



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:59 AM UTC

PDB ID : 4B7D / pdb_00004b7d
Title : PikC bound to the 10-DML analog with the 3-(N,N-dimethylamino) propanoate anchoring group
Authors : Podust, L.M.
Deposited on : 2012-08-17
Resolution : 1.89 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

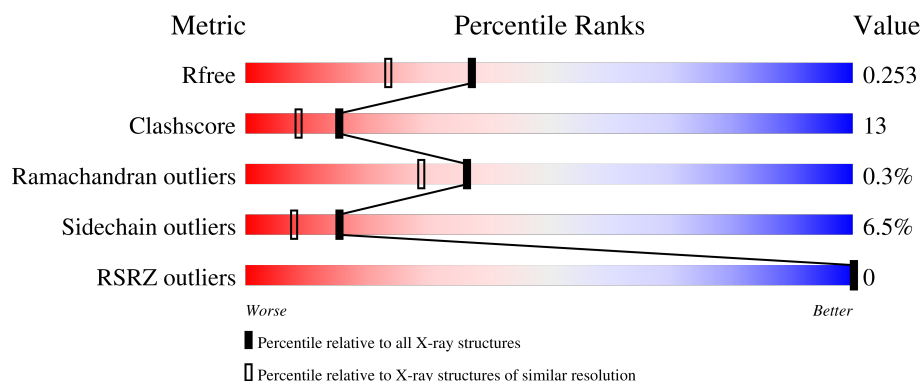
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	B	436	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6719 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 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3038	1919	546	560	13			
1	B	393	Total	C	N	O	S	0	3	0
			3075	1939	554	569	13			

There are 40 discrepancies between the modelled and reference sequences:

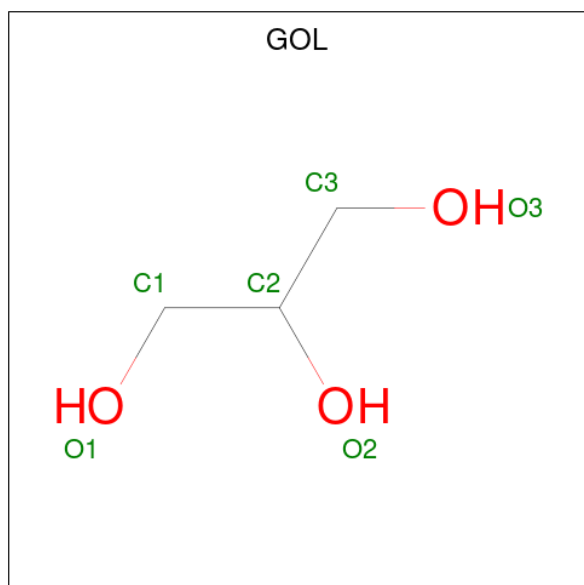
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O87605
A	-18	GLY	-	expression tag	UNP O87605
A	-17	SER	-	expression tag	UNP O87605
A	-16	SER	-	expression tag	UNP O87605
A	-15	HIS	-	expression tag	UNP O87605
A	-14	HIS	-	expression tag	UNP O87605
A	-13	HIS	-	expression tag	UNP O87605
A	-12	HIS	-	expression tag	UNP O87605
A	-11	HIS	-	expression tag	UNP O87605
A	-10	HIS	-	expression tag	UNP O87605
A	-9	SER	-	expression tag	UNP O87605
A	-8	SER	-	expression tag	UNP O87605
A	-7	GLY	-	expression tag	UNP O87605
A	-6	LEU	-	expression tag	UNP O87605
A	-5	VAL	-	expression tag	UNP O87605
A	-4	PRO	-	expression tag	UNP O87605
A	-3	ARG	-	expression tag	UNP O87605
A	-2	GLY	-	expression tag	UNP O87605
A	-1	SER	-	expression tag	UNP O87605
A	0	HIS	-	expression tag	UNP O87605
B	-19	MET	-	expression tag	UNP O87605
B	-18	GLY	-	expression tag	UNP O87605
B	-17	SER	-	expression tag	UNP O87605
B	-16	SER	-	expression tag	UNP O87605
B	-15	HIS	-	expression tag	UNP O87605

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O87605
B	-13	HIS	-	expression tag	UNP O87605
B	-12	HIS	-	expression tag	UNP O87605
B	-11	HIS	-	expression tag	UNP O87605
B	-10	HIS	-	expression tag	UNP O87605
B	-9	SER	-	expression tag	UNP O87605
B	-8	SER	-	expression tag	UNP O87605
B	-7	GLY	-	expression tag	UNP O87605
B	-6	LEU	-	expression tag	UNP O87605
B	-5	VAL	-	expression tag	UNP O87605
B	-4	PRO	-	expression tag	UNP O87605
B	-3	ARG	-	expression tag	UNP O87605
B	-2	GLY	-	expression tag	UNP O87605
B	-1	SER	-	expression tag	UNP O87605
B	0	HIS	-	expression tag	UNP O87605

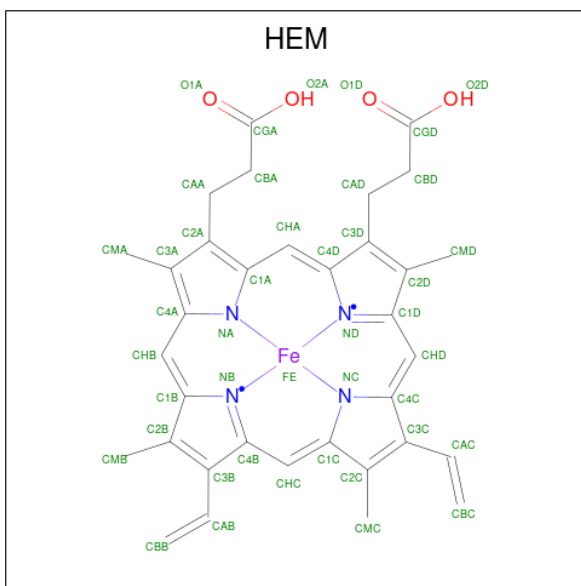
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

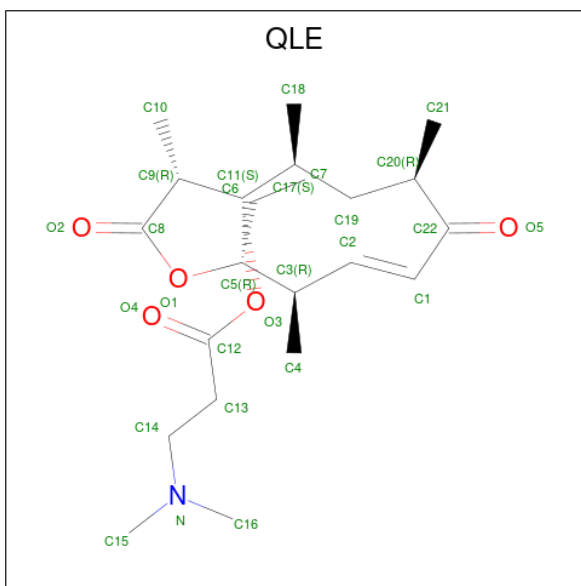
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is [(3R,4S,5S,7R,9E,11R,12R)-12-ethyl-3,5,7,11-tetramethyl-2,8-bis(oxidanylidene)-1-oxacyclododec-9-en-4-yl] 3-(dimethylamino)propanoate (CCD ID: QLE) (formula: $C_{22}H_{37}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	22	1	5		
4	B	1	Total	C	N	O	0	0
			28	22	1	5		

- Molecule 5 is water.

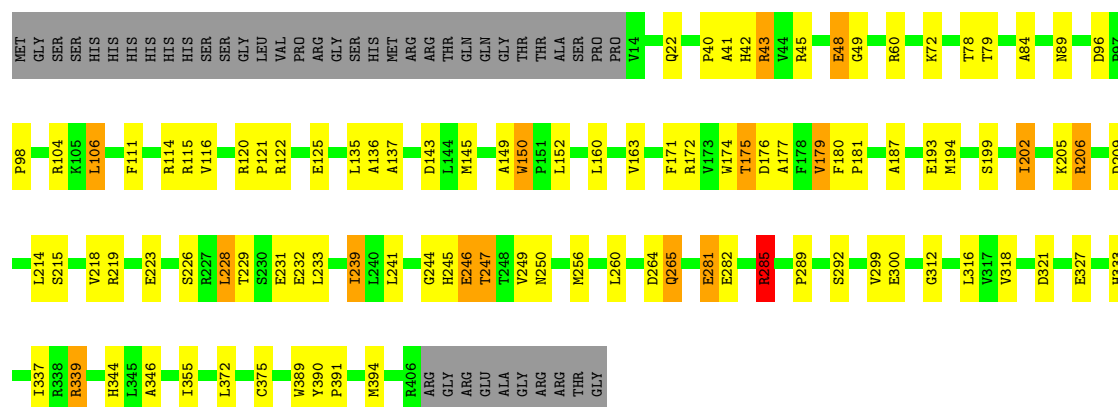
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		
5	B	220	Total	O	0	0
			220	220		

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.

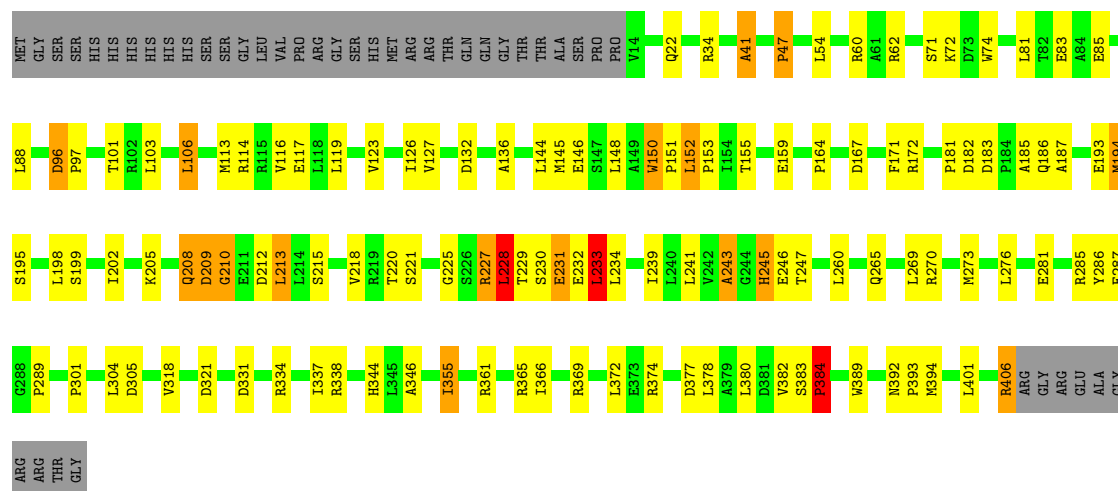
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain A: 



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	36.77Å 58.04Å 96.42Å 79.96° 79.52° 88.73°	Depositor
Resolution (Å)	93.37 – 1.89 93.37 – 1.89	Depositor EDS
% Data completeness (in resolution range)	93.9 (93.37-1.89) 93.9 (93.37-1.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.257 0.199 , 0.253	Depositor DCC
R_{free} test set	2967 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.188 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6719	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, QLE, HEM

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	1.30	6/3109 (0.2%)	1.29	25/4244 (0.6%)
1	B	1.33	9/3146 (0.3%)	1.26	12/4292 (0.3%)
All	All	1.31	15/6255 (0.2%)	1.27	37/8536 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	ILE	CA-CB	8.26	1.65	1.54
1	B	331	ASP	C-O	-7.48	1.20	1.23
1	B	245	HIS	CA-C	6.30	1.55	1.52
1	A	250	ASN	C-O	-6.15	1.16	1.24
1	A	152	LEU	CA-C	6.07	1.59	1.52
1	B	150	TRP	CA-C	5.84	1.59	1.52
1	B	355	ILE	CA-CB	5.75	1.62	1.54
1	B	243	ALA	CA-CB	-5.42	1.44	1.53
1	B	285	ARG	C-O	5.41	1.30	1.24
1	A	239	ILE	CA-CB	5.37	1.60	1.54
1	B	338	ARG	N-CA	5.26	1.52	1.46
1	A	281	GLU	C-O	-5.26	1.18	1.24
1	A	316	LEU	N-CA	5.15	1.52	1.46
1	A	209	ASP	CA-C	5.06	1.59	1.53
1	B	97	PRO	CA-C	5.01	1.54	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	NE-CZ-NH2	-8.71	111.36	119.20
1	A	96	ASP	CA-C-N	-7.65	114.08	119.66
1	A	96	ASP	C-N-CA	-7.65	114.08	119.66
1	A	375	CYS	CA-C-N	-7.40	112.36	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	CYS	C-N-CA	-7.40	112.36	119.76
1	A	48	GLU	N-CA-C	6.92	121.17	112.87
1	B	152	LEU	CA-C-N	-6.90	111.22	119.84
1	B	152	LEU	C-N-CA	-6.90	111.22	119.84
1	A	89	ASN	N-CA-C	6.58	120.91	113.01
1	A	150	TRP	CA-C-N	-6.52	112.28	119.19
1	A	150	TRP	C-N-CA	-6.52	112.28	119.19
1	B	209	ASP	N-CA-C	6.31	120.10	111.39
1	B	123	VAL	N-CA-C	-6.21	104.45	110.72
1	A	300	GLU	CA-C-N	-5.86	113.73	119.76
1	A	300	GLU	C-N-CA	-5.86	113.73	119.76
1	A	199	SER	N-CA-C	-5.76	104.90	111.07
1	A	299	VAL	N-CA-C	-5.74	104.92	110.72
1	B	210	GLY	N-CA-C	5.71	119.84	112.54
1	A	79	THR	CA-C-N	-5.67	114.09	119.76
1	A	79	THR	C-N-CA	-5.67	114.09	119.76
1	A	285	ARG	CB-CG-CD	-5.52	98.61	111.30
1	A	246	GLU	N-CA-C	5.50	120.39	111.37
1	A	285	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	228	LEU	N-CA-C	5.45	117.10	107.61
1	B	233	LEU	N-CA-C	-5.38	104.84	111.40
1	A	206	ARG	CB-CA-C	-5.37	103.19	109.80
1	A	179	VAL	CB-CA-C	5.37	118.70	111.94
1	A	285	ARG	CG-CD-NE	-5.28	100.38	112.00
1	B	41	ALA	N-CA-C	5.26	118.00	108.69
1	B	132	ASP	CB-CA-C	-5.21	102.09	110.74
1	A	209	ASP	N-CA-C	5.17	118.56	111.54
1	B	228	LEU	N-CA-C	5.16	115.97	107.20
1	B	96	ASP	CA-C-N	-5.09	115.94	119.66
1	B	96	ASP	C-N-CA	-5.09	115.94	119.66
1	B	136	ALA	N-CA-C	-5.09	107.02	113.18
1	A	247	THR	CB-CA-C	-5.05	102.40	110.79
1	A	265	GLN	N-CA-C	-5.01	105.48	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3038	0	2998	75	0
1	B	3075	0	3045	88	0
2	A	6	0	8	1	0
2	B	12	0	16	2	0
3	A	43	0	30	9	0
3	B	43	0	30	3	0
4	A	28	0	37	10	0
4	B	28	0	37	6	0
5	A	226	0	0	6	0
5	B	220	0	0	13	0
All	All	6719	0	6201	168	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 13.

All (168) 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:394:MET:HE2	4:A:1408:QLE:C21	1.85	1.05
1:A:171:PHE:HD1	1:A:194:MET:HE2	1.26	0.98
1:A:264:ASP:HB2	5:A:2167:HOH:O	1.69	0.93
1:B:34:ARG:HD2	5:B:2022:HOH:O	1.69	0.93
1:A:175:THR:HG21	1:A:245:HIS:HE1	1.32	0.91
1:B:394:MET:HE1	2:B:1406:GOL:H12	1.54	0.90
1:A:111:PHE:CE1	3:A:1407:HEM:HBC1	2.06	0.90
1:A:344:HIS:HD2	1:A:346:ALA:H	1.18	0.89
1:B:239:ILE:HD12	3:B:1407:HEM:HMD3	1.53	0.87
1:A:171:PHE:CD1	1:A:194:MET:HE2	2.10	0.86
1:B:406:ARG:C	5:B:2219:HOH:O	2.18	0.86
1:A:394:MET:HE2	4:A:1408:QLE:H213	1.57	0.85
1:A:150:TRP:CZ2	1:A:172:ARG:HB2	2.12	0.83
1:A:394:MET:HE2	4:A:1408:QLE:H211	1.59	0.83
1:A:282:GLU:OE1	1:A:285:ARG:HD3	1.78	0.81
1:B:344:HIS:HD2	1:B:346:ALA:H	1.26	0.81
1:B:394:MET:HE2	4:B:1408:QLE:H213	1.65	0.78
1:B:301:PRO:HG3	5:B:2185:HOH:O	1.82	0.77
1:A:104:ARG:NH1	3:A:1407:HEM:O2D	2.18	0.75
1:B:394:MET:HE2	4:B:1408:QLE:C21	2.18	0.73
1:A:43:ARG:HH11	1:A:43:ARG:HB3	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:MET:CE	4:A:1408:QLE:C21	2.67	0.73
1:A:111:PHE:CZ	3:A:1407:HEM:HBC1	2.24	0.72
1:A:344:HIS:CD2	1:A:346:ALA:H	2.07	0.71
1:B:221:SER:O	1:B:225:GLY:HA2	1.90	0.71
1:A:394:MET:CE	4:A:1408:QLE:H213	2.23	0.69
1:B:22:GLN:HE22	1:B:389:TRP:H	1.39	0.67
1:A:163:VAL:HG11	1:A:171:PHE:HE2	1.59	0.67
1:B:229:THR:HB	1:B:232:GLU:HG3	1.77	0.66
1:B:144:LEU:HD23	1:B:401:LEU:HD23	1.78	0.65
1:A:256:MET:O	1:A:260:LEU:HG	1.97	0.65
1:A:22:GLN:HE22	1:A:389:TRP:H	1.46	0.64
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.80	0.63
1:A:175:THR:HG21	1:A:245:HIS:CE1	2.24	0.63
1:B:229:THR:HG22	1:B:230:SER:N	2.13	0.63
1:A:111:PHE:CE1	3:A:1407:HEM:CBC	2.81	0.62
1:B:273:MET:O	1:B:273:MET:HG3	2.00	0.62
1:B:247[A]:THR:HG21	4:B:1408:QLE:HA	1.79	0.62
1:B:227[A]:ARG:HB2	1:B:227[A]:ARG:HH11	1.66	0.61
1:A:394:MET:CE	4:A:1408:QLE:H211	2.30	0.61
1:B:227[A]:ARG:HH11	1:B:227[A]:ARG:CB	2.14	0.60
1:B:228:LEU:HD12	1:B:232:GLU:HB2	1.82	0.60
1:A:282:GLU:OE1	1:A:285:ARG:CD	2.49	0.59
1:A:205:LYS:HD2	1:A:215[A]:SER:OG	2.01	0.59
1:B:113:MET:O	1:B:117:GLU:HB2	2.03	0.58
1:B:220:THR:HG23	1:B:227[A]:ARG:HH12	1.68	0.58
1:A:40:PRO:HB2	1:A:60:ARG:HG2	1.85	0.58
1:A:163:VAL:HG11	1:A:171:PHE:CE2	2.39	0.58
1:B:60:ARG:NH2	1:B:305:ASP:HB2	2.19	0.57
1:B:85:GLU:HB3	4:B:1408:QLE:H163	1.85	0.57
1:B:334:ARG:HH11	1:B:334:ARG:HG3	1.70	0.56
1:B:146:GLU:OE2	1:B:172:ARG:NH2	2.35	0.56
1:A:181:PRO:HG3	1:A:187:ALA:HB2	1.87	0.56
1:B:210:GLY:CA	5:B:2140:HOH:O	2.54	0.55
1:B:183:ASP:OD2	1:B:185:ALA:HB3	2.06	0.55
1:B:212:ASP:OD1	1:B:212:ASP:C	2.49	0.55
1:B:60:ARG:HH22	1:B:305:ASP:HB2	1.71	0.55
1:B:164:PRO:HG2	1:B:167:ASP:OD2	2.06	0.55
1:B:213:LEU:O	1:B:213:LEU:HD12	2.07	0.55
1:A:116:VAL:HG12	5:A:2102:HOH:O	2.07	0.55
1:B:241:LEU:O	1:B:245:HIS:HB3	2.07	0.55
1:A:48:GLU:HG3	5:A:2040:HOH:O	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD23	1:A:233:LEU:HD13	1.90	0.54
1:B:88:LEU:HD21	1:B:195:SER:OG	2.07	0.54
1:B:171:PHE:CD1	1:B:194:MET:HE2	2.42	0.54
1:B:406:ARG:CZ	1:B:406:ARG:HB3	2.35	0.54
1:A:43:ARG:HB3	1:A:43:ARG:NH1	2.21	0.53
1:A:163:VAL:CG1	1:A:171:PHE:HE2	2.20	0.53
1:A:145:MET:HA	1:A:149:ALA:HB3	1.91	0.53
1:A:122:ARG:NH1	1:A:125:GLU:OE1	2.41	0.52
1:A:78:THR:HG23	1:A:312:GLY:HA3	1.92	0.52
1:B:289:PRO:HG2	3:B:1407:HEM:HMB2	1.92	0.52
1:B:227[A]:ARG:CB	1:B:227[A]:ARG:NH1	2.73	0.51
1:A:171:PHE:O	1:A:175:THR:HB	2.09	0.51
1:A:174:TRP:NE1	1:A:193:GLU:HG2	2.26	0.51
1:B:361:ARG:O	1:B:365:ARG:HG3	2.10	0.51
1:B:182:ASP:HB2	1:B:186:GLN:OE1	2.10	0.51
1:A:333:HIS:HE1	5:A:2022:HOH:O	1.93	0.51
1:A:265:GLN:NE2	1:A:337:ILE:H	2.09	0.50
1:A:202:ILE:HG13	1:A:214:LEU:HD11	1.94	0.50
1:B:74:TRP:CD2	1:B:81:LEU:HD21	2.46	0.50
1:B:229:THR:CG2	1:B:230:SER:N	2.75	0.50
1:B:265:GLN:NE2	1:B:337:ILE:HG12	2.27	0.50
1:A:175:THR:CG2	1:A:246:GLU:OE1	2.60	0.49
1:A:228:LEU:CD2	1:A:233:LEU:HD13	2.42	0.49
1:A:244:GLY:HA2	3:A:1407:HEM:HMC2	1.93	0.49
1:B:208:GLN:HB2	5:B:2078:HOH:O	2.11	0.49
1:B:182:ASP:CB	1:B:186:GLN:OE1	2.60	0.49
1:B:181:PRO:HB3	1:B:187:ALA:HB2	1.94	0.49
3:A:1407:HEM:C2D	4:A:1408:QLE:H71C	2.47	0.49
1:B:155:THR:O	1:B:159:GLU:HG3	2.12	0.49
1:B:392:ASN:N	5:B:2218:HOH:O	2.45	0.49
1:A:174:TRP:HB2	1:A:194:MET:HE3	1.94	0.48
1:A:318:VAL:HG12	1:A:321:ASP:H	1.78	0.48
4:B:1408:QLE:H9	4:B:1408:QLE:H192	1.69	0.48
1:A:106:LEU:CD2	1:A:228:LEU:HD13	2.43	0.48
1:B:183:ASP:OD1	1:B:186:GLN:HB2	2.14	0.48
1:B:71:SER:OG	1:B:96:ASP:OD2	2.27	0.47
1:B:127:VAL:HG21	1:B:366:ILE:HG22	1.95	0.47
1:B:198:LEU:O	1:B:202:ILE:HG13	2.14	0.47
1:B:227[A]:ARG:NH1	1:B:227[A]:ARG:HB3	2.29	0.47
1:B:318:VAL:HG12	1:B:321:ASP:H	1.79	0.47
1:A:45:ARG:HB2	1:A:45:ARG:CZ	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HD11	3:A:1407:HEM:HMD2	1.96	0.47
1:A:179:VAL:HG12	1:A:180:PHE:CZ	2.50	0.47
1:B:243:ALA:HA	1:B:247[A]:THR:HG23	1.96	0.47
1:B:265:GLN:NE2	1:B:337:ILE:H	2.14	0.46
1:B:229:THR:HG22	1:B:231:GLU:H	1.80	0.46
1:B:269:LEU:HD11	1:B:276:LEU:HA	1.97	0.46
1:B:334:ARG:HG3	1:B:334:ARG:NH1	2.30	0.46
1:B:106:LEU:CD2	1:B:228:LEU:HD22	2.46	0.46
1:B:281:GLU:OE1	1:B:344:HIS:HE1	1.98	0.46
1:B:383[B]:SER:O	1:B:384:PRO:C	2.59	0.46
1:B:286:TYR:CD2	1:B:287:GLU:HG2	2.52	0.45
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.99	0.45
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.85	0.45
1:A:98:PRO:HD2	5:A:2091:HOH:O	2.17	0.45
1:A:202:ILE:HG23	1:A:218:VAL:HG22	1.99	0.45
3:A:1407:HEM:C3D	4:A:1408:QLE:H71C	2.52	0.45
1:B:205:LYS:HD2	1:B:215:SER:OG	2.17	0.45
1:A:41:ALA:C	1:A:42:HIS:CD2	2.95	0.45
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.98	0.45
1:B:210:GLY:HA3	5:B:2140:HOH:O	2.17	0.44
1:A:135:LEU:O	1:A:137:ALA:N	2.50	0.44
3:B:1407:HEM:HMB2	3:B:1407:HEM:HBB2	1.99	0.44
1:A:390:TYR:HA	1:A:391:PRO:HD3	1.91	0.44
1:B:304:LEU:O	1:B:305:ASP:C	2.60	0.44
1:B:41:ALA:HA	1:B:54:LEU:O	2.17	0.44
1:A:229:THR:OG1	1:A:232:GLU:HG3	2.18	0.44
1:B:34:ARG:NH2	5:B:2023:HOH:O	2.51	0.44
1:A:150:TRP:CE3	1:A:249:VAL:HG21	2.53	0.43
1:B:234:LEU:HA	1:B:234:LEU:HD12	1.74	0.43
1:A:344:HIS:CD2	1:A:344:HIS:C	2.97	0.43
1:B:270:ARG:NH1	5:B:2159:HOH:O	2.50	0.43
1:B:119:LEU:HD23	5:B:2106:HOH:O	2.19	0.43
1:B:273:MET:HG2	1:B:369:ARG:CZ	2.48	0.43
1:B:374:ARG:HD3	5:B:2112:HOH:O	2.18	0.42
1:A:84:ALA:HA	5:A:2037:HOH:O	2.19	0.42
1:A:285:ARG:HD2	1:A:339:ARG:HD2	2.01	0.42
1:B:245:HIS:CG	1:B:246:GLU:N	2.87	0.42
1:A:143:ASP:OD1	1:A:143:ASP:C	2.62	0.42
1:B:270:ARG:HH12	1:B:377:ASP:HA	1.85	0.42
1:A:45:ARG:HD3	1:A:49:GLY:HA2	2.01	0.42
1:B:383[A]:SER:O	1:B:384:PRO:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1408:QLE:H43C	4:A:1408:QLE:H1	1.78	0.42
1:B:145:MET:HE2	1:B:145:MET:HB2	1.47	0.42
1:B:150:TRP:CE3	1:B:151:PRO:HG3	2.54	0.42
1:A:239:ILE:HD11	4:A:1408:QLE:H102	2.01	0.42
1:A:245:HIS:ND1	1:A:246:GLU:N	2.68	0.42
1:B:193:GLU:O	1:B:194:MET:C	2.63	0.42
1:B:243:ALA:HB2	4:B:1408:QLE:H62C	2.02	0.42
1:A:145:MET:HE2	1:A:145:MET:HB2	1.75	0.41
1:B:103:LEU:O	1:B:106:LEU:HB2	2.21	0.41
1:B:62:ARG:HD3	5:B:2050:HOH:O	2.19	0.41
1:B:394:MET:HE1	2:B:1406:GOL:C1	2.39	0.41
1:B:380:LEU:HD23	1:B:384:PRO:HD3	2.02	0.41
1:A:177:ALA:O	1:A:181:PRO:HB3	2.20	0.41
1:A:394:MET:HE1	2:A:1406:GOL:H31	2.03	0.41
1:B:270:ARG:CZ	5:B:2156:HOH:O	2.68	0.41
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.93	0.41
1:A:174:TRP:CB	1:A:194:MET:HE3	2.51	0.40
1:A:289:PRO:HG2	3:A:1407:HEM:HMB2	2.03	0.40
1:B:47:PRO:HD2	1:B:393:PRO:HD3	2.02	0.40
1:B:260:LEU:HD21	1:B:378:LEU:HG	2.03	0.40
1:A:355:ILE:HD13	1:A:355:ILE:HG21	1.92	0.40
1:B:148:LEU:C	1:B:151:PRO:HD2	2.47	0.40
1:A:135:LEU:C	1:A:137:ALA:N	2.80	0.40
1:A:292:SER:HB2	1:A:394:MET:HA	2.04	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	392/436 (90%)	374 (95%)	17 (4%)	1 (0%)	36 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	394/436 (90%)	372 (94%)	21 (5%)	1 (0%)	36	29
All	All	786/872 (90%)	746 (95%)	38 (5%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
1	B	384	PRO

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	314/355 (88%)	295 (94%)	19 (6%)	17	9
1	B	321/355 (90%)	298 (93%)	23 (7%)	13	6
All	All	635/710 (89%)	593 (93%)	42 (7%)	15	8

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	72	LYS
1	A	106	LEU
1	A	114	ARG
1	A	115	ARG
1	A	160	LEU
1	A	175	THR
1	A	176	ASP
1	A	202	ILE
1	A	206	ARG
1	A	219	ARG
1	A	223	GLU
1	A	226	SER
1	A	231	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	THR
1	A	285	ARG
1	A	327	GLU
1	A	339	ARG
1	A	372	LEU
1	B	47	PRO
1	B	72	LYS
1	B	83	GLU
1	B	101	THR
1	B	106	LEU
1	B	114	ARG
1	B	116	VAL
1	B	194	MET
1	B	199	SER
1	B	208	GLN
1	B	209	ASP
1	B	213	LEU
1	B	218	VAL
1	B	227[A]	ARG
1	B	227[B]	ARG
1	B	228	LEU
1	B	231	GLU
1	B	233	LEU
1	B	355	ILE
1	B	372	LEU
1	B	382	VAL
1	B	384	PRO
1	B	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	265	GLN
1	A	344	HIS
1	A	349	HIS
1	B	22	GLN
1	B	89	ASN
1	B	90	HIS
1	B	188	GLN
1	B	208	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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$
4	QLE	A	1408	-	28,28,28	1.50	2 (7%)	34,38,38	1.91	8 (23%)
2	GOL	A	1406	-	5,5,5	0.73	0	5,5,5	1.03	0
2	GOL	B	1409	-	5,5,5	0.81	0	5,5,5	1.29	0
3	HEM	A	1407	1	50,50,50	2.12	10 (20%)	67,82,82	1.63	11 (16%)
3	HEM	B	1407	1	50,50,50	2.12	11 (22%)	67,82,82	1.68	12 (17%)
4	QLE	B	1408	-	28,28,28	1.35	2 (7%)	34,38,38	1.94	8 (23%)
2	GOL	B	1406	-	5,5,5	0.41	0	5,5,5	1.39	1 (20%)

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
4	QLE	A	1408	-	-	3/44/44/44	0/0/1/1
2	GOL	A	1406	-	-	2/4/4/4	-
2	GOL	B	1409	-	-	2/4/4/4	-
3	HEM	A	1407	1	-	4/14/54/54	-
3	HEM	B	1407	1	-	2/14/54/54	-
4	QLE	B	1408	-	-	6/44/44/44	0/0/1/1
2	GOL	B	1406	-	-	3/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1407	HEM	C3D-C2D	6.78	1.51	1.36
3	A	1407	HEM	FE-ND	6.63	2.15	1.94
3	B	1407	HEM	C3D-C2D	6.39	1.50	1.36
3	B	1407	HEM	FE-ND	5.81	2.12	1.94
4	A	1408	QLE	O1-C8	5.72	1.47	1.34
3	A	1407	HEM	FE-NC	5.62	2.13	1.95
4	B	1408	QLE	O1-C8	5.00	1.45	1.34
3	B	1407	HEM	FE-NB	4.82	2.09	1.94
3	B	1407	HEM	FE-NA	4.26	2.09	1.95
4	A	1408	QLE	O3-C12	4.09	1.45	1.34
3	B	1407	HEM	FE-NC	4.06	2.08	1.95
4	B	1408	QLE	O3-C12	3.78	1.45	1.34
3	A	1407	HEM	FE-NA	3.76	2.07	1.95
3	A	1407	HEM	CMB-C2B	3.67	1.58	1.50
3	A	1407	HEM	FE-NB	3.57	2.05	1.94
3	B	1407	HEM	CMA-C3A	3.07	1.57	1.50
3	A	1407	HEM	CMA-C3A	2.84	1.56	1.50
3	B	1407	HEM	CAB-C3B	2.62	1.54	1.47
3	A	1407	HEM	CMD-C2D	2.54	1.56	1.50
3	B	1407	HEM	CMC-C2C	2.37	1.55	1.50
3	B	1407	HEM	CMB-C2B	2.29	1.55	1.50
3	A	1407	HEM	CMC-C2C	2.28	1.55	1.50
3	B	1407	HEM	C4C-NC	-2.18	1.35	1.39
3	B	1407	HEM	CMD-C2D	2.15	1.55	1.50
3	A	1407	HEM	C4D-C3D	2.15	1.48	1.45

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1407	HEM	C4D-ND-C1D	6.57	112.99	105.21
3	B	1407	HEM	C4D-ND-C1D	6.52	112.93	105.21
4	B	1408	QLE	C13-C14-N	-6.42	104.79	113.50
4	A	1408	QLE	O5-C22-C20	-5.68	111.75	121.40
4	A	1408	QLE	C13-C14-N	-4.75	107.06	113.50
3	B	1407	HEM	CMD-C2D-C1D	4.42	131.94	125.03
4	B	1408	QLE	O1-C8-C9	3.95	119.97	111.53
4	B	1408	QLE	O5-C22-C20	-3.77	114.99	121.40
4	B	1408	QLE	C4-C3-C2	3.74	118.36	109.91
3	A	1407	HEM	CBD-CAD-C3D	-3.68	102.35	112.53
3	B	1407	HEM	O1A-CGA-CBA	-3.64	111.55	123.09
4	A	1408	QLE	O3-C12-C13	3.32	118.67	111.48
4	A	1408	QLE	O1-C8-C9	3.27	118.51	111.53
4	B	1408	QLE	O1-C8-O2	-3.10	118.35	123.95
3	A	1407	HEM	C1B-NB-C4B	3.06	108.83	105.21
3	A	1407	HEM	C4C-C3C-C2C	2.96	109.38	106.81
3	B	1407	HEM	C4C-C3C-C2C	2.84	109.27	106.81
4	A	1408	QLE	O3-C12-O4	-2.73	117.32	123.70
3	A	1407	HEM	C3B-C4B-NB	-2.73	107.51	109.47
3	B	1407	HEM	C4C-NC-C1C	2.70	110.22	105.82
3	B	1407	HEM	C3D-C4D-ND	-2.69	107.22	110.17
4	B	1408	QLE	C3-C2-C1	2.62	133.23	126.30
3	B	1407	HEM	CBD-CAD-C3D	-2.56	105.45	112.53
3	B	1407	HEM	C2A-C1A-NA	-2.51	107.36	110.15
3	A	1407	HEM	CHC-C4B-NB	2.50	127.12	124.42
3	B	1407	HEM	C1B-NB-C4B	2.44	108.09	105.21
3	B	1407	HEM	O2A-CGA-CBA	2.37	121.50	114.00
2	B	1406	GOL	O3-C3-C2	-2.28	100.13	110.38
4	A	1408	QLE	C15-N-C14	-2.27	101.75	110.75
4	B	1408	QLE	C10-C9-C11	-2.25	107.97	113.00
3	B	1407	HEM	C1D-C2D-C3D	-2.20	104.67	106.98
3	A	1407	HEM	O2A-CGA-CBA	2.18	120.89	114.00
4	A	1408	QLE	C3-C2-C1	-2.18	120.54	126.30
4	B	1408	QLE	O3-C12-O4	-2.15	118.67	123.70
3	B	1407	HEM	CHA-C4D-ND	2.14	127.02	124.37
3	A	1407	HEM	C4B-C3B-C2B	2.10	109.21	107.28
3	A	1407	HEM	C4C-NC-C1C	2.08	109.21	105.82
3	A	1407	HEM	CBC-CAC-C3C	-2.06	117.22	127.53
4	A	1408	QLE	C11-C9-C8	2.06	114.09	109.93
3	A	1407	HEM	C3D-C4D-ND	-2.01	107.97	110.17

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1406	GOL	O1-C1-C2-C3
2	B	1406	GOL	O1-C1-C2-C3
2	B	1409	GOL	C1-C2-C3-O3
3	A	1407	HEM	C2C-C3C-CAC-CBC
3	A	1407	HEM	C4C-C3C-CAC-CBC
3	B	1407	HEM	C2C-C3C-CAC-CBC
3	B	1407	HEM	C4C-C3C-CAC-CBC
2	A	1406	GOL	O1-C1-C2-O2
2	B	1406	GOL	O1-C1-C2-O2
2	B	1409	GOL	O2-C2-C3-O3
2	B	1406	GOL	O2-C2-C3-O3
4	A	1408	QLE	C1-C2-C3-C4
4	A	1408	QLE	C12-C13-C14-N
4	B	1408	QLE	O2-C8-O1-C5
3	A	1407	HEM	CAA-CBA-CGA-O2A
3	A	1407	HEM	CAA-CBA-CGA-O1A
4	B	1408	QLE	C12-C13-C14-N
4	B	1408	QLE	C1-C2-C3-C4
4	A	1408	QLE	O2-C8-O1-C5
4	B	1408	QLE	O1-C8-C9-C11
4	B	1408	QLE	C9-C8-O1-C5
4	B	1408	QLE	O2-C8-C9-C11

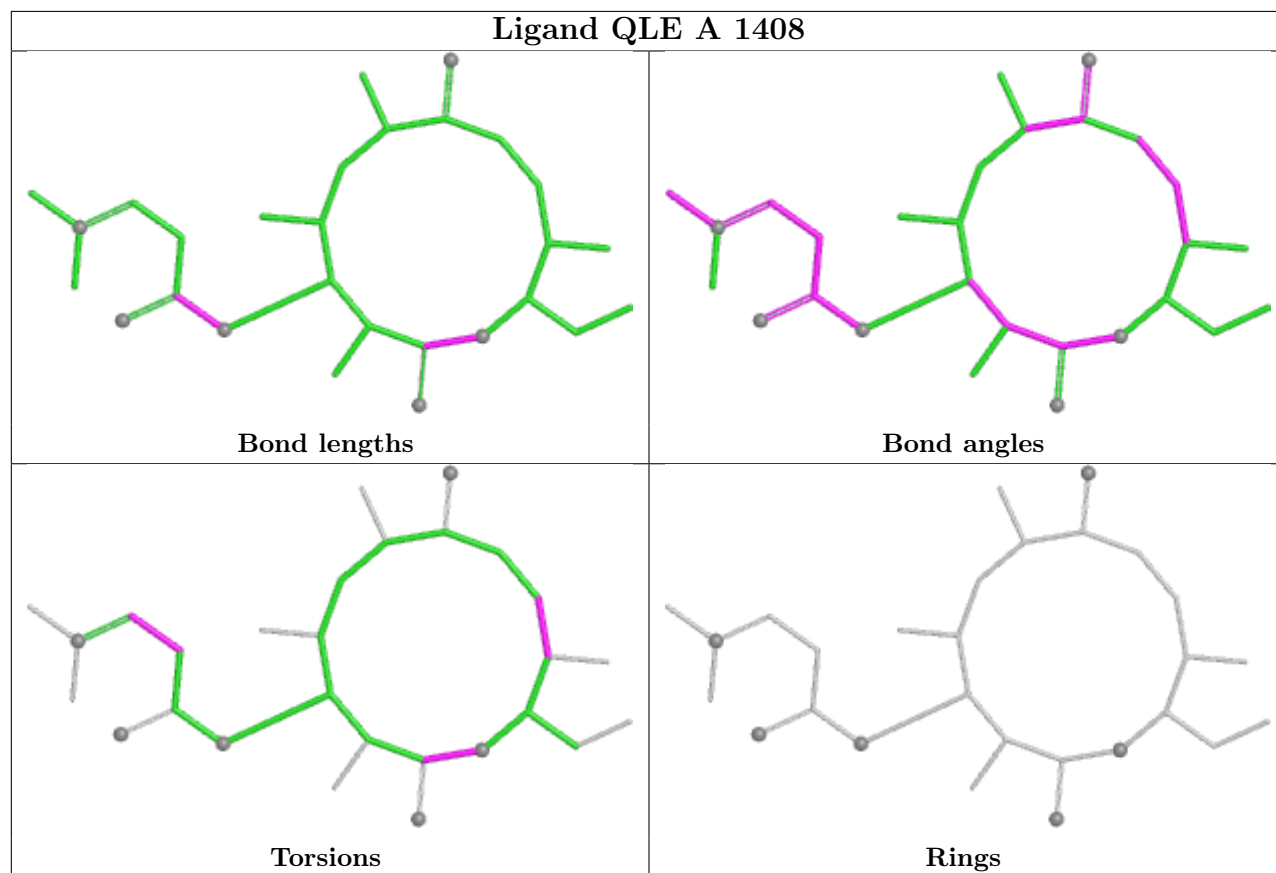
There are no ring outliers.

6 monomers are involved in 29 short contacts:

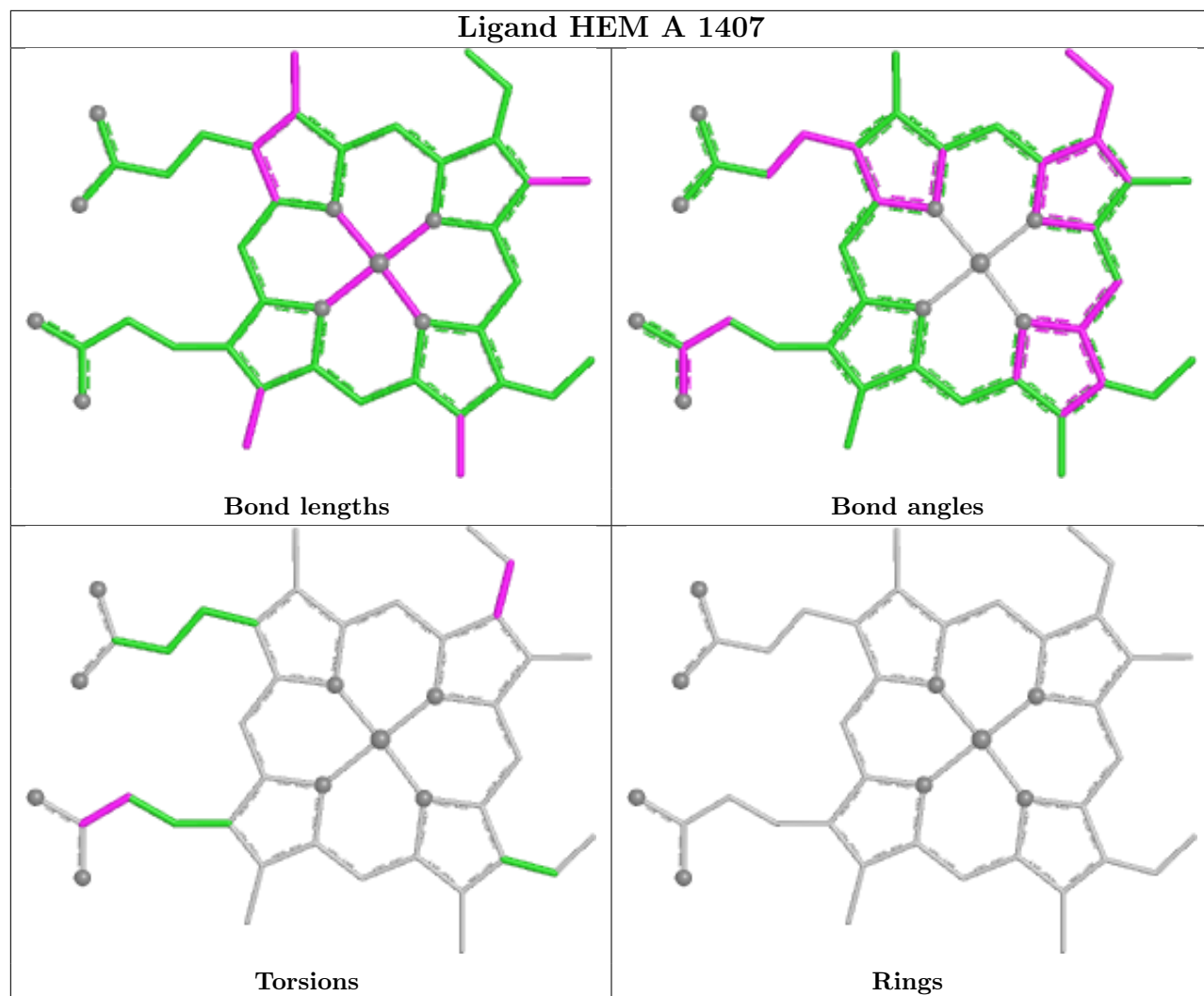
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1408	QLE	10	0
2	A	1406	GOL	1	0
3	A	1407	HEM	9	0
3	B	1407	HEM	3	0
4	B	1408	QLE	6	0
2	B	1406	GOL	2	0

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

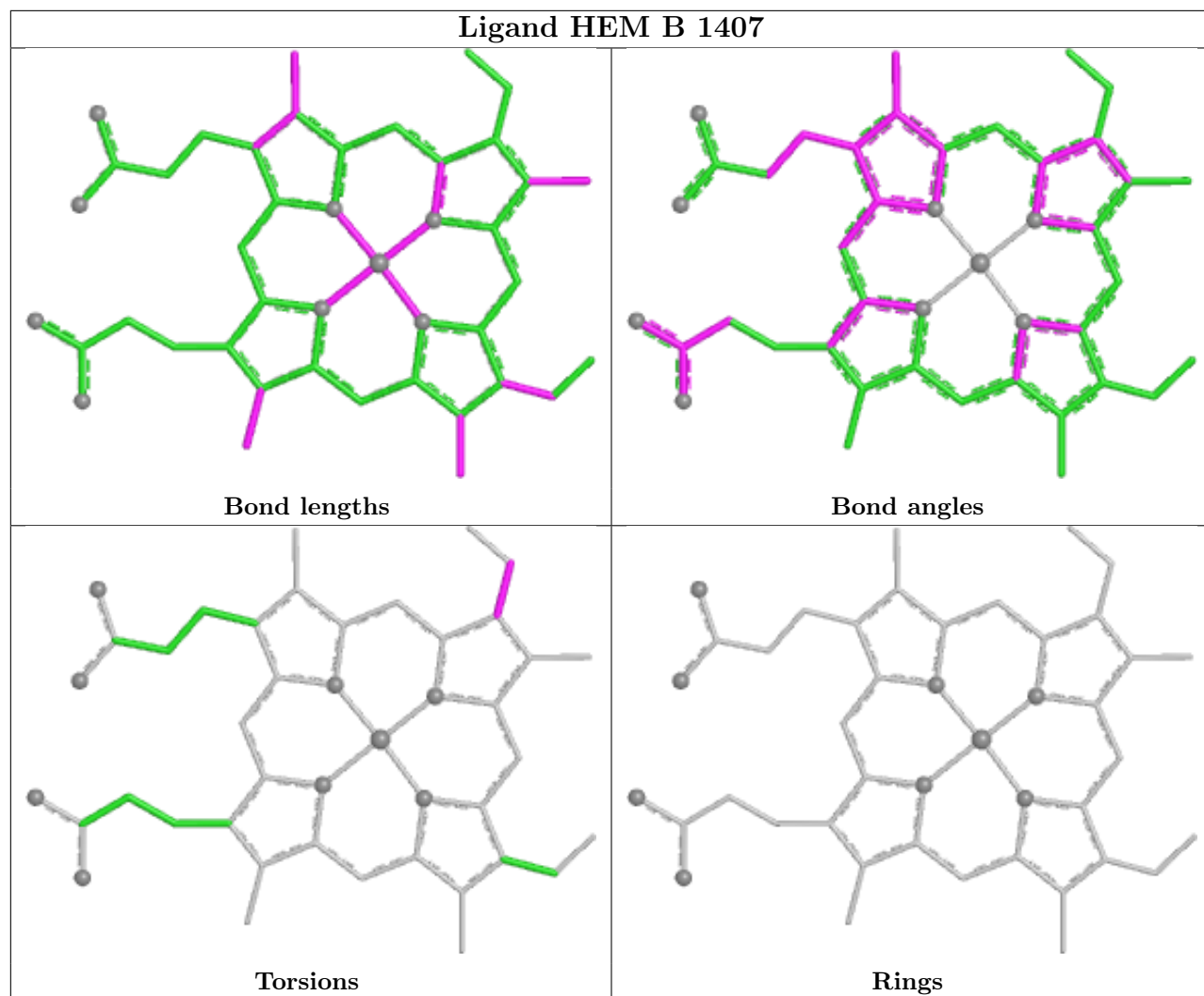
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

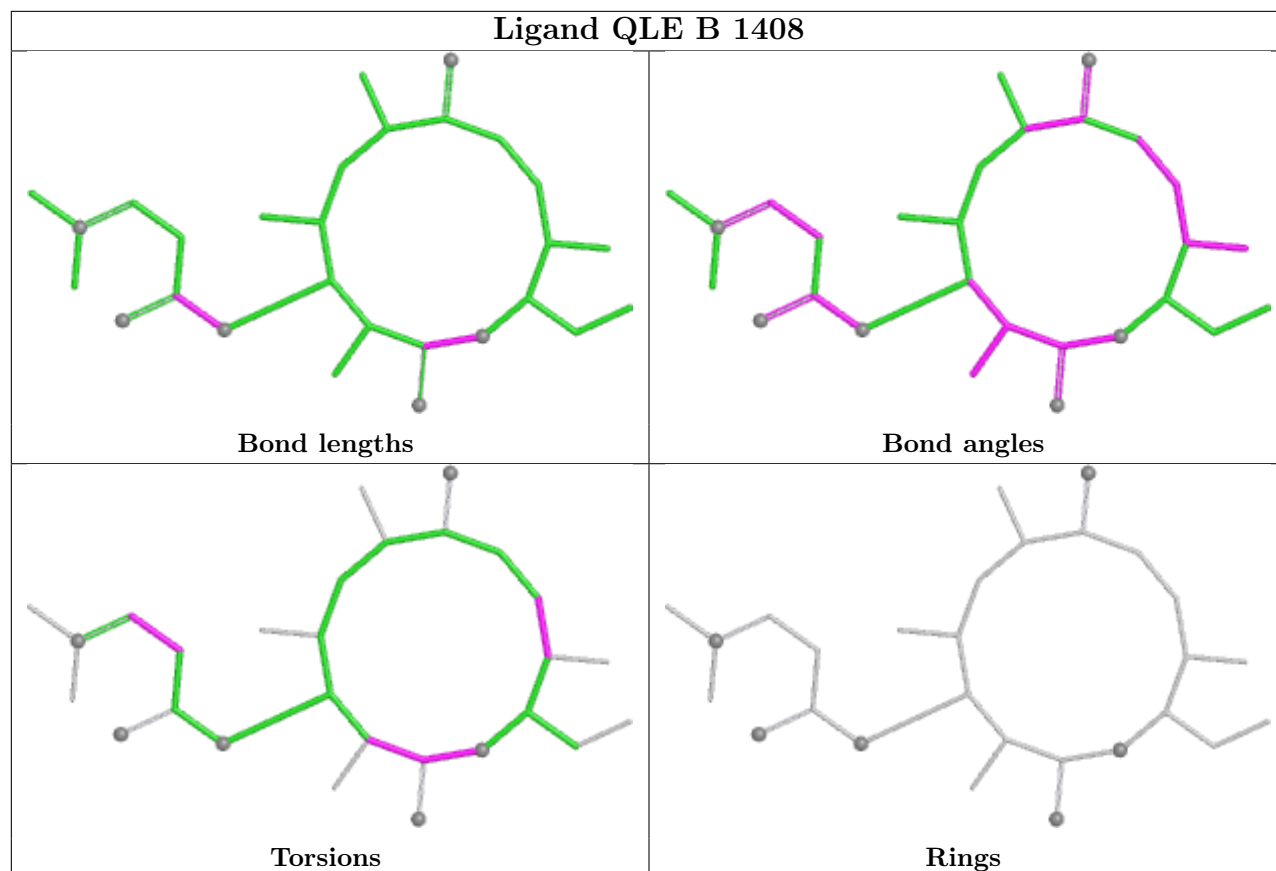


Ligand HEM A 1407



Ligand HEM B 1407





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	393/436 (90%)	-1.29	0 100 100	13, 28, 47, 55	1 (0%)
1	B	393/436 (90%)	-1.26	0 100 100	11, 29, 51, 68	3 (0%)
All	All	786/872 (90%)	-1.28	0 100 100	11, 29, 50, 68	4 (0%)

There are no RSRZ outliers to report.

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](#)

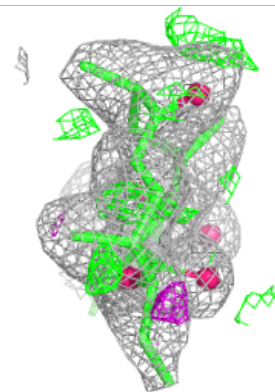
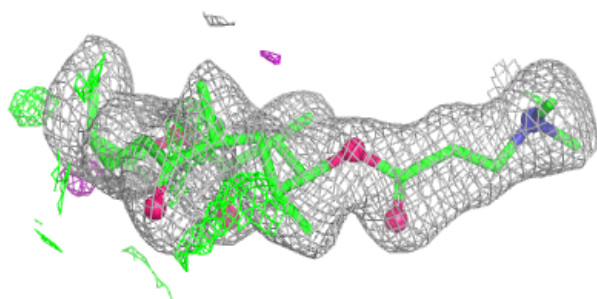
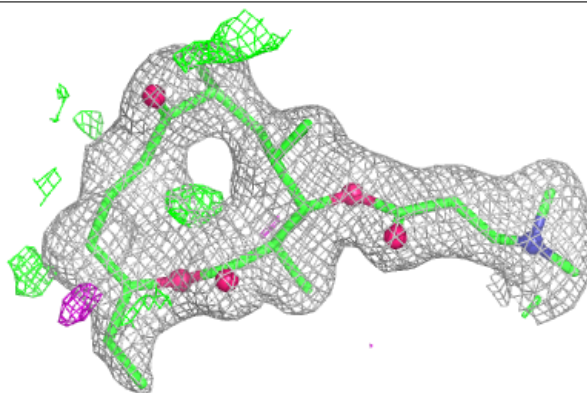
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QLE	A	1408	28/28	0.98	0.04	21,31,35,36	0
2	GOL	B	1406	6/6	0.99	0.04	25,36,38,44	0
2	GOL	B	1409	6/6	0.99	0.03	37,40,41,46	0
2	GOL	A	1406	6/6	0.99	0.05	20,31,37,39	0
4	QLE	B	1408	28/28	0.99	0.03	21,27,32,34	0
3	HEM	A	1407	43/43	1.00	0.02	12,17,21,32	0
3	HEM	B	1407	43/43	1.00	0.02	10,17,20,26	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.

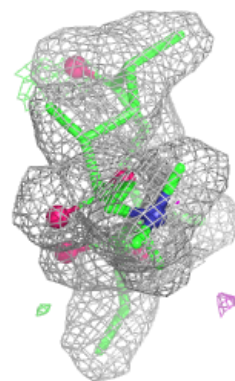
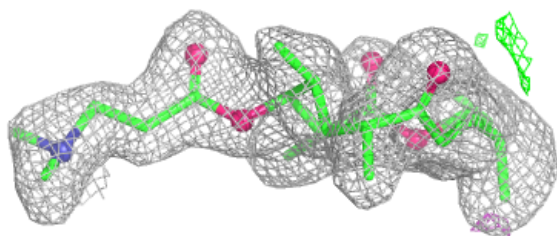
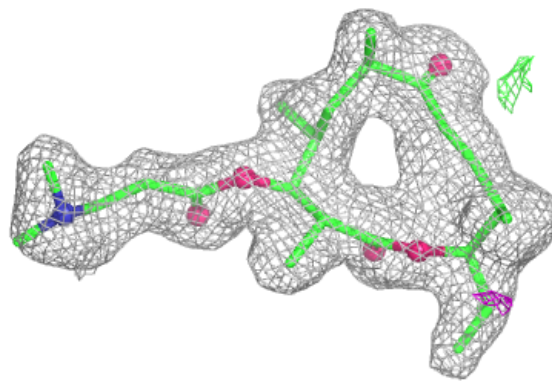
Electron density around QLE A 1408:

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



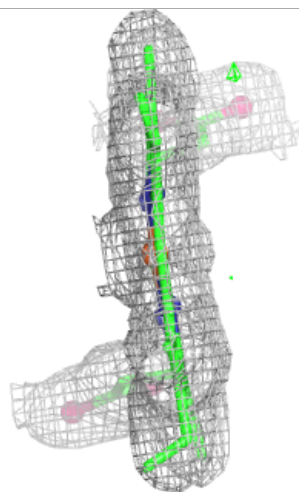
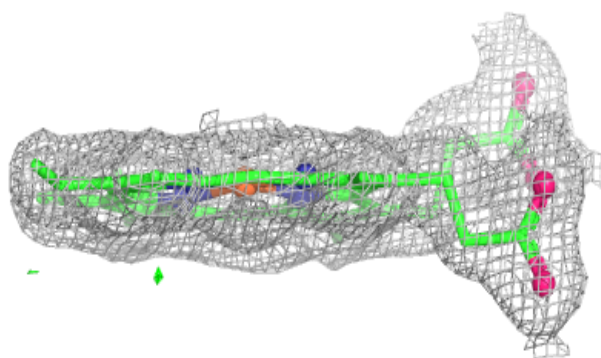
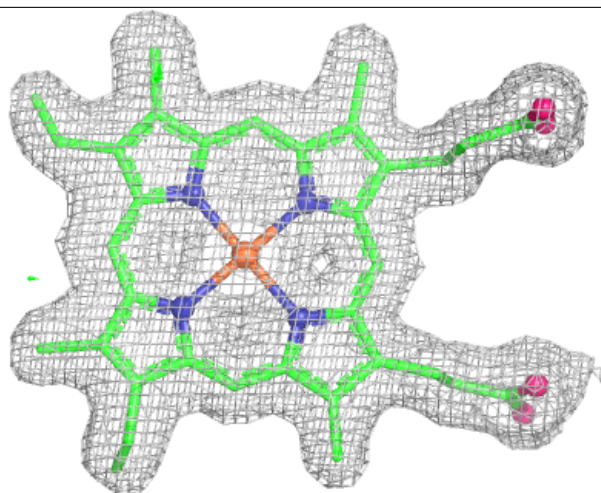
Electron density around QLE B 1408:

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



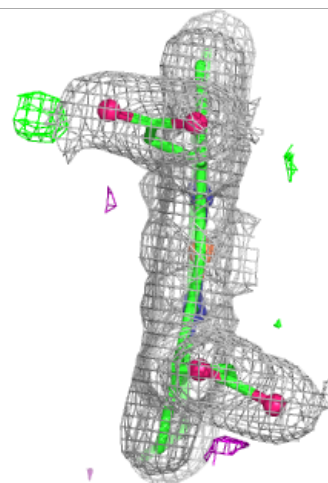
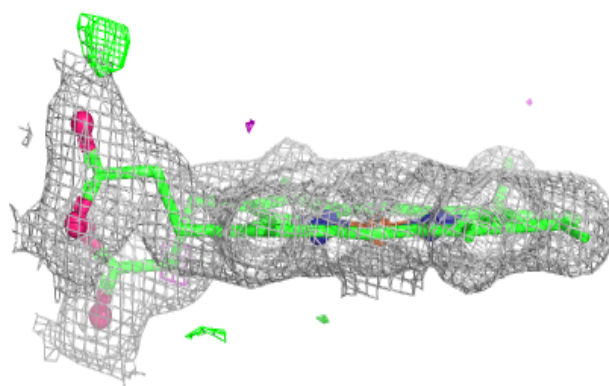
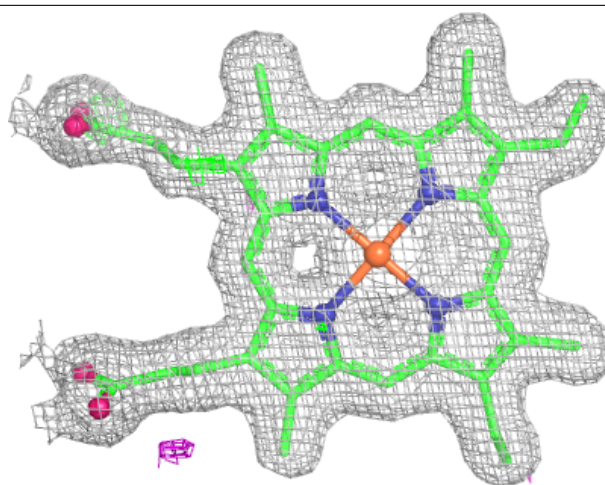
Electron density around HEM A 1407:

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



Electron density around HEM B 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.