



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:49 PM UTC

PDB ID : 2C6H / pdb_00002c6h
Title : Crystal structure of YC-17-bound cytochrome P450 PikC (CYP107L1)
Authors : Sherman, D.H.; Li, S.; Yermalitskaya, L.V.; Kim, Y.; Smith, J.A.; Waterman, M.R.; Podust, L.M.
Deposited on : 2005-11-09
Resolution : 2.35 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

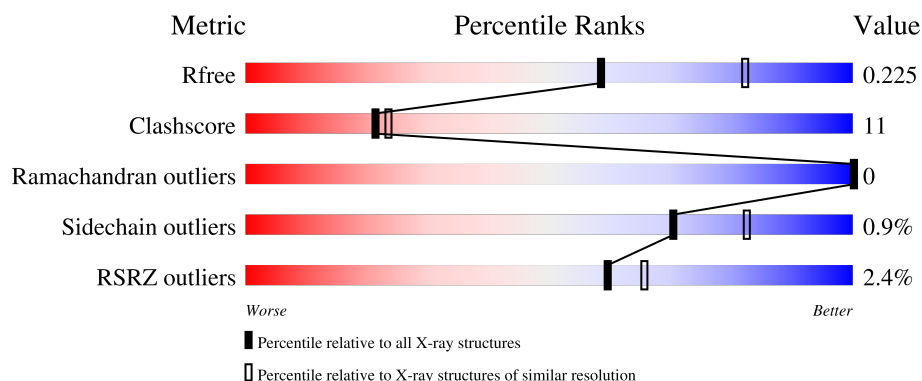
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

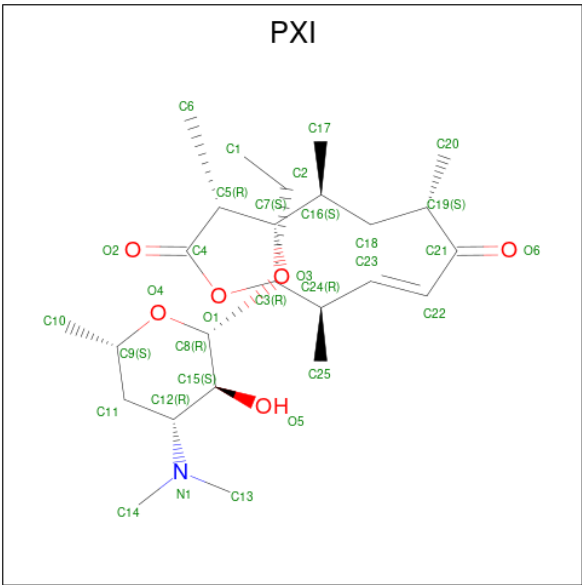
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

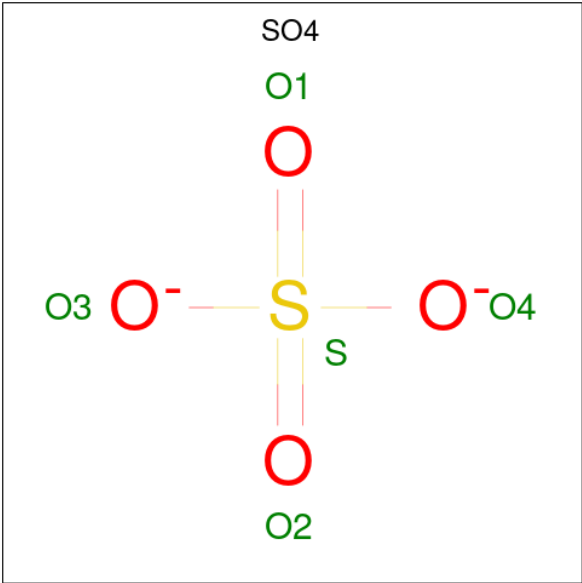
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	436	68% 21% • 10%
1	B	436	3% 70% 20% • 9%



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	25	1	6		
3	B	1	Total	C	N	O	0	0
			32	25	1	6		

- 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	A	1	Total	O	S	0	0
			5	4	1		

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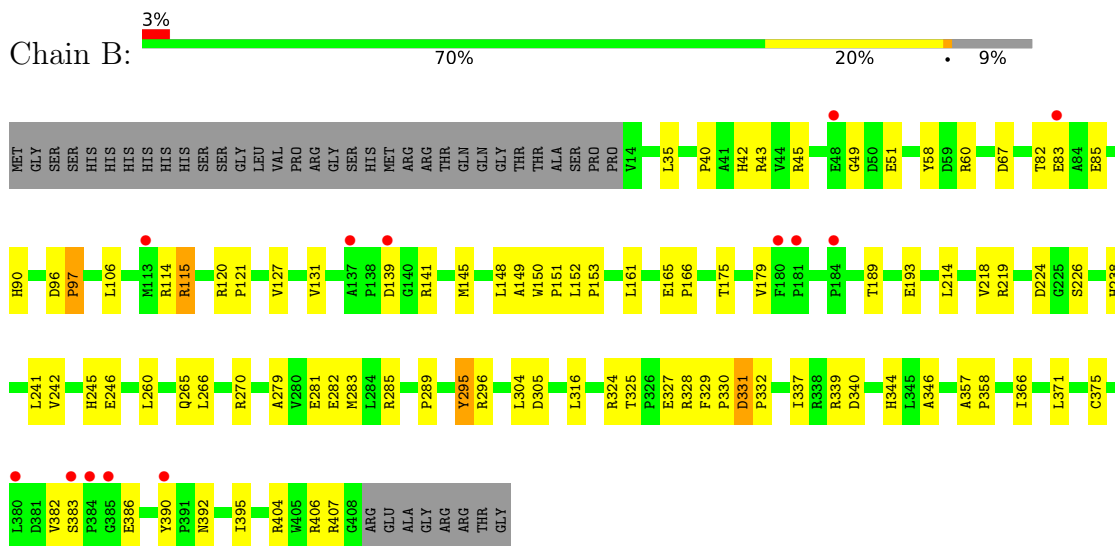
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total	O	0	0
			109	109		
5	B	107	Total	O	0	0
			107	107		

- Molecule 1: CYTOCHROME P450 MONOOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.46Å 104.70Å 153.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.35 49.56 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.56-2.35) 94.1 (49.56-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.231 0.190 , 0.225	Depositor DCC
R_{free} test set	7488 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6492	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.67% 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: SO4, HEM, PXI

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	0.43	1/3113 (0.0%)	0.93	18/4249 (0.4%)
1	B	0.43	1/3129 (0.0%)	0.95	11/4270 (0.3%)
All	All	0.43	2/6242 (0.0%)	0.94	29/8519 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	407	ARG	C-N	-5.47	1.25	1.33
1	A	406	ARG	C-N	-5.34	1.25	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	TYR	CA-C-N	8.28	127.58	118.97
1	A	390	TYR	C-N-CA	8.28	127.58	118.97
1	B	325	THR	CA-C-N	6.64	126.89	119.32
1	B	325	THR	C-N-CA	6.64	126.89	119.32
1	B	242	VAL	N-CA-C	6.51	117.14	110.82
1	A	331	ASP	CA-C-N	6.21	127.60	119.84
1	A	331	ASP	C-N-CA	6.21	127.60	119.84
1	B	331	ASP	CA-C-N	6.17	126.35	119.32
1	B	331	ASP	C-N-CA	6.17	126.35	119.32
1	B	295	TYR	N-CA-C	5.91	118.92	110.24
1	A	395	ILE	N-CA-C	5.88	116.34	108.11
1	B	67	ASP	CA-C-N	5.78	125.46	119.56
1	B	67	ASP	C-N-CA	5.78	125.46	119.56
1	A	262	HIS	CA-C-N	5.68	126.94	119.84
1	A	262	HIS	C-N-CA	5.68	126.94	119.84
1	B	97	PRO	N-CA-C	-5.47	104.73	110.58
1	A	107	VAL	N-CA-C	5.44	118.42	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	TYR	CA-C-N	5.42	124.94	119.19
1	B	390	TYR	C-N-CA	5.42	124.94	119.19
1	A	111	PHE	N-CA-C	5.33	119.09	112.59
1	A	392	ASN	CA-C-N	5.33	124.84	119.19
1	A	392	ASN	C-N-CA	5.33	124.84	119.19
1	A	295	TYR	N-CA-C	5.21	118.03	110.42
1	A	233	LEU	N-CA-C	-5.14	105.57	111.07
1	A	58	TYR	N-CA-C	5.08	117.21	111.11
1	A	92	MET	N-CA-C	5.07	116.81	111.28
1	A	137	ALA	CA-C-N	5.06	125.34	119.47
1	A	137	ALA	C-N-CA	5.06	125.34	119.47
1	A	172	ARG	N-CA-C	-5.05	105.78	111.28

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	3043	0	3006	58	0
1	B	3058	0	3019	77	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
3	A	32	0	43	2	0
3	B	32	0	43	0	0
4	A	20	0	0	1	0
4	B	5	0	0	0	0
5	A	109	0	0	3	0
5	B	107	0	0	5	0
All	All	6492	0	6171	136	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 11.

All (136) 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:B:45:ARG:HE	1:B:49:GLY:HA2	1.20	1.04
1:B:406:ARG:HB3	1:B:406:ARG:NH1	1.90	0.86
1:B:43:ARG:HH12	1:B:51:GLU:HB3	1.43	0.83
1:B:406:ARG:HB3	1:B:406:ARG:HH11	1.42	0.83
1:B:114:ARG:HG3	5:B:2033:HOH:O	1.82	0.78
1:B:58:TYR:CD2	1:B:328:ARG:HG3	2.20	0.76
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.67	0.75
1:A:58:TYR:CD2	1:A:328:ARG:HG3	2.20	0.75
1:B:45:ARG:NE	1:B:49:GLY:HA2	2.00	0.73
1:A:22:GLN:HE22	1:A:389:TRP:H	1.38	0.70
1:B:265:GLN:NE2	1:B:337:ILE:H	1.91	0.69
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.74	0.69
1:B:139:ASP:OD2	1:B:141:ARG:HB2	1.94	0.67
1:A:189:THR:O	1:A:193:GLU:HG3	1.94	0.66
1:B:83:GLU:CD	1:B:83:GLU:H	2.03	0.66
1:B:344:HIS:HD2	1:B:346:ALA:H	1.44	0.65
1:A:82:THR:OG1	1:A:85:GLU:HG3	1.95	0.65
1:A:139:ASP:OD2	1:A:141:ARG:HB2	1.97	0.65
1:A:344:HIS:HD2	1:A:346:ALA:H	1.43	0.65
1:A:58:TYR:CG	1:A:328:ARG:HG3	2.31	0.65
1:B:82:THR:OG1	1:B:85:GLU:HG3	1.98	0.64
1:A:60:ARG:HD2	1:A:304:LEU:HD22	1.80	0.63
1:A:273:MET:HE2	1:A:369:ARG:CZ	2.27	0.63
1:B:90:HIS:HB2	5:B:2063:HOH:O	1.99	0.63
1:B:175:THR:HG23	5:B:2107:HOH:O	1.98	0.61
1:B:224:ASP:OD1	1:B:226:SER:HB3	2.01	0.60
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.83	0.60
1:B:282:GLU:OE1	1:B:285:ARG:HD2	2.03	0.59
1:B:141:ARG:HH22	1:B:404:ARG:NH1	2.00	0.59
1:B:150:TRP:HB3	1:B:151:PRO:HD3	1.85	0.57
1:A:150:TRP:CZ2	1:A:172:ARG:HB2	2.39	0.57
1:A:242:VAL:HG11	3:A:1408:PXI:H173	1.85	0.57
1:A:114:ARG:HH11	1:A:114:ARG:HG3	1.70	0.57
1:A:46:THR:OG1	1:A:50:ASP:HB2	2.05	0.56
1:B:392:ASN:HB3	1:B:395:ILE:HG22	1.87	0.56
1:A:48:GLU:H	1:A:48:GLU:CD	2.14	0.55
1:B:60:ARG:NH2	1:B:305:ASP:OD1	2.39	0.55
1:A:382:VAL:HG22	1:A:386:GLU:HB2	1.89	0.54
1:A:35:LEU:HB3	1:A:42:HIS:CD2	2.42	0.54
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.73	0.54
1:A:224:ASP:OD1	1:A:226:SER:HB3	2.07	0.54
1:A:177:ALA:O	1:A:181:PRO:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:C	1:A:276:LEU:HD13	2.33	0.53
1:B:43:ARG:NH1	1:B:51:GLU:HB3	2.19	0.53
1:B:120:ARG:HB3	1:B:121:PRO:HD3	1.91	0.53
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.92	0.52
1:B:265:GLN:HE21	1:B:337:ILE:H	1.58	0.52
1:B:329:PHE:O	1:B:332:PRO:HG3	2.10	0.52
1:B:406:ARG:NH1	1:B:406:ARG:CB	2.70	0.52
1:B:279:ALA:O	1:B:283:MET:HG3	2.09	0.52
1:B:127:VAL:HG21	1:B:366:ILE:HG22	1.93	0.51
1:A:29:TYR:HB2	1:A:30:PRO:HD3	1.91	0.51
1:A:339:ARG:HG2	1:A:340:ASP:N	2.26	0.51
1:B:45:ARG:HE	1:B:49:GLY:CA	2.07	0.50
1:B:382:VAL:HG22	1:B:383:SER:N	2.26	0.50
1:A:161:LEU:HD12	1:A:241:LEU:CD2	2.42	0.50
1:B:357:ALA:HB3	1:B:358:PRO:HD3	1.94	0.50
1:B:295:TYR:CD1	1:B:316:LEU:HD21	2.46	0.49
1:B:295:TYR:CE1	1:B:316:LEU:HD21	2.47	0.49
1:B:214:LEU:O	1:B:218:VAL:HG23	2.13	0.49
1:B:161:LEU:CD1	1:B:241:LEU:HG	2.43	0.49
1:B:371:LEU:O	1:B:375:CYS:HB2	2.13	0.49
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.27	0.48
1:A:282:GLU:HG3	1:A:335:PHE:CE1	2.48	0.48
1:B:35:LEU:HB3	1:B:42:HIS:CD2	2.49	0.48
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.95	0.48
1:B:339:ARG:HG2	1:B:340:ASP:N	2.29	0.48
1:A:331:ASP:N	1:A:332:PRO:HD3	2.29	0.47
1:A:161:LEU:HD23	1:A:213:LEU:HB3	1.95	0.47
1:B:331:ASP:N	1:B:332:PRO:HD3	2.28	0.47
1:A:265:GLN:NE2	1:A:337:ILE:H	2.13	0.46
1:A:279:ALA:O	1:A:283:MET:HG3	2.15	0.46
1:B:285:ARG:NH2	1:B:332:PRO:O	2.33	0.46
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.81	0.46
1:B:344:HIS:CD2	1:B:346:ALA:HB3	2.51	0.46
1:B:175:THR:HG22	1:B:246:GLU:OE1	2.16	0.45
1:B:60:ARG:HD2	1:B:304:LEU:HD22	1.97	0.45
1:B:127:VAL:O	1:B:131:VAL:HG23	2.16	0.45
1:B:189:THR:O	1:B:193:GLU:HG3	2.15	0.45
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.31	0.45
1:A:341:THR:O	1:A:342:ALA:C	2.60	0.45
1:B:327:GLU:H	1:B:327:GLU:CD	2.25	0.45
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:HH11	1:B:115:ARG:HB2	1.81	0.45
1:B:296:ARG:HH11	1:B:296:ARG:HG3	1.82	0.45
1:B:358:PRO:HD2	5:B:2098:HOH:O	2.16	0.44
1:A:344:HIS:HD2	1:A:346:ALA:N	2.13	0.44
1:B:179:VAL:HG21	1:B:246:GLU:CD	2.42	0.44
1:B:281:GLU:OE1	1:B:344:HIS:HE1	2.00	0.44
1:A:99:ARG:HB2	4:A:1431:SO4:O1	2.16	0.44
1:B:382:VAL:HG22	1:B:386:GLU:HB2	1.98	0.44
1:A:265:GLN:NE2	1:A:337:ILE:HG12	2.33	0.44
1:B:165:GLU:HB3	1:B:166:PRO:HD3	1.98	0.44
1:B:330:PRO:O	1:B:331:ASP:C	2.61	0.44
1:A:334:ARG:HH11	1:A:336:ASP:HB2	1.83	0.44
1:A:256:MET:HE2	1:A:371:LEU:HD13	1.99	0.44
1:A:334:ARG:HH11	1:A:334:ARG:HG2	1.82	0.44
1:B:260:LEU:HD23	1:B:266:LEU:HD22	1.99	0.44
1:A:227:ARG:HB3	5:A:2055:HOH:O	2.18	0.43
1:A:334:ARG:NH1	1:A:336:ASP:HB2	2.32	0.43
1:A:292:SER:HB2	1:A:394:MET:HA	2.01	0.43
1:B:175:THR:HG21	1:B:245:HIS:HD2	1.82	0.43
1:A:286:TYR:CD2	1:A:287:GLU:HG2	2.53	0.43
1:B:289:PRO:O	1:B:395:ILE:HD12	2.19	0.43
1:A:291:GLU:HB3	1:A:393:PRO:O	2.19	0.43
1:B:344:HIS:CD2	1:B:346:ALA:H	2.31	0.43
1:A:103:LEU:O	1:A:106:LEU:HB2	2.18	0.43
1:B:395:ILE:HG23	1:B:395:ILE:O	2.18	0.42
1:A:43:ARG:NH2	1:A:313:ASP:OD2	2.52	0.42
1:B:324:ARG:HA	1:B:332:PRO:HB3	2.02	0.42
2:A:1407:HEM:CMA	2:A:1407:HEM:HBA2	2.50	0.42
1:B:40:PRO:HB2	1:B:60:ARG:HG2	2.00	0.42
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.20	0.42
1:A:41:ALA:HA	1:A:54:LEU:O	2.20	0.42
1:B:219:ARG:HG2	5:B:2057:HOH:O	2.20	0.42
1:A:40:PRO:HB2	1:A:60:ARG:HG2	2.02	0.42
1:B:150:TRP:CD1	1:B:245:HIS:HE1	2.39	0.41
1:B:282:GLU:OE1	1:B:282:GLU:HA	2.20	0.41
1:B:150:TRP:N	1:B:151:PRO:CD	2.83	0.41
1:A:137:ALA:HA	1:A:138:PRO:HD3	1.91	0.41
1:A:273:MET:HE1	1:A:276:LEU:HD23	2.02	0.41
1:B:382:VAL:HG23	1:B:386:GLU:OE1	2.21	0.41
1:A:256:MET:O	1:A:260:LEU:HG	2.20	0.41
1:A:380:LEU:HD23	1:A:402:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD12	1:B:241:LEU:CD2	2.50	0.41
1:A:200:ARG:NE	5:A:2042:HOH:O	2.38	0.41
1:A:344:HIS:CD2	1:A:346:ALA:H	2.32	0.41
1:B:145:MET:HA	1:B:149:ALA:HB3	2.01	0.41
1:B:265:GLN:HE21	1:B:337:ILE:HG23	1.84	0.41
1:B:148:LEU:C	1:B:151:PRO:HD2	2.46	0.41
1:A:251:LEU:HD22	2:A:1407:HEM:HBB1	2.02	0.40
1:A:358:PRO:HD2	5:A:2095:HOH:O	2.21	0.40
1:B:58:TYR:CG	1:B:328:ARG:HG3	2.56	0.40
1:A:243:ALA:HA	3:A:1408:PXI:O2	2.20	0.40
1:B:344:HIS:HD2	1:B:346:ALA:N	2.14	0.40
1:B:96:ASP:HB3	1:B:97:PRO:HD2	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	392/436 (90%)	379 (97%)	13 (3%)	0	100	100
1	B	393/436 (90%)	384 (98%)	9 (2%)	0	100	100
All	All	785/872 (90%)	763 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	317/355 (89%)	314 (99%)	3 (1%)	70	82
1	B	319/355 (90%)	316 (99%)	3 (1%)	70	82
All	All	636/710 (90%)	630 (99%)	6 (1%)	70	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	A	238	HIS
1	A	380	LEU
1	B	106	LEU
1	B	115	ARG
1	B	238	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	91	ASN
1	A	188	GLN
1	A	208	GLN
1	A	265	GLN
1	A	344	HIS
1	B	22	GLN
1	B	89	ASN
1	B	124	GLN
1	B	186	GLN
1	B	188	GLN
1	B	245	HIS
1	B	265	GLN
1	B	344	HIS
1	B	349	HIS

5.3.3 RNA ⓘ

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	A	1407	1	50,50,50	1.32	7 (14%)	67,82,82	1.05	5 (7%)
4	SO4	B	1433	-	4,4,4	0.38	0	6,6,6	0.09	0
4	SO4	A	1432	-	4,4,4	0.44	0	6,6,6	0.14	0
3	PXI	A	1408	-	33,33,33	2.12	6 (18%)	42,47,47	2.32	12 (28%)
2	HEM	B	1408	1	50,50,50	1.25	6 (12%)	67,82,82	1.25	8 (11%)
4	SO4	A	1431	-	4,4,4	0.37	0	6,6,6	0.12	0
4	SO4	A	1434	-	4,4,4	0.40	0	6,6,6	0.13	0
3	PXI	B	1409	-	33,33,33	2.09	8 (24%)	42,47,47	2.30	12 (28%)
4	SO4	A	1430	-	4,4,4	0.41	0	6,6,6	0.07	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
3	PXI	B	1409	-	-	14/43/59/59	0/1/2/2
3	PXI	A	1408	-	-	16/43/59/59	0/1/2/2
2	HEM	B	1408	1	-	5/14/54/54	-
2	HEM	A	1407	1	-	4/14/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1408	PXI	C19-C21	6.35	1.61	1.51
3	B	1409	PXI	C19-C21	6.25	1.61	1.51
3	B	1409	PXI	C16-C7	6.06	1.64	1.53
3	A	1408	PXI	C16-C7	6.00	1.63	1.53
3	A	1408	PXI	C24-C3	4.08	1.63	1.53
3	B	1409	PXI	C24-C3	3.69	1.62	1.53
3	A	1408	PXI	C15-C12	3.48	1.60	1.53
2	B	1408	HEM	CAC-C3C	-3.26	1.38	1.47
2	A	1407	HEM	CAC-C3C	-3.15	1.39	1.47
2	A	1407	HEM	CBB-CAB	3.10	1.45	1.30
3	B	1409	PXI	C15-C12	2.91	1.59	1.53
2	A	1407	HEM	CBC-CAC	2.81	1.43	1.30
2	B	1408	HEM	CAB-C3B	-2.73	1.40	1.47
2	B	1408	HEM	CBC-CAC	2.51	1.42	1.30
2	B	1408	HEM	CBB-CAB	2.50	1.42	1.30
2	A	1407	HEM	FE-NB	2.47	2.02	1.94
3	A	1408	PXI	O4-C9	2.46	1.48	1.44
2	A	1407	HEM	CAB-C3B	-2.37	1.41	1.47
2	B	1408	HEM	FE-NA	2.30	2.02	1.95
2	A	1407	HEM	FE-ND	2.23	2.01	1.94
3	B	1409	PXI	O4-C9	2.18	1.48	1.44
3	B	1409	PXI	C5-C7	2.17	1.59	1.54
3	B	1409	PXI	C11-C9	2.13	1.55	1.52
3	A	1408	PXI	C5-C7	2.12	1.59	1.54
3	B	1409	PXI	O3-C7	2.07	1.49	1.43
2	B	1408	HEM	CMB-C2B	2.06	1.55	1.50
2	A	1407	HEM	C4D-ND	-2.02	1.36	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1409	PXI	C3-O1-C4	7.61	129.36	117.85
3	A	1408	PXI	C3-O1-C4	7.53	129.23	117.85
3	A	1408	PXI	O3-C7-C5	-7.23	98.98	111.16
3	B	1409	PXI	O3-C7-C5	-6.61	100.02	111.16
3	B	1409	PXI	O1-C3-C2	4.59	114.20	106.90
3	B	1409	PXI	C19-C18-C16	4.36	122.90	115.09
3	A	1408	PXI	C19-C18-C16	3.81	121.93	115.09
3	A	1408	PXI	O1-C3-C2	3.67	112.73	106.90
2	B	1408	HEM	CAA-C2A-C1A	3.46	131.70	124.94
3	A	1408	PXI	C10-C9-C11	-3.39	108.14	113.27
3	A	1408	PXI	C8-O3-C7	3.25	125.68	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1409	PXI	C10-C9-C11	-3.12	108.56	113.27
2	B	1408	HEM	CAD-C3D-C4D	3.11	130.12	124.70
3	A	1408	PXI	C25-C24-C23	-2.98	103.16	109.91
3	B	1409	PXI	C25-C24-C23	-2.94	103.25	109.91
3	B	1409	PXI	C8-O3-C7	2.93	124.92	117.98
3	A	1408	PXI	C7-C5-C4	2.86	115.70	109.93
3	A	1408	PXI	C13-N1-C12	-2.86	104.92	113.15
2	B	1408	HEM	C3B-C4B-NB	2.85	111.51	109.47
2	B	1408	HEM	CMC-C2C-C1C	2.78	129.62	124.73
3	A	1408	PXI	C17-C16-C7	2.68	115.52	111.14
3	B	1409	PXI	C13-N1-C12	-2.65	105.53	113.15
3	B	1409	PXI	C7-C5-C4	2.62	115.21	109.93
3	A	1408	PXI	C6-C5-C7	-2.56	107.27	113.00
3	B	1409	PXI	C6-C5-C7	-2.45	107.52	113.00
2	B	1408	HEM	CAA-C2A-C3A	-2.43	121.62	127.07
2	A	1407	HEM	C2D-C1D-ND	2.42	112.70	109.90
2	B	1408	HEM	CAD-C3D-C2D	-2.40	123.37	127.87
2	B	1408	HEM	CHC-C1C-NC	-2.31	121.93	124.45
3	B	1409	PXI	C17-C16-C7	2.26	114.84	111.14
2	A	1407	HEM	C3B-C4B-NB	2.24	111.08	109.47
2	B	1408	HEM	CMA-C3A-C4A	2.24	128.82	125.42
3	A	1408	PXI	O3-C8-O4	2.23	116.57	110.69
2	A	1407	HEM	CAD-C3D-C4D	2.19	128.51	124.70
2	A	1407	HEM	C3C-C2C-C1C	-2.14	105.02	107.05
2	A	1407	HEM	C2B-C1B-NB	2.12	112.28	109.84
3	B	1409	PXI	C18-C19-C21	2.01	115.43	110.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1408	HEM	C2C-C3C-CAC-CBC
2	B	1408	HEM	C4C-C3C-CAC-CBC
3	A	1408	PXI	C23-C24-C3-O1
3	A	1408	PXI	O4-C8-O3-C7
3	A	1408	PXI	C11-C12-N1-C13
3	A	1408	PXI	C11-C12-N1-C14
3	A	1408	PXI	C15-C12-N1-C13
3	A	1408	PXI	C7-C16-C18-C19
3	A	1408	PXI	C16-C18-C19-C20
3	A	1408	PXI	C16-C18-C19-C21
3	B	1409	PXI	C23-C24-C3-O1

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Mol	Chain	Res	Type	Atoms
3	B	1409	PXI	O4-C8-O3-C7
3	B	1409	PXI	C11-C12-N1-C13
3	B	1409	PXI	C11-C12-N1-C14
3	B	1409	PXI	C15-C12-N1-C13
3	B	1409	PXI	C7-C16-C18-C19
3	B	1409	PXI	C16-C18-C19-C20
3	B	1409	PXI	C16-C18-C19-C21
3	A	1408	PXI	C22-C23-C24-C25
3	B	1409	PXI	C22-C23-C24-C25
3	A	1408	PXI	C15-C12-N1-C14
3	B	1409	PXI	C15-C12-N1-C14
2	A	1407	HEM	C3A-C2A-CAA-CBA
3	A	1408	PXI	C19-C21-C22-C23
3	B	1409	PXI	C19-C21-C22-C23
3	A	1408	PXI	C25-C24-C3-C2
3	A	1408	PXI	C25-C24-C3-O1
3	A	1408	PXI	O6-C21-C22-C23
3	B	1409	PXI	O6-C21-C22-C23
3	A	1408	PXI	C17-C16-C18-C19
3	B	1409	PXI	C17-C16-C18-C19
2	A	1407	HEM	C2C-C3C-CAC-CBC
2	B	1408	HEM	C2B-C3B-CAB-CBB
3	A	1408	PXI	C23-C24-C3-C2
2	A	1407	HEM	C1A-C2A-CAA-CBA
3	B	1409	PXI	C25-C24-C3-O1
2	A	1407	HEM	C4C-C3C-CAC-CBC
2	B	1408	HEM	CAA-CBA-CGA-O2A
2	B	1408	HEM	CAA-CBA-CGA-O1A

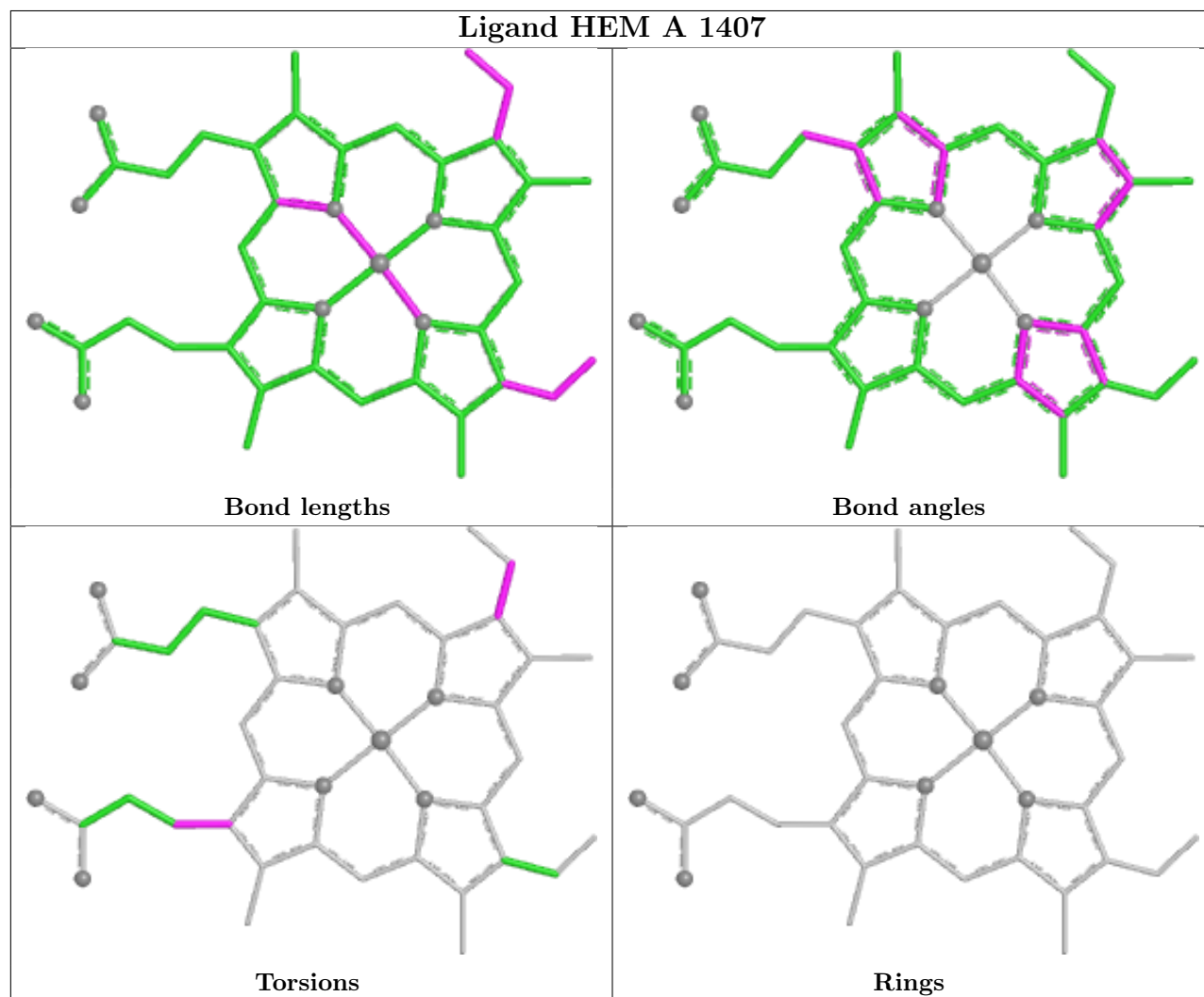
There are no ring outliers.

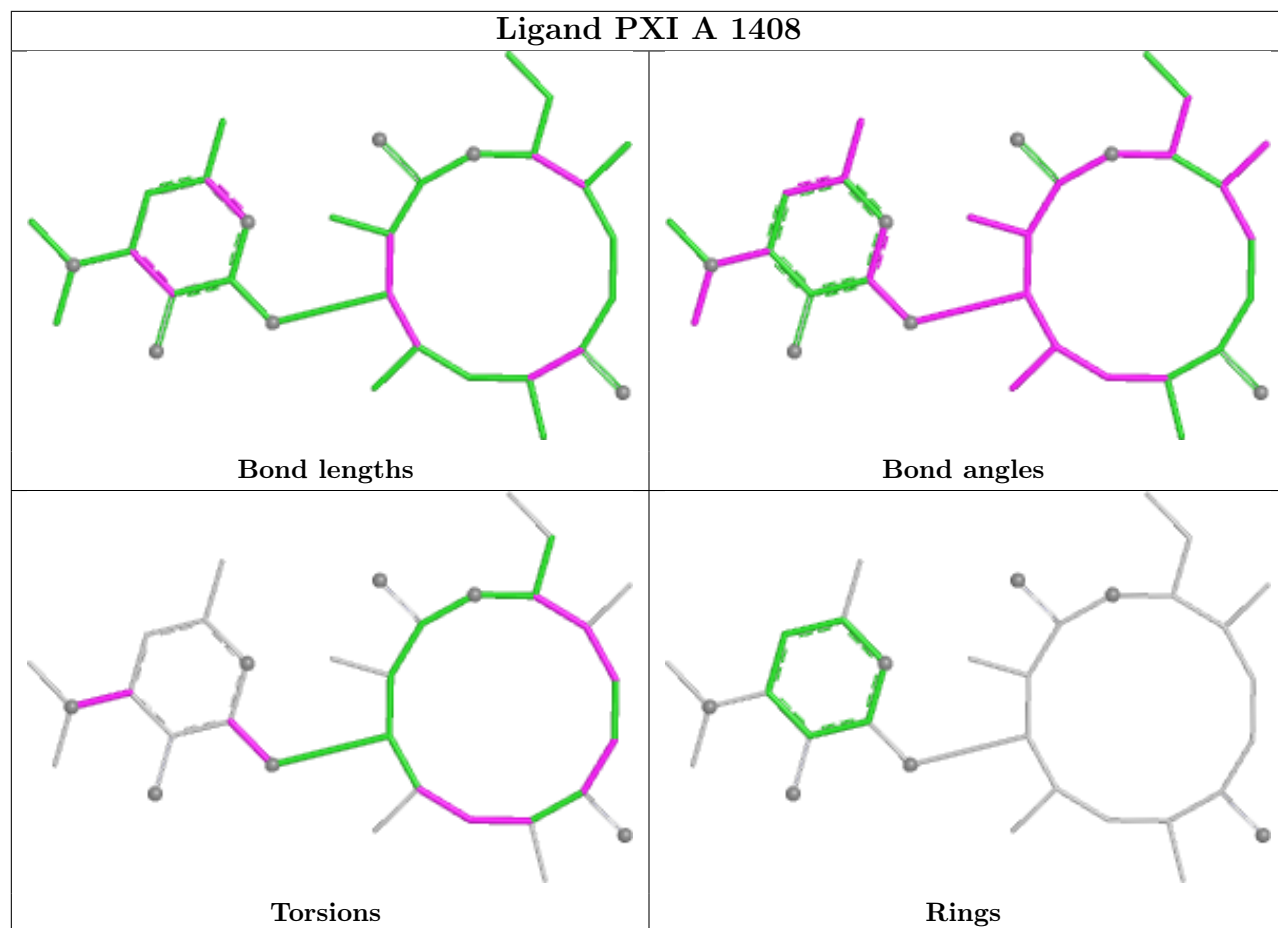
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1407	HEM	2	0
3	A	1408	PXI	2	0
4	A	1431	SO4	1	0

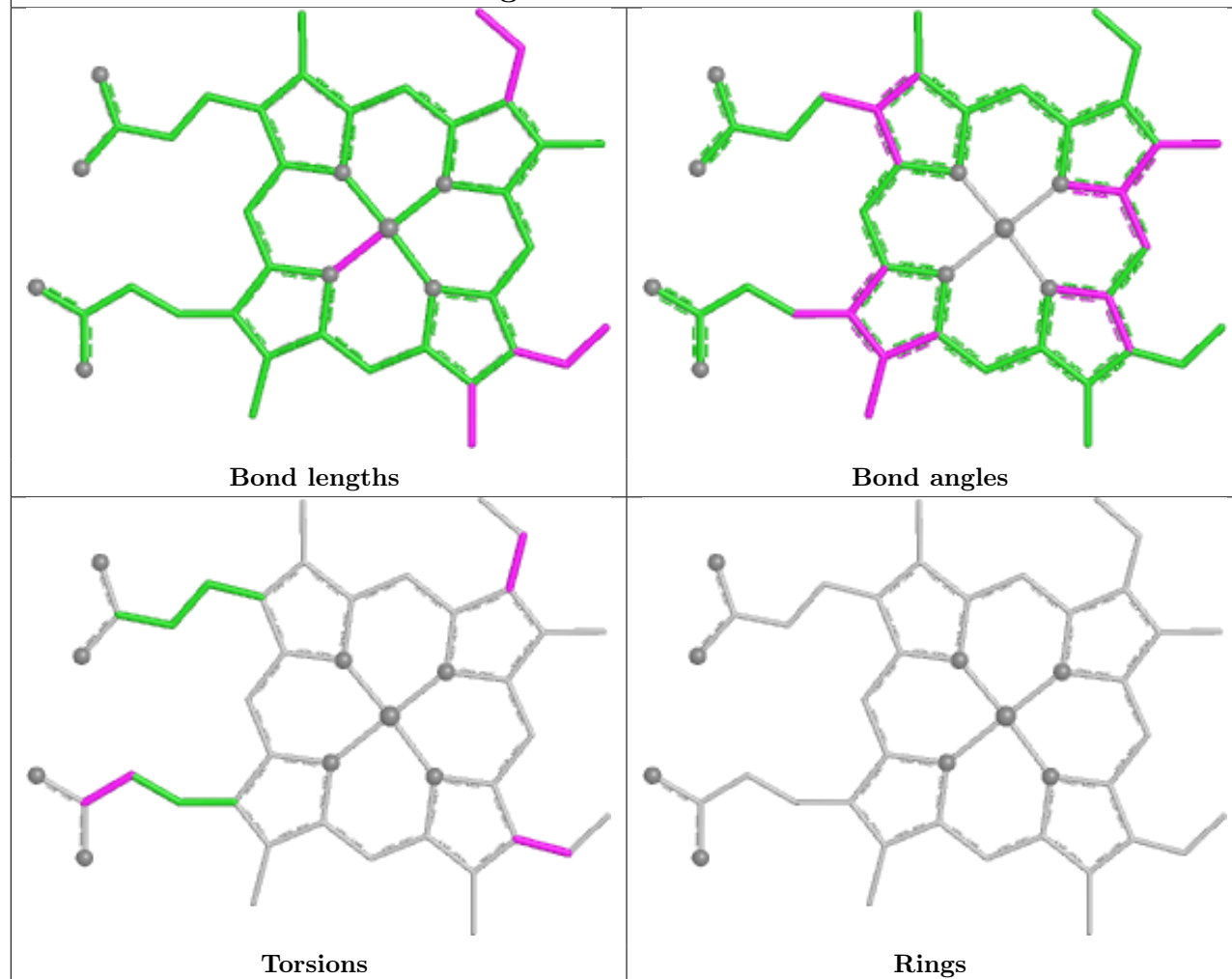
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

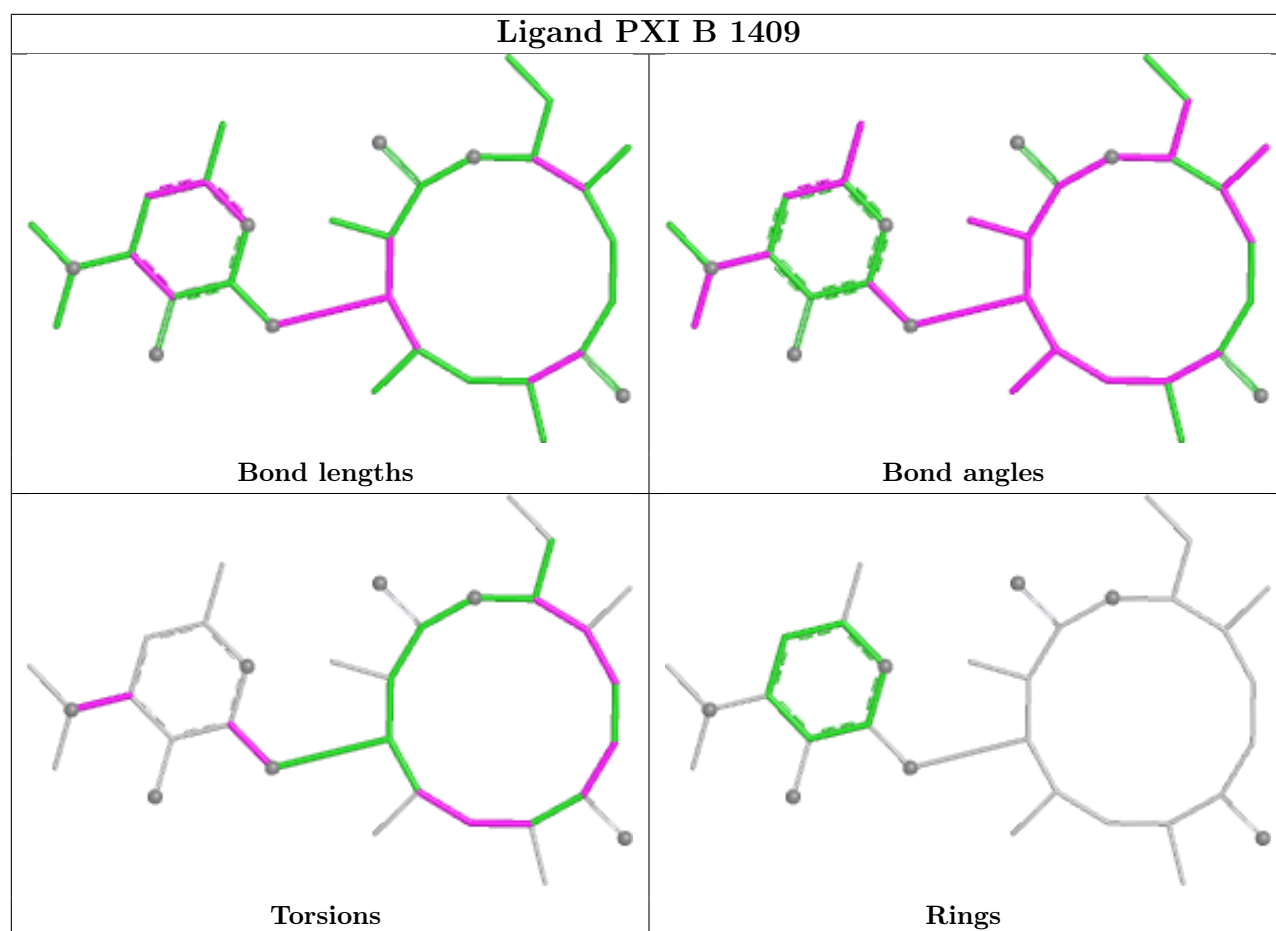
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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 HEM B 1408





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	394/436 (90%)	0.04	6 (1%) 72 77	13, 28, 48, 59	0
1	B	395/436 (90%)	0.14	13 (3%) 49 56	14, 29, 54, 69	0
All	All	789/872 (90%)	0.09	19 (2%) 59 66	13, 28, 51, 69	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	390	TYR	3.5
1	B	180	PHE	3.2
1	A	14	VAL	3.1
1	A	407	ARG	3.0
1	B	385	GLY	2.7
1	B	184	PRO	2.6
1	B	380	LEU	2.6
1	B	113	MET	2.6
1	B	137	ALA	2.5
1	A	114	ARG	2.4
1	A	150	TRP	2.4
1	B	139	ASP	2.3
1	B	384	PRO	2.3
1	B	48	GLU	2.2
1	B	383	SER	2.2
1	B	181	PRO	2.1
1	A	303	ASP	2.1
1	A	34	ARG	2.0
1	B	83	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

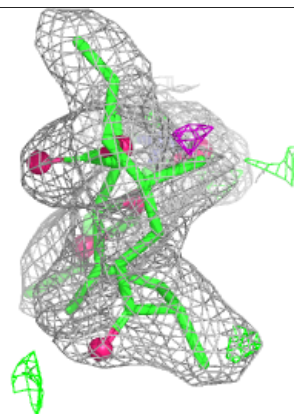
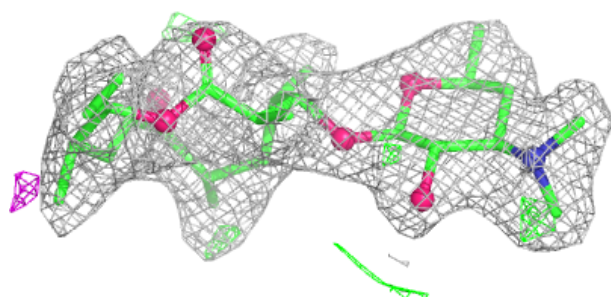
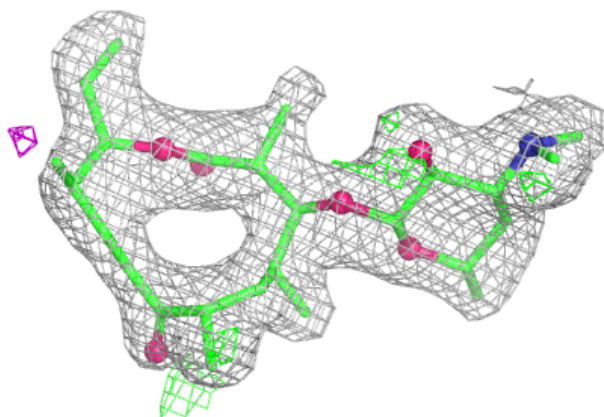
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1432	5/5	0.83	0.22	81,82,83,83	0
4	SO4	A	1434	5/5	0.85	0.16	80,80,81,82	0
4	SO4	A	1431	5/5	0.87	0.17	71,71,72,72	0
4	SO4	A	1430	5/5	0.88	0.14	71,72,73,73	0
3	PXI	A	1408	32/32	0.90	0.12	25,30,36,38	0
4	SO4	B	1433	5/5	0.90	0.15	68,69,70,71	0
3	PXI	B	1409	32/32	0.91	0.11	26,31,36,37	0
2	HEM	B	1408	43/43	0.98	0.06	12,19,22,23	0
2	HEM	A	1407	43/43	0.98	0.05	9,15,19,21	0

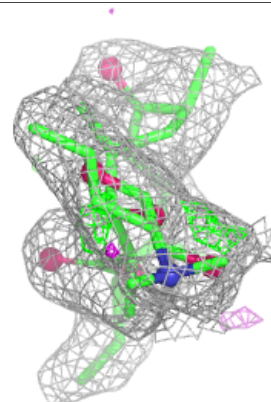
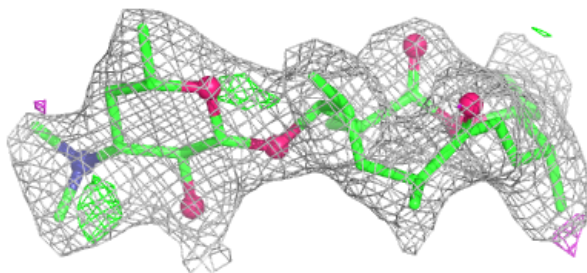
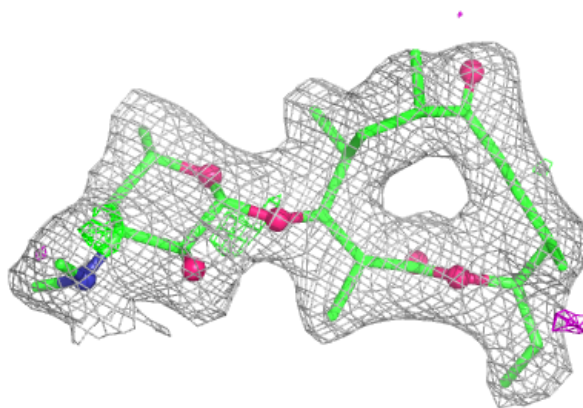
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PXI A 1408:

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

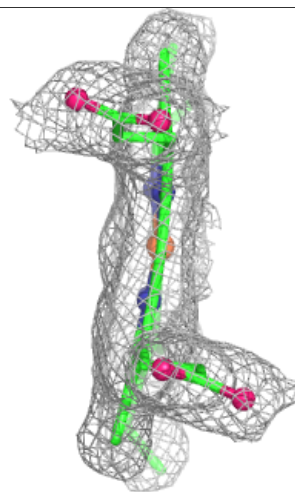
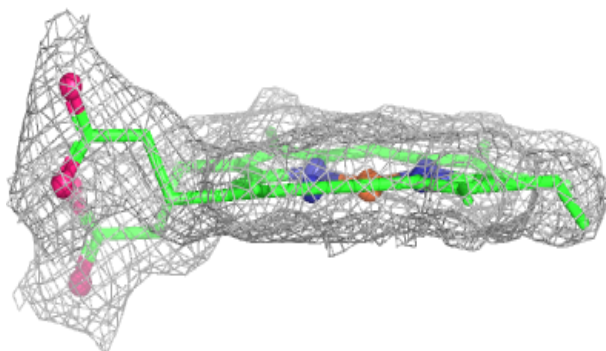
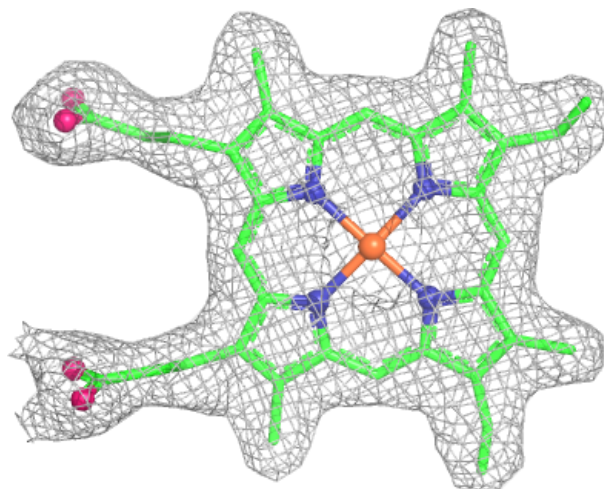
**Electron density around PXI B 1409:**

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



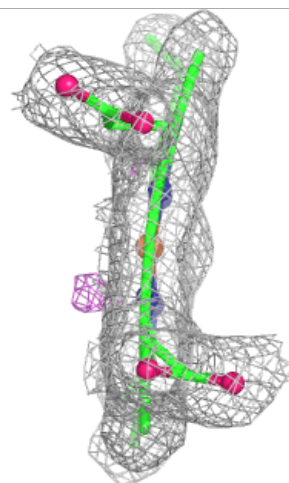
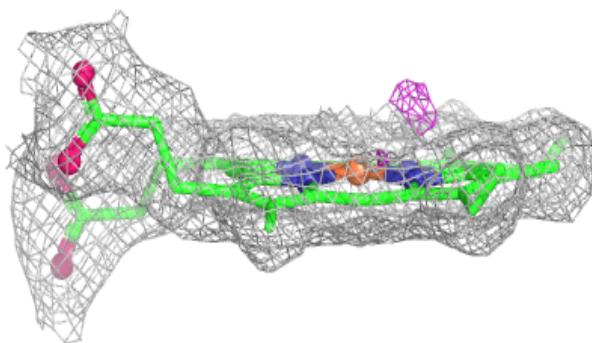
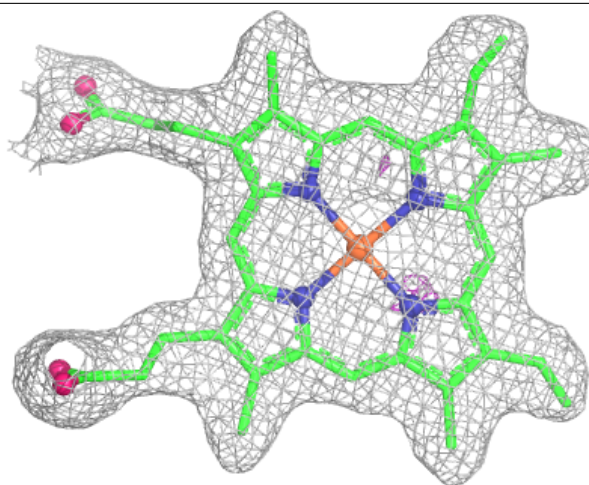
Electron density around HEM B 1408:

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



Electron density around HEM A 1407:

$2mF_o-DF_c$ (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.