



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:18 AM UTC

PDB ID : 7KVK / pdb_00007kvk
Title : Human CYP3A4 bound to an inhibitor
Authors : Sevrioukova, I.
Deposited on : 2020-11-28
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

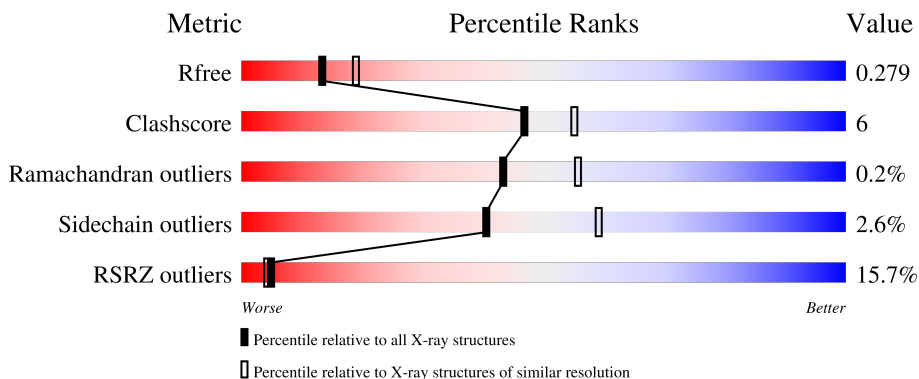
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	9% 81% 11% • 6%
1	B	487	20% 74% 17% • 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7480 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	459	Total	C	N	O	S	0	3	0
			3704	2409	612	658	25			
1	B	445	Total	C	N	O	S	0	1	0
			3574	2333	581	636	24			

There are 52 discrepancies between the modelled and reference sequences:

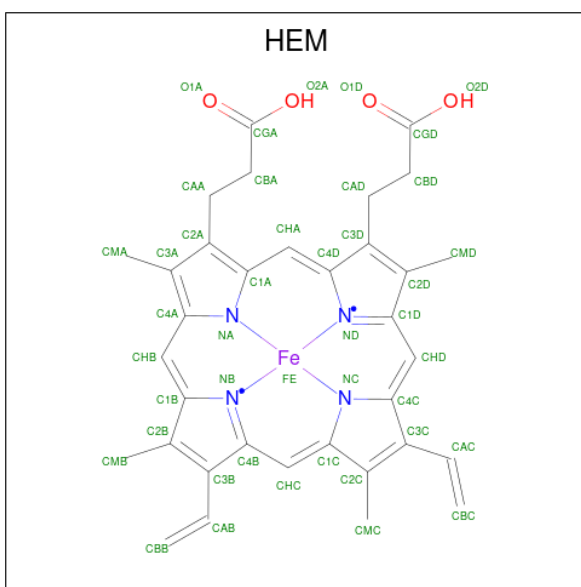
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	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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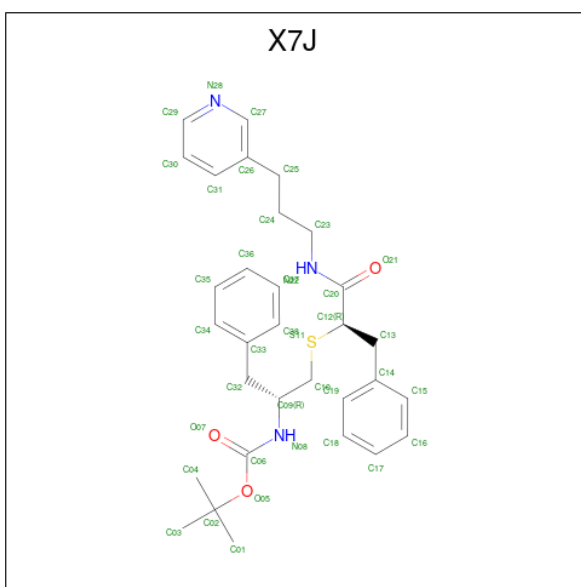
Chain	Residue	Modelled	Actual	Comment	Reference
A	507	HIS	-	expression tag	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is tert-butyl [(2R)-1-[(2R)-1-oxo-3-phenyl-1-[3-(pyridin-3-yl)propyl]amino}propan-2-yl]sulfanyl}-3-phenylpropan-2-yl]carbamate (CCD ID: X7J) (formula: C₃₁H₃₉N₃O₃S) (labeled as "Ligand of Interest" by depositor).



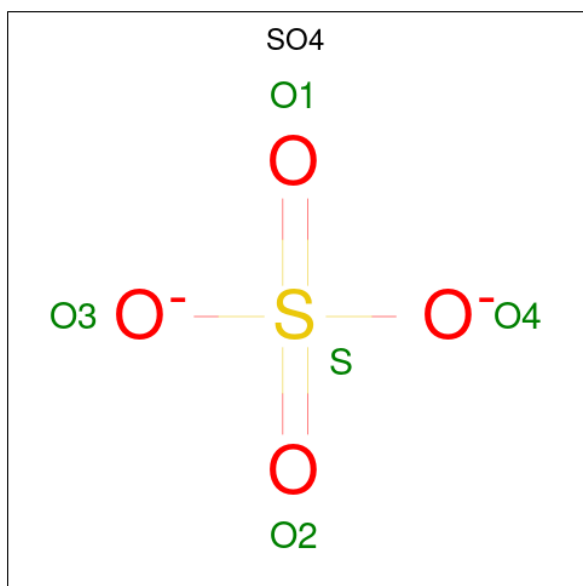
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			38	31	3	3	1		

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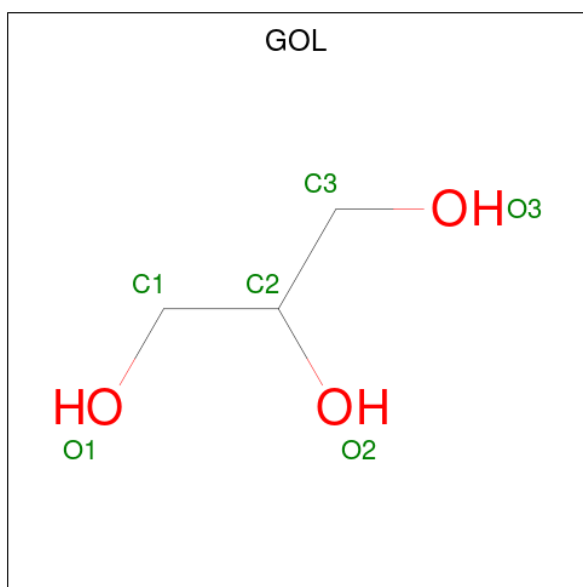
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			38	31	3	3	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



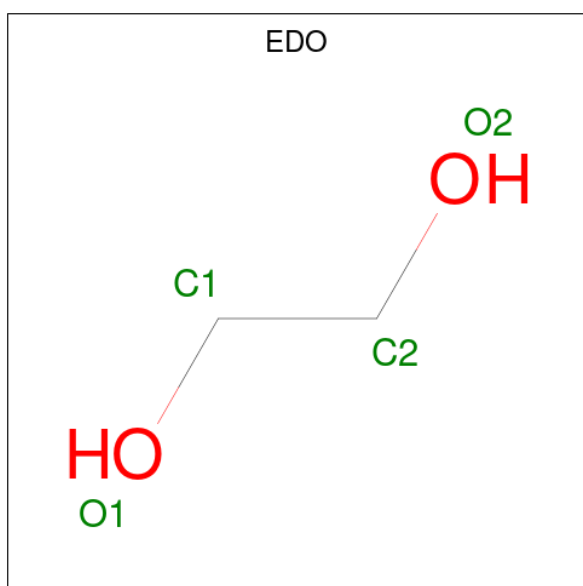
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total 12	O 12	0	0
7	B	2	Total 2	O 2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.59Å 98.50Å 127.12Å 90.00° 142.59° 90.00°	Depositor
Resolution (Å)	63.43 – 2.55 63.43 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.43-2.55) 99.6 (63.43-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.237 , 0.276 0.240 , 0.279	Depositor DCC
R_{free} test set	1965 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7480	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: GOL, HEM, X7J, SO4, 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	0.18	0/3804	0.30	0/5147
1	B	0.23	2/3664 (0.1%)	0.36	6/4958 (0.1%)
All	All	0.21	2/7468 (0.0%)	0.33	6/10105 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	LYS	C-N	7.59	1.44	1.33
1	B	67	LYS	C-N	-5.41	1.25	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	GLY	O-C-N	-5.78	119.32	123.08
1	B	71	VAL	O-C-N	-5.62	117.00	123.07
1	B	69	GLY	CA-C-N	5.42	131.49	121.52
1	B	69	GLY	C-N-CA	5.42	131.49	121.52
1	B	68	TYR	CA-C-N	-5.38	117.29	121.86
1	B	68	TYR	C-N-CA	-5.38	117.29	121.86

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	3704	0	3781	41	0
1	B	3574	0	3656	40	0
2	A	43	0	30	6	0
2	B	43	0	30	5	0
3	A	38	0	0	0	0
3	B	38	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	A	12	0	16	1	0
6	A	4	0	6	1	0
7	A	12	0	0	0	0
7	B	2	0	0	0	0
All	All	7480	0	7519	85	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 6.

All (85) 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)
2:B:601:HEM:HBC2	2:B:601:HEM:HHH	1.67	0.75
2:A:601:HEM:HHH	2:A:601:HEM:HBC2	1.67	0.74
1:A:288:LYS:HB2	1:A:289:ALA:HB2	1.73	0.71
1:B:410:GLU:O	1:B:418:ARG:NH2	2.24	0.71
1:B:50:ILE:HG21	1:B:225:VAL:HG22	1.82	0.62
1:A:154:ASP:OD1	1:A:458:ARG:NH2	2.33	0.61
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.84	0.60
1:B:135:PRO:HA	1:B:138:THR:HG23	1.84	0.59
1:B:223:ILE:HB	1:B:230:ILE:HD11	1.84	0.59
1:A:28:HIS:CD2	1:A:28:HIS:N	2.71	0.58
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.86	0.56
1:B:121:ALA:O	1:B:440:ARG:NH2	2.37	0.56
1:A:218:PRO:O	1:A:222:SER:N	2.37	0.56
1:B:305:ALA:O	1:B:309:THR:OG1	2.21	0.56
1:B:302:PHE:CD2	2:B:601:HEM:HBC1	2.41	0.55
1:B:182:ASP:OD2	1:B:195:SER:OG	2.21	0.55
1:B:103:THR:O	1:B:440:ARG:NH1	2.35	0.54
1:B:193:ILE:HG12	1:B:194:ASP:H	1.73	0.53
1:A:410:GLU:O	1:A:418:ARG:NH2	2.38	0.53
1:B:160:LEU:HD21	1:B:175:VAL:HG11	1.91	0.53
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.90	0.53
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LYS:NZ	1:B:86:ASP:HB2	2.24	0.53
1:A:159:ASN:ND2	1:A:197:ASN:OD1	2.36	0.52
1:A:258:GLU:OE1	1:A:259:SER:N	2.40	0.52
1:A:482:LEU:H	1:A:482:LEU:HD23	1.73	0.52
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.92	0.51
1:B:435:PHE:HB3	1:B:442:CYS:HB3	1.92	0.51
1:B:233:LEU:HB3	1:B:238:ILE:HB	1.92	0.51
1:B:130:ARG:NH2	1:B:441:ASN:OD1	2.45	0.50
1:B:172:LEU:HD11	1:B:491:LEU:HD12	1.94	0.50
1:A:324:HIS:NE2	4:A:603:SO4:O4	2.41	0.50
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.93	0.49
1:B:397:PRO:HB2	1:B:400:ALA:HB3	1.94	0.49
1:A:27:THR:OG1	1:A:28:HIS:N	2.45	0.49
1:A:50:ILE:HD13	1:A:221:LEU:HD11	1.93	0.49
1:A:28:HIS:CD2	1:A:28:HIS:H	2.31	0.48
1:A:232:ILE:O	1:A:236:LEU:HG	2.13	0.48
1:A:29:SER:C	1:A:31:GLY:H	2.22	0.48
1:A:58:CYS:H	5:A:605:GOL:H12	1.78	0.47
1:A:471:THR:OG1	1:A:490:VAL:O	2.21	0.47
1:B:229:LEU:HD22	1:B:232:ILE:HD12	1.97	0.47
1:B:250:ARG:HA	1:B:296:VAL:HG11	1.96	0.46
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.97	0.46
1:B:84:ILE:HB	1:B:89:MET:HE3	1.97	0.46
1:B:46:PHE:HB3	1:B:226:PHE:CE1	2.50	0.46
1:B:109:GLY:HA2	1:B:111:VAL:HG13	1.96	0.46
1:B:248:PHE:HA	1:B:251:LYS:HE2	1.97	0.46
1:B:452:MET:SD	2:B:601:HEM:HBB1	2.55	0.46
1:A:237:ASN:O	1:A:237:ASN:ND2	2.42	0.46
1:A:290:LEU:HD23	1:A:294:GLU:HB2	1.98	0.46
1:A:197:ASN:HA	1:A:198:ASN:HB3	1.98	0.45
1:A:65:HIS:CE1	6:A:606:EDO:H12	2.51	0.45
1:B:436:GLY:HA3	2:B:601:HEM:HBA1	1.98	0.45
1:A:302:PHE:CD2	2:A:601:HEM:HBC1	2.52	0.44
1:A:29:SER:C	1:A:31:GLY:N	2.76	0.44
1:A:102:PHE:HB3	1:A:375:ARG:HB3	1.99	0.44
1:A:84:ILE:HB	1:A:89:MET:HE3	1.98	0.43
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.53	0.43
1:A:93:VAL:HG13	1:A:102:PHE:CG	2.53	0.43
1:B:146:VAL:HB	1:B:147:PRO:HD3	2.01	0.43
1:A:277[B]:ASP:OD1	1:A:278:SER:N	2.52	0.43
1:B:101:VAL:HG21	1:B:381:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HD3	1:A:469:LYS:HA	1.81	0.42
1:B:116:SER:O	1:B:298:GLN:NE2	2.49	0.42
1:B:332:GLN:HG2	1:B:460:LEU:HB3	2.02	0.42
1:B:478:SER:N	1:B:484:GLN:O	2.40	0.42
1:B:199:PRO:HB2	1:B:200:GLN:H	1.66	0.42
1:A:226:PHE:HB3	1:A:228:PHE:CZ	2.54	0.42
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.88	0.42
1:A:29:SER:O	1:A:31:GLY:N	2.53	0.41
1:B:420:SER:O	1:B:424:ALA:N	2.51	0.41
1:A:219:PHE:HE2	1:A:240:VAL:HG12	1.86	0.41
1:A:294:GLU:O	1:A:298:GLN:HG2	2.19	0.41
1:B:97:GLU:OE1	1:B:100:SER:OG	2.26	0.41
1:B:469:LYS:HA	1:B:469:LYS:HD3	1.82	0.41
1:B:71:VAL:HG21	1:B:386:MET:HE1	2.03	0.41
1:A:180:SER:HB3	1:A:306:GLY:O	2.21	0.41
1:A:375:ARG:HH22	2:A:601:HEM:CGA	2.32	0.41
1:A:373:LEU:HB2	1:A:396:ILE:HB	2.03	0.40
1:A:201:ASP:OD2	1:A:203:PHE:HB2	2.21	0.40
1:A:203:PHE:HA	1:A:248:PHE:HE2	1.86	0.40
1:B:61:ASP:OD1	1:B:372:ARG:NH2	2.54	0.40
1:B:401:LEU:HB3	1:B:431:ILE:HG23	2.03	0.40
1:A:441:ASN:HA	2:A:601:HEM:HBA2	2.03	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	456/487 (94%)	429 (94%)	25 (6%)	2 (0%)	30	39
1	B	438/487 (90%)	419 (96%)	19 (4%)	0	100	100
All	All	894/974 (92%)	848 (95%)	44 (5%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	30	HIS

5.3.2 Protein sidechains ⓘ

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	420/441 (95%)	408 (97%)	12 (3%)	37	55
1	B	405/441 (92%)	396 (98%)	9 (2%)	45	64
All	All	825/882 (94%)	804 (98%)	21 (2%)	40	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	HIS
1	A	29	SER
1	A	127	LYS
1	A	163	GLU
1	A	212	ARG
1	A	215	PHE
1	A	226	PHE
1	A	237	ASN
1	A	258	GLU
1	A	268	ARG
1	A	288	LYS
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	237	ASN
1	B	293	LEU
1	B	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	472	GLN
1	B	78	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	601	3	50,50,50	1.44	7 (14%)	67,82,82	1.16	5 (7%)
4	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.07	0
2	HEM	A	601	3,1	50,50,50	1.43	8 (16%)	67,82,82	1.15	4 (5%)
3	X7J	A	602	2	39,40,40	1.64	6 (15%)	46,52,52	1.61	4 (8%)
3	X7J	B	603	2	39,40,40	1.76	7 (17%)	46,52,52	1.75	8 (17%)
5	GOL	A	604	-	5,5,5	0.39	0	5,5,5	0.31	0
5	GOL	A	605	-	5,5,5	0.37	0	5,5,5	0.21	0
6	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.27	0
4	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.08	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	B	601	3	-	2/14/54/54	-
2	HEM	A	601	3,1	-	1/14/54/54	-
3	X7J	A	602	2	-	11/33/33/33	0/3/3/3
3	X7J	B	603	2	-	13/33/33/33	0/3/3/3
5	GOL	A	604	-	-	0/4/4/4	-
5	GOL	A	605	-	-	2/4/4/4	-
6	EDO	A	606	-	-	0/1/1/1	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	X7J	C12-S11	6.06	1.89	1.83
3	A	602	X7J	C12-S11	5.70	1.89	1.83
3	B	603	X7J	C10-S11	5.14	1.87	1.82
3	A	602	X7J	C10-S11	4.59	1.86	1.82
2	B	601	HEM	FE-NB	3.46	2.05	1.94
2	A	601	HEM	FE-NB	3.38	2.05	1.94
2	B	601	HEM	FE-NC	3.30	2.06	1.95
2	A	601	HEM	FE-NC	3.26	2.05	1.95
2	B	601	HEM	FE-ND	3.20	2.04	1.94
2	A	601	HEM	FE-ND	3.20	2.04	1.94
2	B	601	HEM	FE-NA	3.18	2.05	1.95
2	A	601	HEM	FE-NA	3.16	2.05	1.95
2	A	601	HEM	CAB-C3B	3.12	1.55	1.47
2	B	601	HEM	CAB-C3B	3.09	1.55	1.47
2	B	601	HEM	CAC-C3C	2.97	1.55	1.47
2	A	601	HEM	CAC-C3C	2.96	1.55	1.47
3	A	602	X7J	O05-C02	-2.79	1.43	1.48
3	B	603	X7J	C06-N08	2.59	1.41	1.34
3	B	603	X7J	O05-C06	2.55	1.39	1.34
3	B	603	X7J	C20-N22	2.55	1.39	1.33
3	A	602	X7J	C20-N22	2.52	1.39	1.33
3	A	602	X7J	O05-C06	2.39	1.39	1.34
3	B	603	X7J	C32-C09	2.30	1.58	1.53
3	B	603	X7J	O05-C02	-2.26	1.44	1.48
3	A	602	X7J	C06-N08	2.24	1.40	1.34
2	A	601	HEM	CMB-C2B	2.14	1.55	1.50
2	B	601	HEM	CMB-C2B	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	CMD-C2D	2.03	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	X7J	O05-C06-N08	6.20	120.19	110.03
3	A	602	X7J	O05-C06-N08	5.70	119.36	110.03
3	A	602	X7J	O05-C06-O07	-5.10	116.58	125.64
3	B	603	X7J	O05-C06-O07	-4.91	116.92	125.64
3	B	603	X7J	C09-N08-C06	3.18	127.12	122.23
2	A	601	HEM	C4D-ND-C1D	2.49	108.15	105.21
2	B	601	HEM	C4D-ND-C1D	2.48	108.15	105.21
3	A	602	X7J	O21-C20-N22	-2.47	117.75	122.98
3	B	603	X7J	O21-C20-N22	-2.44	117.83	122.98
3	B	603	X7J	C02-O05-C06	2.40	124.61	120.97
3	B	603	X7J	O07-C06-N08	-2.30	121.10	124.86
2	A	601	HEM	C1B-NB-C4B	2.27	107.90	105.21
2	B	601	HEM	C1B-NB-C4B	2.24	107.86	105.21
3	A	602	X7J	O07-C06-N08	-2.19	121.27	124.86
2	B	601	HEM	C3B-C2B-C1B	2.15	108.03	106.41
2	B	601	HEM	C3D-C4D-ND	-2.14	107.83	110.17
2	A	601	HEM	C3D-C4D-ND	-2.13	107.83	110.17
3	B	603	X7J	C01-C02-C04	-2.07	105.96	111.13
2	A	601	HEM	C3B-C2B-C1B	2.07	107.96	106.41
2	B	601	HEM	C2A-C1A-NA	-2.06	107.87	110.15
3	B	603	X7J	C32-C09-N08	2.05	114.23	110.34

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	X7J	O05-C06-N08-C09
3	A	602	X7J	N08-C06-O05-C02
3	B	603	X7J	C10-C09-N08-C06
3	B	603	X7J	C32-C09-N08-C06
5	A	605	GOL	O1-C1-C2-C3
3	A	602	X7J	C01-C02-O05-C06
3	A	602	X7J	C03-C02-O05-C06
3	A	602	X7J	C04-C02-O05-C06
3	B	603	X7J	O07-C06-O05-C02
3	A	602	X7J	O07-C06-N08-C09
3	A	602	X7J	O07-C06-O05-C02

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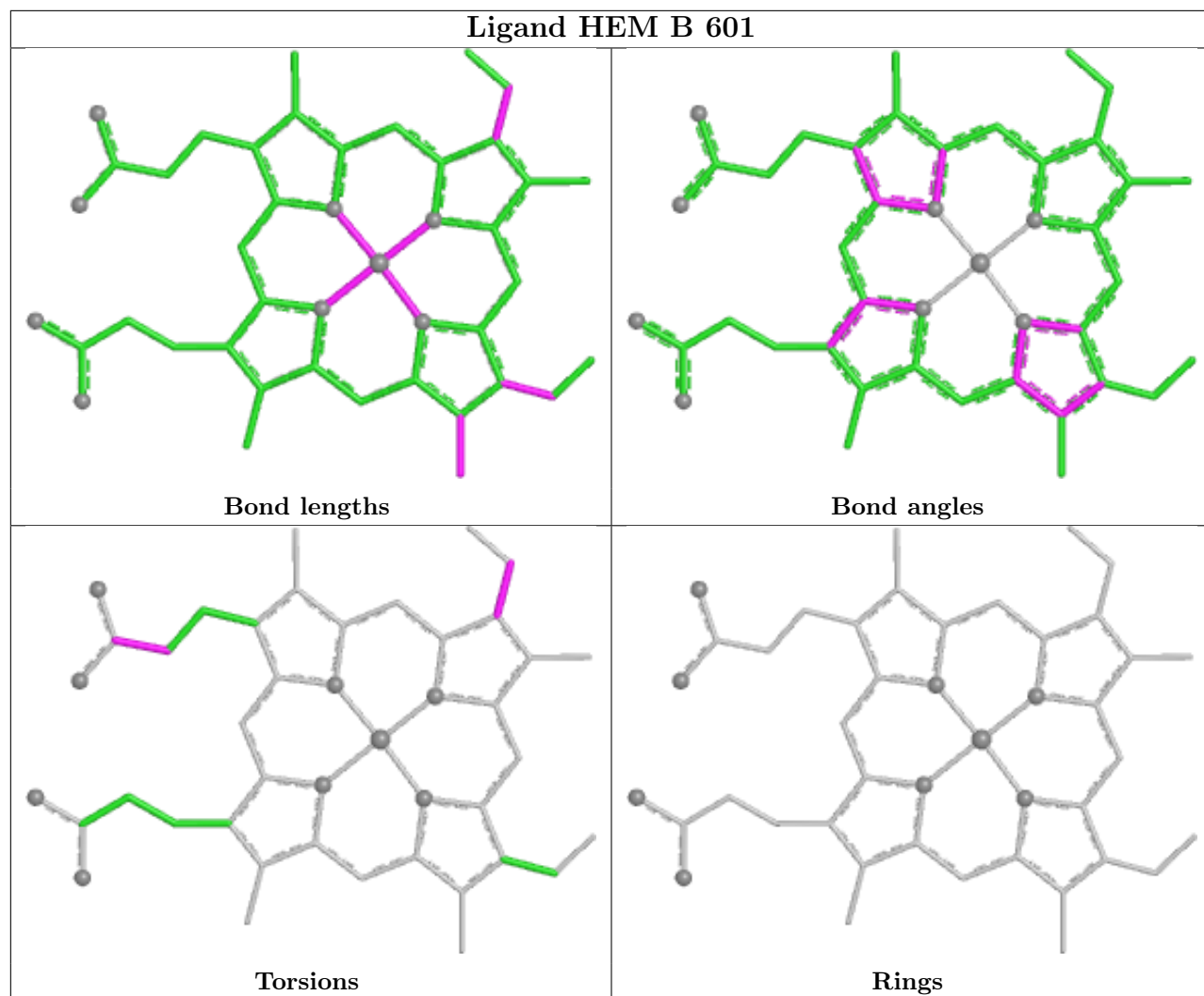
Mol	Chain	Res	Type	Atoms
3	B	603	X7J	C04-C02-O05-C06
3	B	603	X7J	C01-C02-O05-C06
3	B	603	X7J	C03-C02-O05-C06
3	B	603	X7J	N08-C06-O05-C02
3	A	602	X7J	C23-C24-C25-C26
3	B	603	X7J	N22-C23-C24-C25
3	A	602	X7J	N22-C23-C24-C25
5	A	605	GOL	O1-C1-C2-O2
2	A	601	HEM	C4C-C3C-CAC-CBC
2	B	601	HEM	C4C-C3C-CAC-CBC
3	B	603	X7J	O07-C06-N08-C09
3	A	602	X7J	N08-C09-C10-S11
3	B	603	X7J	N08-C09-C10-S11
3	A	602	X7J	C32-C09-C10-S11
3	B	603	X7J	C32-C09-C10-S11
3	B	603	X7J	O05-C06-N08-C09
3	B	603	X7J	C23-C24-C25-C26
2	B	601	HEM	CAD-CBD-CGD-O2D

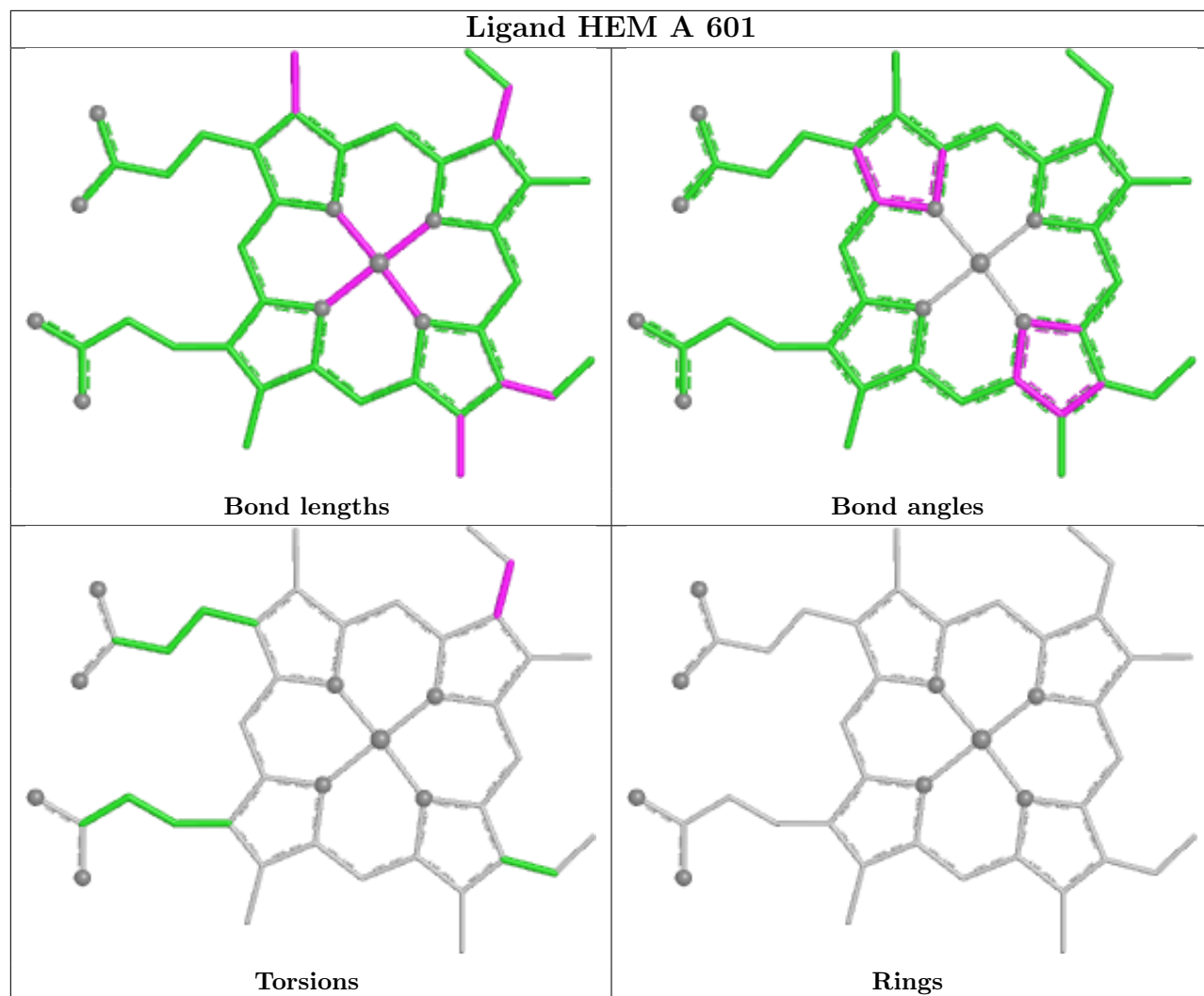
There are no ring outliers.

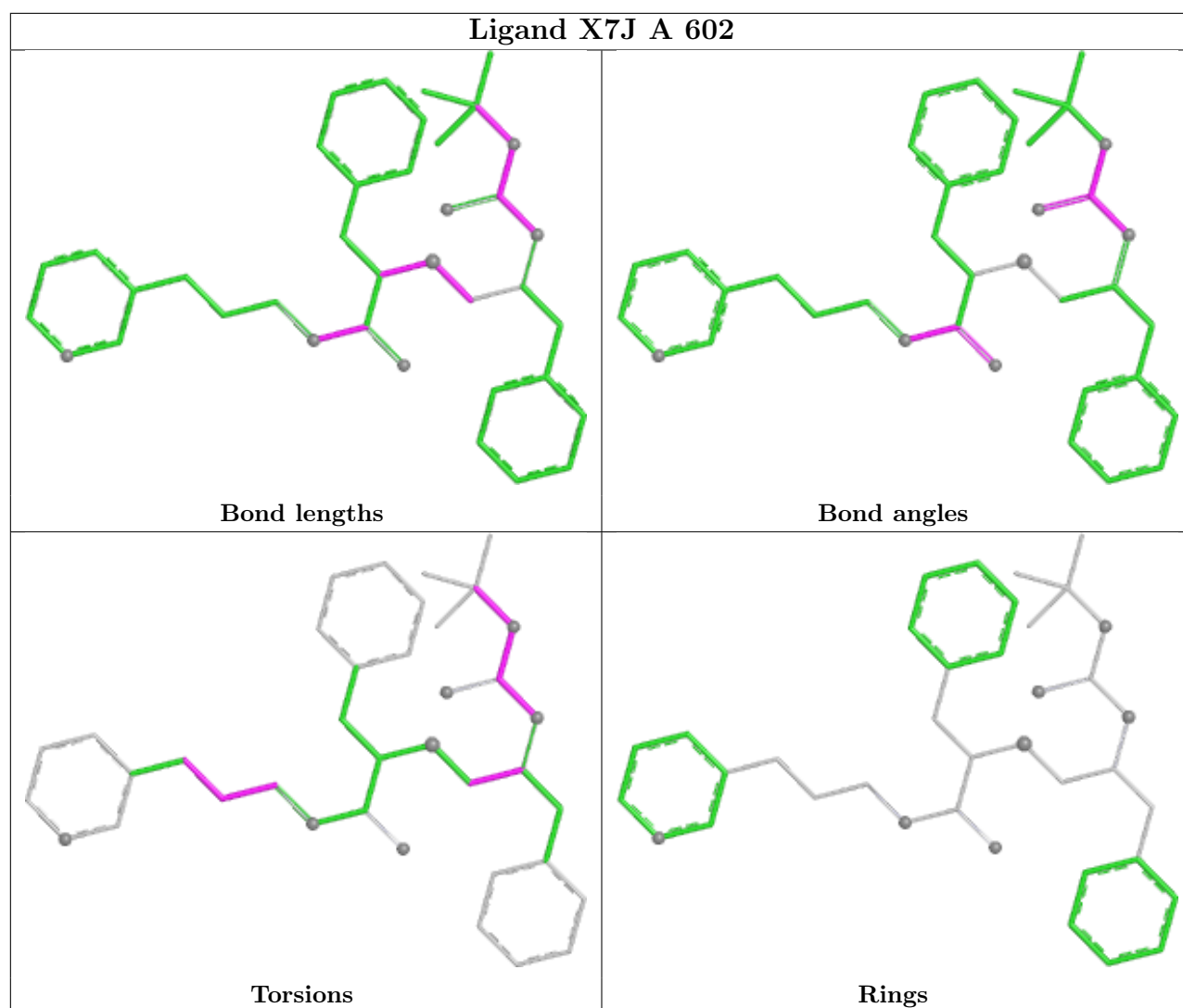
5 monomers are involved in 14 short contacts:

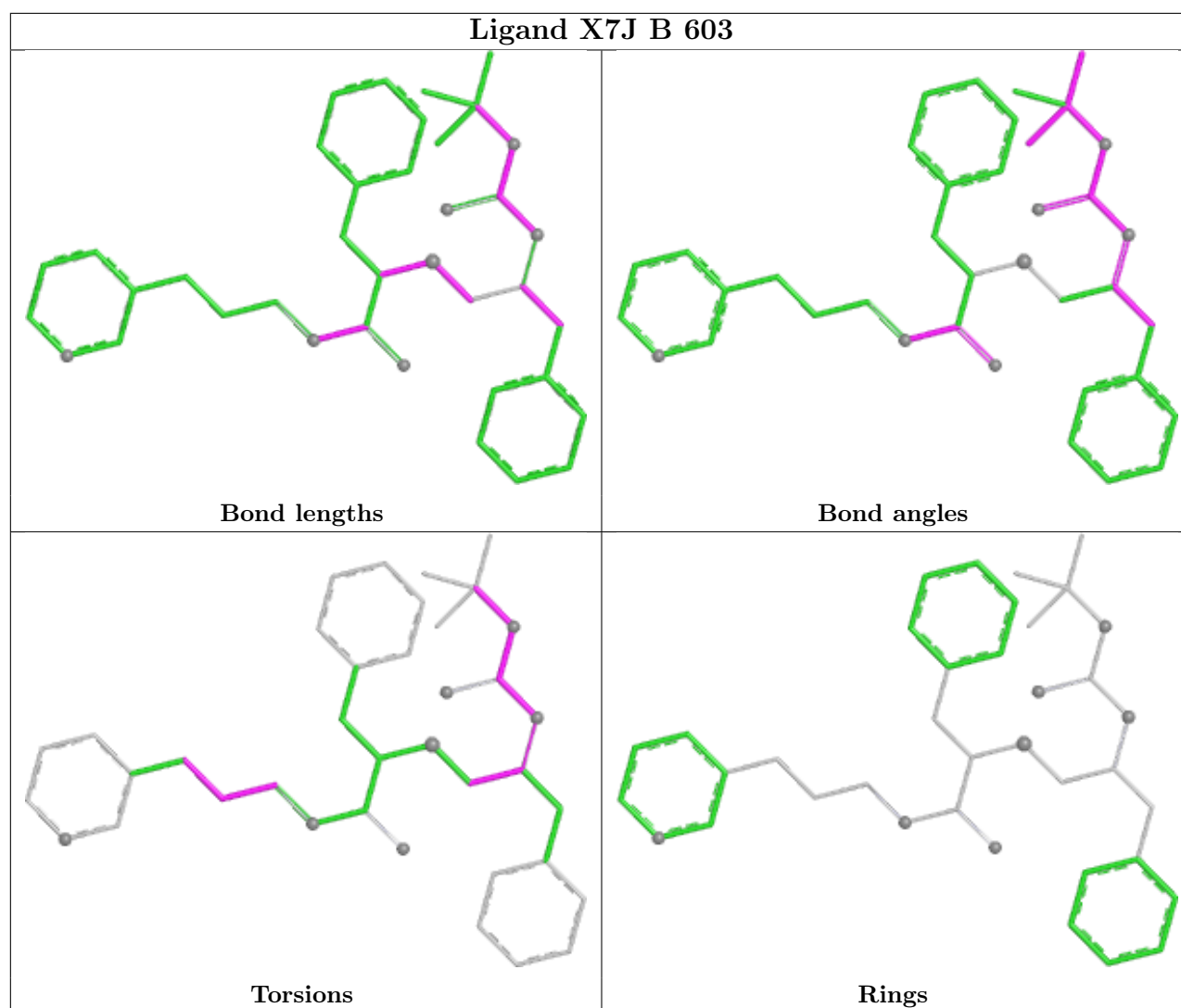
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	5	0
4	A	603	SO4	1	0
2	A	601	HEM	6	0
5	A	605	GOL	1	0
6	A	606	EDO	1	0

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	459/487 (94%)	0.81	43 (9%) 14 13	34, 84, 137, 204	3 (0%)
1	B	445/487 (91%)	1.38	99 (22%) 2 2	58, 131, 184, 221	1 (0%)
All	All	904/974 (92%)	1.09	142 (15%) 5 4	34, 103, 176, 221	4 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	PHE	8.7
1	B	226	PHE	7.0
1	B	249	LEU	6.1
1	B	156	LEU	5.6
1	B	225	VAL	5.5
1	B	236	LEU	5.1
1	A	225	VAL	4.7
1	B	352[A]	GLN	4.6
1	A	229	LEU	4.3
1	B	232	ILE	4.3
1	B	457	ILE	4.3
1	B	118	ILE	4.2
1	B	229	LEU	4.1
1	B	233	LEU	3.9
1	A	228	PHE	3.8
1	A	223	ILE	3.8
1	B	221	LEU	3.8
1	B	369	ILE	3.8
1	B	253	VAL	3.7
1	B	479	LEU	3.7
1	A	479	LEU	3.6
1	B	424	ALA	3.6
1	A	421	ALA	3.6
1	B	154	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	179	TYR	3.5
1	B	241	PHE	3.5
1	B	345	PRO	3.4
1	B	456	LEU	3.3
1	A	412	GLU	3.3
1	B	153	GLY	3.3
1	B	215	PHE	3.2
1	B	57	PHE	3.2
1	B	211	LEU	3.2
1	A	196	LEU	3.2
1	B	317	ILE	3.2
1	B	111	VAL	3.1
1	B	220	PHE	3.1
1	A	158	ARG	3.1
1	A	108	PHE	3.0
1	A	27	THR	3.0
1	B	256	MET	3.0
1	B	353	MET	3.0
1	A	287	HIS	3.0
1	A	142	LEU	3.0
1	B	224	THR	2.9
1	B	133	LEU	2.9
1	B	160	LEU	2.9
1	B	228	PHE	2.9
1	B	210	LEU	2.9
1	B	120	ILE	2.9
1	B	240	VAL	2.9
1	B	223	ILE	2.9
1	B	113	PHE	2.9
1	A	222	SER	2.8
1	B	186	SER	2.8
1	B	222	SER	2.8
1	A	235	VAL	2.8
1	B	218	PRO	2.8
1	B	302	PHE	2.8
1	B	187	THR	2.8
1	A	236	LEU	2.8
1	A	192	ASN	2.7
1	A	259	SER	2.7
1	B	346	THR	2.7
1	B	448	ALA	2.7
1	B	295	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	213	PHE	2.7
1	B	489	VAL	2.7
1	B	298	GLN	2.7
1	A	193	ILE	2.6
1	A	139	SER	2.6
1	B	231	PRO	2.6
1	B	50	ILE	2.6
1	B	269	VAL	2.6
1	B	355	TYR	2.6
1	A	224	THR	2.6
1	B	407	TYR	2.6
1	B	230	ILE	2.5
1	B	465	PHE	2.5
1	B	207	THR	2.5
1	A	227	PRO	2.5
1	B	199	PRO	2.5
1	B	102	PHE	2.5
1	A	267	HIS	2.5
1	B	119	SER	2.5
1	B	354	GLU	2.4
1	B	417	GLU	2.4
1	A	210	LEU	2.4
1	B	219	PHE	2.4
1	B	459	VAL	2.4
1	B	450	MET	2.4
1	A	211	LEU	2.4
1	B	367	PHE	2.4
1	A	256	MET	2.4
1	B	145	MET	2.4
1	A	189	PHE	2.4
1	B	488	PRO	2.3
1	A	135	PRO	2.3
1	B	185	THR	2.3
1	B	276	ILE	2.3
1	B	46	PHE	2.3
1	B	190	GLY	2.3
1	B	216	LEU	2.3
1	B	289	ALA	2.3
1	B	136	THR	2.3
1	A	50	ILE	2.3
1	B	184	ILE	2.3
1	A	254	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	349	THR	2.2
1	B	301	ILE	2.2
1	B	427	ILE	2.2
1	B	425	ASP	2.2
1	A	424	ALA	2.2
1	A	216	LEU	2.2
1	A	215	PHE	2.2
1	B	146	VAL	2.2
1	B	235	VAL	2.2
1	B	467	PRO	2.2
1	B	54	HIS	2.2
1	A	166	THR	2.2
1	A	220	PHE	2.2
1	B	170	VAL	2.2
1	B	310	THR	2.2
1	B	318	MET	2.1
1	B	129	LEU	2.1
1	B	306	GLY	2.1
1	B	412	GLU	2.1
1	A	425	ASP	2.1
1	A	213	PHE	2.1
1	B	387	PHE	2.1
1	A	493	VAL	2.1
1	B	347	TYR	2.1
1	B	296	VAL	2.1
1	A	349	THR	2.1
1	A	348	ASP	2.1
1	B	452	MET	2.1
1	A	111	VAL	2.0
1	A	302	PHE	2.0
1	B	290	LEU	2.0
1	B	455	ALA	2.0
1	B	166	THR	2.0
1	B	114	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

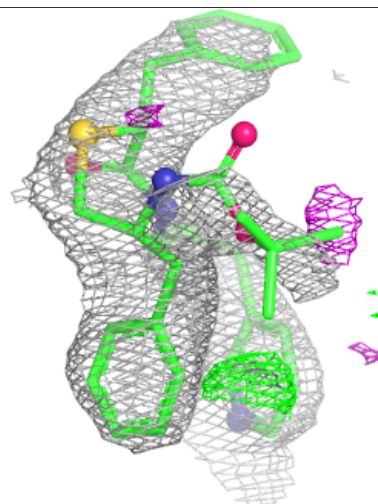
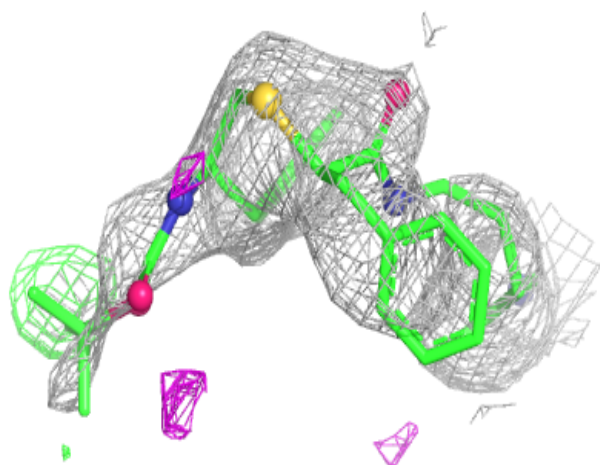
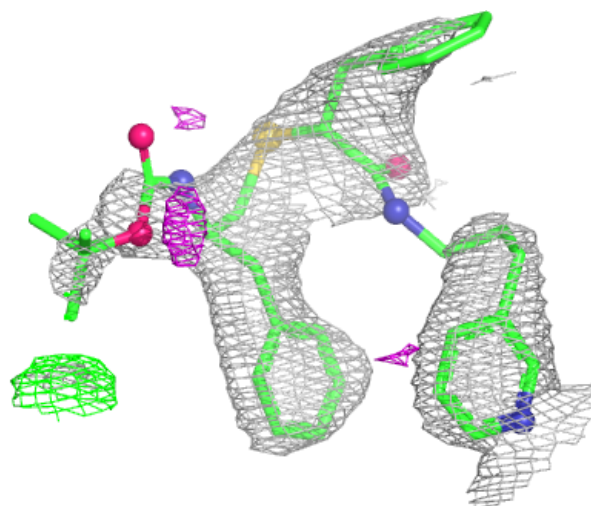
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	602	5/5	0.32	0.12	197,199,202,202	0
3	X7J	B	603	38/38	0.79	0.21	85,126,177,181	0
6	EDO	A	606	4/4	0.85	0.15	94,108,115,118	0
5	GOL	A	604	6/6	0.87	0.15	105,111,116,122	0
4	SO4	A	603	5/5	0.88	0.08	87,92,93,103	5
5	GOL	A	605	6/6	0.89	0.11	91,94,105,106	0
3	X7J	A	602	38/38	0.91	0.18	51,94,154,178	0
2	HEM	B	601	43/43	0.97	0.09	65,82,98,102	0
2	HEM	A	601	43/43	0.98	0.08	38,51,65,78	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.

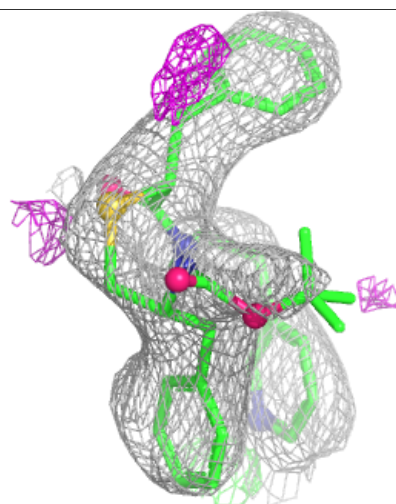
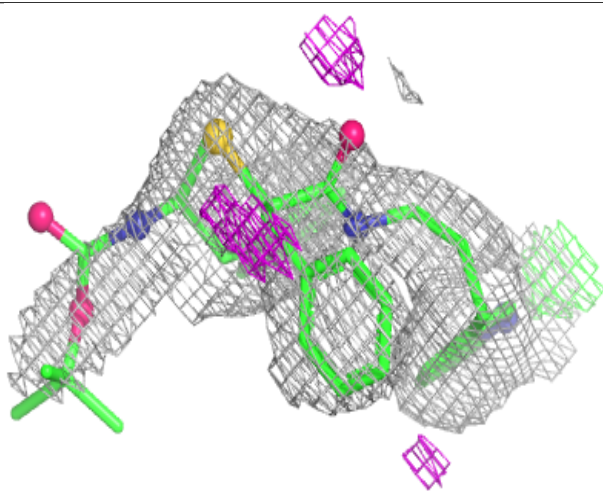
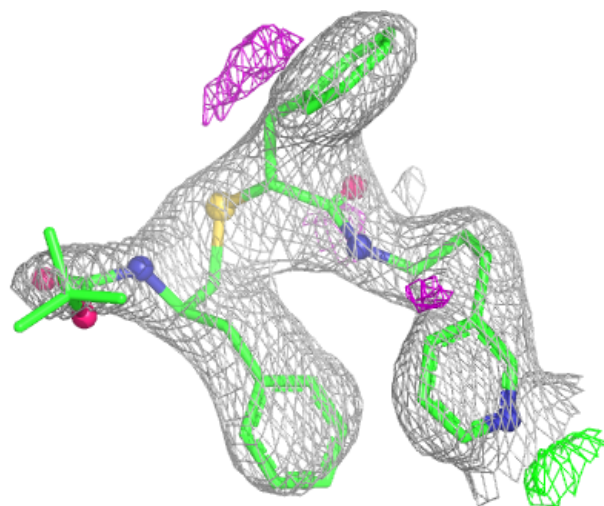
Electron density around X7J B 603:

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



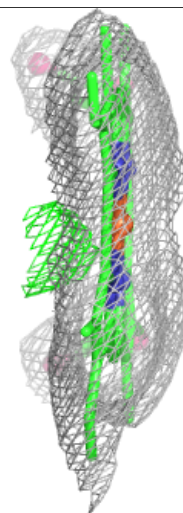
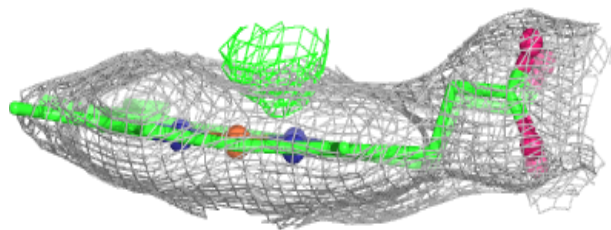
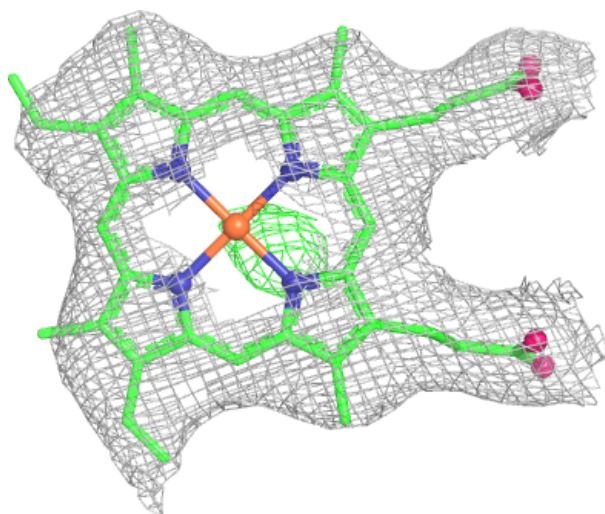
Electron density around X7J A 602:

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



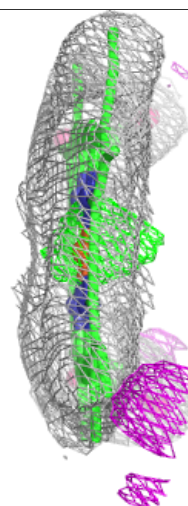
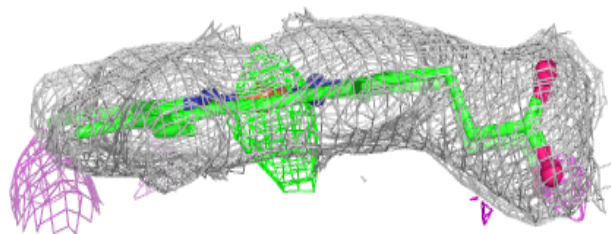
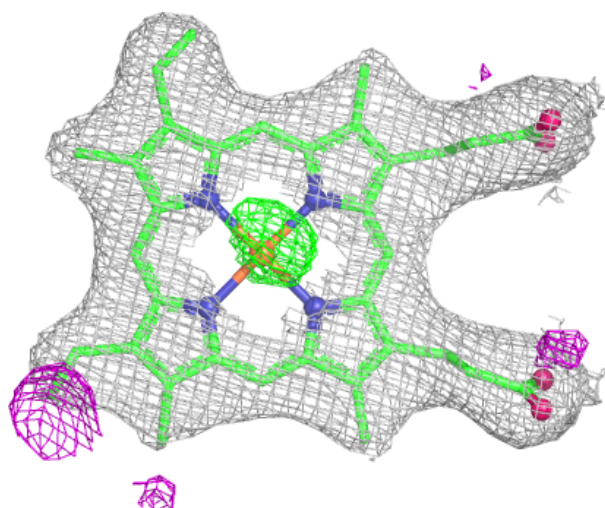
Electron density around HEM B 601:

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



Electron density around HEM 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.