



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2021 – 04:07 PM EST

PDB ID : 7KVO
Title : Human CYP3A4 bound to an inhibitor
Authors : Sevrioukova, I.
Deposited on : 2020-11-28
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

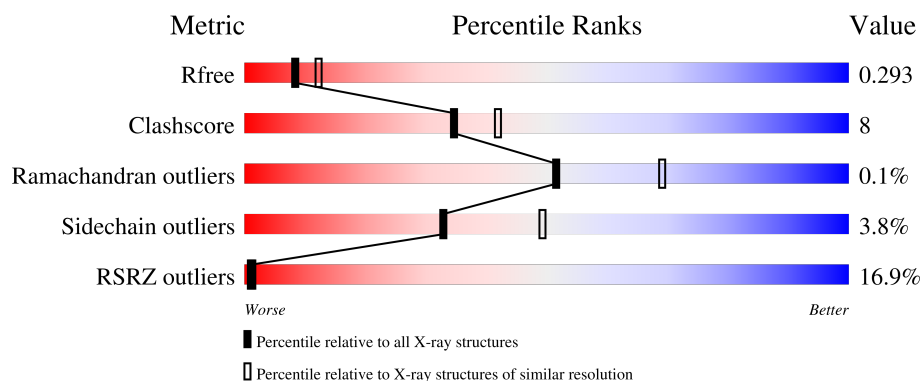
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 $\leq 5\%$. 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	<div> <div>5%</div> <div>75%</div> <div>17%</div> <div>6%</div> </div>
1	B	487	<div> <div>26%</div> <div>71%</div> <div>19%</div> <div>9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7467 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	4	0
			3710	2417	612	656	25			
1	B	445	Total	C	N	O	S	0	1	0
			3582	2339	583	636	24			

There are 48 discrepancies between the modelled and reference sequences:

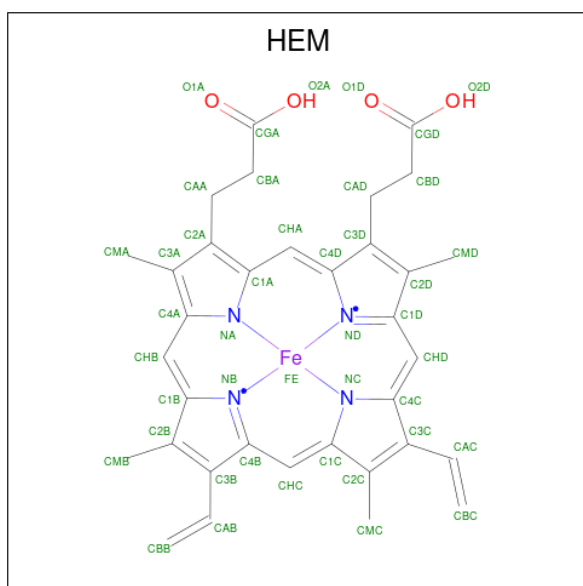
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	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
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

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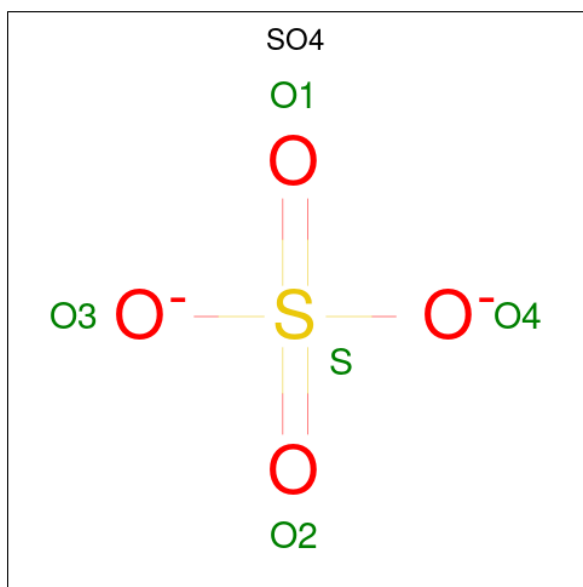
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	GLU	deletion	UNP P08684
B	?	-	THR	deletion	UNP P08684
B	?	-	TRP	deletion	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

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



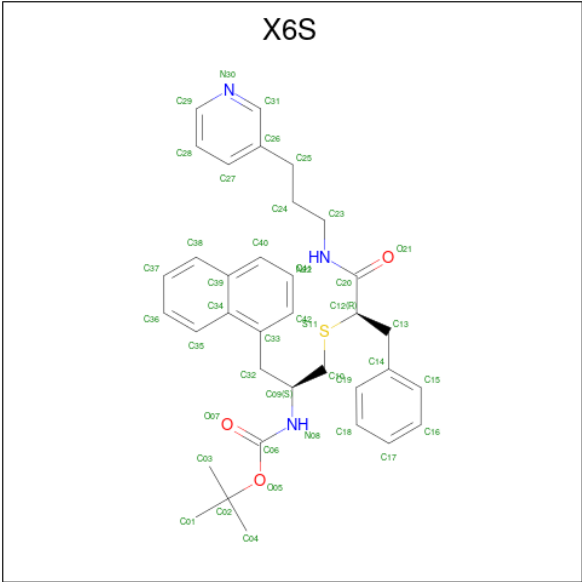
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is tert-butyl [(2S)-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: X6S) (formula: C₃₅H₄₁N₃O₃S) (labeled as "Ligand of Interest" by depositor).

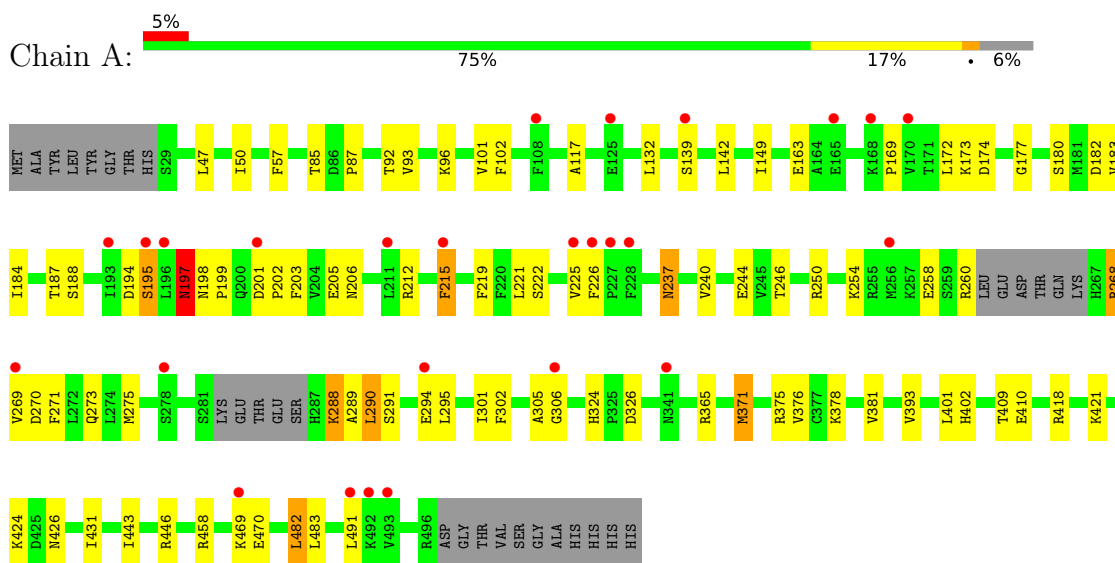


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			42	35	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			42	35	3	3	1		

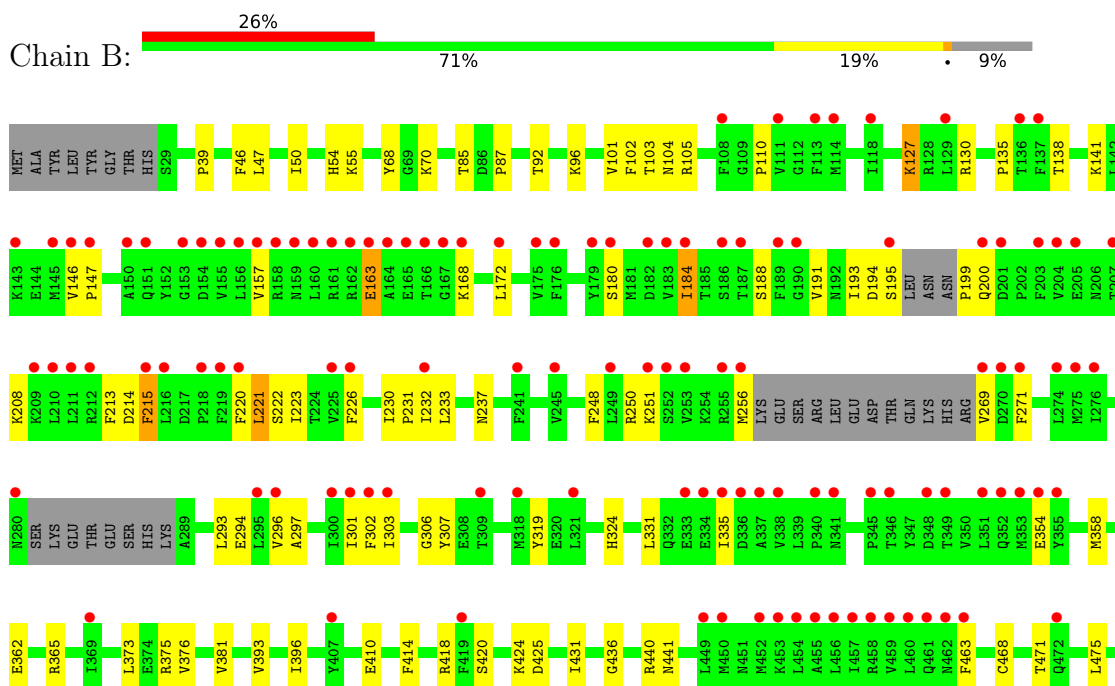
3 Residue-property plots [i](#)

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



• Molecule 1: Cytochrome P450 3A4



S478	L479	G480	G481	L482	V489	V490	L491	K492	V493	E494	S495	R496	ASP	GLY	THR	VAL	SER	GLY	ALA	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.88Å 98.08Å 126.77Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	49.04 – 2.65 49.04 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.04-2.65) 99.7 (49.04-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.241 , 0.293 0.244 , 0.293	Depositor DCC
R_{free} test set	1685 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	90.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, X6S, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	1/3810 (0.0%)	0.43	0/5151
1	B	0.25	0/3672	0.40	0/4966
All	All	0.26	1/7482 (0.0%)	0.42	0/10117

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	ASP	C-N	-5.34	1.21	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3803	64	0
1	B	3582	0	3671	57	0
2	A	43	0	30	4	0
2	B	43	0	30	6	0
3	A	5	0	0	1	0
4	A	42	0	0	1	0
4	B	42	0	0	0	0
All	All	7467	0	7534	124	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 8.

All (124) 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:197:ASN:HA	1:A:198:ASN:HB3	1.43	0.98
1:A:288:LYS:HB2	1:A:289:ALA:HB2	1.61	0.82
2:A:601:HEM:HBC2	2:A:601:HEM:HHD	1.67	0.76
1:A:268:ARG:CZ	1:A:270:ASP:HB3	2.16	0.75
1:A:187:THR:O	1:A:268:ARG:NH2	2.20	0.74
1:A:139:SER:HB3	1:A:446[A]:ARG:HH22	1.52	0.73
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.71	0.72
1:B:482:LEU:H	1:B:482:LEU:HD23	1.56	0.71
1:A:270:ASP:H	1:A:273:GLN:HB2	1.56	0.69
1:A:194:ASP:OD2	1:A:197:ASN:ND2	2.25	0.69
1:A:268:ARG:NH2	1:A:270:ASP:HB3	2.08	0.68
1:A:197:ASN:HA	1:A:198:ASN:CB	2.11	0.64
1:A:87:PRO:HG3	1:A:431:ILE:HD11	1.78	0.64
1:B:223:ILE:HB	1:B:230:ILE:HD11	1.80	0.63
1:A:482:LEU:H	1:A:482:LEU:HD23	1.63	0.63
1:A:202:PRO:O	1:A:206:ASN:ND2	2.22	0.62
1:A:237:ASN:ND2	1:A:237:ASN:O	2.31	0.62
1:A:268:ARG:NH2	1:A:270:ASP:CB	2.61	0.62
1:B:373:LEU:HB2	1:B:396:ILE:HB	1.80	0.62
1:A:92:THR:HA	1:A:96:LYS:HB2	1.82	0.62
1:B:410:GLU:O	1:B:418:ARG:NH2	2.33	0.61
1:B:47:LEU:HD22	1:B:50:ILE:HD11	1.85	0.59
1:B:103:THR:O	1:B:440:ARG:NH1	2.35	0.58
1:B:248:PHE:HA	1:B:251:LYS:HE2	1.86	0.57
1:A:117:ALA:HB1	1:A:301:ILE:HG13	1.87	0.56
1:A:169:PRO:HG2	1:A:470:GLU:OE2	2.06	0.56
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.88	0.55
1:B:302:PHE:CD2	2:B:601:HEM:HBC1	2.41	0.55
1:A:409:THR:O	1:A:418:ARG:NH1	2.36	0.54
1:A:225:VAL:HG23	1:A:226[A]:PHE:CD2	2.43	0.54
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.90	0.53
1:A:222:SER:HA	1:A:225:VAL:HG22	1.89	0.53
1:B:180:SER:HB3	1:B:307:TYR:HA	1.89	0.53
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.90	0.53
1:B:420:SER:O	1:B:424:LYS:N	2.40	0.53
1:A:446[A]:ARG:NH2	1:B:425:ASP:OD1	2.40	0.53
1:A:246:THR:O	1:A:250:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.92	0.52
1:B:188:SER:HA	1:B:271:PHE:HB3	1.93	0.51
1:B:39:PRO:HB2	1:B:68:TYR:HD2	1.75	0.51
1:A:219:PHE:HE2	1:A:240:VAL:HG12	1.75	0.51
1:B:130:ARG:NH2	1:B:441:ASN:OD1	2.44	0.51
1:B:163:GLU:HG3	1:B:168:LYS:HD2	1.92	0.51
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.91	0.51
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.93	0.50
1:A:326:ASP:N	1:A:326:ASP:OD1	2.44	0.50
1:A:270:ASP:O	1:A:273:GLN:N	2.45	0.49
1:B:105:ARG:HH21	2:B:601:HEM:HAA1	1.78	0.49
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.95	0.48
1:B:194:ASP:OD1	1:B:195:SER:N	2.47	0.47
1:A:275:MET:HB3	1:A:295:LEU:HD12	1.95	0.47
1:B:54:HIS:CD2	1:B:55:LYS:HG3	2.50	0.47
1:B:471:THR:OG1	1:B:490:VAL:O	2.20	0.47
1:B:135:PRO:HA	1:B:138:THR:HG23	1.97	0.47
1:A:132:LEU:HD21	1:A:290:LEU:HD12	1.96	0.46
1:B:70:LYS:O	1:B:85:THR:OG1	2.21	0.46
1:A:198:ASN:N	1:A:199:PRO:HD3	2.30	0.46
1:A:305:ALA:HB2	4:A:603:X6S:C25	2.45	0.46
1:B:92:THR:HA	1:B:96:LYS:HB2	1.98	0.46
1:A:197:ASN:CA	1:A:198:ASN:CB	2.89	0.46
1:A:302:PHE:CD2	2:A:601:HEM:HBC1	2.50	0.46
1:B:478:SER:C	1:B:480:GLY:H	2.19	0.46
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.96	0.46
1:A:215:PHE:O	1:A:221:LEU:HG	2.15	0.46
1:B:191:VAL:HG21	1:B:256:MET:HG2	1.98	0.46
1:B:302:PHE:CG	2:B:601:HEM:HBC1	2.51	0.46
1:B:39:PRO:HB2	1:B:68:TYR:CD2	2.51	0.46
1:A:182:ASP:N	1:A:182:ASP:OD1	2.49	0.45
1:A:57:PHE:HB2	1:A:371:MET:HE3	1.97	0.45
1:A:180:SER:HB3	1:A:306:GLY:O	2.17	0.45
1:A:187:THR:C	1:A:268:ARG:HH22	2.13	0.45
1:A:469:LYS:HD3	1:A:469:LYS:HA	1.71	0.45
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.97	0.45
1:B:362:GLU:OE1	1:B:365:ARG:NH2	2.50	0.45
1:B:87:PRO:HG3	1:B:431:ILE:HD11	1.99	0.45
1:B:436:GLY:HA3	2:B:601:HEM:HBA1	1.99	0.45
1:B:146:VAL:HB	1:B:147:PRO:HD3	1.99	0.45
1:A:324:HIS:NE2	3:A:602:SO4:O4	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HA	1:B:440:ARG:NH1	2.32	0.45
1:B:250:ARG:HA	1:B:296:VAL:HG11	1.99	0.45
1:A:149:ILE:HG12	1:A:183:VAL:HG13	1.98	0.44
1:A:376:VAL:HG22	1:A:393:VAL:HG22	1.98	0.44
1:B:110:PRO:HG3	1:B:233:LEU:HB2	1.99	0.44
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.30	0.44
1:B:214:ASP:OD1	1:B:214:ASP:N	2.41	0.44
1:B:319:TYR:CZ	1:B:475:LEU:HB2	2.53	0.44
1:A:184:ILE:HA	1:A:184:ILE:HD12	1.84	0.43
1:B:222:SER:O	1:B:226:PHE:N	2.32	0.43
1:B:230:ILE:HB	1:B:231:PRO:HD3	2.00	0.43
1:A:421:LYS:HA	1:A:424:LYS:HE3	1.99	0.43
1:A:101:VAL:HG21	1:A:381:VAL:HG11	2.01	0.43
1:B:141:LYS:HE2	1:B:269:VAL:HB	2.00	0.43
1:A:195:SER:C	1:A:197:ASN:H	2.21	0.43
1:A:93:VAL:HG13	1:A:102:PHE:CG	2.54	0.43
1:B:376:VAL:HG22	1:B:393:VAL:HG22	2.01	0.43
1:B:324:HIS:CE1	1:B:414:PHE:HB3	2.53	0.43
1:A:173:LYS:O	1:A:177:GLY:N	2.48	0.42
1:B:297:ALA:O	1:B:301:ILE:HG12	2.19	0.42
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.87	0.42
1:A:101:VAL:HA	1:A:378:LYS:HG2	2.01	0.42
1:B:127:LYS:HB2	1:B:127:LYS:HE2	1.74	0.42
1:B:46:PHE:HB3	1:B:226:PHE:CE1	2.55	0.42
1:B:157:VAL:HG13	1:B:463:PHE:CE2	2.54	0.42
1:B:354:GLU:HG2	1:B:358:MET:SD	2.60	0.42
1:A:201:ASP:OD2	1:A:203:PHE:HB2	2.20	0.42
1:A:371:MET:SD	1:A:483:LEU:HB2	2.60	0.42
1:A:194:ASP:CG	1:A:197:ASN:ND2	2.73	0.41
1:A:410:GLU:O	1:A:418:ARG:NH2	2.52	0.41
1:B:215:PHE:O	1:B:221:LEU:HG	2.20	0.41
1:A:250:ARG:HG2	1:A:254:LYS:HE3	2.02	0.41
1:A:85:THR:HB	1:A:401:LEU:HD21	2.02	0.41
1:B:199:PRO:HB2	1:B:200:GLN:H	1.65	0.41
1:A:288:LYS:HA	1:A:289:ALA:HA	1.89	0.41
1:B:294:GLU:HG3	1:B:294:GLU:H	1.72	0.41
1:A:188:SER:HB3	1:A:271:PHE:CD2	2.55	0.41
1:A:365:ARG:NH1	1:A:402:HIS:O	2.54	0.41
1:B:213:PHE:CE1	1:B:220:PHE:HB3	2.55	0.41
1:A:291:SER:HB3	1:A:294:GLU:HG3	2.03	0.41
1:B:157:VAL:HG13	1:B:463:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HA	1:A:424:LYS:HG2	2.03	0.41
1:A:195:SER:C	1:A:197:ASN:N	2.73	0.40
1:B:208:LYS:HB2	1:B:208:LYS:HE3	1.92	0.40
1:A:188:SER:HB3	1:A:271:PHE:HD2	1.86	0.40
1:B:331:LEU:O	1:B:335:ILE:HG13	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	455/487 (93%)	424 (93%)	30 (7%)	1 (0%)	47	64
1	B	438/487 (90%)	416 (95%)	22 (5%)	0	100	100
All	All	893/974 (92%)	840 (94%)	52 (6%)	1 (0%)	51	69

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/443 (95%)	402 (95%)	20 (5%)	26	40
1	B	407/443 (92%)	396 (97%)	11 (3%)	44	63
All	All	829/886 (94%)	798 (96%)	31 (4%)	33	50

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LEU
1	A	163	GLU
1	A	195	SER
1	A	197	ASN
1	A	205	GLU
1	A	212	ARG
1	A	215	PHE
1	A	237	ASN
1	A	244	GLU
1	A	258	GLU
1	A	260	ARG
1	A	268	ARG
1	A	269	VAL
1	A	288	LYS
1	A	290	LEU
1	A	371	MET
1	A	426	ASN
1	A	443	ILE
1	A	458	ARG
1	A	482	LEU
1	B	127	LYS
1	B	163	GLU
1	B	184	ILE
1	B	193	ILE
1	B	215	PHE
1	B	221	LEU
1	B	232	ILE
1	B	237	ASN
1	B	293	LEU
1	B	468	CYS
1	B	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
3	SO4	A	602	-	4,4,4	0.15	0	6,6,6	0.05	0
4	X6S	B	602	2	44,45,45	1.52	6 (13%)	52,60,60	1.33	8 (15%)
2	HEM	A	601	1,4	27,50,50	1.89	4 (14%)	17,82,82	1.50	1 (5%)
2	HEM	B	601	1,4	27,50,50	1.89	4 (14%)	17,82,82	1.54	4 (23%)
4	X6S	A	603	2	44,45,45	1.42	6 (13%)	52,60,60	1.31	7 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	X6S	B	602	2	-	11/33/33/33	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1,4	-	0/6/54/54	-
2	HEM	B	601	1,4	-	0/6/54/54	-
4	X6S	A	603	2	-	11/33/33/33	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	X6S	C12-S11	5.51	1.89	1.83
4	B	602	X6S	C10-S11	4.77	1.87	1.82
2	B	601	HEM	C3C-C2C	-4.69	1.33	1.40
4	A	603	X6S	C12-S11	4.55	1.88	1.83
2	A	601	HEM	C3C-C2C	-4.49	1.34	1.40
4	A	603	X6S	C10-S11	4.26	1.86	1.82
4	B	602	X6S	C20-N22	3.86	1.42	1.33
2	A	601	HEM	C3C-CAC	3.82	1.55	1.47
2	B	601	HEM	C3B-C2B	-3.80	1.35	1.40
2	A	601	HEM	C3B-CAB	3.80	1.55	1.47
2	B	601	HEM	C3B-CAB	3.77	1.55	1.47
4	A	603	X6S	C20-N22	3.67	1.41	1.33
2	B	601	HEM	C3C-CAC	3.61	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.55	1.35	1.40
4	A	603	X6S	C06-N08	2.73	1.41	1.34
4	B	602	X6S	C06-N08	2.71	1.41	1.34
4	A	603	X6S	O05-C06	2.40	1.39	1.34
4	B	602	X6S	O05-C06	2.28	1.39	1.34
4	B	602	X6S	C32-C09	2.02	1.58	1.53
4	A	603	X6S	C32-C09	2.01	1.58	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	X6S	O21-C20-N22	-3.54	115.40	122.99
4	B	602	X6S	O21-C20-N22	-3.48	115.52	122.99
4	A	603	X6S	O05-C06-N08	3.46	115.84	110.02
4	B	602	X6S	O05-C06-N08	3.33	115.61	110.02
4	B	602	X6S	C23-C24-C25	2.82	117.96	112.95
4	A	603	X6S	O05-C06-O07	-2.81	120.49	125.62
4	B	602	X6S	O05-C06-O07	-2.78	120.56	125.62
2	A	601	HEM	CMB-C2B-C3B	2.71	129.74	124.68
2	B	601	HEM	CAD-CBD-CGD	-2.59	108.33	112.67
4	B	602	X6S	C23-N22-C20	2.50	127.06	122.59
2	B	601	HEM	CAA-CBA-CGA	-2.39	108.66	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	CMA-C3A-C4A	-2.38	124.81	128.46
4	B	602	X6S	C40-C39-C38	-2.32	117.76	123.19
4	A	603	X6S	C23-N22-C20	2.28	126.66	122.59
4	A	603	X6S	C23-C24-C25	2.28	117.01	112.95
4	A	603	X6S	C40-C39-C38	-2.26	117.91	123.19
2	B	601	HEM	CMB-C2B-C3B	2.14	128.69	124.68
4	B	602	X6S	C02-O05-C06	-2.11	117.74	120.99
4	B	602	X6S	C38-C39-C34	2.11	121.89	119.12
4	A	603	X6S	C38-C39-C34	2.09	121.88	119.12

There are no chirality outliers.

All (22) torsion outliers are listed below:

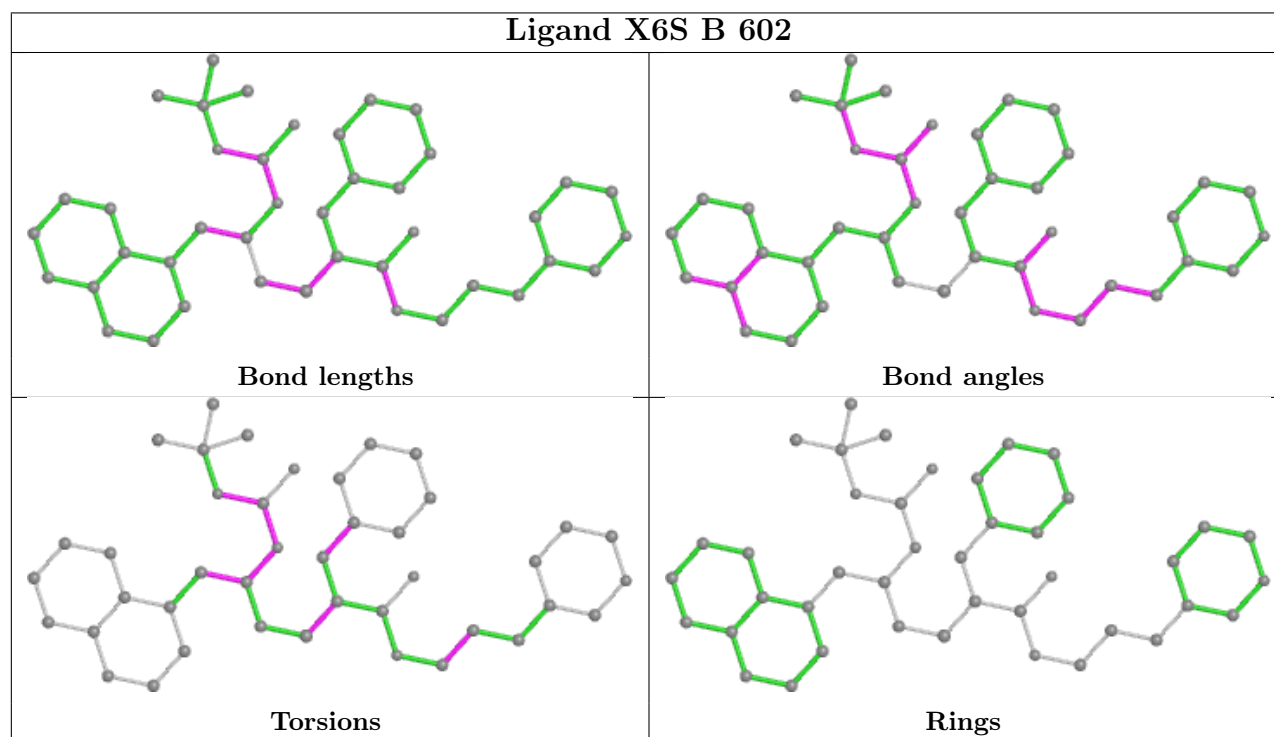
Mol	Chain	Res	Type	Atoms
4	B	602	X6S	C10-C09-C32-C33
4	B	602	X6S	N08-C09-C32-C33
4	B	602	X6S	C32-C09-N08-C06
4	A	603	X6S	C10-C09-C32-C33
4	A	603	X6S	N08-C09-C32-C33
4	A	603	X6S	C32-C09-N08-C06
4	B	602	X6S	O07-C06-O05-C02
4	A	603	X6S	O07-C06-O05-C02
4	B	602	X6S	N08-C06-O05-C02
4	A	603	X6S	N08-C06-O05-C02
4	B	602	X6S	N22-C23-C24-C25
4	B	602	X6S	C20-C12-S11-C10
4	A	603	X6S	C20-C12-S11-C10
4	A	603	X6S	N22-C23-C24-C25
4	A	603	X6S	C12-C13-C14-C15
4	A	603	X6S	C12-C13-C14-C19
4	B	602	X6S	O05-C06-N08-C09
4	A	603	X6S	O05-C06-N08-C09
4	B	602	X6S	O07-C06-N08-C09
4	B	602	X6S	C12-C13-C14-C19
4	A	603	X6S	O07-C06-N08-C09
4	B	602	X6S	C12-C13-C14-C15

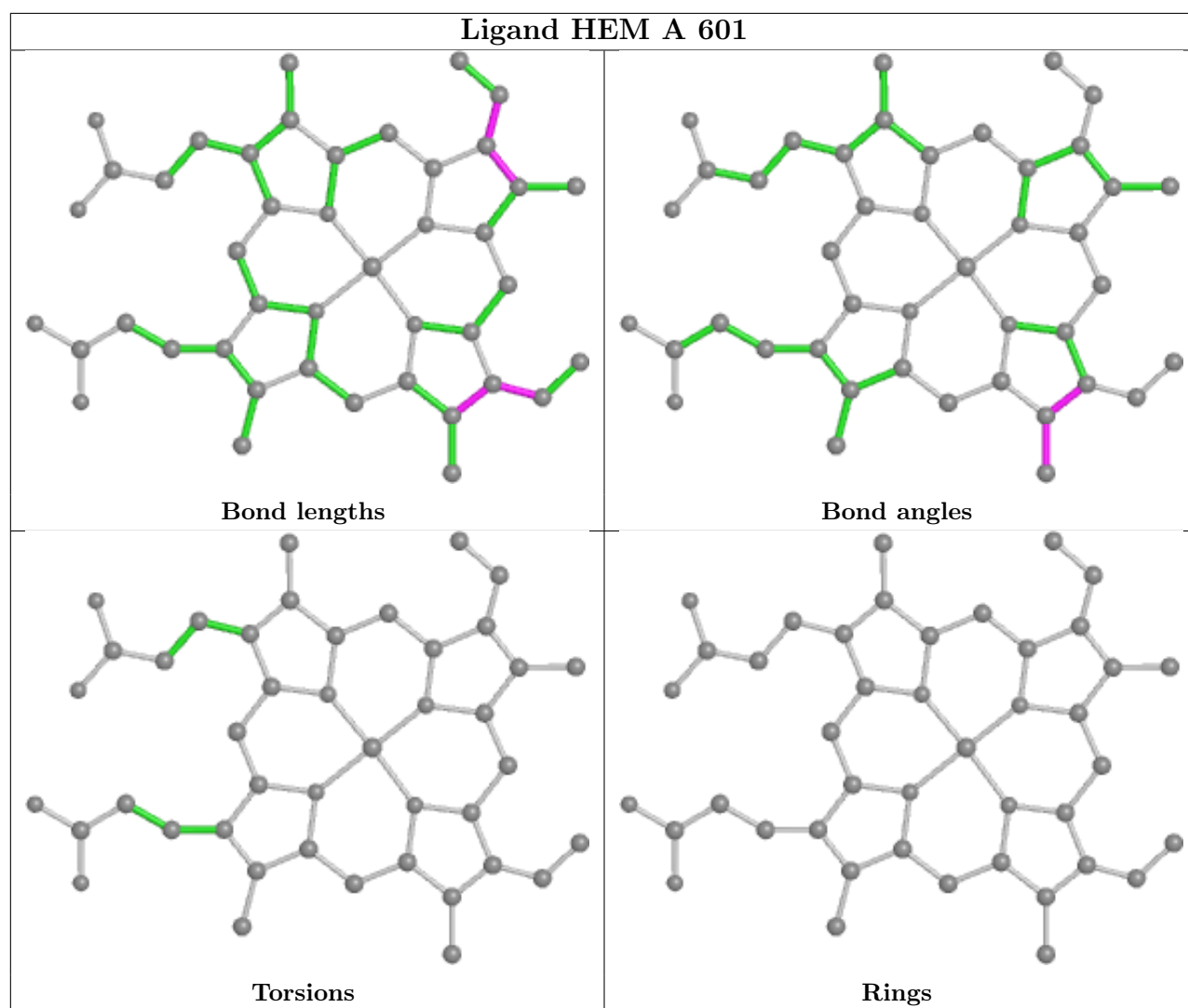
There are no ring outliers.

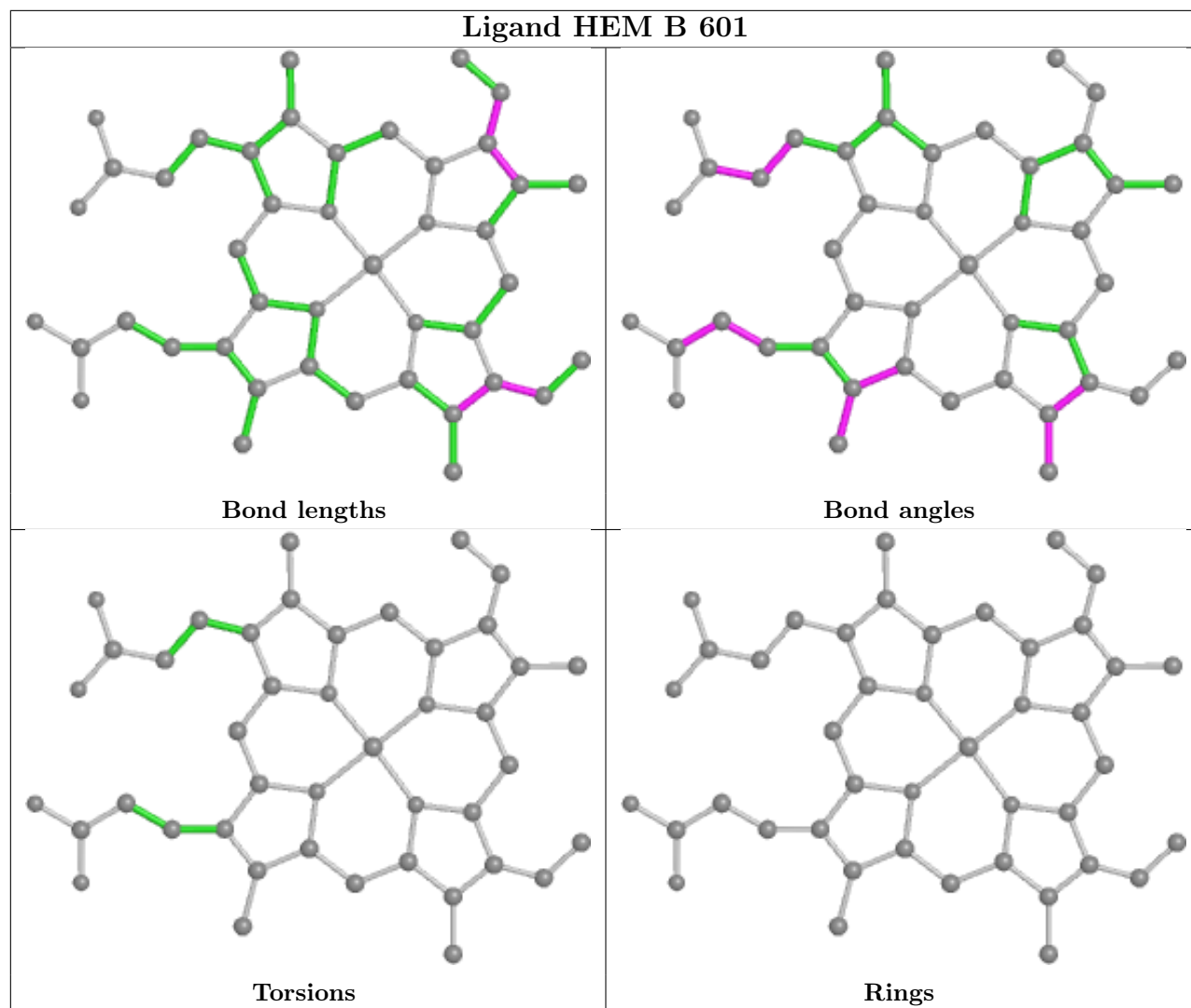
4 monomers are involved in 12 short contacts:

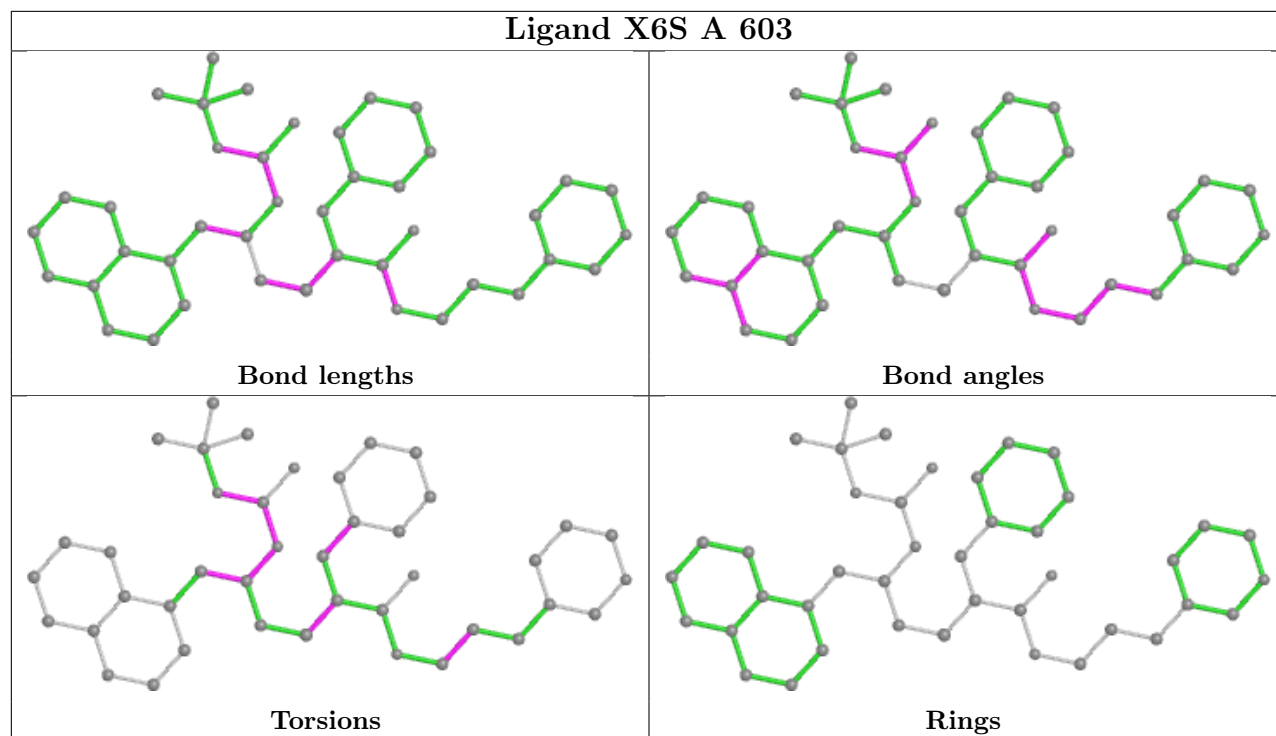
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	SO4	1	0
2	A	601	HEM	4	0
2	B	601	HEM	6	0
4	A	603	X6S	1	0

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 than 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.









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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	457/487 (93%)	0.36	26 (5%) 23 20	58, 98, 173, 214	0
1	B	445/487 (91%)	1.65	126 (28%) 0 0	73, 155, 247, 307	0
All	All	902/974 (92%)	1.00	152 (16%) 1 1	58, 124, 225, 307	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	MET	17.2
1	B	190	GLY	16.9
1	B	457	ILE	16.6
1	B	153	GLY	16.1
1	B	154	ASP	12.7
1	B	456	LEU	12.6
1	B	160	LEU	12.0
1	B	146	VAL	11.9
1	B	345	PRO	10.1
1	B	253	VAL	9.8
1	B	150	ALA	9.8
1	B	187	THR	9.6
1	B	157	VAL	9.5
1	B	156	LEU	9.4
1	B	147	PRO	9.4
1	B	158	ARG	9.2
1	B	145	MET	8.8
1	B	249	LEU	8.5
1	B	179	TYR	8.1
1	B	209	LYS	8.0
1	B	460	LEU	7.5
1	B	210	LEU	7.4
1	B	137	PHE	7.3
1	B	161	ARG	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	LEU	6.7
1	B	496	ARG	6.6
1	B	303	ILE	6.6
1	B	186	SER	6.6
1	B	336	ASP	6.6
1	B	183	VAL	6.5
1	B	203	PHE	6.5
1	B	493	VAL	6.4
1	B	452	MET	6.2
1	B	302	PHE	6.2
1	A	195	SER	6.0
1	B	338	VAL	5.9
1	B	334	GLU	5.8
1	B	204	VAL	5.8
1	B	172	LEU	5.6
1	B	168	LYS	5.4
1	B	340	PRO	5.2
1	B	175	VAL	5.0
1	B	458	ARG	4.9
1	B	255	ARG	4.8
1	B	341	ASN	4.8
1	B	136	THR	4.7
1	B	454	LEU	4.6
1	B	461	GLN	4.6
1	B	164	ALA	4.6
1	B	241	PHE	4.5
1	A	196	LEU	4.5
1	B	269	VAL	4.4
1	B	270	ASP	4.3
1	B	459	VAL	4.3
1	B	159	ASN	4.3
1	A	225	VAL	4.2
1	B	333	GLU	4.1
1	B	349	THR	4.1
1	B	195	SER	4.1
1	A	165	GLU	4.0
1	A	228	PHE	3.9
1	B	205	GLU	3.9
1	B	352[A]	GLN	3.8
1	B	220	PHE	3.8
1	B	180	SER	3.8
1	B	494	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	111	VAL	3.8
1	B	353	MET	3.7
1	A	215	PHE	3.7
1	B	462	ASN	3.7
1	B	212	ARG	3.6
1	B	215	PHE	3.6
1	B	271	PHE	3.6
1	B	162	ARG	3.5
1	A	469	LYS	3.5
1	B	335	ILE	3.5
1	A	227	PRO	3.4
1	B	296	VAL	3.4
1	B	276	ILE	3.4
1	B	354	GLU	3.4
1	B	166	THR	3.4
1	A	256	MET	3.3
1	B	355	TYR	3.3
1	B	491	LEU	3.3
1	B	114	MET	3.3
1	B	176	PHE	3.3
1	B	252	SER	3.2
1	A	306	GLY	3.2
1	B	348	ASP	3.2
1	B	337	ALA	3.2
1	B	151	GLN	3.2
1	B	184	ILE	3.2
1	B	495	SER	3.1
1	B	163	GLU	3.1
1	B	450	MET	3.1
1	B	155	VAL	3.1
1	B	280	ASN	3.1
1	B	218	PRO	3.1
1	B	200	GLN	3.0
1	A	193	ILE	3.0
1	B	472	GLN	3.0
1	B	113	PHE	3.0
1	B	201	ASP	3.0
1	B	165	GLU	3.0
1	B	211	LEU	2.9
1	B	108	PHE	2.9
1	A	168	LYS	2.9
1	A	170	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	493	VAL	2.8
1	B	407	TYR	2.8
1	A	491	LEU	2.8
1	B	189	PHE	2.8
1	B	463	PHE	2.7
1	A	278	SER	2.7
1	B	143	LYS	2.7
1	B	251	LYS	2.6
1	B	129	LEU	2.6
1	B	167	GLY	2.6
1	B	419	PHE	2.6
1	B	453	LYS	2.6
1	A	226[A]	PHE	2.5
1	B	232	ILE	2.5
1	B	369	ILE	2.5
1	B	226	PHE	2.5
1	B	321	LEU	2.5
1	B	245	VAL	2.5
1	B	182	ASP	2.5
1	A	269	VAL	2.5
1	A	341	ASN	2.4
1	A	492	LYS	2.4
1	B	118	ILE	2.4
1	A	201	ASP	2.3
1	B	351	LEU	2.3
1	B	449	LEU	2.3
1	B	301	ILE	2.3
1	A	294	GLU	2.3
1	A	125	GLU	2.2
1	A	139	SER	2.2
1	B	346	THR	2.2
1	B	225	VAL	2.1
1	B	300	ILE	2.1
1	A	211	LEU	2.1
1	B	274	LEU	2.1
1	B	455	ALA	2.1
1	B	309	THR	2.1
1	B	318	MET	2.1
1	B	219	PHE	2.1
1	B	207	THR	2.1
1	B	275	MET	2.1
1	A	108	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	295	LEU	2.0
1	B	489	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

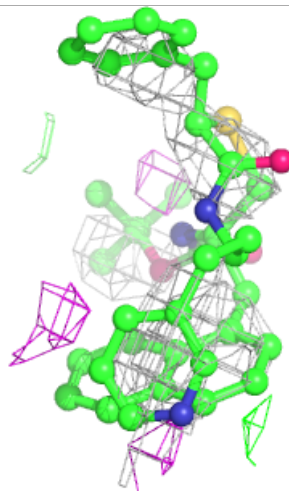
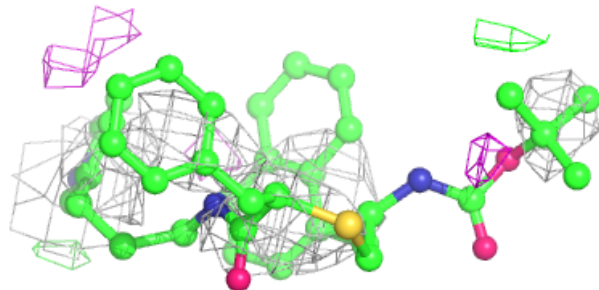
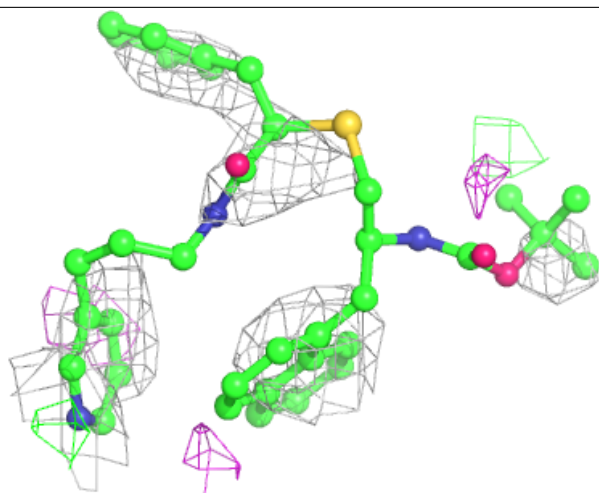
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	602	5/5	0.81	0.14	187,192,195,196	0
4	X6S	B	602	42/42	0.83	0.63	132,176,209,231	0
4	X6S	A	603	42/42	0.86	0.49	116,169,197,198	0
2	HEM	A	601	43/43	0.96	0.23	48,62,77,92	0
2	HEM	B	601	43/43	0.98	0.19	72,95,122,142	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.

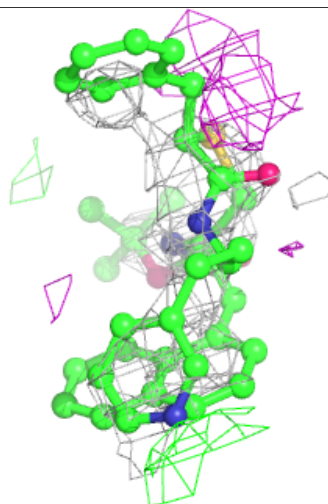
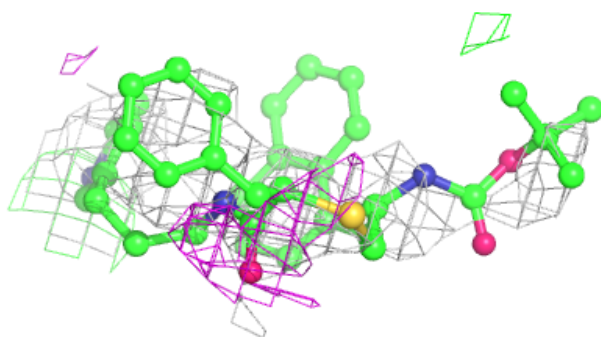
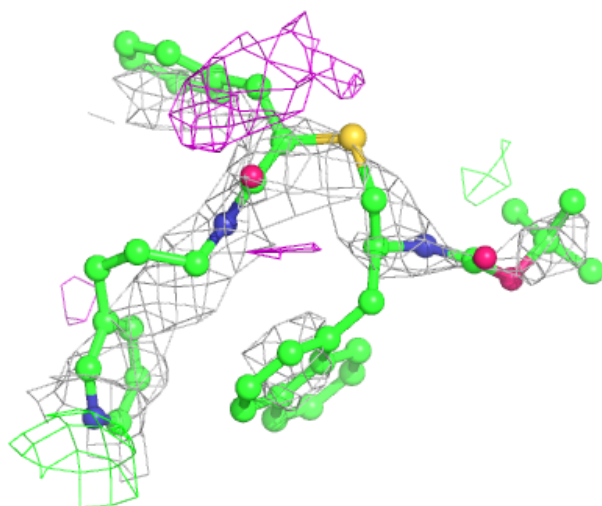
Electron density around X6S B 602:

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



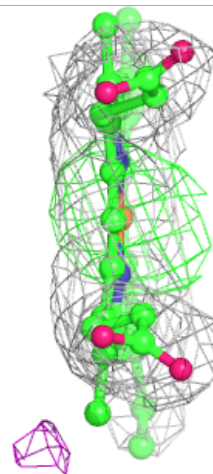
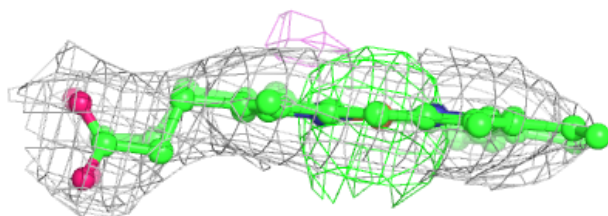
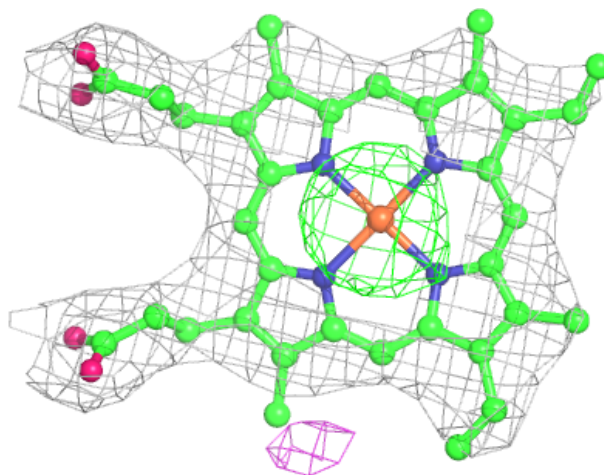
Electron density around X6S A 603:

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



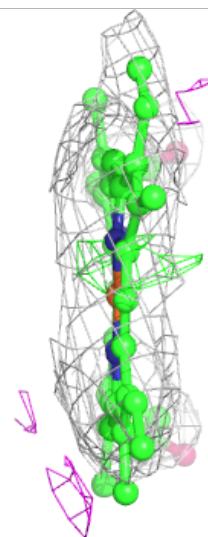
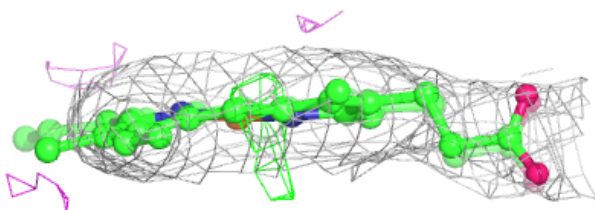
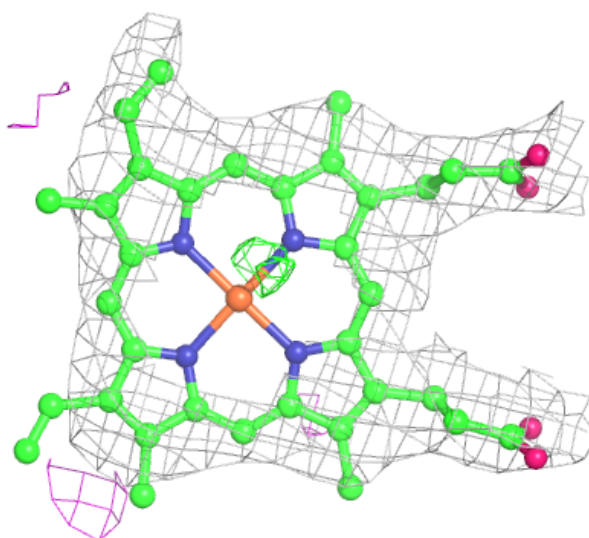
Electron density around HEM A 601:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.