.46	119.92	126.72
2	B	601	HEM	CHC-C4B-C3B	-2.45	120.81	124.57
2	C	601	HEM	CMD-C2D-C1D	2.40	128.69	125.04
2	D	601	HEM	CHC-C4B-C3B	-2.37	120.94	124.57
3	C	602	7AW	C09-C08-C07	-2.35	108.44	113.78
3	C	602	7AW	C25-C24-N22	-2.33	109.60	113.60
2	C	601	HEM	CAD-C3D-C4D	2.30	128.67	124.66
2	B	601	HEM	CHA-C4D-C3D	-2.22	121.16	125.33
2	C	601	HEM	CHB-C1B-C2B	-2.22	120.58	126.72
3	D	602	7AW	C18-N19-C20	2.17	126.72	122.39
3	D	602	7AW	C09-C08-C07	-2.17	108.85	113.78
2	C	601	HEM	C4D-C3D-C2D	-2.16	103.74	106.90
2	A	601	HEM	CMC-C2C-C3C	2.16	128.72	124.68
2	B	601	HEM	CHA-C4D-ND	-2.16	121.71	124.38
2	D	601	HEM	CHB-C1B-NB	-2.16	121.72	124.38
3	A	602	7AW	C25-C24-N22	-2.16	109.90	113.60
3	D	602	7AW	C33-C18-C16	-2.15	106.00	111.38
2	C	601	HEM	C4A-C3A-C2A	-2.13	105.52	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CHB-C1B-NB	-2.10	121.79	124.38
2	D	601	HEM	CHA-C4D-C3D	-2.09	121.40	125.33
2	C	601	HEM	CHA-C4D-ND	-2.02	121.89	124.38

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	C2B-C3B-CAB-CBB
2	D	601	HEM	C2B-C3B-CAB-CBB
3	A	602	7AW	C03-C04-N36-C37
3	A	602	7AW	C02-C03-C04-C05
3	A	602	7AW	N36-C04-C05-C06
3	A	602	7AW	C03-C04-C05-C06
3	A	602	7AW	C06-C07-C08-C09
3	A	602	7AW	N15-C07-C08-C09
3	A	602	7AW	O21-C20-N19-C18
3	A	602	7AW	N22-C20-N19-C18
3	A	602	7AW	N19-C20-N22-C23
3	A	602	7AW	N19-C20-N22-C24
3	A	602	7AW	O21-C20-N22-C23
3	A	602	7AW	O21-C20-N22-C24
3	B	602	7AW	C03-C04-N36-C37
3	B	602	7AW	C02-C03-C04-C05
3	B	602	7AW	C04-C05-C06-C07
3	B	602	7AW	C06-C07-C08-C09
3	B	602	7AW	N15-C07-C08-C09
3	B	602	7AW	O21-C20-N19-C18
3	B	602	7AW	N22-C20-N19-C18
3	B	602	7AW	N19-C20-N22-C23
3	B	602	7AW	N19-C20-N22-C24
3	B	602	7AW	O21-C20-N22-C23
3	B	602	7AW	O21-C20-N22-C24
3	C	602	7AW	C03-C04-N36-C37
3	C	602	7AW	N36-C04-C05-C06
3	C	602	7AW	C03-C04-C05-C06
3	C	602	7AW	C06-C07-C08-C09
3	C	602	7AW	N15-C07-C08-C09
3	C	602	7AW	C16-C18-C33-C35
3	C	602	7AW	C16-C18-C33-C34
3	C	602	7AW	O21-C20-N19-C18
3	C	602	7AW	N22-C20-N19-C18

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Mol	Chain	Res	Type	Atoms
3	C	602	7AW	N19-C20-N22-C23
3	C	602	7AW	N19-C20-N22-C24
3	C	602	7AW	O21-C20-N22-C23
3	C	602	7AW	O21-C20-N22-C24
3	D	602	7AW	C03-C04-N36-C37
3	D	602	7AW	N36-C04-C05-C06
3	D	602	7AW	C03-C04-C05-C06
3	D	602	7AW	C06-C07-C08-C09
3	D	602	7AW	N15-C07-C08-C09
3	D	602	7AW	O21-C20-N19-C18
3	D	602	7AW	N22-C20-N19-C18
3	D	602	7AW	N19-C20-N22-C23
3	D	602	7AW	N19-C20-N22-C24
3	D	602	7AW	O21-C20-N22-C23
3	D	602	7AW	O21-C20-N22-C24
3	C	602	7AW	O17-C16-N15-C07
3	D	602	7AW	O17-C16-N15-C07
3	D	602	7AW	C18-C16-N15-C07
3	D	602	7AW	N19-C18-C33-C35
3	B	602	7AW	O39-C37-N36-C04
3	C	602	7AW	C18-C16-N15-C07
3	D	602	7AW	O38-C37-O39-C40
3	D	602	7AW	C16-C18-C33-C35
3	D	602	7AW	N36-C37-O39-C40
3	C	602	7AW	N19-C18-C33-C35
3	D	602	7AW	N19-C18-C33-C34
3	C	602	7AW	N19-C18-C33-C34
3	B	602	7AW	C18-C16-N15-C07
3	D	602	7AW	C16-C18-C33-C34
3	B	602	7AW	O38-C37-N36-C04
3	A	602	7AW	N19-C18-C33-C34
3	B	602	7AW	O17-C16-N15-C07
3	A	602	7AW	C16-C18-C33-C34
3	A	602	7AW	C16-C18-C33-C35
3	B	602	7AW	C02-C03-C04-N36
3	A	602	7AW	N19-C18-C33-C35
3	A	602	7AW	O39-C37-N36-C04
3	A	602	7AW	O38-C37-N36-C04
3	C	602	7AW	O38-C37-O39-C40
3	C	602	7AW	N36-C37-O39-C40
3	B	602	7AW	C01-C02-C03-C04
2	C	601	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	D	601	HEM	C4B-C3B-CAB-CBB
3	A	602	7AW	C01-C02-C03-C04
3	C	602	7AW	C01-C02-C03-C04
3	A	602	7AW	C33-C18-N19-C20
3	C	602	7AW	C02-C03-C04-C05
3	D	602	7AW	C02-C03-C04-C05
3	A	602	7AW	C02-C03-C04-N36
3	B	602	7AW	C05-C04-N36-C37
2	C	601	HEM	C2A-CAA-CBA-CGA
3	A	602	7AW	N32-C28-C29-C30
3	C	602	7AW	N32-C28-C29-C31
2	B	601	HEM	CAD-CBD-CGD-O2D
2	B	601	HEM	CAD-CBD-CGD-O1D
2	D	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAD-CBD-CGD-O2D

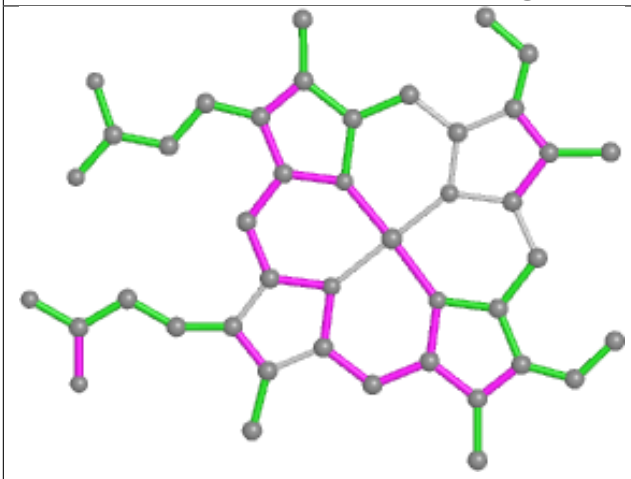
There are no ring outliers.

8 monomers are involved in 38 short contacts:

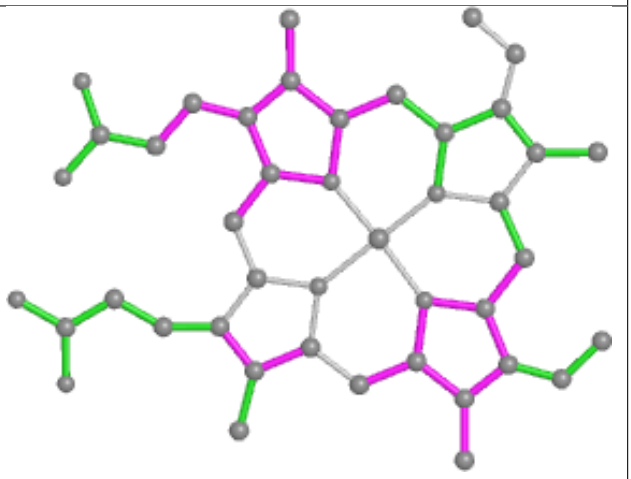
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	8	0
3	C	602	7AW	4	0
3	A	602	7AW	8	0
2	B	601	HEM	4	0
2	A	601	HEM	8	0
3	D	602	7AW	4	0
3	B	602	7AW	5	0
2	D	601	HEM	11	0

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.

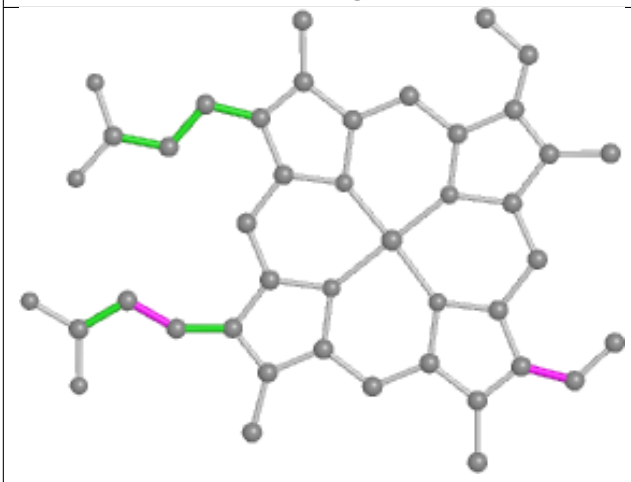
Ligand HEM C 601



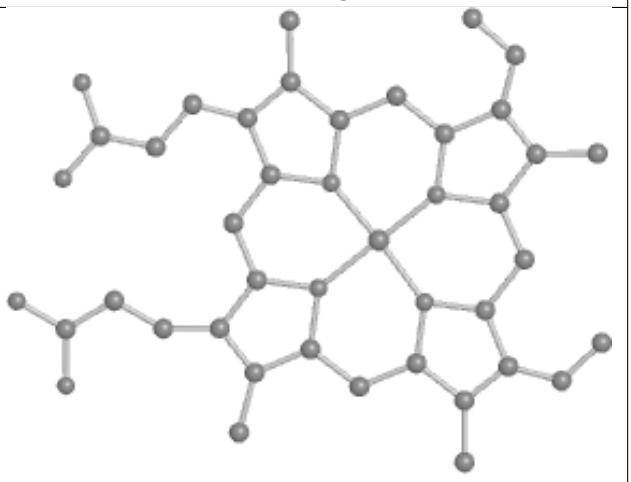
Bond lengths



Bond angles

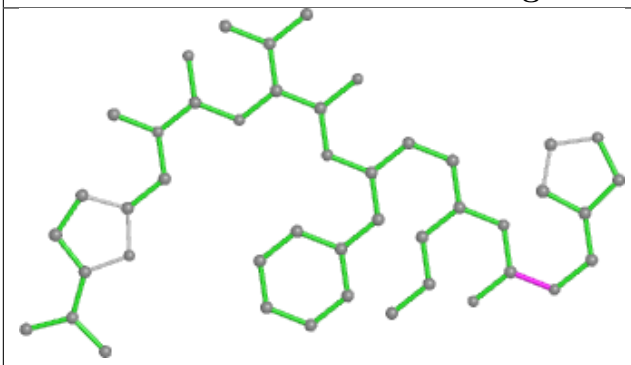


Torsions

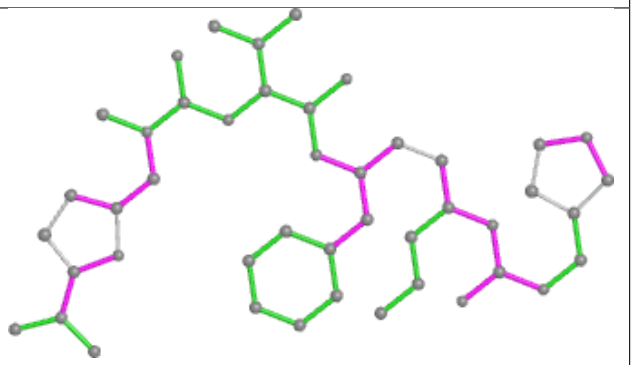


Rings

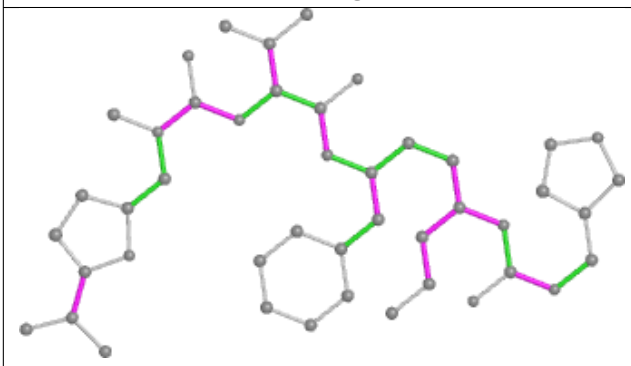
Ligand 7AW C 602



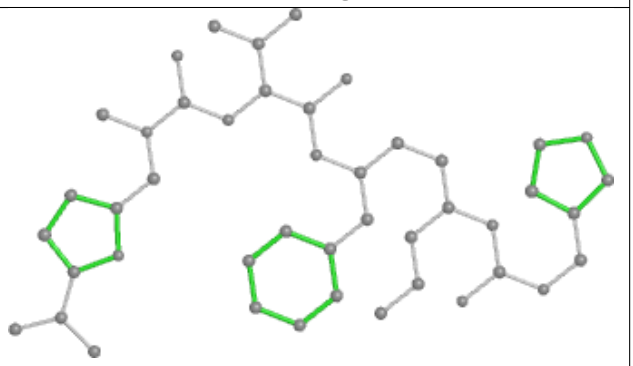
Bond lengths



Bond angles

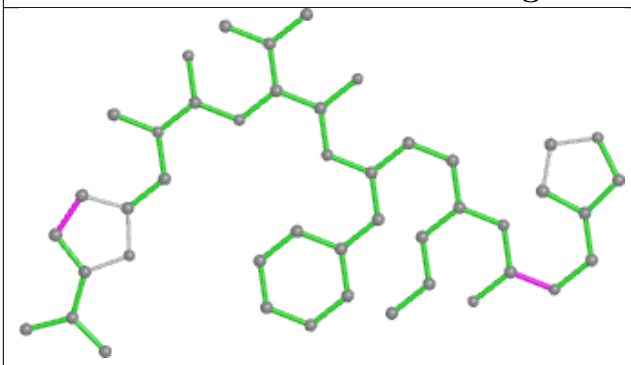


Torsions

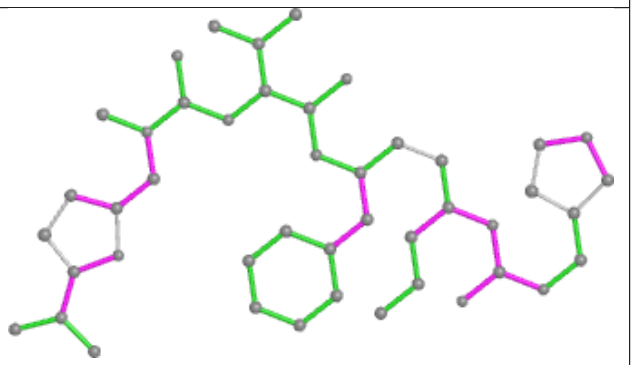


Rings

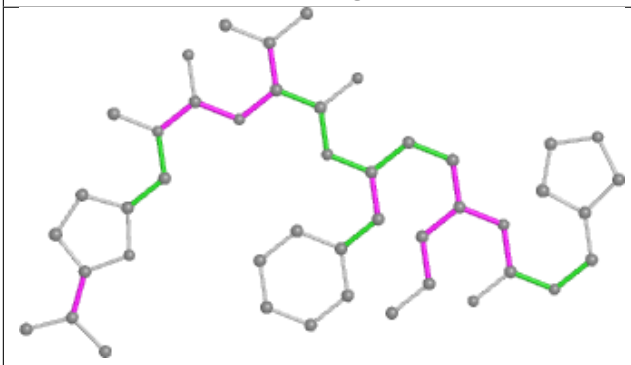
Ligand 7AW A 602



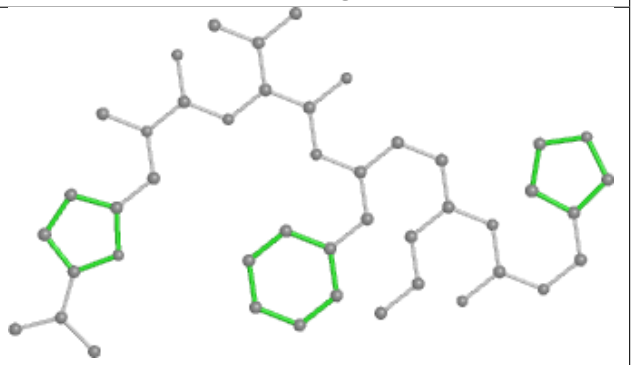
Bond lengths



Bond angles

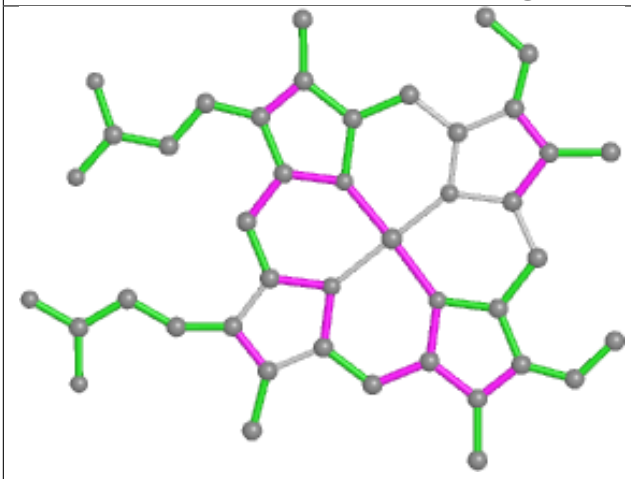


Torsions

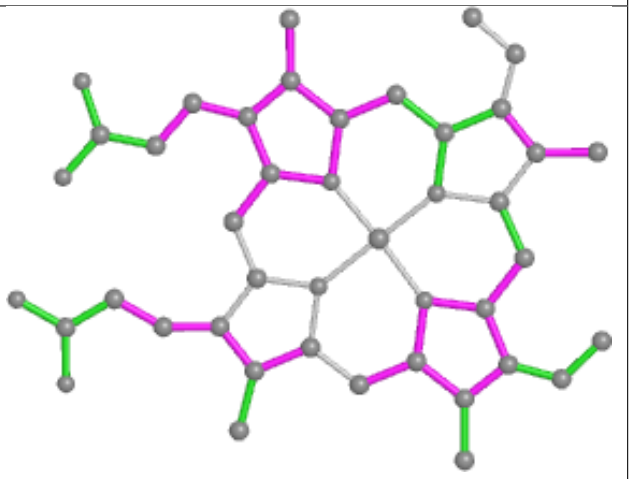


Rings

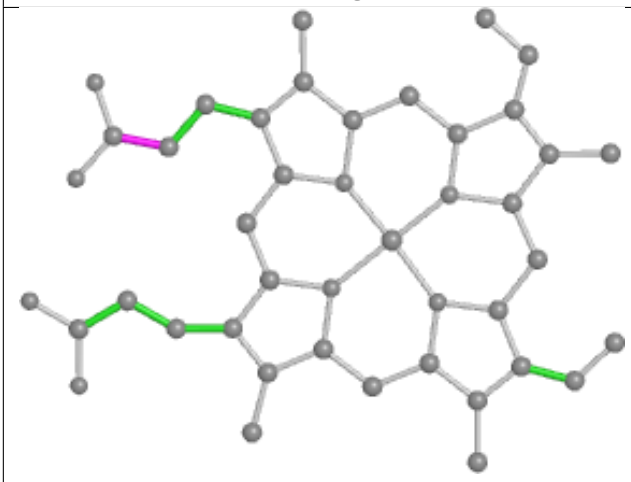
Ligand HEM B 601



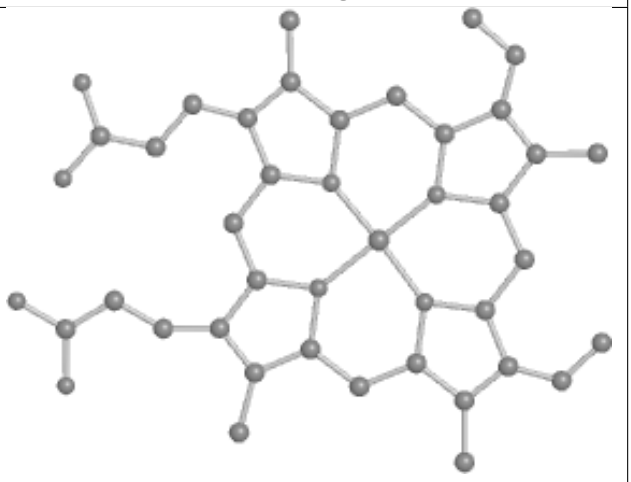
Bond lengths



Bond angles

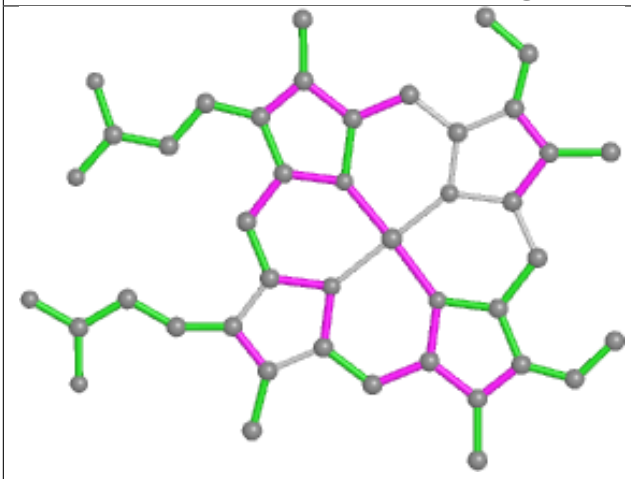


Torsions

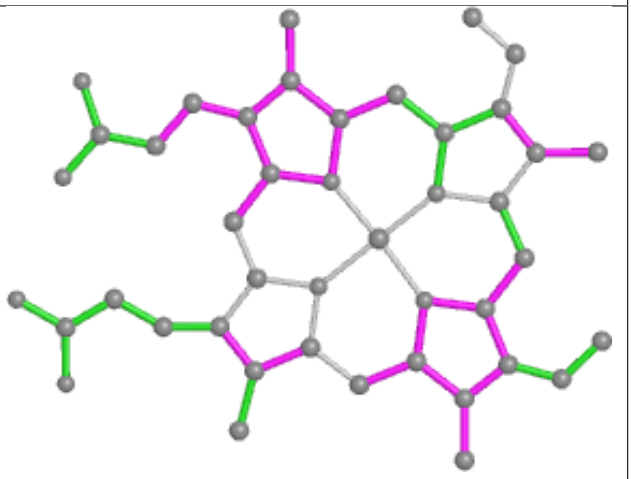


Rings

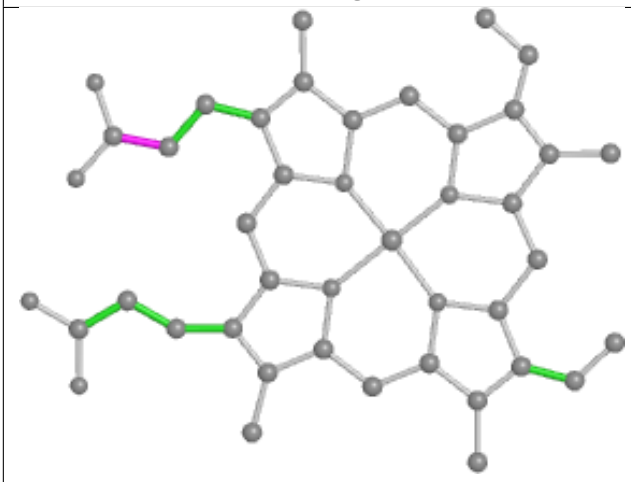
Ligand HEM A 601



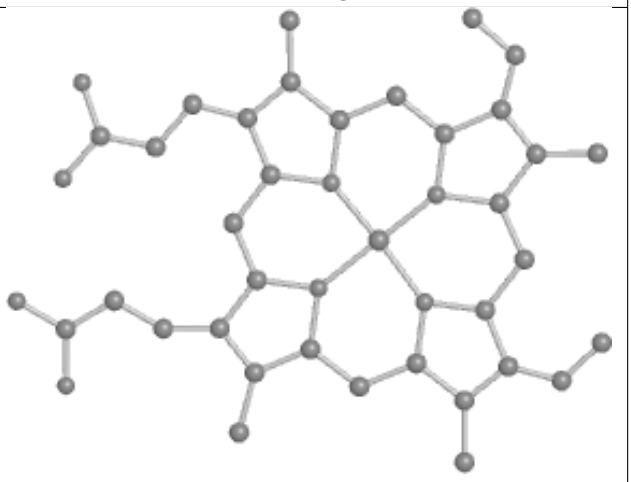
Bond lengths



Bond angles

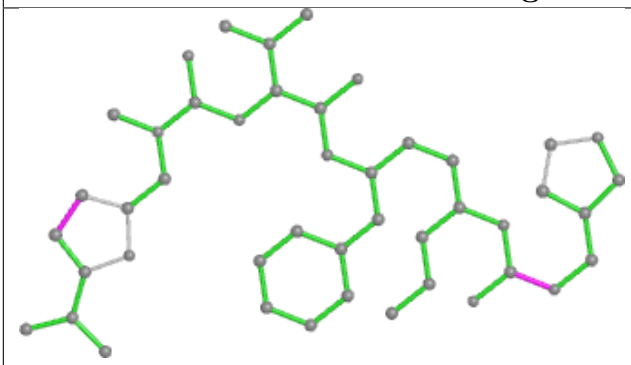


Torsions

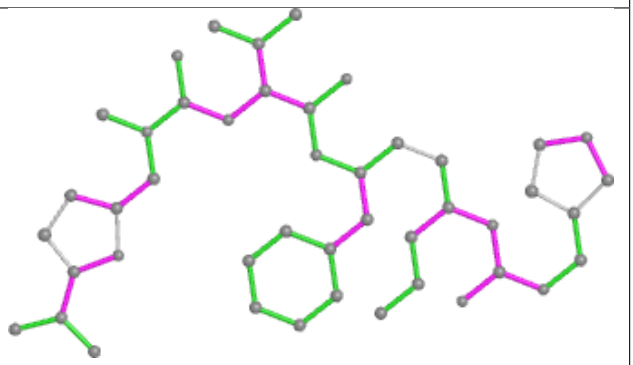


Rings

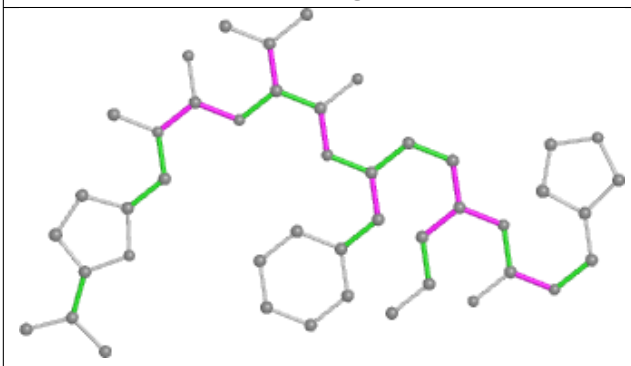
Ligand 7AW D 602



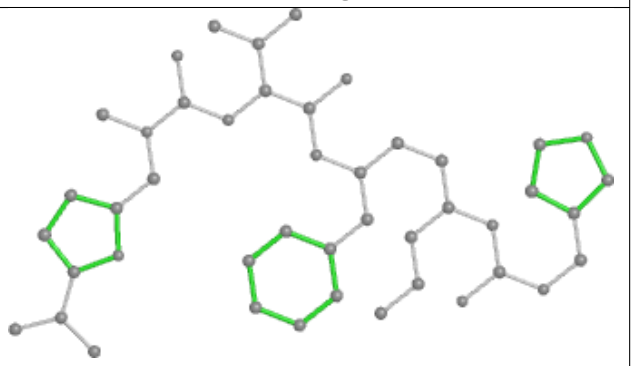
Bond lengths



Bond angles

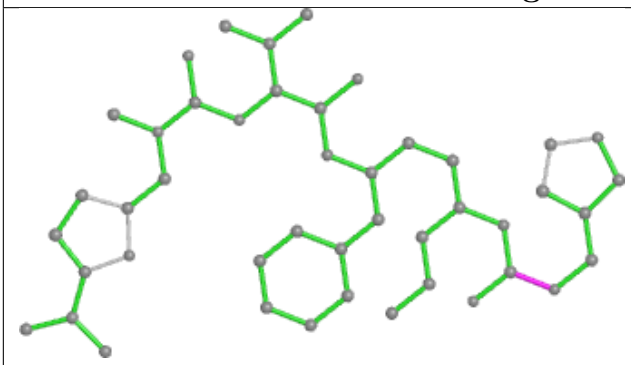


Torsions

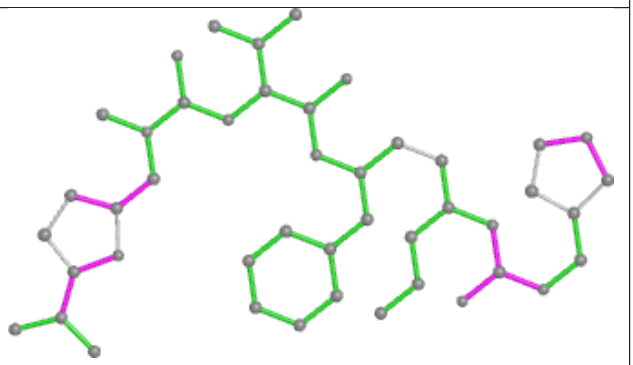


Rings

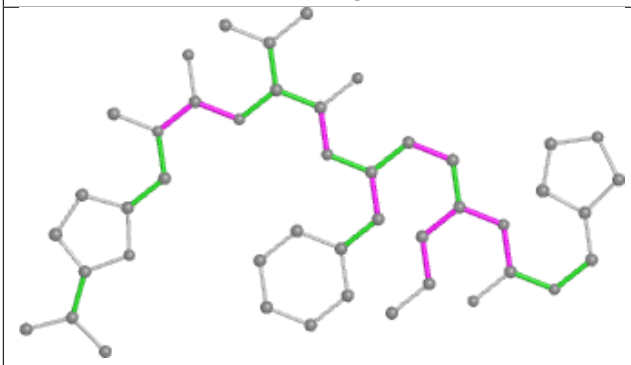
Ligand 7AW B 602



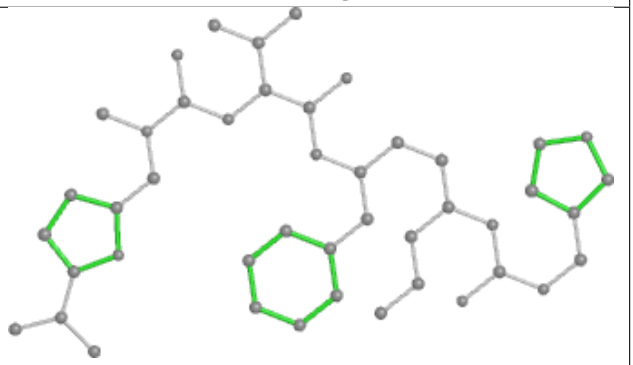
Bond lengths



Bond angles

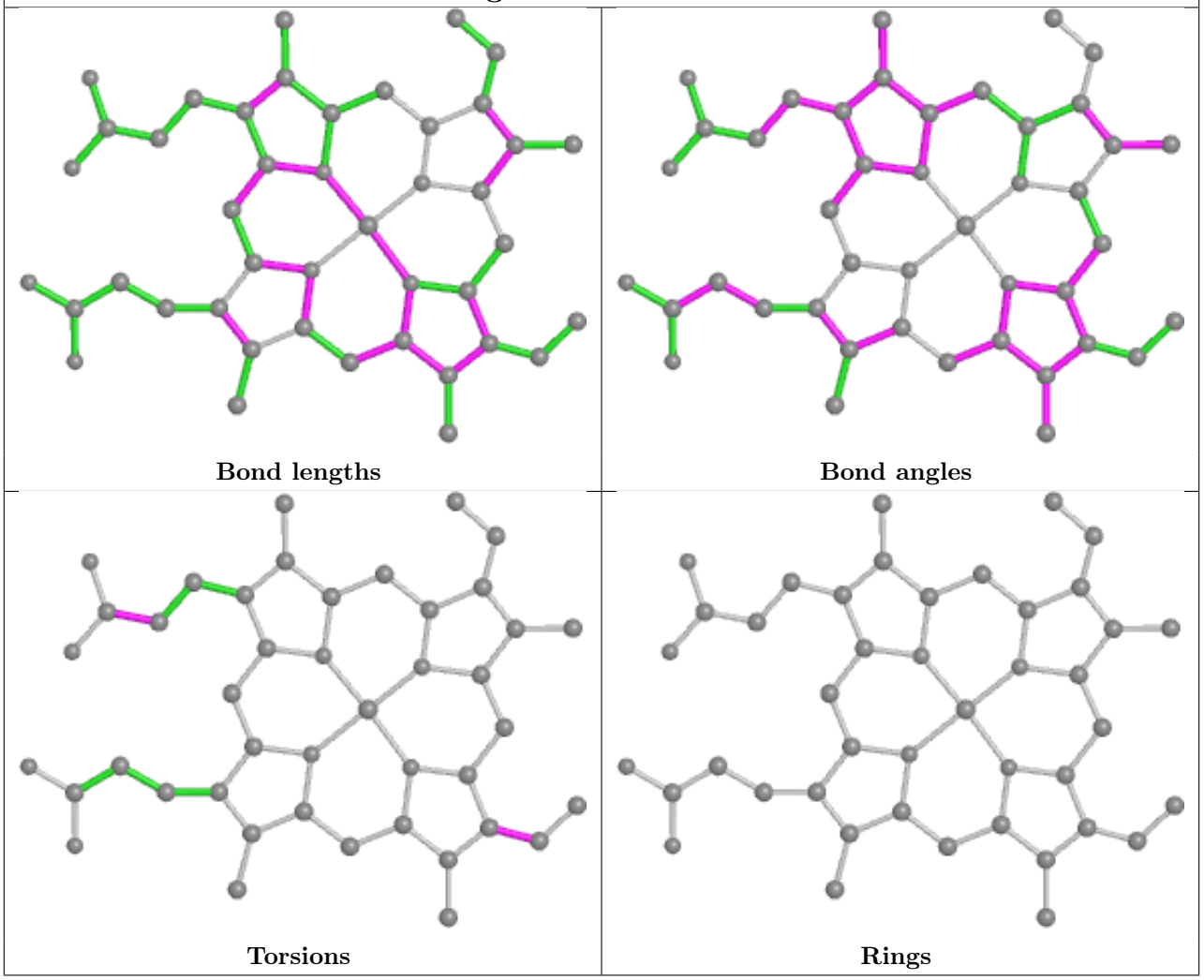


Torsions



Rings

Ligand HEM D 601



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	458/487 (94%)	0.33	12 (2%)	56	54	35, 57, 80, 103	0
1	B	457/487 (93%)	0.18	15 (3%)	46	45	35, 58, 80, 110	0
1	C	458/487 (94%)	0.26	23 (5%)	28	27	36, 59, 85, 104	0
1	D	458/487 (94%)	0.46	26 (5%)	23	22	38, 61, 87, 113	0
All	All	1831/1948 (93%)	0.31	76 (4%)	36	35	35, 59, 84, 113	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	PHE	4.5
1	B	280	ASN	4.5
1	D	481	GLY	4.4
1	B	212	ARG	4.1
1	C	468	CYS	3.6
1	D	422	LYS	3.6
1	D	341	ASN	3.5
1	C	341	ASN	3.3
1	D	337	ALA	3.3
1	D	473	ILE	3.2
1	A	422	LYS	3.2
1	A	55	LYS	3.2
1	A	331	LEU	3.1
1	D	264	THR	3.1
1	D	385	GLY	3.1
1	D	321	LEU	3.1
1	C	215	PHE	3.1
1	C	255	ARG	3.1
1	D	382	GLU	3.0
1	C	216	LEU	3.0
1	D	215	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	225	VAL	2.9
1	D	165	GLU	2.8
1	D	494	GLU	2.8
1	D	262	GLU	2.7
1	D	289	ALA	2.7
1	D	495	SER	2.7
1	B	35	LYS	2.7
1	D	340	PRO	2.7
1	C	191	VAL	2.6
1	B	259	SER	2.6
1	C	492	LYS	2.6
1	B	171	THR	2.6
1	C	469	LYS	2.6
1	B	37	GLY	2.6
1	C	267	HIS	2.5
1	D	443	ILE	2.5
1	C	386	MET	2.5
1	B	492	LYS	2.5
1	A	34	LYS	2.5
1	C	227	PRO	2.5
1	B	487	LYS	2.5
1	A	235	VAL	2.4
1	D	164	ALA	2.4
1	D	413	LYS	2.4
1	C	170	VAL	2.4
1	C	479	LEU	2.4
1	C	212	ARG	2.4
1	D	463	PHE	2.3
1	C	481	GLY	2.3
1	C	425	ASP	2.3
1	A	492	LYS	2.3
1	B	289	ALA	2.3
1	C	167	GLY	2.2
1	A	410	GLU	2.2
1	C	166	THR	2.2
1	D	335	ILE	2.2
1	D	280	ASN	2.2
1	D	69	GLY	2.2
1	B	36	LEU	2.2
1	B	277	ASP	2.2
1	B	469	LYS	2.1
1	B	225	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	2.1
1	A	470	GLU	2.1
1	B	157	VAL	2.1
1	C	225	VAL	2.1
1	C	384	ASN	2.1
1	C	34	LYS	2.1
1	A	468	CYS	2.1
1	C	262	GLU	2.0
1	A	254	LYS	2.0
1	D	474	PRO	2.0
1	B	30	HIS	2.0
1	A	289	ALA	2.0
1	D	424	LYS	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.

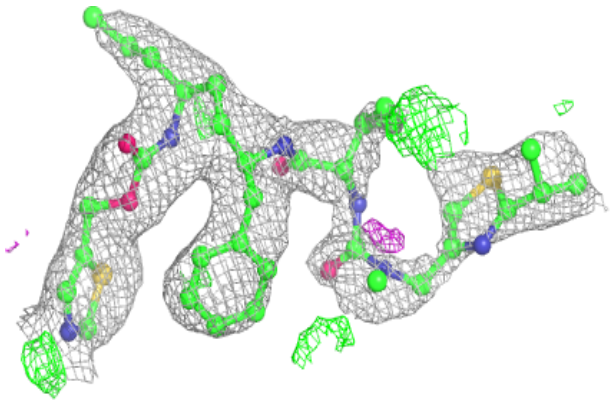
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	7AW	D	602	45/45	0.88	0.24	53,78,106,110	0
3	7AW	B	602	45/45	0.91	0.20	55,72,154,157	0
3	7AW	A	602	45/45	0.92	0.22	51,68,94,95	0
3	7AW	C	602	45/45	0.94	0.21	42,68,120,121	0
2	HEM	A	601	43/43	0.98	0.21	31,35,39,40	0
2	HEM	B	601	43/43	0.98	0.17	36,45,49,50	0
2	HEM	C	601	43/43	0.98	0.17	38,40,43,44	0
2	HEM	D	601	43/43	0.98	0.20	42,44,46,47	0

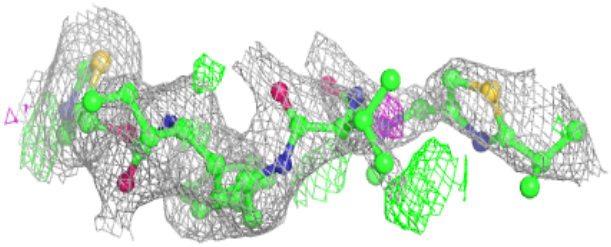
The following is a graphical depiction of the model fit to experimental electron density of all

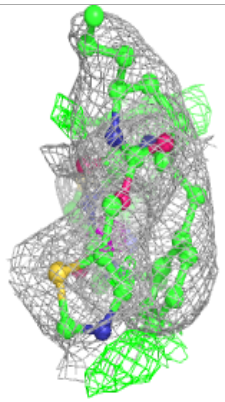
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 7AW D 602:

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

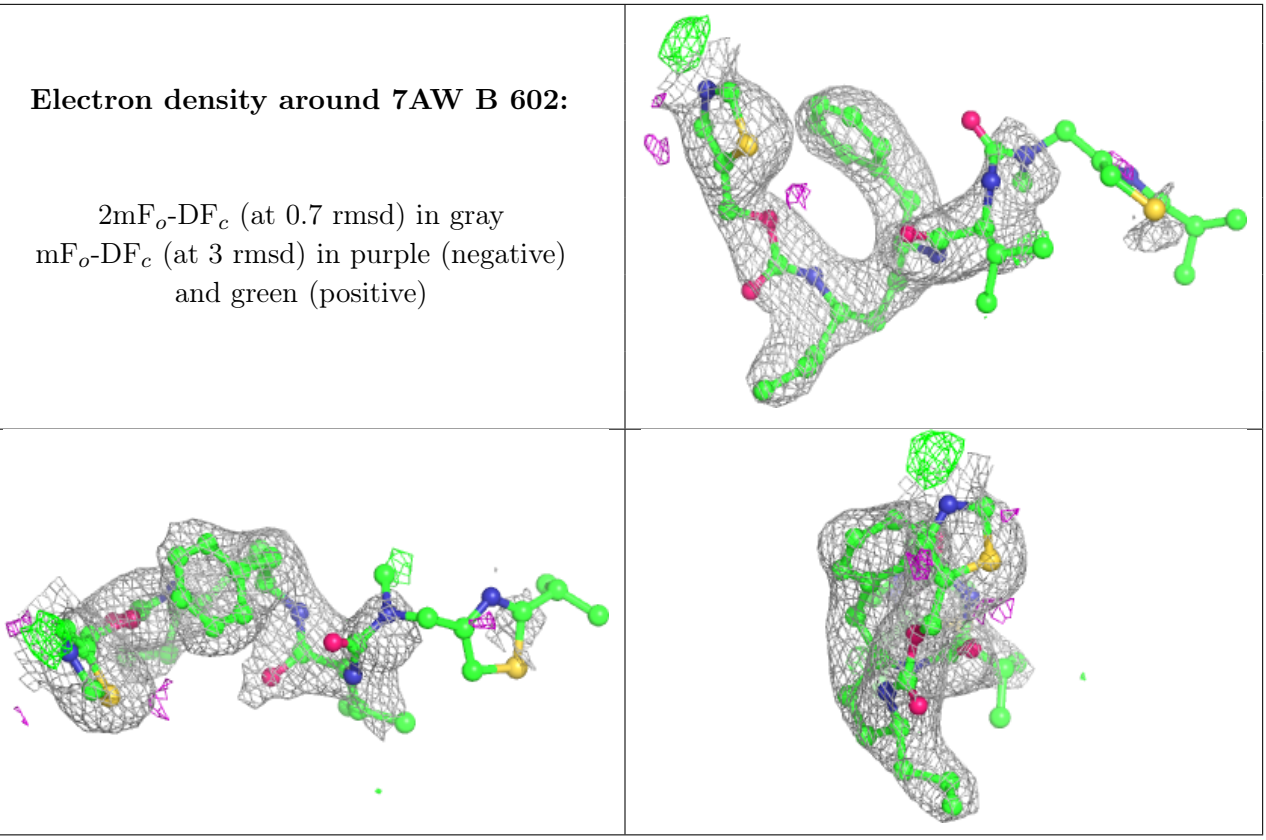






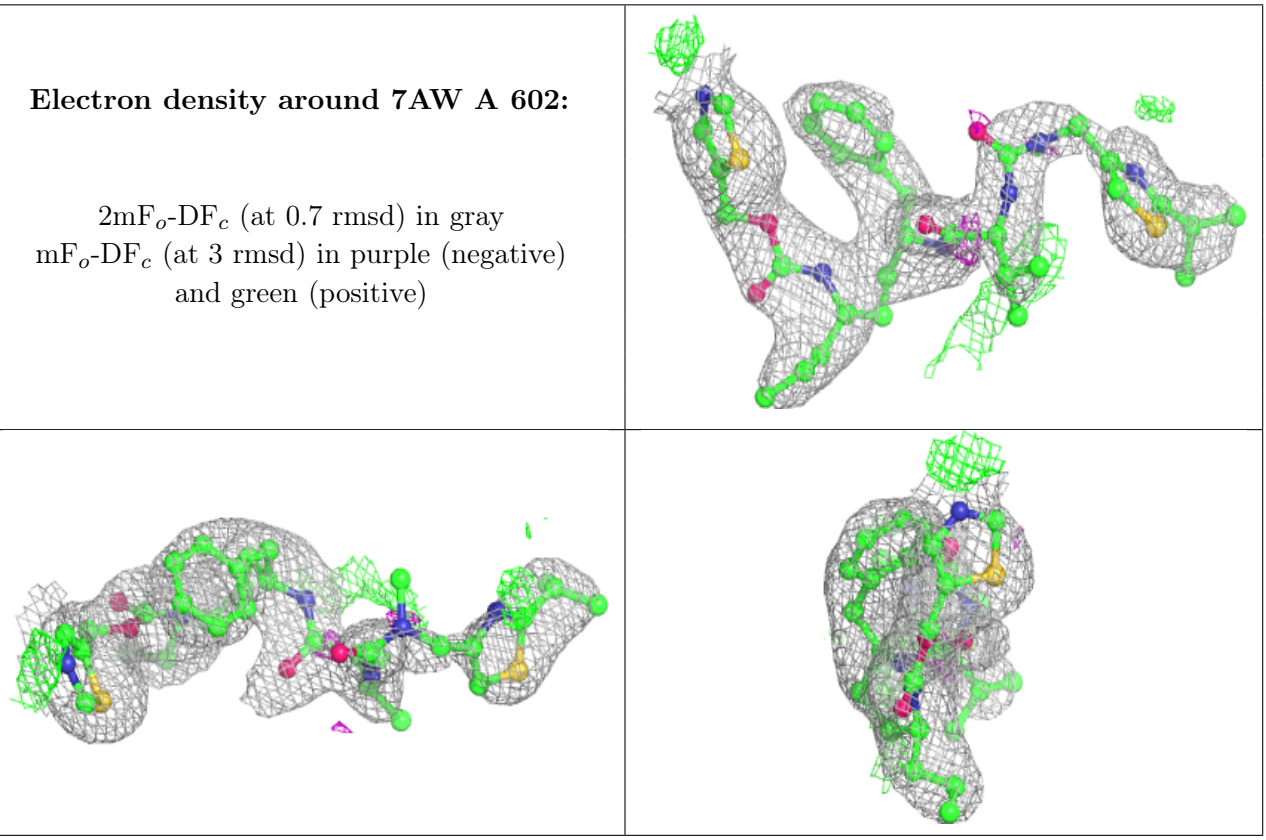
Electron density around 7AW B 602:

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



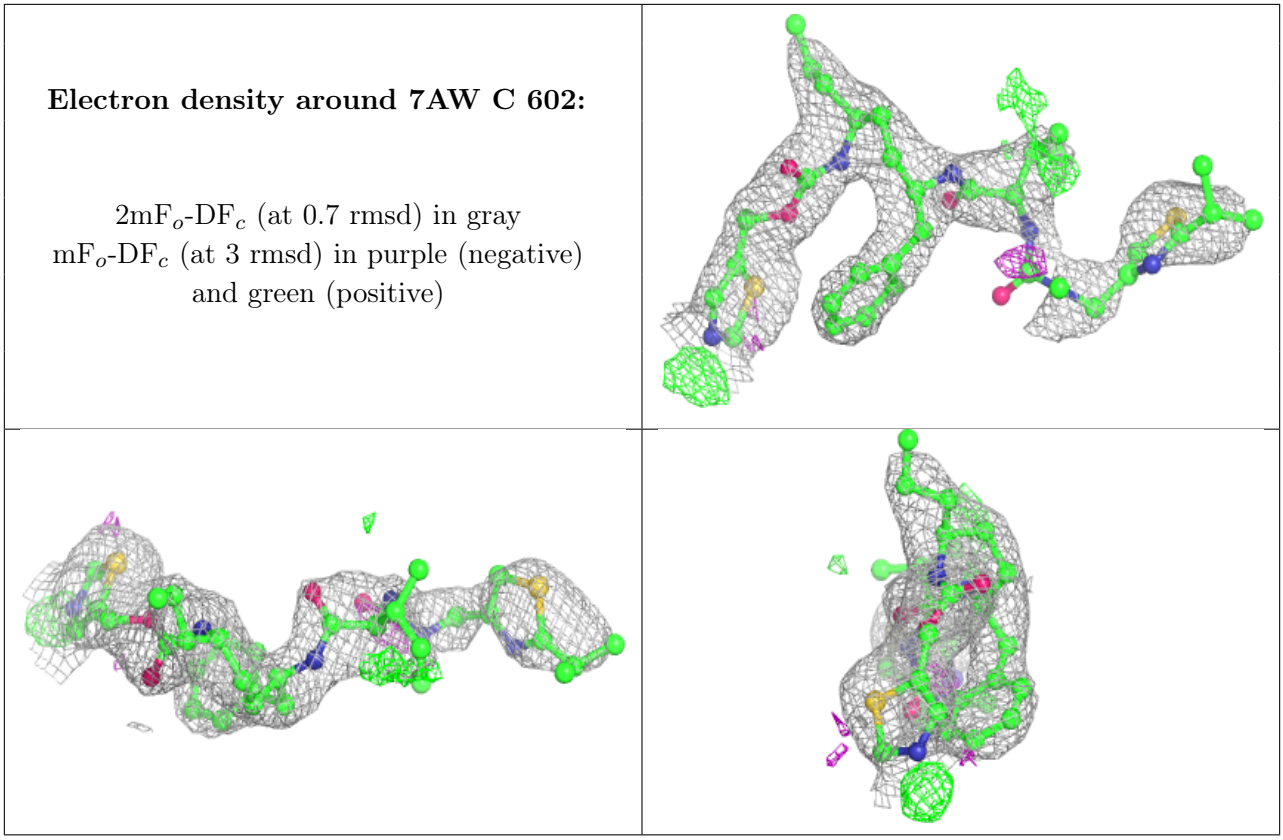
Electron density around 7AW A 602:

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



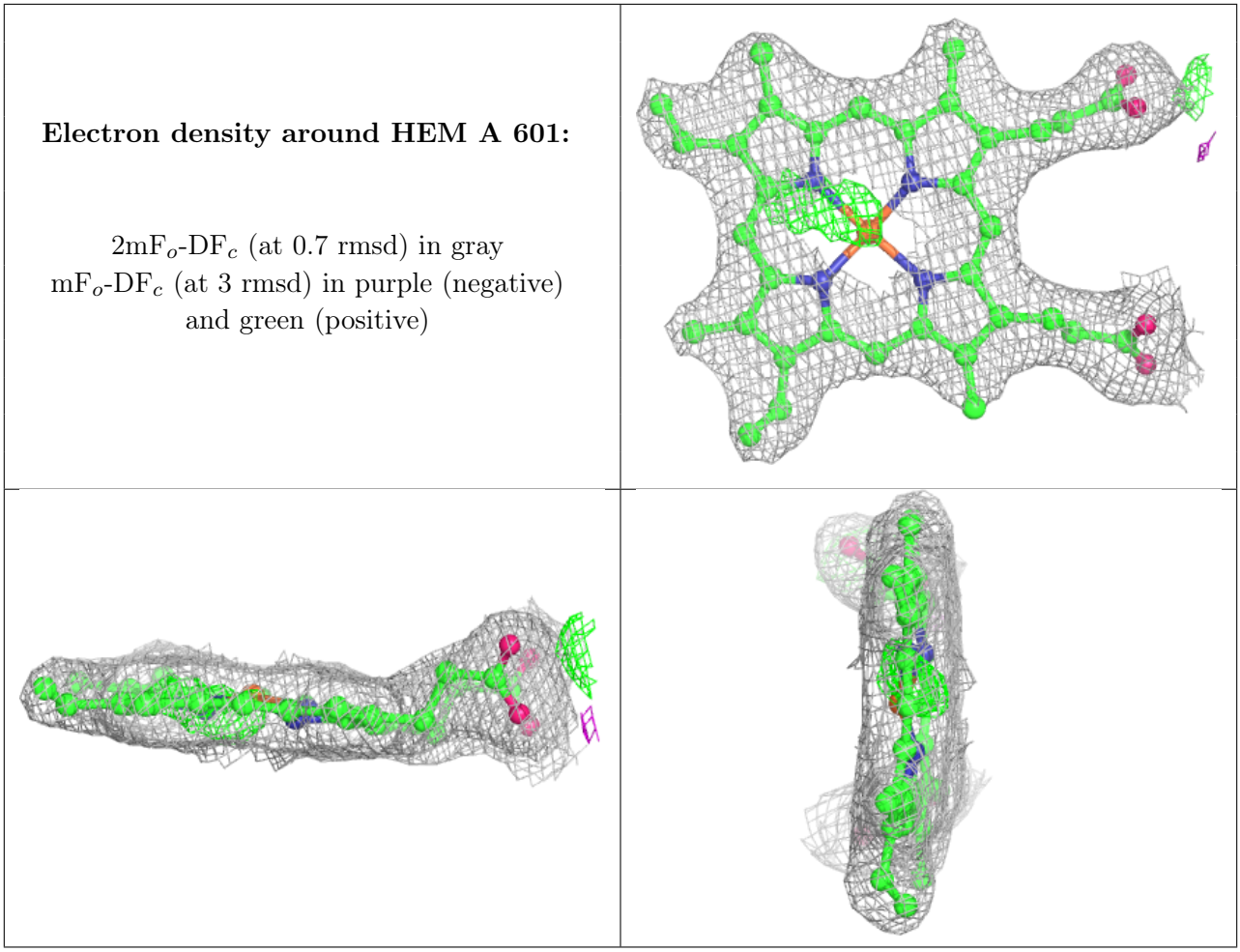
Electron density around 7AW C 602:

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



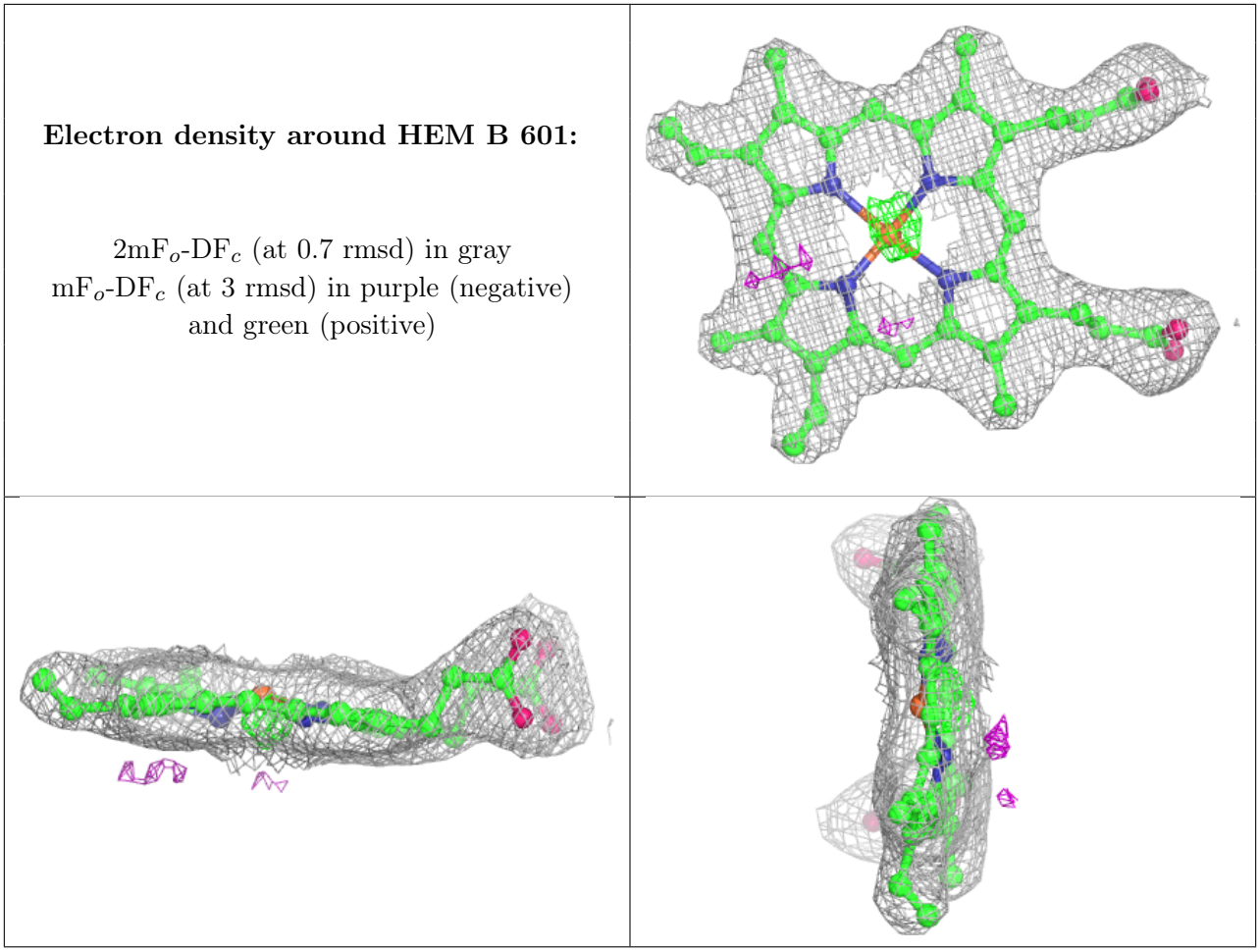
Electron density around HEM A 601:

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



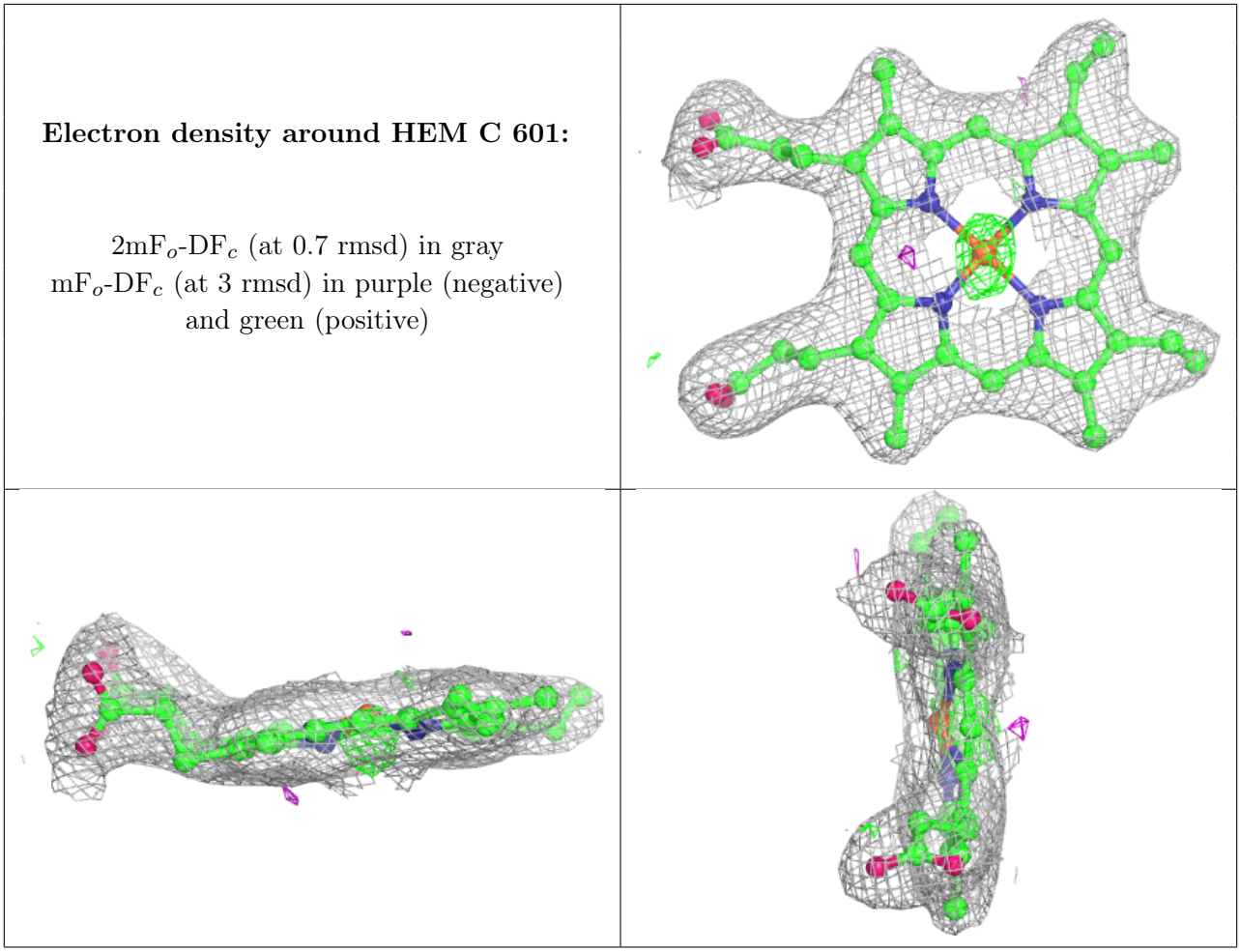
Electron density around HEM B 601:

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



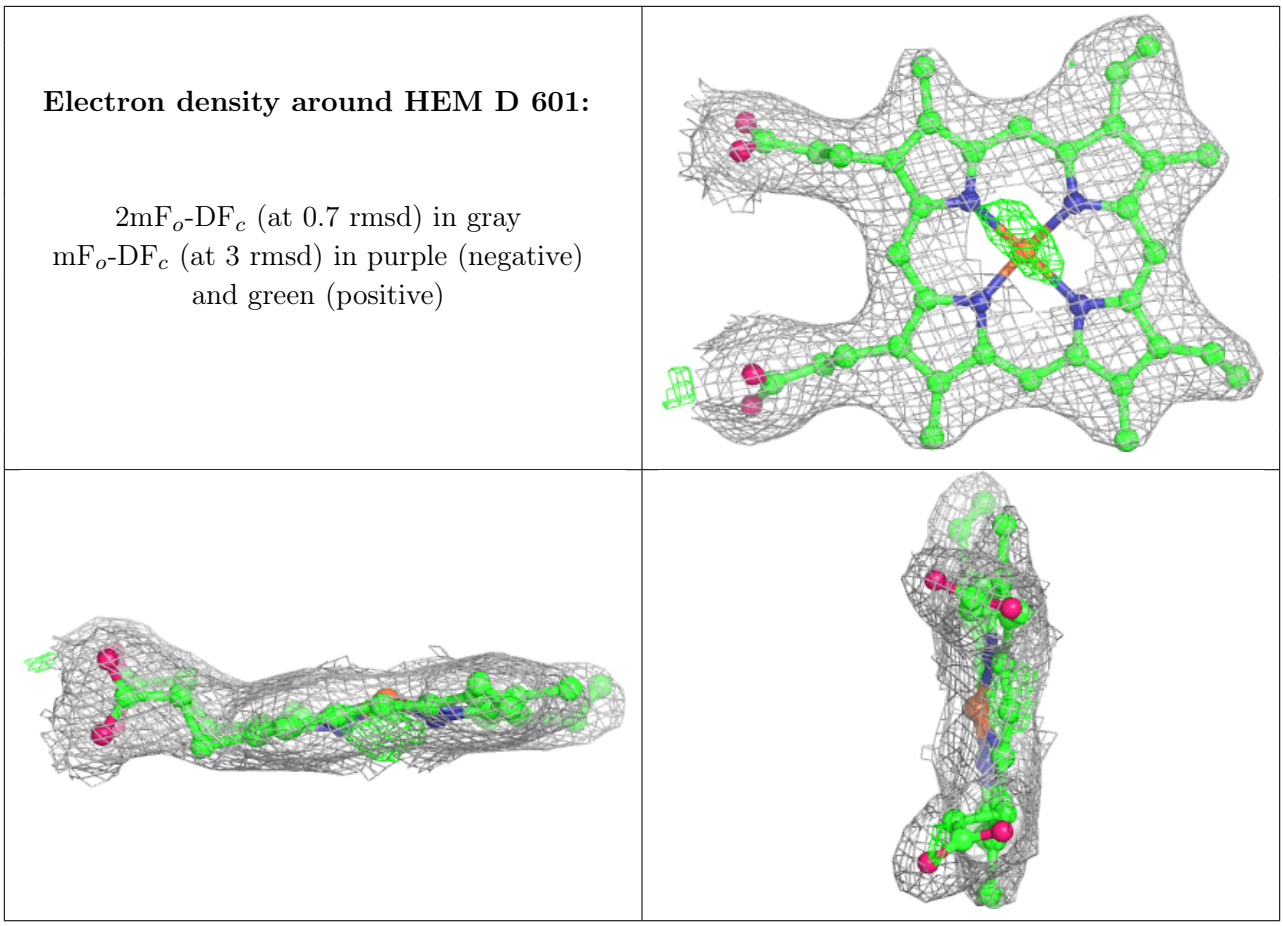
Electron density around HEM C 601:

$2mF_o$-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 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.