



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:17 PM BST

PDB ID : 7PRC
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (DG-420315 (TRIAZINE) COMPLEX)
Authors : Lancaster, C.R.D.; Michel, H.
Deposited on : 1997-08-01
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

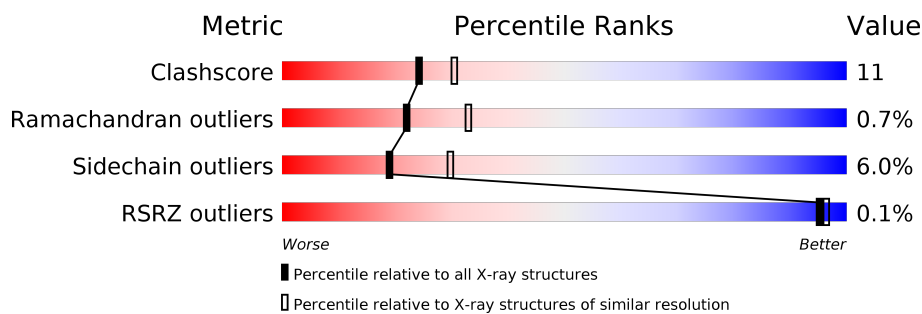
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.65 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))
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 ≥ 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	C	336	
2	L	273	
3	M	323	
4	H	258	

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
7	BPB	L	402	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10476 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	51	1	0
			2607	1642	467	480	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	14	0	0
			2171	1459	350	355	7			

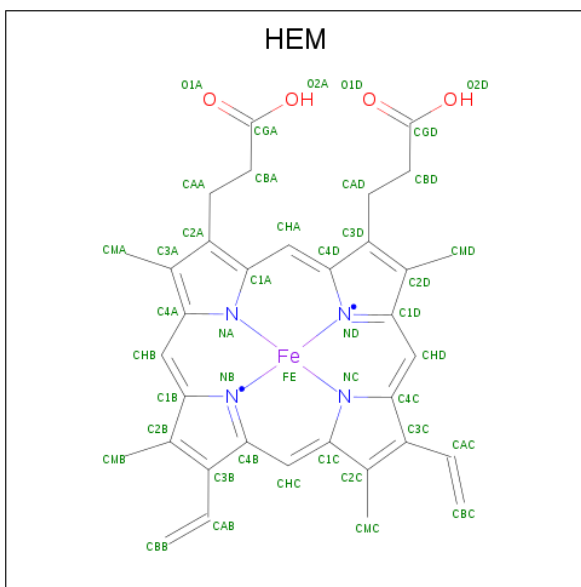
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	19	2	0
			2577	1720	421	425	11			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

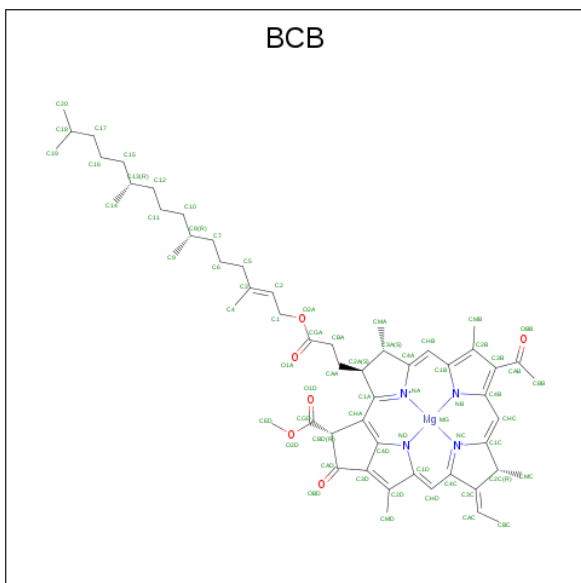
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	122	0	0
			2018	1292	344	380	2			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



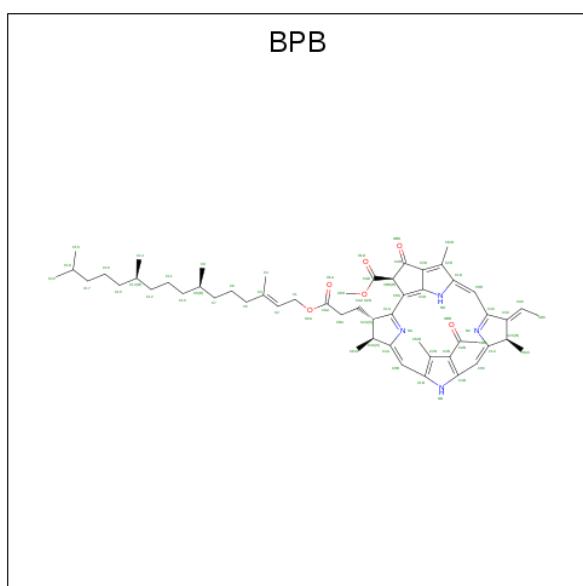
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_6$).



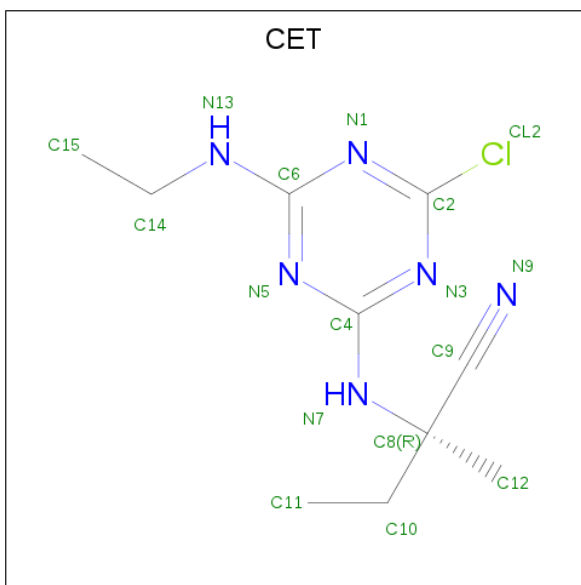
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



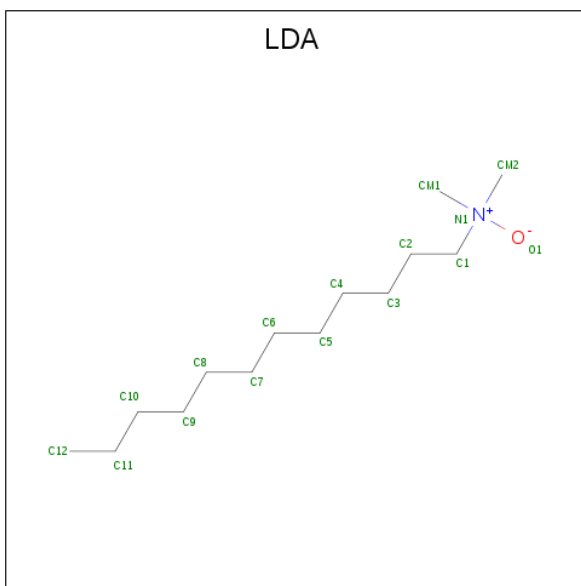
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	7	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is 2-CHLORO-4-ETHYLAMINO-6-(R(+)-2'-CYANO-4-BUTYLAMINO)-1,3,5-TRIAZINE (three-letter code: CET) (formula: $C_{10}H_{15}ClN_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	Cl	N	0	0
			17	10	1	6		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $\text{C}_{14}\text{H}_{31}\text{NO}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total 16	C 14	N 1	O 1	0	0
9	M	1	Total 16	C 14	N 1	O 1	0	0

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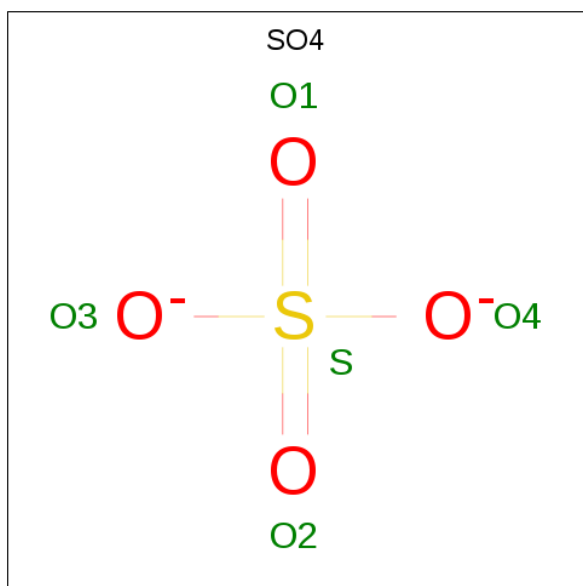
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	5	0
			16	14	1	1		
9	M	1	Total	C	N	O	4	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

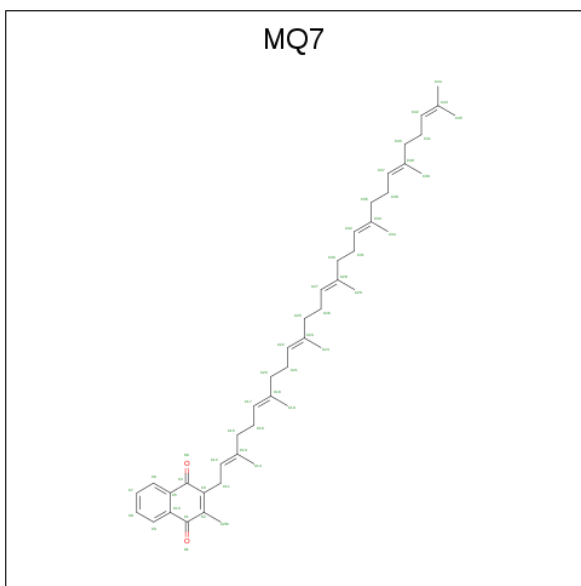
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



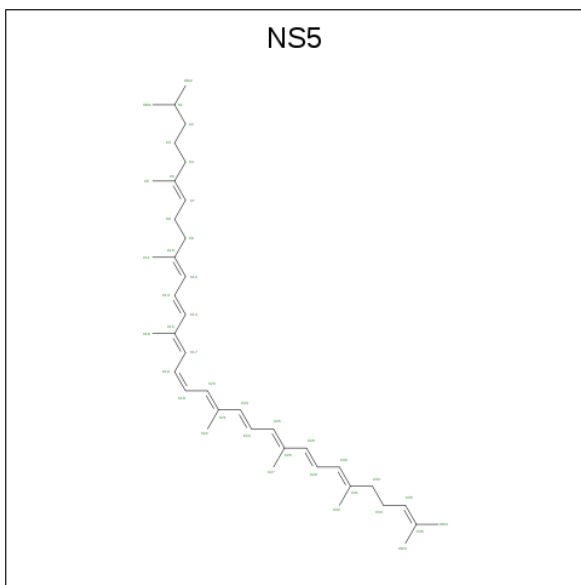
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	O	S	0	0
			5	4	1		
11	M	1	Total	O	S	0	0
			5	4	1		
11	M	1	Total	O	S	0	0
			5	4	1		
11	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



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

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C	4	0
			40	40		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	118	Total 118	O 118	0	0
14	L	55	Total 55	O 55	0	0
14	M	78	Total 78	O 78	0	0
14	H	64	Total 64	O 64	0	0

- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

R293	R146	C1
C308	Y147	T8
P315	L148	T12
A319	F449	R15
L322	P150	S18
K323	T151	M19
E327	P153	G20
L328	E158	L23
G329	T159	K29
P330	V163	Y38
I331	E164	G49
K332	R165	P50
ALA	V166	P51
ALA	E167	V52
LYS	T168	V55
	R169	Y56
	S170	X60
	V173	L65
	T174	T66
	R175	E57
	Y179	F70
	T180	I77
	A181	X80
	Y182	D92
	Y187	N95
	D188	Y102
	P189	P103
	R202	Y104
	V203	R108
	Y227	R109
	L232	M110
	M233	L111
	T252	R115
	K258	W121
	W269	T122
	M273	Q123
	L277	Y133
	N280	P142
	S288	
	L289	
	P290	
	A291	
	S292	

- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Y148	W156	W159	F160	G161	Y162	W166	W167	H168	S178	F181	V182	M185	L193	S196	X205	T208	Y215	D218	V219	V220	E230	A237	T240	T249	P253	R257	H272	S273										
A1	L2	L3	S4	F5	R12	L16	P22	D23	P24	G45	L49	A52	P57	D60	P61	L71	L80	L81	G84	F85	W100	R103	I107	S108	R109	I113	G114	W115	L119	A120	F121	P124	R135	P136	L139	G143	F146	P147

- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

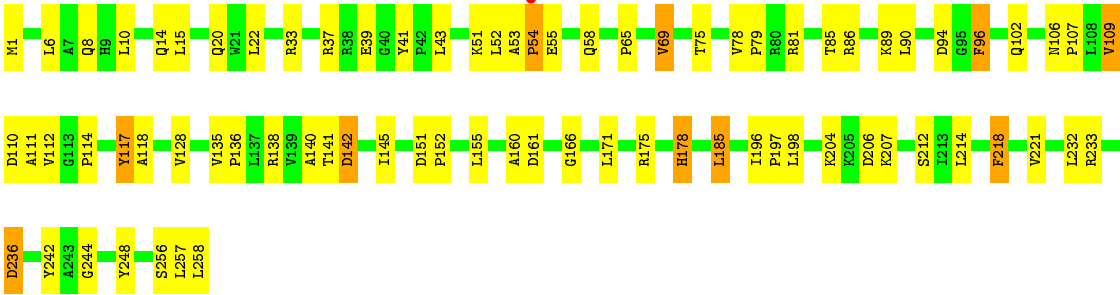
W292	W178	A1
Y293	I181	I10
	D182	Q11
V297	W183	I17
A307	L184	
	G192	S20
A311	N193	W37
T312	F194	I38
P313	Y195	G39
L318	H200	R40
P319	G201	
G320	F202	L51
A321	S203	P61
P322	I204	
K323	G205	F71
		N72
	Y208	M73
		D80
	F214	P81
	H217	L82
		Q83
	I221	L91
	L222	
	A223	X97
	R231	
	E232	L107
	I233	
	I236	G111
		M112
		N113
	R239	L114
	G240	M115
	T241	
		S126
	R245	S133
	F249	R134
		A135
	W252	R136
		G141
	F256	I144
	H257	
	A258	N147
	E261	
	S262	F154
	R265	C157
	M275	C160
		I161
	V289	H162
	D290	R163
	F293	

- Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:

70%

26%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50 Å 223.50 Å 113.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65 29.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (10.00-2.65) 87.0 (29.74-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.61 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.231 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10476	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: LDA, BPB, BCB, CET, FE2, SO4, MQ7, HEM, FME, NS5

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	0.55	0/2674	0.67	2/3645 (0.1%)
2	L	0.58	0/2259	0.62	0/3084
3	M	0.58	0/2683	0.62	0/3669
4	H	0.67	2/2055 (0.1%)	0.86	4/2807 (0.1%)
All	All	0.59	2/9671 (0.0%)	0.69	6/13205 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
2	L	0	7
3	M	0	5
4	H	0	2
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	54	PRO	C-N	14.77	1.68	1.34
4	H	52	LEU	C-N	-6.29	1.19	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	52	LEU	O-C-N	-18.31	93.41	122.70
4	H	52	LEU	CA-C-N	13.07	145.95	117.20
4	H	52	LEU	C-N-CA	8.96	144.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	53	ALA	CB-CA-C	-6.78	99.92	110.10
1	C	50	PRO	CB-CA-C	-5.63	97.93	112.00
1	C	329	GLY	C-N-CD	-5.03	109.53	120.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	ARG	Sidechain
1	C	187	TYR	Sidechain
1	C	202	ARG	Sidechain
1	C	227	TYR	Sidechain
4	H	117	TYR	Sidechain
4	H	218	PHE	Sidechain
2	L	103	ARG	Sidechain
2	L	148	TYR	Sidechain
2	L	160	PHE	Sidechain
2	L	162	TYR	Sidechain
2	L	215	TYR	Sidechain
2	L	257	ARG	Sidechain
2	L	85	PHE	Sidechain
3	M	154	PHE	Sidechain
3	M	231	ARG	Sidechain
3	M	249	PHE	Sidechain
3	M	265	ARG	Sidechain
3	M	61	PHE	Sidechain

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	C	2607	0	2575	54	0
2	L	2171	0	2098	46	0
3	M	2577	0	2468	60	0
4	H	2018	0	2019	51	0
5	C	172	0	120	6	0
6	L	132	0	144	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	132	0	144	14	0
7	L	130	0	148	18	0
8	L	17	0	15	1	0
9	H	16	0	31	1	0
9	L	16	0	31	0	0
9	M	64	0	124	5	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	2	0
12	M	48	0	64	1	0
13	M	40	0	60	7	0
14	C	118	0	0	3	0
14	H	64	0	0	0	0
14	L	55	0	0	1	0
14	M	78	0	0	2	0
All	All	10476	0	10041	216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (216) 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)
4:H:54:PRO:C	4:H:55:GLU:N	1.68	1.44
7:L:402:BPB:HBBB	7:L:402:BPB:HHC	1.54	0.90
6:M:805:BCB:HBB2	6:M:805:BCB:HHC	1.57	0.85
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.09	0.83
2:L:181:PHE:HB3	7:L:401:BPB:CBB	2.10	0.81
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.65	0.78
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.67	0.76
1:C:152:LEU:HB3	1:C:164:GLU:HG2	1.69	0.75
7:L:401:BPB:H4B	6:M:806:BCB:H172	1.69	0.75
9:M:701:LDA:HM21	9:M:705:LDA:H22	1.71	0.73
1:C:123[A]:GLN:HG3	1:C:269:TRP:CE3	2.24	0.73
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.26	0.71
2:L:178:SER:O	2:L:182:VAL:HG23	1.91	0.70
3:M:160:CYS:SG	13:M:600:NS5:C31	2.80	0.69
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.76	0.68
3:M:160:CYS:SG	13:M:600:NS5:H332	2.34	0.68
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.73	0.67
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LYS:HG2	3:M:307:ALA:HB2	1.77	0.66
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.60	0.65
1:C:323:LYS:HD3	1:C:323:LYS:H	1.62	0.65
6:M:805:BCB:CBB	6:M:805:BCB:HHC	2.26	0.64
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.80	0.64
2:L:208:THR:HG21	4:H:128:VAL:HG23	1.79	0.64
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.79	0.64
1:C:52:VAL:HG13	1:C:65:LEU:O	1.98	0.64
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.32	0.63
3:M:195:TYR:CE2	6:M:806:BCB:HMC2	2.34	0.63
7:L:401:BPB:HHC	7:L:401:BPB:HBBB	1.80	0.63
6:L:302:BCB:OBB	6:L:302:BCB:HHC	1.99	0.63
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.80	0.63
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.80	0.63
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.81	0.62
4:H:107:PRO:HA	4:H:110:ASP:HB2	1.82	0.62
3:M:160:CYS:SG	13:M:600:NS5:H322	2.40	0.61
1:C:323:LYS:H	1:C:323:LYS:CD	2.14	0.61
3:M:195:TYR:CZ	6:M:806:BCB:HMC2	2.36	0.61
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.36	0.60
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.36	0.60
2:L:185:MET:SD	6:M:805:BCB:H41	2.41	0.60
6:M:805:BCB:HBB3	6:M:806:BCB:H41	1.83	0.60
3:M:231:ARG:HD2	14:M:1013:HOH:O	2.02	0.59
2:L:230:HIS:CD2	3:M:221:ILE:HG13	2.37	0.59
7:L:401:BPB:HBBB	7:L:401:BPB:CHC	2.33	0.58
3:M:136:ARG:HE	3:M:136:ARG:HA	1.69	0.58
1:C:8:THR:HB	1:C:23:LEU:HB2	1.86	0.58
4:H:37:ARG:HG2	4:H:41:TYR:CZ	2.39	0.57
4:H:86:ARG:NH2	4:H:111:ALA:O	2.36	0.57
2:L:215:TYR:O	2:L:219:VAL:HG23	2.03	0.57
1:C:56:TYR:HB3	5:C:337:HEM:O2A	2.04	0.57
2:L:181:PHE:HB3	7:L:401:BPB:HBB	1.86	0.57
7:L:402:BPB:HBB	3:M:208:TYR:CD2	2.40	0.57
1:C:121:TRP:HA	1:C:123[A]:GLN:HE21	1.70	0.57
4:H:136:PRO:HG2	4:H:138:ARG:HG2	1.86	0.57
1:C:189:PRO:HB3	1:C:232:LEU:HA	1.86	0.56
6:L:302:BCB:HMC1	6:L:302:BCB:HBC3	1.88	0.56
2:L:181:PHE:CD2	7:L:401:BPB:HBB	2.41	0.56
8:L:502:CET:H101	8:L:502:CET:N3	2.21	0.56
7:L:401:BPB:HMDA	3:M:147:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:55:GLU:HB3	4:H:58:GLN:HG3	1.88	0.55
4:H:90:LEU:HA	4:H:102:GLN:O	2.06	0.55
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.41	0.55
2:L:124:PRO:HB2	6:L:302:BCB:H93	1.89	0.54
6:L:304:BCB:HHC	6:L:304:BCB:OBB	2.07	0.54
3:M:192:GLY:O	3:M:193:ASN:HB3	2.06	0.54
4:H:166:GLY:HA3	4:H:185:LEU:HD12	1.89	0.54
2:L:220:VAL:HG11	7:L:401:BPB:HEDA	1.89	0.54
3:M:204:ILE:HG12	6:M:806:BCB:HMB3	1.90	0.54
4:H:218:PHE:HA	4:H:221:VAL:HG23	1.89	0.54
4:H:114:PRO:HB2	4:H:244:GLY:HA2	1.90	0.53
2:L:109:ARG:HD2	14:L:1243:HOH:O	2.08	0.53
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.72	0.53
7:L:401:BPB:HBCA	3:M:275:MET:HG2	1.90	0.53
4:H:152:PRO:HD2	4:H:171:LEU:HD11	1.90	0.53
1:C:170:SER:HB2	3:M:83:GLN:HG3	1.90	0.53
2:L:185:MET:SD	6:M:805:BCB:C4	2.97	0.52
1:C:323:LYS:HD3	1:C:323:LYS:N	2.25	0.52
2:L:139:LEU:HD21	2:L:253:PRO:HD3	1.92	0.52
2:L:12:ARG:HD3	4:H:102:GLN:NE2	2.26	0.51
6:L:304:BCB:HMB1	6:L:304:BCB:CBB	2.41	0.51
1:C:319:ALA:HB2	14:C:1169:HOH:O	2.11	0.51
4:H:233:ARG:O	4:H:233:ARG:HG2	2.11	0.50
1:C:50:PRO:HB2	1:C:55:VAL:HG23	1.91	0.50
2:L:193:LEU:HB2	3:M:144:ILE:HD11	1.94	0.50
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.47	0.50
4:H:155:LEU:HD22	4:H:206:ASP:C	2.32	0.50
2:L:81:LEU:HD23	2:L:85:PHE:CE2	2.47	0.50
3:M:289:VAL:HG11	3:M:292:TRP:CD2	2.47	0.50
3:M:160:CYS:SG	13:M:600:NS5:C30	3.00	0.50
2:L:124:PRO:HB2	6:L:302:BCB:C9	2.42	0.50
3:M:160:CYS:SG	13:M:600:NS5:C32	2.99	0.50
1:C:252:THR:HG23	1:C:252:THR:O	2.11	0.49
2:L:166:ASN:OD1	2:L:168:HIS:HB2	2.12	0.49
1:C:123[A]:GLN:HG3	1:C:269:TRP:CD2	2.47	0.49
4:H:106:ASN:ND2	4:H:109:VAL:HG23	2.28	0.49
6:L:302:BCB:HMB1	6:L:302:BCB:CBB	2.42	0.49
4:H:145:ILE:HD13	4:H:151:ASP:HA	1.95	0.49
3:M:160:CYS:SG	13:M:600:NS5:C33	2.99	0.49
4:H:65:PRO:HA	4:H:79:PRO:HD2	1.95	0.49
2:L:205:LYS:HA	4:H:69:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:256:PHE:HB2	4:H:33:ARG:NH2	2.27	0.49
1:C:146:ARG:NH2	1:C:150:PRO:HA	2.28	0.48
4:H:65:PRO:HG3	9:H:703:LDA:H82	1.95	0.48
4:H:204:LYS:HB2	4:H:207:LYS:O	2.13	0.48
4:H:37:ARG:HG2	4:H:41:TYR:CE1	2.48	0.48
4:H:54:PRO:C	4:H:55:GLU:CA	2.73	0.48
4:H:96:PHE:H	4:H:96:PHE:HD1	1.61	0.48
1:C:65:LEU:HD11	1:C:327:GLU:CG	2.40	0.48
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.95	0.48
3:M:73:MET:HE3	3:M:91:LEU:HB2	1.95	0.48
2:L:148:TYR:CE1	7:L:402:BPB:H14	2.48	0.48
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.48	0.48
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.49	0.47
6:M:806:BCB:HBD	6:M:806:BCB:HAA2	1.97	0.47
3:M:160:CYS:C	3:M:163:PRO:HD2	2.35	0.47
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.97	0.47
4:H:145:ILE:CD1	4:H:151:ASP:HA	2.45	0.47
1:C:52:VAL:HA	1:C:55:VAL:HB	1.97	0.47
2:L:22:PHE:HA	2:L:24:PHE:HE1	1.79	0.47
2:L:1:ALA:N	4:H:43:LEU:HB3	2.30	0.47
6:L:302:BCB:HBB3	6:M:805:BCB:HMD2	1.96	0.47
2:L:16:LEU:HD12	2:L:16:LEU:HA	1.63	0.47
3:M:154:PHE:O	3:M:157:CYS:HB2	2.14	0.47
6:M:806:BCB:HBB3	6:M:806:BCB:HMB1	1.96	0.47
3:M:289:VAL:HG11	3:M:292:TRP:CE3	2.50	0.46
1:C:115:ARG:HA	1:C:328:LEU:O	2.15	0.46
3:M:293:TYR:O	3:M:297:VAL:HG23	2.16	0.46
2:L:196:SER:HB2	3:M:141:GLY:O	2.15	0.46
2:L:237:ALA:HA	2:L:240:ILE:HD12	1.97	0.46
1:C:123[A]:GLN:H	1:C:123[A]:GLN:NE2	2.14	0.46
1:C:179:TYR:HB2	14:C:914:HOH:O	2.14	0.46
4:H:78:VAL:HA	4:H:79:PRO:C	2.36	0.46
2:L:113:ILE:HB	3:M:223:ALA:O	2.16	0.46
1:C:233:MET:HB3	5:C:339:HEM:C4B	2.51	0.46
2:L:45:GLY:O	2:L:49:ILE:HG13	2.16	0.46
7:L:401:BPB:C1B	6:M:805:BCB:H42	2.46	0.46
2:L:3:LEU:HD13	2:L:5:PHE:CZ	2.51	0.46
3:M:133:SER:OG	9:M:704:LDA:HM12	2.17	0.45
1:C:49:GLY:HA3	1:C:50:PRO:HD3	1.63	0.45
1:C:273:MET:O	1:C:277:LEU:HG	2.16	0.45
4:H:96:PHE:CD1	4:H:96:PHE:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:LEU:HD23	2:L:85:PHE:HE2	1.80	0.45
1:C:50:PRO:HB2	1:C:55:VAL:CG2	2.47	0.45
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.98	0.45
1:C:104:TYR:HE1	1:C:108:ARG:NH2	2.15	0.45
4:H:90:LEU:HD21	4:H:112:VAL:HB	1.99	0.45
1:C:110:MET:HB3	5:C:338:HEM:C4B	2.52	0.44
1:C:70:PHE:HE2	5:C:337:HEM:C2A	2.35	0.44
1:C:108:ARG:NH1	5:C:337:HEM:O2D	2.50	0.44
4:H:6:LEU:HA	4:H:6:LEU:HD23	1.77	0.44
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.99	0.44
1:C:163:VAL:HB	2:L:273:SER:O	2.17	0.44
1:C:181:ALA:O	1:C:182:TYR:HB2	2.18	0.44
3:M:10:ILE:CG2	4:H:145:ILE:HG23	2.48	0.44
2:L:107:ILE:HG23	3:M:252:TRP:HE3	1.83	0.44
6:M:805:BCB:HBA2	6:M:805:BCB:C4A	2.47	0.44
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.53	0.44
1:C:92:ASP:HB3	1:C:95:ASN:O	2.18	0.43
3:M:112:TRP:CZ2	9:M:706:LDA:H51	2.53	0.43
3:M:241:THR:O	3:M:245:ARG:HG3	2.18	0.43
1:C:173:VAL:HG13	14:C:1137:HOH:O	2.18	0.43
4:H:106:ASN:CG	4:H:109:VAL:HG23	2.39	0.43
4:H:196:ILE:HD12	4:H:242:TYR:CE1	2.53	0.43
3:M:262:SER:O	3:M:265:ARG:HB2	2.18	0.43
1:C:109:ARG:NH2	1:C:280:ASN:O	2.52	0.43
2:L:115:TRP:CD1	2:L:115:TRP:N	2.86	0.43
1:C:308:CYS:O	1:C:315:PRO:HB3	2.18	0.43
4:H:114:PRO:HD2	4:H:248:TYR:CE2	2.53	0.43
13:M:600:NS5:H29	13:M:600:NS5:H271	1.71	0.43
7:L:401:BPB:H7A	7:L:401:BPB:H4	2.00	0.43
3:M:162:HIS:HD2	14:M:913:HOH:O	2.02	0.43
3:M:240:GLY:HA2	4:H:118:ALA:CB	2.49	0.43
4:H:142:ASP:OD1	4:H:142:ASP:N	2.50	0.43
3:M:183:TRP:CE3	3:M:184:LEU:HD23	2.53	0.43
3:M:239:ARG:HD3	4:H:39:GLU:OE1	2.18	0.43
1:C:111:LEU:HD23	5:C:338:HEM:CBB	2.49	0.43
2:L:52:ALA:HB2	2:L:85:PHE:CG	2.53	0.43
3:M:112:TRP:O	3:M:115:MET:HB2	2.19	0.43
4:H:10:LEU:HD21	4:H:15:LEU:HD21	2.01	0.42
3:M:233:ILE:O	3:M:236:ILE:HB	2.19	0.42
1:C:12:THR:OG1	1:C:20:GLY:HA2	2.19	0.42
2:L:80:LEU:HD12	2:L:80:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LEU:HD11	1:C:330:PRO:HD3	2.00	0.42
3:M:217:HIS:CE1	3:M:221:ILE:HD11	2.55	0.42
4:H:135:VAL:HG23	4:H:140:ALA:HB2	2.01	0.42
4:H:69:VAL:HA	4:H:75:THR:HG22	2.01	0.42
2:L:60:ASP:HA	2:L:61:PRO:HD3	1.80	0.42
3:M:11:GLN:OE1	3:M:39:GLY:HA3	2.20	0.42
2:L:100:TRP:CH2	12:M:501:MQ7:H301	2.55	0.42
6:L:304:BCB:H62	6:L:304:BCB:H92	1.75	0.42
3:M:1:ALA:N	11:M:803:SO4:S	2.85	0.42
11:M:804:SO4:O4	9:M:704:LDA:H22	2.20	0.42
3:M:17:ILE:HG13	4:H:178:HIS:CE1	2.55	0.42
2:L:121:PHE:O	2:L:124:PRO:HG2	2.19	0.42
3:M:318:LEU:HB2	3:M:321:ALA:HB2	2.02	0.42
1:C:77:ILE:HD11	1:C:111:LEU:HD21	2.02	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.55	0.41
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.56	0.41
3:M:236:ILE:HG12	3:M:261:GLU:HB2	2.01	0.41
6:L:304:BCB:HBB3	6:L:304:BCB:HMB1	2.02	0.41
3:M:311:ALA:O	3:M:313:PRO:HD3	2.20	0.41
1:C:153:PRO:HG2	1:C:158:GLU:HB2	2.03	0.41
1:C:329:GLY:HA2	1:C:330:PRO:C	2.41	0.41
7:L:401:BPB:H4	7:L:401:BPB:C7	2.50	0.41
1:C:123[A]:GLN:CD	1:C:123[A]:GLN:H	2.24	0.41
1:C:289:LEU:HD22	1:C:293:ARG:HG3	2.01	0.41
3:M:258:ALA:HB1	3:M:262:SER:OG	2.21	0.41
4:H:232:LEU:HA	4:H:232:LEU:HD23	1.89	0.40
3:M:205:GLY:HA3	9:M:701:LDA:H121	2.03	0.40
3:M:318:LEU:HA	3:M:319:PRO:HD2	1.64	0.40
3:M:80:ASP:HA	3:M:81:PRO:HD2	1.87	0.40
7:L:401:BPB:H6	7:L:401:BPB:H4	1.96	0.40
4:H:196:ILE:HG13	4:H:197:PRO:HD2	2.03	0.40
2:L:159:ASN:O	2:L:160:PHE:C	2.58	0.40
1:C:60:LYS:HB2	1:C:108:ARG:NH1	2.36	0.40
3:M:202:PHE:CZ	4:H:20:GLN:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/336 (98%)	314 (95%)	14 (4%)	3 (1%)	17	26
2	L	271/273 (99%)	255 (94%)	14 (5%)	2 (1%)	22	33
3	M	323/323 (100%)	308 (95%)	12 (4%)	3 (1%)	17	26
4	H	256/258 (99%)	241 (94%)	15 (6%)	0	100	100
All	All	1181/1190 (99%)	1118 (95%)	55 (5%)	8 (1%)	22	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	51	LEU
3	M	193	ASN
2	L	57	PRO
1	C	67	GLU
2	L	23	ASP
1	C	148	LEU
3	M	319	PRO
1	C	330	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	C	281/282 (100%)	263 (94%)	18 (6%)	17	27
2	L	218/218 (100%)	212 (97%)	6 (3%)	43	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	251/249 (101%)	238 (95%)	13 (5%)	23	36
4	H	212/212 (100%)	190 (90%)	22 (10%)	7	10
All	All	962/961 (100%)	903 (94%)	59 (6%)	19	29

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	29	LYS
1	C	38	TYR
1	C	115	ARG
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	142	PRO
1	C	146	ARG
1	C	159	THR
1	C	166	VAL
1	C	168	THR
1	C	169	ARG
1	C	170	SER
1	C	203	VAL
1	C	288	SER
1	C	292	SER
1	C	322	LEU
1	C	323	LYS
2	L	4	SER
2	L	16	LEU
2	L	119	LEU
2	L	160	PHE
2	L	249	ILE
2	L	272	TRP
3	M	20	SER
3	M	37	TRP
3	M	40	LYS
3	M	71	PHE
3	M	97	LYS
3	M	114	LEU
3	M	115	MET
3	M	126	SER
3	M	136	ARG
3	M	181	ILE

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Mol	Chain	Res	Type
3	M	203	SER
3	M	214	PHE
3	M	290	ASP
4	H	8	GLN
4	H	14	GLN
4	H	22	LEU
4	H	51	LYS
4	H	69	VAL
4	H	81	ARG
4	H	85	THR
4	H	89	LYS
4	H	94	ASP
4	H	96	PHE
4	H	109	VAL
4	H	141	THR
4	H	142	ASP
4	H	175	ARG
4	H	178	HIS
4	H	185	LEU
4	H	198	LEU
4	H	212	SER
4	H	236	ASP
4	H	256	SER
4	H	257	LEU
4	H	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
2	L	214	GLN
2	L	239	ASN
3	M	147	ASN
4	H	102	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	$\# Z > 2$
4	FME	H	1	4	8,9,10	0.61	0	7,9,11	2.81	2 (28%)

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	FME	H	1	4	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	O1-CN-N	-5.63	110.45	125.27
4	H	1	FME	CA-N-CN	-4.04	116.60	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	$\# Z > 2$
9	LDA	M	706	-	12,15,15	2.19	1 (8%)	14,17,17	0.50	0
8	CET	L	502	-	16,17,17	1.34	2 (12%)	21,23,23	0.89	1 (4%)
5	HEM	C	340	1	27,50,50	1.94	8 (29%)	17,82,82	1.48	3 (17%)
9	LDA	M	701	-	12,15,15	2.49	1 (8%)	14,17,17	0.71	0
9	LDA	H	703	-	12,15,15	2.27	1 (8%)	14,17,17	0.68	0
5	HEM	C	337	1	27,50,50	1.79	5 (18%)	17,82,82	0.94	1 (5%)
12	MQ7	M	501	-	49,49,49	1.49	12 (24%)	60,63,63	1.74	12 (20%)
5	HEM	C	338	1	27,50,50	1.54	4 (14%)	17,82,82	1.27	2 (11%)
9	LDA	M	704	-	12,15,15	1.93	1 (8%)	14,17,17	0.54	0
9	LDA	M	705	-	12,15,15	2.19	1 (8%)	14,17,17	0.50	0
11	SO4	M	802	-	4,4,4	0.57	0	6,6,6	0.83	0
9	LDA	L	702	-	12,15,15	2.27	1 (8%)	14,17,17	0.54	0
7	BPB	L	402	-	64,70,70	1.39	9 (14%)	64,101,101	1.63	9 (14%)
6	BCB	M	805	3	60,74,74	3.77	25 (41%)	48,115,115	2.87	18 (37%)
11	SO4	H	801	-	4,4,4	0.55	0	6,6,6	0.33	0
11	SO4	M	803	-	4,4,4	0.67	0	6,6,6	0.78	0
13	NS5	M	600	-	39,39,39	0.81	1 (2%)	44,46,46	1.20	6 (13%)
11	SO4	M	804	-	4,4,4	0.90	0	6,6,6	0.70	0
6	BCB	L	304	2	60,74,74	3.86	24 (40%)	48,115,115	2.56	17 (35%)
7	BPB	L	401	-	64,70,70	1.21	8 (12%)	64,101,101	2.04	14 (21%)
6	BCB	L	302	2	60,74,74	3.68	21 (35%)	48,115,115	2.38	14 (29%)
6	BCB	M	806	3	60,74,74	3.58	22 (36%)	48,115,115	2.92	16 (33%)
5	HEM	C	339	1	27,50,50	1.76	6 (22%)	17,82,82	1.66	5 (29%)

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
9	LDA	M	706	-	-	4/13/13/13	-
8	CET	L	502	-	-	0/11/14/14	0/1/1/1
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
5	HEM	C	338	1	-	0/6/54/54	-
5	HEM	C	339	1	-	0/6/54/54	-
7	BPB	L	401	-	-	8/47/105/105	0/5/6/6
5	HEM	C	337	1	-	0/6/54/54	-
9	LDA	M	704	-	-	6/13/13/13	-
6	BCB	M	805	3	-	12/41/177/177	-
5	HEM	C	340	1	-	0/6/54/54	-
9	LDA	M	705	-	-	1/13/13/13	-
9	LDA	M	701	-	-	5/13/13/13	-
13	NS5	M	600	-	-	14/43/43/43	-
6	BCB	L	304	2	-	11/41/177/177	-
9	LDA	L	702	-	-	4/13/13/13	-
9	LDA	H	703	-	-	3/13/13/13	-
6	BCB	L	302	2	-	9/41/177/177	-
6	BCB	M	806	3	-	14/41/177/177	-
7	BPB	L	402	-	1/1/18/23	5/47/105/105	0/5/6/6

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	304	BCB	C1A-CHA	-10.41	1.37	1.54
6	L	302	BCB	C1A-CHA	-9.79	1.38	1.54
6	M	805	BCB	CHB-C1B	-9.29	1.38	1.53
6	L	304	BCB	CHD-C4C	-9.27	1.37	1.53
6	M	805	BCB	CHD-C1D	-9.09	1.39	1.53
6	M	805	BCB	C1A-CHA	-8.94	1.40	1.54
6	L	304	BCB	CHD-C1D	-8.83	1.39	1.53
6	L	304	BCB	CHB-C1B	-8.71	1.39	1.53
6	L	304	BCB	CHC-C4B	-8.66	1.39	1.53
9	M	701	LDA	O1-N1	-8.57	1.22	1.42
6	L	302	BCB	CHD-C1D	-8.56	1.40	1.53
6	M	805	BCB	CHC-C4B	-8.51	1.40	1.53
6	M	806	BCB	CHB-C1B	-8.38	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	805	BCB	CHD-C4C	-7.94	1.40	1.53
6	M	806	BCB	CHD-C1D	-7.89	1.41	1.53
6	L	304	BCB	C3D-C2D	-7.83	1.34	1.55
6	L	302	BCB	CHC-C4B	-7.83	1.41	1.53
9	H	703	LDA	O1-N1	-7.82	1.23	1.42
9	L	702	LDA	O1-N1	-7.79	1.23	1.42
6	M	806	BCB	C1A-CHA	-7.75	1.41	1.54
6	L	302	BCB	CHB-C1B	-7.71	1.41	1.53
6	M	806	BCB	CHC-C4B	-7.70	1.41	1.53
9	M	705	LDA	O1-N1	-7.56	1.24	1.42
9	M	706	LDA	O1-N1	-7.53	1.24	1.42
6	L	302	BCB	CHD-C4C	-7.36	1.41	1.53
6	L	302	BCB	C3B-C2B	-7.15	1.36	1.55
6	M	806	BCB	CHD-C4C	-7.13	1.41	1.53
6	L	304	BCB	C3B-C2B	-6.99	1.37	1.55
6	L	302	BCB	C3D-C2D	-6.97	1.37	1.55
6	M	806	BCB	C3B-C2B	-6.94	1.37	1.55
6	M	805	BCB	C3B-C2B	-6.89	1.37	1.55
6	M	806	BCB	C3B-CAB	-6.80	1.44	1.52
6	M	806	BCB	C4D-ND	-6.79	1.36	1.50
6	M	806	BCB	C3D-C2D	-6.75	1.37	1.55
9	M	704	LDA	O1-N1	-6.62	1.26	1.42
6	L	302	BCB	C4D-ND	-6.51	1.36	1.50
6	M	805	BCB	C3D-C2D	-6.46	1.38	1.55
6	L	304	BCB	C4D-ND	-6.45	1.36	1.50
6	M	805	BCB	CHB-C4A	-6.40	1.38	1.52
6	M	805	BCB	C4D-ND	-6.31	1.37	1.50
6	L	304	BCB	CHC-C1C	-6.09	1.38	1.52
6	L	302	BCB	C3B-CAB	-6.08	1.45	1.52
6	L	304	BCB	CHB-C4A	-6.07	1.38	1.52
6	M	805	BCB	C1D-ND	-6.03	1.37	1.50
6	M	806	BCB	CHB-C4A	-5.92	1.39	1.52
6	L	304	BCB	C3B-CAB	-5.88	1.45	1.52
6	L	302	BCB	C1D-ND	-5.87	1.37	1.50
6	L	302	BCB	CHB-C4A	-5.79	1.39	1.52
6	L	304	BCB	C1D-ND	-5.79	1.38	1.50
6	L	302	BCB	C4B-NB	-5.74	1.38	1.50
6	M	806	BCB	C4B-NB	-5.74	1.38	1.50
6	M	805	BCB	C1B-NB	-5.69	1.38	1.50
6	L	304	BCB	C4B-NB	-5.66	1.38	1.50
6	M	806	BCB	C1D-ND	-5.61	1.38	1.50
6	L	302	BCB	C1B-NB	-5.59	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	805	BCB	C2B-C1B	-5.58	1.43	1.53
6	L	302	BCB	CHC-C1C	-5.51	1.40	1.52
6	M	805	BCB	CHC-C1C	-5.47	1.40	1.52
6	M	805	BCB	C4B-NB	-5.42	1.38	1.50
6	M	806	BCB	C1B-NB	-5.41	1.38	1.50
7	L	402	BPB	C3B-C4B	5.34	1.48	1.41
6	M	806	BCB	C2B-C1B	-5.31	1.43	1.53
6	L	304	BCB	C1B-NB	-5.27	1.39	1.50
6	L	302	BCB	C2B-C1B	-4.80	1.44	1.53
7	L	402	BPB	O2D-CED	-4.64	1.34	1.45
6	M	805	BCB	C3B-CAB	-4.63	1.47	1.52
6	M	806	BCB	CHC-C1C	-4.59	1.42	1.52
7	L	401	BPB	O2A-CGA	4.56	1.46	1.33
5	C	337	HEM	C3B-C2B	-4.51	1.34	1.40
6	M	805	BCB	C1-C2	-4.25	1.36	1.49
5	C	340	HEM	CAD-C3D	-4.22	1.44	1.52
6	M	805	BCB	O2D-CED	-4.13	1.35	1.45
5	C	340	HEM	CBC-CAC	4.12	1.56	1.29
6	L	302	BCB	O2D-CED	-4.10	1.35	1.45
6	L	304	BCB	C2D-C1D	-4.04	1.46	1.53
6	L	304	BCB	C2B-C1B	-4.04	1.46	1.53
5	C	339	HEM	CBC-CAC	3.90	1.55	1.29
5	C	339	HEM	CBB-CAB	3.81	1.54	1.29
6	L	302	BCB	C2D-C1D	-3.78	1.46	1.53
6	L	304	BCB	C3D-CAD	-3.77	1.44	1.51
5	C	337	HEM	C3C-C2C	-3.63	1.35	1.40
5	C	337	HEM	CBB-CAB	3.60	1.53	1.29
6	M	806	BCB	C3D-CAD	-3.60	1.44	1.51
8	L	502	CET	C9-N9	3.60	1.19	1.14
6	M	805	BCB	C2D-C1D	-3.55	1.46	1.53
5	C	337	HEM	CBC-CAC	3.53	1.52	1.29
5	C	338	HEM	CBC-CAC	3.49	1.52	1.29
6	L	302	BCB	C4C-C3C	-3.45	1.40	1.50
12	M	501	MQ7	C11-C12	-3.45	1.45	1.50
6	M	806	BCB	C2D-C1D	-3.43	1.47	1.53
6	M	806	BCB	C4C-C3C	-3.41	1.40	1.50
5	C	339	HEM	C3C-CAC	3.37	1.54	1.47
6	L	302	BCB	O2D-CGD	3.32	1.41	1.33
5	C	340	HEM	C3B-C2B	-3.30	1.35	1.40
5	C	340	HEM	C3C-CAC	3.28	1.54	1.47
5	C	338	HEM	C3C-C2C	-3.28	1.35	1.40
5	C	340	HEM	CBB-CAB	3.27	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	302	BCB	C3D-CAD	-3.25	1.45	1.51
6	M	805	BCB	C3D-CAD	-3.22	1.45	1.51
7	L	402	BPB	CMD-C2D	3.21	1.57	1.50
5	C	339	HEM	C3B-C2B	-3.19	1.35	1.40
12	M	501	MQ7	C32-C33	3.18	1.40	1.33
5	C	338	HEM	CBB-CAB	3.17	1.50	1.29
5	C	338	HEM	C3B-C2B	-3.16	1.36	1.40
6	L	302	BCB	C1-C2	-3.14	1.39	1.49
5	C	339	HEM	C3B-CAB	3.14	1.54	1.47
5	C	340	HEM	C3B-CAB	3.12	1.54	1.47
6	L	304	BCB	C4C-C3C	-3.10	1.41	1.50
7	L	401	BPB	C3B-C4B	3.04	1.45	1.41
5	C	339	HEM	C3C-C2C	-3.01	1.36	1.40
6	M	805	BCB	O2A-CGA	2.88	1.41	1.33
12	M	501	MQ7	C21-C22	-2.86	1.41	1.50
7	L	401	BPB	C2-C3	2.80	1.39	1.33
7	L	402	BPB	O2D-CGD	2.77	1.40	1.33
7	L	401	BPB	O2D-CGD	2.75	1.39	1.33
6	M	805	BCB	C4C-C3C	-2.74	1.42	1.50
6	L	304	BCB	O2D-CGD	2.71	1.39	1.33
6	M	806	BCB	C4A-C3A	-2.67	1.50	1.53
6	M	806	BCB	CAA-CBA	-2.66	1.44	1.52
13	M	600	NS5	C22-C21	-2.66	1.45	1.50
7	L	402	BPB	C2-C3	2.62	1.39	1.33
6	L	304	BCB	C1A-C2A	-2.59	1.50	1.53
8	L	502	CET	C8-C9	-2.57	1.47	1.49
6	M	806	BCB	C2-C3	2.50	1.39	1.33
12	M	501	MQ7	C37-C38	2.49	1.39	1.33
6	L	304	BCB	C2A-C3A	-2.47	1.50	1.54
12	M	501	MQ7	C42-C43	2.46	1.39	1.32
12	M	501	MQ7	C27-C28	2.45	1.38	1.33
6	L	304	BCB	O2D-CED	-2.43	1.39	1.45
12	M	501	MQ7	C10-C5	-2.42	1.36	1.40
12	M	501	MQ7	C17-C18	2.41	1.38	1.33
5	C	340	HEM	C3C-C2C	-2.40	1.37	1.40
7	L	402	BPB	C4C-C3C	-2.39	1.40	1.45
7	L	402	BPB	O2A-CGA	2.38	1.40	1.33
6	L	304	BCB	C2-C3	2.38	1.38	1.33
7	L	401	BPB	CAC-C3C	2.32	1.39	1.33
6	M	805	BCB	O2D-CGD	2.31	1.38	1.33
6	M	805	BCB	C1A-C2A	-2.29	1.51	1.53
7	L	401	BPB	C4D-ND	2.29	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	806	BCB	O2D-CGD	2.25	1.38	1.33
12	M	501	MQ7	C19-C18	2.23	1.56	1.50
7	L	401	BPB	C4C-C3C	-2.23	1.40	1.45
7	L	402	BPB	CMB-C2B	2.20	1.56	1.51
12	M	501	MQ7	C16-C17	-2.16	1.43	1.50
5	C	340	HEM	CAA-C2A	-2.16	1.48	1.52
7	L	402	BPB	C1-C2	-2.13	1.42	1.49
6	M	805	BCB	C2-C3	2.11	1.38	1.33
5	C	337	HEM	CMD-C2D	2.07	1.55	1.51
6	L	304	BCB	CMD-C2D	-2.06	1.49	1.53
12	M	501	MQ7	C22-C23	2.03	1.37	1.33
7	L	401	BPB	C3B-C2B	-2.02	1.35	1.39
6	M	805	BCB	C2A-C3A	-2.01	1.51	1.54
12	M	501	MQ7	C12-C13	2.01	1.37	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	806	BCB	CMB-C2B-C3B	8.96	136.54	114.29
6	M	805	BCB	CBB-CAB-C3B	8.60	125.58	116.80
7	L	401	BPB	O2D-CGD-CBD	7.52	124.63	111.27
6	M	806	BCB	OBB-CAB-C3B	7.42	129.34	121.52
6	M	805	BCB	C1D-CHD-C4C	7.41	128.16	112.37
6	L	304	BCB	C1D-CHD-C4C	7.21	127.73	112.37
6	M	806	BCB	C1D-CHD-C4C	7.18	127.67	112.37
6	M	805	BCB	CMB-C2B-C3B	6.91	131.46	114.29
6	L	302	BCB	C1D-CHD-C4C	6.81	126.87	112.37
6	L	304	BCB	CMB-C2B-C3B	6.61	130.70	114.29
6	L	302	BCB	CMB-C2B-C3B	6.57	130.60	114.29
7	L	401	BPB	OBB-CAB-C3B	6.52	131.56	119.99
7	L	402	BPB	O2D-CGD-CBD	6.47	122.77	111.27
6	L	304	BCB	CMD-C2D-C3D	5.80	128.69	114.29
6	L	302	BCB	CMD-C2D-C3D	5.64	128.30	114.29
6	L	304	BCB	O2D-CGD-CBD	5.53	124.09	111.11
6	M	805	BCB	CMD-C2D-C3D	5.41	127.72	114.29
7	L	401	BPB	CED-O2D-CGD	5.34	128.01	115.94
6	L	304	BCB	O1D-CGD-CBD	-5.25	114.14	124.54
6	M	806	BCB	CMD-C2D-C3D	5.18	127.17	114.29
7	L	402	BPB	O1D-CGD-CBD	-5.05	114.15	124.48
7	L	401	BPB	O1D-CGD-CBD	-4.84	114.58	124.48
6	M	806	BCB	CHA-CBD-CGD	-4.80	104.16	115.02
6	L	302	BCB	CHA-CBD-CGD	-4.74	104.28	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	501	MQ7	C29-C28-C30	-4.70	107.36	115.27
6	M	806	BCB	O2D-CGD-CBD	4.63	121.99	111.11
12	M	501	MQ7	C41-C42-C43	4.62	143.52	127.75
6	M	805	BCB	OBB-CAB-C3B	-4.60	116.67	121.52
6	M	806	BCB	O1D-CGD-CBD	-4.58	115.47	124.54
6	M	805	BCB	C1-C2-C3	4.40	133.65	126.04
6	M	805	BCB	CHA-CBD-CGD	-4.34	105.20	115.02
6	M	805	BCB	C4-C3-C5	4.28	122.47	115.27
7	L	401	BPB	CBB-CAB-C3B	-4.23	107.77	120.34
6	M	806	BCB	CBB-CAB-C3B	-4.23	112.48	116.80
6	M	806	BCB	O2A-CGA-CBA	4.20	125.10	111.91
13	M	600	NS5	C19-C20-C21	-4.17	121.36	127.31
6	M	805	BCB	O1D-CGD-CBD	-4.16	116.31	124.54
6	M	805	BCB	O2D-CGD-CBD	4.13	120.82	111.11
6	L	302	BCB	O1D-CGD-CBD	-4.13	116.36	124.54
7	L	401	BPB	C4B-C3B-CAB	-4.11	118.27	127.19
12	M	501	MQ7	C25-C23-C22	4.01	129.24	121.12
12	M	501	MQ7	C35-C33-C32	4.01	129.23	121.12
5	C	340	HEM	CBD-CAD-C3D	3.97	119.78	112.48
6	L	304	BCB	CHA-CBD-CGD	-3.85	106.31	115.02
6	M	806	BCB	C1-C2-C3	-3.81	119.46	126.04
6	L	302	BCB	OBB-CAB-C3B	3.78	125.50	121.52
6	L	302	BCB	CED-O2D-CGD	-3.70	107.56	115.94
6	M	806	BCB	CHC-C4B-C3B	3.70	127.24	118.17
12	M	501	MQ7	C34-C33-C35	-3.52	109.36	115.27
7	L	402	BPB	C3C-C2C-C1C	3.43	105.39	100.72
6	L	304	BCB	O2A-CGA-CBA	3.39	122.53	111.91
6	M	806	BCB	O2A-CGA-O1A	-3.39	115.05	123.59
12	M	501	MQ7	C24-C23-C25	-3.33	109.68	115.27
5	C	339	HEM	CMB-C2B-C3B	3.32	130.90	124.68
12	M	501	MQ7	C40-C41-C42	-3.32	100.96	111.88
6	M	806	BCB	CHC-C1C-C2C	3.30	127.15	117.19
5	C	339	HEM	CMD-C2D-C1D	-3.25	123.47	128.46
6	M	805	BCB	CHC-C4B-C3B	3.20	126.02	118.17
6	M	805	BCB	O2A-CGA-CBA	3.11	121.66	111.91
6	L	304	BCB	CHC-C4B-C3B	3.09	125.76	118.17
6	L	304	BCB	OBB-CAB-C3B	3.09	124.78	121.52
12	M	501	MQ7	C30-C28-C27	3.06	127.31	121.12
6	L	302	BCB	O2D-CGD-CBD	3.04	118.24	111.11
7	L	402	BPB	C4B-C3B-CAB	-3.01	120.65	127.19
6	L	302	BCB	CHC-C4B-C3B	3.01	125.55	118.17
7	L	401	BPB	C3C-C2C-C1C	2.96	104.75	100.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	805	BCB	C5-C3-C2	-2.96	115.13	121.12
5	C	338	HEM	CBA-CAA-C2A	-2.95	107.05	112.49
5	C	337	HEM	CMC-C2C-C3C	2.91	130.12	124.68
6	L	302	BCB	OBD-CAD-C3D	2.88	131.80	126.73
6	L	302	BCB	CHC-C1C-C2C	2.88	125.89	117.19
6	M	805	BCB	CHC-C1C-C2C	2.88	125.88	117.19
6	L	304	BCB	CHC-C1C-C2C	2.87	125.86	117.19
6	L	302	BCB	OBD-CAD-CBD	-2.86	120.64	127.49
6	M	805	BCB	OBD-CAD-CBD	-2.80	120.78	127.49
6	L	304	BCB	C3B-C4B-NB	2.79	108.84	103.75
6	L	304	BCB	OBD-CAD-CBD	-2.78	120.83	127.49
13	M	600	NS5	C23-C21-C20	2.77	123.18	118.94
6	M	806	BCB	OBD-CAD-CBD	-2.76	120.87	127.49
12	M	501	MQ7	C21-C20-C18	-2.66	104.23	112.98
6	L	304	BCB	CBA-CAA-C2A	-2.63	112.15	115.72
6	L	302	BCB	C3B-C4B-NB	2.60	108.50	103.75
7	L	401	BPB	C6-C5-C3	2.59	120.25	113.45
13	M	600	NS5	C22-C21-C23	-2.56	114.05	118.08
6	M	805	BCB	OBD-CAD-C3D	2.56	131.23	126.73
7	L	402	BPB	C4-C3-C5	-2.54	111.00	115.27
6	L	304	BCB	C1-C2-C3	-2.52	121.68	126.04
5	C	340	HEM	CBA-CAA-C2A	2.51	117.11	112.49
12	M	501	MQ7	C31-C32-C33	2.50	133.69	127.66
7	L	402	BPB	O2A-CGA-O1A	-2.50	117.28	123.59
13	M	600	NS5	C19-C18-C17	2.48	128.56	123.47
7	L	402	BPB	O2A-CGA-CBA	2.44	119.55	111.91
12	M	501	MQ7	C44-C43-C42	2.39	129.56	122.65
8	L	502	CET	C11-C10-C8	-2.39	108.98	115.07
7	L	401	BPB	CBD-CHA-C1A	2.38	130.63	126.84
5	C	338	HEM	CMD-C2D-C1D	-2.36	124.84	128.46
7	L	401	BPB	CBD-CHA-C4D	-2.34	105.90	108.54
13	M	600	NS5	C18-C19-C20	2.33	128.24	123.47
5	C	339	HEM	CAA-C2A-C3A	-2.31	120.60	127.25
7	L	401	BPB	C10-C8-C7	2.31	124.30	112.13
7	L	402	BPB	CBD-CHA-C4D	-2.31	105.94	108.54
5	C	339	HEM	CBD-CAD-C3D	2.27	116.67	112.48
6	M	806	BCB	C3B-C4B-NB	2.26	107.87	103.75
5	C	339	HEM	CMD-C2D-C3D	2.25	129.19	124.94
6	L	304	BCB	OBD-CAD-C3D	2.18	130.58	126.73
6	M	806	BCB	OBD-CAD-C3D	2.17	130.56	126.73
6	L	304	BCB	C4-C3-C5	-2.15	111.66	115.27
5	C	340	HEM	CAD-C3D-C2D	2.14	133.39	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	805	BCB	C3B-C4B-NB	2.13	107.63	103.75
6	L	304	BCB	O2A-CGA-O1A	-2.12	118.23	123.59
7	L	402	BPB	CBD-CHA-C1A	2.11	130.21	126.84
12	M	501	MQ7	C21-C22-C23	-2.11	122.59	127.66
7	L	401	BPB	C1-C2-C3	2.08	129.63	126.04
7	L	401	BPB	C3C-C4C-NC	2.06	112.88	109.58
6	L	302	BCB	C15-C13-C12	-2.06	101.29	112.13
7	L	401	BPB	CAA-C2A-C1A	-2.05	105.44	112.19
13	M	600	NS5	C16-C15-C14	-2.02	114.89	118.08
6	M	805	BCB	OBB-CAB-CBB	-2.02	117.57	121.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	402	BPB	C13

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	706	LDA	N1-C1-C2-C3
9	M	704	LDA	C2-C1-N1-CM1
9	M	704	LDA	N1-C1-C2-C3
6	M	805	BCB	C3A-C2A-CAA-CBA
6	M	805	BCB	C2-C3-C5-C6
13	M	600	NS5	C20-C21-C23-C24
13	M	600	NS5	C22-C21-C23-C24
13	M	600	NS5	C29-C30-C31-C33
13	M	600	NS5	C30-C31-C33-C34
6	L	304	BCB	C2B-C3B-CAB-OBB
6	L	304	BCB	C2B-C3B-CAB-CBB
6	L	302	BCB	C2B-C3B-CAB-OBB
6	L	302	BCB	C2B-C3B-CAB-CBB
6	L	302	BCB	C4-C3-C5-C6
6	M	806	BCB	C2B-C3B-CAB-OBB
6	M	806	BCB	C2B-C3B-CAB-CBB
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D
6	L	302	BCB	O1D-CGD-O2D-CED
6	L	302	BCB	CBD-CGD-O2D-CED
6	M	805	BCB	C4-C3-C5-C6
7	L	401	BPB	CBD-CGD-O2D-CED
7	L	401	BPB	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	L	401	BPB	C2-C3-C5-C6
6	L	302	BCB	C2-C3-C5-C6
13	M	600	NS5	C7-C8-C9-C10
6	M	806	BCB	C13-C15-C16-C17
9	H	703	LDA	C3-C4-C5-C6
13	M	600	NS5	C2-C3-C4-C5
6	M	806	BCB	C8-C10-C11-C12
6	M	806	BCB	O1D-CGD-O2D-CED
6	L	302	BCB	C15-C16-C17-C18
13	M	600	NS5	C12-C13-C14-C15
13	M	600	NS5	C16-C15-C17-C18
13	M	600	NS5	C24-C25-C26-C27
6	M	805	BCB	C15-C16-C17-C18
6	L	304	BCB	C16-C17-C18-C20
7	L	402	BPB	C4-C3-C5-C6
6	M	806	BCB	C2A-CAA-CBA-CGA
7	L	401	BPB	O1A-CGA-O2A-C1
6	M	806	BCB	CBD-CGD-O2D-CED
7	L	402	BPB	O2A-C1-C2-C3
6	M	805	BCB	C3-C5-C6-C7
7	L	401	BPB	CBA-CGA-O2A-C1
7	L	401	BPB	O1D-CGD-O2D-CED
6	M	806	BCB	C15-C16-C17-C18
9	M	706	LDA	C6-C7-C8-C9
6	M	805	BCB	C6-C7-C8-C10
9	M	706	LDA	C1-C2-C3-C4
9	M	704	LDA	C4-C5-C6-C7
6	L	304	BCB	C16-C17-C18-C19
9	M	701	LDA	C2-C3-C4-C5
9	L	702	LDA	C3-C4-C5-C6
9	M	704	LDA	C5-C6-C7-C8
7	L	401	BPB	C5-C6-C7-C8
13	M	600	NS5	C3-C4-C5-C6
6	M	805	BCB	C11-C12-C13-C15
6	L	304	BCB	C12-C13-C15-C16
6	M	805	BCB	C4B-C3B-CAB-OBB
6	M	805	BCB	C4B-C3B-CAB-CBB
6	M	805	BCB	C6-C7-C8-C9
6	L	304	BCB	C14-C13-C15-C16
9	L	702	LDA	N1-C1-C2-C3
6	M	805	BCB	C10-C11-C12-C13
9	H	703	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
9	M	701	LDA	C11-C10-C9-C8
6	L	304	BCB	C8-C10-C11-C12
9	L	702	LDA	C1-C2-C3-C4
7	L	401	BPB	CAD-CBD-CGD-O2D
9	M	701	LDA	C9-C10-C11-C12
9	H	703	LDA	C7-C8-C9-C10
6	M	806	BCB	C11-C10-C8-C7
9	M	704	LDA	C6-C7-C8-C9
9	L	702	LDA	C2-C3-C4-C5
9	M	701	LDA	C7-C8-C9-C10
7	L	402	BPB	C10-C11-C12-C13
13	M	600	NS5	C31-C33-C34-C35
6	M	805	BCB	C11-C12-C13-C14
6	M	806	BCB	C11-C10-C8-C9
9	M	701	LDA	C1-C2-C3-C4
13	M	600	NS5	C28-C29-C30-C31
7	L	402	BPB	C2-C3-C5-C6
6	M	806	BCB	C6-C7-C8-C10
6	L	304	BCB	CHA-CBD-CGD-O1D
12	M	501	MQ7	C34-C33-C35-C36
13	M	600	NS5	C3-C4-C5-C7
9	M	706	LDA	C7-C8-C9-C10
9	M	705	LDA	C9-C10-C11-C12
7	L	402	BPB	CAD-CBD-CGD-O2D
12	M	501	MQ7	C32-C33-C35-C36
6	L	304	BCB	C3A-C2A-CAA-CBA
6	L	304	BCB	CHA-CBD-CGD-O2D
6	L	302	BCB	CAD-CBD-CGD-O1D
6	L	302	BCB	C16-C17-C18-C20
9	M	704	LDA	C2-C1-N1-O1
13	M	600	NS5	C32-C31-C33-C34
6	M	806	BCB	C11-C12-C13-C15
6	L	304	BCB	C13-C15-C16-C17

There are no ring outliers.

19 monomers are involved in 61 short contacts:

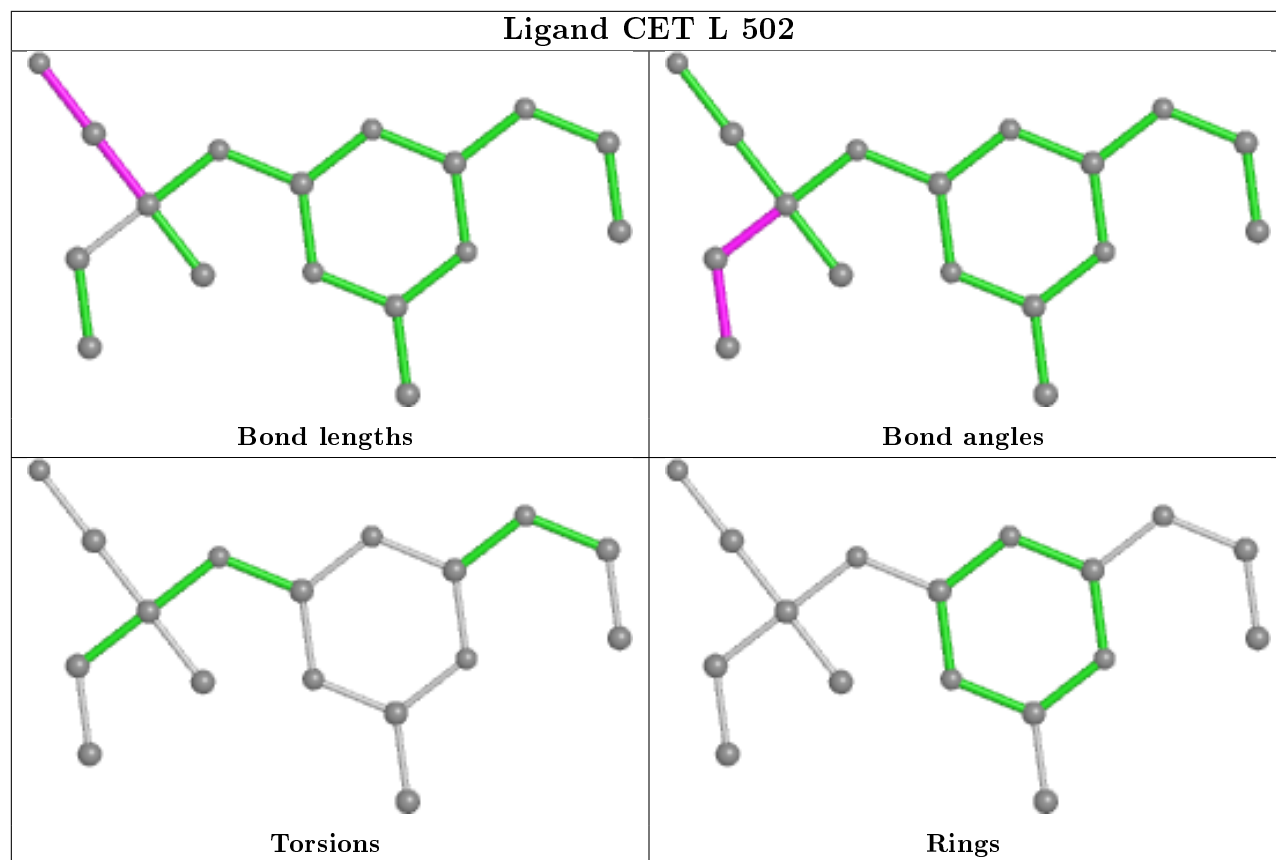
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	706	LDA	1	0
8	L	502	CET	1	0
9	M	701	LDA	2	0
9	H	703	LDA	1	0

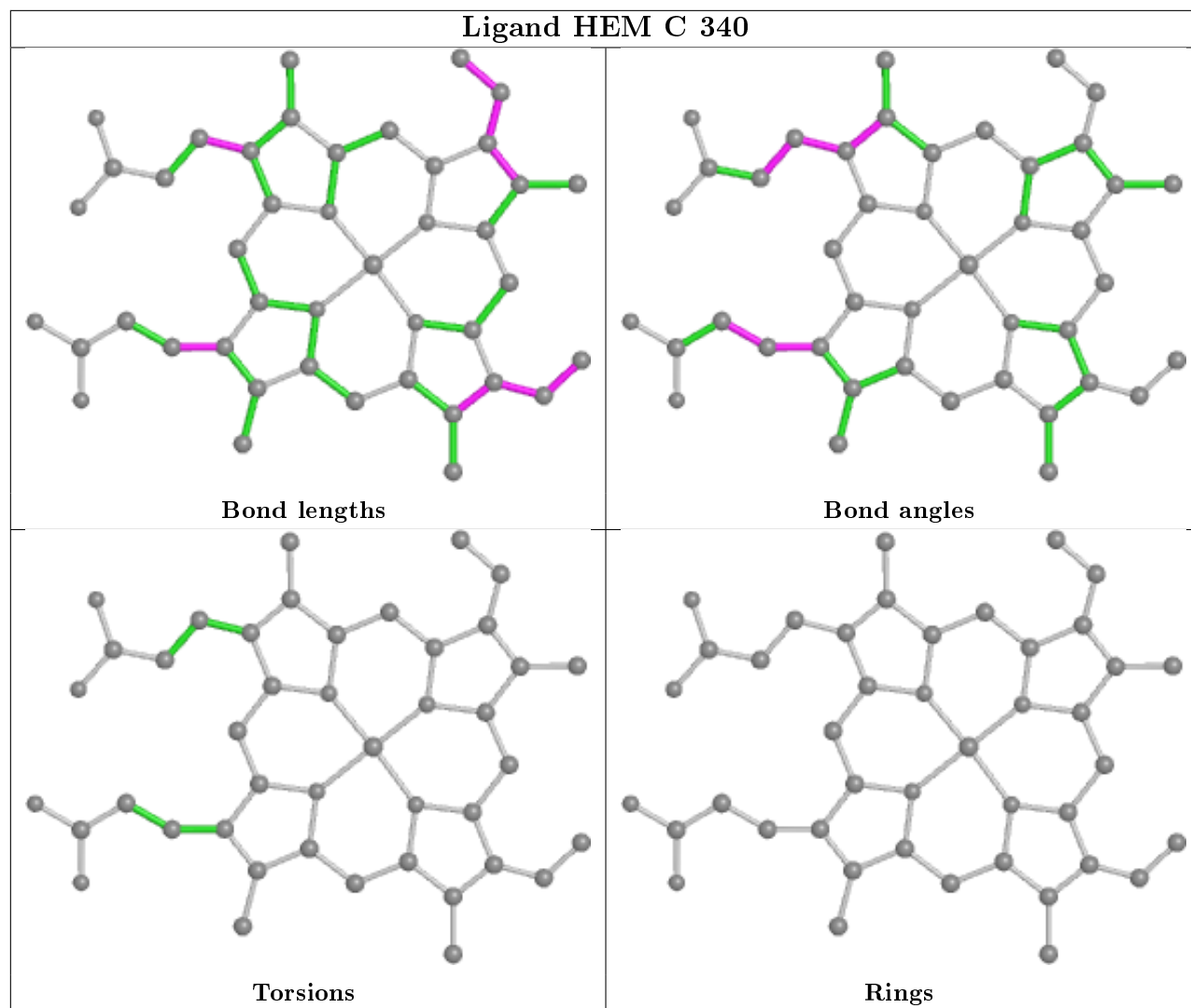
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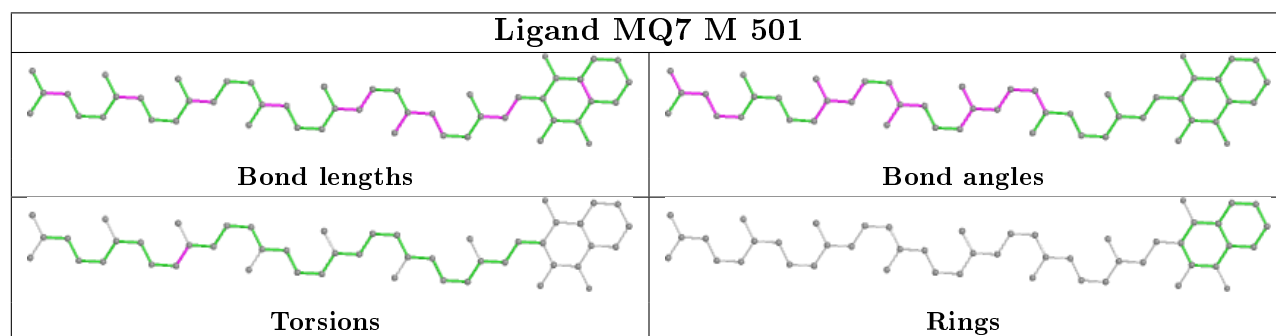
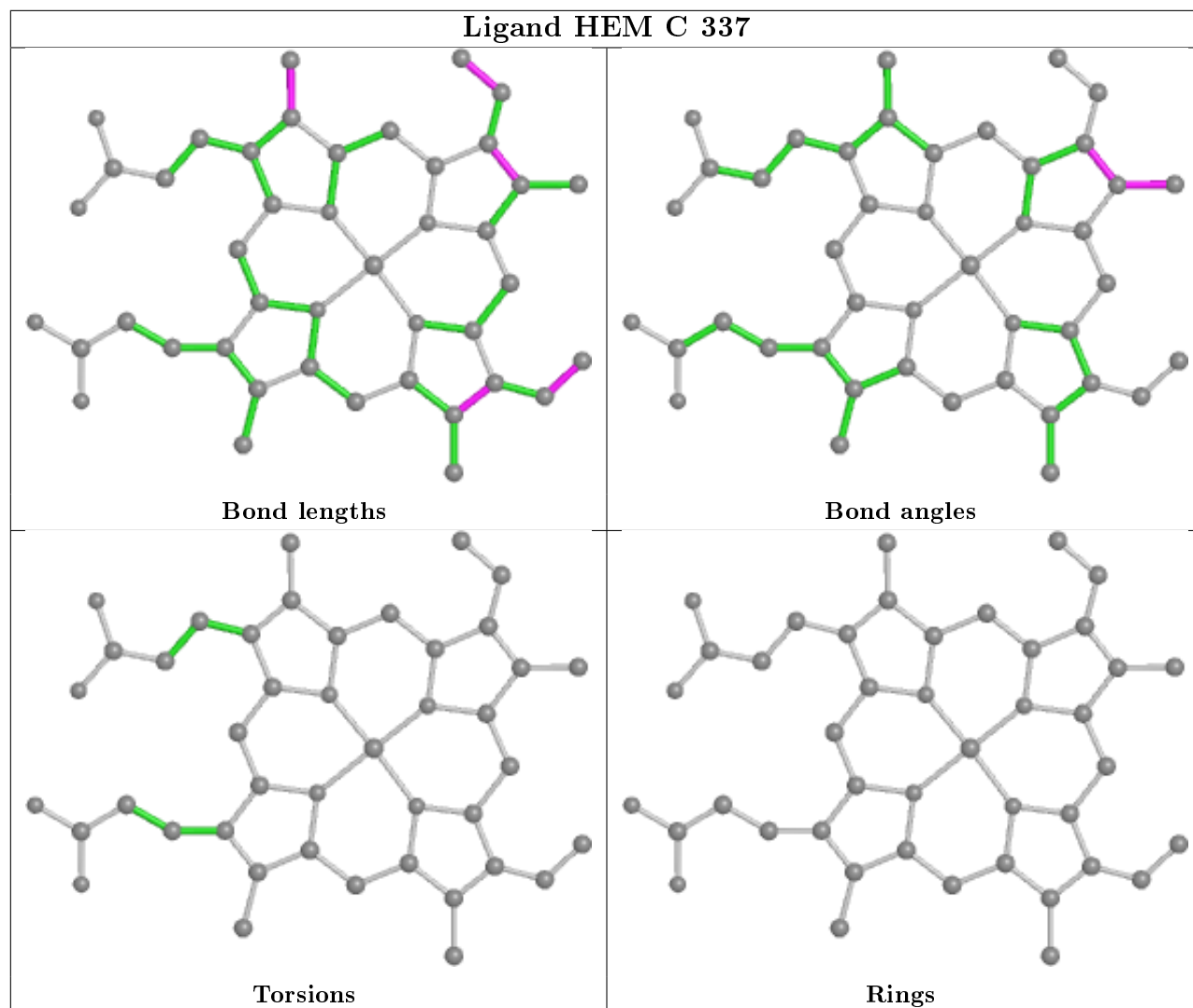
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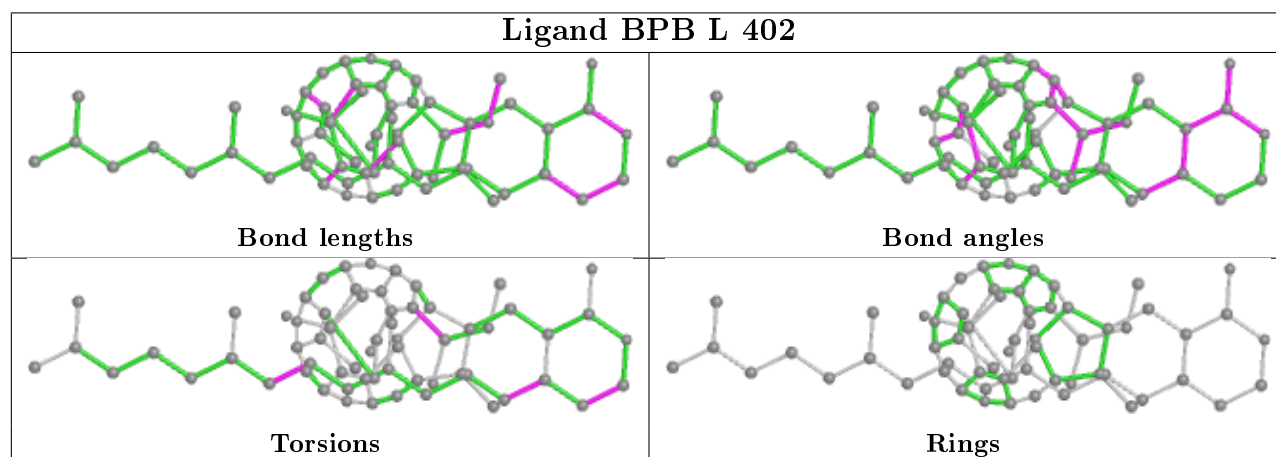
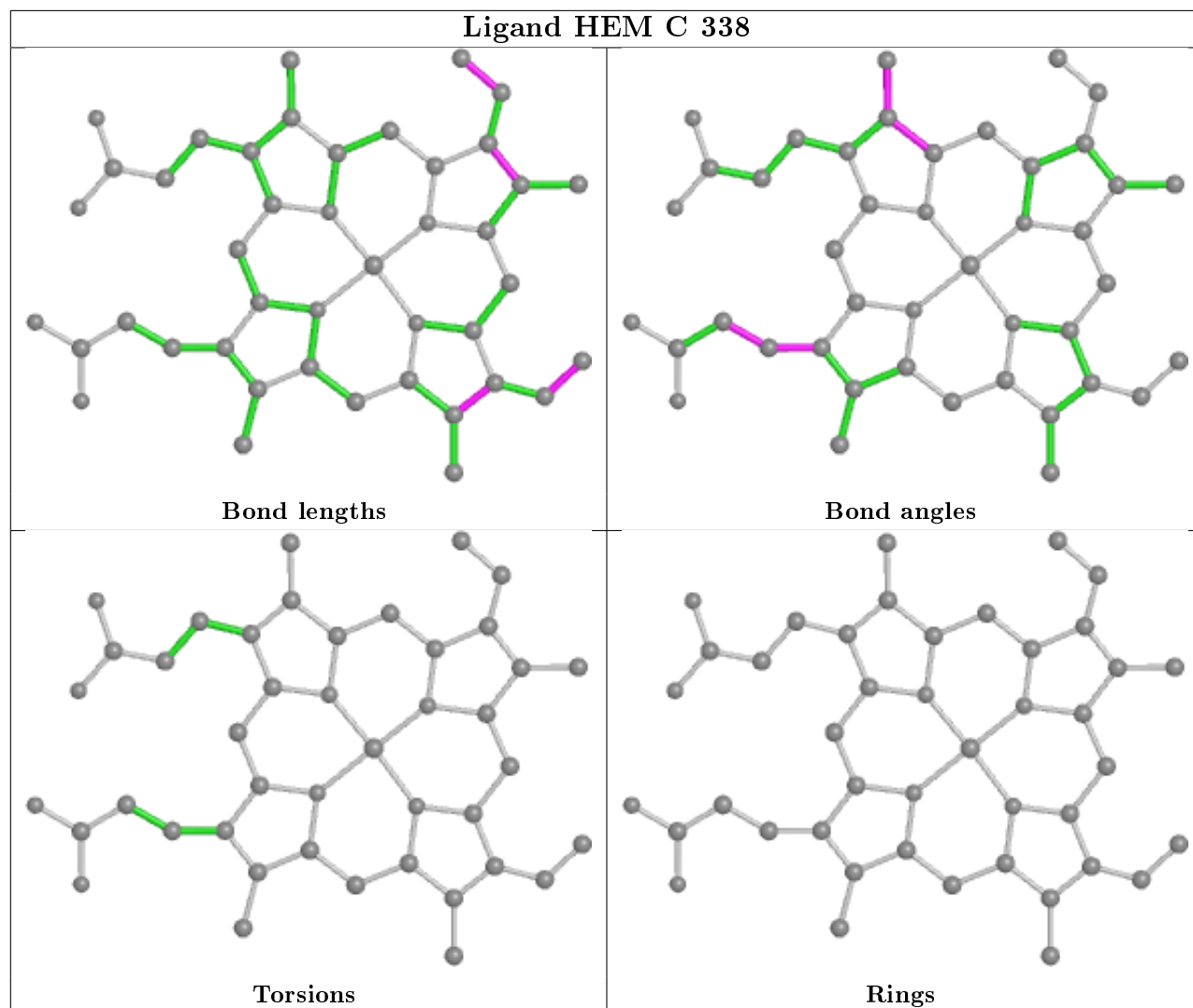
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	337	HEM	3	0
12	M	501	MQ7	1	0
5	C	338	HEM	2	0
9	M	704	LDA	2	0
9	M	705	LDA	1	0
7	L	402	BPB	5	0
6	M	805	BCB	8	0
11	M	803	SO4	1	0
13	M	600	NS5	7	0
11	M	804	SO4	1	0
6	L	304	BCB	4	0
7	L	401	BPB	13	0
6	L	302	BCB	6	0
6	M	806	BCB	7	0
5	C	339	HEM	1	0

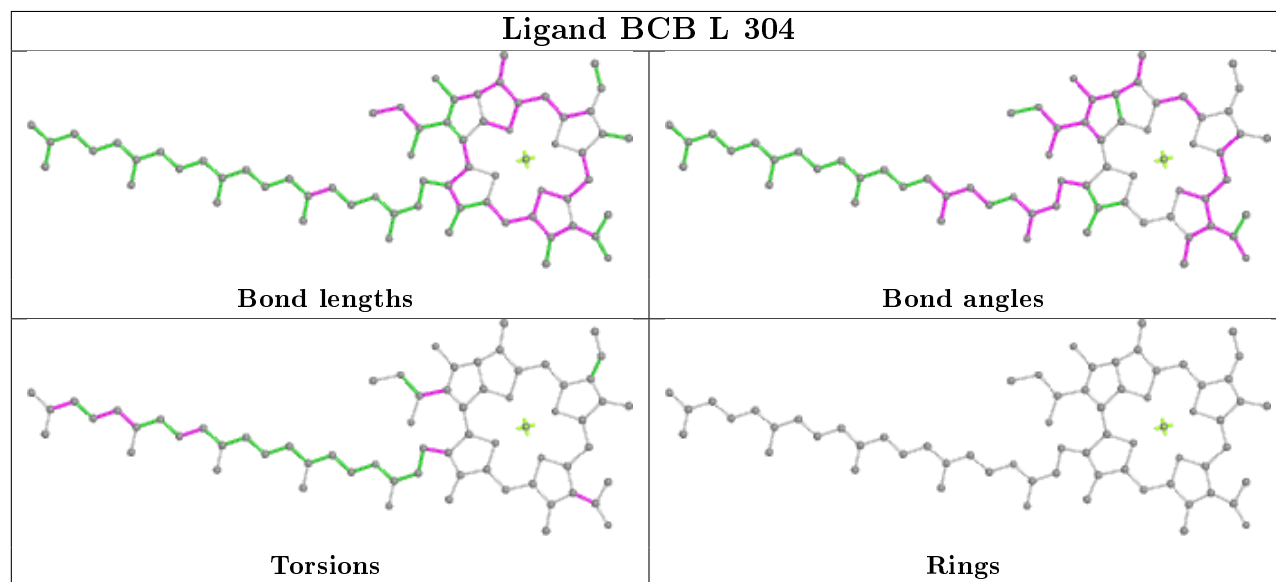
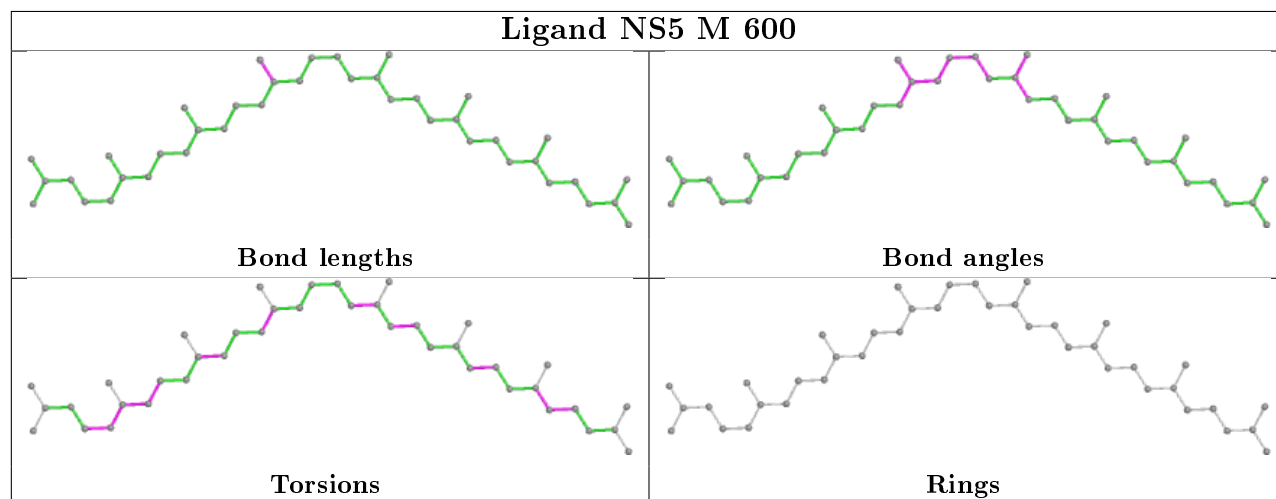
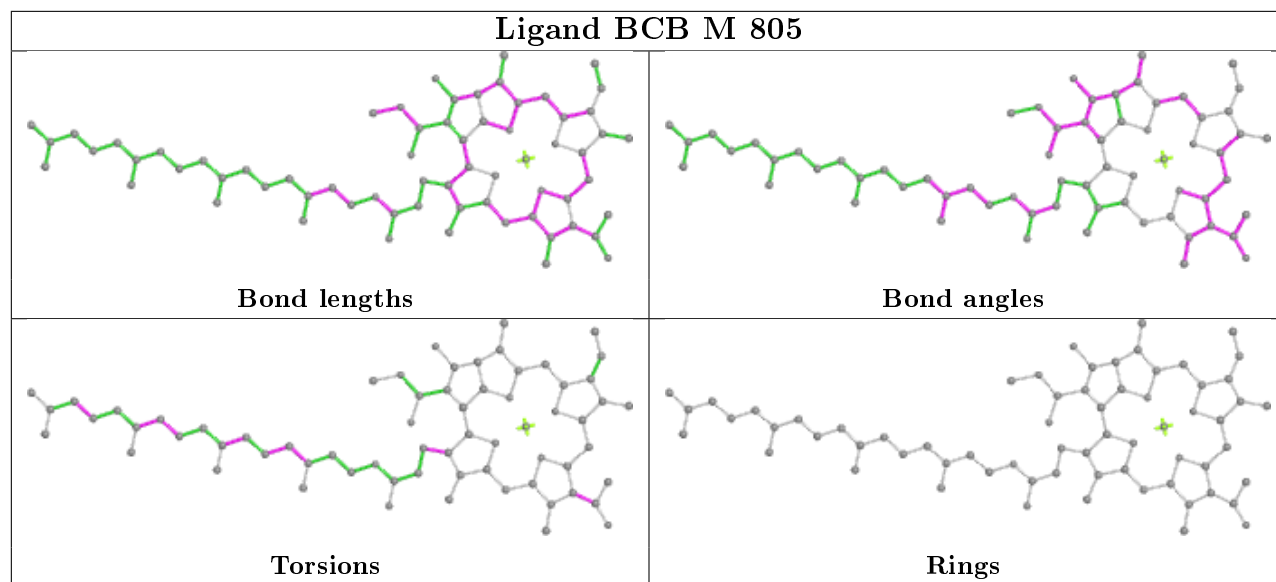
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

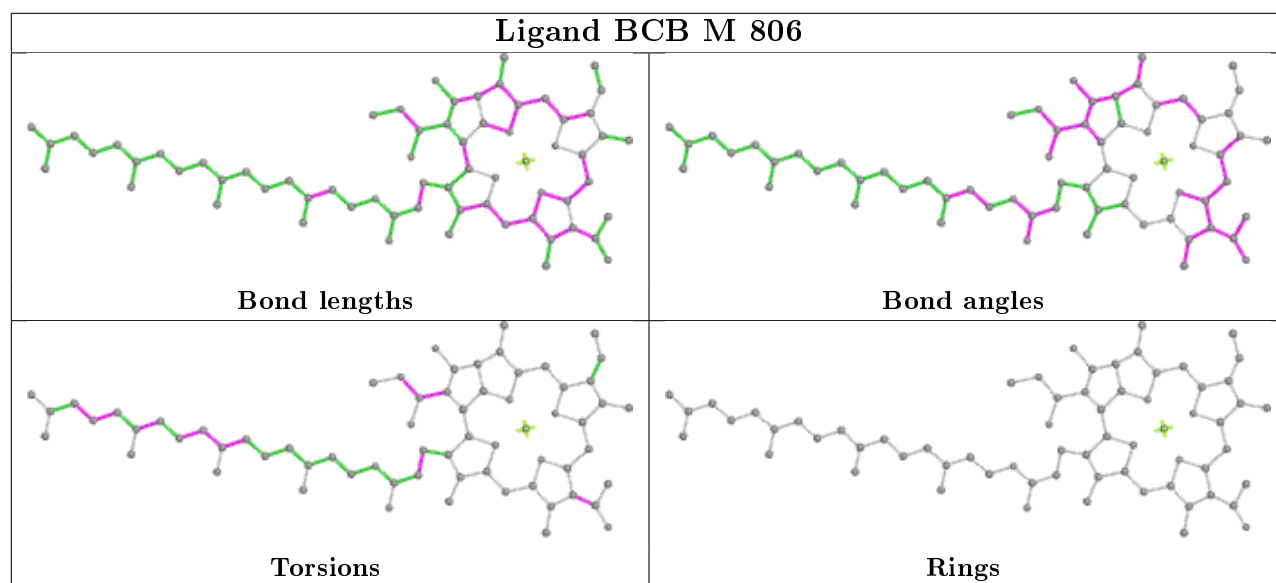
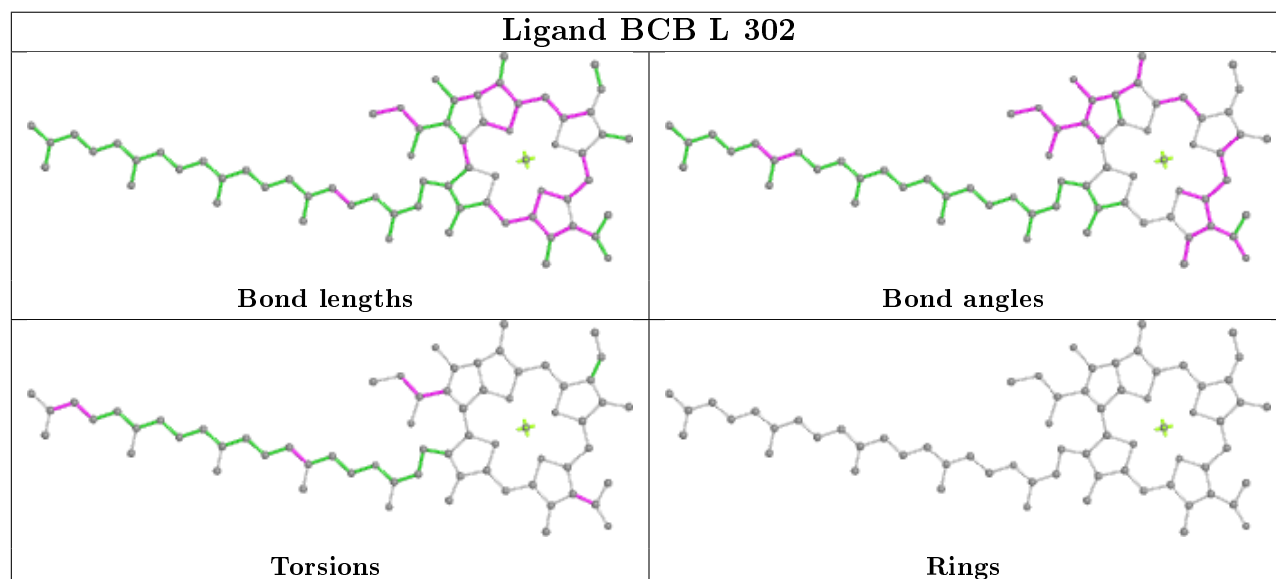
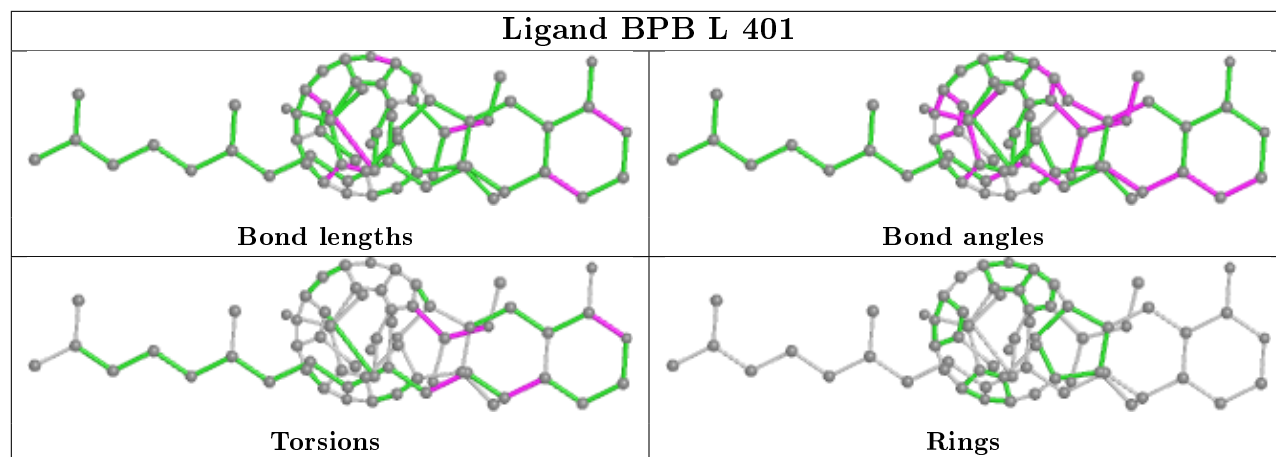


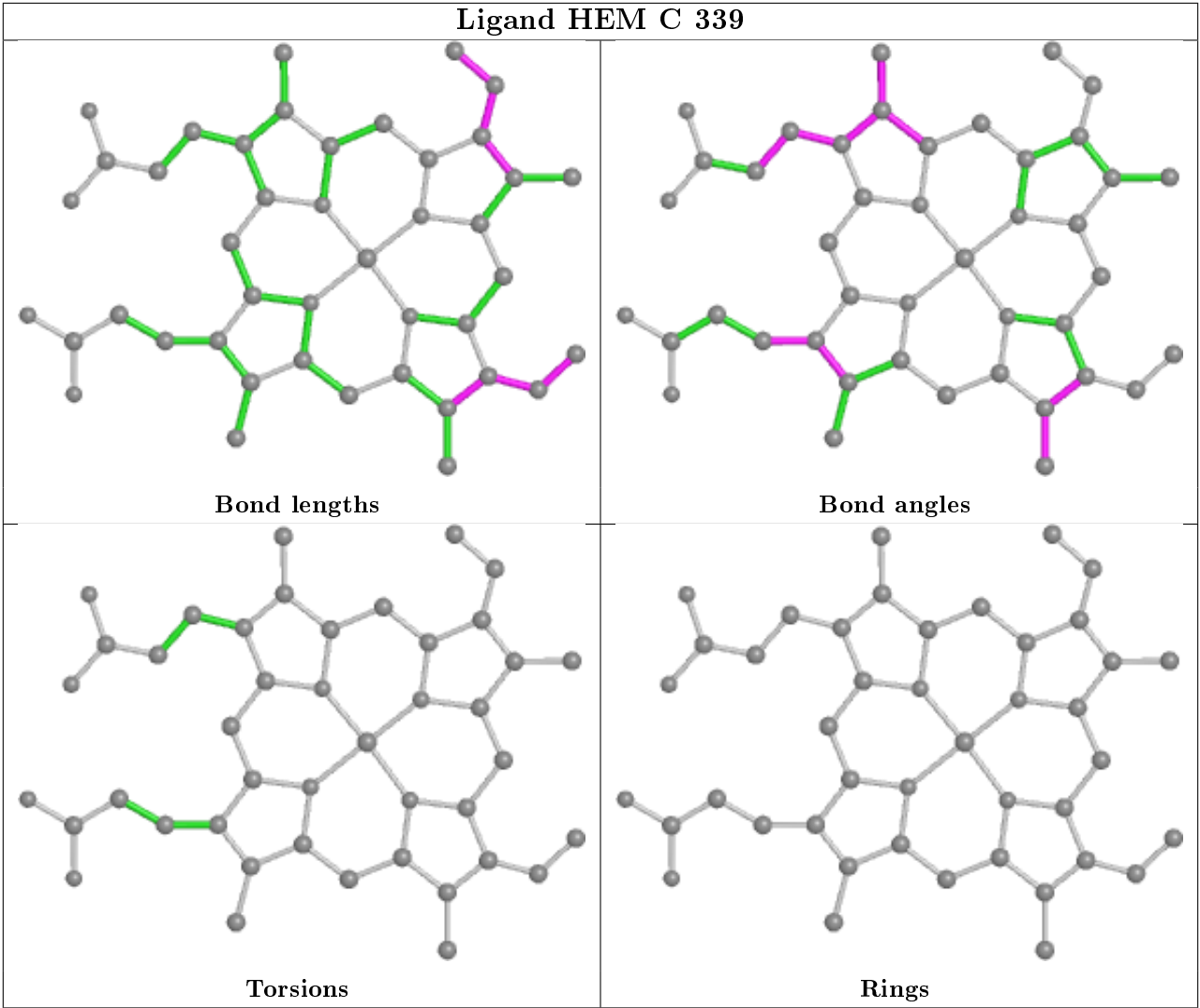












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	54:PRO	C	55:GLU	N	1.68

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	52:LEU	C	53:ALA	N	1.19

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(Å²)	Q<0.9	
1	C	332/336 (98%)	-0.77	0	100	100	4, 20, 44, 66	18 (5%)
2	L	273/273 (100%)	-0.91	0	100	100	4, 16, 41, 61	6 (2%)
3	M	323/323 (100%)	-0.78	0	100	100	4, 18, 48, 60	10 (3%)
4	H	249/258 (96%)	-0.65	1 (0%)	92	93	6, 27, 58, 76	19 (7%)
All	All	1177/1190 (98%)	-0.78	1 (0%)	95	96	4, 20, 48, 76	53 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [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	FME	H	1	10/11	0.96	0.10	23,30,40,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

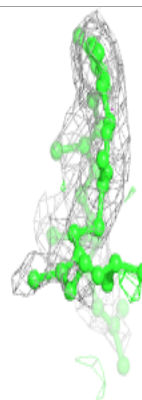
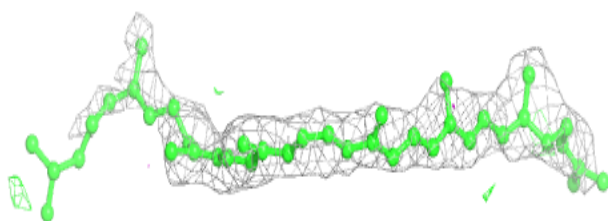
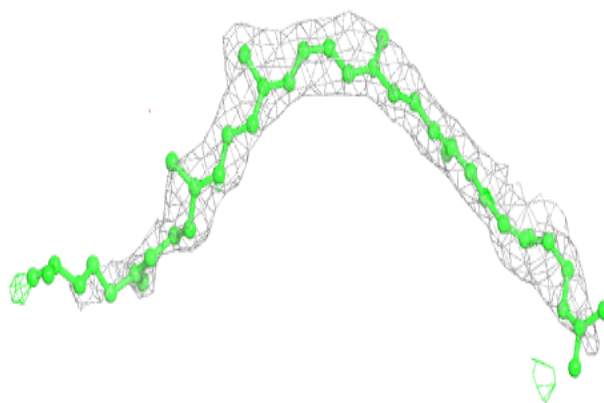
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	LDA	L	702	16/16	0.73	0.38	17,45,71,72	0
9	LDA	M	706	16/16	0.77	0.36	68,71,72,73	4
9	LDA	M	705	16/16	0.80	0.23	53,58,69,69	5
9	LDA	M	704	16/16	0.80	0.34	55,59,79,81	0
13	NS5	M	600	40/40	0.84	0.23	23,40,76,76	4
9	LDA	H	703	16/16	0.93	0.22	27,38,57,58	0
12	MQ7	M	501	48/48	0.94	0.13	3,15,34,38	0
11	SO4	M	803	5/5	0.95	0.18	73,74,76,77	0
6	BCB	M	805	66/66	0.95	0.12	2,15,44,46	0
7	BPB	L	401	65/65	0.95	0.13	2,21,70,70	7
9	LDA	M	701	16/16	0.96	0.11	11,21,24,27	0
5	HEM	C	337	43/43	0.97	0.10	8,21,30,39	0
5	HEM	C	340	43/43	0.97	0.11	5,13,30,44	0
5	HEM	C	338	43/43	0.97	0.14	11,22,28,33	0
7	BPB	L	402	65/65	0.97	0.10	2,6,13,17	0
6	BCB	L	302	66/66	0.97	0.11	2,8,15,19	0
6	BCB	M	806	66/66	0.97	0.12	2,10,25,29	0
6	BCB	L	304	66/66	0.98	0.12	2,6,21,27	0
8	CET	L	502	17/17	0.98	0.11	10,18,21,25	0
11	SO4	H	801	5/5	0.98	0.09	56,56,57,57	0
11	SO4	M	804	5/5	0.98	0.12	39,39,44,44	0
5	HEM	C	339	43/43	0.98	0.10	2,10,15,23	0
10	FE2	M	500	1/1	0.99	0.04	16,16,16,16	0
11	SO4	M	802	5/5	0.99	0.09	21,24,27,28	0

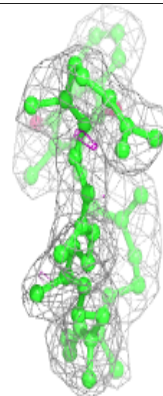
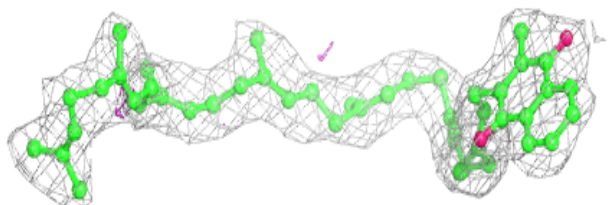
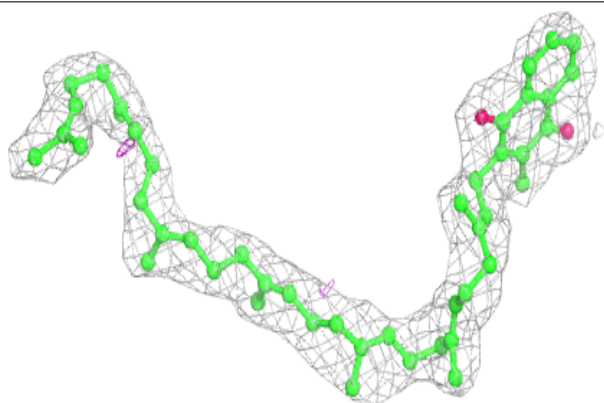
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS5 M 600:

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

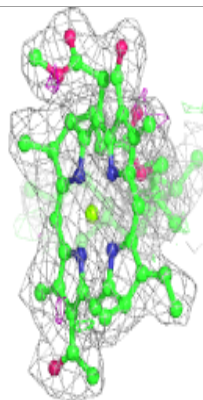
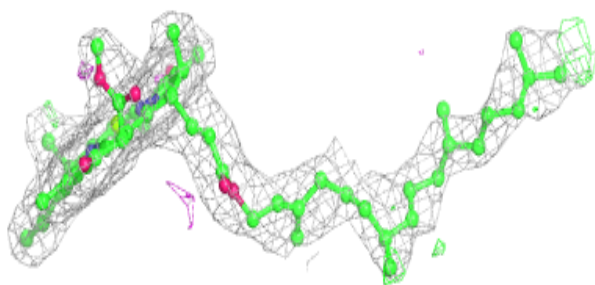
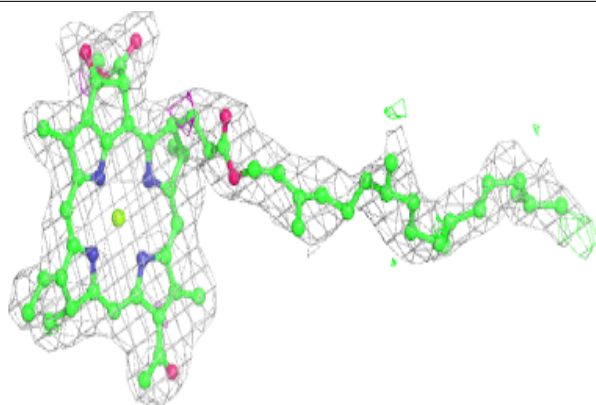
**Electron density around MQ7 M 501:**

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

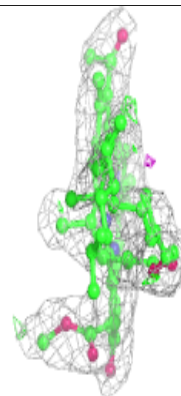
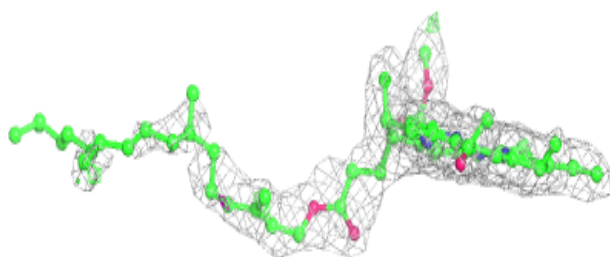
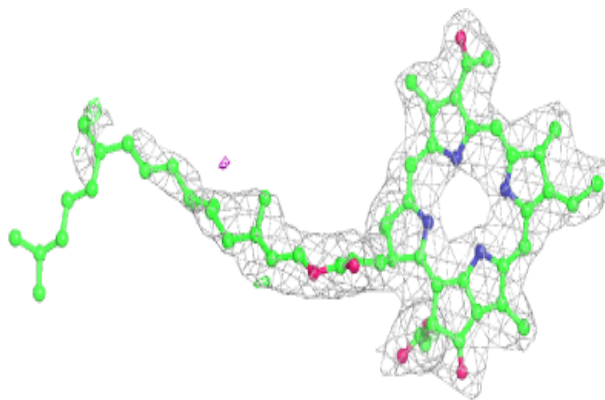


Electron density around BCB M 805:

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

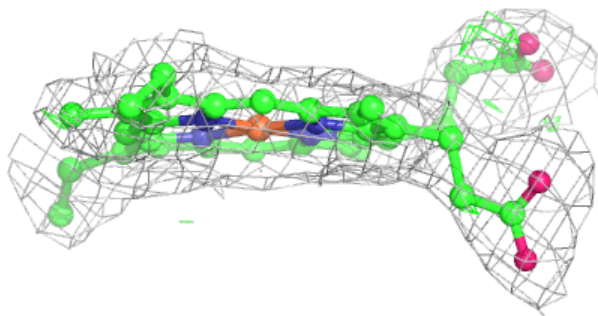
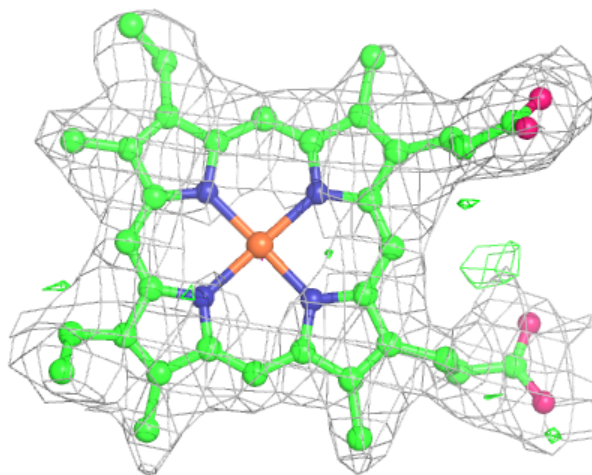
**Electron density around BPB L 401:**

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



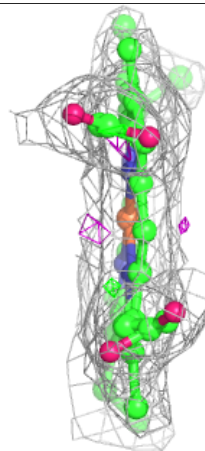
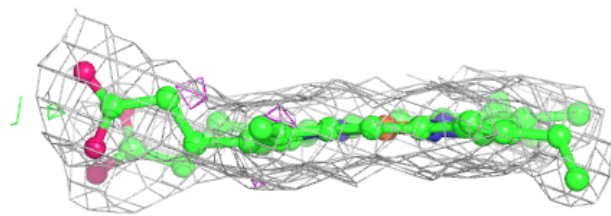
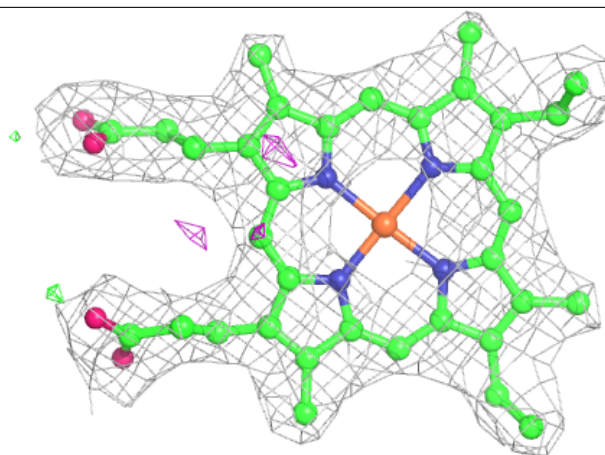
Electron density around HEM C 337:

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



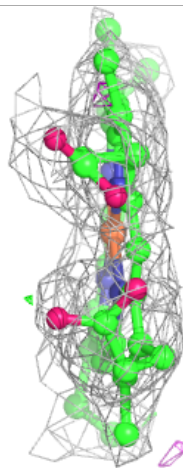
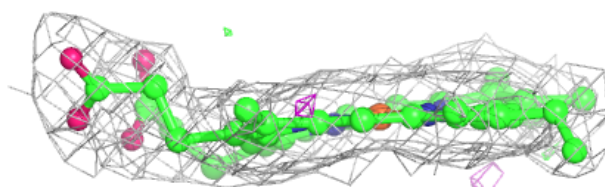
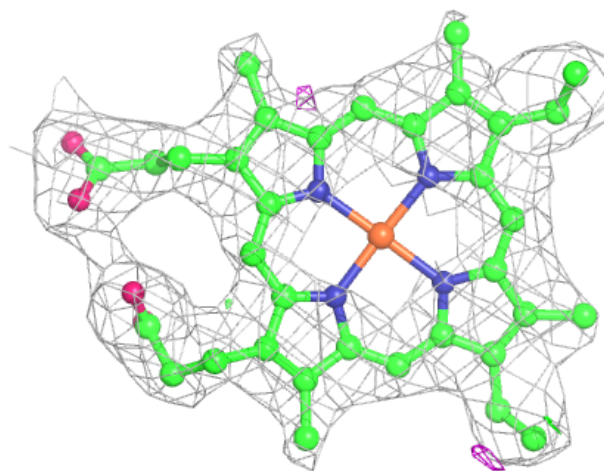
Electron density around HEM C 340:

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



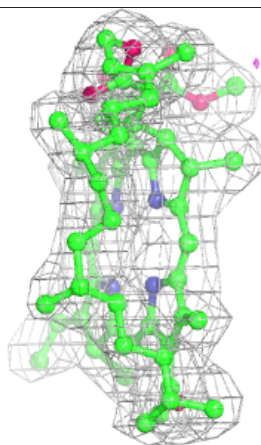
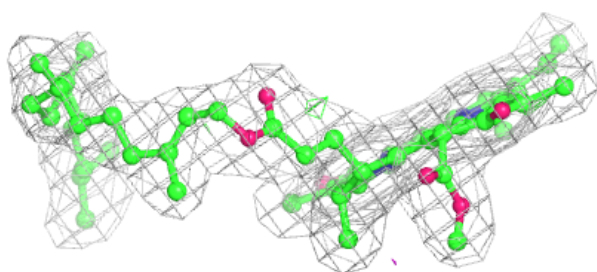
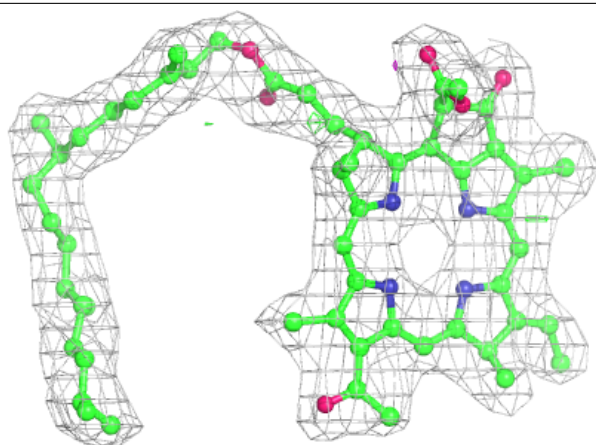
Electron density around HEM C 338:

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

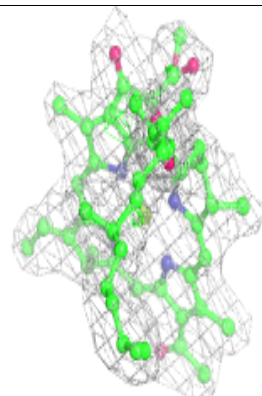
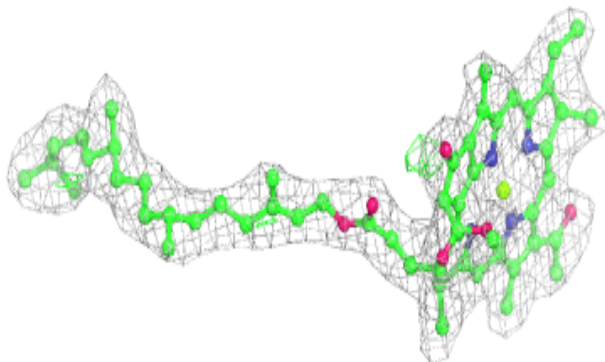
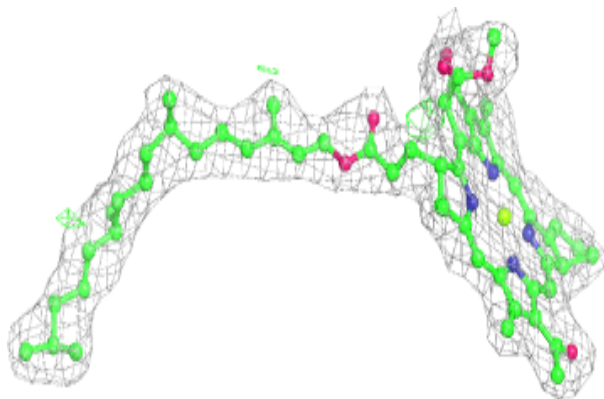


Electron density around BPB L 402:

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

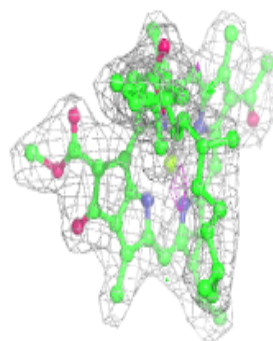
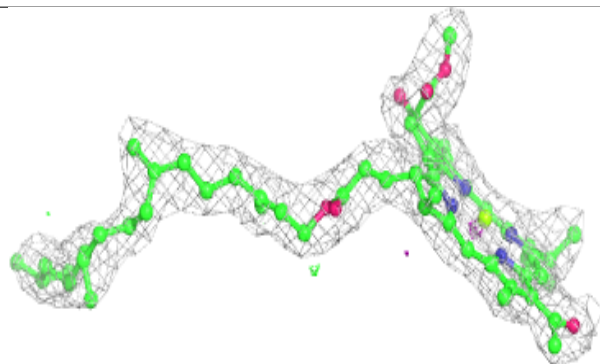
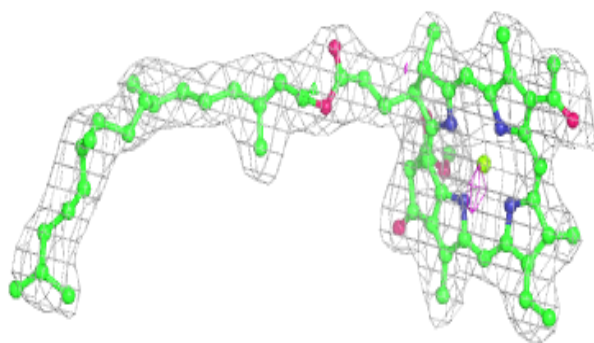
**Electron density around BCB L 302:**

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

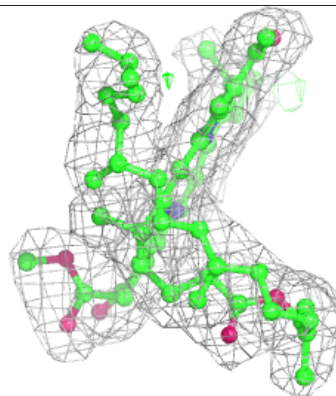
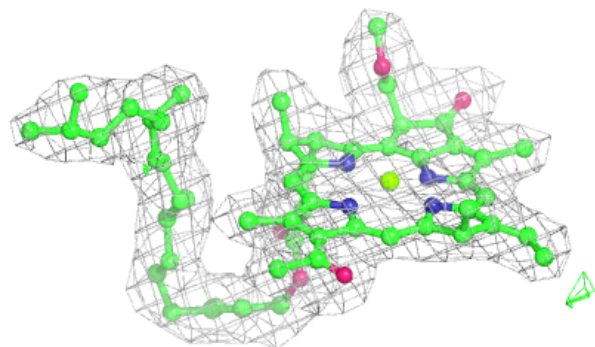
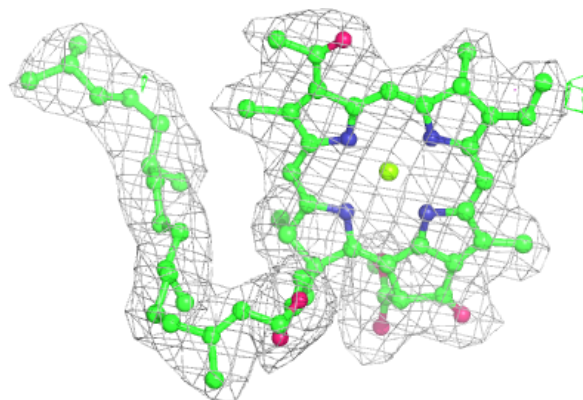


Electron density around BCB M 806:

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

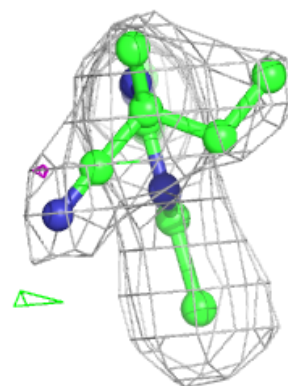
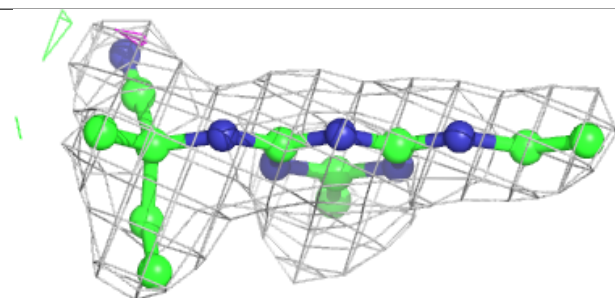
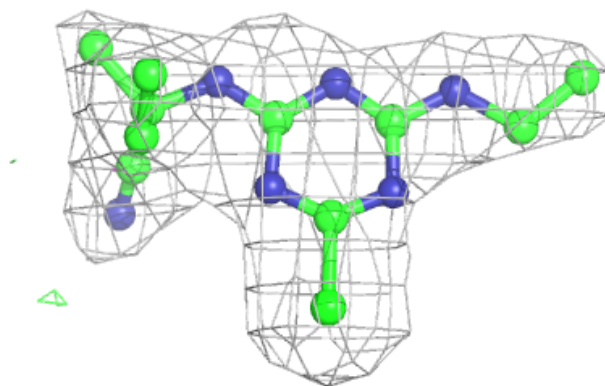
**Electron density around BCB L 304:**

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



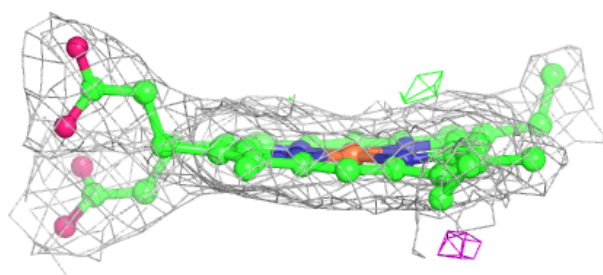
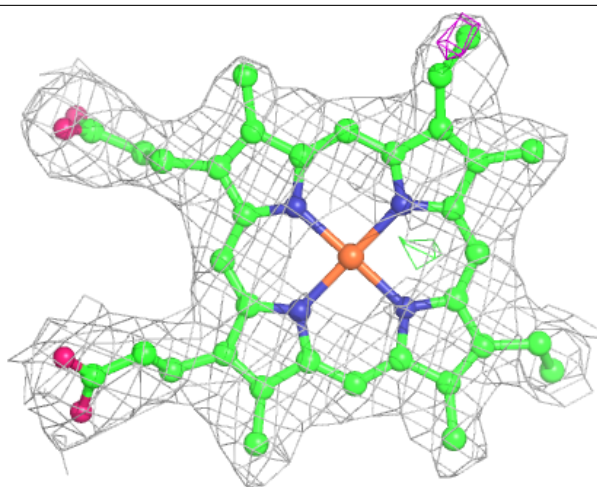
Electron density around CET L 502:

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



Electron density around HEM C 339:

$2mF_o-DF_c$ (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.