



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2021 – 04:07 PM EST

PDB ID : 7KVK
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 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

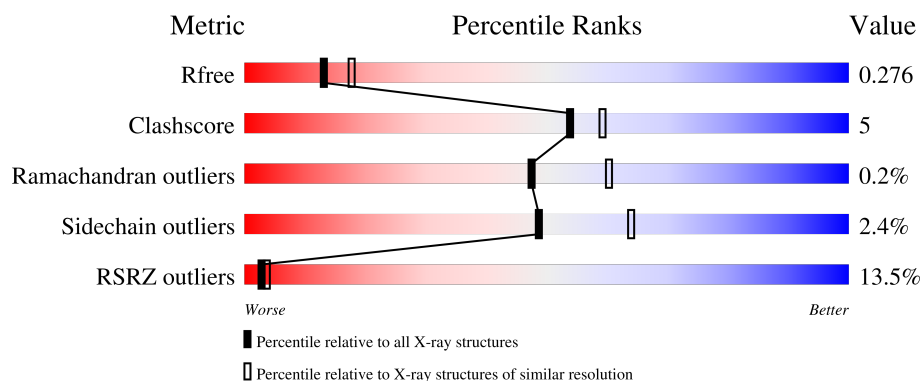
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	
1	B	487	

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:

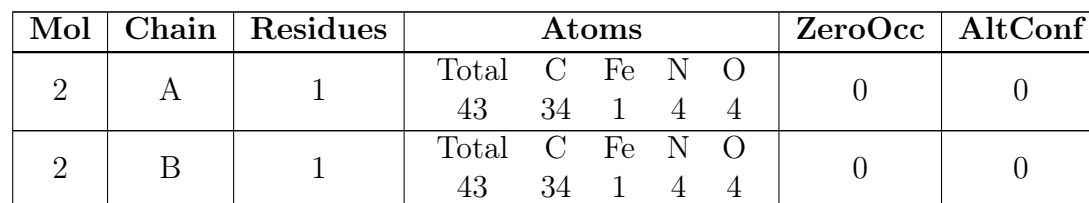
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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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 (three-letter code: SO4) (formula: O₄S).



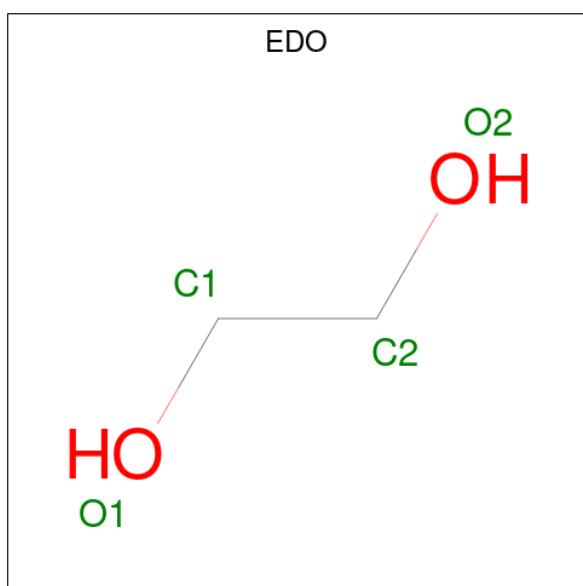
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: 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 (three-letter code: 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 0.238 , 0.276	Depositor DCC
R_{free} test set	1959 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 , 72.4	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, X7J, EDO, HEM, 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	0.26	0/3804	0.40	0/5147
1	B	0.28	0/3664	0.41	0/4958
All	All	0.27	0/7468	0.40	0/10105

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	3704	0	3781	39	0
1	B	3574	0	3656	37	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	2	0	0	0	0
All	All	7480	0	7519	80	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 5.

All (80) 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:HBC2	2:A:601:HEM:HHH	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:N	1:A:28:HIS:CD2	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:302:PHE:CD2	2:B:601:HEM:HBC1	2.41	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:HMB2	2:A:601:HEM:HBB2	1.90	0.53
1:B:184:ILE:HG21	1:B:303:ILE:HA	1.90	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:28:HIS:CD2	2.31	0.48
1:A:232:ILE:O	1:A:236:LEU:HG	2.13	0.48
1:A:58:CYS:H	5:A:605:GOL:H12	1.78	0.47
1:B:229:LEU:HD22	1:B:232:ILE:HD12	1.97	0.47
1:A:471:THR:OG1	1:A:490:VAL:O	2.21	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: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:ND2	1:A:237:ASN:O	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:102:PHE:HB3	1:A:375:ARG:HB3	1.99	0.44
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:A:29:SER:C	1:A:31:GLY:H	2.22	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
1:B:182:ASP:OD2	1:B:195:SER:OG	2.21	0.42
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:469:LYS:HA	1:B:469:LYS:HD3	1.82	0.41
1:B:97:GLU:OE1	1:B:100:SER:OG	2.26	0.41
1:A:180:SER:HB3	1:A:306:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:PHE:HA	1:A:248:PHE:HE2	1.86	0.40
1:A:201:ASP:OD2	1:A:203:PHE:HB2	2.21	0.40
1:B:401:LEU:HB3	1:B:431:ILE:HG23	2.03	0.40
1:B:61:ASP:OD1	1:B:372:ARG:NH2	2.54	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%)	34	46
1	B	438/487 (90%)	419 (96%)	19 (4%)	0	100	100
All	All	894/974 (92%)	848 (95%)	44 (5%)	2 (0%)	47	60

All (2) Ramachandran outliers are listed below:

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

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	420/441 (95%)	409 (97%)	11 (3%)	46	61
1	B	405/441 (92%)	396 (98%)	9 (2%)	52	66
All	All	825/882 (94%)	805 (98%)	20 (2%)	49	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS

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 [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$
6	EDO	A	606	-	3,3,3	0.47	0	2,2,2	0.22	0
4	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.04	0
3	X7J	A	602	2	39,40,40	1.60	6 (15%)	45,52,52	1.58	4 (8%)
2	HEM	B	601	3	27,50,50	1.88	4 (14%)	17,82,82	1.44	1 (5%)
5	GOL	A	604	-	5,5,5	0.39	0	5,5,5	0.28	0
3	X7J	B	603	2	39,40,40	1.71	7 (17%)	45,52,52	1.72	7 (15%)
2	HEM	A	601	1,3	27,50,50	1.87	5 (18%)	17,82,82	1.43	2 (11%)
5	GOL	A	605	-	5,5,5	0.36	0	5,5,5	0.18	0
4	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.05	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
6	EDO	A	606	-	-	0/1/1/1	-
3	X7J	A	602	2	-	11/33/33/33	0/3/3/3
2	HEM	B	601	3	-	0/6/54/54	-
5	GOL	A	604	-	-	0/4/4/4	-
3	X7J	B	603	2	-	12/33/33/33	0/3/3/3
2	HEM	A	601	1,3	-	0/6/54/54	-
5	GOL	A	605	-	-	2/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	X7J	C12-S11	6.07	1.89	1.83
3	A	602	X7J	C12-S11	5.71	1.89	1.83
3	B	603	X7J	C10-S11	4.80	1.87	1.82
2	B	601	HEM	C3C-C2C	-4.59	1.34	1.40
2	A	601	HEM	C3C-C2C	-4.53	1.34	1.40
3	A	602	X7J	C10-S11	4.29	1.86	1.82
2	A	601	HEM	C3B-CAB	3.81	1.55	1.47
2	B	601	HEM	C3B-CAB	3.78	1.55	1.47
2	B	601	HEM	C3B-C2B	-3.74	1.35	1.40
2	B	601	HEM	C3C-CAC	3.66	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.65	1.35	1.40
2	A	601	HEM	C3C-CAC	3.65	1.55	1.47
3	B	603	X7J	C20-N22	2.74	1.39	1.33
3	A	602	X7J	C20-N22	2.71	1.39	1.33
3	A	602	X7J	O05-C02	-2.68	1.43	1.48
3	B	603	X7J	C06-N08	2.62	1.41	1.34
3	B	603	X7J	O05-C06	2.44	1.39	1.34
3	A	602	X7J	O05-C06	2.29	1.39	1.34
3	A	602	X7J	C06-N08	2.26	1.40	1.34
3	B	603	X7J	C32-C09	2.19	1.58	1.53
3	B	603	X7J	O05-C02	-2.17	1.44	1.48
2	A	601	HEM	CAA-C2A	2.10	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	X7J	O05-C06-N08	6.05	120.19	110.02
3	A	602	X7J	O05-C06-N08	5.56	119.36	110.02
3	A	602	X7J	O05-C06-O07	-4.96	116.58	125.62
3	B	603	X7J	O05-C06-O07	-4.77	116.92	125.62
3	B	603	X7J	C09-N08-C06	3.12	127.12	122.30
3	A	602	X7J	O21-C20-N22	-2.44	117.75	122.99
3	B	603	X7J	O21-C20-N22	-2.41	117.83	122.99
3	B	603	X7J	C02-O05-C06	2.35	124.61	120.99
3	B	603	X7J	O07-C06-N08	-2.29	121.10	124.85
2	B	601	HEM	CMB-C2B-C3B	2.26	128.91	124.68
2	A	601	HEM	CMB-C2B-C3B	2.22	128.83	124.68
3	A	602	X7J	O07-C06-N08	-2.19	121.27	124.85
2	A	601	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
3	B	603	X7J	C32-C09-N08	2.00	114.23	110.39

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	X7J	O05-C06-N08-C09
3	A	602	X7J	O07-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	C03-C02-O05-C06
3	A	602	X7J	C01-C02-O05-C06
3	A	602	X7J	C04-C02-O05-C06
3	B	603	X7J	O07-C06-O05-C02
3	B	603	X7J	C01-C02-O05-C06
3	A	602	X7J	O07-C06-O05-C02
3	B	603	X7J	C03-C02-O05-C06
3	B	603	X7J	C04-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
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

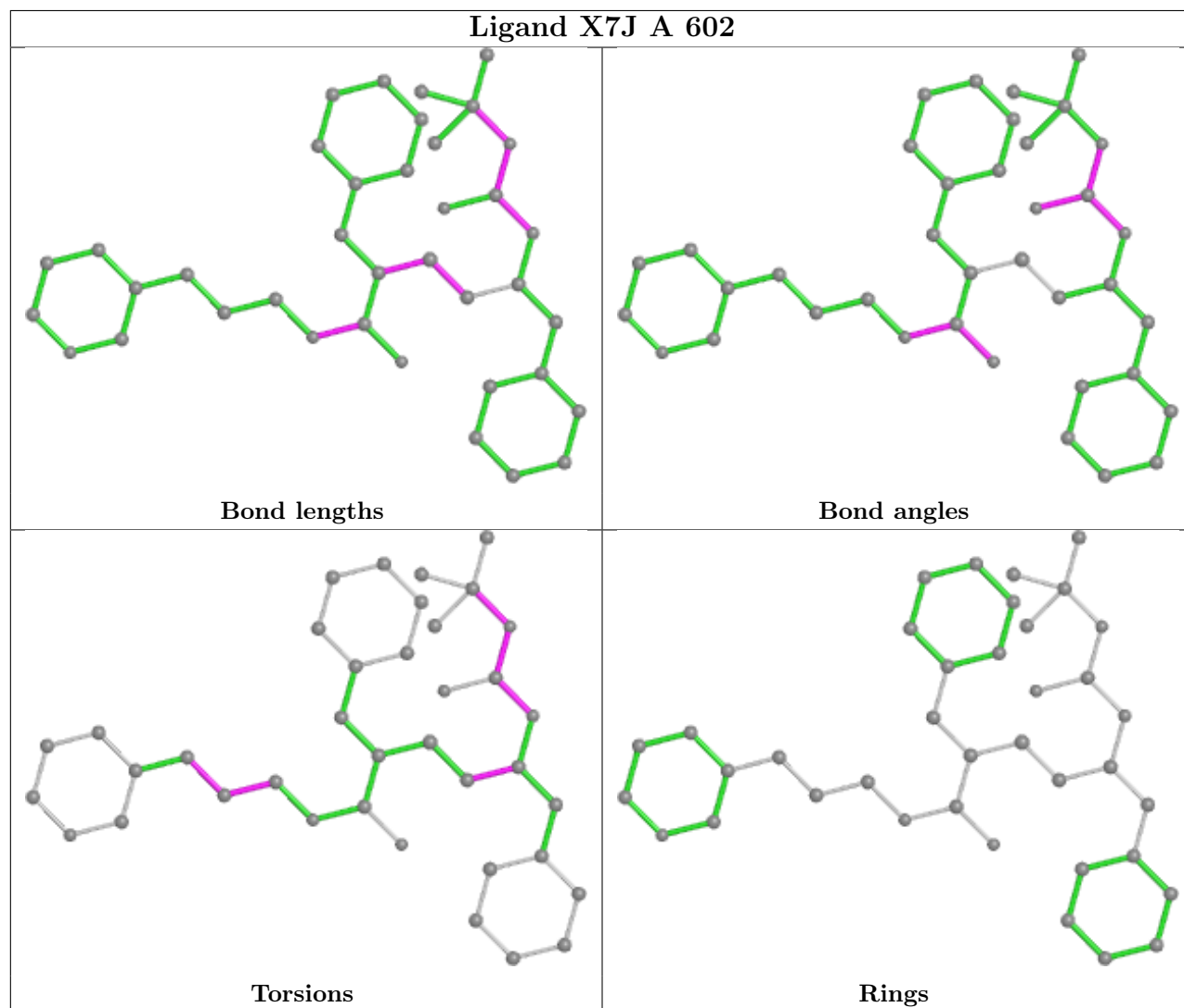
There are no ring outliers.

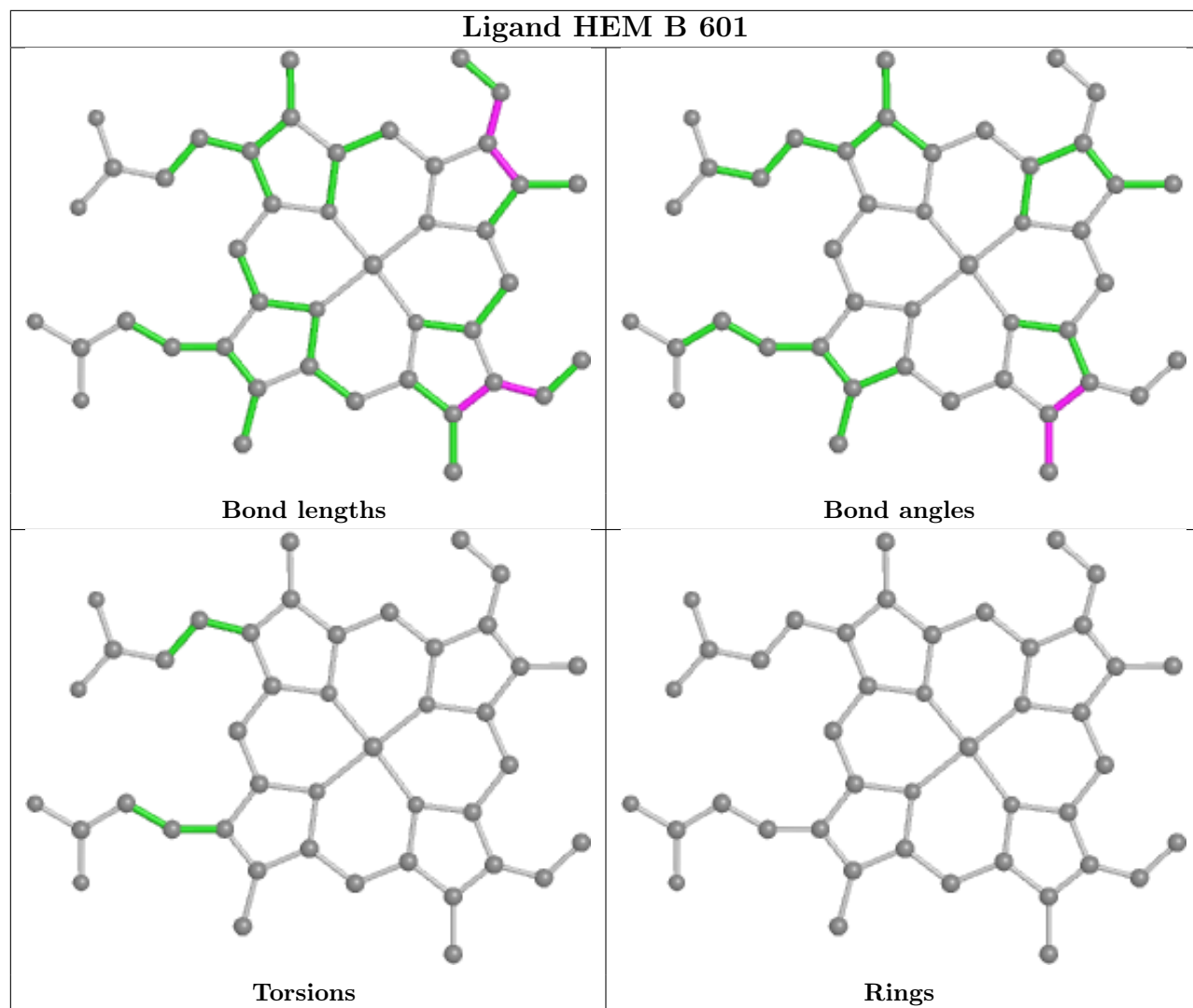
5 monomers are involved in 14 short contacts:

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

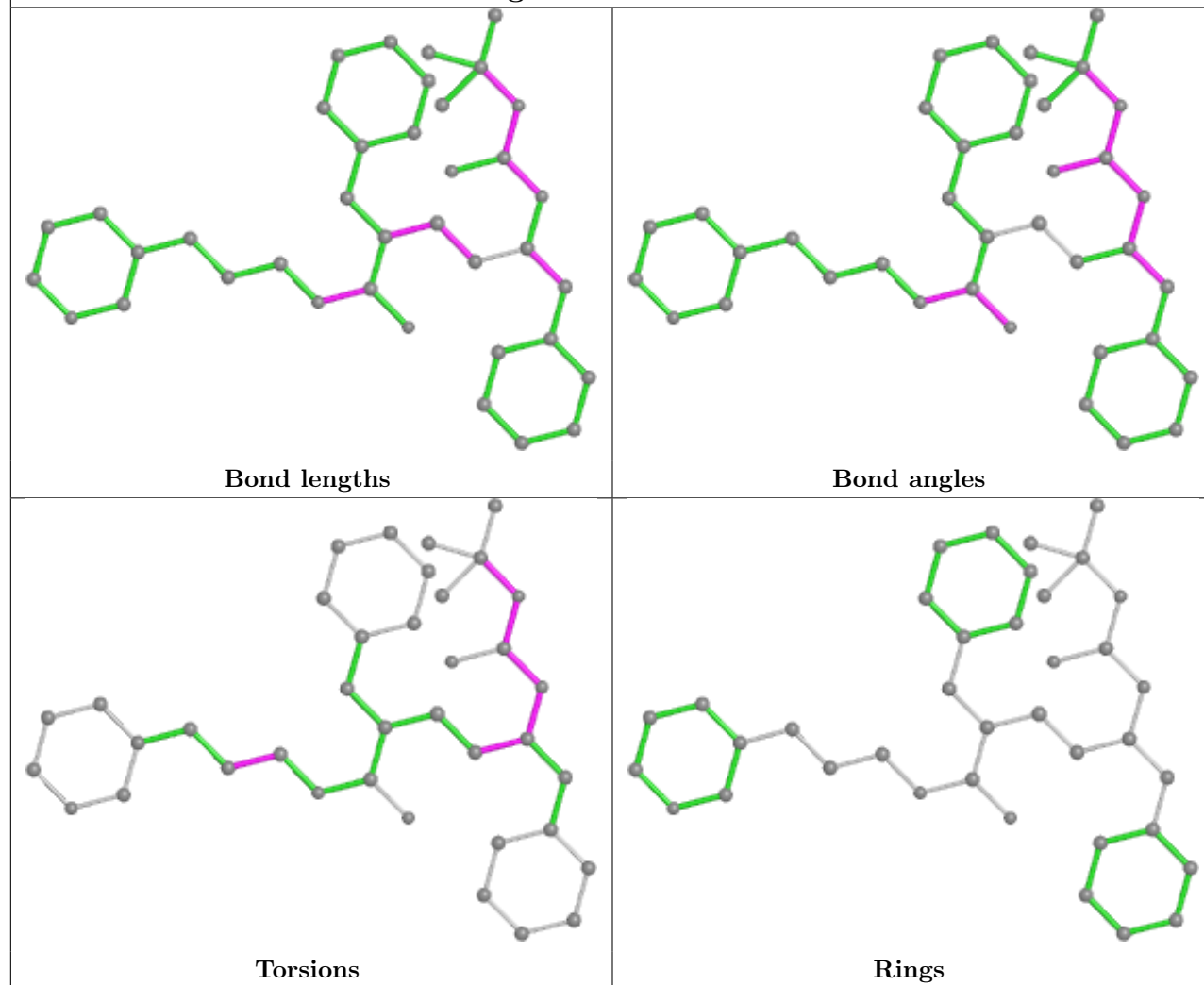
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

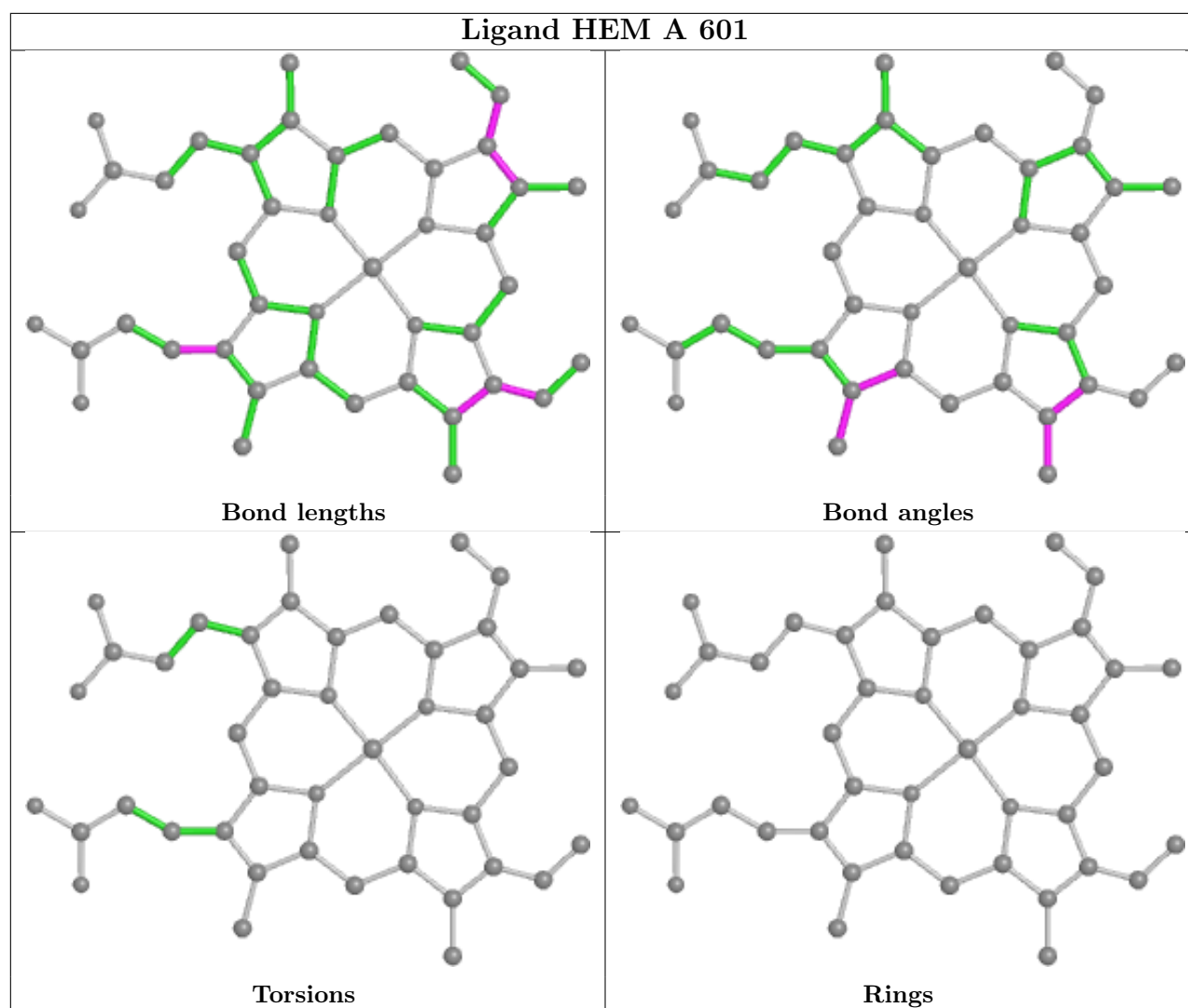
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand X7J B 603





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%)	0.18	16 (3%)	44 51	48, 84, 137, 204	0
1	B	445/487 (91%)	1.14	106 (23%)	0 0	58, 131, 184, 221	0
All	All	904/974 (92%)	0.65	122 (13%)	3 4	48, 104, 176, 221	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	LEU	14.2
1	B	345	PRO	9.1
1	B	457	ILE	8.0
1	B	190	GLY	7.8
1	B	256	MET	7.8
1	B	341	ASN	7.3
1	B	156	LEU	7.0
1	B	253	VAL	6.9
1	A	226	PHE	6.6
1	B	154	ASP	6.5
1	B	111	VAL	6.5
1	B	153	GLY	5.7
1	B	160	LEU	5.6
1	B	210	LEU	5.6
1	B	352[A]	GLN	5.4
1	A	479	LEU	5.4
1	B	215	PHE	5.2
1	B	209	LYS	5.1
1	B	179	TYR	4.9
1	B	118	ILE	4.9
1	B	161	ARG	4.8
1	B	340	PRO	4.8
1	B	166	THR	4.7
1	B	164	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	251	LYS	4.6
1	B	296	VAL	4.5
1	B	133	LEU	4.5
1	B	226	PHE	4.4
1	B	145	MET	4.4
1	A	158	ARG	4.3
1	B	225	VAL	4.2
1	B	189	PHE	4.2
1	B	184	ILE	4.1
1	B	276	ILE	4.1
1	A	167	GLY	3.9
1	B	216	LEU	3.9
1	B	207	THR	3.9
1	B	303	ILE	3.8
1	B	280	ASN	3.8
1	A	469	LYS	3.8
1	B	302	PHE	3.8
1	B	203	PHE	3.7
1	B	493	VAL	3.7
1	B	163	GLU	3.7
1	B	456	LEU	3.7
1	B	158	ARG	3.7
1	B	336	ASP	3.6
1	B	479	LEU	3.6
1	B	241	PHE	3.6
1	B	128	ARG	3.6
1	B	290	LEU	3.6
1	B	221	LEU	3.6
1	A	216	LEU	3.5
1	B	132	LEU	3.5
1	B	300	ILE	3.4
1	B	292	ASP	3.4
1	B	245	VAL	3.4
1	B	187	THR	3.2
1	B	205	GLU	3.2
1	B	201	ASP	3.2
1	B	353	MET	3.2
1	B	114	MET	3.2
1	B	146	VAL	3.1
1	B	234	GLU	3.1
1	B	137	PHE	3.0
1	B	129	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	236	LEU	3.0
1	B	274	LEU	3.0
1	B	349	THR	2.9
1	B	459	VAL	2.9
1	B	220	PHE	2.9
1	B	147	PRO	2.9
1	B	269	VAL	2.8
1	B	136	THR	2.8
1	B	168	LYS	2.8
1	B	271	PHE	2.8
1	B	337	ALA	2.8
1	B	223	ILE	2.8
1	B	295	LEU	2.8
1	B	334	GLU	2.7
1	A	229	LEU	2.7
1	A	281	SER	2.7
1	B	57	PHE	2.7
1	B	186	SER	2.7
1	B	172	LEU	2.6
1	B	135	PRO	2.6
1	A	196	LEU	2.6
1	B	183	VAL	2.5
1	B	113	PHE	2.5
1	B	232	ILE	2.5
1	B	348	ASP	2.5
1	B	335	ILE	2.4
1	B	165	GLU	2.4
1	A	168	LYS	2.4
1	B	218	PRO	2.3
1	A	223	ILE	2.3
1	B	495	SER	2.3
1	B	175	VAL	2.3
1	B	140	GLY	2.3
1	B	325	PRO	2.3
1	B	212	ARG	2.3
1	B	230	ILE	2.3
1	B	167	GLY	2.2
1	B	317	ILE	2.2
1	A	228	PHE	2.2
1	B	213	PHE	2.2
1	B	278	SER	2.2
1	B	452	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	116	SER	2.2
1	B	354	GLU	2.2
1	B	119	SER	2.1
1	B	412	GLU	2.1
1	A	210	LEU	2.1
1	B	236	LEU	2.1
1	B	200	GLN	2.1
1	B	487	LYS	2.1
1	B	461	GLN	2.1
1	A	170	VAL	2.1
1	A	227	PRO	2.1
1	B	120	ILE	2.1
1	B	491	LEU	2.0
1	B	244	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

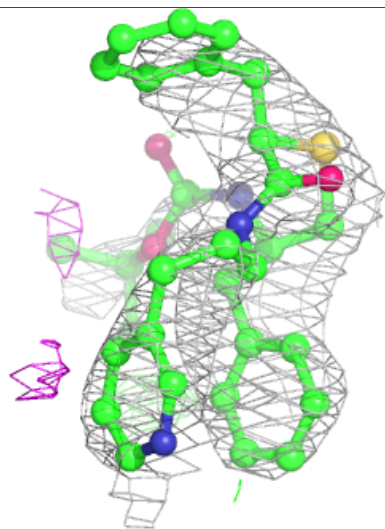
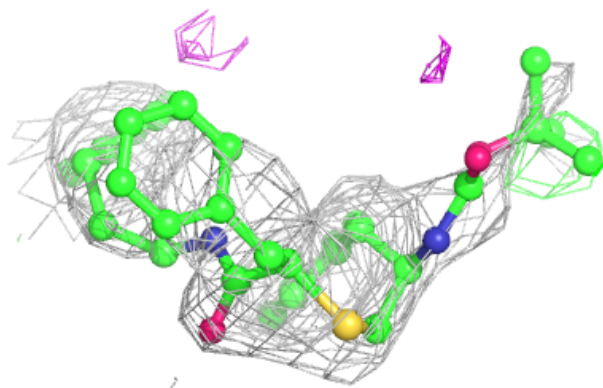
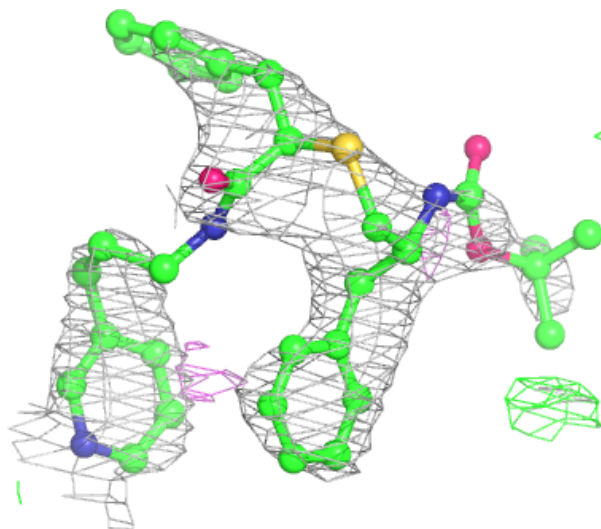
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	606	4/4	0.81	0.22	94,108,115,118	0
3	X7J	B	603	38/38	0.84	0.30	85,126,177,181	0
5	GOL	A	605	6/6	0.88	0.33	91,94,105,106	0
4	SO4	B	602	5/5	0.89	0.18	197,199,202,202	0
4	SO4	A	603	5/5	0.92	0.13	87,92,93,103	5
3	X7J	A	602	38/38	0.92	0.27	51,94,154,178	0
5	GOL	A	604	6/6	0.92	0.29	105,111,116,122	0
2	HEM	B	601	43/43	0.97	0.16	65,82,98,102	0
2	HEM	A	601	43/43	0.97	0.19	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.

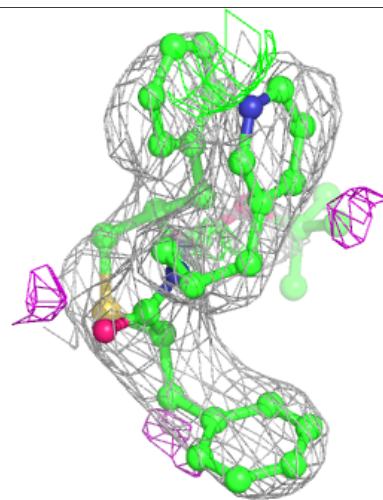
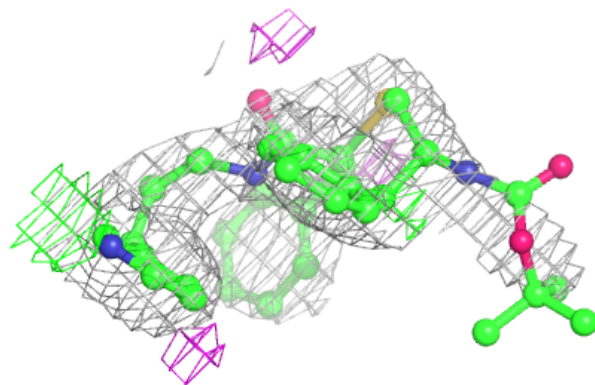
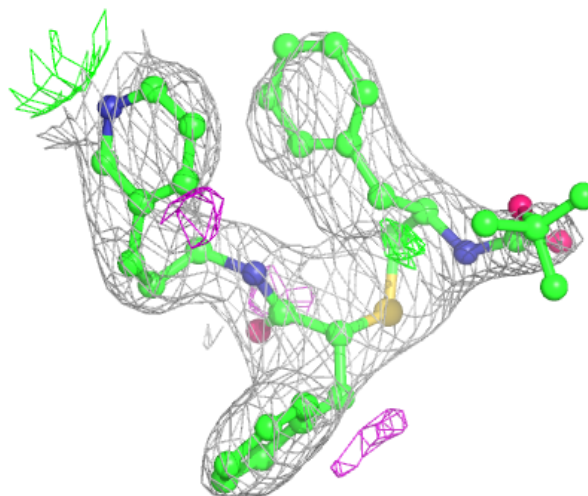
Electron density around X7J B 603:

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



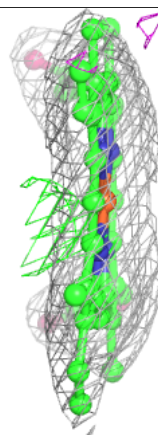
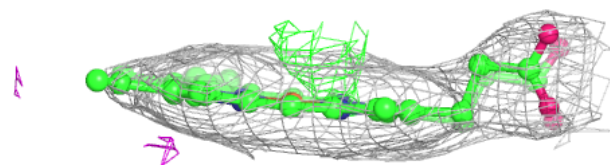
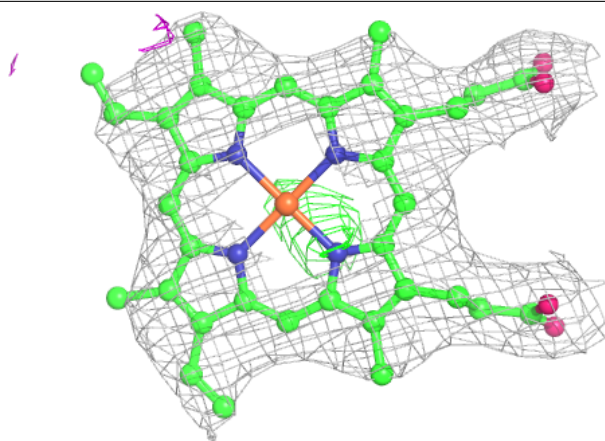
Electron density around X7J A 602:

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



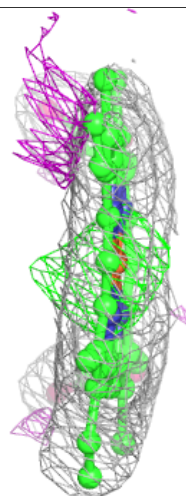
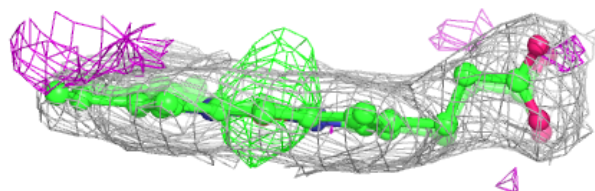
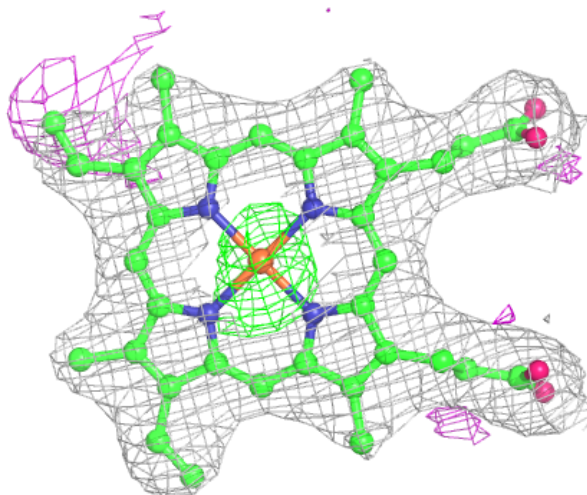
Electron density around HEM B 601:

$2mF_o - DF_c$ (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 [i](#)

There are no such residues in this entry.