Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 01:15 PM EDT

PDB ID	:	7KVS
Title	:	Human CYP3A4 bound to an inhibitor
Authors	:	Sevrioukova, I.
Deposited on	:	2020-11-28
Resolution	:	2.50 Å(reported)

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

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

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

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

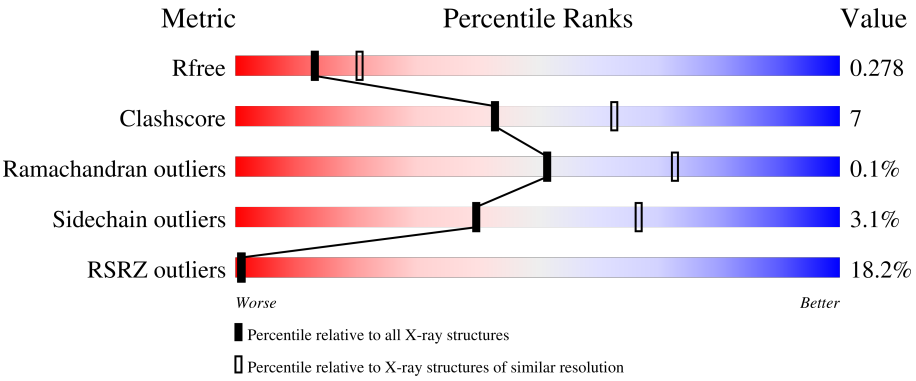
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	6% 79% 14% • 6%
1	B	487	28% 77% 13% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	X74	A	605	-	-	-	X
6	X74	B	603	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7470 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	457	Total	C	N	O	S	0	3	0
			3689	2404	606	654	25			
1	B	441	Total	C	N	O	S	0	1	0
			3539	2313	572	630	24			

There are 52 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	421	ALA	LYS	engineered mutation	UNP P08684
A	424	ALA	LYS	engineered mutation	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684

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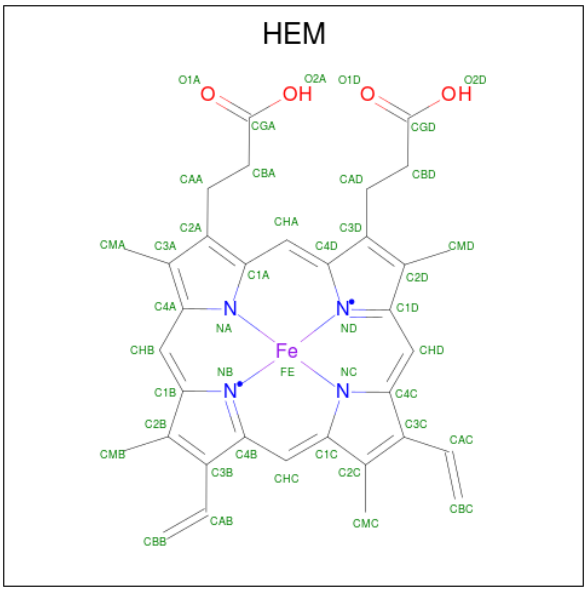
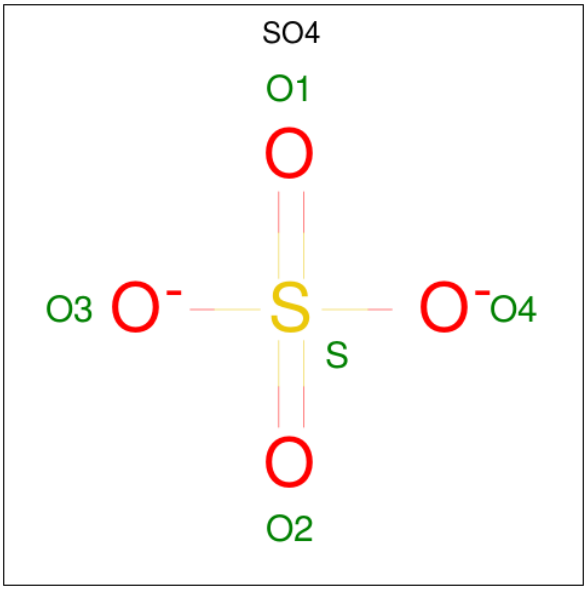
Chain	Residue	Modelled	Actual	Comment	Reference
A	507	HIS	-	expression tag	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	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	421	ALA	LYS	engineered mutation	UNP P08684
B	424	ALA	LYS	engineered mutation	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

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



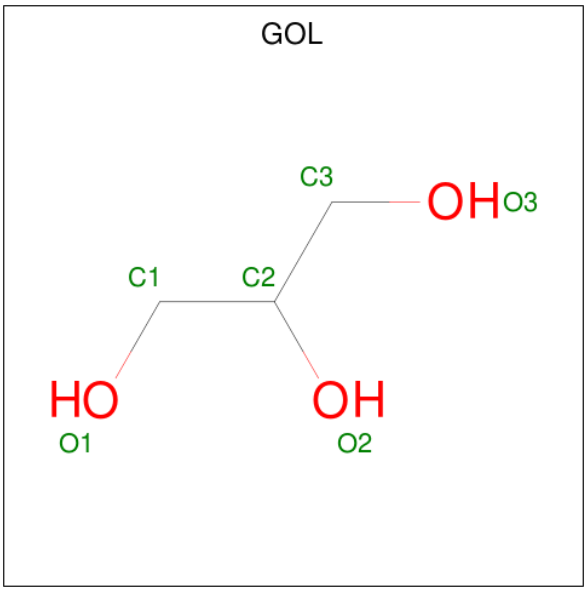
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



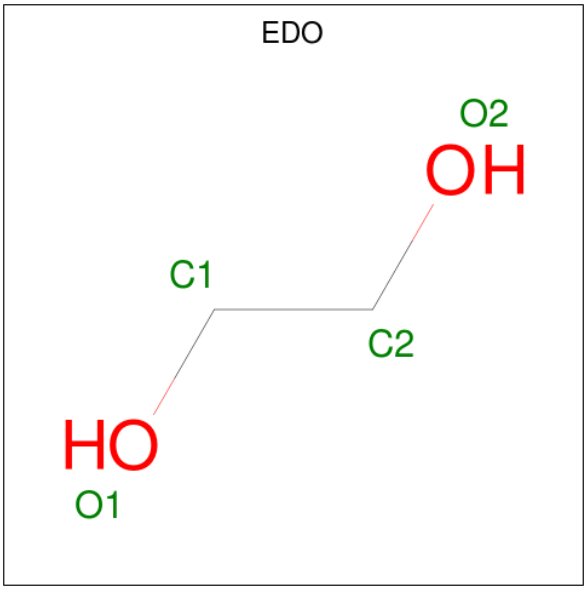
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



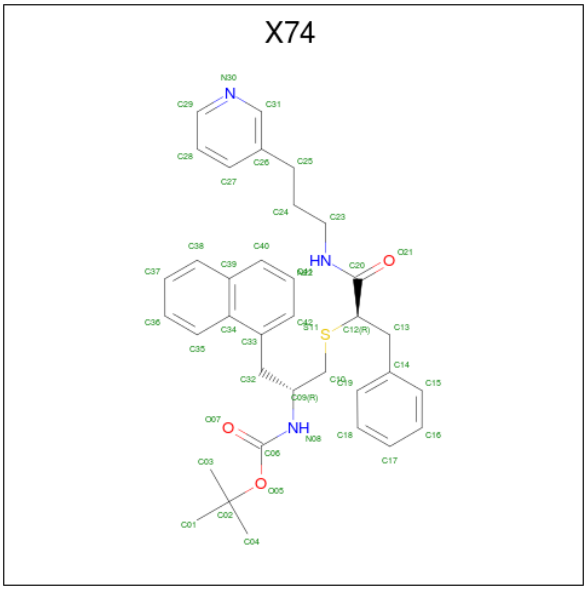
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is tert-butyl [(2R)-1-(naphthalen-1-yl)-3-{[(2R)-1-oxo-3-phenyl-1-{[3-(pyridin-3-yl)propyl]amino}propan-2-yl]sulfanyl}propan-2-yl]carbamate (three-letter code: X74) (formula: $C_{35}H_{41}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			42	35	3	3	1		
6	B	1	Total	C	N	O	S	0	0
			42	35	3	3	1		

- Molecule 7 is water.

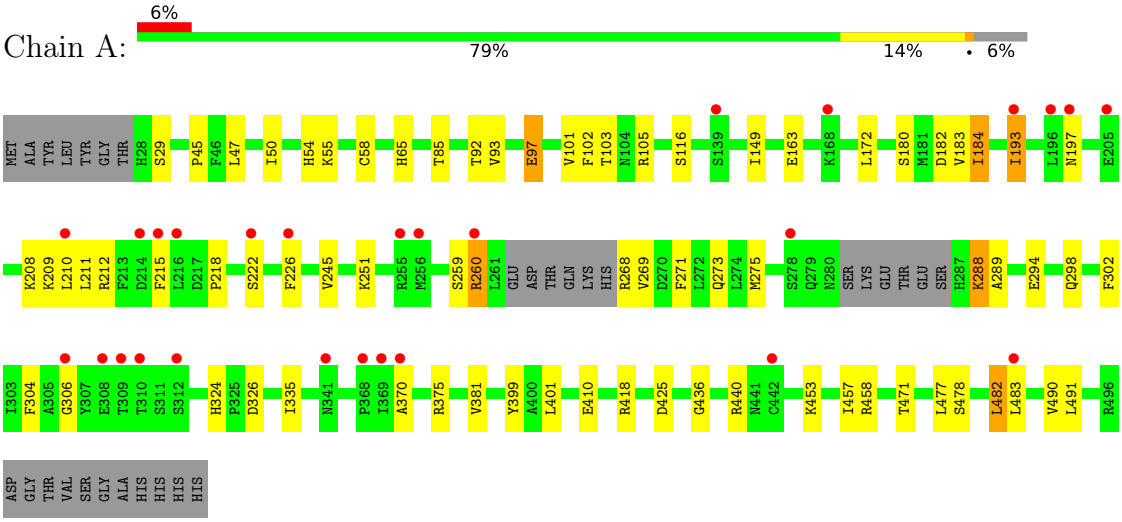
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	38	Total	O	0	0
			38	38		
7	B	9	Total	O	0	0
			9	9		

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.

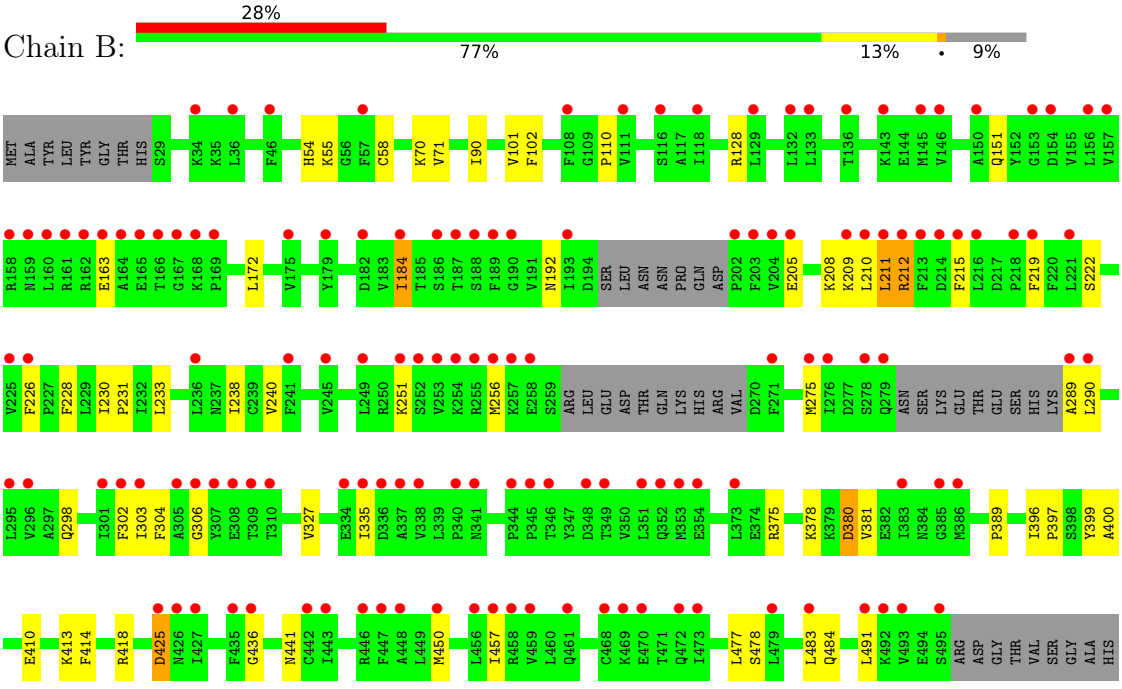
• Molecule 1: Cytochrome P450 3A4

Chain A:



• Molecule 1: Cytochrome P450 3A4

Chain B:




HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.51Å 98.22Å 93.48Å 90.00° 124.37° 90.00°	Depositor
Resolution (Å)	38.58 – 2.50 38.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.58-2.50) 97.3 (38.58-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.235 , 0.275 0.239 , 0.278	Depositor DCC
R_{free} test set	1832 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 84.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7470	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: GOL, SO4, HEM, X74, EDO

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	0.27	0/3788	0.42	0/5125
1	B	0.24	0/3628	0.39	0/4907
All	All	0.25	0/7416	0.41	0/10032

There are no bond length outliers.

There are no bond angle outliers.

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	3689	0	3780	51	0
1	B	3539	0	3624	47	0
2	A	43	0	30	6	0
2	B	43	0	30	5	0
3	A	5	0	0	1	0
4	A	6	0	8	1	0
4	B	6	0	8	0	0
5	A	8	0	12	0	0
6	A	42	0	0	2	0
6	B	42	0	0	1	0
7	A	38	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	9	0	0	2	0
All	All	7470	0	7492	102	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 (102) 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:211:LEU:HD22	1:A:304:PHE:HZ	1.16	1.09
1:B:211:LEU:HD13	1:B:212:ARG:H	1.18	1.04
1:B:211:LEU:HD12	1:B:211:LEU:H	1.33	0.94
1:A:211:LEU:HD22	1:A:304:PHE:CZ	2.08	0.82
1:B:211:LEU:CD1	1:B:212:ARG:H	1.92	0.82
2:B:602:HEM:HBC2	2:B:602:HEM:HHD	1.68	0.76
2:A:601:HEM:HHD	2:A:601:HEM:HBC2	1.69	0.75
1:A:184:ILE:HG13	1:A:306:GLY:HA3	1.68	0.74
1:B:211:LEU:HD12	1:B:211:LEU:N	2.01	0.73
1:B:410:GLU:O	1:B:418:ARG:NH2	2.26	0.68
1:B:233:LEU:HB3	1:B:238:ILE:HB	1.77	0.66
1:A:288:LYS:HB2	1:A:289:ALA:HB2	1.79	0.64
1:B:211:LEU:HG	1:B:304:PHE:CE1	2.33	0.64
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.81	0.63
1:A:211:LEU:HB2	1:A:304:PHE:CE1	2.35	0.62
1:A:410:GLU:O	1:A:418:ARG:NH2	2.34	0.61
1:B:90:ILE:HG23	1:B:396:ILE:HD13	1.84	0.58
1:B:211:LEU:HD13	1:B:212:ARG:N	2.03	0.58
1:A:211:LEU:HD13	6:A:605:X74:C16	2.33	0.58
1:A:211:LEU:CD2	1:A:304:PHE:HZ	2.04	0.57
1:B:128:ARG:NH2	1:B:289:ALA:O	2.39	0.56
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.88	0.55
1:A:269:VAL:O	1:A:269:VAL:HG12	2.07	0.55
1:B:192:ASN:ND2	7:B:704:HOH:O	2.40	0.55
1:A:103:THR:O	1:A:440:ARG:NH1	2.38	0.54
1:B:302:PHE:CD2	2:B:602:HEM:HBC1	2.42	0.54
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.89	0.54
2:B:602:HEM:HMB2	2:B:602:HEM:HBB2	1.88	0.54
1:B:397:PRO:HB2	1:B:400:ALA:HB3	1.90	0.54
1:B:441:ASN:HA	2:B:602:HEM:HBA2	1.89	0.53
1:A:47:LEU:HD22	1:A:50[A]:ILE:HD11	1.91	0.53
1:A:65:HIS:CD2	1:A:85:THR:HG21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.91	0.53
1:B:211:LEU:CD1	1:B:212:ARG:N	2.69	0.52
1:B:233:LEU:HD22	1:B:238:ILE:HD12	1.90	0.52
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.91	0.51
1:A:302:PHE:CD2	2:A:601:HEM:HBC1	2.46	0.50
1:B:211:LEU:HG	1:B:304:PHE:CZ	2.46	0.50
1:B:335:ILE:HD13	1:B:457:ILE:HA	1.92	0.50
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.92	0.50
1:A:482:LEU:H	1:A:482:LEU:HD23	1.76	0.50
1:A:105:ARG:HH21	2:A:601:HEM:HAA1	1.76	0.50
1:A:259:SER:HB3	1:A:260:ARG:HD2	1.93	0.49
1:A:65:HIS:HD2	1:A:85:THR:HG21	1.76	0.49
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.93	0.49
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.95	0.48
1:A:92:THR:HG22	1:A:97:GLU:HG3	1.95	0.48
1:B:211:LEU:HD23	1:B:304:PHE:HZ	1.78	0.48
1:B:477:LEU:HD13	1:B:483:LEU:HD11	1.96	0.47
1:A:54:HIS:CD2	1:A:55:LYS:HG3	2.48	0.47
1:B:222:SER:O	1:B:226:PHE:N	2.36	0.47
1:A:85:THR:HB	1:A:401:LEU:HD21	1.96	0.47
1:A:193:ILE:H	1:A:193:ILE:HG13	1.51	0.47
1:A:269:VAL:HA	1:A:273:GLN:HG2	1.96	0.47
1:A:324:HIS:NE2	3:A:602:SO4:O4	2.48	0.46
1:A:208:LYS:C	1:A:210:LEU:H	2.19	0.46
1:A:149:ILE:HG12	1:A:183:VAL:HG13	1.98	0.46
1:A:425:ASP:OD1	1:A:425:ASP:N	2.46	0.46
1:B:70:LYS:HG3	1:B:71:VAL:HG23	1.97	0.46
1:A:93:VAL:HG13	1:A:102:PHE:CG	2.51	0.45
1:A:211:LEU:CD1	6:A:605:X74:C16	2.95	0.45
1:A:209:LYS:HG3	1:A:245:VAL:HG11	1.97	0.45
1:B:436:GLY:HA3	2:B:602:HEM:HBA1	1.97	0.45
1:B:478:SER:N	1:B:484:GLN:O	2.37	0.45
1:A:477:LEU:HD13	1:A:483:LEU:HD11	1.98	0.44
1:B:230:ILE:HB	1:B:231:PRO:HD3	1.99	0.44
1:A:478:SER:O	4:A:603:GOL:H32	2.17	0.44
1:A:326:ASP:N	1:A:326:ASP:OD1	2.51	0.44
1:B:110:PRO:HG3	1:B:233:LEU:HB2	1.99	0.44
1:B:151:GLN:NE2	7:B:704:HOH:O	2.50	0.44
1:B:413:LYS:HD2	1:B:413:LYS:HA	1.72	0.44
1:A:218:PRO:O	1:A:222:SER:N	2.46	0.43
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ASP:OD1	1:B:425:ASP:N	2.35	0.43
1:B:58:CYS:HB3	1:B:399:TYR:CD2	2.53	0.43
1:A:116:SER:O	1:A:298:GLN:NE2	2.48	0.43
1:B:211:LEU:CD1	1:B:211:LEU:N	2.73	0.43
1:A:180:SER:HB3	1:A:306:GLY:O	2.18	0.43
1:A:268:ARG:NH2	1:A:273:GLN:OE1	2.41	0.43
1:A:453:LYS:NZ	7:A:708:HOH:O	2.36	0.43
1:B:210:LEU:HG	6:B:603:X74:C17	2.49	0.43
1:A:288:LYS:HA	1:A:289:ALA:HA	1.80	0.42
1:A:102:PHE:HB3	1:A:375:ARG:HB3	2.00	0.42
1:B:101:VAL:HA	1:B:378:LYS:HG2	2.02	0.42
1:A:211:LEU:HB2	1:A:304:PHE:CZ	2.53	0.42
1:A:294:GLU:O	1:A:298:GLN:HG2	2.20	0.42
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.55	0.42
1:A:370:ALA:HB3	7:A:720:HOH:O	2.20	0.41
1:B:211:LEU:CD2	1:B:304:PHE:HZ	2.32	0.41
1:B:54:HIS:CD2	1:B:55:LYS:HG3	2.56	0.41
1:B:275:MET:HE2	1:B:290:LEU:HD21	2.02	0.41
1:B:327:VAL:HG11	1:B:414:PHE:HE2	1.85	0.41
1:B:208:LYS:HB2	1:B:208:LYS:HE3	1.58	0.41
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.32	0.41
1:A:45:PRO:O	1:A:47:LEU:N	2.51	0.41
1:A:271:PHE:O	1:A:275:MET:HG3	2.21	0.41
1:A:471:THR:OG1	1:A:490:VAL:O	2.26	0.41
1:B:219:PHE:CE2	1:B:240:VAL:HG12	2.56	0.40
1:A:335:ILE:HD13	1:A:457:ILE:HA	2.03	0.40
1:B:205:GLU:O	1:B:209:LYS:HG2	2.21	0.40
1:B:380:ASP:OD1	1:B:389:PRO:HA	2.22	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	454/487 (93%)	426 (94%)	27 (6%)	1 (0%)	47 68
1	B	434/487 (89%)	410 (94%)	24 (6%)	0	100 100
All	All	888/974 (91%)	836 (94%)	51 (6%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASN

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	419/441 (95%)	405 (97%)	14 (3%)	38 64
1	B	401/441 (91%)	390 (97%)	11 (3%)	44 71
All	All	820/882 (93%)	795 (97%)	25 (3%)	40 68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	97	GLU
1	A	163	GLU
1	A	182	ASP
1	A	184	ILE
1	A	193	ILE
1	A	212	ARG
1	A	215	PHE
1	A	226	PHE
1	A	251	LYS
1	A	260	ARG
1	A	288	LYS
1	A	458	ARG
1	A	482	LEU
1	B	163	GLU

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Mol	Chain	Res	Type
1	B	184	ILE
1	B	211	LEU
1	B	212	ARG
1	B	215	PHE
1	B	228	PHE
1	B	251	LYS
1	B	256	MET
1	B	380	ASP
1	B	425	ASP
1	B	450	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS

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)

9 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	A	601	1,6	41,50,50	1.51	5 (12%)	45,82,82	1.42	6 (13%)
2	HEM	B	602	1,6	41,50,50	1.51	5 (12%)	45,82,82	1.41	7 (15%)
3	SO4	A	602	-	4,4,4	0.15	0	6,6,6	0.04	0
5	EDO	A	606	-	3,3,3	0.45	0	2,2,2	0.35	0
6	X74	A	605	2	44,45,45	1.27	5 (11%)	52,60,60	1.68	11 (21%)
4	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.20	0
6	X74	B	603	2	44,45,45	1.28	6 (13%)	52,60,60	1.69	11 (21%)
5	EDO	A	604	-	3,3,3	0.46	0	2,2,2	0.31	0
4	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.27	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
2	HEM	A	601	1,6	-	0/12/54/54	-
2	HEM	B	602	1,6	-	0/12/54/54	-
5	EDO	A	606	-	-	0/1/1/1	-
6	X74	A	605	2	-	10/33/33/33	0/4/4/4
4	GOL	A	603	-	-	2/4/4/4	-
6	X74	B	603	2	-	13/33/33/33	0/4/4/4
5	EDO	A	604	-	-	1/1/1/1	-
4	GOL	B	601	-	-	4/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-C2C	-4.62	1.34	1.40
2	B	602	HEM	C3C-C2C	-4.56	1.34	1.40
6	B	603	X74	C06-N08	3.71	1.43	1.34
2	B	602	HEM	C3C-CAC	3.68	1.55	1.47
2	A	601	HEM	C3C-CAC	3.66	1.55	1.47
6	A	605	X74	C06-N08	3.66	1.43	1.34
2	B	602	HEM	CAB-C3B	3.04	1.55	1.47
2	A	601	HEM	CAB-C3B	3.02	1.55	1.47
6	B	603	X74	O05-C06	2.97	1.40	1.34
6	A	605	X74	O05-C06	2.95	1.40	1.34
6	A	605	X74	C32-C09	2.94	1.60	1.53
6	B	603	X74	C32-C09	2.79	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	X74	O21-C20	2.26	1.27	1.23
6	B	603	X74	O21-C20	2.26	1.27	1.23
2	A	601	HEM	CAA-C2A	2.12	1.55	1.52
2	B	602	HEM	CAA-C2A	2.10	1.55	1.52
6	A	605	X74	C41-C42	2.10	1.43	1.38
2	B	602	HEM	CMB-C2B	2.05	1.55	1.50
2	A	601	HEM	CMB-C2B	2.03	1.55	1.50
6	B	603	X74	C12-S11	2.01	1.85	1.83
6	B	603	X74	C41-C42	2.01	1.43	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	603	X74	O05-C06-N08	4.59	117.74	110.02
6	A	605	X74	O05-C06-N08	4.50	117.58	110.02
6	B	603	X74	O05-C06-O07	-3.77	118.74	125.62
6	A	605	X74	O05-C06-O07	-3.76	118.76	125.62
6	B	603	X74	C23-C24-C25	3.56	119.28	112.95
6	B	603	X74	C23-N22-C20	3.39	128.63	122.59
6	A	605	X74	C23-N22-C20	3.36	128.58	122.59
6	A	605	X74	C23-C24-C25	3.24	118.71	112.95
2	B	602	HEM	C4C-CHD-C1D	3.16	126.73	122.56
2	A	601	HEM	C4C-CHD-C1D	3.06	126.59	122.56
2	A	601	HEM	C4D-ND-C1D	3.01	108.18	105.07
2	B	602	HEM	C4D-ND-C1D	2.96	108.13	105.07
6	B	603	X74	O21-C20-C12	-2.92	117.38	121.61
2	A	601	HEM	C4B-CHC-C1C	2.89	126.37	122.56
6	A	605	X74	O21-C20-C12	-2.88	117.44	121.61
2	B	602	HEM	C4B-CHC-C1C	2.84	126.31	122.56
6	A	605	X74	C27-C26-C31	-2.71	113.12	117.10
6	B	603	X74	C27-C26-C31	-2.71	113.12	117.10
2	A	601	HEM	C1B-NB-C4B	2.69	107.85	105.07
2	B	602	HEM	C1B-NB-C4B	2.66	107.82	105.07
6	A	605	X74	C09-N08-C06	2.52	126.19	122.30
6	B	603	X74	C16-C15-C14	2.51	124.48	120.63
6	B	603	X74	O21-C20-N22	-2.49	117.64	122.99
6	A	605	X74	O21-C20-N22	-2.46	117.72	122.99
6	A	605	X74	C16-C15-C14	2.45	124.40	120.63
6	B	603	X74	O05-C02-C03	2.28	116.21	107.20
6	A	605	X74	C36-C35-C34	2.27	124.04	120.89
6	A	605	X74	O05-C02-C03	2.27	116.17	107.20
6	B	603	X74	C36-C35-C34	2.25	124.02	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	C3D-C4D-ND	-2.13	107.80	110.17
2	B	602	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
2	B	602	HEM	C3D-C4D-ND	-2.09	107.84	110.17
2	B	602	HEM	C3B-C2B-C1B	2.02	107.98	106.49
6	B	603	X74	C09-N08-C06	2.01	125.40	122.30
2	A	601	HEM	C3B-C2B-C1B	2.01	107.98	106.49

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	GOL	O1-C1-C2-C3
4	B	601	GOL	O1-C1-C2-C3
6	A	605	X74	N08-C06-O05-C02
6	A	605	X74	O07-C06-O05-C02
6	A	605	X74	C10-C09-C32-C33
6	A	605	X74	N08-C09-C32-C33
6	A	605	X74	C20-C12-S11-C10
6	A	605	X74	C09-C32-C33-C34
6	B	603	X74	C10-C09-C32-C33
6	B	603	X74	N08-C09-C32-C33
6	B	603	X74	C10-C09-N08-C06
6	B	603	X74	C32-C09-N08-C06
6	B	603	X74	C20-C12-S11-C10
6	B	603	X74	C09-C32-C33-C34
6	B	603	X74	O07-C06-O05-C02
6	B	603	X74	N08-C06-O05-C02
4	B	601	GOL	C1-C2-C3-O3
6	A	605	X74	C09-C32-C33-C42
6	B	603	X74	C09-C32-C33-C42
4	A	603	GOL	O1-C1-C2-O2
4	B	601	GOL	O1-C1-C2-O2
5	A	604	EDO	O1-C1-C2-O2
6	B	603	X74	N22-C23-C24-C25
6	A	605	X74	C10-C09-N08-C06
6	B	603	X74	O05-C06-N08-C09
6	A	605	X74	S11-C12-C13-C14
6	B	603	X74	O07-C06-N08-C09
6	A	605	X74	C32-C09-N08-C06
4	B	601	GOL	O2-C2-C3-O3
6	B	603	X74	S11-C12-C13-C14

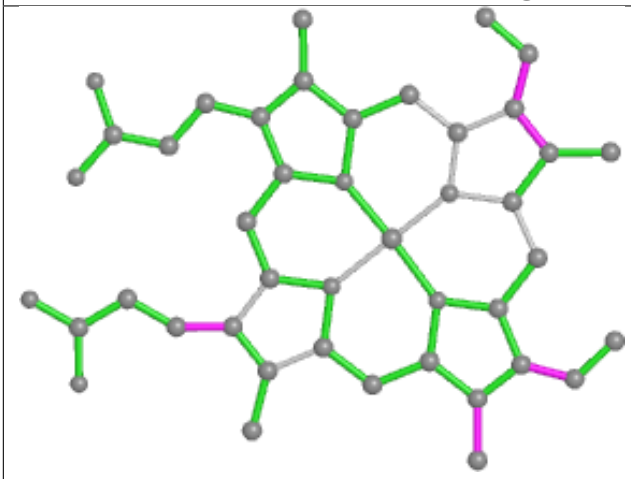
There are no ring outliers.

6 monomers are involved in 16 short contacts:

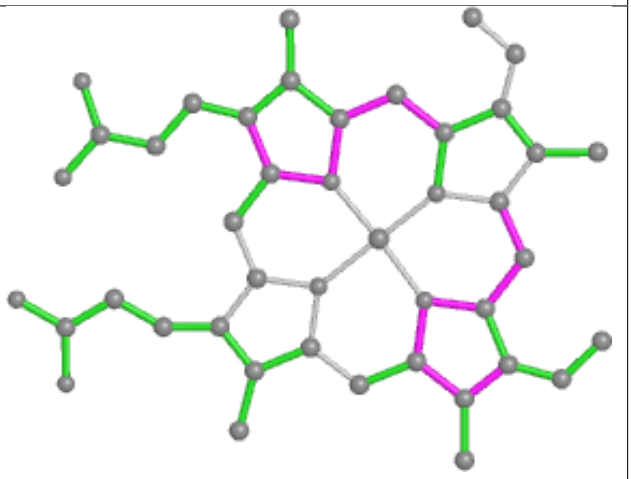
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	6	0
2	B	602	HEM	5	0
3	A	602	SO4	1	0
6	A	605	X74	2	0
4	A	603	GOL	1	0
6	B	603	X74	1	0

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

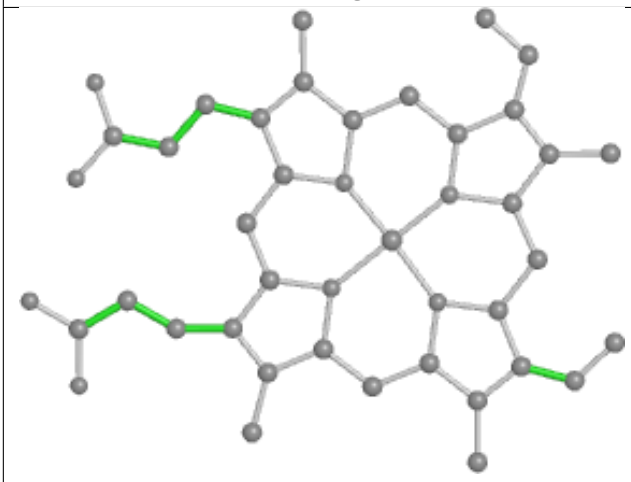
Ligand HEM A 601



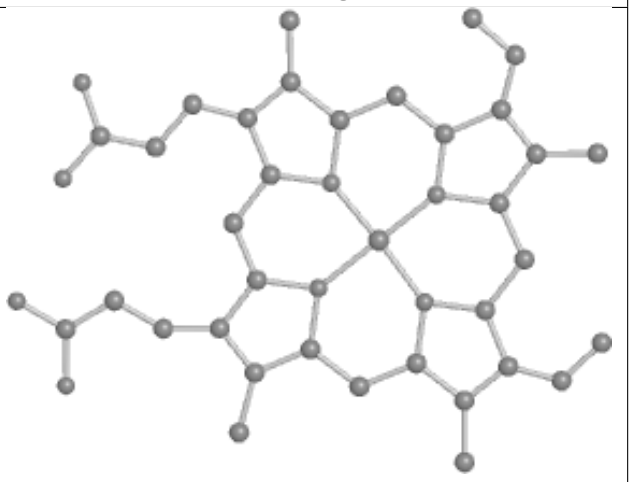
Bond lengths



Bond angles

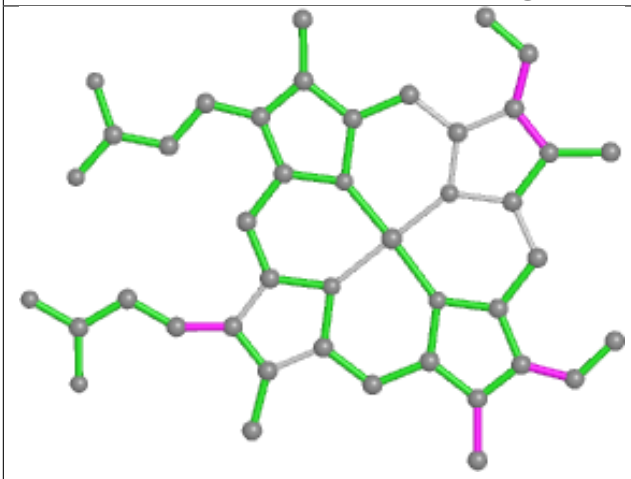


Torsions

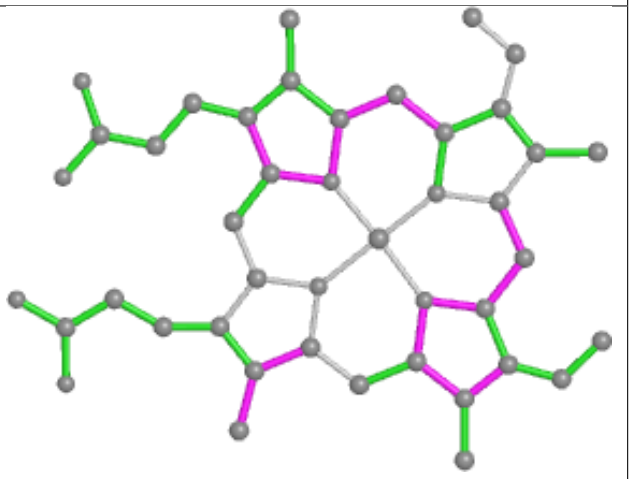


Rings

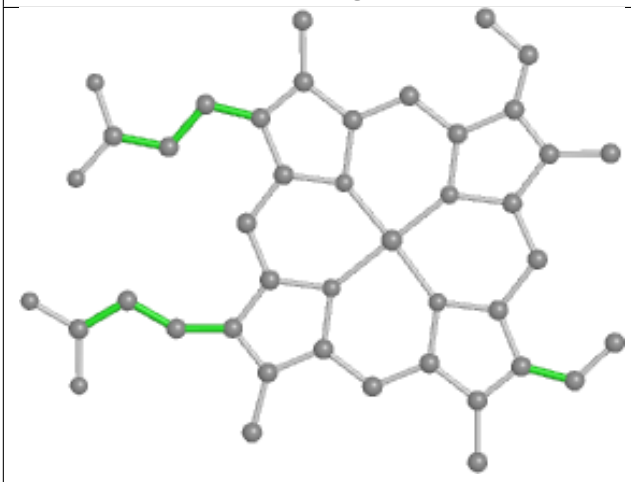
Ligand HEM B 602



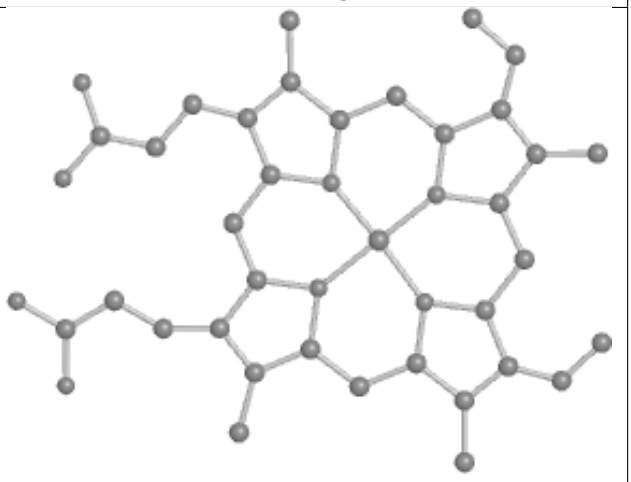
Bond lengths



Bond angles

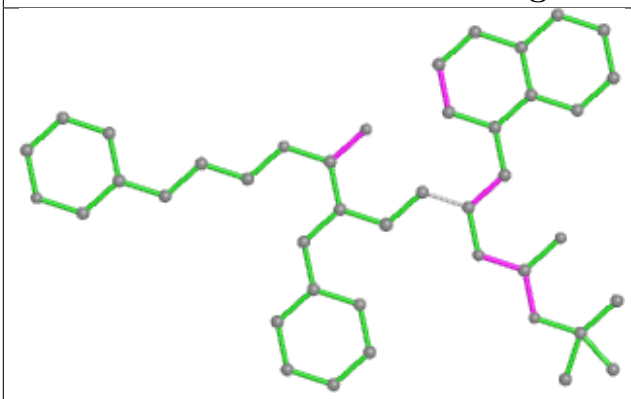


Torsions

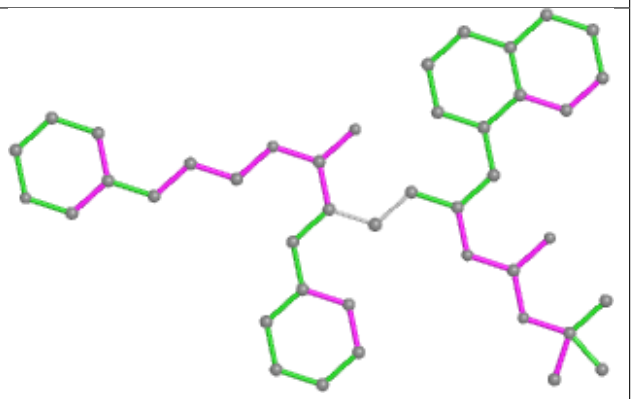


Rings

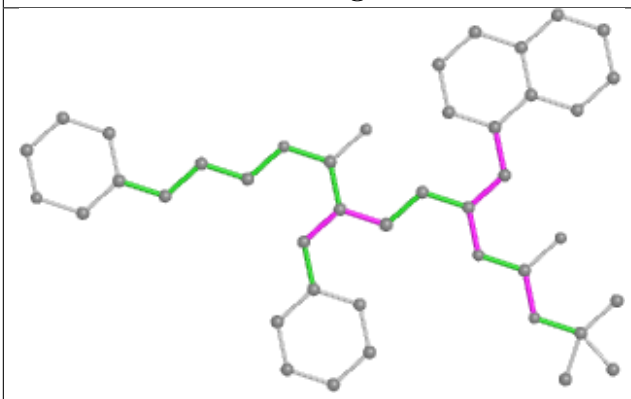
Ligand X74 A 605



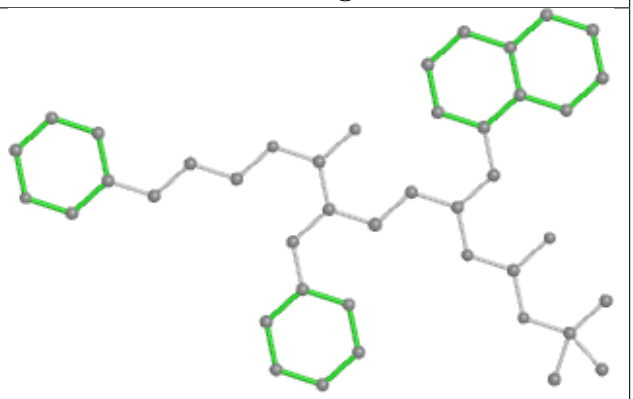
Bond lengths



Bond angles

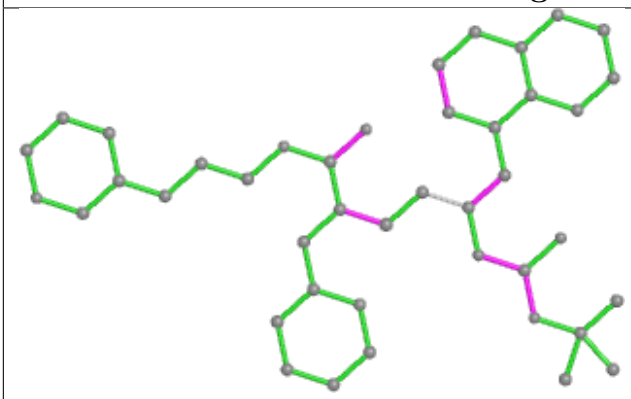


Torsions

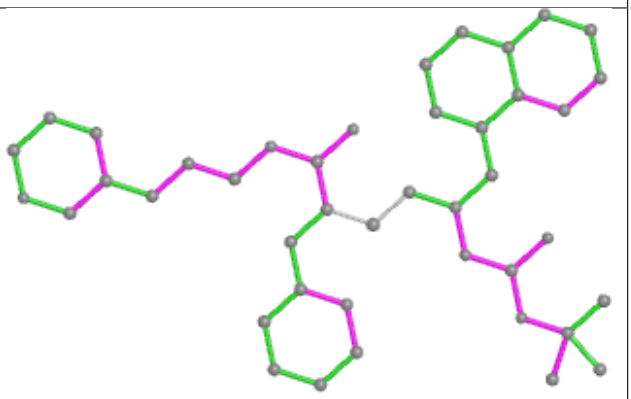


Rings

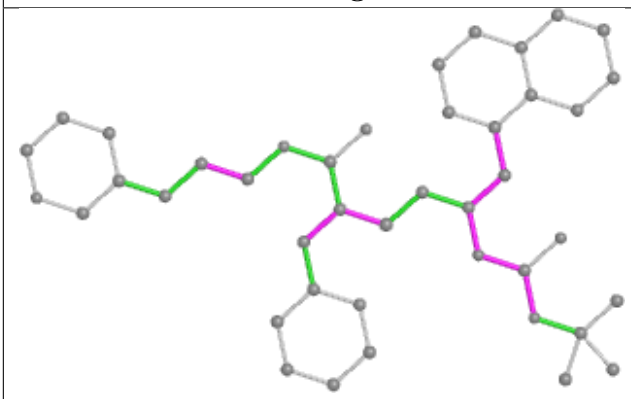
Ligand X74 B 603



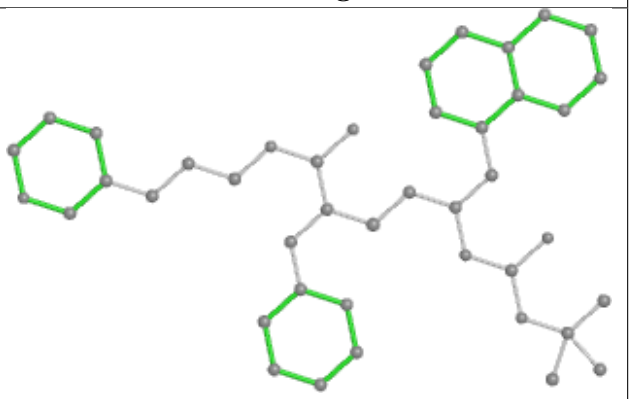
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	457/487 (93%)	0.36	27 (5%) 22 23	54, 94, 159, 233	0
1	B	441/487 (90%)	1.49	136 (30%) 0 0	68, 149, 226, 270	0
All	All	898/974 (92%)	0.92	163 (18%) 1 1	54, 114, 209, 270	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	LEU	20.3
1	B	253	VAL	11.4
1	B	209	LYS	11.2
1	B	190	GLY	10.4
1	B	457	ILE	9.4
1	B	160	LEU	8.3
1	A	216	LEU	8.3
1	B	161	ARG	7.6
1	B	256	MET	7.5
1	B	164	ALA	7.0
1	A	226	PHE	6.7
1	B	212	ARG	6.6
1	B	158	ARG	6.5
1	B	479	LEU	6.5
1	B	245	VAL	6.2
1	B	249	LEU	6.1
1	B	168	LYS	6.0
1	B	211	LEU	5.7
1	B	493	VAL	5.6
1	B	278	SER	5.5
1	B	189	PHE	5.4
1	B	255	ARG	5.4
1	B	251	LYS	5.4
1	B	214	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	210	LEU	5.2
1	B	154	ASP	5.1
1	A	196	LEU	5.0
1	A	168	LYS	4.9
1	B	215	PHE	4.9
1	B	226	PHE	4.8
1	B	461	GLN	4.7
1	B	491	LEU	4.6
1	B	306	GLY	4.5
1	B	179	TYR	4.5
1	B	352	GLN	4.5
1	B	156	LEU	4.4
1	A	369	ILE	4.4
1	B	427	ILE	4.4
1	B	302	PHE	4.3
1	A	193	ILE	4.3
1	B	341	ASN	4.3
1	B	295	LEU	4.3
1	A	215	PHE	4.2
1	B	213	PHE	4.2
1	B	218	PRO	4.2
1	B	162	ARG	4.1
1	B	349	THR	4.0
1	B	290	LEU	4.0
1	B	348	ASP	4.0
1	B	204	VAL	4.0
1	A	309	THR	3.9
1	A	214	ASP	3.9
1	B	469	LYS	3.9
1	B	132	LEU	3.9
1	B	305	ALA	3.7
1	B	337	ALA	3.7
1	B	257	LYS	3.7
1	B	275	MET	3.6
1	B	258	GLU	3.6
1	B	202	PRO	3.6
1	B	36	LEU	3.6
1	B	289	ALA	3.6
1	B	336	ASP	3.6
1	B	205	GLU	3.6
1	B	442	CYS	3.5
1	B	276	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	385	GLY	3.4
1	B	338	VAL	3.4
1	B	150	ALA	3.3
1	B	166	THR	3.3
1	B	345	PRO	3.3
1	B	334	GLU	3.3
1	B	133	LEU	3.3
1	B	254	LYS	3.2
1	B	187	THR	3.1
1	A	205	GLU	3.1
1	B	203	PHE	3.1
1	B	271	PHE	3.1
1	B	340	PRO	3.1
1	A	260	ARG	3.0
1	B	307	TYR	3.0
1	B	188	SER	3.0
1	B	163	GLU	3.0
1	B	296	VAL	3.0
1	B	221	LEU	3.0
1	A	310	THR	3.0
1	B	165	GLU	2.9
1	B	159	ASN	2.9
1	A	197	ASN	2.9
1	B	129	LEU	2.9
1	B	456	LEU	2.9
1	B	383	ILE	2.8
1	A	442	CYS	2.8
1	B	143	LYS	2.8
1	B	458	ARG	2.8
1	B	241	PHE	2.7
1	B	470	GLU	2.7
1	B	146	VAL	2.7
1	B	303	ILE	2.7
1	B	435	PHE	2.7
1	A	483	LEU	2.6
1	B	386	MET	2.6
1	B	111	VAL	2.6
1	B	153	GLY	2.6
1	B	483	LEU	2.6
1	B	353	MET	2.6
1	A	139	SER	2.6
1	B	446	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	473	ILE	2.6
1	A	222	SER	2.5
1	B	169	PRO	2.5
1	B	193	ILE	2.5
1	B	116[A]	SER	2.5
1	B	354	GLU	2.5
1	B	182	ASP	2.5
1	B	436	GLY	2.5
1	B	301	ILE	2.5
1	B	468	CYS	2.4
1	A	278	SER	2.4
1	B	492	LYS	2.4
1	B	426	ASN	2.4
1	B	351	LEU	2.4
1	B	46	PHE	2.4
1	B	219	PHE	2.4
1	B	157	VAL	2.3
1	B	136	THR	2.3
1	A	210	LEU	2.3
1	B	118	ILE	2.3
1	B	447	PHE	2.3
1	A	341	ASN	2.3
1	B	175	VAL	2.3
1	B	145	MET	2.3
1	B	335	ILE	2.3
1	A	312	SER	2.3
1	B	252	SER	2.3
1	B	34	LYS	2.3
1	B	225	VAL	2.2
1	A	256	MET	2.2
1	B	450	MET	2.2
1	B	425	ASP	2.2
1	B	459	VAL	2.2
1	B	448	ALA	2.2
1	B	308	GLU	2.2
1	B	373	LEU	2.2
1	B	495	SER	2.2
1	A	308	GLU	2.2
1	B	184	ILE	2.2
1	B	443	ILE	2.2
1	B	279	GLN	2.2
1	B	346	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	57	PHE	2.2
1	A	370	ALA	2.1
1	A	255	ARG	2.1
1	B	309	THR	2.1
1	B	310	THR	2.1
1	B	167	GLY	2.1
1	B	186	SER	2.1
1	B	344	PRO	2.1
1	B	108	PHE	2.1
1	B	236	LEU	2.1
1	A	306	GLY	2.1
1	B	472	GLN	2.0
1	A	368	PRO	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)

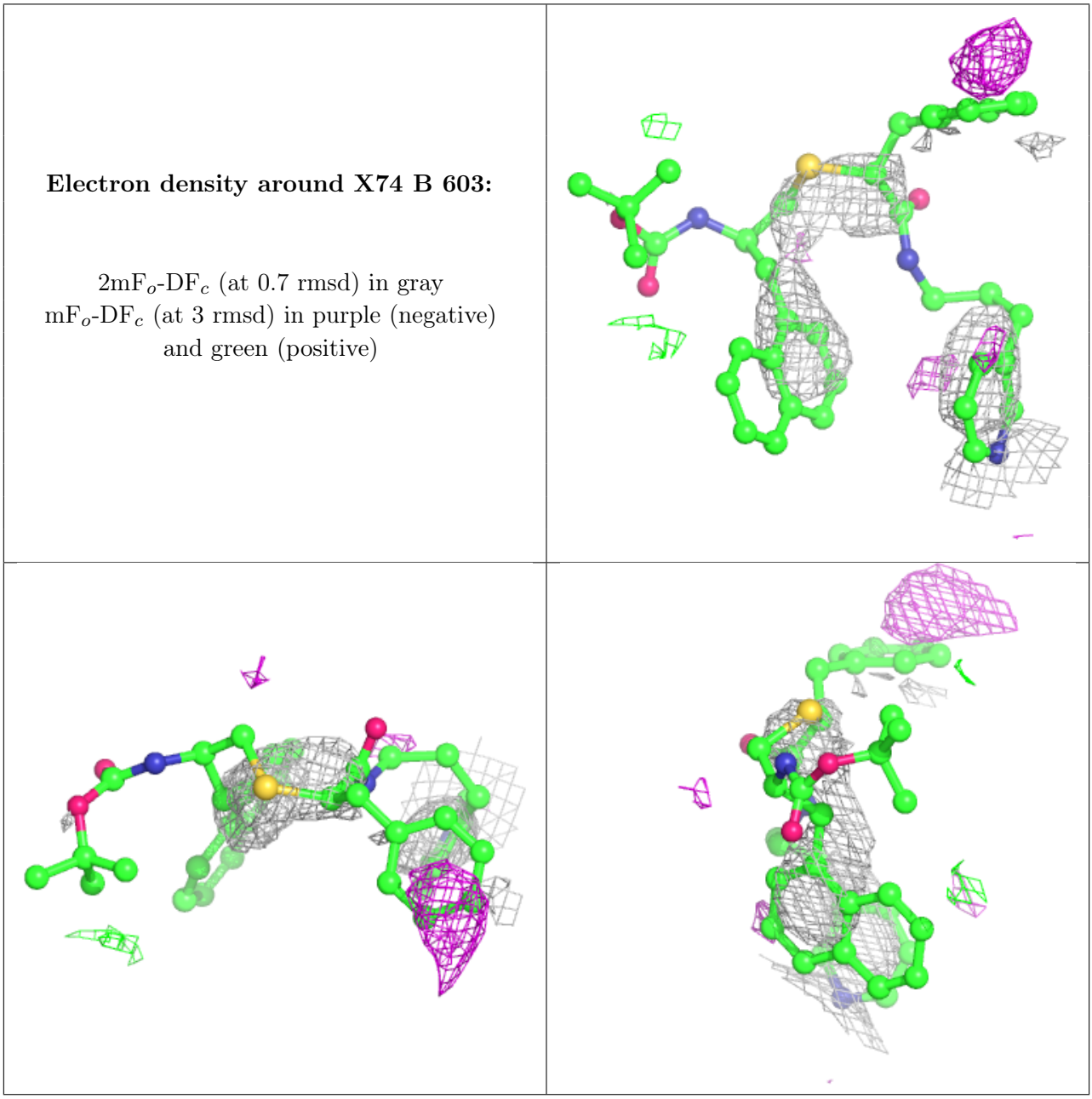
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	EDO	A	604	4/4	0.70	0.27	113,121,129,130	0
6	X74	B	603	42/42	0.71	0.45	129,184,213,222	0
5	EDO	A	606	4/4	0.73	0.30	91,92,103,111	0
6	X74	A	605	42/42	0.80	0.41	80,132,169,174	0
4	GOL	A	603	6/6	0.83	0.45	107,112,116,129	0
3	SO4	A	602	5/5	0.91	0.16	116,117,124,134	5
4	GOL	B	601	6/6	0.91	0.23	125,130,133,140	0
2	HEM	B	602	43/43	0.98	0.22	71,87,113,123	0
2	HEM	A	601	43/43	0.98	0.25	45,54,73,78	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.

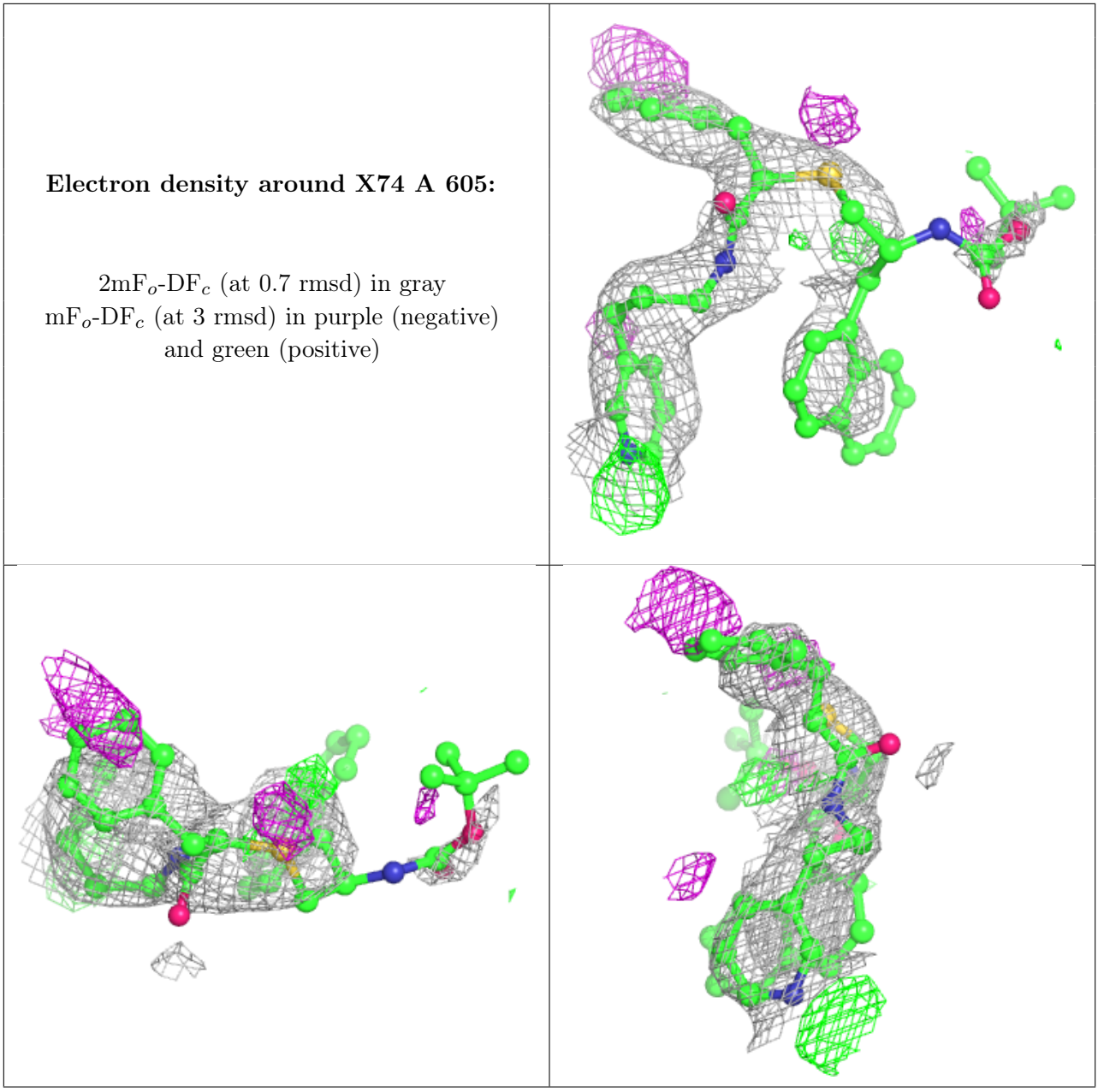
Electron density around X74 B 603:

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



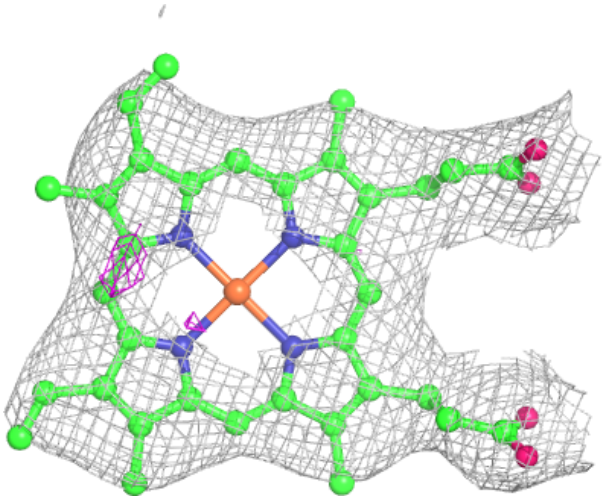
Electron density around X74 A 605:

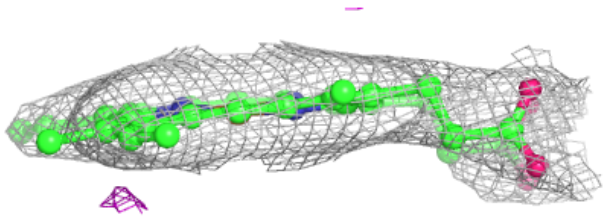
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

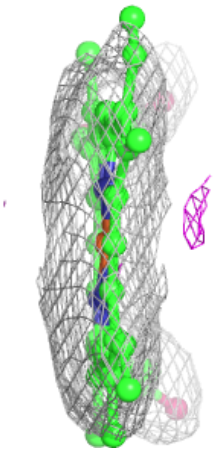


Electron density around HEM B 602:

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

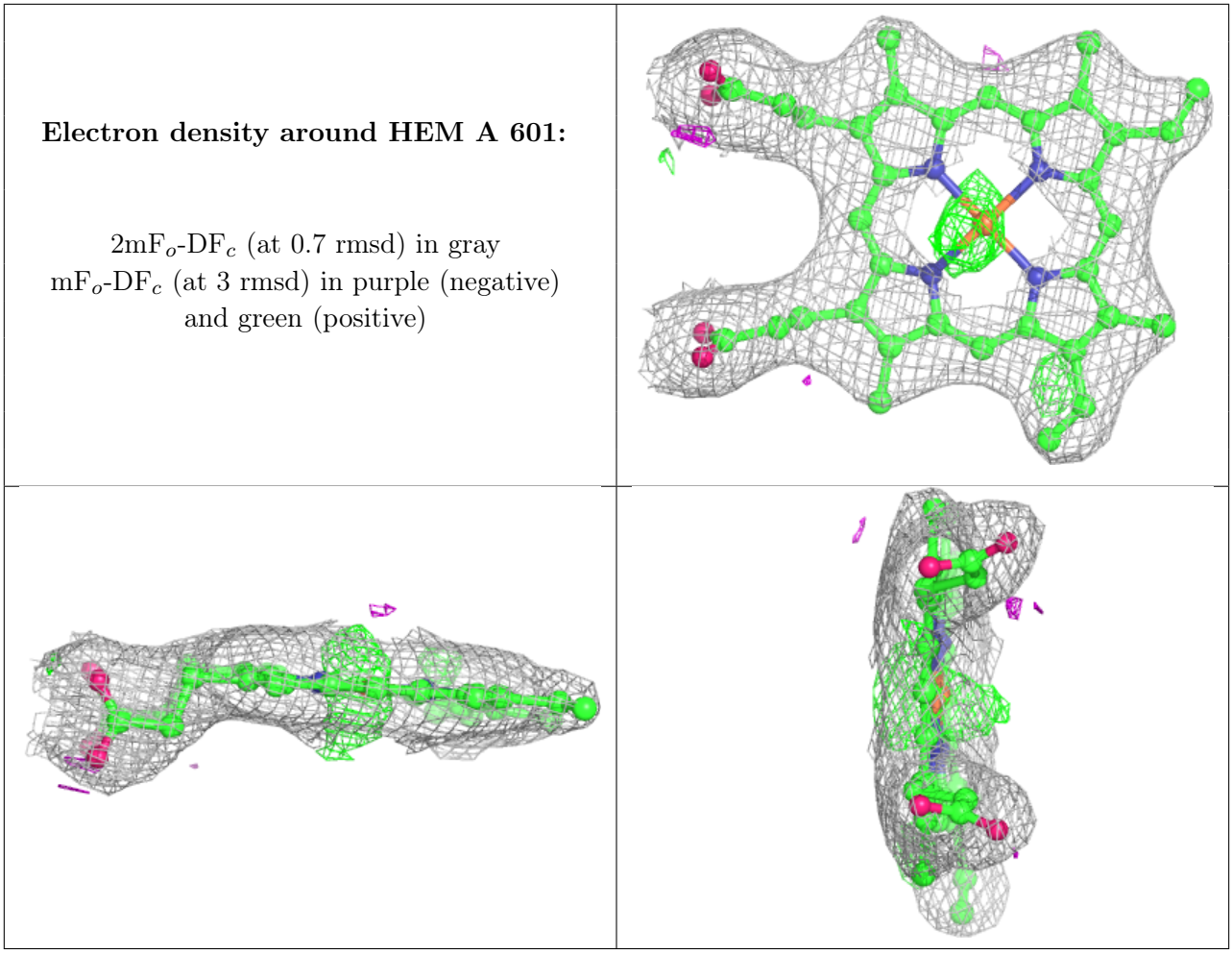






Electron density around HEM A 601:

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



6.5 Other polymers

There are no such residues in this entry.