



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:25 pm BST

PDB ID : 2CD8  
Title : Crystal structure of YC-17-bound cytochrome P450 PikC (CYP107L1)  
Authors : Yermalitskaya, L.I.; Kim, Y.; Sherman, D.H.; Waterman, M.R.; Podust, L.M.  
Deposited on : 2006-01-20  
Resolution : 1.70 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](mailto: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.

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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 : 2.11  
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) : 2.11

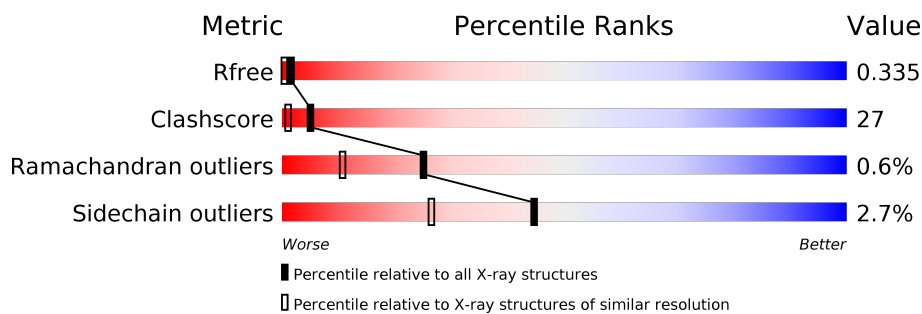
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	436	
1	B	436	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6456 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 MONOOXYGENASE.

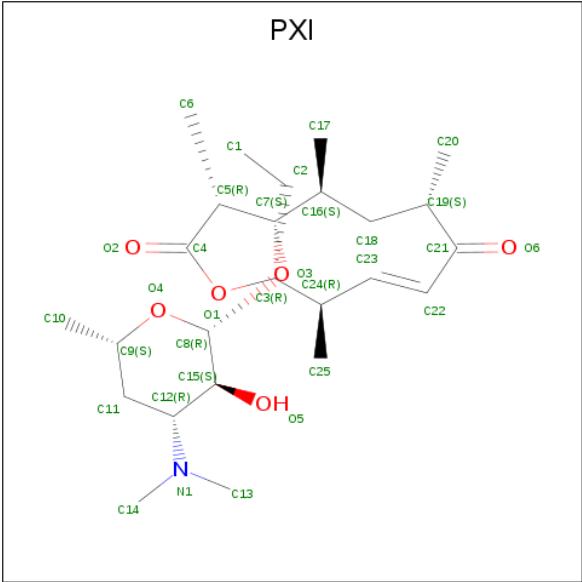
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	1
			3024	1904	543	564	13			
1	B	393	Total	C	N	O	S	0	0	1
			3027	1910	545	559	13			

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



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

- Molecule 3 is 4-{{[4-(DIMETHYLAMINO)-3-HYDROXY-6-METHYLTETRAHYDRO-2H-PYRAN-2-YL]OXY}}-12-ETHYL-3,5,7,11-TETRAMETHYLOXACYCLODODEC-9-ENE-2,8-DIONE (three-letter code: PXI) (formula:  $C_{25}H_{43}NO_6$ ).



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		

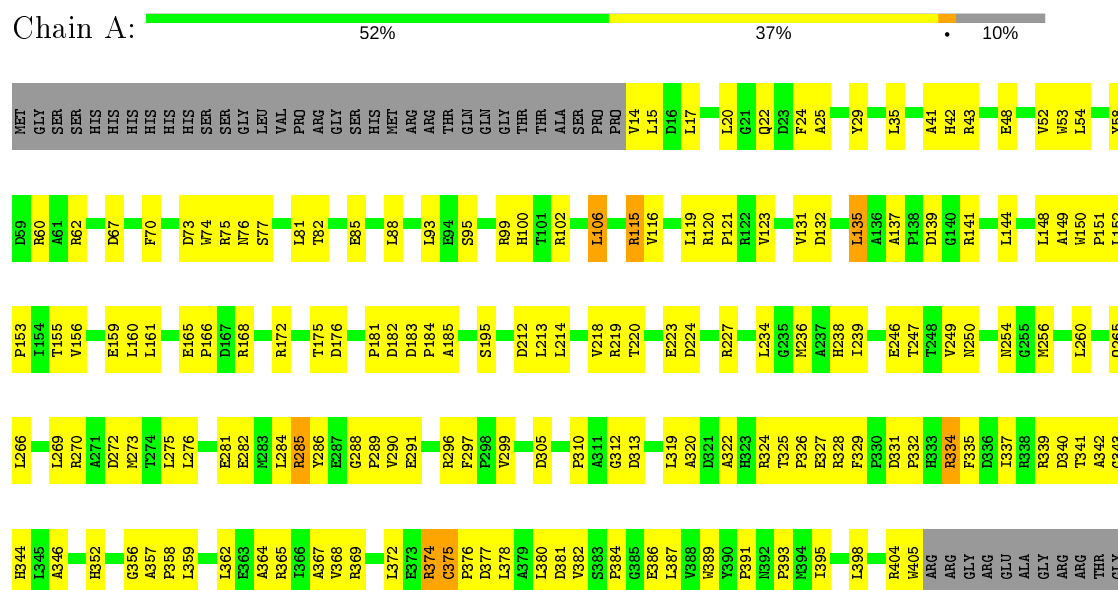
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	116	Total	O	0	0
			116	116		

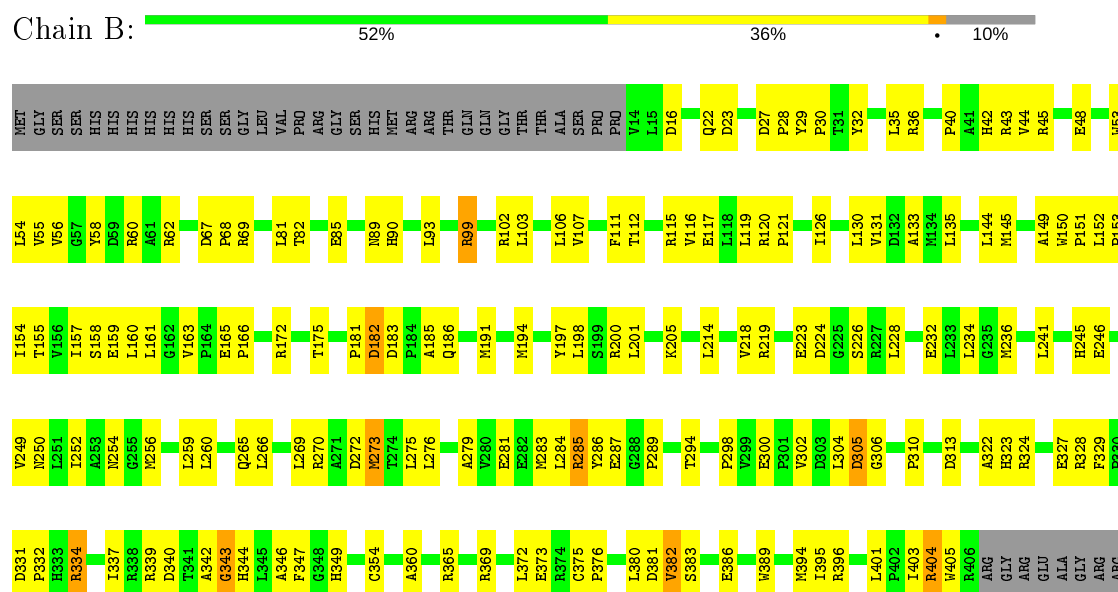
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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 MONOOXYGENASE



#### • Molecule 1: CYTOCHROME P450 MONOOXYGENASE



TER  
GLY

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.40Å 92.10Å 67.57Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	39.84 – 1.70 39.84 – 1.65	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.84-1.70) 95.3 (39.84-1.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.290 , 0.333 0.292 , 0.335	Depositor DCC
$R_{free}$ test set	8535 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 22.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6456	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.38	0/3092	0.63	0/4219
1	B	0.36	0/3097	0.62	0/4228
All	All	0.37	0/6189	0.62	0/8447

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	3024	0	2994	172	0
1	B	3027	0	2995	164	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	32	0	43	1	0
3	B	32	0	43	5	0
4	A	139	0	0	25	0
4	B	116	0	0	16	0
All	All	6456	0	6135	336	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 27.



All (336) 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:285:ARG:HB3	1:A:285:ARG:HH11	1.09	1.09
1:B:119:LEU:HD13	1:B:160:LEU:HD11	1.51	0.92
1:A:285:ARG:HB3	1:A:285:ARG:NH1	1.84	0.92
1:B:40:PRO:HG3	1:B:305:ASP:HB2	1.54	0.89
1:B:150:TRP:HB3	1:B:151:PRO:HD3	1.52	0.88
1:A:329:PHE:O	1:A:332:PRO:HG3	1.76	0.85
1:A:265:GLN:HE21	1:A:337:ILE:H	1.21	0.83
1:B:16:ASP:HA	1:B:45:ARG:HB3	1.58	0.82
1:B:382:VAL:HG22	1:B:383:SER:H	1.43	0.82
1:A:175:THR:CG2	1:A:246:GLU:HG2	2.11	0.81
1:B:102:ARG:O	1:B:106:LEU:HD13	1.81	0.80
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.61	0.80
1:B:250:ASN:HB3	4:B:2076:HOH:O	1.81	0.79
1:A:95:SER:CB	1:A:99:ARG:HD2	2.13	0.79
1:B:107:VAL:HG22	4:B:2044:HOH:O	1.83	0.79
1:B:181:PRO:HB2	1:B:186:GLN:HB3	1.63	0.78
1:A:95:SER:HB3	1:A:99:ARG:HH11	1.49	0.77
1:B:197:TYR:HD1	1:B:200:ARG:HH12	1.30	0.77
1:A:175:THR:HG22	1:A:246:GLU:HG2	1.67	0.77
1:A:95:SER:HB2	1:A:99:ARG:HD2	1.67	0.77
1:B:381:ASP:OD2	1:B:404:ARG:HB3	1.85	0.77
1:A:319:LEU:HB3	4:A:2121:HOH:O	1.83	0.77
1:A:288:GLY:HA3	4:A:2102:HOH:O	1.85	0.77
1:B:22:GLN:HE22	1:B:389:TRP:H	1.30	0.77
1:A:265:GLN:NE2	1:A:337:ILE:H	1.82	0.77
1:B:35:LEU:HB3	1:B:42:HIS:CD2	2.20	0.76
1:B:395:ILE:HD12	1:B:395:ILE:N	2.00	0.76
1:A:219:ARG:O	1:A:223:GLU:HG3	1.86	0.76
1:B:131:VAL:O	1:B:135:LEU:HG	1.87	0.75
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.70	0.74
1:A:289:PRO:O	1:A:395:ILE:HD12	1.88	0.74
1:B:81:LEU:CD2	1:B:85:GLU:HB2	2.17	0.74
1:B:205:LYS:HG3	1:B:214:LEU:HD12	1.71	0.73
1:A:344:HIS:HD2	1:A:346:ALA:H	1.35	0.73
1:B:294:THR:HA	1:B:394:MET:HE1	1.68	0.73
1:B:119:LEU:HD22	1:B:160:LEU:HD21	1.71	0.72
1:A:106:LEU:HD11	1:A:220:THR:HG21	1.71	0.72
1:B:120:ARG:HB3	1:B:121:PRO:HD3	1.72	0.72
1:B:85:GLU:HG2	1:B:191:MET:SD	2.29	0.72
1:B:165:GLU:HB3	1:B:166:PRO:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:HG3	1:A:335:PHE:CE1	2.26	0.70
1:B:90:HIS:ND1	1:B:99:ARG:NH2	2.41	0.69
1:A:328:ARG:HG3	1:A:329:PHE:CD1	2.28	0.69
1:B:339:ARG:HG2	1:B:340:ASP:N	2.08	0.69
1:A:327:GLU:H	1:A:327:GLU:CD	1.97	0.68
1:B:334:ARG:HA	1:B:334:ARG:CZ	2.23	0.67
1:B:329:PHE:O	1:B:332:PRO:HG3	1.95	0.67
1:B:32:TYR:HA	1:B:35:LEU:HD12	1.76	0.67
1:B:44:VAL:HG11	1:B:54:LEU:HD12	1.77	0.67
1:B:294:THR:HA	1:B:394:MET:CE	2.25	0.67
1:B:246:GLU:HG3	3:B:420:PXI:O6	1.95	0.66
1:A:250:ASN:HD22	1:A:395:ILE:HD11	1.60	0.66
1:A:324:ARG:O	1:A:326:PRO:HD3	1.96	0.66
1:B:28:PRO:HB2	1:B:32:TYR:CE1	2.31	0.65
1:A:43:ARG:HG2	4:A:2019:HOH:O	1.96	0.65
1:B:289:PRO:HA	4:B:2076:HOH:O	1.96	0.65
1:B:144:LEU:HD21	1:B:256:MET:HG3	1.77	0.65
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.79	0.65
1:B:376:PRO:HG2	1:B:405:TRP:HB2	1.78	0.65
1:B:331:ASP:N	1:B:332:PRO:HD3	2.12	0.64
1:B:327:GLU:H	1:B:327:GLU:CD	2.00	0.64
1:B:182:ASP:OD1	1:B:186:GLN:NE2	2.30	0.64
1:B:145:MET:HA	1:B:149:ALA:HB3	1.79	0.64
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.79	0.64
1:A:62:ARG:HH11	1:A:62:ARG:HG2	1.62	0.63
1:B:310:PRO:HG2	1:B:313:ASP:OD2	1.98	0.63
1:B:265:GLN:HE21	1:B:337:ILE:H	1.45	0.63
1:B:376:PRO:HG2	1:B:405:TRP:O	1.99	0.63
1:B:81:LEU:HD23	1:B:85:GLU:HB2	1.80	0.63
1:A:150:TRP:CE2	1:A:172:ARG:HD2	2.33	0.63
1:A:22:GLN:HE22	1:A:389:TRP:H	1.46	0.63
1:A:139:ASP:O	1:A:141:ARG:HG3	2.00	0.62
1:B:254:ASN:ND2	4:B:2076:HOH:O	2.33	0.61
1:A:29:TYR:HE2	1:A:320:ALA:HB1	1.65	0.61
1:A:339:ARG:NE	4:A:2117:HOH:O	2.31	0.61
1:B:69:ARG:HD3	4:B:2020:HOH:O	2.01	0.60
1:A:132:ASP:OD1	1:A:374:ARG:NH1	2.34	0.60
1:A:285:ARG:HD2	1:A:329:PHE:CE2	2.37	0.60
1:B:44:VAL:HG11	1:B:54:LEU:CD1	2.32	0.60
1:B:103:LEU:HD21	4:B:2075:HOH:O	2.01	0.60
1:B:214:LEU:O	1:B:218:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH1	1:A:115:ARG:HB2	2.17	0.60
1:B:276:LEU:CD1	1:B:365:ARG:HG2	2.31	0.59
1:B:58:TYR:HD1	1:B:322:ALA:HB1	1.67	0.59
1:A:260:LEU:HD21	1:A:378:LEU:HG	1.85	0.59
1:B:197:TYR:HA	1:B:200:ARG:NH1	2.18	0.59
1:A:282:GLU:OE1	1:A:285:ARG:NH1	2.35	0.59
1:B:286:TYR:CD2	1:B:287:GLU:HG2	2.37	0.58
1:A:273:MET:HE3	1:A:369:ARG:HG3	1.85	0.58
1:A:266:LEU:HD13	1:A:266:LEU:O	2.04	0.58
1:A:165:GLU:HA	1:A:168:ARG:NE	2.18	0.57
1:A:285:ARG:NH2	4:A:2117:HOH:O	2.36	0.57
1:B:150:TRP:CZ2	1:B:172:ARG:HB2	2.39	0.57
1:A:135:LEU:N	1:A:135:LEU:HD23	2.20	0.57
1:A:276:LEU:HD11	1:A:365:ARG:HB3	1.87	0.57
1:A:29:TYR:CE2	1:A:320:ALA:HB1	2.40	0.57
1:A:328:ARG:HG3	1:A:329:PHE:CE1	2.40	0.56
1:A:135:LEU:HD12	1:A:374:ARG:CZ	2.35	0.56
1:A:35:LEU:HB3	1:A:42:HIS:CD2	2.40	0.56
1:B:214:LEU:HD13	1:B:218:VAL:HG23	1.88	0.56
1:B:260:LEU:HB3	1:B:380:LEU:HG	1.86	0.56
1:B:285:ARG:NH2	1:B:332:PRO:O	2.35	0.56
1:A:137:ALA:C	1:A:139:ASP:H	2.08	0.56
1:A:266:LEU:HD13	1:A:266:LEU:C	2.26	0.56
1:A:250:ASN:O	1:A:254:ASN:HB2	2.06	0.56
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.87	0.56
1:A:227:ARG:HH11	1:A:227:ARG:HG2	1.71	0.56
1:B:382:VAL:HG22	1:B:383:SER:N	2.19	0.56
1:B:298:PRO:HD2	1:B:313:ASP:O	2.06	0.56
1:B:82:THR:OG1	1:B:85:GLU:HG3	2.06	0.56
1:A:376:PRO:HG2	1:A:377:ASP:H	1.71	0.55
1:B:224:ASP:C	1:B:226:SER:H	2.08	0.55
1:B:245:HIS:O	1:B:249:VAL:HG23	2.05	0.55
1:A:150:TRP:O	1:A:153:PRO:HD2	2.06	0.55
1:B:133:ALA:HB3	4:B:2052:HOH:O	2.06	0.55
1:B:69:ARG:CZ	1:B:302:VAL:HG13	2.37	0.55
1:B:250:ASN:O	1:B:254:ASN:HB2	2.07	0.55
1:A:175:THR:HG23	4:A:2139:HOH:O	2.07	0.55
1:B:344:HIS:HD2	1:B:346:ALA:H	1.54	0.55
1:B:112:THR:O	1:B:116:VAL:HG13	2.07	0.54
1:B:285:ARG:NH2	1:B:324:ARG:HD3	2.22	0.54
1:B:200:ARG:HB2	1:B:200:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:NH1	1:B:349:HIS:NE2	2.55	0.54
1:A:17:LEU:HA	1:A:20:LEU:HD12	1.90	0.54
1:A:344:HIS:CD2	1:A:346:ALA:HB3	2.42	0.54
1:A:352:HIS:NE2	4:A:2125:HOH:O	2.34	0.54
1:B:360:ALA:HB1	2:B:419:HEM:CBB	2.38	0.54
1:A:82:THR:OG1	1:A:85:GLU:HG3	2.08	0.53
1:B:150:TRP:O	1:B:153:PRO:HD2	2.08	0.53
1:B:81:LEU:HD21	1:B:85:GLU:HB2	1.89	0.53
1:A:156:VAL:O	1:A:160:LEU:HG	2.09	0.53
1:A:181:PRO:HB2	1:A:183:ASP:O	2.08	0.53
1:A:88:LEU:HD21	1:A:195:SER:HB2	1.89	0.53
1:B:60:ARG:CZ	1:B:304:LEU:HD22	2.39	0.53
1:B:175:THR:HG23	1:B:246:GLU:OE2	2.09	0.53
1:A:155:THR:O	1:A:159:GLU:HG3	2.09	0.52
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.91	0.52
1:A:381:ASP:HB2	1:A:404:ARG:HB3	1.91	0.52
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.24	0.52
1:A:272:ASP:HB3	1:A:275:LEU:CD1	2.39	0.52
1:A:331:ASP:N	1:A:332:PRO:HD3	2.24	0.52
1:A:247:THR:O	1:A:289:PRO:HG3	2.09	0.52
1:A:282:GLU:HA	1:A:282:GLU:OE1	2.09	0.52
1:B:194:MET:O	1:B:198:LEU:HG	2.09	0.52
1:A:175:THR:HG22	1:A:246:GLU:CG	2.39	0.52
1:B:276:LEU:HD13	1:B:276:LEU:C	2.30	0.52
1:B:22:GLN:NE2	1:B:389:TRP:H	2.05	0.52
1:A:290:VAL:HG12	1:A:319:LEU:HD12	1.91	0.52
1:B:183:ASP:OD1	1:B:185:ALA:HB3	2.10	0.52
1:A:310:PRO:HG2	1:A:313:ASP:CG	2.30	0.51
1:B:161:LEU:HD13	1:B:241:LEU:HG	1.92	0.51
1:B:48:GLU:N	4:B:2011:HOH:O	2.42	0.51
1:A:260:LEU:HB3	1:A:380:LEU:HG	1.93	0.51
1:B:327:GLU:HB3	4:B:2091:HOH:O	2.10	0.51
1:A:41:ALA:HA	1:A:54:LEU:O	2.10	0.51
1:B:376:PRO:HG3	4:B:2115:HOH:O	2.09	0.51
1:A:381:ASP:HA	1:A:404:ARG:HH11	1.76	0.51
1:A:328:ARG:NE	4:A:2113:HOH:O	2.43	0.51
1:A:250:ASN:HB2	1:A:289:PRO:HB3	1.92	0.51
1:A:405:TRP:N	4:A:2137:HOH:O	2.44	0.51
1:B:150:TRP:CB	1:B:151:PRO:HD3	2.35	0.51
1:A:74:TRP:CE3	1:A:81:LEU:HG	2.46	0.51
1:B:272:ASP:HB3	1:B:275:LEU:HG	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:HG2	1:A:340:ASP:N	2.24	0.50
1:A:364:ALA:O	1:A:368:VAL:HG23	2.11	0.50
1:A:319:LEU:HD13	4:A:2121:HOH:O	2.10	0.50
1:A:324:ARG:HA	1:A:332:PRO:HB3	1.94	0.50
1:A:346:ALA:HA	4:A:2121:HOH:O	2.11	0.50
1:B:347:PHE:HB3	1:B:354:CYS:HB3	1.94	0.50
1:B:260:LEU:HA	1:B:266:LEU:HD22	1.94	0.50
1:A:276:LEU:HD11	1:A:365:ARG:CB	2.42	0.49
1:A:334:ARG:CZ	1:A:335:PHE:O	2.60	0.49
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.95	0.49
1:B:273:MET:HE2	1:B:369:ARG:CZ	2.42	0.49
1:B:395:ILE:CD1	1:B:395:ILE:N	2.71	0.49
1:A:341:THR:O	1:A:342:ALA:C	2.51	0.49
1:A:224:ASP:OD2	1:A:227:ARG:HB2	2.12	0.49
1:A:234:LEU:HD23	4:A:2038:HOH:O	2.13	0.49
1:A:246:GLU:HA	1:A:246:GLU:OE1	2.13	0.49
1:A:67:ASP:HB3	1:A:70:PHE:HD1	1.78	0.49
1:B:252:ILE:O	1:B:256:MET:HG2	2.13	0.49
1:B:150:TRP:NE1	1:B:172:ARG:HG3	2.28	0.48
1:B:89:ASN:HB3	3:B:420:PXI:H141	1.94	0.48
1:A:352:HIS:HB2	4:A:2123:HOH:O	2.13	0.48
1:A:82:THR:HB	4:A:2073:HOH:O	2.12	0.48
1:B:276:LEU:HD11	1:B:365:ARG:HG2	1.95	0.48
1:A:135:LEU:HD12	1:A:374:ARG:NH2	2.29	0.48
1:A:272:ASP:HB3	1:A:275:LEU:HD11	1.95	0.48
1:A:73:ASP:CG	1:A:75:ARG:HE	2.18	0.48
1:B:155:THR:HG22	1:B:159:GLU:OE2	2.13	0.48
1:B:394:MET:C	1:B:395:ILE:HD12	2.34	0.48
1:A:25:ALA:HB2	1:A:391:PRO:HA	1.96	0.47
1:B:157:ILE:O	1:B:161:LEU:HB2	2.14	0.47
1:B:310:PRO:HG2	1:B:313:ASP:CG	2.34	0.47
1:B:158:SER:HB3	1:B:163:VAL:HB	1.97	0.47
1:A:153:PRO:HB2	4:A:2061:HOH:O	2.14	0.47
1:A:328:ARG:O	1:A:328:ARG:HD3	2.14	0.47
1:B:373:GLU:N	1:B:373:GLU:OE1	2.47	0.47
1:A:389:TRP:CZ2	1:A:398:LEU:HD21	2.49	0.47
1:A:150:TRP:NE1	1:A:172:ARG:HD2	2.29	0.47
1:A:181:PRO:C	1:A:183:ASP:H	2.17	0.47
1:B:115:ARG:HG3	4:B:2047:HOH:O	2.15	0.47
1:A:359:LEU:HD23	2:A:419:HEM:HBC2	1.95	0.47
1:B:198:LEU:HB2	1:B:234:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD23	1:B:401:LEU:HD23	1.96	0.47
1:B:40:PRO:O	1:B:55:VAL:HA	2.15	0.47
1:B:35:LEU:HB3	1:B:42:HIS:HD2	1.72	0.47
1:A:344:HIS:HD2	1:A:346:ALA:N	2.09	0.46
1:A:381:ASP:HA	1:A:404:ARG:NH1	2.30	0.46
1:A:339:ARG:NH2	4:A:2117:HOH:O	2.48	0.46
1:A:266:LEU:CD2	1:A:372:LEU:HD11	2.45	0.46
1:A:290:VAL:CG1	1:A:319:LEU:HD12	2.45	0.46
1:A:62:ARG:NH1	1:A:62:ARG:HG2	2.29	0.46
1:A:43:ARG:O	1:A:43:ARG:HG3	2.15	0.46
1:B:334:ARG:NH1	1:B:334:ARG:HA	2.31	0.46
1:A:285:ARG:HH12	1:A:286:TYR:HB2	1.81	0.46
1:A:384:PRO:O	1:A:387:LEU:HB2	2.15	0.46
1:B:126:ILE:O	1:B:130:LEU:HG	2.15	0.46
1:A:183:ASP:C	1:A:185:ALA:H	2.18	0.46
1:A:369:ARG:NH2	4:A:2130:HOH:O	2.48	0.46
1:B:150:TRP:HE3	1:B:151:PRO:HG3	1.80	0.46
1:B:81:LEU:HD21	1:B:85:GLU:CB	2.45	0.46
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.98	0.46
1:A:144:LEU:HD21	1:A:256:MET:HG3	1.98	0.46
1:A:284:LEU:HB3	1:A:346:ALA:CB	2.46	0.46
1:B:150:TRP:HB3	1:B:151:PRO:CD	2.34	0.45
1:B:93:LEU:HB3	4:B:2036:HOH:O	2.15	0.45
1:B:67:ASP:HA	1:B:68:PRO:HD3	1.84	0.45
1:A:148:LEU:HD21	1:A:367:ALA:HB1	1.99	0.45
1:B:246:GLU:CD	1:B:246:GLU:H	2.20	0.45
1:B:191:MET:HG2	3:B:420:PXI:H101	1.98	0.45
1:A:183:ASP:OD1	1:A:184:PRO:HD2	2.17	0.45
1:B:106:LEU:CD1	4:B:2042:HOH:O	2.64	0.45
1:B:304:LEU:C	1:B:306:GLY:H	2.20	0.45
1:A:382:VAL:HG22	1:A:386:GLU:HB3	1.98	0.44
1:A:291:GLU:HB3	1:A:393:PRO:O	2.17	0.44
1:B:27:ASP:O	1:B:30:PRO:HD2	2.16	0.44
1:A:58:TYR:HA	1:A:322:ALA:HB1	1.99	0.44
1:B:328:ARG:NH2	1:B:343:GLY:HA3	2.33	0.44
1:A:161:LEU:HD13	1:A:213:LEU:HB3	1.98	0.44
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.83	0.44
1:A:165:GLU:HA	1:A:168:ARG:CZ	2.47	0.44
1:A:305:ASP:O	1:A:305:ASP:OD1	2.35	0.44
1:B:154:ILE:N	4:B:2056:HOH:O	2.43	0.44
1:B:43:ARG:CZ	1:B:53:TRP:HZ2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ASP:O	1:A:275:LEU:HD12	2.17	0.44
1:A:389:TRP:CD2	1:A:398:LEU:HD23	2.53	0.44
1:B:219:ARG:O	1:B:223:GLU:HG3	2.18	0.44
1:B:36:ARG:HA	1:B:56:VAL:CG2	2.48	0.44
1:A:149:ALA:O	1:A:249:VAL:HG22	2.18	0.44
1:B:228:LEU:HD12	1:B:232:GLU:CB	2.48	0.44
1:A:15:LEU:HD11	1:A:20:LEU:HD11	1.99	0.44
1:B:181:PRO:C	1:B:183:ASP:N	2.69	0.44
1:B:36:ARG:HA	1:B:56:VAL:HG23	1.99	0.44
1:B:181:PRO:C	1:B:183:ASP:H	2.20	0.44
1:B:259:LEU:HG	1:B:266:LEU:HB2	2.00	0.44
1:B:273:MET:O	1:B:276:LEU:HB2	2.17	0.44
1:A:346:ALA:CB	4:A:2102:HOH:O	2.65	0.43
1:A:266:LEU:HD21	1:A:372:LEU:HD11	2.00	0.43
1:B:300:GLU:O	1:B:302:VAL:HG23	2.18	0.43
1:A:116:VAL:HG12	1:A:362:LEU:HD22	2.00	0.43
1:A:182:ASP:O	1:A:183:ASP:HB2	2.19	0.43
1:A:102:ARG:NH1	1:A:227:ARG:O	2.51	0.43
1:A:358:PRO:HD2	4:A:2127:HOH:O	2.17	0.43
1:A:131:VAL:O	1:A:135:LEU:HG	2.18	0.43
1:A:165:GLU:HA	1:A:168:ARG:CD	2.49	0.43
1:B:331:ASP:N	1:B:332:PRO:CD	2.79	0.43
1:B:152:LEU:CB	1:B:153:PRO:HD3	2.37	0.43
1:B:214:LEU:HD13	1:B:218:VAL:CG2	2.49	0.43
1:B:279:ALA:O	1:B:283:MET:HG3	2.18	0.43
1:B:281:GLU:HA	1:B:284:LEU:HD12	1.99	0.43
1:A:296:ARG:HH11	1:A:296:ARG:HG3	1.84	0.43
1:A:334:ARG:NH1	1:A:335:PHE:O	2.52	0.43
1:A:356:GLY:HA2	4:A:2127:HOH:O	2.18	0.43
1:A:375:CYS:HA	1:A:376:PRO:HD2	1.86	0.43
1:B:111:PHE:CE2	2:B:419:HEM:HBC1	2.54	0.43
1:B:285:ARG:O	1:B:323:HIS:HB3	2.18	0.43
1:A:236:MET:O	1:A:239:ILE:HG22	2.19	0.43
1:A:100:HIS:CD2	1:A:352:HIS:CE1	3.07	0.43
1:A:52:VAL:HG23	1:A:53:TRP:N	2.32	0.43
1:B:285:ARG:HH21	1:B:324:ARG:HD3	1.84	0.43
1:B:382:VAL:HG21	1:B:386:GLU:OE1	2.19	0.42
1:A:214:LEU:O	1:A:218:VAL:HG23	2.19	0.42
1:A:269:LEU:HD11	1:A:276:LEU:HA	2.01	0.42
1:B:29:TYR:HB2	1:B:30:PRO:HD3	2.01	0.42
1:B:369:ARG:NH1	1:B:373:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:N	4:B:2098:HOH:O	2.52	0.42
1:A:115:ARG:HB2	1:A:115:ARG:HH11	1.84	0.42
1:A:14:VAL:N	4:A:2001:HOH:O	2.52	0.42
1:A:95:SER:HB3	1:A:99:ARG:HD2	1.96	0.42
1:B:32:TYR:O	1:B:35:LEU:HB2	2.20	0.42
1:B:85:GLU:HB3	3:B:420:PXI:H132	2.00	0.42
1:A:270:ARG:NH2	1:A:375:CYS:O	2.53	0.42
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.35	0.42
1:B:375:CYS:HA	1:B:376:PRO:HD2	1.90	0.42
1:B:273:MET:HE1	1:B:276:LEU:HD23	2.02	0.42
1:A:150:TRP:N	1:A:151:PRO:CD	2.83	0.41
1:A:131:VAL:CG1	1:A:374:ARG:HD3	2.50	0.41
1:B:102:ARG:O	1:B:106:LEU:CD1	2.60	0.41
1:B:85:GLU:O	3:B:420:PXI:H143	2.20	0.41
1:A:325:THR:HG22	1:A:327:GLU:OE1	2.19	0.41
1:B:381:ASP:HB2	1:B:403:ILE:C	2.39	0.41
1:B:372:LEU:HB2	1:B:373:GLU:OE1	2.20	0.41
1:A:119:LEU:O	1:A:123:VAL:HG23	2.20	0.41
1:A:334:ARG:NH2	1:A:335:PHE:O	2.53	0.41
1:B:266:LEU:O	1:B:270:ARG:HG3	2.20	0.41
1:B:272:ASP:HB3	1:B:275:LEU:CD1	2.51	0.41
1:B:254:ASN:ND2	1:B:396:ARG:O	2.48	0.41
1:B:117:GLU:O	1:B:117:GLU:HG3	2.21	0.41
1:A:137:ALA:C	1:A:139:ASP:N	2.74	0.41
1:A:20:LEU:HB3	1:A:24:PHE:HB2	2.03	0.41
1:A:77:SER:HB2	1:A:297:PHE:CD2	2.56	0.41
1:B:224:ASP:C	1:B:226:SER:N	2.74	0.41
1:A:328:ARG:HA	4:A:2113:HOH:O	2.19	0.41
1:B:157:ILE:HG13	1:B:161:LEU:HD12	2.03	0.41
1:A:299:VAL:O	1:A:299:VAL:HG12	2.22	0.41
1:A:116:VAL:HA	4:A:2054:HOH:O	2.21	0.40
1:A:212:ASP:HA	4:A:2064:HOH:O	2.19	0.40
1:A:290:VAL:HG13	3:A:420:PXI:H252	2.02	0.40
1:A:324:ARG:HA	1:A:332:PRO:CB	2.52	0.40
1:A:339:ARG:CZ	4:A:2117:HOH:O	2.67	0.40
1:A:43:ARG:HA	1:A:52:VAL:O	2.21	0.40
1:B:119:LEU:O	1:B:120:ARG:C	2.58	0.40
1:B:201:LEU:O	1:B:205:LYS:HG2	2.21	0.40
1:A:331:ASP:O	1:A:334:ARG:HB3	2.20	0.40
1:A:76:ASN:O	1:A:312:GLY:HA2	2.22	0.40
1:B:273:MET:CE	1:B:276:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLY:O	1:A:344:HIS:C	2.59	0.40
1:B:165:GLU:N	1:B:166:PRO:CD	2.84	0.40
1:B:161:LEU:CD1	1:B:241:LEU:HG	2.52	0.40
1:B:269:LEU:HD11	1:B:276:LEU:HA	2.03	0.40
1:A:175:THR:HG21	1:A:246:GLU:HG2	1.96	0.40
1:A:282:GLU:CA	1:A:282:GLU:OE1	2.70	0.40
1:A:93:LEU:HA	2:A:419:HEM:O1D	2.21	0.40
1:B:48:GLU:HB2	4:B:2011:HOH:O	2.20	0.40
1:B:276:LEU:HD11	1:B:365:ARG:CB	2.52	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	390/436 (89%)	360 (92%)	28 (7%)	2 (0%)	29	13
1	B	391/436 (90%)	350 (90%)	38 (10%)	3 (1%)	19	6
All	All	781/872 (90%)	710 (91%)	66 (8%)	5 (1%)	25	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	382	VAL
1	A	374	ARG
1	B	273	MET
1	A	375	CYS
1	B	343	GLY

### 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	316/355 (89%)	307 (97%)	9 (3%)	43	25
1	B	314/355 (88%)	306 (98%)	8 (2%)	47	29
All	All	630/710 (89%)	613 (97%)	17 (3%)	44	26

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	60	ARG
1	A	106	LEU
1	A	115	ARG
1	A	135	LEU
1	A	176	ASP
1	A	238	HIS
1	A	285	ARG
1	A	334	ARG
1	B	23	ASP
1	B	99	ARG
1	B	182	ASP
1	B	236	MET
1	B	285	ARG
1	B	305	ASP
1	B	334	ARG
1	B	404	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	208	GLN
1	A	250	ASN
1	A	265	GLN

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Mol	Chain	Res	Type
1	A	344	HIS
1	B	22	GLN
1	B	42	HIS
1	B	89	ASN
1	B	188	GLN
1	B	208	GLN
1	B	238	HIS
1	B	265	GLN
1	B	344	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 ⓘ

There are no carbohydrates 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$
2	HEM	B	419	1	27,50,50	1.76	6 (22%)	17,82,82	1.80	6 (35%)
2	HEM	A	419	1	27,50,50	1.87	7 (25%)	17,82,82	1.49	5 (29%)
3	PXI	A	420	-	33,33,33	1.87	7 (21%)	40,47,47	2.08	9 (22%)
3	PXI	B	420	-	33,33,33	2.03	5 (15%)	40,47,47	2.11	12 (30%)

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	419	1	-	0/6/54/54	-
2	HEM	A	419	1	-	1/6/54/54	-
3	PXI	A	420	-	-	16/43/59/59	0/1/2/2
3	PXI	B	420	-	-	15/43/59/59	0/1/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	420	PXI	C19-C21	6.45	1.62	1.51
3	B	420	PXI	C16-C7	5.87	1.63	1.53
3	A	420	PXI	C19-C21	5.70	1.61	1.51
3	A	420	PXI	C16-C7	4.59	1.61	1.53
2	B	419	HEM	C3C-CAC	-4.46	1.38	1.47
2	A	419	HEM	C1A-NA	4.38	1.45	1.36
3	A	420	PXI	C24-C3	4.01	1.63	1.53
3	B	420	PXI	C24-C3	3.85	1.62	1.53
2	A	419	HEM	C4A-NA	3.72	1.43	1.36
2	B	419	HEM	C3B-CAB	-3.52	1.40	1.47
2	A	419	HEM	C3C-CAC	-2.99	1.41	1.47
3	A	420	PXI	C11-C9	2.95	1.57	1.51
2	A	419	HEM	C1B-C2B	2.92	1.49	1.42
3	B	420	PXI	C11-C9	2.85	1.56	1.51
2	B	419	HEM	C1B-C2B	2.64	1.48	1.42
2	B	419	HEM	C1A-NA	2.61	1.41	1.36
2	A	419	HEM	CBC-CAC	2.59	1.46	1.29
3	B	420	PXI	O4-C9	2.53	1.49	1.44
2	A	419	HEM	CBB-CAB	2.51	1.45	1.29
2	A	419	HEM	CMB-C2B	2.37	1.57	1.51
3	A	420	PXI	C5-C4	-2.28	1.46	1.51
2	B	419	HEM	CBB-CAB	2.12	1.43	1.29
3	A	420	PXI	C15-C12	2.06	1.58	1.53
2	B	419	HEM	C4B-NB	2.05	1.40	1.36
3	A	420	PXI	O4-C9	2.01	1.48	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	420	PXI	C3-O1-C4	7.61	129.32	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	420	PXI	C3-O1-C4	6.88	128.21	117.89
3	A	420	PXI	O3-C7-C5	-6.01	100.68	111.14
3	B	420	PXI	O3-C7-C5	-5.49	101.59	111.14
3	B	420	PXI	C7-C5-C4	3.57	117.30	110.01
3	A	420	PXI	C7-C5-C4	3.35	116.86	110.01
2	B	419	HEM	C3B-C4B-NB	3.25	113.41	109.21
3	B	420	PXI	C10-C9-C11	-3.06	108.59	113.40
3	B	420	PXI	O1-C3-C2	2.97	111.67	106.92
2	B	419	HEM	C4A-C3A-C2A	2.93	109.03	107.00
2	B	419	HEM	CMC-C2C-C3C	2.87	130.05	124.68
3	B	420	PXI	C6-C5-C7	-2.85	106.46	112.92
3	B	420	PXI	C25-C24-C23	-2.85	103.10	109.99
2	A	419	HEM	C4A-C3A-C2A	-2.72	105.10	107.00
3	A	420	PXI	O3-C8-O4	2.72	118.26	110.67
3	A	420	PXI	C25-C24-C23	-2.69	103.48	109.99
3	B	420	PXI	C13-N1-C12	-2.59	105.33	113.11
2	A	419	HEM	CMA-C3A-C4A	-2.58	124.49	128.46
3	B	420	PXI	O3-C8-O4	2.57	117.85	110.67
2	B	419	HEM	CAA-C2A-C3A	-2.54	119.95	127.25
3	A	420	PXI	C6-C5-C7	-2.49	107.27	112.92
3	A	420	PXI	C10-C9-C11	-2.47	109.53	113.40
3	A	420	PXI	C13-N1-C12	-2.41	105.87	113.11
3	A	420	PXI	O1-C3-C2	2.28	110.56	106.92
3	B	420	PXI	C19-C21-C22	2.25	123.95	118.29
3	B	420	PXI	C9-C11-C12	-2.25	106.52	110.46
2	B	419	HEM	CMD-C2D-C1D	-2.23	125.03	128.46
2	B	419	HEM	C1D-C2D-C3D	2.15	108.49	107.00
2	A	419	HEM	CBA-CAA-C2A	-2.12	108.58	112.49
3	B	420	PXI	C8-C15-C12	-2.11	105.73	109.19
2	A	419	HEM	CMB-C2B-C3B	2.09	128.59	124.68
2	A	419	HEM	CMC-C2C-C3C	2.09	128.59	124.68

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	420	PXI	C23-C24-C3-O1
3	A	420	PXI	C11-C12-N1-C13
3	A	420	PXI	C11-C12-N1-C14
3	A	420	PXI	C15-C12-N1-C13
3	A	420	PXI	C15-C12-N1-C14
3	A	420	PXI	C16-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
3	B	420	PXI	C23-C24-C3-O1
3	B	420	PXI	C11-C12-N1-C13
3	B	420	PXI	C11-C12-N1-C14
3	B	420	PXI	C15-C12-N1-C13
3	B	420	PXI	C15-C12-N1-C14
3	A	420	PXI	O4-C8-O3-C7
3	B	420	PXI	O4-C8-O3-C7
3	A	420	PXI	C22-C23-C24-C25
3	B	420	PXI	C22-C23-C24-C25
3	B	420	PXI	O6-C21-C22-C23
3	B	420	PXI	C6-C5-C7-O3
3	A	420	PXI	C19-C21-C22-C23
3	B	420	PXI	C19-C21-C22-C23
3	B	420	PXI	C16-C18-C19-C21
3	A	420	PXI	C25-C24-C3-C2
3	A	420	PXI	C25-C24-C3-O1
3	B	420	PXI	C16-C18-C19-C20
3	A	420	PXI	O6-C21-C22-C23
3	A	420	PXI	C23-C24-C3-C2
3	B	420	PXI	C23-C24-C3-C2
2	A	419	HEM	C3A-C2A-CAA-CBA
3	A	420	PXI	C16-C18-C19-C20
3	B	420	PXI	C25-C24-C3-O1
3	A	420	PXI	C17-C16-C18-C19
3	A	420	PXI	C7-C16-C18-C19
3	B	420	PXI	C4-C5-C7-C16

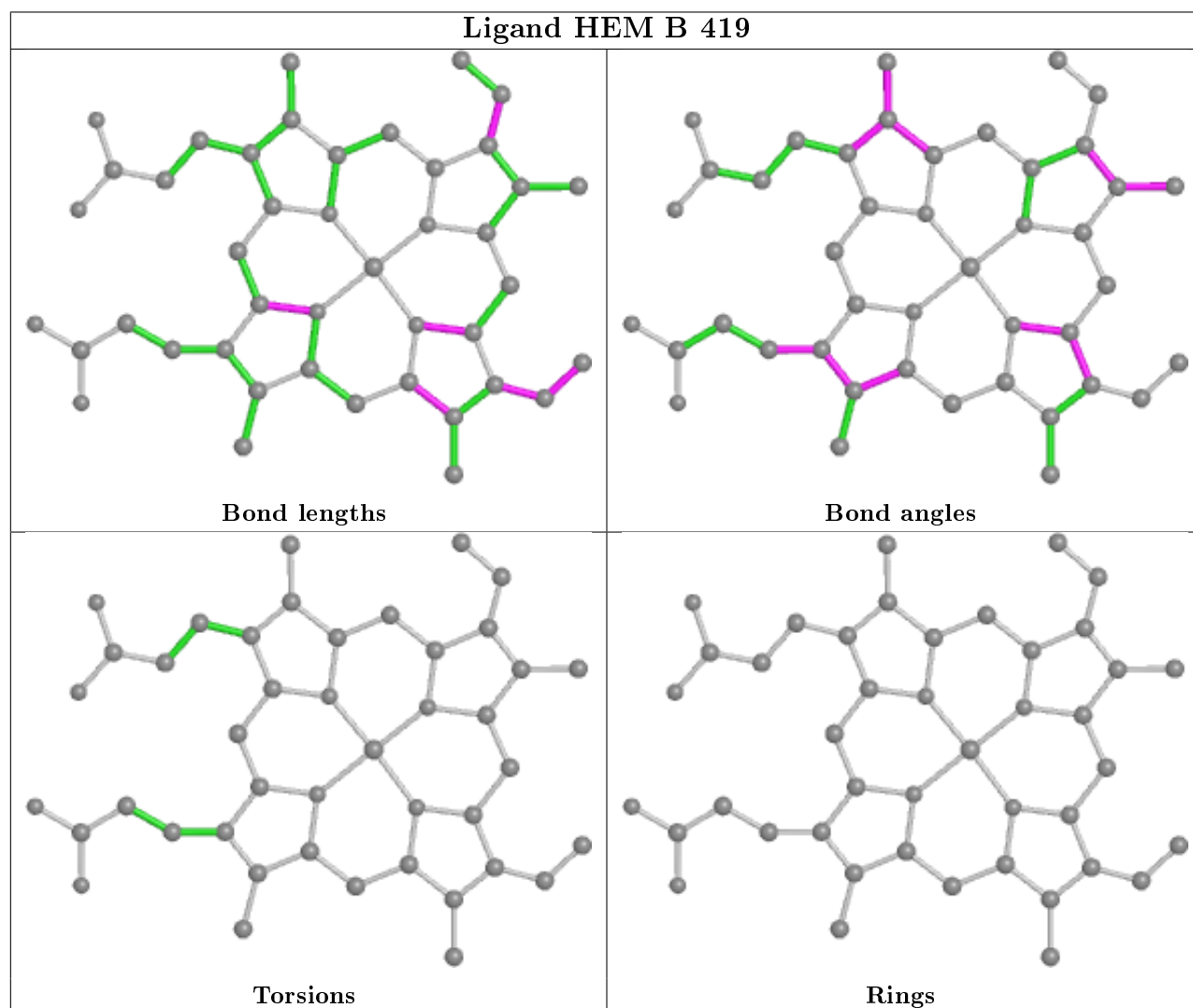
There are no ring outliers.

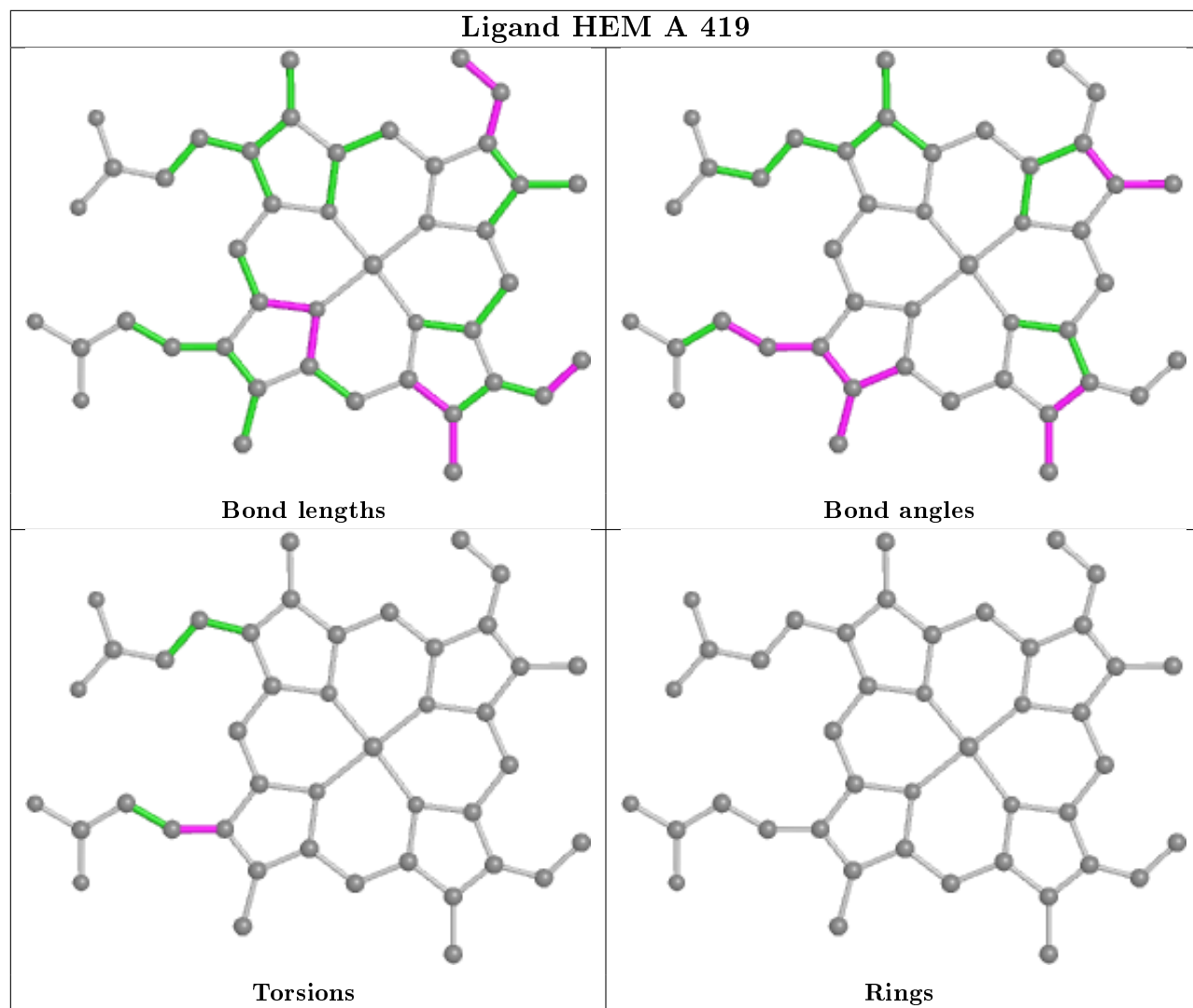
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	419	HEM	2	0
2	A	419	HEM	2	0
3	A	420	PXI	1	0
3	B	420	PXI	5	0

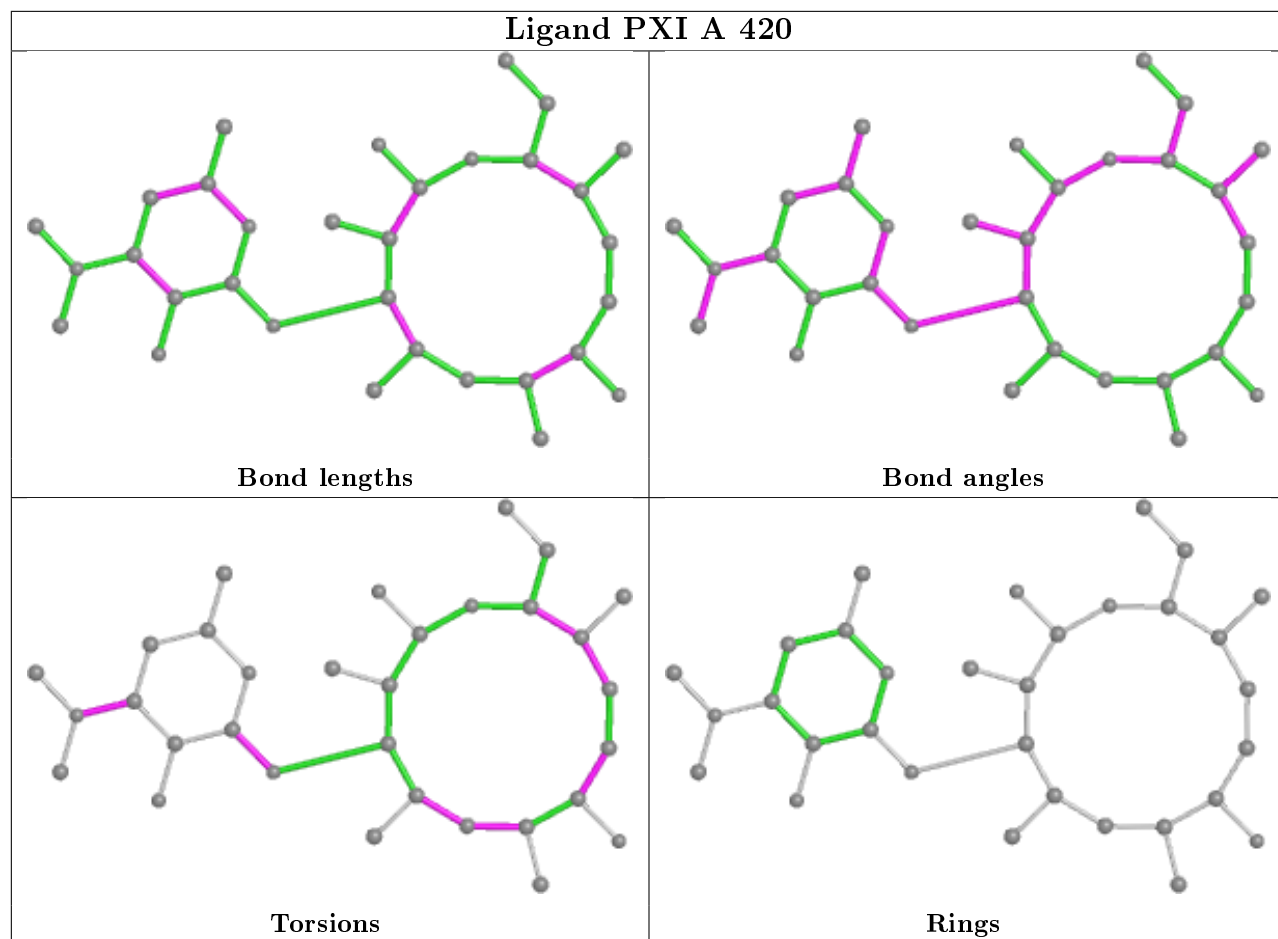
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

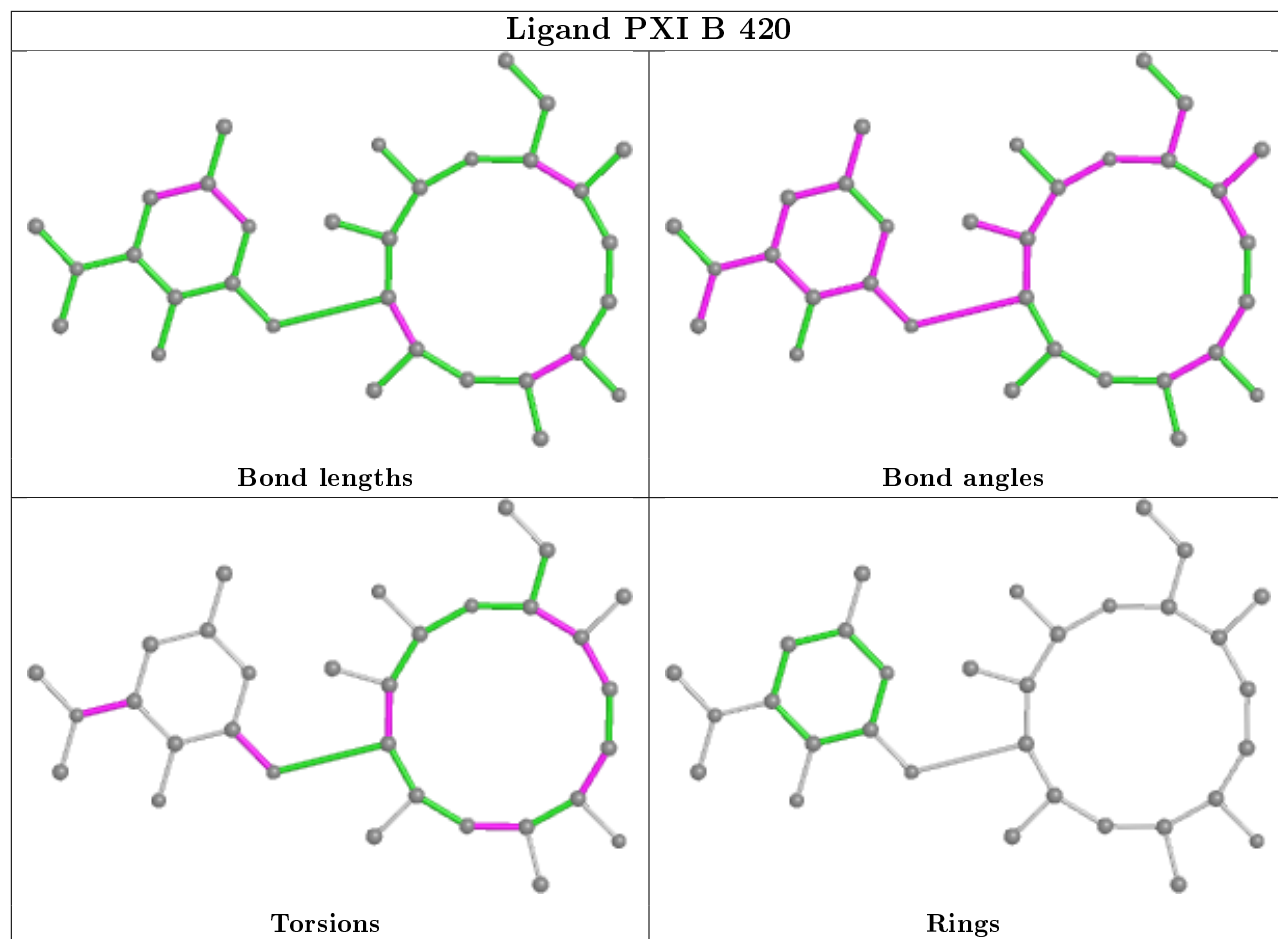
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

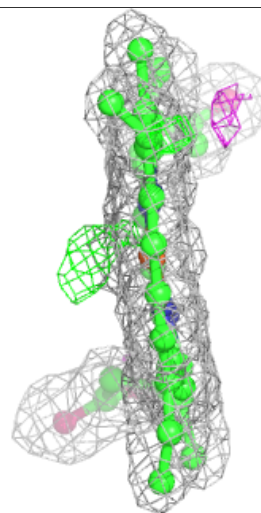
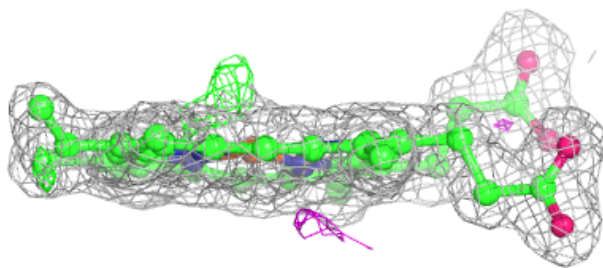
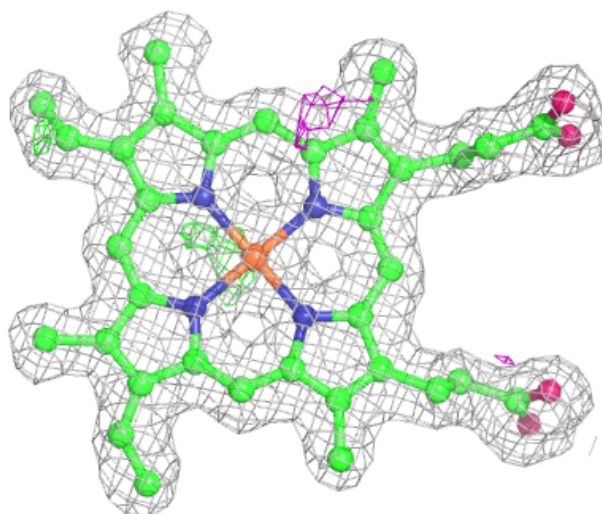
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

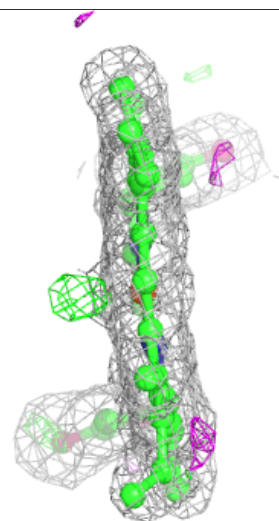
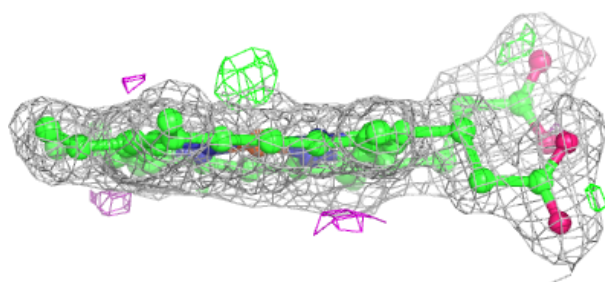
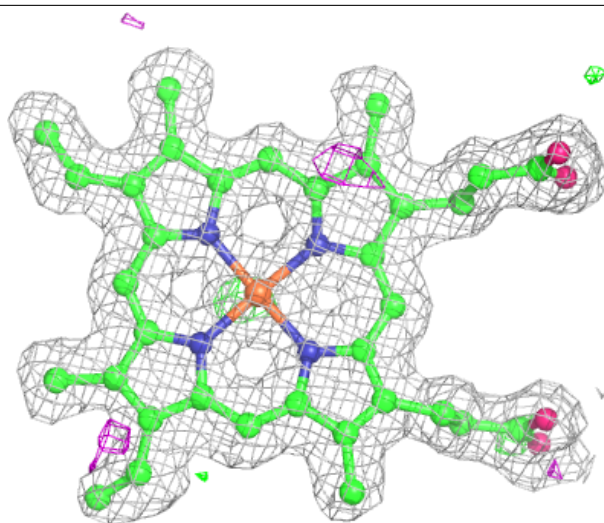
**Electron density around HEM B 419:**

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



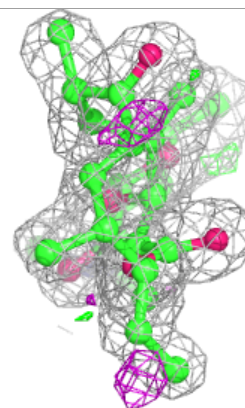
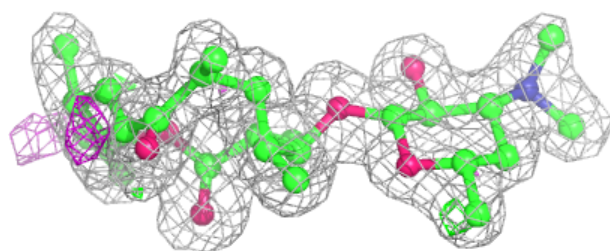
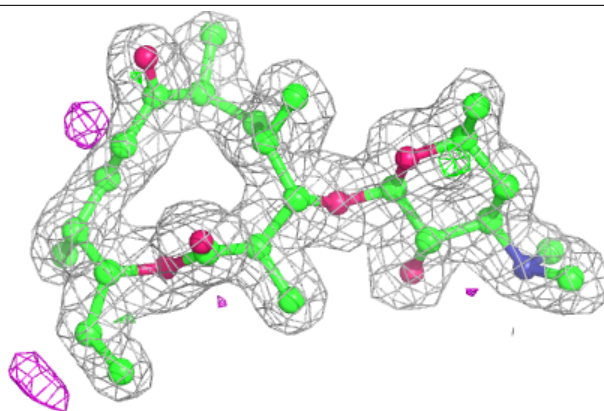
**Electron density around HEM A 419:**

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

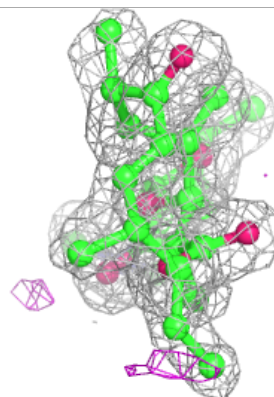
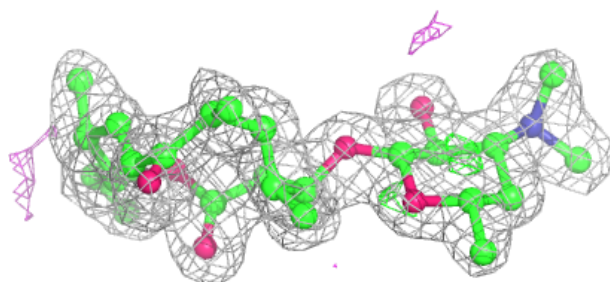
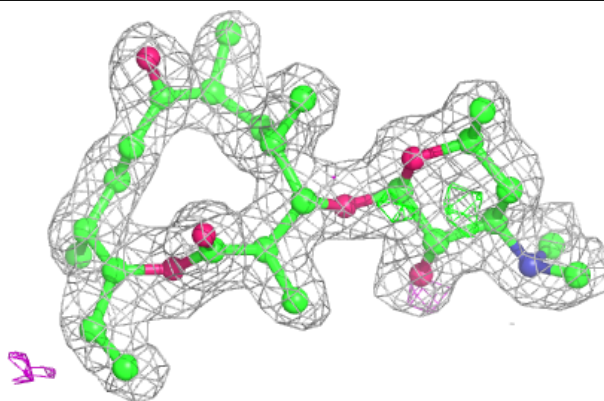


**Electron density around PXI A 420:**

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

**Electron density around PXI B 420:**

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



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.