



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

PDB ID : 4AC5 / pdb_00004ac5
Title : Lipidic sponge phase crystal structure of the Bl. viridis reaction centre solved using serial femtosecond crystallography
Authors : Johansson, L.C.; Arnlund, D.; White, T.A.; Katona, G.; DePonte, D.P.; Weierstall, U.; Doak, R.B.; Shoeman, R.L.; Lomb, L.; Malmerberg, E.; Davidsson, J.; Nass, K.; Liang, M.; Andreasson, J.; Aquila, A.; Bajt, S.; Barthelmess, M.; Barty, A.; Bogan, M.J.; Bostedt, C.; Bozek, J.D.; Caleman, C.; Coffee, R.; Coppola, N.; Ekeberg, T.; Epp, S.W.; Erk, B.; Fleckenstein, H.; Foucar, L.; Graafsma, H.; Gumprecht, L.; Hajdu, J.; Hampton, C.Y.; Hartmann, R.; Hartmann, A.; Hauser, G.; Hirsemann, H.; Holl, P.; Hunter, M.S.; Kassemeyer, S.; Kimmel, N.; Kirian, R.A.; Maia, F.R.N.C.; Marchesini, S.; Martin, A.V.; Reich, C.; Rolles, D.; Rudek, B.; Rudenko, A.; Schlichting, I.; Schulz, J.; Seibert, M.M.; Sierra, R.; Soltau, H.; Starodub, D.; Stellato, F.; Stern, S.; Struder, L.; Timneanu, N.; Ullrich, J.; Wahlgren, W.Y.; Wang, X.; Weidenspointner, G.; Wunderer, C.; Fromme, P.; Chapman, H.N.; Spence, J.C.H.; Neutze, R.
Deposited on : 2011-12-14
Resolution : 8.20 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>.

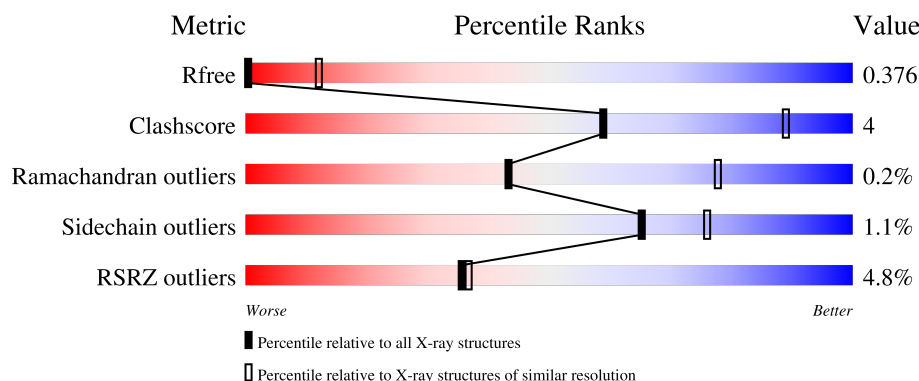
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.20 Å.

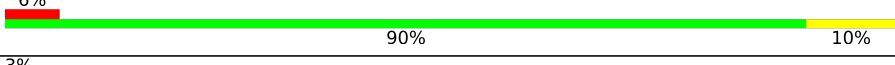
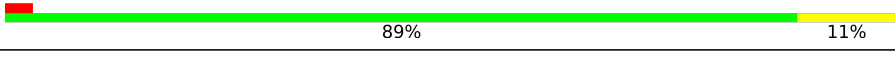
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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.

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

Mol	Chain	Length	Quality of chain
1	C	336	
2	H	258	
3	L	274	
4	M	324	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCB	L	1274	X	-	-	-
6	BCB	L	1275	X	-	-	-
6	BCB	M	1324	X	-	-	-
6	BCB	M	1325	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9835 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 PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2590	1632	464	476	18			

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	243	Total	C	N	O	S	0	0	0
			1886	1209	326	349	2			

- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	0	0
			2161	1452	350	352	7			

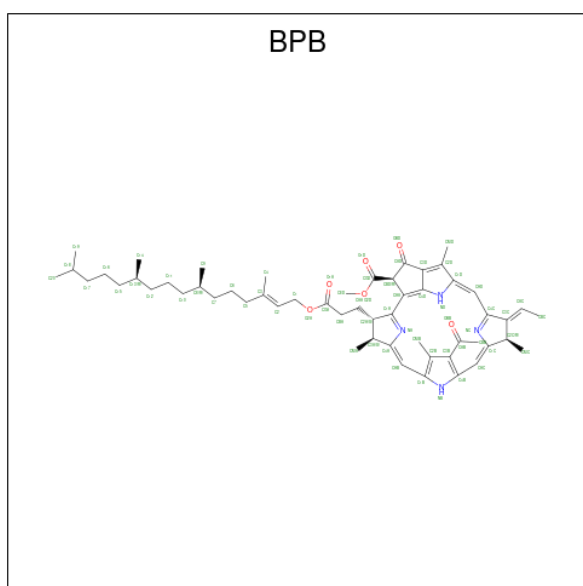
- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).

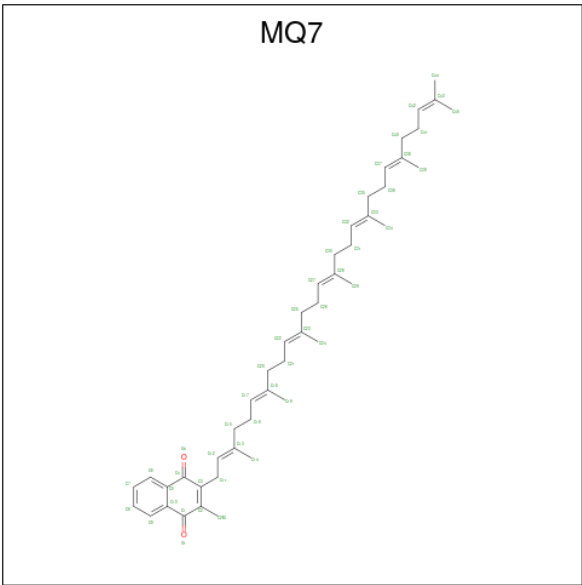


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is FE (II) ION (CCD ID: FE2) (formula: Fe).

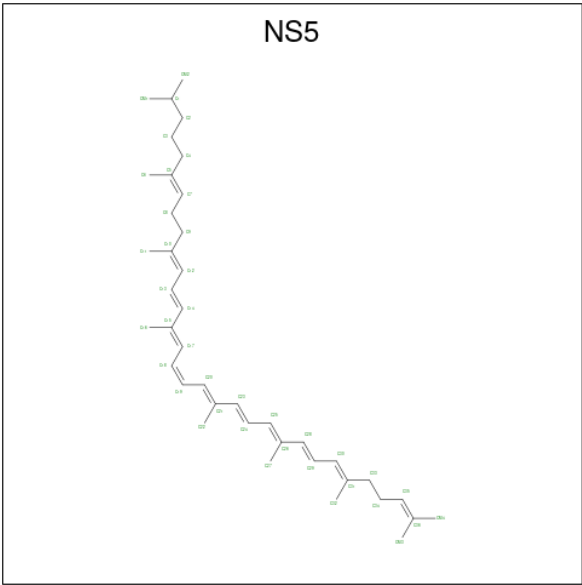
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	C	O	0
			48	46	2	

- Molecule 10 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).

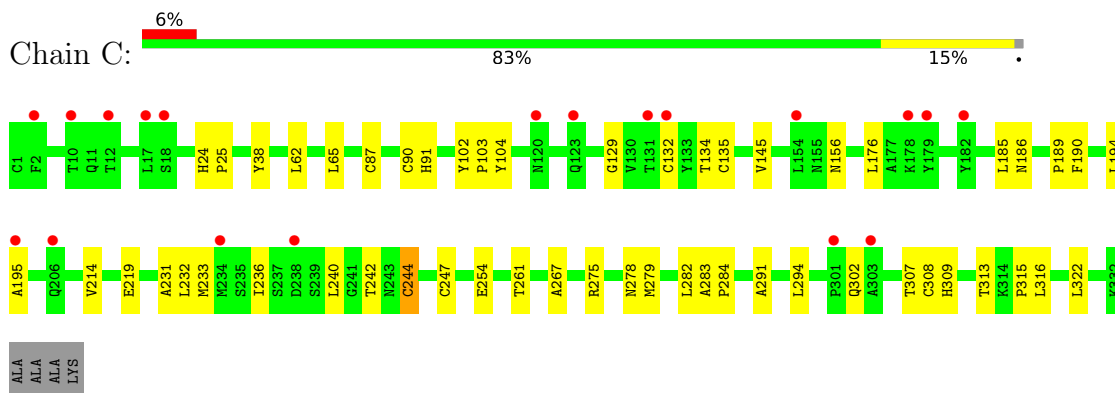


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	C		0
			40	40		

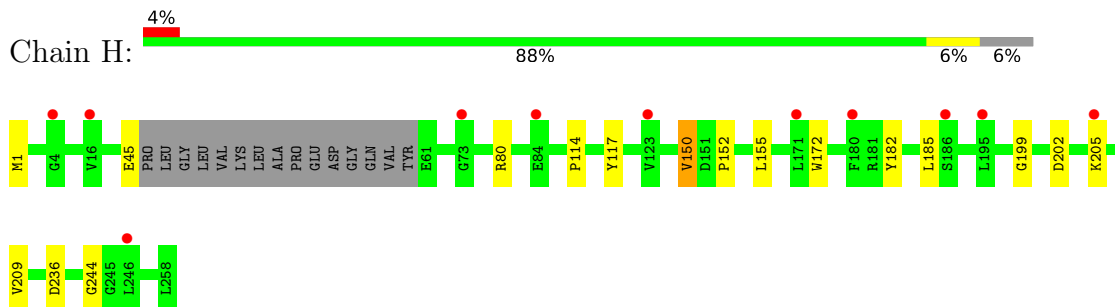
3 Residue-property plots

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.

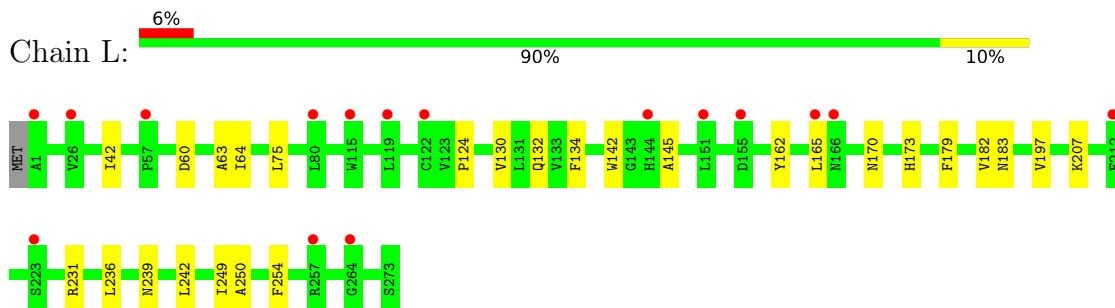
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



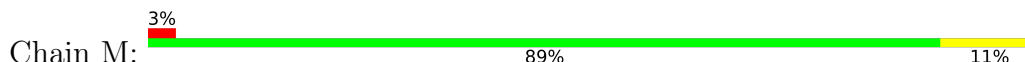
- Molecule 2: REACTION CENTER PROTEIN H CHAIN

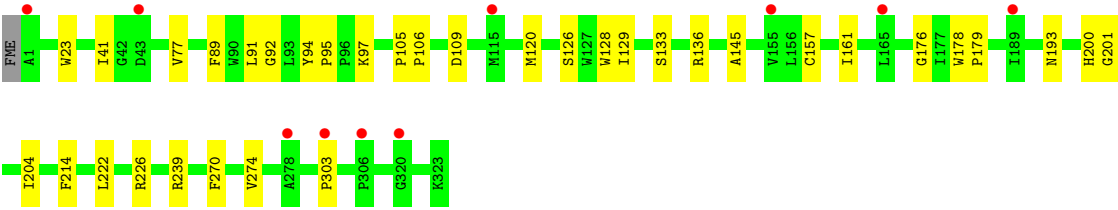


- Molecule 3: REACTION CENTER PROTEIN L CHAIN



- Molecule 4: REACTION CENTER PROTEIN M CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.50Å 84.60Å 375.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 8.20 46.10 – 8.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.10-8.20) 96.5 (46.10-8.20)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 8.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.351 , 0.384 0.343 , 0.376	Depositor DCC
R_{free} test set	95 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	-2.7	Xtriage
Anisotropy	-13.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 192.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NS5, BCB, BPB, FME, FE2, MQ7

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	C	0.43	0/2657	0.78	0/3624
2	H	0.46	0/1919	0.73	0/2621
3	L	0.42	0/2248	0.78	0/3069
4	M	0.43	0/2652	0.77	0/3630
All	All	0.44	0/9476	0.77	0/12944

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 [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	C	2590	0	2561	35	0
2	H	1886	0	1880	8	0
3	L	2161	0	2089	15	0
4	M	2548	0	2432	20	0
5	C	172	0	120	10	0
6	L	132	0	144	7	0
6	M	131	0	140	4	0
7	L	65	0	74	4	0
7	M	61	0	63	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	48	0	64	0	0
10	M	40	0	60	3	0
All	All	9835	0	9627	86	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 4.

All (86) 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)
6:M:1325:BCB:HBD	6:M:1325:BCB:HAA1	1.62	0.80
1:C:247:CYS:SG	5:C:1335:HEM:HAC	2.24	0.78
1:C:308:CYS:SG	5:C:1336:HEM:HAC	2.25	0.76
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.69	0.73
3:L:239:ASN:HA	3:L:242:LEU:HB2	1.76	0.66
4:M:176:GLY:H	10:M:1329:NS5:H14	1.60	0.65
1:C:176:LEU:HD21	1:C:186:ASN:HA	1.78	0.64
3:L:130:VAL:HA	3:L:134:PHE:HB2	1.80	0.62
1:C:278:ASN:HA	1:C:282:LEU:HB2	1.82	0.62
3:L:179:PHE:HA	3:L:182:VAL:HG12	1.81	0.62
6:M:1325:BCB:HAA1	6:M:1325:BCB:CBD	2.29	0.61
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.82	0.61
6:L:1275:BCB:OBD	4:M:201:GLY:HA2	1.99	0.61
1:C:244:CYS:SG	5:C:1335:HEM:HAB	2.41	0.61
3:L:132:GLN:OE1	3:L:145:ALA:HB1	2.03	0.57
4:M:77:VAL:HG13	4:M:91:LEU:HD21	1.89	0.55
1:C:236:ILE:CG2	5:C:1335:HEM:HBC2	2.37	0.55
1:C:195:ALA:HA	1:C:278:ASN:HD22	1.72	0.54
2:H:172:TRP:HB2	2:H:182:TYR:HB2	1.90	0.53
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.43	0.53
4:M:157:CYS:HA	4:M:161:ILE:HB	1.91	0.52
3:L:170:ASN:HB3	3:L:173:HIS:HB3	1.91	0.52
1:C:135:CYS:SG	5:C:1334:HEM:HAC	2.49	0.52
1:C:267:ALA:HB2	5:C:1336:HEM:HMA1	1.92	0.50
3:L:124:PRO:HB2	6:L:1274:BCB:H71	1.94	0.50
1:C:244:CYS:SG	3:L:162:TYR:HB3	2.52	0.49
4:M:270:PHE:O	4:M:274:VAL:HG23	2.13	0.49
3:L:250:ALA:HA	3:L:254:PHE:HB2	1.95	0.49
1:C:190:PHE:HZ	1:C:302:GLN:HB2	1.77	0.48
3:L:183:ASN:HD22	3:L:236:LEU:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HB3	1:C:65:LEU:HD12	1.95	0.48
1:C:132:CYS:SG	5:C:1334:HEM:HAB	2.54	0.48
6:L:1274:BCB:H112	6:L:1275:BCB:HBB2	1.96	0.47
2:H:199:GLY:HA3	4:M:226:ARG:HG2	1.97	0.47
10:M:1329:NS5:H82	10:M:1329:NS5:H61	1.68	0.47
3:L:231:ARG:HA	4:M:222:LEU:HD11	1.97	0.47
2:H:152:PRO:HA	2:H:155:LEU:HD12	1.97	0.46
4:M:178:TRP:N	4:M:179:PRO:CD	2.78	0.46
1:C:240:LEU:HB3	1:C:313:THR:HA	1.97	0.46
6:L:1274:BCB:H122	7:L:1276:BPB:HAA	1.97	0.46
2:H:114:PRO:HG2	2:H:244:GLY:HA2	1.98	0.46
1:C:38:TYR:CE2	1:C:316:LEU:HD13	2.51	0.46
1:C:185:LEU:HD13	1:C:231:ALA:HA	1.98	0.45
1:C:190:PHE:HA	1:C:194:LEU:HB2	1.99	0.45
3:L:42:ILE:HG12	7:L:1276:BPB:H6A	1.99	0.45
4:M:89:PHE:HB3	4:M:178:TRP:NE1	2.32	0.45
4:M:128:TRP:NE1	4:M:145:ALA:O	2.45	0.45
3:L:75:LEU:HA	3:L:142:TRP:CD1	2.52	0.45
2:H:150:VAL:HG11	2:H:205:LYS:HA	1.98	0.45
1:C:134:THR:HG23	1:C:316:LEU:HD12	1.99	0.45
1:C:283:ALA:H	1:C:284:PRO:HD3	1.82	0.45
1:C:91:HIS:CE1	1:C:104:TYR:HE2	2.35	0.44
1:C:145:VAL:HG22	1:C:156:ASN:HD22	1.82	0.44
1:C:247:CYS:HA	1:C:261:THR:OG1	2.17	0.44
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.99	0.44
4:M:120:MET:HA	6:M:1325:BCB:H202	1.98	0.44
1:C:233:MET:HB3	5:C:1335:HEM:C3B	2.53	0.44
1:C:24:HIS:HA	1:C:25:PRO:HD3	1.85	0.43
6:M:1325:BCB:H3A	6:M:1325:BCB:HBA1	1.76	0.43
7:L:1276:BPB:HHC	7:L:1276:BPB:CBB	2.42	0.43
1:C:90:CYS:SG	5:C:1333:HEM:CAC	3.06	0.43
1:C:189:PRO:CB	1:C:232:LEU:HA	2.49	0.43
1:C:254:GLU:H	1:C:254:GLU:CD	2.27	0.43
3:L:63:ALA:HA	4:M:303:PRO:HB3	2.01	0.43
1:C:214:VAL:HA	1:C:219:GLU:HB3	2.01	0.43
3:L:197:VAL:HG13	3:L:207:LYS:HB2	2.00	0.42
10:M:1329:NS5:H18	10:M:1329:NS5:H161	1.71	0.42
4:M:23:TRP:HZ2	4:M:133:SER:HB2	1.84	0.42
4:M:94:TYR:HA	4:M:95:PRO:HD3	1.93	0.42
6:L:1275:BCB:HAA2	6:L:1275:BCB:H93	2.00	0.41
4:M:97:LYS:H	4:M:109:ASP:CG	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:105:PRO:HA	4:M:106:PRO:HD3	1.96	0.41
1:C:247:CYS:SG	5:C:1335:HEM:CAC	3.04	0.41
7:M:1326:BPB:H9B	7:M:1326:BPB:H11A	1.94	0.41
2:H:80:ARG:HG2	4:M:239:ARG:HH12	1.86	0.41
1:C:275:ARG:HB3	1:C:279:MET:HE2	2.02	0.41
1:C:291:ALA:HA	1:C:294:LEU:HD12	2.01	0.41
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.56	0.40
3:L:60:ASP:O	3:L:64:ILE:HG13	2.21	0.40
4:M:92:GLY:HA3	4:M:179:PRO:HG2	2.03	0.40
1:C:102:TYR:N	1:C:103:PRO:CD	2.85	0.40
1:C:240:LEU:HB2	1:C:242:THR:HG22	2.04	0.40
6:L:1274:BCB:HBD	6:L:1274:BCB:HAA1	2.03	0.40
6:L:1275:BCB:HMB1	6:L:1275:BCB:HBB3	2.04	0.40
1:C:129:GLY:HA3	1:C:322:LEU:HD13	2.03	0.40
4:M:126:SER:HA	4:M:129:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	311 (94%)	19 (6%)	0	100	100
2	H	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
3	L	271/274 (99%)	253 (93%)	17 (6%)	1 (0%)	30	67
4	M	321/324 (99%)	309 (96%)	11 (3%)	1 (0%)	36	72
All	All	1161/1192 (97%)	1102 (95%)	57 (5%)	2 (0%)	43	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	165	LEU
4	M	193	ASN

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	C	278/282 (99%)	275 (99%)	3 (1%)	65	76
2	H	194/212 (92%)	191 (98%)	3 (2%)	57	72
3	L	216/219 (99%)	215 (100%)	1 (0%)	81	83
4	M	247/249 (99%)	244 (99%)	3 (1%)	63	75
All	All	935/962 (97%)	925 (99%)	10 (1%)	65	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	87	CYS
1	C	244	CYS
1	C	307	THR
2	H	45	GLU
2	H	150	VAL
2	H	185	LEU
3	L	249	ILE
4	M	41	ILE
4	M	136	ARG
4	M	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	156	ASN
1	C	186	ASN
1	C	200	GLN
1	C	263	GLN
1	C	278	ASN

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Mol	Chain	Res	Type
2	H	8	GLN
2	H	178	HIS
2	H	217	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	FME	H	1	2	8,9,10	0.74	0	8,9,11	3.18	3 (37%)

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	FME	H	1	2	-	5/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-8.28	110.09	122.82
2	H	1	FME	O1-CN-N	-2.11	119.86	125.32
2	H	1	FME	CE-SD-CG	2.01	110.70	100.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA
2	H	1	FME	CB-CA-N-CN
2	H	1	FME	N-CA-CB-CG
2	H	1	FME	C-CA-CB-CG
2	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
5	HEM	C	1334	1	50,50,50	1.91	11 (22%)	67,82,82	1.24	3 (4%)
5	HEM	C	1336	1	50,50,50	1.98	11 (22%)	67,82,82	1.25	4 (5%)
6	BCB	M	1325	4	60,74,74	3.14	17 (28%)	59,115,115	2.71	17 (28%)
6	BCB	L	1274	3	60,74,74	3.12	17 (28%)	59,115,115	2.67	19 (32%)
10	NS5	M	1329	-	39,39,39	2.07	5 (12%)	46,46,46	2.39	17 (36%)
6	BCB	M	1324	-	59,73,74	3.10	17 (28%)	57,113,115	2.70	19 (33%)
7	BPB	L	1276	-	57,70,70	2.60	13 (22%)	55,101,101	2.77	18 (32%)
6	BCB	L	1275	-	60,74,74	3.11	17 (28%)	59,115,115	2.47	16 (27%)
7	BPB	M	1326	-	53,66,70	2.71	13 (24%)	50,96,101	2.85	17 (34%)
5	HEM	C	1335	1	50,50,50	1.95	10 (20%)	67,82,82	1.26	3 (4%)
9	MQ7	M	1328	-	49,49,49	1.54	2 (4%)	61,63,63	1.21	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEM	C	1333	1	50,50,50	2.02	11 (22%)	67,82,82	1.28	4 (5%)

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
5	HEM	C	1334	1	-	9/14/54/54	-
5	HEM	C	1336	1	-	5/14/54/54	-
6	BCB	M	1325	4	3/3/21/26	24/37/137/137	-
6	BCB	L	1274	3	3/3/21/26	17/37/137/137	-
10	NS5	M	1329	-	-	16/43/43/43	-
6	BCB	M	1324	-	3/3/20/26	21/36/136/137	-
7	BPB	L	1276	-	-	19/37/105/105	0/5/6/6
6	BCB	L	1275	-	3/3/21/26	14/37/137/137	-
7	BPB	M	1326	-	-	13/33/101/105	0/5/6/6
5	HEM	C	1335	1	-	8/14/54/54	-
9	MQ7	M	1328	-	-	3/41/61/61	0/2/2/2
5	HEM	C	1333	1	-	7/14/54/54	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1326	BPB	C1B-C2B	9.11	1.49	1.39
7	L	1276	BPB	C1B-C2B	8.91	1.49	1.39
6	L	1275	BCB	C1B-C2B	8.78	1.49	1.39
6	L	1274	BCB	C1B-C2B	8.74	1.49	1.39
6	M	1325	BCB	C1B-C2B	8.66	1.49	1.39
7	M	1326	BPB	C1D-C2D	8.64	1.49	1.39
6	M	1324	BCB	C1B-C2B	8.58	1.49	1.39
6	L	1275	BCB	CHC-C1C	8.36	1.48	1.38
9	M	1328	MQ7	C3-C2	8.35	1.50	1.35
6	L	1274	BCB	C1A-CHA	8.27	1.49	1.40
6	M	1324	BCB	C1D-C2D	8.22	1.48	1.39
6	M	1325	BCB	C1D-C2D	8.22	1.48	1.39
7	L	1276	BPB	C1D-C2D	8.19	1.48	1.39
6	M	1325	BCB	C1A-CHA	8.17	1.49	1.40
6	M	1325	BCB	CHC-C1C	8.15	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1336	HEM	C3D-C2D	8.06	1.54	1.36
5	C	1333	HEM	C3D-C2D	8.05	1.54	1.36
6	L	1275	BCB	C1D-C2D	8.04	1.48	1.39
5	C	1334	HEM	C3D-C2D	8.01	1.54	1.36
6	L	1274	BCB	CHC-C1C	7.92	1.48	1.38
6	L	1274	BCB	C1D-C2D	7.89	1.48	1.39
5	C	1335	HEM	C3D-C2D	7.88	1.53	1.36
6	M	1324	BCB	C1A-CHA	7.84	1.48	1.40
6	M	1324	BCB	CHC-C1C	7.83	1.48	1.38
6	L	1275	BCB	C1A-CHA	7.78	1.48	1.40
10	M	1329	NS5	C29-C28	7.11	1.53	1.34
10	M	1329	NS5	C35-C36	6.94	1.53	1.32
10	M	1329	NS5	C9-C8	-5.98	1.34	1.53
5	C	1333	HEM	FE-ND	5.89	2.13	1.94
7	M	1326	BPB	C4D-CHA	5.58	1.47	1.39
6	M	1325	BCB	CHC-C4B	5.45	1.48	1.39
6	L	1275	BCB	CHC-C4B	5.45	1.48	1.39
9	M	1328	MQ7	C10-C5	5.43	1.49	1.40
5	C	1336	HEM	FE-ND	5.41	2.11	1.94
6	M	1324	BCB	CHC-C4B	5.41	1.48	1.39
6	L	1274	BCB	CHC-C4B	5.39	1.48	1.39
6	M	1325	BCB	C3D-C2D	5.37	1.48	1.39
6	L	1274	BCB	O2D-CGD	5.37	1.46	1.33
6	M	1324	BCB	C3D-C2D	5.37	1.48	1.39
6	L	1275	BCB	C3D-C2D	5.36	1.48	1.39
7	L	1276	BPB	C4D-CHA	5.35	1.47	1.39
7	M	1326	BPB	C3D-C2D	5.35	1.48	1.39
6	L	1274	BCB	C3D-C2D	5.34	1.48	1.39
6	M	1325	BCB	CHD-C1D	5.33	1.48	1.39
6	L	1275	BCB	CHD-C1D	5.33	1.48	1.39
6	M	1325	BCB	O2D-CGD	5.32	1.46	1.33
7	M	1326	BPB	O2D-CGD	5.23	1.46	1.33
6	L	1275	BCB	C3B-C2B	5.22	1.48	1.39
6	L	1275	BCB	O2D-CGD	5.21	1.46	1.33
6	M	1324	BCB	CHD-C1D	5.21	1.48	1.39
6	M	1325	BCB	OBD-CAD	5.20	1.29	1.22
5	C	1335	HEM	FE-ND	5.19	2.10	1.94
7	L	1276	BPB	O2D-CGD	5.19	1.46	1.33
6	M	1324	BCB	O2D-CGD	5.18	1.46	1.33
7	M	1326	BPB	OBD-CAD	5.16	1.29	1.22
6	L	1274	BCB	OBD-CAD	5.14	1.29	1.22
7	L	1276	BPB	C3D-C2D	5.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1324	BCB	OBD-CAD	5.11	1.29	1.22
7	L	1276	BPB	OBD-CAD	5.05	1.28	1.22
6	L	1274	BCB	C3B-C2B	5.02	1.48	1.39
6	L	1274	BCB	CHD-C1D	5.02	1.47	1.39
6	L	1274	BCB	C3B-C4B	4.97	1.49	1.41
6	M	1325	BCB	C3B-C2B	4.97	1.48	1.39
6	L	1275	BCB	CHB-C1B	4.92	1.47	1.39
6	M	1324	BCB	CHB-C4A	-4.91	1.32	1.38
6	L	1275	BCB	C3B-C4B	4.88	1.49	1.41
7	L	1276	BPB	C3B-C4B	4.84	1.49	1.41
6	M	1325	BCB	C3B-C4B	4.80	1.49	1.41
6	L	1275	BCB	OBD-CAD	4.78	1.28	1.22
7	L	1276	BPB	C3B-C2B	4.77	1.47	1.39
6	M	1325	BCB	C3A-C2A	-4.73	1.50	1.54
6	L	1275	BCB	CHD-C4C	4.72	1.48	1.39
6	M	1325	BCB	CHB-C4A	-4.66	1.33	1.38
6	M	1324	BCB	CHD-C4C	4.63	1.48	1.39
7	M	1326	BPB	C3B-C2B	4.60	1.47	1.39
6	L	1274	BCB	O2A-CGA	4.60	1.46	1.33
6	M	1324	BCB	C3B-C4B	4.60	1.48	1.41
5	C	1334	HEM	FE-ND	4.59	2.09	1.94
6	L	1274	BCB	CHB-C4A	-4.53	1.33	1.38
6	M	1325	BCB	CHD-C4C	4.52	1.48	1.39
6	L	1275	BCB	O2A-CGA	4.51	1.46	1.33
7	M	1326	BPB	C3B-C4B	4.47	1.48	1.41
6	M	1324	BCB	C3A-C2A	-4.41	1.50	1.54
6	L	1274	BCB	CHD-C4C	4.39	1.47	1.39
6	M	1325	BCB	O2A-CGA	4.39	1.46	1.33
6	L	1274	BCB	CHB-C1B	4.37	1.46	1.39
7	M	1326	BPB	O2A-CGA	4.36	1.46	1.33
6	M	1324	BCB	C3B-C2B	4.35	1.47	1.39
7	L	1276	BPB	O2A-CGA	4.35	1.46	1.33
6	M	1324	BCB	O2A-CGA	4.34	1.46	1.33
6	L	1274	BCB	C3A-C2A	-4.34	1.51	1.54
5	C	1333	HEM	FE-NB	4.29	2.08	1.94
6	M	1325	BCB	CHB-C1B	4.28	1.46	1.39
6	L	1275	BCB	CHB-C4A	-4.18	1.33	1.38
6	M	1324	BCB	CHB-C1B	4.11	1.46	1.39
5	C	1336	HEM	FE-NB	3.98	2.07	1.94
5	C	1335	HEM	FE-NB	3.93	2.07	1.94
5	C	1335	HEM	FE-NA	3.91	2.08	1.95
5	C	1334	HEM	FE-NB	3.83	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1334	HEM	FE-NA	3.75	2.07	1.95
5	C	1336	HEM	FE-NC	3.73	2.07	1.95
5	C	1333	HEM	FE-NA	3.71	2.07	1.95
7	L	1276	BPB	C3A-C2A	-3.62	1.51	1.54
5	C	1336	HEM	FE-NA	3.58	2.07	1.95
5	C	1333	HEM	FE-NC	3.53	2.06	1.95
6	L	1275	BCB	C3A-C2A	-3.46	1.51	1.54
5	C	1335	HEM	FE-NC	3.45	2.06	1.95
7	L	1276	BPB	C4C-NC	-3.39	1.27	1.37
7	M	1326	BPB	C4C-NC	-3.35	1.27	1.37
7	L	1276	BPB	CHA-CBD	-3.18	1.47	1.51
6	L	1274	BCB	CHA-CBD	-3.16	1.48	1.51
7	M	1326	BPB	C3A-C2A	-3.16	1.52	1.54
5	C	1334	HEM	FE-NC	3.14	2.05	1.95
5	C	1333	HEM	CAC-C3C	2.98	1.55	1.47
5	C	1336	HEM	CAB-C3B	2.97	1.55	1.47
7	M	1326	BPB	CHA-CBD	-2.97	1.48	1.51
6	M	1325	BCB	CHA-CBD	-2.93	1.48	1.51
5	C	1333	HEM	CAB-C3B	2.91	1.55	1.47
5	C	1334	HEM	CAB-C3B	2.88	1.55	1.47
6	L	1275	BCB	CHA-CBD	-2.86	1.48	1.51
5	C	1336	HEM	CAC-C3C	2.86	1.55	1.47
5	C	1334	HEM	CAC-C3C	2.85	1.55	1.47
5	C	1335	HEM	CAB-C3B	2.84	1.55	1.47
5	C	1335	HEM	CAC-C3C	2.82	1.54	1.47
10	M	1329	NS5	C28-C26	2.80	1.51	1.46
10	M	1329	NS5	C29-C30	2.77	1.51	1.43
6	M	1324	BCB	CHA-CBD	-2.68	1.48	1.51
5	C	1333	HEM	CMB-C2B	2.21	1.55	1.50
5	C	1333	HEM	CMC-C2C	2.21	1.55	1.50
5	C	1333	HEM	CMA-C3A	2.20	1.55	1.50
5	C	1334	HEM	CMB-C2B	2.17	1.55	1.50
5	C	1334	HEM	CMA-C3A	2.17	1.55	1.50
5	C	1336	HEM	CMB-C2B	2.17	1.55	1.50
7	L	1276	BPB	C1D-ND	-2.16	1.34	1.38
5	C	1334	HEM	CMC-C2C	2.13	1.55	1.50
7	M	1326	BPB	C1D-ND	-2.13	1.34	1.38
5	C	1335	HEM	CMA-C3A	2.11	1.55	1.50
5	C	1335	HEM	CMC-C2C	2.11	1.55	1.50
5	C	1336	HEM	CMD-C2D	2.10	1.55	1.50
5	C	1336	HEM	CMC-C2C	2.09	1.55	1.50
5	C	1335	HEM	CMB-C2B	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1334	HEM	CMD-C2D	2.07	1.55	1.50
5	C	1333	HEM	CMD-C2D	2.07	1.55	1.50
5	C	1336	HEM	CMA-C3A	2.02	1.54	1.50

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1324	BCB	C4B-CHC-C1C	9.82	127.64	121.32
7	L	1276	BPB	C3D-C4D-ND	9.78	120.25	107.71
7	M	1326	BPB	C3D-C4D-ND	9.64	120.07	107.71
6	M	1325	BCB	O2D-CGD-CBD	9.54	121.42	110.95
6	M	1324	BCB	O2D-CGD-CBD	8.81	120.63	110.95
6	L	1274	BCB	C4B-CHC-C1C	8.71	126.92	121.32
7	M	1326	BPB	O2D-CGD-CBD	8.66	120.46	110.95
6	M	1325	BCB	C4B-CHC-C1C	8.61	126.86	121.32
7	L	1276	BPB	O2D-CGD-CBD	8.40	120.17	110.95
6	L	1275	BCB	O2D-CGD-CBD	8.36	120.13	110.95
6	L	1274	BCB	O2D-CGD-CBD	8.29	120.05	110.95
7	L	1276	BPB	C2B-C1B-NB	7.95	115.18	109.43
6	L	1275	BCB	C4B-CHC-C1C	7.88	126.39	121.32
6	L	1274	BCB	C1B-CHB-C4A	7.55	126.18	121.32
7	M	1326	BPB	C2B-C1B-NB	7.34	114.74	109.43
6	M	1325	BCB	C1B-CHB-C4A	6.65	125.60	121.32
6	L	1275	BCB	C3D-CAD-CBD	6.44	116.08	107.61
6	M	1325	BCB	C3D-CAD-CBD	6.09	115.62	107.61
6	M	1324	BCB	C3D-CAD-CBD	5.95	115.44	107.61
7	L	1276	BPB	C4D-ND-C1D	-5.91	101.79	108.87
6	M	1324	BCB	CHA-C1A-C2A	-5.86	119.55	133.31
5	C	1335	HEM	C4D-ND-C1D	5.82	112.09	105.21
5	C	1333	HEM	C4D-ND-C1D	5.76	112.03	105.21
6	L	1274	BCB	C3D-CAD-CBD	5.73	115.15	107.61
5	C	1334	HEM	C4D-ND-C1D	5.49	111.71	105.21
7	M	1326	BPB	C4D-ND-C1D	-5.47	102.32	108.87
6	M	1325	BCB	CHA-C1A-C2A	-5.47	120.47	133.31
5	C	1336	HEM	C4D-ND-C1D	5.44	111.65	105.21
10	M	1329	NS5	C19-C20-C21	-5.40	119.71	127.28
6	L	1275	BCB	CHA-C1A-C2A	-5.30	120.86	133.31
7	L	1276	BPB	OBD-CAD-C3D	-5.20	119.78	127.89
10	M	1329	NS5	C18-C17-C15	-5.20	119.99	127.28
10	M	1329	NS5	C30-C29-C28	-5.09	108.46	123.20
7	M	1326	BPB	OBD-CAD-C3D	-5.05	120.02	127.89
6	L	1274	BCB	CHA-C1A-C2A	-5.04	121.48	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	1329	NS5	C34-C35-C36	-4.75	111.80	127.64
6	M	1324	BCB	C1B-CHB-C4A	4.65	124.32	121.32
10	M	1329	NS5	C29-C28-C26	-4.64	113.65	126.36
6	L	1275	BCB	OBD-CAD-C3D	-4.25	121.27	127.89
6	M	1324	BCB	C3D-C4D-ND	4.15	119.59	112.94
10	M	1329	NS5	C8-C9-C10	4.11	126.81	113.19
7	L	1276	BPB	OBD-CAD-CBD	-4.06	119.86	125.82
7	M	1326	BPB	OBD-CAD-CBD	-3.97	120.00	125.82
6	M	1325	BCB	C3D-C4D-CHA	3.96	114.55	108.54
6	L	1274	BCB	C3D-C4D-ND	3.95	119.28	112.94
6	L	1275	BCB	C3D-C4D-CHA	3.92	114.50	108.54
6	M	1325	BCB	OBD-CAD-C3D	-3.89	121.83	127.89
6	L	1274	BCB	C3D-C4D-CHA	3.87	114.43	108.54
6	M	1325	BCB	C3D-C4D-ND	3.81	119.05	112.94
6	L	1275	BCB	C3D-C4D-ND	3.80	119.04	112.94
6	M	1324	BCB	OBD-CAD-C3D	-3.77	122.01	127.89
6	L	1275	BCB	CMD-C2D-C3D	-3.70	117.28	124.68
10	M	1329	NS5	CM3-C36-C35	-3.68	111.63	122.66
10	M	1329	NS5	CM4-C36-C35	-3.63	111.75	122.66
6	M	1324	BCB	C3D-C4D-CHA	3.59	114.00	108.54
6	M	1324	BCB	CMD-C2D-C3D	-3.58	117.54	124.68
7	M	1326	BPB	CMD-C2D-C3D	-3.56	117.56	124.68
6	M	1325	BCB	CMD-C2D-C3D	-3.56	117.58	124.68
7	L	1276	BPB	C2D-C1D-ND	3.54	111.99	109.43
6	L	1274	BCB	OBD-CAD-C3D	-3.54	122.37	127.89
7	L	1276	BPB	CMD-C2D-C3D	-3.50	117.69	124.68
6	M	1325	BCB	O2D-CGD-O1D	-3.37	117.29	123.85
6	L	1274	BCB	CMD-C2D-C3D	-3.33	118.04	124.68
6	M	1325	BCB	CMB-C2B-C3B	3.28	131.24	124.68
10	M	1329	NS5	C13-C12-C10	-3.25	123.12	127.69
6	L	1275	BCB	O1D-CGD-CBD	-3.21	119.86	124.72
6	L	1274	BCB	C4-C3-C5	3.21	120.80	115.23
6	L	1274	BCB	CMB-C2B-C3B	3.20	131.08	124.68
7	M	1326	BPB	O1D-CGD-CBD	-3.19	119.89	124.72
10	M	1329	NS5	C24-C25-C26	-3.14	122.88	127.28
6	M	1324	BCB	O1D-CGD-CBD	-3.14	119.97	124.72
6	L	1275	BCB	CMB-C2B-C3B	3.13	130.93	124.68
10	M	1329	NS5	C11-C10-C9	3.10	120.60	115.23
6	L	1274	BCB	O1D-CGD-CBD	-3.09	120.03	124.72
7	L	1276	BPB	C3B-C4B-NB	3.08	112.53	108.05
6	L	1275	BCB	C1B-CHB-C4A	3.07	123.30	121.32
9	M	1328	MQ7	C14-C13-C15	3.06	120.53	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1274	BCB	O2A-CGA-CBA	3.01	121.02	111.83
6	M	1324	BCB	CHC-C1C-C2C	-3.01	114.63	122.69
7	M	1326	BPB	C4A-C3A-C2A	-3.00	99.98	102.84
7	M	1326	BPB	C3B-C4B-NB	2.96	112.35	108.05
7	L	1276	BPB	O1D-CGD-CBD	-2.95	120.24	124.72
7	M	1326	BPB	C2D-C1D-ND	2.89	111.52	109.43
6	L	1274	BCB	CHC-C1C-C2C	-2.85	115.05	122.69
10	M	1329	NS5	C9-C8-C7	2.69	125.31	112.02
6	M	1325	BCB	CHC-C1C-C2C	-2.68	115.50	122.69
10	M	1329	NS5	C8-C7-C5	-2.65	121.57	127.62
6	L	1275	BCB	CHC-C1C-C2C	-2.63	115.64	122.69
7	L	1276	BPB	C4A-C3A-C2A	-2.62	100.35	102.84
7	L	1276	BPB	CMB-C2B-C3B	2.61	129.90	124.68
6	M	1325	BCB	O2A-CGA-CBA	2.61	119.78	111.83
7	M	1326	BPB	O2A-CGA-CBA	2.52	119.51	111.83
6	L	1275	BCB	O2A-CGA-CBA	2.51	119.49	111.83
5	C	1333	HEM	C1B-NB-C4B	2.50	108.17	105.21
10	M	1329	NS5	C29-C30-C31	-2.46	124.22	127.69
5	C	1334	HEM	C1B-NB-C4B	2.45	108.11	105.21
6	M	1325	BCB	C4-C3-C5	2.44	119.46	115.23
9	M	1328	MQ7	C34-C33-C35	2.41	119.42	115.23
5	C	1333	HEM	C3B-C4B-NB	-2.41	107.74	109.47
6	M	1324	BCB	O2A-CGA-CBA	2.40	119.17	111.83
10	M	1329	NS5	C32-C31-C33	2.38	119.36	115.23
6	L	1274	BCB	C1A-CHA-C4D	2.36	122.92	118.98
9	M	1328	MQ7	C19-C18-C20	2.35	119.31	115.23
6	M	1324	BCB	C4D-ND-C1D	-2.34	103.44	105.22
5	C	1336	HEM	C1B-NB-C4B	2.34	107.98	105.21
7	M	1326	BPB	C4-C3-C5	2.34	119.28	115.23
6	L	1275	BCB	CED-O2D-CGD	2.33	121.21	115.92
6	M	1324	BCB	CMB-C2B-C3B	2.33	129.34	124.68
6	L	1275	BCB	C4-C3-C5	2.32	119.26	115.23
5	C	1335	HEM	C1B-NB-C4B	2.32	107.95	105.21
6	M	1324	BCB	O2D-CGD-O1D	-2.28	119.41	123.85
6	L	1274	BCB	OBD-CAD-CBD	-2.28	122.48	125.82
7	L	1276	BPB	C1-O2A-CGA	2.28	122.16	116.65
6	M	1325	BCB	O1D-CGD-CBD	-2.27	121.29	124.72
6	M	1325	BCB	OBD-CAD-CBD	-2.26	122.50	125.82
7	M	1326	BPB	CMB-C2B-C3B	2.26	129.19	124.68
10	M	1329	NS5	C6-C5-C4	2.24	119.12	115.23
6	M	1324	BCB	OBD-CAD-CBD	-2.23	122.56	125.82
9	M	1328	MQ7	C24-C23-C25	2.22	119.08	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1328	MQ7	C11-C3-C2	-2.21	121.10	124.89
6	M	1324	BCB	C4C-CHD-C1D	2.21	123.97	116.07
7	L	1276	BPB	O2D-CGD-O1D	-2.19	119.58	123.85
6	M	1324	BCB	C4-C3-C5	2.18	119.01	115.23
7	L	1276	BPB	O2A-CGA-CBA	2.18	118.47	111.83
9	M	1328	MQ7	C39-C38-C40	2.17	119.00	115.23
6	L	1275	BCB	OBD-CAD-CBD	-2.16	122.66	125.82
7	M	1326	BPB	O2D-CGD-O1D	-2.16	119.65	123.85
9	M	1328	MQ7	C2M-C2-C3	-2.15	120.92	124.45
7	L	1276	BPB	C4B-NB-C1B	-2.15	105.69	108.82
7	M	1326	BPB	CED-O2D-CGD	2.14	120.77	115.92
9	M	1328	MQ7	C29-C28-C30	2.11	118.88	115.23
7	L	1276	BPB	CMA-C3A-C4A	-2.10	110.08	114.61
5	C	1336	HEM	C3B-C2B-C1B	2.09	107.98	106.41
5	C	1335	HEM	C3B-C4B-NB	-2.08	107.97	109.47
6	M	1325	BCB	C1A-CHA-C4D	2.07	122.44	118.98
10	M	1329	NS5	C24-C23-C21	-2.06	120.72	126.36
5	C	1336	HEM	C2A-C1A-NA	-2.05	107.87	110.15
5	C	1334	HEM	C3B-C4B-NB	-2.05	108.00	109.47
7	M	1326	BPB	C4B-NB-C1B	-2.04	105.84	108.82
6	L	1274	BCB	O2A-CGA-O1A	-2.04	118.53	123.63
7	L	1276	BPB	CED-O2D-CGD	2.03	120.53	115.92
6	L	1274	BCB	O2D-CGD-O1D	-2.03	119.90	123.85
6	L	1274	BCB	CED-O2D-CGD	2.01	120.48	115.92
5	C	1333	HEM	C2A-C1A-NA	-2.01	107.92	110.15
6	M	1324	BCB	CED-O2D-CGD	2.01	120.47	115.92

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1274	BCB	NA
6	L	1274	BCB	ND
6	L	1274	BCB	NC
6	L	1275	BCB	NA
6	L	1275	BCB	ND
6	L	1275	BCB	NC
6	M	1324	BCB	NA
6	M	1324	BCB	ND
6	M	1324	BCB	NC
6	M	1325	BCB	NA
6	M	1325	BCB	ND
6	M	1325	BCB	NC

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1333	HEM	C3D-CAD-CBD-CGD
5	C	1334	HEM	C2C-C3C-CAC-CBC
5	C	1335	HEM	C2B-C3B-CAB-CBB
5	C	1336	HEM	C2C-C3C-CAC-CBC
5	C	1336	HEM	C4C-C3C-CAC-CBC
6	L	1274	BCB	C2C-C3C-CAC-CBC
6	L	1274	BCB	C4C-C3C-CAC-CBC
6	L	1274	BCB	CBD-CGD-O2D-CED
6	L	1275	BCB	C2C-C3C-CAC-CBC
6	L	1275	BCB	C4C-C3C-CAC-CBC
6	M	1324	BCB	C1A-C2A-CAA-CBA
6	M	1324	BCB	C3A-C2A-CAA-CBA
6	M	1324	BCB	C2C-C3C-CAC-CBC
6	M	1324	BCB	C4C-C3C-CAC-CBC
6	M	1325	BCB	C2C-C3C-CAC-CBC
6	M	1325	BCB	C4C-C3C-CAC-CBC
6	M	1325	BCB	CAD-CBD-CGD-O1D
6	M	1325	BCB	CAD-CBD-CGD-O2D
6	M	1325	BCB	CBD-CGD-O2D-CED
7	L	1276	BPB	C2C-C3C-CAC-CBC
7	L	1276	BPB	C4C-C3C-CAC-CBC
7	M	1326	BPB	CBD-CGD-O2D-CED
7	M	1326	BPB	C2C-C3C-CAC-CBC
7	M	1326	BPB	C4C-C3C-CAC-CBC
10	M	1329	NS5	C10-C12-C13-C14
10	M	1329	NS5	C25-C26-C28-C29
10	M	1329	NS5	C27-C26-C28-C29
6	M	1324	BCB	CBD-CGD-O2D-CED
7	L	1276	BPB	CBD-CGD-O2D-CED
10	M	1329	NS5	C34-C35-C36-CM3
10	M	1329	NS5	C34-C35-C36-CM4
7	L	1276	BPB	O1D-CGD-O2D-CED
6	L	1274	BCB	O1D-CGD-O2D-CED
6	M	1324	BCB	C3-C5-C6-C7
6	M	1325	BCB	O1D-CGD-O2D-CED
7	M	1326	BPB	O1D-CGD-O2D-CED
6	M	1324	BCB	O1D-CGD-O2D-CED
6	L	1274	BCB	C4-C3-C5-C6
6	L	1274	BCB	C2-C3-C5-C6
9	M	1328	MQ7	C18-C20-C21-C22
10	M	1329	NS5	C31-C33-C34-C35
6	M	1325	BCB	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
7	M	1326	BPB	C11-C10-C8-C9
10	M	1329	NS5	C7-C8-C9-C10
6	M	1325	BCB	C10-C11-C12-C13
6	M	1325	BCB	O1A-CGA-O2A-C1
7	M	1326	BPB	C5-C6-C7-C8
6	M	1324	BCB	C13-C15-C16-C17
6	M	1325	BCB	C15-C16-C17-C18
7	L	1276	BPB	C13-C15-C16-C17
7	L	1276	BPB	C5-C6-C7-C8
10	M	1329	NS5	C1-C2-C3-C4
6	M	1324	BCB	C10-C11-C12-C13
7	L	1276	BPB	C8-C10-C11-C12
7	L	1276	BPB	C3-C5-C6-C7
7	L	1276	BPB	C15-C16-C17-C18
7	M	1326	BPB	C8-C10-C11-C12
10	M	1329	NS5	C2-C3-C4-C5
9	M	1328	MQ7	C38-C40-C41-C42
10	M	1329	NS5	C13-C14-C15-C16
10	M	1329	NS5	C13-C14-C15-C17
6	L	1274	BCB	C16-C17-C18-C19
6	L	1274	BCB	C16-C17-C18-C20
10	M	1329	NS5	CM2-C1-C2-C3
6	M	1325	BCB	C5-C6-C7-C8
7	L	1276	BPB	C3A-C2A-CAA-CBA
10	M	1329	NS5	CM1-C1-C2-C3
7	M	1326	BPB	C12-C13-C15-C16
5	C	1333	HEM	C2B-C3B-CAB-CBB
5	C	1333	HEM	C4B-C3B-CAB-CBB
5	C	1335	HEM	C4B-C3B-CAB-CBB
6	L	1275	BCB	C16-C17-C18-C20
5	C	1334	HEM	C3D-CAD-CBD-CGD
6	L	1274	BCB	C8-C10-C11-C12
7	L	1276	BPB	C11-C12-C13-C15
6	L	1275	BCB	C11-C12-C13-C14
7	M	1326	BPB	C14-C13-C15-C16
6	L	1275	BCB	C16-C17-C18-C19
6	L	1275	BCB	C15-C16-C17-C18
7	L	1276	BPB	C11-C12-C13-C14
6	L	1274	BCB	C12-C13-C15-C16
6	L	1275	BCB	C11-C10-C8-C7
6	M	1325	BCB	C6-C7-C8-C10
6	M	1325	BCB	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
7	M	1326	BPB	C6-C7-C8-C10
6	M	1324	BCB	C16-C17-C18-C19
10	M	1329	NS5	C28-C29-C30-C31
7	L	1276	BPB	C1A-C2A-CAA-CBA
6	M	1324	BCB	C15-C16-C17-C18
6	M	1325	BCB	C6-C7-C8-C9
7	M	1326	BPB	C6-C7-C8-C9
6	M	1325	BCB	C16-C17-C18-C19
6	M	1324	BCB	C11-C10-C8-C7
6	M	1325	BCB	C11-C10-C8-C7
7	L	1276	BPB	C6-C7-C8-C10
7	L	1276	BPB	C4-C3-C5-C6
5	C	1334	HEM	C2B-C3B-CAB-CBB
5	C	1335	HEM	C2C-C3C-CAC-CBC
5	C	1334	HEM	C4C-C3C-CAC-CBC
6	L	1274	BCB	C14-C13-C15-C16
6	L	1275	BCB	CBD-CGD-O2D-CED
6	L	1275	BCB	C11-C12-C13-C15
6	M	1324	BCB	C6-C7-C8-C10
6	M	1324	BCB	C11-C12-C13-C15
6	M	1324	BCB	C12-C13-C15-C16
6	L	1275	BCB	C14-C13-C15-C16
6	M	1324	BCB	C11-C10-C8-C9
6	M	1325	BCB	C11-C10-C8-C9
6	M	1325	BCB	C14-C13-C15-C16
7	L	1276	BPB	C6-C7-C8-C9
6	M	1325	BCB	C16-C17-C18-C20
7	L	1276	BPB	C2-C3-C5-C6
10	M	1329	NS5	C22-C21-C23-C24
5	C	1336	HEM	C3D-CAD-CBD-CGD
6	M	1324	BCB	C14-C13-C15-C16
6	L	1275	BCB	O1D-CGD-O2D-CED
6	L	1274	BCB	C11-C10-C8-C9
6	L	1275	BCB	C11-C10-C8-C9
6	M	1324	BCB	C11-C12-C13-C14
5	C	1334	HEM	C4B-C3B-CAB-CBB
5	C	1335	HEM	C4C-C3C-CAC-CBC
6	M	1324	BCB	C4-C3-C5-C6
5	C	1335	HEM	CAA-CBA-CGA-O1A
6	M	1324	BCB	C6-C7-C8-C9
5	C	1334	HEM	CAA-CBA-CGA-O1A
5	C	1335	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	L	1275	BCB	C1A-C2A-CAA-CBA
6	M	1324	BCB	C2-C3-C5-C6
5	C	1333	HEM	CAA-CBA-CGA-O1A
5	C	1334	HEM	CAD-CBD-CGD-O2D
6	L	1274	BCB	C11-C10-C8-C7
5	C	1333	HEM	CAA-CBA-CGA-O2A
5	C	1333	HEM	CAD-CBD-CGD-O2D
6	L	1274	BCB	C5-C6-C7-C8
5	C	1334	HEM	CAD-CBD-CGD-O1D
5	C	1333	HEM	CAD-CBD-CGD-O1D
5	C	1334	HEM	CAA-CBA-CGA-O2A
6	L	1275	BCB	C3-C5-C6-C7
6	L	1274	BCB	CHA-CBD-CGD-O1D
6	M	1325	BCB	CHA-CBD-CGD-O1D
6	M	1325	BCB	CHA-CBD-CGD-O2D
5	C	1336	HEM	CAD-CBD-CGD-O2D
7	M	1326	BPB	C11-C10-C8-C7
5	C	1336	HEM	CAD-CBD-CGD-O1D
7	L	1276	BPB	C11-C10-C8-C9
7	M	1326	BPB	C3A-C2A-CAA-CBA
9	M	1328	MQ7	C39-C38-C40-C41
6	M	1325	BCB	C2A-CAA-CBA-CGA
7	L	1276	BPB	C11-C10-C8-C7
5	C	1335	HEM	CAD-CBD-CGD-O2D
10	M	1329	NS5	C20-C21-C23-C24
6	L	1274	BCB	C6-C7-C8-C10
6	L	1274	BCB	C11-C12-C13-C15
5	C	1335	HEM	CAD-CBD-CGD-O1D
6	M	1325	BCB	C13-C15-C16-C17
6	M	1325	BCB	C11-C12-C13-C14

There are no ring outliers.

10 monomers are involved in 28 short contacts:

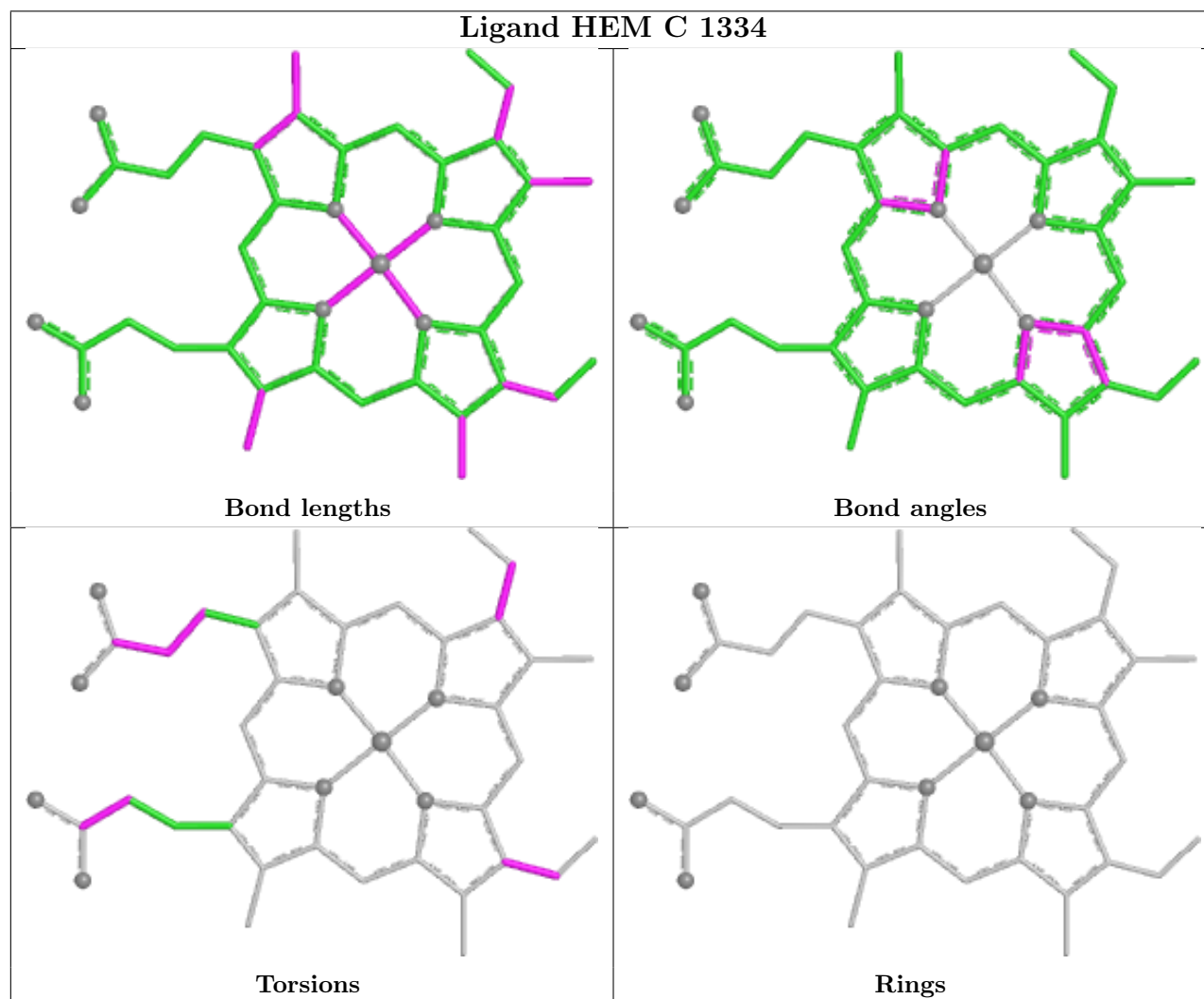
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1334	HEM	2	0
5	C	1336	HEM	2	0
6	M	1325	BCB	4	0
6	L	1274	BCB	4	0
10	M	1329	NS5	3	0
7	L	1276	BPB	4	0
6	L	1275	BCB	4	0

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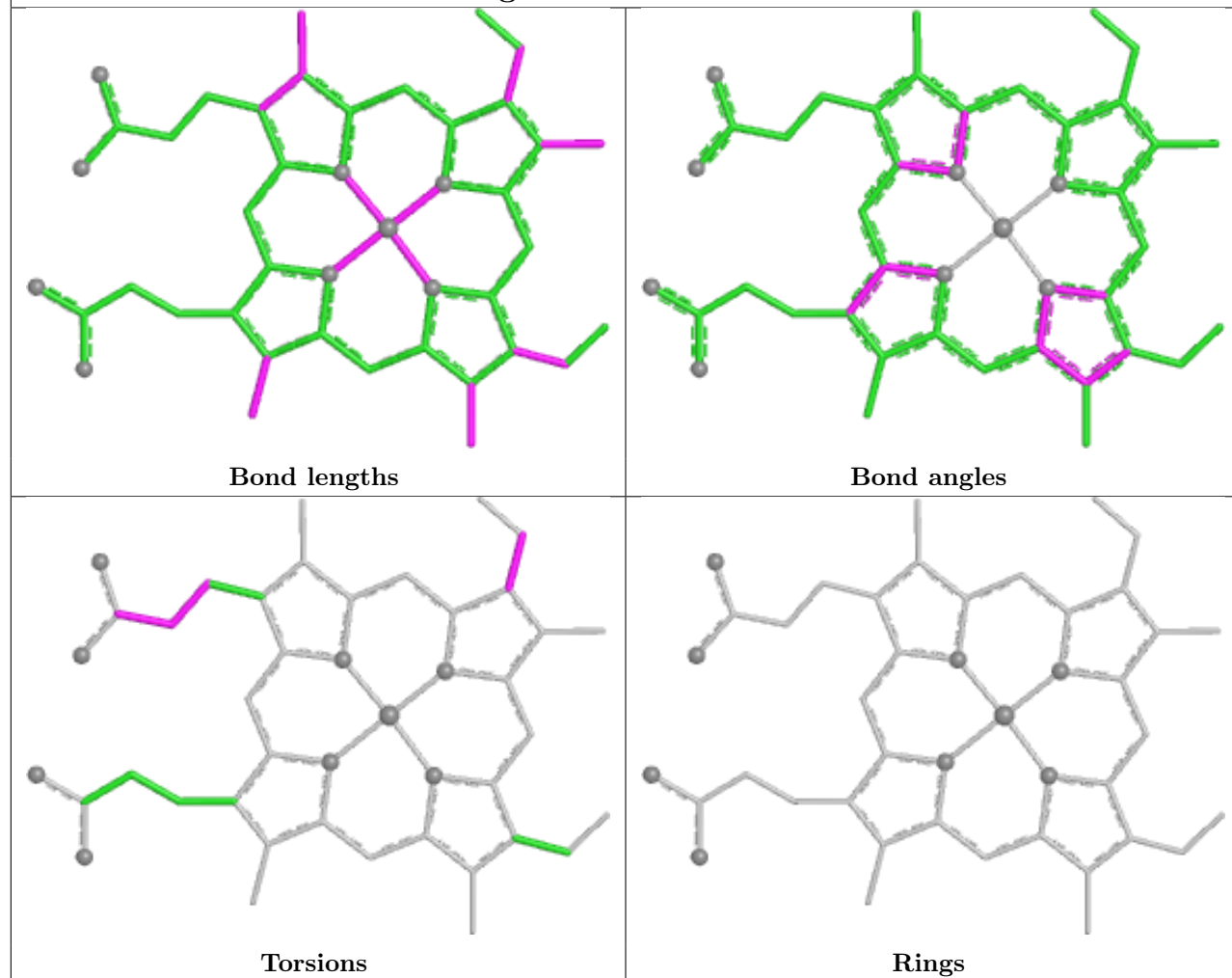
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1326	BPB	1	0
5	C	1335	HEM	5	0
5	C	1333	HEM	1	0

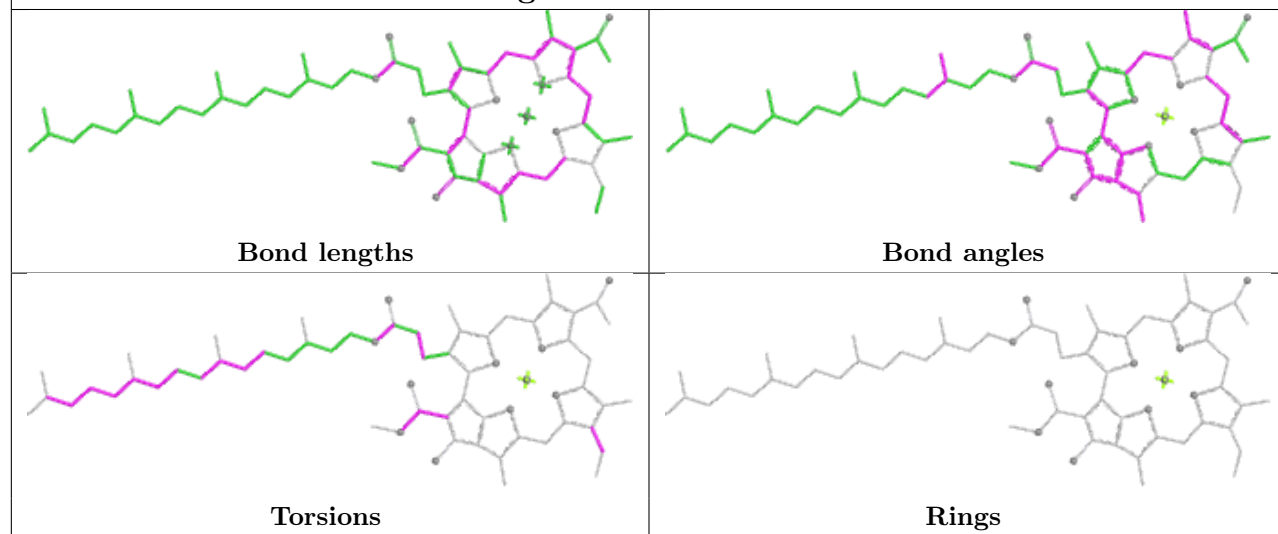
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

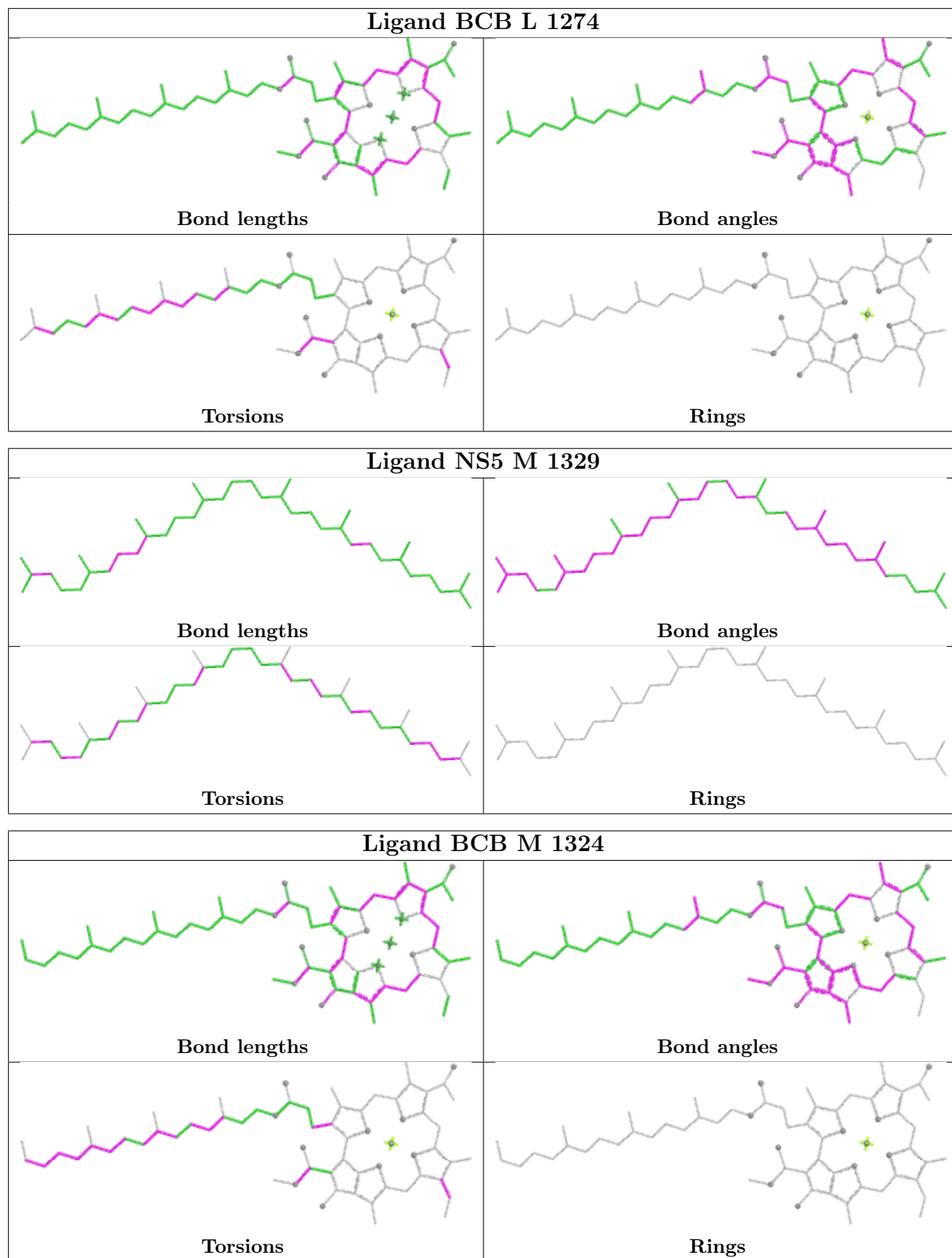


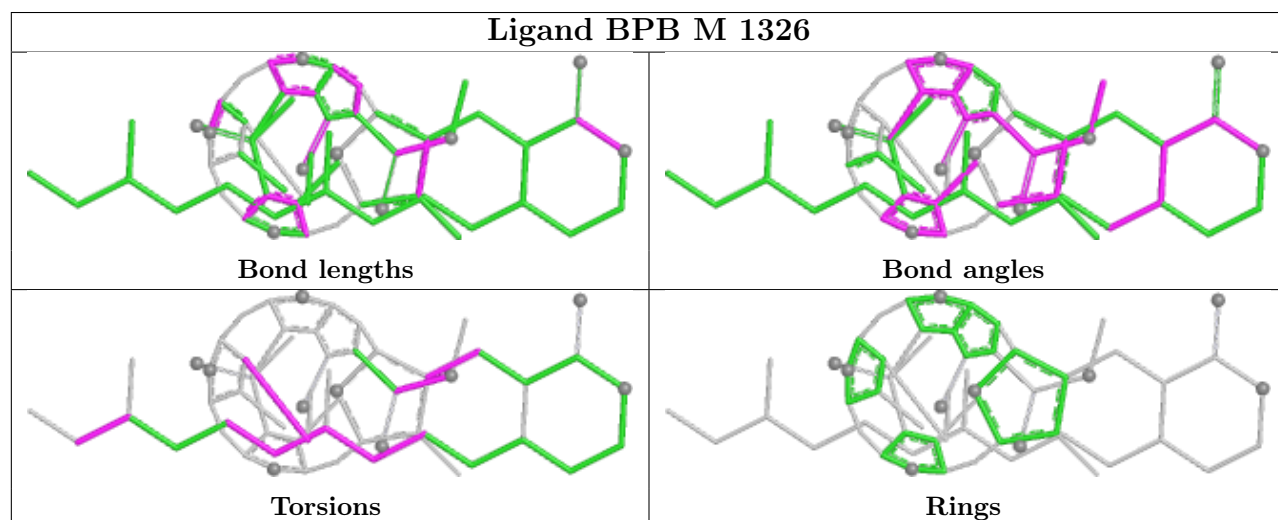
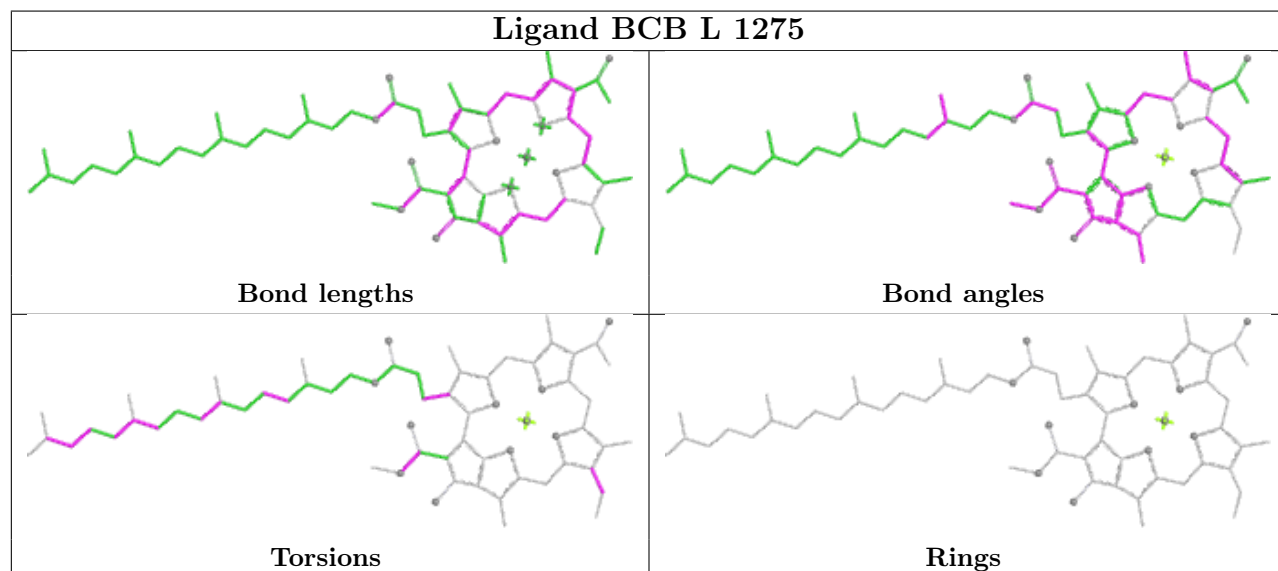
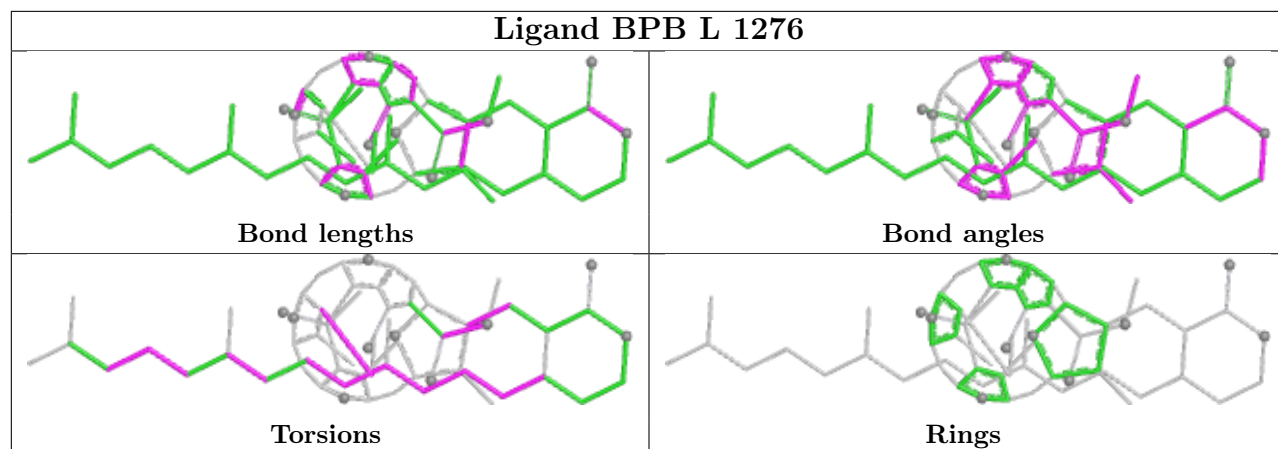
Ligand HEM C 1336



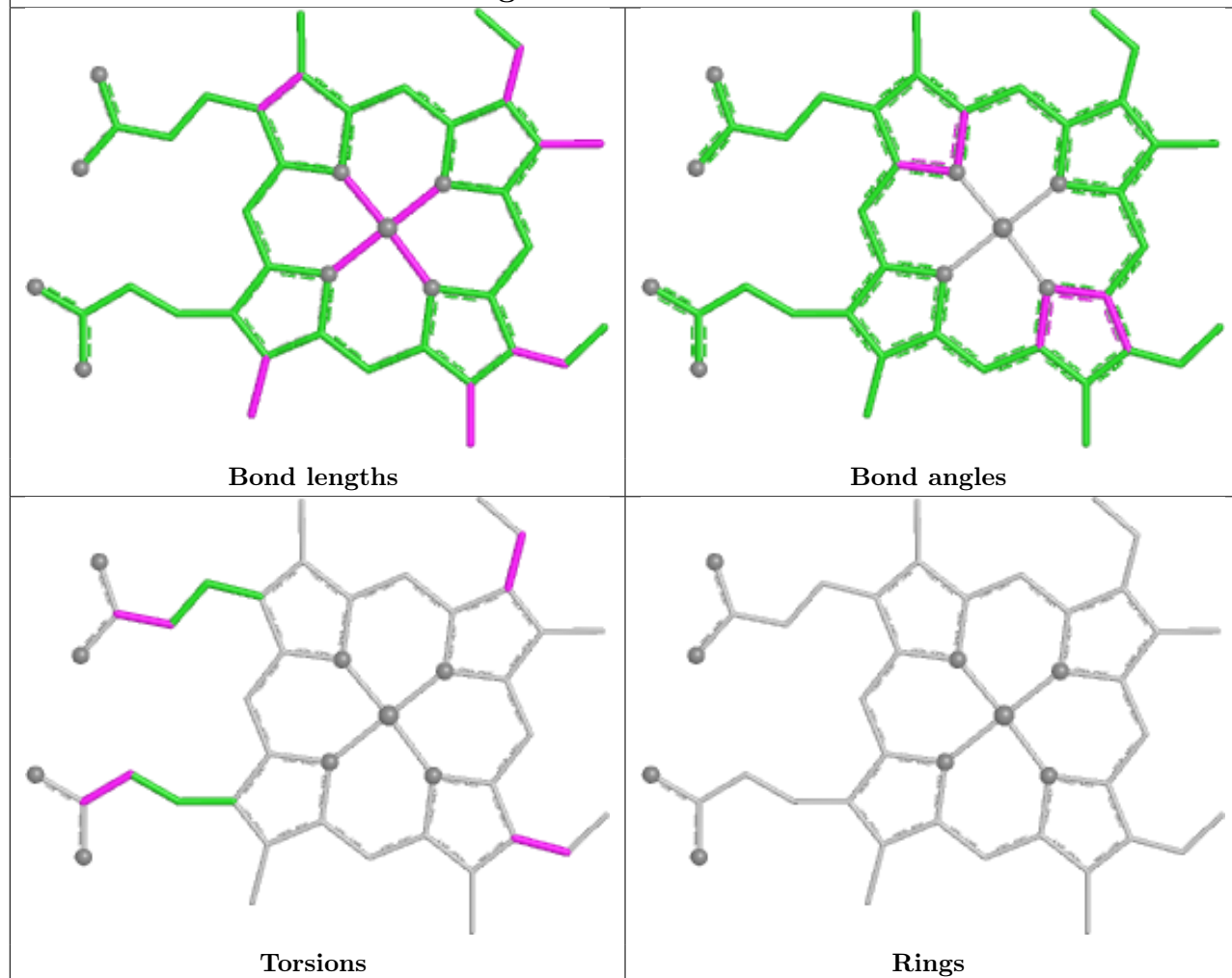
Ligand BCB M 1325



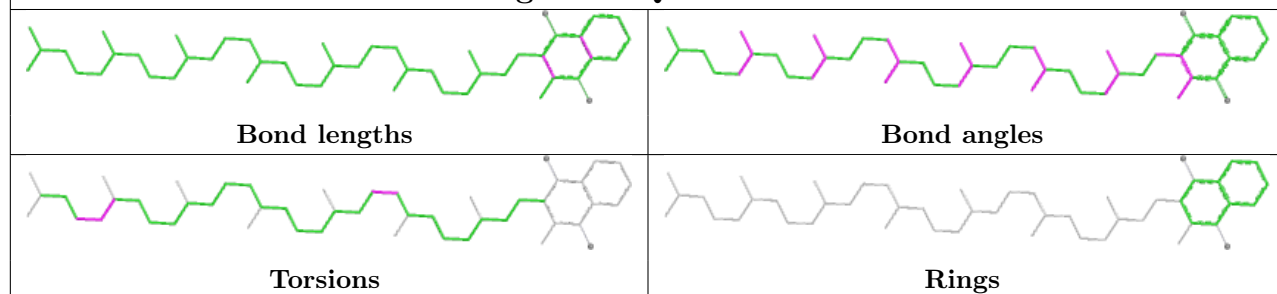


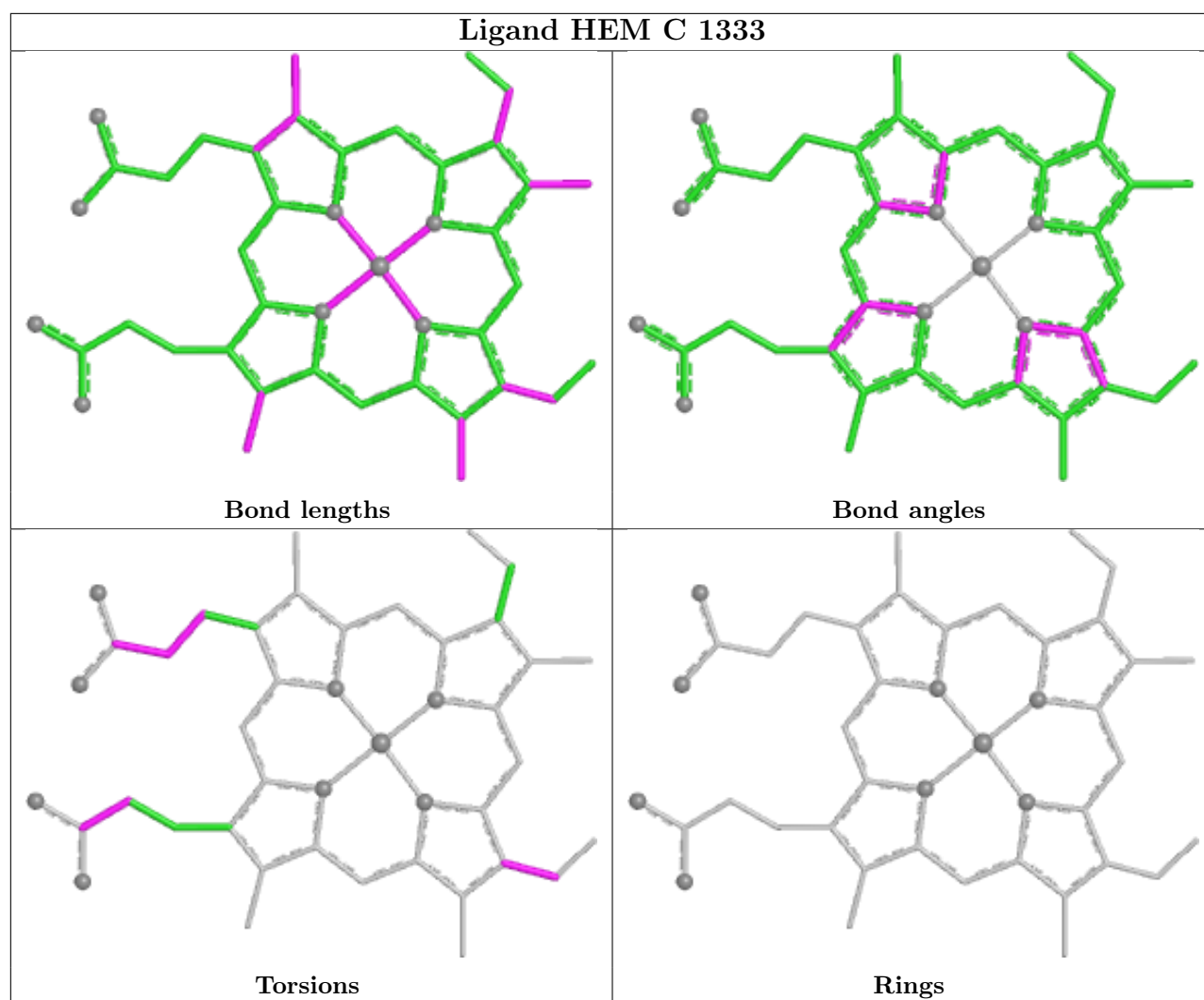


Ligand HEM C 1335



Ligand MQ7 M 1328





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	C	332/336 (98%)	0.14	19 (5%)	29 33	12, 15, 19, 21	0
2	H	242/258 (93%)	0.14	11 (4%)	38 38	12, 16, 25, 26	0
3	L	273/274 (99%)	0.31	16 (5%)	28 33	10, 15, 21, 22	0
4	M	323/324 (99%)	-0.12	10 (3%)	51 46	11, 15, 20, 20	0
All	All	1170/1192 (98%)	0.11	56 (4%)	35 37	10, 15, 21, 26	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	178	LYS	8.9
2	H	195	LEU	7.5
3	L	144	HIS	6.3
1	C	179	TYR	6.2
3	L	115	TRP	5.8
3	L	166	ASN	5.5
1	C	10	THR	5.4
4	M	306	PRO	5.4
1	C	206	GLN	5.3
3	L	223	SER	4.8
1	C	303	ALA	4.8
1	C	17	LEU	4.6
3	L	264	GLY	4.6
2	H	84	GLU	4.4
2	H	246	LEU	4.2
1	C	131	THR	4.2
3	L	151	LEU	4.1
3	L	165	LEU	4.0
1	C	182	TYR	4.0
1	C	12	THR	3.9
4	M	43	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	171	LEU	3.6
1	C	238	ASP	3.5
3	L	1	ALA	3.4
1	C	132	CYS	3.3
2	H	205	LYS	3.2
3	L	80	LEU	3.2
4	M	320	GLY	3.2
4	M	115	MET	3.1
1	C	154	LEU	3.1
4	M	165	LEU	3.1
2	H	16	VAL	3.0
1	C	234	MET	2.9
2	H	180	PHE	2.9
2	H	4	GLY	2.9
3	L	212	GLU	2.9
1	C	301	PRO	2.8
1	C	120	ASN	2.8
3	L	119	LEU	2.8
2	H	123	VAL	2.8
3	L	26	VAL	2.7
2	H	73	GLY	2.5
3	L	155	ASP	2.5
4	M	303	PRO	2.5
1	C	123	GLN	2.5
4	M	1	ALA	2.4
4	M	155	VAL	2.3
2	H	186	SER	2.3
1	C	195	ALA	2.2
1	C	2	PHE	2.2
3	L	257	ARG	2.2
3	L	122	CYS	2.2
4	M	278	ALA	2.1
4	M	189	ILE	2.1
1	C	18	SER	2.1
3	L	57	PRO	2.0

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

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
2	FME	H	1	10/11	0.76	0.18	18,18,18,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

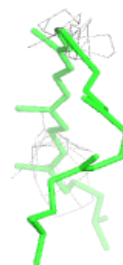
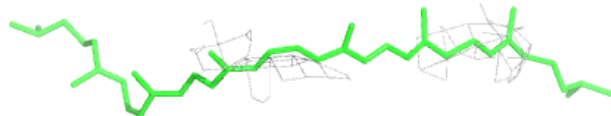
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
10	NS5	M	1329	40/40	0.85	0.18	27,28,30,30	0
6	BCB	M	1324	65/66	0.86	0.14	16,16,16,17	0
6	BCB	L	1275	66/66	0.87	0.18	19,20,21,21	0
9	MQ7	M	1328	48/48	0.90	0.19	9,9,10,10	0
7	BPB	M	1326	61/65	0.91	0.13	26,26,27,27	0
7	BPB	L	1276	65/65	0.92	0.17	2,2,4,4	0
6	BCB	M	1325	66/66	0.92	0.12	12,12,15,15	0
6	BCB	L	1274	66/66	0.93	0.14	29,29,30,30	0
5	HEM	C	1334	43/43	0.95	0.13	2,2,2,2	0
5	HEM	C	1336	43/43	0.96	0.11	2,2,2,2	0
5	HEM	C	1333	43/43	0.96	0.09	15,16,16,16	0
5	HEM	C	1335	43/43	0.96	0.11	4,4,4,4	0
8	FE2	M	1327	1/1	1.00	0.00	2,2,2,2	0

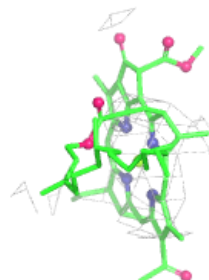
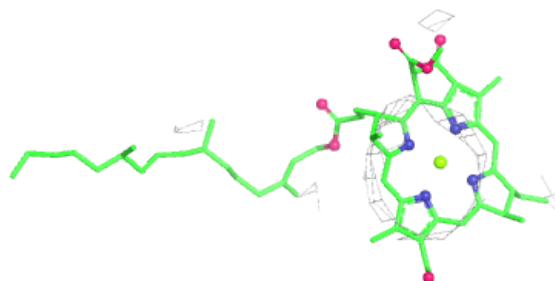
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS5 M 1329:

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

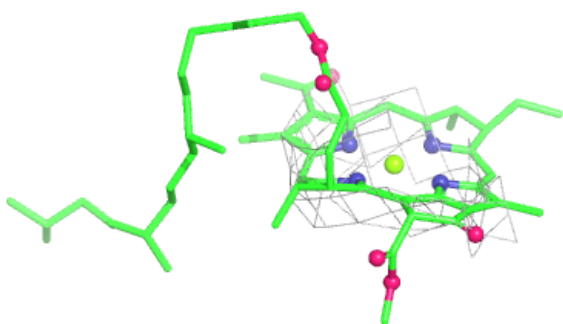
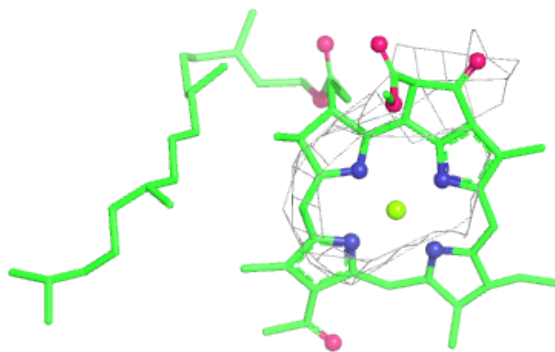
**Electron density around BCB M 1324:**

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

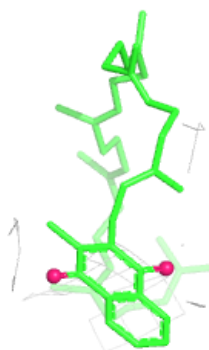
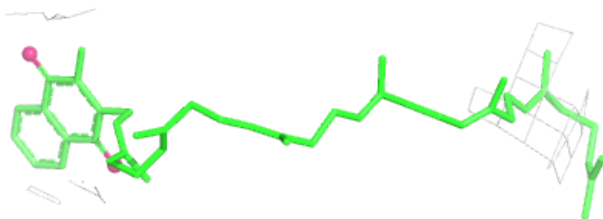
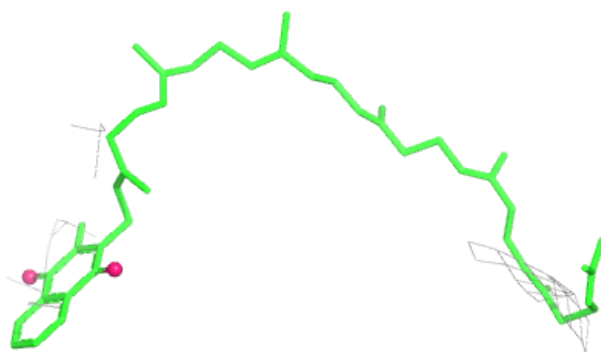


Electron density around BCB L 1275:

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

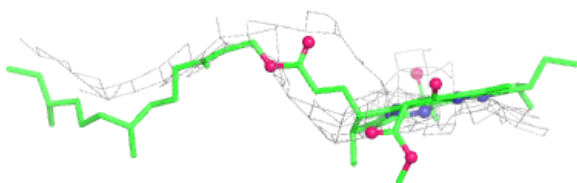
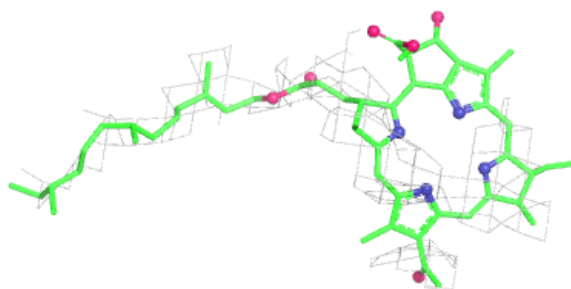
**Electron density around MQ7 M 1328:**

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



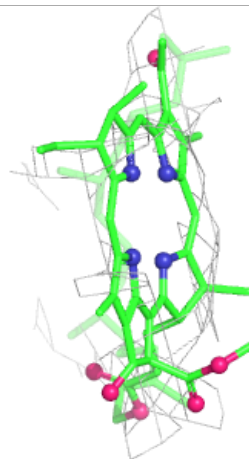
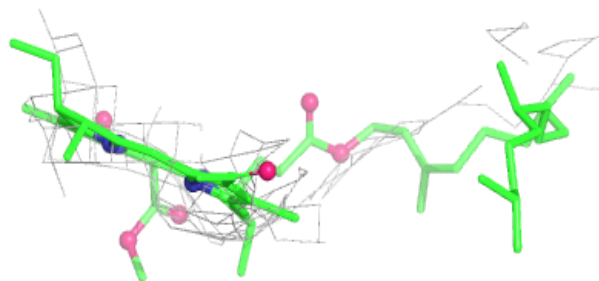
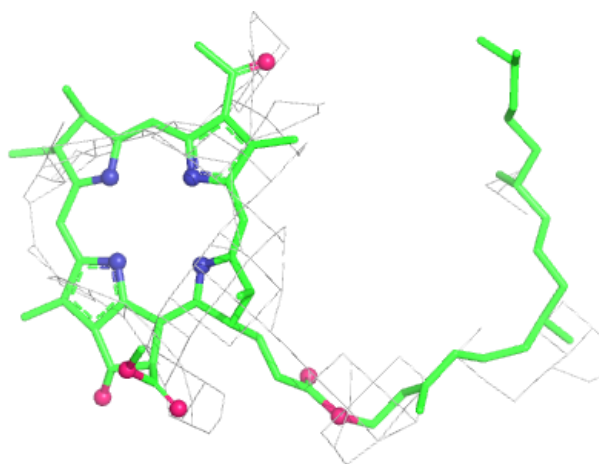
Electron density around BPB M 1326:

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



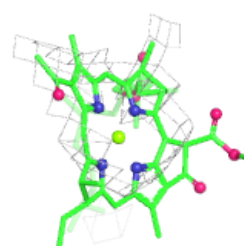
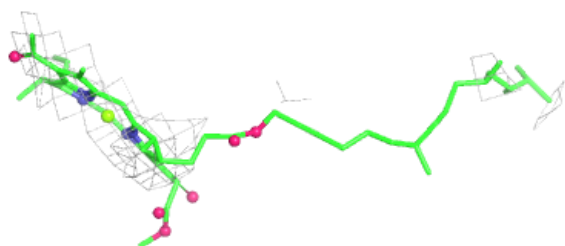
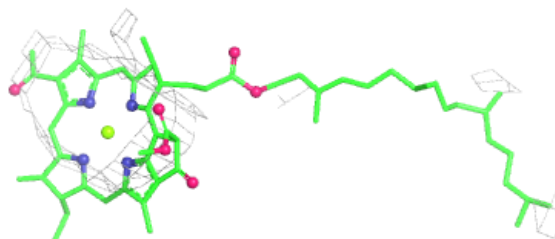
Electron density around BPB L 1276:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

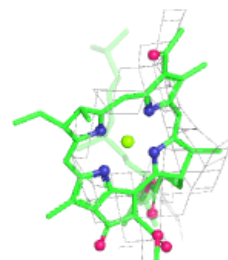


Electron density around BCB M 1325:

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

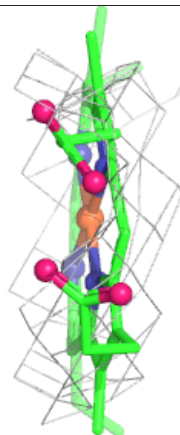
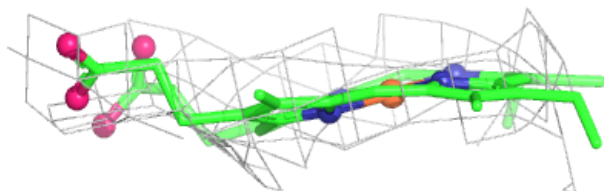
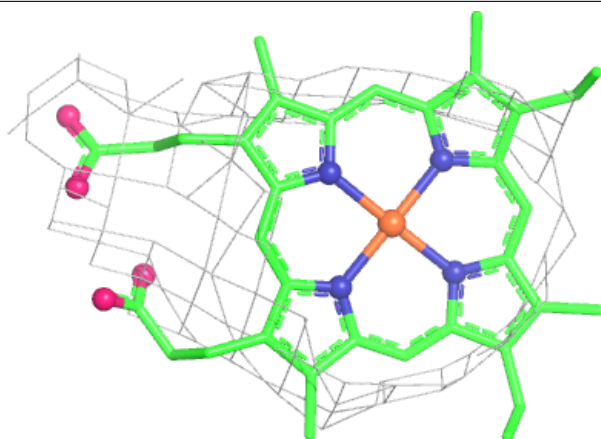
**Electron density around BCB L 1274:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



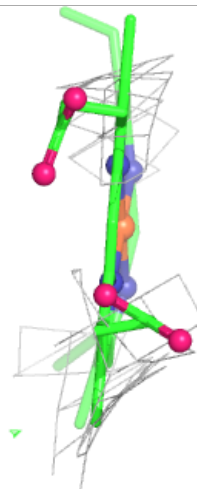
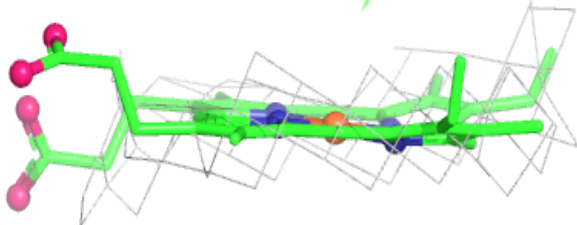
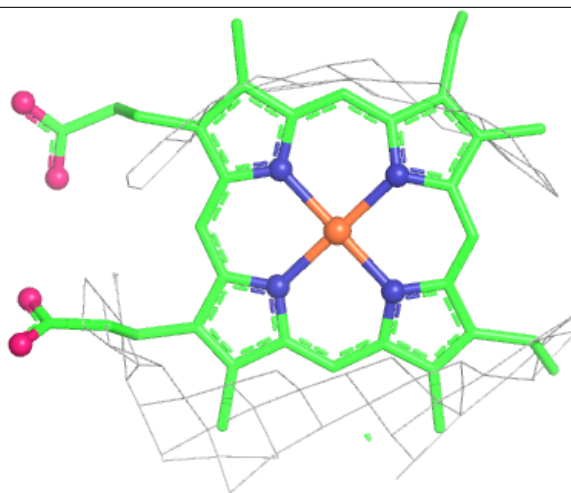
Electron density around HEM C 1334:

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



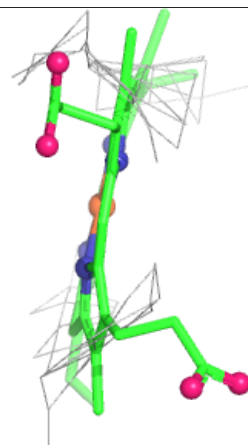
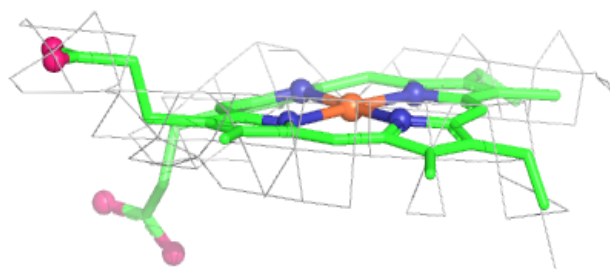
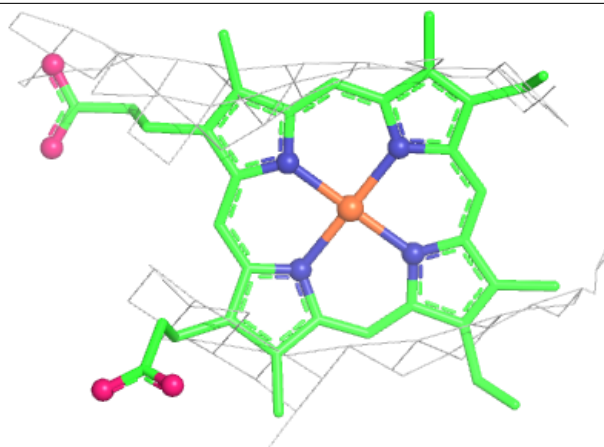
Electron density around HEM C 1336:

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



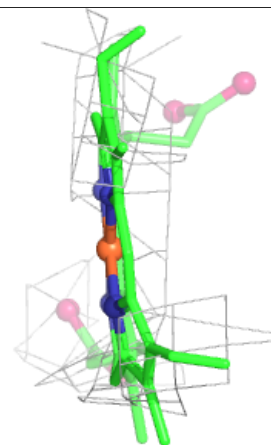
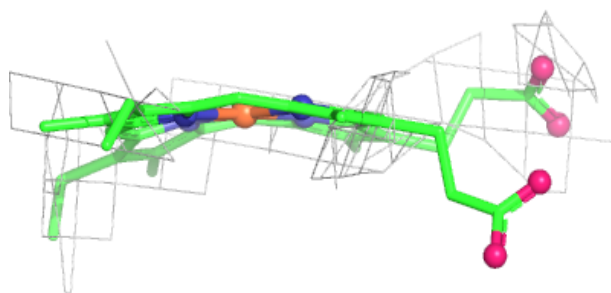
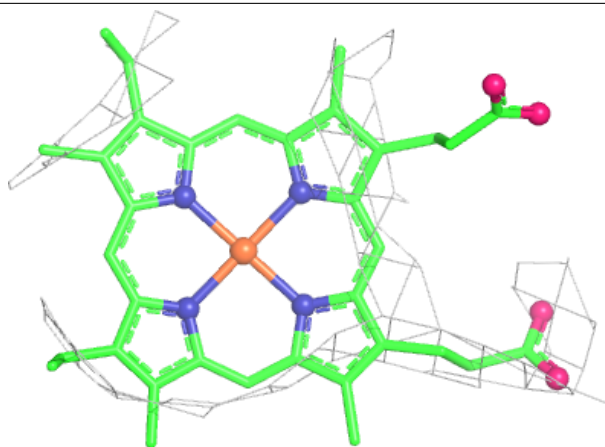
Electron density around HEM C 1333:

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



Electron density around HEM C 1335:

$2mF_o-DF_c$ (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.