



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2021 – 04:04 PM EST

PDB ID : 7KVH
Title : Human CYP3A4 bound to an inhibitor
Authors : Sevrioukova, I.
Deposited on : 2020-11-28
Resolution : 2.79 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

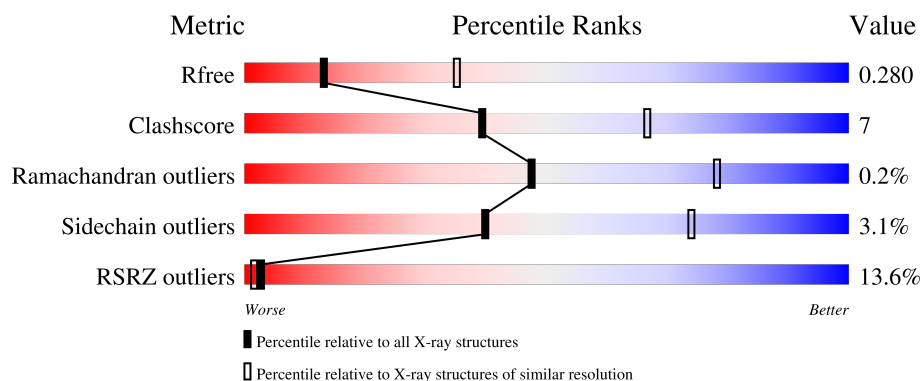
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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>6%</div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div>
1	B	487	<div> <div>19%</div> <div>74%</div> <div>15%</div> <div>• 9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7383 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	454	Total	C	N	O	S	0	1	0
			3657	2383	600	650	24			
1	B	441	Total	C	N	O	S	0	1	0
			3540	2310	576	630	24			

There are 48 discrepancies between the modelled and reference sequences:

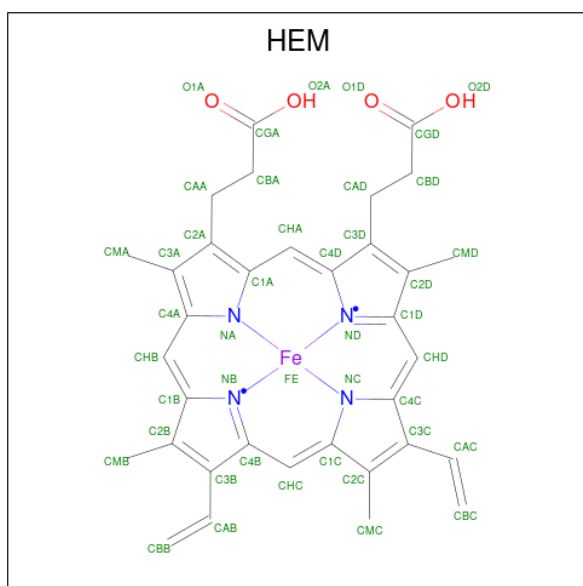
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP P08684
A	?	-	ILE	deletion	UNP P08684
A	?	-	PRO	deletion	UNP P08684
A	?	-	ASP	deletion	UNP P08684
A	?	-	LEU	deletion	UNP P08684
A	?	-	ALA	deletion	UNP P08684
A	?	-	MET	deletion	UNP P08684
A	?	-	GLU	deletion	UNP P08684
A	?	-	THR	deletion	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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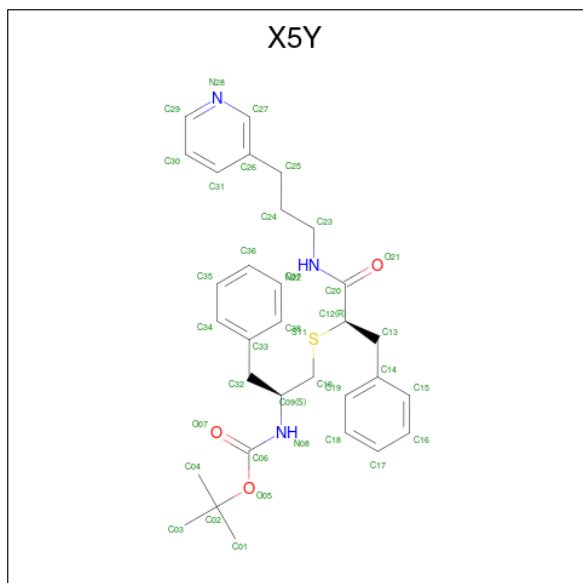
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	deletion	UNP P08684
B	?	-	PRO	deletion	UNP P08684
B	?	-	ASP	deletion	UNP P08684
B	?	-	LEU	deletion	UNP P08684
B	?	-	ALA	deletion	UNP P08684
B	?	-	MET	deletion	UNP P08684
B	?	-	GLU	deletion	UNP P08684
B	?	-	THR	deletion	UNP P08684
B	?	-	TRP	deletion	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 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 [(2S)-1-{[(2R)-1-oxo-3-phenyl-1-{[3-(pyridin-3-yl)propyl]amino}propan-2-yl]sulfanyl}-3-phenylpropan-2-yl]carbamate (three-letter code: X5Y) (formula: C₃₁H₃₉N₃O₃S) (labeled as "Ligand of Interest" by depositor).



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

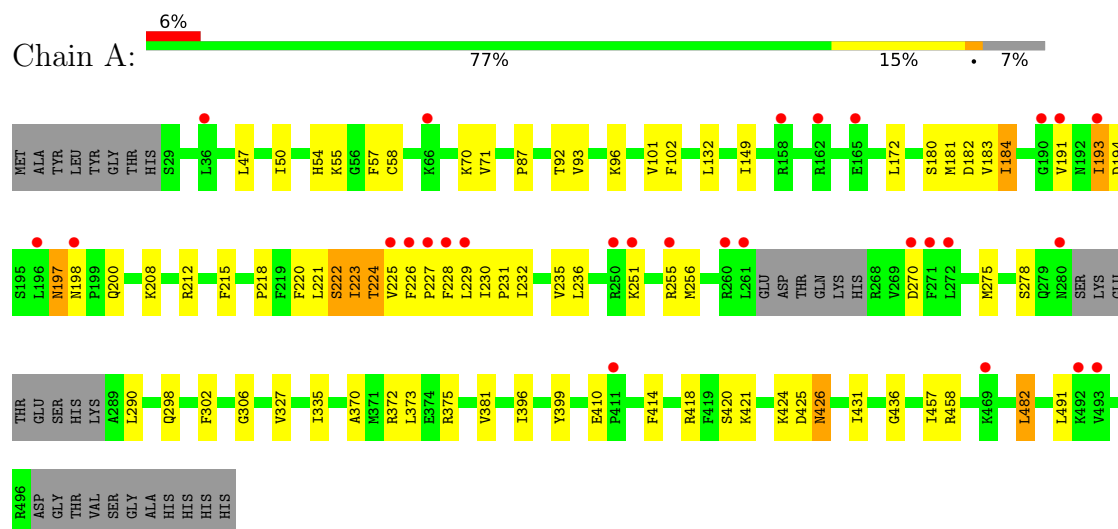
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	9	Total	O	0	0
			9	9		

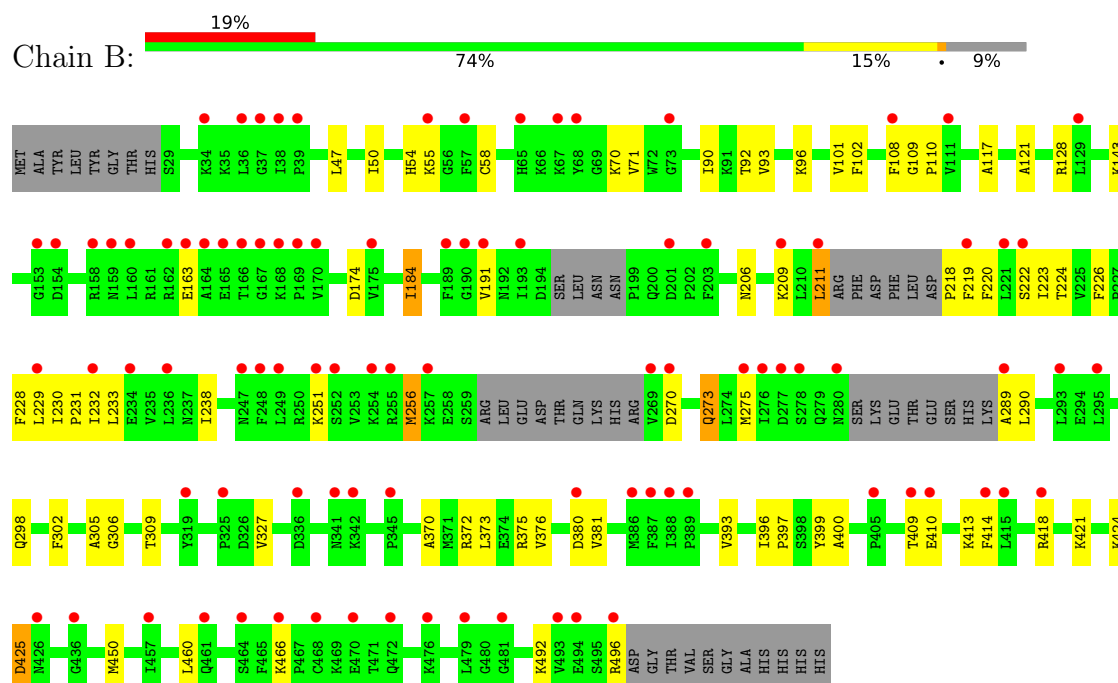
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.94Å 94.81Å 93.17Å 90.00° 123.73° 90.00°	Depositor
Resolution (Å)	39.55 – 2.79 39.56 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.55-2.79) 96.5 (39.56-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.238 , 0.278 0.239 , 0.280	Depositor DCC
R_{free} test set	2101 reflections (7.87%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.009 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7383	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: HEM, X5Y

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	0/3748	0.42	0/5069
1	B	0.25	0/3627	0.40	0/4902
All	All	0.25	0/7375	0.41	0/9971

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	3657	0	3752	61	0
1	B	3540	0	3637	45	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	38	0	0	0	0
3	B	38	0	0	0	0
4	A	15	0	0	0	0
4	B	9	0	0	0	0
All	All	7383	0	7449	110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (110) 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:223:ILE:HG22	1:A:229:LEU:HD13	1.48	0.93
1:A:226:PHE:HB2	1:A:229:LEU:HD21	1.60	0.81
1:B:233:LEU:HB3	1:B:238:ILE:HB	1.63	0.81
2:B:601:HEM:HBC2	2:B:601:HEM:HHD	1.67	0.76
1:A:223:ILE:O	1:A:224:THR:OG1	2.05	0.74
2:A:601:HEM:HBC2	2:A:601:HEM:HHD	1.69	0.73
1:A:50:ILE:HG21	1:A:225:VAL:HG22	1.71	0.73
1:A:184:ILE:HG13	1:A:306:GLY:HA3	1.68	0.72
1:A:218:PRO:O	1:A:222:SER:N	2.24	0.71
1:A:50:ILE:HD13	1:A:225:VAL:HG21	1.74	0.69
1:A:223:ILE:HG22	1:A:229:LEU:CD1	2.23	0.68
1:A:410:GLU:O	1:A:418:ARG:NH2	2.28	0.65
1:B:184:ILE:HG13	1:B:306:GLY:HA3	1.81	0.63
1:A:226:PHE:O	1:A:229:LEU:HD11	1.99	0.62
1:B:425:ASP:N	1:B:425:ASP:OD1	2.32	0.61
1:A:230:ILE:HB	1:A:231:PRO:HD3	1.84	0.60
1:B:70:LYS:HG3	1:B:71:VAL:HG23	1.84	0.60
1:B:410:GLU:O	1:B:418:ARG:NH2	2.34	0.59
1:A:421:LYS:HA	1:A:424:LYS:HG2	1.85	0.58
1:A:220:PHE:O	1:A:224:THR:OG1	2.20	0.58
1:A:230:ILE:H	1:A:231:PRO:CD	2.18	0.56
1:A:482:LEU:H	1:A:482:LEU:HD23	1.71	0.55
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.89	0.55
1:A:227:PRO:HD2	1:A:228:PHE:H	1.72	0.54
1:B:128:ARG:NH2	1:B:289:ALA:O	2.41	0.54
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.88	0.54
1:A:223:ILE:HA	1:A:229:LEU:HD11	1.88	0.54
1:A:70:LYS:HG3	1:A:71:VAL:HG23	1.89	0.53
1:B:90:ILE:HG23	1:B:396:ILE:HD13	1.89	0.53
1:B:327:VAL:HG11	1:B:414:PHE:HE2	1.74	0.53
1:A:226:PHE:HB2	1:A:229:LEU:CD2	2.37	0.53
1:A:275:MET:HE2	1:A:290:LEU:HD21	1.90	0.52
1:A:230:ILE:N	1:A:231:PRO:CD	2.72	0.52
1:B:222:SER:O	1:B:226:PHE:N	2.38	0.52
1:B:373:LEU:HB2	1:B:396:ILE:HB	1.93	0.51
1:B:409:THR:O	1:B:418:ARG:NH1	2.38	0.51
1:B:47:LEU:HD22	1:B:50:ILE:HD11	1.93	0.50
1:A:50:ILE:HD13	1:A:225:VAL:CG2	2.41	0.50
1:A:302:PHE:CD2	2:A:601:HEM:HBC1	2.47	0.50
1:B:108:PHE:CZ	1:B:220:PHE:CZ	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:VAL:HG22	1:B:393:VAL:HG22	1.94	0.49
1:A:221:LEU:O	1:A:221:LEU:HD23	2.11	0.49
1:B:233:LEU:HD22	1:B:238:ILE:HD12	1.94	0.49
1:B:302:PHE:CD2	2:B:601:HEM:HBC1	2.48	0.49
1:B:305:ALA:O	1:B:309:THR:OG1	2.21	0.49
1:B:191:VAL:HG21	1:B:256:MET:HG3	1.94	0.49
1:A:149:ILE:HG12	1:A:183:VAL:HG13	1.96	0.48
1:A:373:LEU:HB2	1:A:396:ILE:HB	1.95	0.48
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.95	0.48
1:A:182:ASP:OD1	1:A:194:ASP:HB3	2.13	0.47
1:B:218:PRO:HG2	1:B:219:PHE:H	1.79	0.47
1:A:132:LEU:HD11	1:A:278:SER:HB2	1.96	0.47
1:A:172:LEU:HD11	1:A:491:LEU:HD12	1.95	0.47
1:B:108:PHE:CZ	1:B:220:PHE:HZ	2.32	0.47
1:B:413:LYS:HD2	1:B:413:LYS:HA	1.68	0.47
1:A:92:THR:HA	1:A:96:LYS:HB2	1.96	0.47
1:A:232:ILE:O	1:A:236:LEU:HG	2.14	0.47
1:B:460:LEU:O	1:B:496:ARG:NH1	2.48	0.47
1:B:92:THR:HA	1:B:96:LYS:HB2	1.96	0.47
1:A:220:PHE:HA	1:A:223:ILE:HG12	1.96	0.47
1:B:110:PRO:HG3	1:B:233:LEU:HD12	1.97	0.47
1:B:101:VAL:HG21	1:B:381:VAL:HG11	1.97	0.46
1:A:101:VAL:HG21	1:A:381:VAL:HG11	1.97	0.46
1:B:421:LYS:HA	1:B:424:LYS:HG2	1.96	0.46
1:B:397:PRO:HB2	1:B:400:ALA:HB3	1.97	0.46
1:A:87:PRO:HG3	1:A:431:ILE:HD11	1.98	0.46
1:A:223:ILE:HG13	1:A:224:THR:N	2.31	0.46
1:B:218:PRO:CG	1:B:219:PHE:H	2.29	0.46
1:A:54:HIS:CD2	1:A:55:LYS:HG3	2.51	0.45
1:A:223:ILE:O	1:A:225:VAL:N	2.43	0.45
1:B:117:ALA:O	1:B:121:ALA:N	2.50	0.45
1:B:102:PHE:HB3	1:B:375:ARG:HB3	1.98	0.45
1:A:436:GLY:HA3	2:A:601:HEM:HBA1	1.99	0.45
1:A:57:PHE:CZ	1:A:215:PHE:HZ	2.34	0.44
1:A:426:ASN:N	1:A:426:ASN:OD1	2.51	0.44
1:B:380:ASP:N	1:B:380:ASP:OD1	2.48	0.44
1:A:197:ASN:HA	1:A:198:ASN:HB2	1.99	0.44
1:B:211:LEU:HA	1:B:211:LEU:HD23	1.76	0.44
1:B:230:ILE:HB	1:B:231:PRO:HD3	2.00	0.44
1:B:206:ASN:HA	1:B:209:LYS:HE2	2.00	0.44
1:A:228:PHE:O	1:A:228:PHE:CD1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASP:H	1:B:273:GLN:HB3	1.82	0.43
1:B:466:LYS:HB2	1:B:492:LYS:HE2	2.00	0.43
1:A:58:CYS:HB3	1:A:399:TYR:CD2	2.53	0.43
1:B:58:CYS:HB3	1:B:399:TYR:CD2	2.54	0.43
1:A:420:SER:O	1:A:424:LYS:N	2.50	0.43
1:A:181:MET:HG3	1:A:193:ILE:HD11	2.00	0.42
1:A:93:VAL:HG13	1:A:102:PHE:CG	2.54	0.42
1:A:180:SER:HB3	1:A:306:GLY:O	2.20	0.42
1:A:191:VAL:HG21	1:A:256:MET:HG3	2.01	0.42
1:A:227:PRO:CD	1:A:228:PHE:H	2.32	0.42
1:B:370:ALA:O	1:B:372:ARG:N	2.47	0.42
1:B:93:VAL:HG13	1:B:102:PHE:CG	2.54	0.42
1:A:197:ASN:HA	1:A:198:ASN:CB	2.49	0.42
1:A:327:VAL:HG11	1:A:414:PHE:HE2	1.85	0.42
1:A:57:PHE:CE1	1:A:215:PHE:HZ	2.38	0.41
1:B:108:PHE:CE1	1:B:220:PHE:CE1	3.08	0.41
1:A:370:ALA:O	1:A:372:ARG:N	2.46	0.41
1:A:232:ILE:O	1:A:235:VAL:HG12	2.21	0.41
1:B:109:GLY:O	1:B:223:ILE:HD13	2.21	0.41
1:A:102:PHE:HB3	1:A:375:ARG:HB3	2.02	0.41
1:A:193:ILE:HG13	1:A:193:ILE:H	1.71	0.41
1:A:335:ILE:HD13	1:A:457:ILE:HA	2.02	0.41
1:B:54:HIS:CD2	1:B:55:LYS:HG3	2.56	0.41
1:B:275:MET:HE2	1:B:290:LEU:HD21	2.03	0.40
1:A:208:LYS:HB2	1:A:208:LYS:HE3	1.89	0.40
1:A:47:LEU:O	1:A:50:ILE:HG12	2.21	0.40
1:B:229:LEU:HD23	1:B:232:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	449/487 (92%)	418 (93%)	29 (6%)	2 (0%)	34	66
1	B	432/487 (89%)	408 (94%)	24 (6%)	0	100	100
All	All	881/974 (90%)	826 (94%)	53 (6%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	223	ILE

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	416/443 (94%)	403 (97%)	13 (3%)	40	74
1	B	403/443 (91%)	391 (97%)	12 (3%)	41	75
All	All	819/886 (92%)	794 (97%)	25 (3%)	40	74

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

Mol	Chain	Res	Type
1	A	184	ILE
1	A	193	ILE
1	A	200	GLN
1	A	212	ARG
1	A	222	SER
1	A	224	THR
1	A	251	LYS
1	A	255	ARG
1	A	270	ASP
1	A	425	ASP
1	A	426	ASN
1	A	458	ARG
1	A	482	LEU
1	B	143	LYS

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Mol	Chain	Res	Type
1	B	163	GLU
1	B	174	ASP
1	B	184	ILE
1	B	211	LEU
1	B	224	THR
1	B	228	PHE
1	B	251	LYS
1	B	256	MET
1	B	273	GLN
1	B	425	ASP
1	B	450	MET

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 ⓘ

4 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	X5Y	A	602	2	39,40,40	1.62	6 (15%)	45,52,52	1.65	6 (13%)
3	X5Y	B	602	2	39,40,40	1.65	6 (15%)	45,52,52	1.60	5 (11%)
2	HEM	B	601	1,3	27,50,50	1.88	4 (14%)	17,82,82	1.45	3 (17%)
2	HEM	A	601	1,3	27,50,50	1.89	4 (14%)	17,82,82	1.44	2 (11%)

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
3	X5Y	A	602	2	-	18/33/33/33	0/3/3/3
3	X5Y	B	602	2	-	21/33/33/33	0/3/3/3
2	HEM	B	601	1,3	-	0/6/54/54	-
2	HEM	A	601	1,3	-	0/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	X5Y	C12-S11	5.88	1.89	1.83
3	A	602	X5Y	C12-S11	5.73	1.89	1.83
2	A	601	HEM	C3C-C2C	-4.65	1.33	1.40
2	B	601	HEM	C3C-C2C	-4.59	1.34	1.40
3	B	602	X5Y	C10-S11	4.56	1.86	1.82
3	A	602	X5Y	C10-S11	4.43	1.86	1.82
2	B	601	HEM	C3B-CAB	3.81	1.55	1.47
2	A	601	HEM	C3B-CAB	3.81	1.55	1.47
2	A	601	HEM	C3C-CAC	3.72	1.55	1.47
2	A	601	HEM	C3B-C2B	-3.72	1.35	1.40
2	B	601	HEM	C3C-CAC	3.68	1.55	1.47
2	B	601	HEM	C3B-C2B	-3.68	1.35	1.40
3	B	602	X5Y	C20-N22	2.71	1.39	1.33
3	A	602	X5Y	C20-N22	2.70	1.39	1.33
3	B	602	X5Y	O05-C02	-2.55	1.43	1.48
3	B	602	X5Y	C06-N08	2.45	1.40	1.34
3	A	602	X5Y	O05-C02	-2.41	1.44	1.48
3	A	602	X5Y	C06-N08	2.40	1.40	1.34
3	A	602	X5Y	O05-C06	2.32	1.39	1.34
3	B	602	X5Y	O05-C06	2.32	1.39	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	X5Y	O05-C06-N08	5.91	119.96	110.02
3	B	602	X5Y	O05-C06-N08	5.90	119.92	110.02
3	A	602	X5Y	O05-C06-O07	-4.81	116.86	125.62
3	B	602	X5Y	O05-C06-O07	-4.69	117.07	125.62
3	A	602	X5Y	C14-C13-C12	2.48	116.88	113.32
3	B	602	X5Y	O21-C20-N22	-2.43	117.77	122.99
3	A	602	X5Y	O21-C20-N22	-2.39	117.86	122.99
2	B	601	HEM	CMB-C2B-C3B	2.27	128.93	124.68
2	A	601	HEM	CMB-C2B-C3B	2.26	128.90	124.68
2	A	601	HEM	CBD-CAD-C3D	-2.16	108.50	112.48
3	B	602	X5Y	C14-C13-C12	2.14	116.39	113.32
3	A	602	X5Y	O07-C06-N08	-2.10	121.40	124.85
2	B	601	HEM	CBD-CAD-C3D	-2.06	108.68	112.48
3	A	602	X5Y	O05-C02-C01	2.02	115.20	107.20
3	B	602	X5Y	O07-C06-N08	-2.01	121.55	124.85
2	B	601	HEM	CMA-C3A-C4A	-2.00	125.39	128.46

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	X5Y	C32-C09-C10-S11
3	A	602	X5Y	N08-C09-C10-S11
3	A	602	X5Y	C09-C10-S11-C12
3	A	602	X5Y	O07-C06-O05-C02
3	A	602	X5Y	C10-C09-C32-C33
3	A	602	X5Y	C20-C12-S11-C10
3	B	602	X5Y	C32-C09-C10-S11
3	B	602	X5Y	N08-C09-C10-S11
3	B	602	X5Y	C09-C10-S11-C12
3	B	602	X5Y	O07-C06-O05-C02
3	B	602	X5Y	C10-C09-C32-C33
3	B	602	X5Y	C20-C12-S11-C10
3	A	602	X5Y	C03-C02-O05-C06
3	A	602	X5Y	C04-C02-O05-C06
3	A	602	X5Y	C01-C02-O05-C06
3	A	602	X5Y	O07-C06-N08-C09
3	B	602	X5Y	O05-C06-N08-C09
3	A	602	X5Y	N08-C06-O05-C02
3	B	602	X5Y	N08-C06-O05-C02
3	A	602	X5Y	O05-C06-N08-C09
3	B	602	X5Y	C01-C02-O05-C06
3	B	602	X5Y	C04-C02-O05-C06

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Mol	Chain	Res	Type	Atoms
3	B	602	X5Y	N08-C09-C32-C33
3	B	602	X5Y	C03-C02-O05-C06
3	A	602	X5Y	C20-C12-C13-C14
3	B	602	X5Y	C20-C12-C13-C14
3	A	602	X5Y	C23-C24-C25-C26
3	B	602	X5Y	C23-C24-C25-C26
3	B	602	X5Y	O07-C06-N08-C09
3	A	602	X5Y	N08-C09-C32-C33
3	A	602	X5Y	N22-C23-C24-C25
3	B	602	X5Y	N22-C23-C24-C25
3	B	602	X5Y	C32-C09-N08-C06
3	A	602	X5Y	C24-C25-C26-C27
3	B	602	X5Y	C24-C25-C26-C27
3	B	602	X5Y	C10-C09-N08-C06
3	B	602	X5Y	C24-C25-C26-C31
3	A	602	X5Y	C24-C25-C26-C31
3	B	602	X5Y	S11-C12-C20-O21

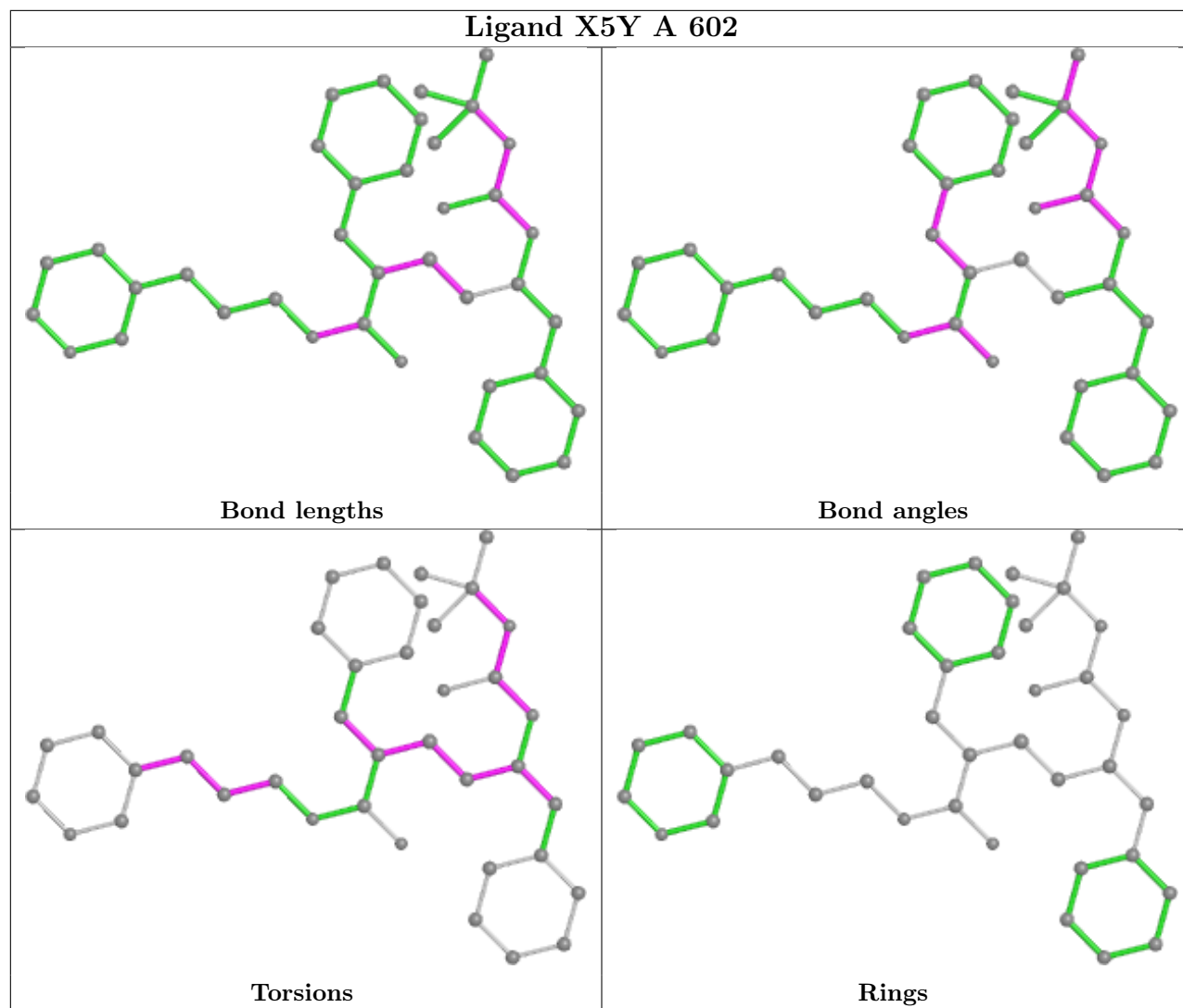
There are no ring outliers.

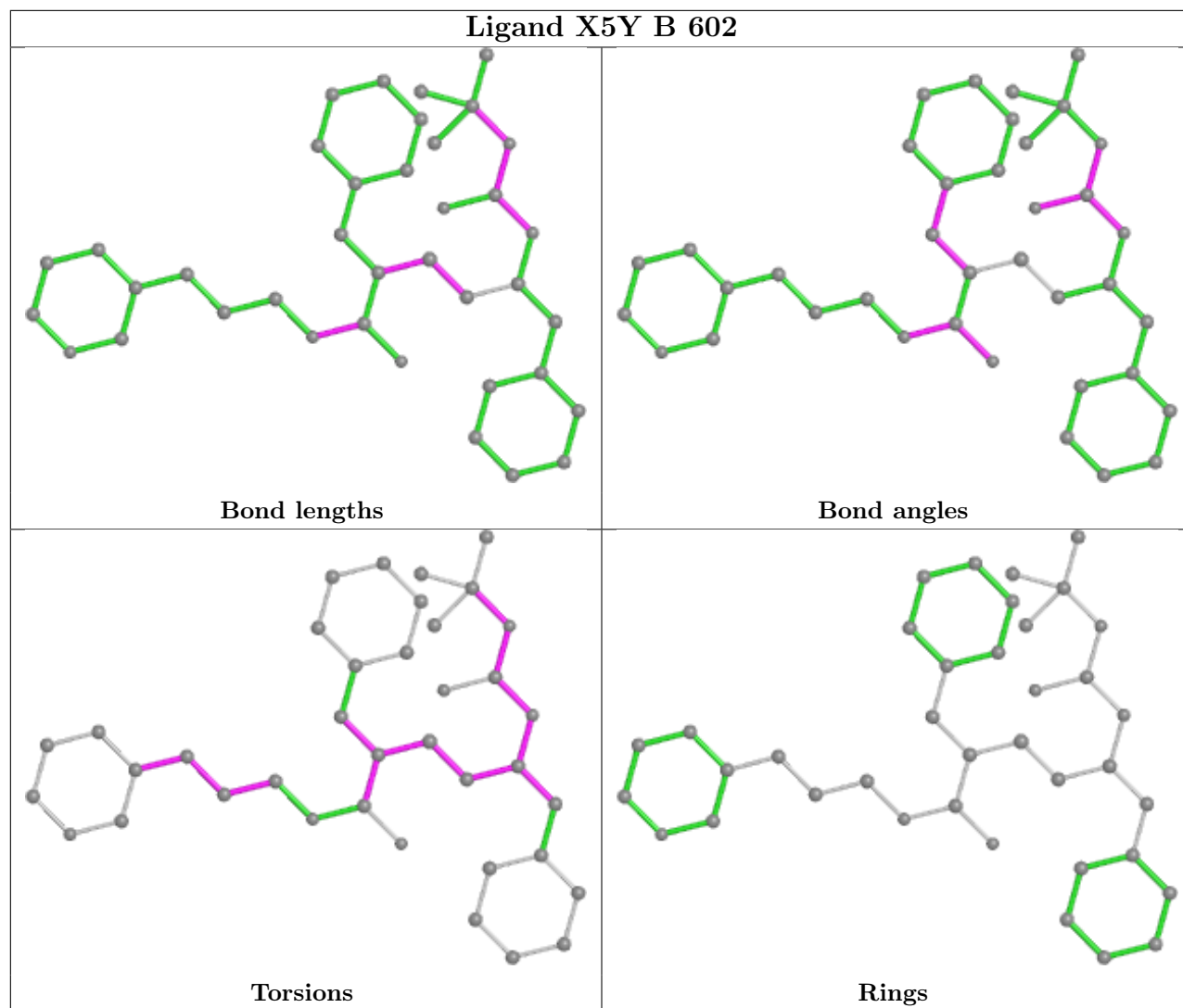
2 monomers are involved in 7 short contacts:

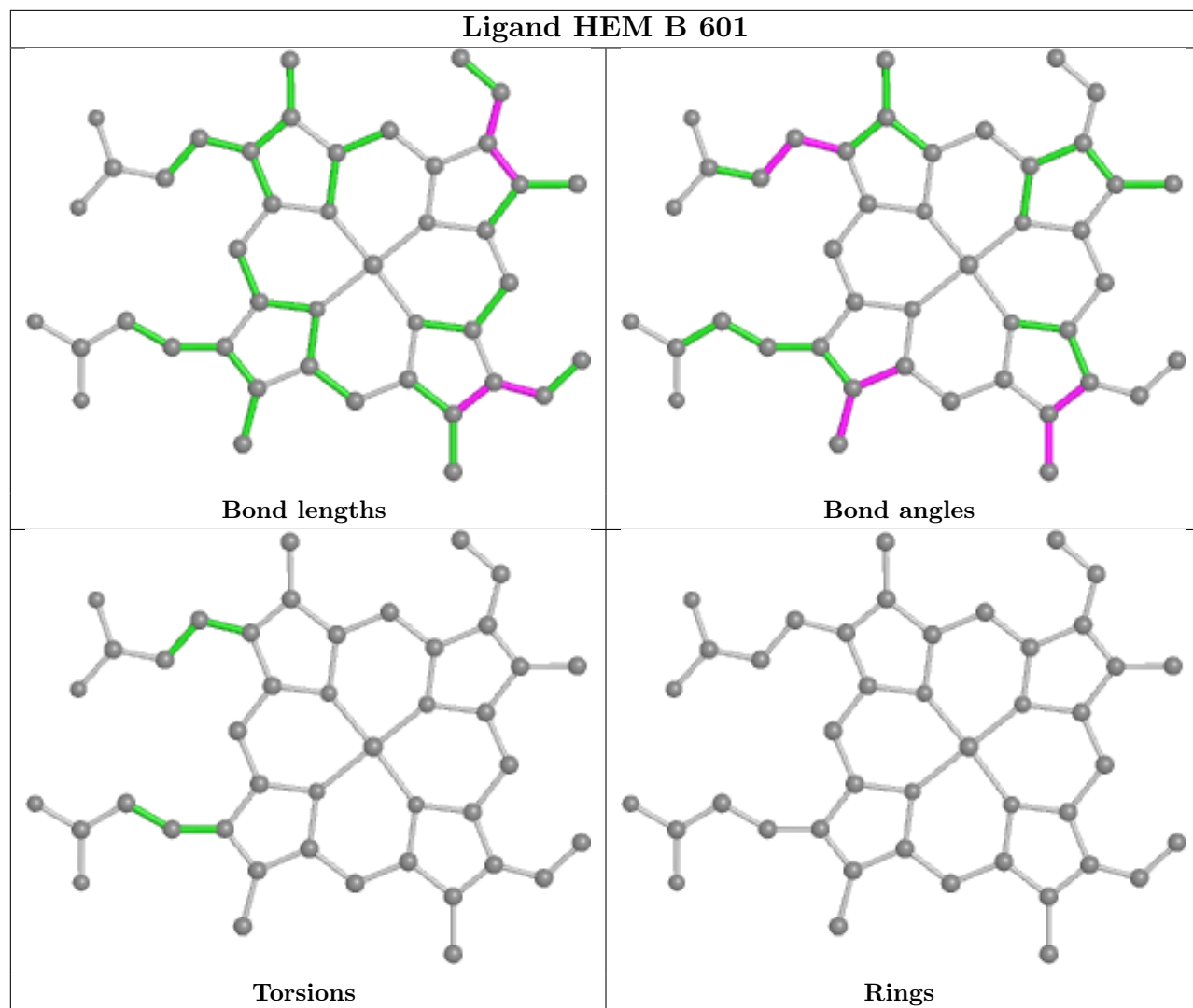
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	3	0
2	A	601	HEM	4	0

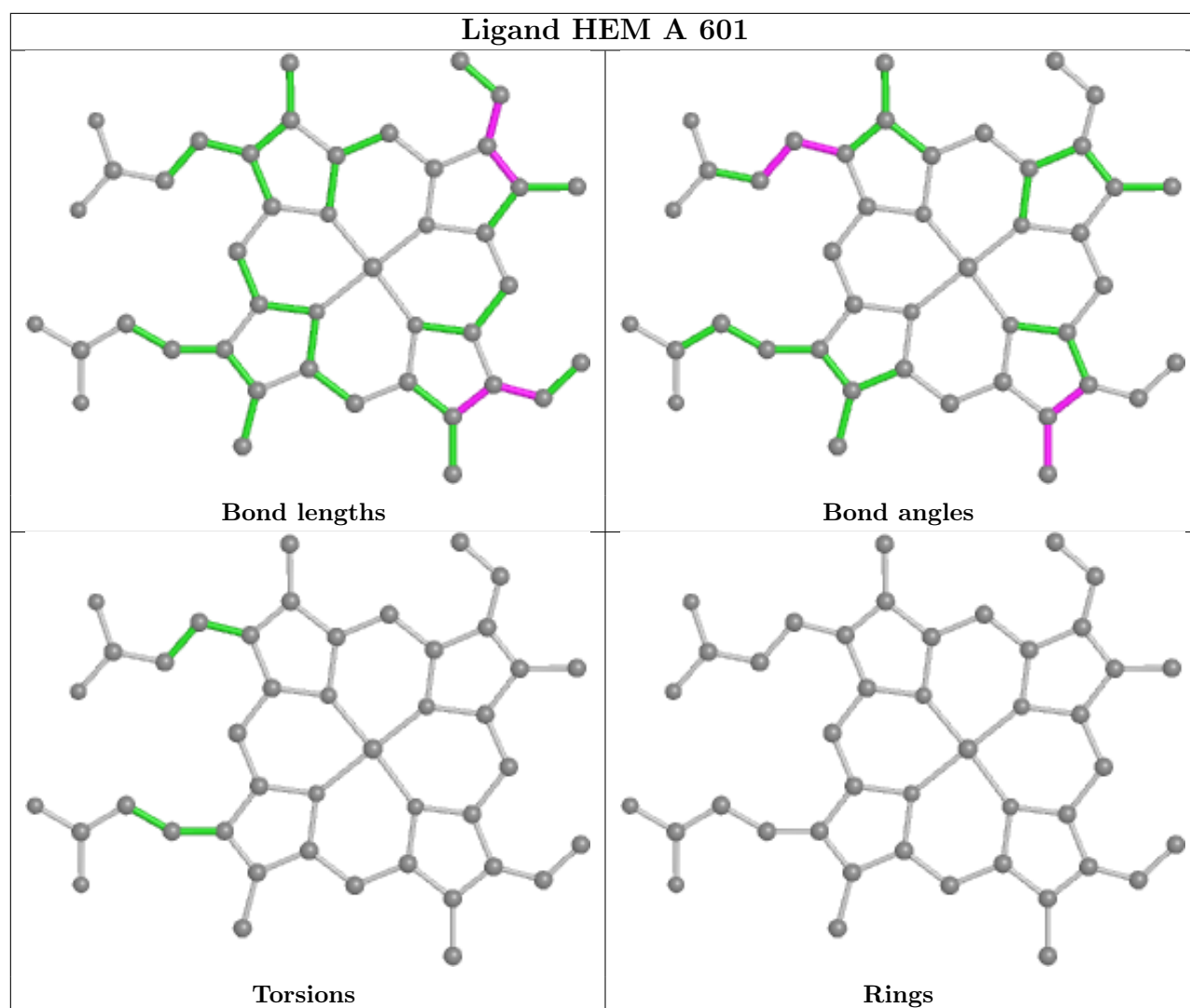
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 X5Y A 602









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	454/487 (93%)	0.54	28 (6%) 20 13	46, 87, 134, 172	0
1	B	441/487 (90%)	1.13	94 (21%) 0 0	64, 109, 150, 210	0
All	All	895/974 (91%)	0.83	122 (13%) 3 1	46, 97, 147, 210	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	221	LEU	5.5
1	B	160	LEU	5.3
1	A	469	LYS	4.9
1	B	278	SER	4.9
1	B	165	GLU	4.8
1	B	481	GLY	4.7
1	B	493	VAL	4.6
1	B	232	ILE	4.6
1	B	36	LEU	4.4
1	B	270	ASP	4.3
1	B	468	CYS	4.2
1	A	165	GLU	4.1
1	B	255	ARG	4.1
1	B	37	GLY	4.1
1	B	496	ARG	4.0
1	B	68	TYR	4.0
1	B	341	ASN	4.0
1	B	289	ALA	3.9
1	B	280	ASN	3.9
1	A	272	LEU	3.9
1	A	228	PHE	3.9
1	B	170	VAL	3.9
1	A	260	ARG	3.8
1	B	342	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	3.7
1	B	415	LEU	3.6
1	B	457	ILE	3.5
1	B	154	ASP	3.5
1	A	158	ARG	3.5
1	B	405	PRO	3.5
1	B	277	ASP	3.5
1	B	169	PRO	3.5
1	B	276	ILE	3.4
1	B	34	LYS	3.4
1	B	111	VAL	3.4
1	B	494	GLU	3.4
1	B	345	PRO	3.3
1	A	411	PRO	3.3
1	B	73	GLY	3.3
1	B	67	LYS	3.3
1	B	476	LYS	3.3
1	B	153	GLY	3.2
1	B	190	GLY	3.2
1	B	251	LYS	3.2
1	B	164	ALA	3.1
1	B	158	ARG	3.1
1	A	271	PHE	3.1
1	B	386	MET	3.1
1	B	191	VAL	3.0
1	B	203	PHE	3.0
1	B	229	LEU	3.0
1	B	269	VAL	3.0
1	A	270	ASP	2.9
1	B	295	LEU	2.9
1	B	166	THR	2.8
1	B	479	LEU	2.8
1	B	319	TYR	2.8
1	A	227	PRO	2.8
1	A	255	ARG	2.8
1	A	226	PHE	2.8
1	B	38	ILE	2.8
1	B	209	LYS	2.7
1	A	162	ARG	2.7
1	B	275	MET	2.7
1	B	249	LEU	2.6
1	A	492	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	57	PHE	2.6
1	B	388	ILE	2.5
1	B	257	LYS	2.5
1	B	470	GLU	2.5
1	B	159	ASN	2.5
1	B	222	SER	2.5
1	B	409	THR	2.4
1	B	389	PRO	2.4
1	A	196	LEU	2.4
1	B	293	LEU	2.4
1	B	219	PHE	2.4
1	A	229	LEU	2.4
1	B	175	VAL	2.4
1	A	36	LEU	2.4
1	A	193	ILE	2.4
1	B	234	GLU	2.4
1	A	191	VAL	2.4
1	B	248	PHE	2.4
1	B	168	LYS	2.3
1	B	247	ASN	2.3
1	B	254	LYS	2.3
1	A	261	LEU	2.3
1	B	167	GLY	2.3
1	B	252	SER	2.3
1	A	250	ARG	2.3
1	B	336	ASP	2.3
1	B	472	GLN	2.3
1	B	201	ASP	2.2
1	B	380	ASP	2.2
1	B	414	PHE	2.2
1	B	426	ASN	2.2
1	B	387	PHE	2.2
1	B	129	LEU	2.2
1	B	464	SER	2.2
1	B	108	PHE	2.2
1	B	39	PRO	2.2
1	A	251	LYS	2.2
1	A	190	GLY	2.2
1	B	162	ARG	2.2
1	B	211	LEU	2.1
1	B	461	GLN	2.1
1	B	163	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	198	ASN	2.1
1	B	65	HIS	2.1
1	B	55	LYS	2.1
1	B	193	ILE	2.1
1	B	236	LEU	2.1
1	B	325	PRO	2.1
1	B	466	LYS	2.1
1	B	189	PHE	2.1
1	B	410	GLU	2.1
1	B	436	GLY	2.1
1	A	493	VAL	2.0
1	B	418	ARG	2.0
1	A	66	LYS	2.0
1	A	280	ASN	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](#)

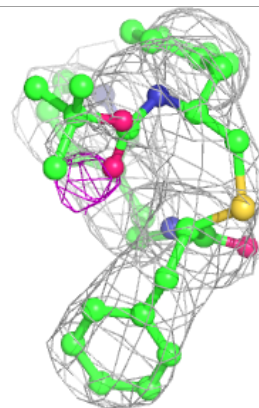
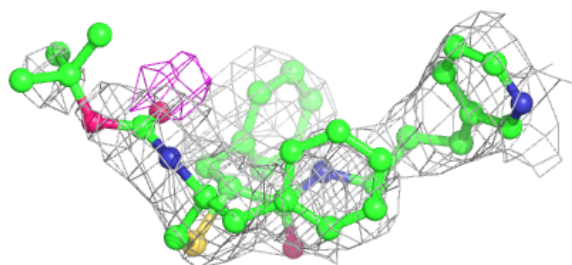
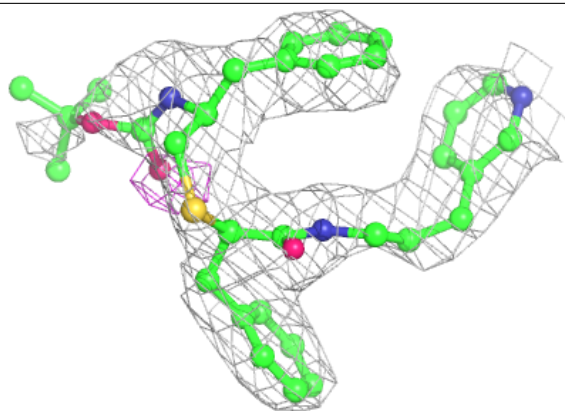
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	X5Y	B	602	38/38	0.87	0.33	75,102,139,152	0
3	X5Y	A	602	38/38	0.90	0.30	57,79,119,139	0
2	HEM	A	601	43/43	0.96	0.24	40,52,76,85	0
2	HEM	B	601	43/43	0.98	0.24	52,55,79,95	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.

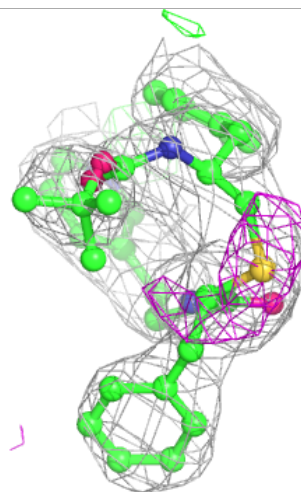
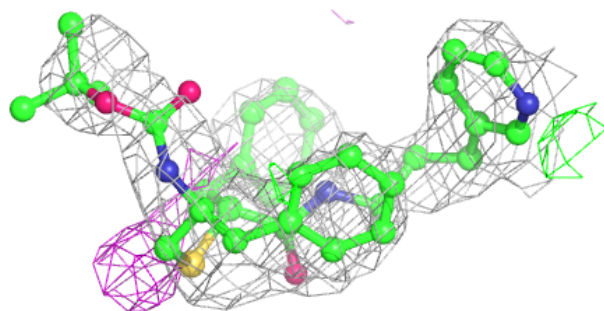
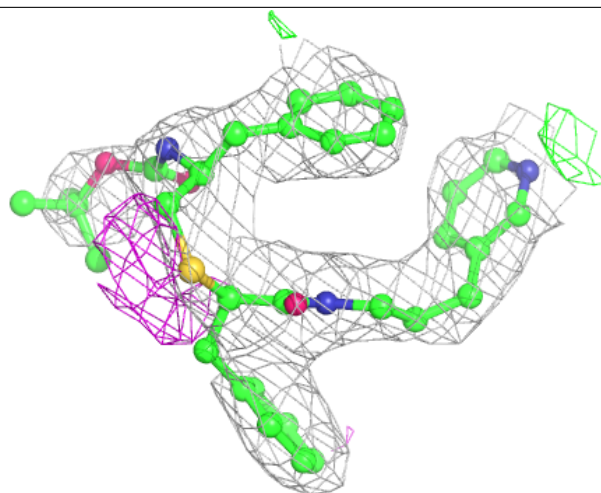
Electron density around X5Y B 602:

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



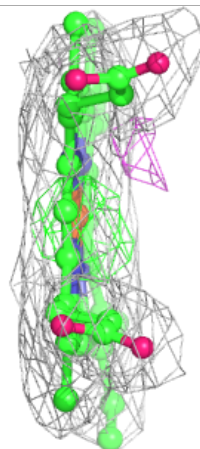
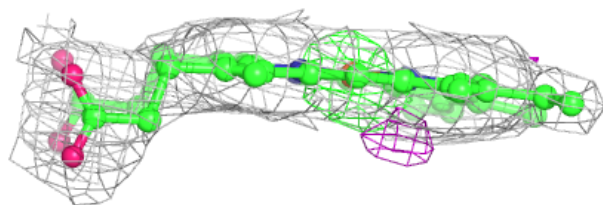
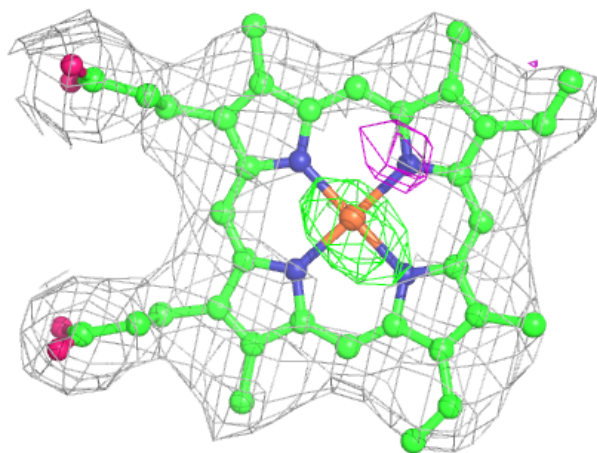
Electron density around X5Y A 602:

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



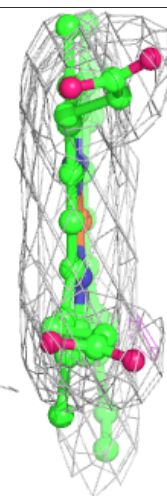
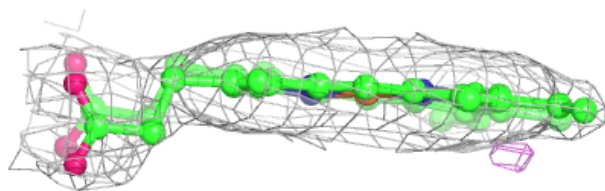
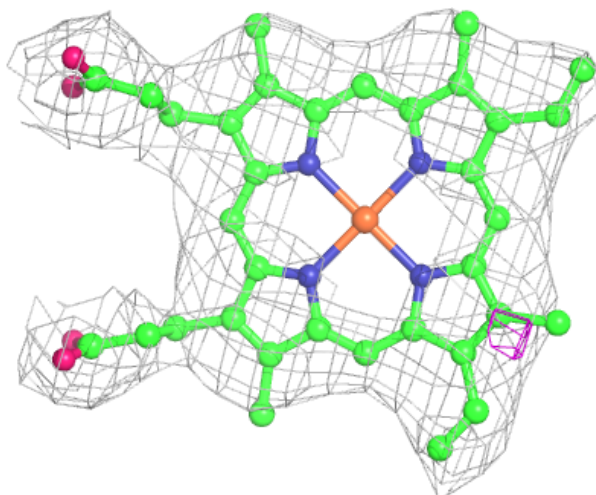
Electron density around HEM A 601:

$2mF_o-DF_c$ (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.