Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2026 – 05:59 PM EDT

PDB ID	:	2PRC / pdb_00002prc
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM RHODOPSEUDOMONAS VIRIDIS (UBIQUINONE-2 COMPLEX)
Authors	:	Lancaster, C.R.D.; Michel, H.
Deposited on	:	1997-07-29
Resolution	:	2.45 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

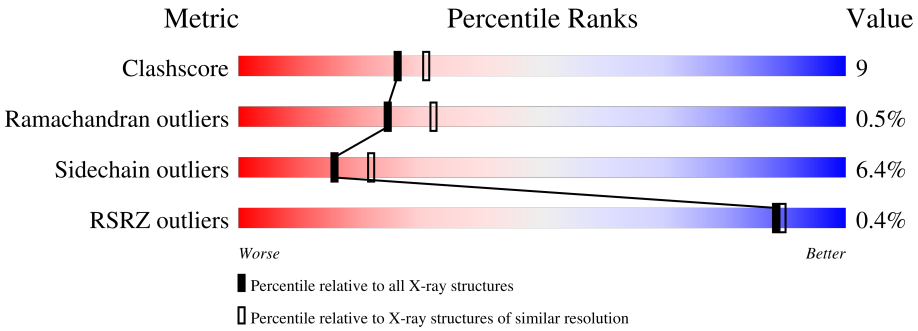
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.45 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	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 <=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	75% 21%
2	L	273	81% 18%
3	M	323	77% 21%
4	H	258	2% 70% 28%

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
5	HEC	C	337	X	-	-	-
5	HEC	C	338	X	-	-	-
5	HEC	C	339	X	-	-	-
5	HEC	C	340	X	-	-	-
6	BCB	L	302	X	-	-	-
6	BCB	L	304	X	-	-	-
6	BCB	M	805	X	-	-	-
6	BCB	M	806	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10528 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
			Total	C	N	O	S			
1	C	332	2630	1655	470	485	20	53	4	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	273	2193	1471	358	357	7	14	2	0

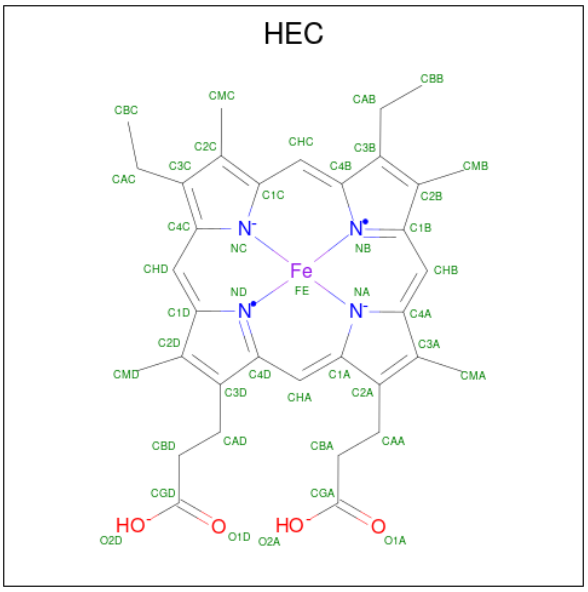
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

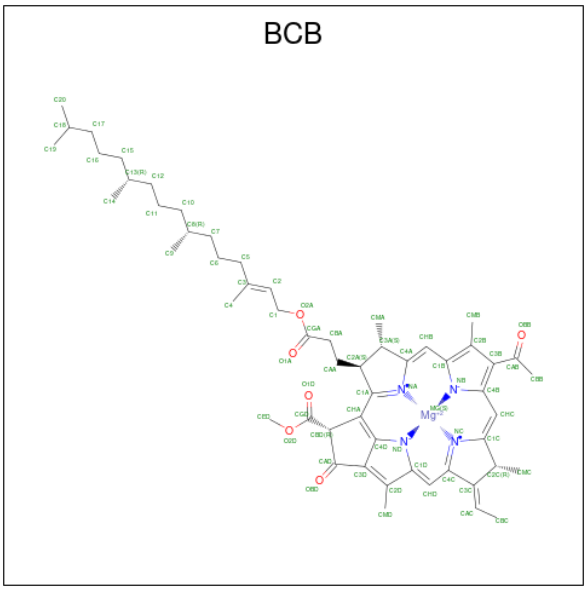
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	258	2018	1292	344	380	2	124	0	0

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



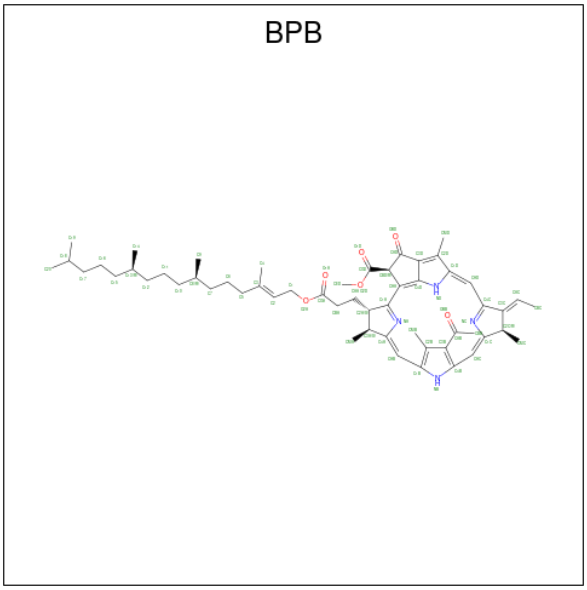
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



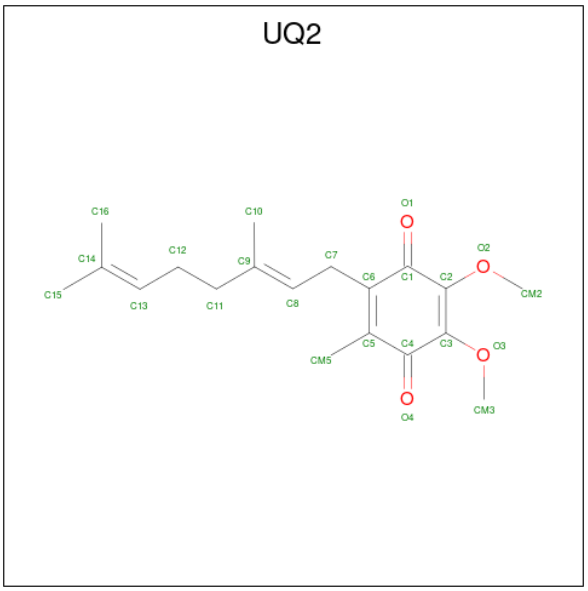
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



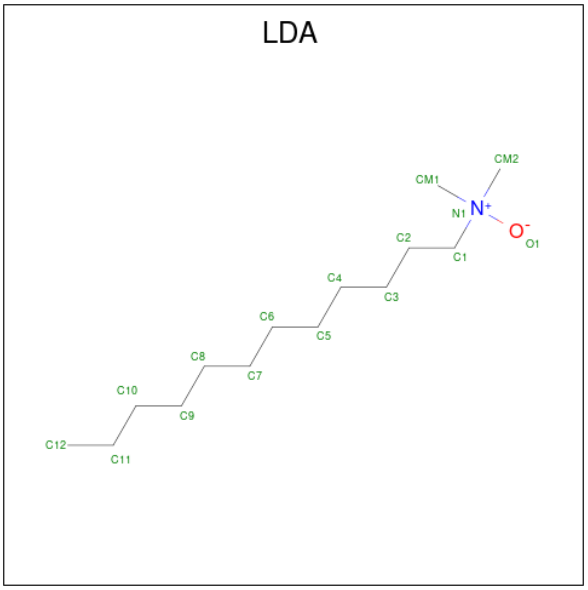
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	7	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

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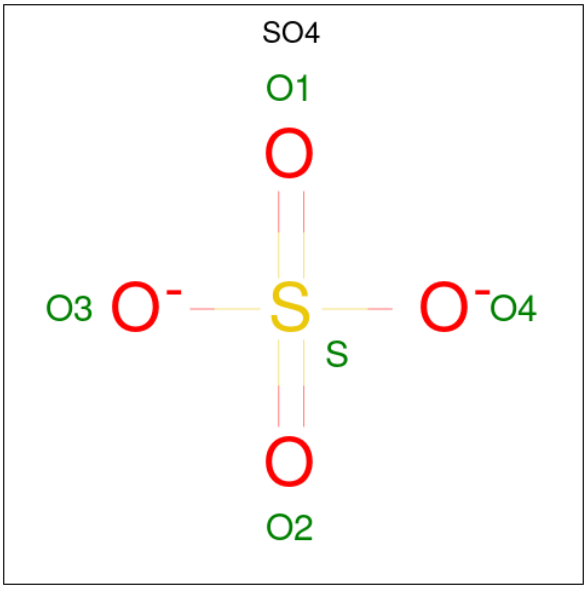
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C N O 16 14 1 1	0	0
9	M	1	Total C N O 16 14 1 1	4	0
9	H	1	Total C N O 16 14 1 1	0	0

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

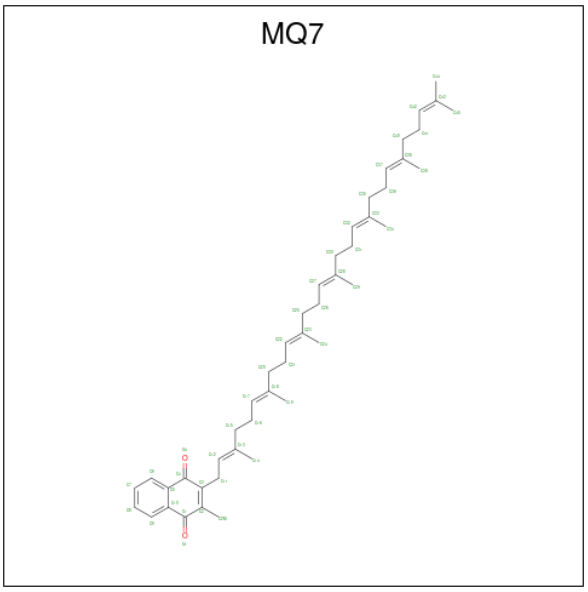
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



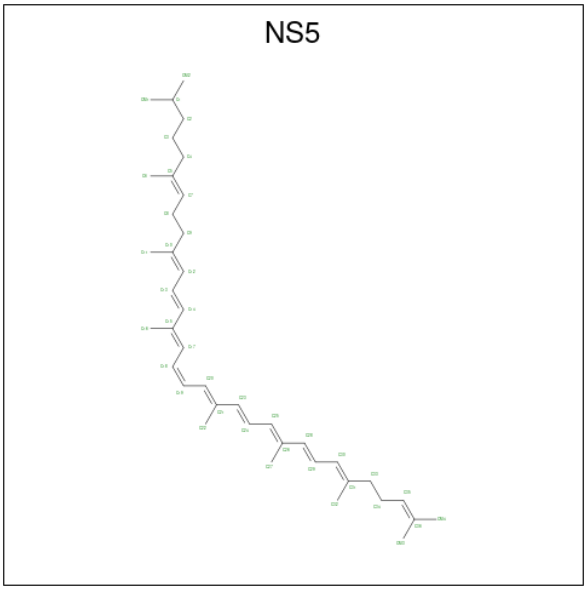
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	M	1	Total O S 5 4 1	0	0
11	H	1	Total O S 5 4 1	0	0

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C 40 40	14	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	121	Total O 121 121	0	0
14	L	48	Total O 48 48	0	0
14	M	76	Total O 76 76	0	0
14	H	71	Total O 71 71	0	0

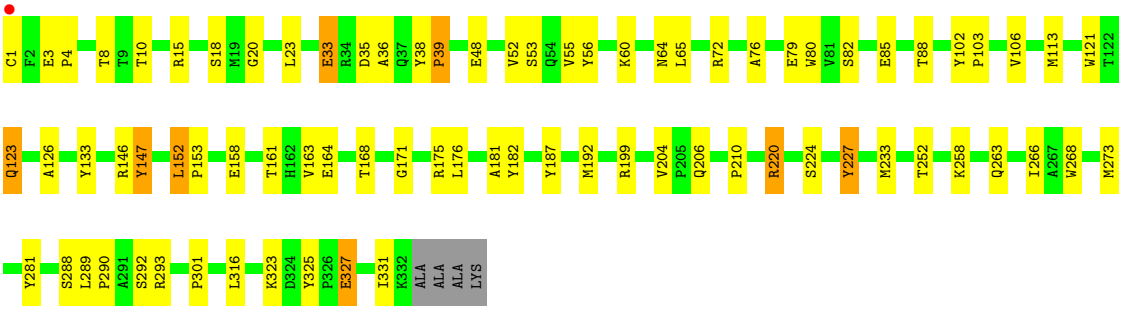
3 Residue-property plots (i)

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

Chain C:

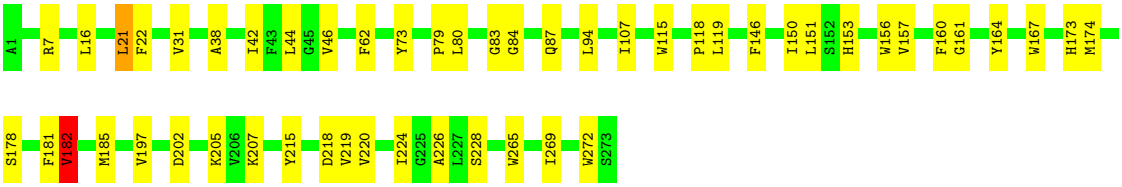




• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain L:





• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

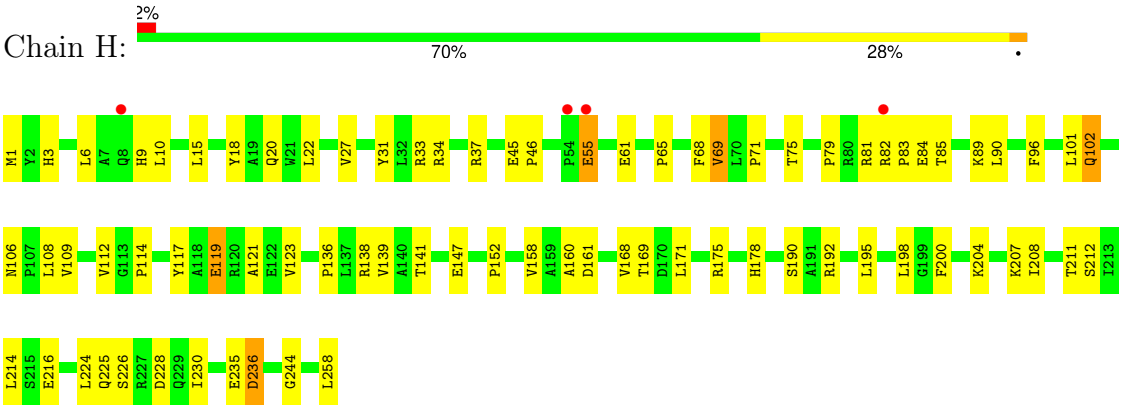
Chain M:





• Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:


2%
70%
28%
M1 Y2 H3 L6 A7 Q8 H9 L10 L15 Y18 A19 Q20 W21 L22 V27 Y31 L32 R33 R34 R37 E45 P46 P54 E55 E61 P65 F68 V69 L70 P71 T75 P79 R80 R81 R82 P83 E84 T85 K89 L90 F96 L101 Q102
N106 P107 L108 V109 V112 G113 P114 Y117 A118 E119 R120 A121 E122 V123 P136 L137 R138 V139 A140 T141 E147 P152 V158 A159 A160 D161 V168 T169 D170 L171 R175 H178 S190 A191 R192 L195 L198 G199 F200 K204 K207 I208 T211 S212 I213
L214 S215 E216 L224 Q225 S226 R227 D228 Q229 I230 E235 D236 G244 L258

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 10.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	76.5 (10.00-2.45) 75.3 (10.00-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.44Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.229 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 93.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HEC, MQ7, NS5, UQ2, LDA, BCB, FME, FE2, BPB

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	0.67	0/2697	0.92	11/3675 (0.3%)
2	L	0.66	0/2281	0.85	2/3112 (0.1%)
3	M	0.64	0/2683	0.90	10/3669 (0.3%)
4	H	0.64	0/2055	0.87	3/2807 (0.1%)
All	All	0.65	0/9716	0.88	26/13263 (0.2%)

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	3
2	L	0	2
4	H	0	1
All	All	0	6

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	80	ASP	CA-C-N	6.83	126.30	118.85
3	M	80	ASP	C-N-CA	6.83	126.30	118.85
1	C	3	GLU	CA-C-N	6.50	124.34	119.66
1	C	3	GLU	C-N-CA	6.50	124.34	119.66
1	C	325	TYR	CA-C-N	6.30	125.93	119.56
1	C	325	TYR	C-N-CA	6.30	125.93	119.56
1	C	4	PRO	CA-C-N	6.10	124.06	119.66
1	C	4	PRO	C-N-CA	6.10	124.06	119.66
2	L	182	VAL	CB-CA-C	-5.80	104.31	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	39	PRO	CA-C-N	5.77	125.74	120.03
1	C	39	PRO	C-N-CA	5.77	125.74	120.03
2	L	202	ASP	CB-CA-C	-5.64	110.05	116.54
4	H	45	GLU	CB-CA-C	-5.58	99.17	110.17
3	M	305	TYR	CA-C-N	5.50	125.45	119.78
3	M	305	TYR	C-N-CA	5.50	125.45	119.78
3	M	302	ALA	N-CA-C	5.48	117.55	109.50
3	M	65	ALA	N-CA-C	-5.38	105.33	111.14
3	M	312	THR	CA-C-N	5.33	125.33	119.89
3	M	312	THR	C-N-CA	5.33	125.33	119.89
4	H	102	GLN	CA-C-N	-5.12	114.64	119.76
4	H	102	GLN	C-N-CA	-5.12	114.64	119.76
1	C	126	ALA	CB-CA-C	-5.12	110.66	116.54
1	C	204	VAL	CA-C-N	5.08	125.02	119.78
1	C	204	VAL	C-N-CA	5.08	125.02	119.78
3	M	9	GLN	N-CA-C	5.07	116.80	111.28
3	M	94	TYR	N-CA-C	5.04	117.00	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	147	TYR	Sidechain
1	C	220	ARG	Sidechain
1	C	227	TYR	Sidechain
4	H	18	TYR	Sidechain
2	L	160	PHE	Sidechain
2	L	164	TYR	Sidechain

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	2630	0	2594	49	0
2	L	2193	0	2122	34	0
3	M	2577	0	2468	53	0
4	H	2018	0	2020	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	172	0	120	3	0
6	L	132	0	144	9	0
6	M	132	0	144	13	0
7	L	65	0	74	6	0
7	M	65	0	74	7	0
8	L	23	0	26	2	0
9	H	16	0	31	1	0
9	L	16	0	31	0	0
9	M	64	0	124	2	0
10	M	1	0	0	0	0
11	H	5	0	0	0	0
11	M	15	0	0	0	0
12	M	48	0	64	0	0
13	M	40	0	60	6	0
14	C	121	0	0	1	0
14	H	71	0	0	0	0
14	L	48	0	0	0	0
14	M	76	0	0	0	0
All	All	10528	0	10096	185	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 9.

All (185) 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)
7:L:402:BPB:HBBB	7:L:402:BPB:HHC	1.42	1.02
7:M:401:BPB:HBBB	7:M:401:BPB:HHC	1.59	0.84
6:M:805:BCB:HHC	6:M:805:BCB:HBB2	1.60	0.84
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.59	0.83
7:L:402:BPB:HHC	7:L:402:BPB:CBB	2.12	0.79
3:M:160:CYS:SG	13:M:600:NS5:H322	2.25	0.76
2:L:181:PHE:HB3	7:M:401:BPB:CBB	2.16	0.75
2:L:226:ALA:HA	8:L:502:UQ2:H3M2	1.70	0.73
6:M:805:BCB:HBB3	6:M:806:BCB:H62	1.73	0.71
1:C:52:VAL:HB	1:C:56:TYR:HD2	1.56	0.68
4:H:10:LEU:HD11	4:H:15:LEU:HG	1.75	0.68
3:M:160:CYS:C	3:M:163:PRO:HD2	2.19	0.68
3:M:23:TRP:CZ2	9:M:704:LDA:HM23	2.29	0.67
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.78	0.66
7:M:401:BPB:HBBB	7:M:401:BPB:CHC	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:275:MET:HA	3:M:275:MET:HE2	1.80	0.63
7:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.81	0.63
2:L:178:SER:O	2:L:182:VAL:HG23	1.99	0.62
1:C:121:TRP:CG	1:C:273:MET:HG3	2.35	0.62
1:C:1[A]:CYS:SG	2:L:265:TRP:HB3	2.40	0.61
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.00	0.61
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.82	0.60
6:M:806:BCB:HAA2	6:M:806:BCB:HBD	1.83	0.60
2:L:181:PHE:HB3	7:M:401:BPB:HBBA	1.83	0.60
3:M:315:PRO:HA	3:M:318:LEU:HG	1.84	0.60
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.37	0.59
1:C:290:PRO:HG2	1:C:293:ARG:HG2	1.83	0.58
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.85	0.58
2:L:205:LYS:HA	4:H:69:VAL:HG22	1.85	0.58
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.83	0.58
2:L:174:MET:HE3	6:M:805:BCB:HED3	1.84	0.58
1:C:224:SER:HA	1:C:227:TYR:HD1	1.69	0.58
1:C:52:VAL:HB	1:C:56:TYR:CD2	2.38	0.57
1:C:52:VAL:HG13	1:C:65:LEU:O	2.05	0.57
1:C:163:VAL:HG12	1:C:171:GLY:HA3	1.85	0.57
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.85	0.56
4:H:136:PRO:HG2	4:H:139:VAL:HG23	1.87	0.56
2:L:21:LEU:HD23	2:L:22:PHE:CZ	2.41	0.56
3:M:226:ARG:HD3	4:H:200:PHE:CZ	2.41	0.56
1:C:181:ALA:O	1:C:182:TYR:HB2	2.06	0.55
1:C:192[A]:MET:O	1:C:199:ARG:HD2	2.05	0.55
1:C:192[B]:MET:O	1:C:199:ARG:HD2	2.05	0.55
1:C:289:LEU:HD22	1:C:293:ARG:HG3	1.88	0.55
3:M:69:ILE:HA	3:M:93:LEU:HD22	1.88	0.55
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.41	0.55
2:L:182:VAL:HG22	6:M:805:BCB:H12	1.88	0.55
2:L:181:PHE:CD2	7:M:401:BPB:HBB	2.42	0.55
3:M:115:MET:HA	3:M:115:MET:HE2	1.89	0.54
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.41	0.54
1:C:153:PRO:HG2	1:C:158:GLU:CB	2.37	0.54
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.41	0.54
1:C:123[A]:GLN:NE2	1:C:123[A]:GLN:H	2.05	0.53
3:M:160:CYS:SG	13:M:600:NS5:C31	2.96	0.53
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.27	0.53
3:M:71:PHE:HB3	9:M:706:LDA:H61	1.90	0.53
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:90:LEU:HA	4:H:102:GLN:O	2.10	0.52
4:H:114:PRO:HB2	4:H:244:GLY:HA2	1.92	0.52
2:L:7[B]:ARG:NH2	4:H:101:LEU:HD21	2.24	0.52
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.91	0.52
3:M:160:CYS:SG	13:M:600:NS5:C30	2.98	0.52
1:C:153:PRO:HG2	1:C:158:GLU:HB2	1.92	0.51
4:H:90:LEU:HB3	4:H:101:LEU:HB3	1.92	0.51
4:H:152:PRO:HD2	4:H:171:LEU:HD11	1.92	0.51
4:H:10:LEU:HD11	4:H:15:LEU:CG	2.39	0.51
1:C:258:LYS:HG2	3:M:307:ALA:HB2	1.93	0.51
2:L:197:VAL:HG13	2:L:207:LYS:HB2	1.93	0.51
3:M:17:ILE:HD11	4:H:178:HIS:HE1	1.76	0.51
1:C:123[A]:GLN:H	1:C:123[A]:GLN:HE21	1.59	0.51
6:M:805:BCB:HBB2	6:M:805:BCB:CHC	2.37	0.51
3:M:160:CYS:SG	13:M:600:NS5:C32	2.98	0.50
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.47	0.50
2:L:73:TYR:CE1	2:L:79:PRO:HD2	2.47	0.50
4:H:139:VAL:HG21	4:H:228:ASP:HB3	1.93	0.50
4:H:152:PRO:O	4:H:168:VAL:HB	2.10	0.50
4:H:82:ARG:HH22	4:H:119:GLU:HB2	1.77	0.50
3:M:231:ARG:HH22	4:H:235:GLU:CD	2.19	0.50
7:L:402:BPB:HBB	3:M:208:TYR:CD2	2.47	0.49
1:C:163:VAL:HG12	1:C:171:GLY:CA	2.42	0.49
3:M:34:TYR:HA	3:M:44:ALA:O	2.13	0.49
1:C:8:THR:HB	1:C:23:LEU:HB2	1.94	0.49
6:L:302:BCB:OBB	6:L:302:BCB:HHC	2.13	0.49
1:C:176:LEU:HD11	1:C:187:TYR:O	2.13	0.49
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.48	0.48
2:L:218:ASP:HB3	3:M:134:ARG:HD2	1.95	0.48
6:M:806:BCB:OBB	6:M:806:BCB:HHC	2.12	0.48
1:C:72:ARG:HG2	1:C:72:ARG:HH11	1.77	0.48
3:M:185:THR:HG22	3:M:189:ILE:HD12	1.96	0.48
2:L:269:ILE:HB	2:L:272:TRP:NE1	2.28	0.48
3:M:11:GLN:NE2	3:M:40:LYS:HG2	2.29	0.48
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.49	0.48
3:M:52:GLY:O	3:M:56:ILE:HD13	2.14	0.47
3:M:195:TYR:CE2	6:M:806:BCB:HMC2	2.49	0.47
1:C:23:LEU:HD22	1:C:23:LEU:N	2.30	0.47
1:C:210:PRO:HB2	4:H:3:HIS:HD2	1.79	0.47
1:C:76:ALA:O	1:C:79[A]:GLU:HG2	2.14	0.47
6:L:304:BCB:HBB2	6:L:304:BCB:HMB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:275:MET:HG2	7:M:401:BPB:HBCA	1.97	0.47
6:M:805:BCB:H41	6:M:805:BCB:H62	1.70	0.47
4:H:138:ARG:HG3	4:H:139:VAL:HG23	1.97	0.47
1:C:52:VAL:HA	1:C:55:VAL:HB	1.97	0.46
3:M:202:PHE:CZ	4:H:20:GLN:HG2	2.50	0.46
4:H:121:ALA:HB1	4:H:123:VAL:HG13	1.96	0.46
2:L:62:PHE:HB3	2:L:151:LEU:HD12	1.97	0.46
4:H:33:ARG:HA	4:H:33:ARG:HD2	1.78	0.46
1:C:72:ARG:HG2	1:C:72:ARG:NH1	2.31	0.46
4:H:6:LEU:HB2	4:H:10:LEU:HG	1.98	0.46
1:C:147:TYR:OH	1:C:301:PRO:HG3	2.16	0.46
4:H:68:PHE:O	4:H:75:THR:HA	2.16	0.46
1:C:10:THR:O	1:C:20:GLY:HA3	2.16	0.46
6:M:806:BCB:HAA2	6:M:806:BCB:CBD	2.45	0.45
2:L:224:ILE:HG12	2:L:228:SER:HB2	1.97	0.45
3:M:107:LEU:HD22	3:M:112:TRP:CE2	2.51	0.45
2:L:107:ILE:HG23	3:M:252:TRP:HE3	1.82	0.45
3:M:62:GLY:O	3:M:66:ILE:HD12	2.17	0.45
1:C:224:SER:HA	1:C:227:TYR:CD1	2.50	0.45
6:M:805:BCB:HHC	6:M:805:BCB:CBB	2.38	0.44
7:M:401:BPB:H6	7:M:401:BPB:H4	1.63	0.44
2:L:94:LEU:HA	2:L:94:LEU:HD23	1.77	0.44
2:L:224:ILE:HG22	8:L:502:UQ2:H8	1.99	0.44
6:L:304:BCB:HMC1	6:L:304:BCB:HBC3	1.99	0.44
3:M:69:ILE:HG12	3:M:93:LEU:HD23	1.99	0.44
1:C:35:ASP:HB3	1:C:316:LEU:HA	1.99	0.44
1:C:263:GLN:HA	1:C:266:ILE:HD12	1.99	0.44
3:M:291:ASN:HB3	3:M:294:LEU:HB2	2.00	0.44
1:C:113:MET:HB2	1:C:281:TYR:CD2	2.52	0.44
3:M:114:LEU:HD11	13:M:600:NS5:H331	2.00	0.44
4:H:37:ARG:HD3	4:H:61:GLU:HG3	2.00	0.44
6:L:302:BCB:H2C	6:M:806:BCB:H2C	1.99	0.44
3:M:80:ASP:HA	3:M:81:PRO:HD3	1.76	0.44
3:M:87:GLN:O	3:M:91:LEU:HG	2.18	0.44
3:M:176:GLY:N	13:M:600:NS5:H13	2.33	0.44
4:H:224:LEU:HD21	4:H:230:ILE:HD12	1.98	0.44
6:M:806:BCB:HMB1	6:M:806:BCB:HHB	1.82	0.43
1:C:192[A]:MET:HE3	1:C:199:ARG:HD3	2.01	0.43
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.53	0.43
4:H:27:VAL:O	4:H:31:TYR:HB3	2.18	0.43
1:C:233:MET:HB3	5:C:339:HEC:C4B	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:BCB:HBB3	7:L:402:BPB:H14	2.00	0.43
6:L:304:BCB:HHC	6:L:304:BCB:OBB	2.18	0.43
4:H:10:LEU:HD11	4:H:15:LEU:CD2	2.48	0.43
4:H:106:ASN:CG	4:H:109:VAL:HG22	2.44	0.43
4:H:136:PRO:HG2	4:H:138:ARG:HG2	2.00	0.43
1:C:33:GLU:O	1:C:36:ALA:HB3	2.19	0.43
7:L:402:BPB:NC	7:L:402:BPB:ND	2.66	0.43
3:M:96:PRO:HG3	3:M:105:PRO:HB3	2.01	0.43
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.01	0.43
4:H:138:ARG:CG	4:H:139:VAL:HG23	2.48	0.43
2:L:153:HIS:O	2:L:157:VAL:HG23	2.18	0.43
9:H:703:LDA:H42	9:H:703:LDA:H11	1.78	0.42
4:H:34:ARG:HG2	4:H:61:GLU:O	2.20	0.42
4:H:190:SER:HB3	4:H:192:ARG:HG2	2.00	0.42
4:H:81:ARG:O	4:H:83:PRO:HD3	2.19	0.42
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.83	0.42
1:C:331:ILE:O	1:C:331:ILE:HG22	2.19	0.42
1:C:268:TRP:CE3	3:M:315:PRO:HB2	2.54	0.42
4:H:204:LYS:HB2	4:H:207:LYS:O	2.20	0.42
3:M:67:LEU:O	3:M:71:PHE:HB2	2.20	0.42
4:H:65:PRO:HA	4:H:79:PRO:HD2	2.02	0.42
1:C:220:ARG:NH2	14:C:362:HOH:O	2.52	0.42
1:C:38:TYR:HD1	1:C:39:PRO:HD2	1.85	0.42
2:L:115:TRP:O	2:L:118:PRO:HG2	2.20	0.42
3:M:233:ILE:O	3:M:236:ILE:HB	2.20	0.42
2:L:161:GLY:HA3	6:L:302:BCB:HAC1	2.03	0.41
3:M:96:PRO:HD3	3:M:110:GLY:HA3	2.01	0.41
1:C:106:VAL:HG11	5:C:338:HEC:HAA2	2.02	0.41
3:M:192:GLY:O	3:M:193:ASN:HB3	2.20	0.41
4:H:90:LEU:HD21	4:H:112:VAL:HB	2.03	0.41
2:L:42:ILE:O	2:L:46:VAL:HG23	2.20	0.41
3:M:63:SER:O	3:M:67:LEU:HG	2.20	0.41
3:M:160:CYS:O	3:M:163:PRO:HD2	2.21	0.41
5:C:339:HEC:HBC3	5:C:339:HEC:HMC1	2.03	0.41
2:L:38:ALA:O	2:L:42:ILE:HG13	2.20	0.41
1:C:153:PRO:HG2	1:C:158:GLU:HB3	2.03	0.41
2:L:150:ILE:O	6:L:304:BCB:HED1	2.21	0.41
3:M:318:LEU:HA	3:M:319:PRO:HD2	1.72	0.41
2:L:205:LYS:HB3	4:H:71:PRO:HA	2.03	0.41
2:L:215:TYR:O	2:L:219:VAL:HG23	2.21	0.41
3:M:162:HIS:HB3	3:M:163:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:11:GLN:OE1	3:M:39:GLY:HA3	2.21	0.41
2:L:146:PHE:HB3	2:L:156:TRP:CE3	2.56	0.40
6:L:302:BCB:H161	6:L:302:BCB:H203	1.82	0.40
3:M:99:GLN:OE1	3:M:99:GLN:HA	2.22	0.40
2:L:83:GLY:O	2:L:87:GLN:HG3	2.21	0.40
3:M:106:PRO:HB2	3:M:108:HIS:CE1	2.57	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	333/336 (99%)	320 (96%)	13 (4%)	0	100	100
2	L	273/273 (100%)	256 (94%)	16 (6%)	1 (0%)	30	37
3	M	323/323 (100%)	310 (96%)	10 (3%)	3 (1%)	14	17
4	H	256/258 (99%)	243 (95%)	11 (4%)	2 (1%)	16	20
All	All	1185/1190 (100%)	1129 (95%)	50 (4%)	6 (0%)	24	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	46	PRO
3	M	322	PRO
4	H	55	GLU
3	M	193	ASN
2	L	31	VAL
3	M	96	PRO

5.3.2 Protein sidechains (i)

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	284/282 (101%)	266 (94%)	18 (6%)	16 23
2	L	220/218 (101%)	213 (97%)	7 (3%)	34 49
3	M	251/249 (101%)	239 (95%)	12 (5%)	23 34
4	H	212/212 (100%)	187 (88%)	25 (12%)	5 4
All	All	967/961 (101%)	905 (94%)	62 (6%)	16 22

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	33	GLU
1	C	48	GLU
1	C	53	SER
1	C	60	LYS
1	C	64	ASN
1	C	88	THR
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	146	ARG
1	C	152	LEU
1	C	168	THR
1	C	206	GLN
1	C	252	THR
1	C	288	SER
1	C	292	SER
1	C	323	LYS
1	C	327	GLU
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	119	LEU
2	L	182	VAL
2	L	185	MET

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Mol	Chain	Res	Type
2	L	220	VAL
3	M	17	ILE
3	M	20	SER
3	M	31	LYS
3	M	40	LYS
3	M	71	PHE
3	M	97	LYS
3	M	114	LEU
3	M	179	PRO
3	M	203	SER
3	M	287	THR
3	M	290	ASP
3	M	323	LYS
4	H	9	HIS
4	H	22	LEU
4	H	55	GLU
4	H	69	VAL
4	H	84	GLU
4	H	85	THR
4	H	89	LYS
4	H	96	PHE
4	H	108	LEU
4	H	119	GLU
4	H	141	THR
4	H	147	GLU
4	H	158	VAL
4	H	169	THR
4	H	175	ARG
4	H	195	LEU
4	H	198	LEU
4	H	208	ILE
4	H	211	THR
4	H	212	SER
4	H	216	GLU
4	H	225	GLN
4	H	226	SER
4	H	236	ASP
4	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	186	ASN
2	L	158	ASN
2	L	214	GLN
2	L	239	ASN
3	M	147	ASN
4	H	58	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	0.66	0	8,9,11	2.95	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
4	FME	H	1	4	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CA-N-CN	-6.31	113.11	122.82
4	H	1	FME	O1-CN-N	-4.50	113.69	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	FME	CE-SD-CG	2.13	111.35	100.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	CA-CB-CG-SD
4	H	1	FME	O1-CN-N-CA
4	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 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	$\#\|Z\| > 2$
5	HEC	C	339	1	50,50,50	1.06	5 (10%)	68,82,82	1.46	6 (8%)
8	UQ2	L	502	-	23,23,23	2.84	6 (26%)	30,31,31	1.38	5 (16%)
7	BPB	L	402	-	57,70,70	1.79	10 (17%)	55,101,101	2.51	14 (25%)
9	LDA	H	703	-	13,15,15	2.49	2 (15%)	14,17,17	0.60	0
5	HEC	C	338	1	50,50,50	1.12	5 (10%)	68,82,82	1.49	9 (13%)
12	MQ7	M	501	-	49,49,49	1.71	17 (34%)	61,63,63	1.31	5 (8%)
11	SO4	H	801	-	4,4,4	0.56	0	6,6,6	0.18	0
9	LDA	M	701	-	13,15,15	2.43	2 (15%)	14,17,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	SO4	M	802	-	4,4,4	0.59	0	6,6,6	0.97	0
6	BCB	M	805	3	68,74,74	1.38	10 (14%)	77,115,115	1.76	12 (15%)
13	NS5	M	600	-	39,39,39	0.76	0	46,46,46	1.27	6 (13%)
5	HEC	C	337	1	50,50,50	1.08	3 (6%)	68,82,82	1.49	9 (13%)
6	BCB	M	806	3	68,74,74	1.21	9 (13%)	77,115,115	2.10	16 (20%)
9	LDA	M	702	-	13,15,15	2.21	1 (7%)	14,17,17	0.49	0
11	SO4	M	803	-	4,4,4	0.53	0	6,6,6	0.59	0
9	LDA	M	704	-	13,15,15	1.88	2 (15%)	14,17,17	0.74	0
6	BCB	L	302	2	68,74,74	1.45	8 (11%)	77,115,115	1.87	17 (22%)
11	SO4	M	804	-	4,4,4	0.85	0	6,6,6	0.68	0
7	BPB	M	401	-	57,70,70	1.67	9 (15%)	55,101,101	2.62	15 (27%)
6	BCB	L	304	2	68,74,74	1.33	7 (10%)	77,115,115	1.96	15 (19%)
9	LDA	L	705	-	13,15,15	2.49	2 (15%)	14,17,17	0.58	0
5	HEC	C	340	1	50,50,50	1.04	4 (8%)	68,82,82	1.45	7 (10%)
9	LDA	M	706	-	13,15,15	2.60	2 (15%)	14,17,17	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	339	1	1/1/3/7	4/14/54/54	-
8	UQ2	L	502	-	-	4/15/39/39	0/1/1/1
7	BPB	L	402	-	-	5/37/105/105	0/5/6/6
9	LDA	H	703	-	-	4/13/13/13	-
5	HEC	C	338	1	1/1/3/7	8/14/54/54	-
12	MQ7	M	501	-	-	2/41/61/61	0/2/2/2
9	LDA	M	701	-	-	2/13/13/13	-
6	BCB	M	805	3	3/3/21/26	18/41/137/137	-
13	NS5	M	600	-	-	15/43/43/43	-
5	HEC	C	337	1	1/1/3/7	9/14/54/54	-
6	BCB	M	806	3	3/3/21/26	7/41/137/137	-
9	LDA	M	702	-	-	3/13/13/13	-
9	LDA	M	704	-	-	3/13/13/13	-
6	BCB	L	302	2	3/3/21/26	6/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPB	M	401	-	-	6/37/105/105	0/5/6/6
6	BCB	L	304	2	3/3/21/26	8/41/137/137	-
9	LDA	L	705	-	-	1/13/13/13	-
5	HEC	C	340	1	1/1/3/7	5/14/54/54	-
9	LDA	M	706	-	-	5/13/13/13	-

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	502	UQ2	C7-C8	-11.73	1.32	1.50
9	M	702	LDA	O1-N1	-7.72	1.23	1.42
9	M	706	LDA	O1-N1	-7.46	1.23	1.42
9	M	701	LDA	O1-N1	-7.44	1.23	1.42
9	L	705	LDA	O1-N1	-7.01	1.25	1.42
9	H	703	LDA	O1-N1	-6.98	1.25	1.42
7	M	401	BPB	C1D-C2D	5.99	1.46	1.39
6	L	304	BCB	MG-NA	5.90	2.20	2.06
9	M	704	LDA	O1-N1	-5.69	1.28	1.42
9	M	706	LDA	C1-N1	-5.60	1.45	1.51
9	H	703	LDA	C1-N1	-5.58	1.45	1.51
6	L	302	BCB	MG-NA	5.55	2.19	2.06
9	L	705	LDA	C1-N1	-5.50	1.45	1.51
6	L	302	BCB	C1-C2	-5.40	1.34	1.49
7	L	402	BPB	C1B-C2B	5.14	1.45	1.39
7	M	401	BPB	C1B-C2B	5.07	1.45	1.39
6	M	805	BCB	MG-NA	5.00	2.18	2.06
7	M	401	BPB	C3A-C2A	-4.82	1.50	1.54
7	L	402	BPB	O2D-CED	-4.59	1.35	1.45
9	M	701	LDA	C1-N1	-4.52	1.46	1.51
7	L	402	BPB	C1D-C2D	4.51	1.44	1.39
5	C	338	HEC	FE-NC	3.99	2.08	1.95
7	L	402	BPB	O2D-CGD	3.97	1.43	1.33
7	L	402	BPB	C3A-C2A	-3.97	1.51	1.54
6	M	805	BCB	O2D-CED	-3.74	1.37	1.45
7	L	402	BPB	C3B-C4B	3.72	1.47	1.41
6	M	805	BCB	O2A-CGA	3.67	1.44	1.33
6	L	302	BCB	O2D-CED	-3.56	1.37	1.45
9	M	704	LDA	C1-N1	-3.53	1.47	1.51
6	L	304	BCB	O2A-CGA	3.52	1.43	1.33
5	C	337	HEC	FE-ND	3.42	2.05	1.94
6	L	304	BCB	O2D-CED	-3.42	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	402	BPB	O2A-CGA	3.35	1.43	1.33
12	M	501	MQ7	C32-C33	3.26	1.40	1.33
7	M	401	BPB	O2A-CGA	3.24	1.42	1.33
5	C	337	HEC	FE-NA	3.14	2.05	1.95
6	L	302	BCB	MG-ND	-3.12	1.99	2.05
6	L	304	BCB	C3B-C4B	3.12	1.47	1.41
12	M	501	MQ7	C10-C5	-3.11	1.35	1.40
8	L	502	UQ2	O3-CM3	-3.09	1.38	1.45
6	M	805	BCB	MG-NB	-3.04	1.99	2.05
5	C	340	HEC	FE-NA	3.00	2.05	1.95
7	L	402	BPB	C2-C3	3.00	1.40	1.33
6	L	302	BCB	O2D-CGD	2.99	1.40	1.33
5	C	338	HEC	FE-NB	2.98	2.04	1.94
6	M	806	BCB	O2D-CED	-2.97	1.38	1.45
6	M	806	BCB	CAA-CBA	-2.97	1.44	1.52
5	C	340	HEC	FE-NB	2.95	2.04	1.94
8	L	502	UQ2	O4-C4	2.89	1.29	1.23
7	M	401	BPB	C2-C3	2.87	1.39	1.33
6	M	806	BCB	C2-C3	2.84	1.39	1.33
12	M	501	MQ7	C17-C18	2.81	1.39	1.33
12	M	501	MQ7	C41-C42	-2.78	1.42	1.50
12	M	501	MQ7	C27-C28	2.73	1.39	1.33
6	L	304	BCB	C2-C3	2.71	1.39	1.33
12	M	501	MQ7	C37-C38	2.70	1.39	1.33
6	M	806	BCB	MG-ND	-2.70	2.00	2.05
12	M	501	MQ7	C26-C27	-2.69	1.42	1.50
7	M	401	BPB	C3B-C4B	2.69	1.45	1.41
7	M	401	BPB	O2D-CGD	2.64	1.39	1.33
7	L	402	BPB	C1-C2	-2.63	1.41	1.49
8	L	502	UQ2	C13-C14	2.60	1.40	1.32
5	C	339	HEC	FE-NC	2.53	2.03	1.95
5	C	339	HEC	FE-NB	2.52	2.02	1.94
12	M	501	MQ7	C21-C22	-2.50	1.42	1.50
7	M	401	BPB	C3B-C2B	-2.47	1.35	1.39
6	M	806	BCB	O2A-CGA	2.47	1.40	1.33
6	M	805	BCB	C2-C3	2.46	1.38	1.33
12	M	501	MQ7	C36-C37	-2.44	1.43	1.50
8	L	502	UQ2	C16-C14	2.44	1.56	1.50
6	M	805	BCB	C3B-C4B	2.43	1.45	1.41
12	M	501	MQ7	C42-C43	2.43	1.39	1.32
5	C	339	HEC	FE-ND	2.42	2.02	1.94
6	L	302	BCB	MG-NC	-2.38	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	402	BPB	C5-C3	2.37	1.56	1.51
12	M	501	MQ7	C11-C12	-2.37	1.46	1.50
6	L	302	BCB	C3B-C4B	2.31	1.45	1.41
5	C	340	HEC	CMD-C2D	2.31	1.55	1.50
12	M	501	MQ7	C12-C13	2.30	1.38	1.33
6	M	806	BCB	C3B-C4B	2.28	1.45	1.41
6	M	805	BCB	O2D-CGD	2.27	1.38	1.33
12	M	501	MQ7	C45-C43	2.21	1.56	1.50
8	L	502	UQ2	CM5-C5	2.21	1.55	1.50
12	M	501	MQ7	C22-C23	2.18	1.38	1.33
6	L	304	BCB	C4C-C3C	-2.17	1.40	1.44
6	M	806	BCB	C1-C2	-2.17	1.43	1.49
12	M	501	MQ7	C16-C17	-2.15	1.43	1.50
5	C	340	HEC	FE-NC	2.14	2.02	1.95
12	M	501	MQ7	C34-C33	2.13	1.55	1.50
6	L	304	BCB	C2C-C3C	-2.12	1.49	1.51
5	C	338	HEC	FE-ND	2.12	2.01	1.94
12	M	501	MQ7	C10-C1	-2.12	1.44	1.48
5	C	337	HEC	CMC-C2C	2.11	1.55	1.50
7	M	401	BPB	C1B-NB	2.11	1.42	1.38
5	C	338	HEC	FE-NA	2.10	2.02	1.95
5	C	339	HEC	CMC-C2C	2.09	1.55	1.50
6	L	302	BCB	C2-C3	2.07	1.37	1.33
6	M	805	BCB	CAC-C3C	2.06	1.38	1.33
6	M	805	BCB	CMD-C2D	2.06	1.55	1.50
6	M	806	BCB	CMD-C2D	2.05	1.55	1.50
6	M	805	BCB	C4-C3	2.04	1.55	1.50
5	C	338	HEC	CHD-C1D	2.03	1.42	1.38
5	C	339	HEC	O2A-CGA	-2.02	1.24	1.30
6	M	806	BCB	O2D-CGD	2.01	1.38	1.33

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BPB	O2D-CGD-CBD	12.75	124.96	110.95
7	L	402	BPB	O2D-CGD-CBD	11.87	123.99	110.95
6	M	805	BCB	C4A-NA-C1A	7.78	110.23	106.68
6	L	302	BCB	C4A-NA-C1A	7.67	110.18	106.68
6	M	806	BCB	C4A-NA-C1A	7.58	110.14	106.68
6	L	304	BCB	C4A-NA-C1A	7.42	110.07	106.68
6	L	304	BCB	O2D-CGD-CBD	7.31	124.00	111.23
7	M	401	BPB	O1D-CGD-CBD	-7.13	113.92	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	806	BCB	CMB-C2B-C1B	-6.66	115.28	125.42
7	L	402	BPB	O1D-CGD-CBD	-6.57	114.76	124.72
7	L	402	BPB	C4D-CHA-CBD	-6.22	105.47	108.45
6	M	805	BCB	O2D-CGD-CBD	6.12	121.93	111.23
6	M	806	BCB	O2D-CGD-CBD	5.84	121.44	111.23
5	C	339	HEC	CAC-C3C-C4C	-5.60	117.22	124.91
5	C	339	HEC	CAC-C3C-C2C	5.53	135.64	126.89
7	M	401	BPB	C4D-CHA-CBD	-5.47	105.83	108.45
5	C	338	HEC	CAC-C3C-C4C	-5.28	117.64	124.91
5	C	339	HEC	CAB-C3B-C4B	-5.27	117.94	124.79
5	C	340	HEC	CBD-CAD-C3D	5.17	126.83	112.53
5	C	338	HEC	CAC-C3C-C2C	5.11	134.97	126.89
6	L	302	BCB	O2D-CGD-CBD	5.05	120.06	111.23
6	L	304	BCB	O1D-CGD-CBD	-4.84	114.97	124.52
5	C	337	HEC	CAB-C3B-C4B	-4.79	118.56	124.79
7	M	401	BPB	C1-C2-C3	4.77	134.01	126.20
5	C	338	HEC	CAB-C3B-C4B	-4.73	118.64	124.79
6	M	806	BCB	C1C-NC-C4C	4.68	108.81	106.68
5	C	340	HEC	CAC-C3C-C2C	4.50	134.00	126.89
5	C	340	HEC	CAC-C3C-C4C	-4.24	119.07	124.91
5	C	337	HEC	CAC-C3C-C2C	4.20	133.54	126.89
6	M	805	BCB	O1D-CGD-CBD	-4.19	116.25	124.52
13	M	600	NS5	C19-C18-C17	4.15	132.01	123.52
6	L	304	BCB	C4-C3-C5	-4.11	108.10	115.23
5	C	337	HEC	CAC-C3C-C4C	-4.10	119.27	124.91
5	C	340	HEC	CAB-C3B-C4B	-4.09	119.47	124.79
6	L	302	BCB	O1D-CGD-CBD	-4.08	116.46	124.52
6	M	806	BCB	O2A-CGA-CBA	4.07	124.25	111.83
6	M	806	BCB	O1D-CGD-CBD	-4.04	116.55	124.52
12	M	501	MQ7	C11-C12-C13	4.03	133.77	126.83
6	M	806	BCB	OBB-CAB-C3B	3.97	127.45	120.43
6	L	304	BCB	C1C-NC-C4C	3.89	108.45	106.68
5	C	339	HEC	CAB-C3B-C2B	3.88	134.68	127.56
8	L	502	UQ2	CM3-O3-C3	3.81	129.86	116.47
7	M	401	BPB	OBD-CAD-CBD	-3.80	120.25	125.82
5	C	337	HEC	CAB-C3B-C2B	3.75	134.46	127.56
5	C	337	HEC	CAA-C2A-C3A	-3.72	120.90	127.87
5	C	338	HEC	CAB-C3B-C2B	3.69	134.34	127.56
13	M	600	NS5	C16-C15-C14	-3.69	112.45	118.09
7	L	402	BPB	OBD-CAD-CBD	-3.69	120.41	125.82
7	M	401	BPB	OBB-CAB-C3B	3.69	126.16	119.99
6	L	304	BCB	O2A-CGA-CBA	3.68	123.04	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	806	BCB	CMB-C2B-C3B	3.68	137.26	125.67
6	L	302	BCB	C1C-NC-C4C	3.64	108.34	106.68
6	M	805	BCB	C1C-NC-C4C	3.60	108.32	106.68
5	C	337	HEC	CAA-C2A-C1A	3.52	132.01	124.85
7	L	402	BPB	CED-O2D-CGD	3.52	123.90	115.92
6	M	806	BCB	CBB-CAB-C3B	-3.49	113.04	120.40
5	C	340	HEC	CAB-C3B-C2B	3.40	133.81	127.56
6	M	805	BCB	O2A-CGA-CBA	3.35	122.06	111.83
6	L	302	BCB	C15-C13-C12	-3.35	95.11	112.07
6	M	805	BCB	C4-C3-C5	3.30	120.96	115.23
6	L	302	BCB	O2A-CGA-CBA	3.30	121.89	111.83
12	M	501	MQ7	C41-C42-C43	3.30	138.63	127.64
13	M	600	NS5	C18-C19-C20	3.27	130.21	123.52
7	M	401	BPB	CMA-C3A-C4A	-3.17	107.77	114.61
7	M	401	BPB	CBB-CAB-C3B	-3.17	110.86	120.34
8	L	502	UQ2	C12-C13-C14	3.16	138.17	127.64
6	L	302	BCB	O2A-CGA-O1A	-3.14	115.77	123.63
12	M	501	MQ7	C26-C25-C23	-3.11	102.89	113.19
6	L	304	BCB	OBB-CAB-C3B	3.09	125.89	120.43
7	L	402	BPB	CMD-C2D-C3D	3.07	130.82	124.68
6	L	304	BCB	CAB-C3B-C2B	3.04	134.06	127.74
6	M	806	BCB	CAB-C3B-C2B	2.96	133.89	127.74
6	L	302	BCB	CAB-C3B-C2B	2.95	133.86	127.74
7	L	402	BPB	C2D-C1D-ND	2.93	111.55	109.43
5	C	338	HEC	CBA-CAA-C2A	-2.85	104.65	112.53
6	L	304	BCB	C5-C3-C2	2.85	127.56	121.17
6	M	806	BCB	O2A-CGA-O1A	-2.83	116.56	123.63
7	L	402	BPB	O2A-CGA-CBA	2.81	120.40	111.83
12	M	501	MQ7	C11-C3-C2	-2.80	120.08	124.89
5	C	337	HEC	CMA-C3A-C4A	2.80	129.66	124.73
7	L	402	BPB	C4D-ND-C1D	-2.74	105.59	108.87
5	C	337	HEC	CBD-CAD-C3D	-2.73	104.98	112.53
7	M	401	BPB	O2A-CGA-CBA	2.73	120.15	111.83
6	L	302	BCB	CMD-C2D-C1D	2.72	129.52	124.73
6	L	302	BCB	C4-C3-C5	2.68	119.87	115.23
6	L	304	BCB	O2A-CGA-O1A	-2.64	117.03	123.63
7	L	402	BPB	CMA-C3A-C4A	-2.62	108.97	114.61
6	M	805	BCB	CAB-C3B-C2B	2.59	133.12	127.74
5	C	340	HEC	CMA-C3A-C4A	2.55	129.22	124.73
6	L	302	BCB	CHD-C1D-ND	-2.53	121.24	124.80
6	L	302	BCB	C2A-C1A-CHA	2.53	128.25	123.87
7	M	401	BPB	C4D-ND-C1D	-2.50	105.88	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	806	BCB	C4-C3-C2	-2.48	117.25	123.63
8	L	502	UQ2	C7-C6-C5	-2.48	120.64	124.89
6	L	302	BCB	CMB-C2B-C1B	-2.45	121.68	125.42
6	L	302	BCB	C1D-ND-C4D	-2.44	104.60	106.31
8	L	502	UQ2	C7-C8-C9	-2.43	122.65	126.83
6	M	805	BCB	O2A-CGA-O1A	-2.42	117.57	123.63
5	C	338	HEC	CAD-C3D-C4D	2.40	128.88	124.70
6	M	806	BCB	CAA-C2A-C1A	-2.37	104.22	111.97
6	M	806	BCB	C3A-C2A-C1A	2.36	104.88	101.34
6	M	806	BCB	C1-C2-C3	-2.34	122.36	126.20
5	C	337	HEC	CMC-C2C-C3C	2.34	130.58	125.62
5	C	338	HEC	CBD-CAD-C3D	2.33	118.98	112.53
8	L	502	UQ2	C10-C9-C11	2.33	119.27	115.23
7	L	402	BPB	O2A-CGA-O1A	-2.33	117.80	123.63
6	L	302	BCB	C1-C2-C3	-2.32	122.40	126.20
6	M	805	BCB	CMB-C2B-C1B	-2.29	121.93	125.42
5	C	340	HEC	CBC-CAC-C3C	2.28	118.61	112.42
7	L	402	BPB	C4A-C3A-C2A	2.25	104.98	102.84
6	L	302	BCB	OBB-CAB-C3B	2.25	124.41	120.43
6	L	304	BCB	C1D-ND-C4D	-2.21	104.76	106.31
7	L	402	BPB	C1A-C2A-C3A	2.20	104.93	102.84
6	L	304	BCB	C1-C2-C3	-2.19	122.61	126.20
6	M	805	BCB	C10-C8-C7	2.19	123.14	112.07
12	M	501	MQ7	C29-C28-C30	-2.17	111.45	115.23
7	M	401	BPB	OBD-CAD-C3D	2.17	131.28	127.89
7	M	401	BPB	CMD-C2D-C3D	2.16	129.01	124.68
6	M	805	BCB	C2A-C1A-CHA	2.16	127.62	123.87
7	M	401	BPB	C3D-C4D-ND	2.16	110.47	107.71
6	L	304	BCB	CBC-CAC-C3C	-2.15	120.86	126.70
5	C	338	HEC	CMC-C2C-C3C	2.13	130.14	125.62
6	L	304	BCB	CBB-CAB-C3B	-2.12	115.93	120.40
13	M	600	NS5	C22-C21-C23	-2.12	114.86	118.09
5	C	339	HEC	CAA-C2A-C3A	-2.11	123.91	127.87
6	M	805	BCB	CHB-C1B-NB	2.11	127.22	124.05
5	C	338	HEC	CAD-C3D-C2D	-2.11	123.92	127.87
7	L	402	BPB	C3D-C4D-ND	2.11	110.41	107.71
6	L	302	BCB	CHB-C1B-NB	2.08	127.16	124.05
13	M	600	NS5	C19-C20-C21	-2.06	124.39	127.28
7	M	401	BPB	O2A-CGA-O1A	-2.05	118.49	123.63
7	M	401	BPB	CED-O2D-CGD	2.05	120.56	115.92
5	C	339	HEC	CAA-C2A-C1A	2.05	129.02	124.85
6	L	304	BCB	C2A-C1A-CHA	2.03	127.39	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	806	BCB	CHD-C1D-ND	-2.00	121.99	124.80
13	M	600	NS5	C14-C15-C17	2.00	122.16	119.01

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	337	HEC	NA
5	C	338	HEC	NA
5	C	339	HEC	NA
5	C	340	HEC	NA
6	L	302	BCB	ND
6	L	302	BCB	NC
6	L	302	BCB	NA
6	L	304	BCB	ND
6	L	304	BCB	NC
6	L	304	BCB	NA
6	M	805	BCB	ND
6	M	805	BCB	NC
6	M	805	BCB	NA
6	M	806	BCB	ND
6	M	806	BCB	NC
6	M	806	BCB	NA

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	805	BCB	C4B-C3B-CAB-CBB
6	M	805	BCB	C2C-C3C-CAC-CBC
6	M	806	BCB	CAD-CBD-CGD-O1D
6	M	806	BCB	CAD-CBD-CGD-O2D
6	M	806	BCB	C14-C13-C15-C16
13	M	600	NS5	C3-C4-C5-C6
13	M	600	NS5	C10-C12-C13-C14
13	M	600	NS5	C13-C14-C15-C16
13	M	600	NS5	C13-C14-C15-C17
6	M	805	BCB	C3-C5-C6-C7
8	L	502	UQ2	C12-C11-C9-C8
5	C	337	HEC	C2B-C3B-CAB-CBB
7	M	401	BPB	C4-C3-C5-C6
8	L	502	UQ2	C12-C11-C9-C10
6	M	805	BCB	C2-C3-C5-C6
7	M	401	BPB	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	L	502	UQ2	C9-C11-C12-C13
13	M	600	NS5	C7-C8-C9-C10
6	L	302	BCB	CBD-CGD-O2D-CED
5	C	338	HEC	C2C-C3C-CAC-CBC
6	L	304	BCB	CBD-CGD-O2D-CED
6	L	302	BCB	C4-C3-C5-C6
6	M	805	BCB	C4-C3-C5-C6
6	L	302	BCB	C2-C3-C5-C6
13	M	600	NS5	C3-C4-C5-C7
6	L	304	BCB	C14-C13-C15-C16
5	C	338	HEC	C2B-C3B-CAB-CBB
6	L	302	BCB	O1D-CGD-O2D-CED
13	M	600	NS5	C22-C21-C23-C24
5	C	339	HEC	C4B-C3B-CAB-CBB
5	C	338	HEC	C4C-C3C-CAC-CBC
5	C	339	HEC	C2B-C3B-CAB-CBB
6	M	806	BCB	C2A-CAA-CBA-CGA
7	L	402	BPB	C8-C10-C11-C12
5	C	338	HEC	C4B-C3B-CAB-CBB
5	C	337	HEC	C4B-C3B-CAB-CBB
6	M	805	BCB	C15-C16-C17-C18
5	C	340	HEC	C2B-C3B-CAB-CBB
6	M	805	BCB	C2B-C3B-CAB-CBB
6	L	304	BCB	C16-C17-C18-C20
9	M	704	LDA	C7-C8-C9-C10
6	L	304	BCB	C16-C17-C18-C19
6	L	304	BCB	O1D-CGD-O2D-CED
5	C	339	HEC	C2C-C3C-CAC-CBC
6	M	805	BCB	C10-C11-C12-C13
9	M	706	LDA	C6-C7-C8-C9
7	L	402	BPB	C16-C17-C18-C19
5	C	340	HEC	C2C-C3C-CAC-CBC
7	M	401	BPB	O1A-CGA-O2A-C1
5	C	337	HEC	C2C-C3C-CAC-CBC
9	M	704	LDA	C2-C3-C4-C5
7	M	401	BPB	CBA-CGA-O2A-C1
9	M	701	LDA	C2-C3-C4-C5
5	C	340	HEC	C4C-C3C-CAC-CBC
9	M	706	LDA	C11-C10-C9-C8
6	M	806	BCB	C13-C15-C16-C17
6	M	805	BCB	C1A-C2A-CAA-CBA
5	C	339	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	M	702	LDA	C2-C3-C4-C5
7	M	401	BPB	C5-C6-C7-C8
13	M	600	NS5	C20-C21-C23-C24
7	L	402	BPB	O2A-C1-C2-C3
6	L	304	BCB	C11-C12-C13-C14
9	M	706	LDA	C5-C6-C7-C8
6	L	304	BCB	C11-C12-C13-C15
6	M	806	BCB	C12-C13-C15-C16
6	M	805	BCB	C3A-C2A-CAA-CBA
7	M	401	BPB	C3-C5-C6-C7
13	M	600	NS5	C17-C18-C19-C20
9	H	703	LDA	C3-C4-C5-C6
7	L	402	BPB	C16-C17-C18-C20
9	M	704	LDA	C3-C4-C5-C6
6	M	806	BCB	CBD-CGD-O2D-CED
13	M	600	NS5	C34-C35-C36-CM3
5	C	340	HEC	C4B-C3B-CAB-CBB
13	M	600	NS5	C23-C24-C25-C26
5	C	337	HEC	C4C-C3C-CAC-CBC
6	M	805	BCB	C11-C10-C8-C7
9	M	701	LDA	C5-C6-C7-C8
6	L	302	BCB	C15-C16-C17-C18
6	M	805	BCB	CAD-CBD-CGD-O1D
9	M	706	LDA	C2-C3-C4-C5
13	M	600	NS5	C14-C15-C17-C18
9	M	702	LDA	C3-C4-C5-C6
6	M	805	BCB	C4B-C3B-CAB-OBB
9	M	702	LDA	C4-C5-C6-C7
5	C	337	HEC	C2A-CAA-CBA-CGA
9	H	703	LDA	C11-C10-C9-C8
5	C	337	HEC	CAA-CBA-CGA-O1A
9	H	703	LDA	C7-C8-C9-C10
6	M	805	BCB	C2B-C3B-CAB-OBB
12	M	501	MQ7	C39-C38-C40-C41
6	M	805	BCB	C6-C7-C8-C10
5	C	337	HEC	CAA-CBA-CGA-O2A
9	H	703	LDA	C5-C6-C7-C8
13	M	600	NS5	C18-C19-C20-C21
5	C	338	HEC	CAA-CBA-CGA-O1A
8	L	502	UQ2	C4-C3-O3-CM3
6	M	805	BCB	C16-C17-C18-C20
5	C	338	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
5	C	338	HEC	CAD-CBD-CGD-O2D
7	L	402	BPB	C4-C3-C5-C6
5	C	338	HEC	CAD-CBD-CGD-O1D
9	M	706	LDA	C9-C10-C11-C12
6	L	304	BCB	C12-C13-C15-C16
9	L	705	LDA	C1-C2-C3-C4
5	C	337	HEC	CAD-CBD-CGD-O2D
5	C	337	HEC	CAD-CBD-CGD-O1D
13	M	600	NS5	C30-C31-C33-C34
12	M	501	MQ7	C37-C38-C40-C41
6	M	805	BCB	CBA-CGA-O2A-C1
6	L	302	BCB	C11-C12-C13-C14
5	C	340	HEC	CAD-CBD-CGD-O2D
13	M	600	NS5	C12-C10-C9-C8
6	M	805	BCB	CAD-CBD-CGD-O2D

There are no ring outliers.

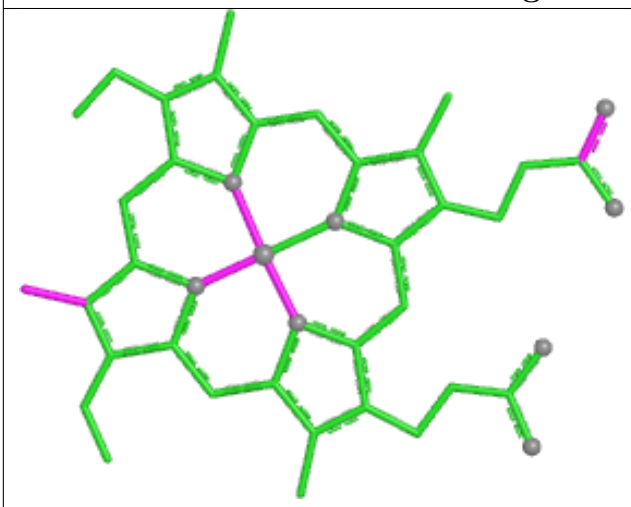
13 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	339	HEC	2	0
8	L	502	UQ2	2	0
7	L	402	BPB	6	0
9	H	703	LDA	1	0
5	C	338	HEC	1	0
6	M	805	BCB	7	0
13	M	600	NS5	6	0
6	M	806	BCB	7	0
9	M	704	LDA	1	0
6	L	302	BCB	4	0
7	M	401	BPB	7	0
6	L	304	BCB	5	0
9	M	706	LDA	1	0

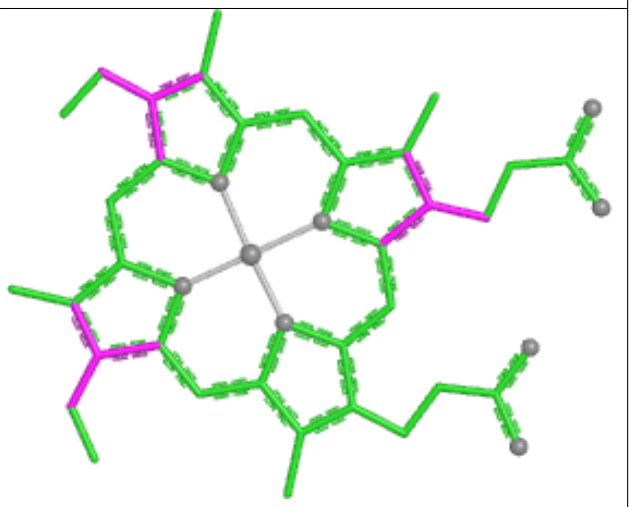
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

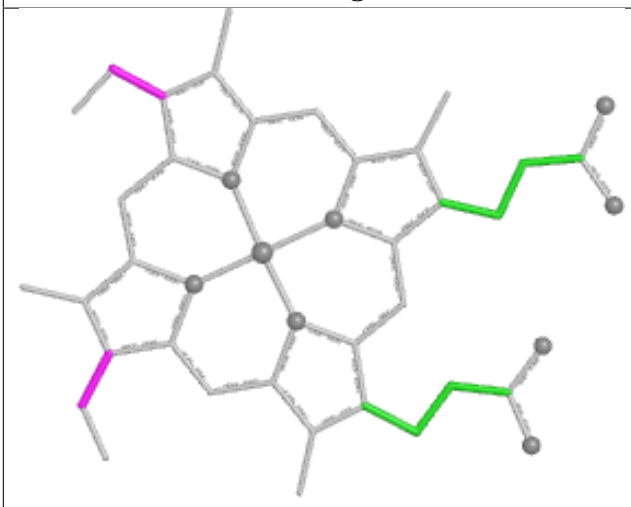
Ligand HEC C 339



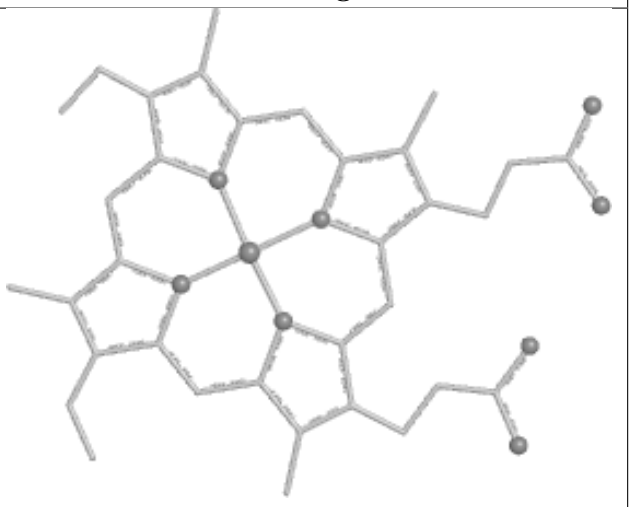
Bond lengths



Bond angles

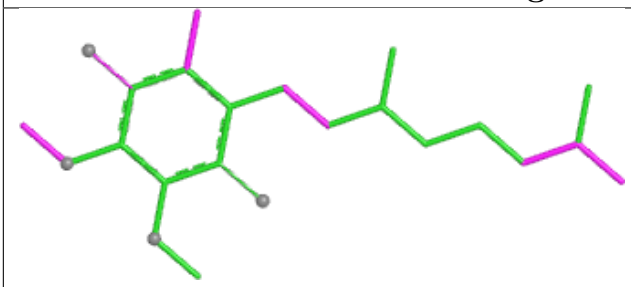


Torsions

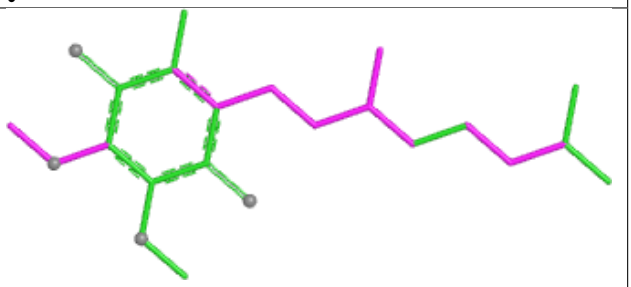


Rings

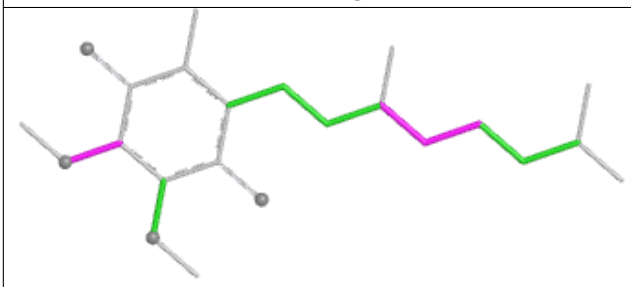
Ligand UQ2 L 502



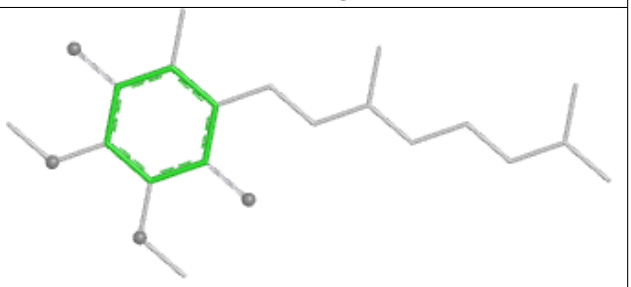
Bond lengths



Bond angles

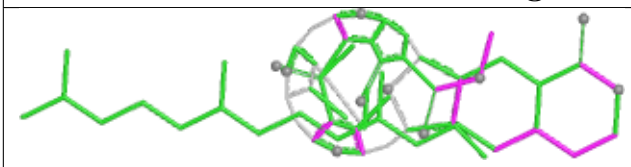


Torsions

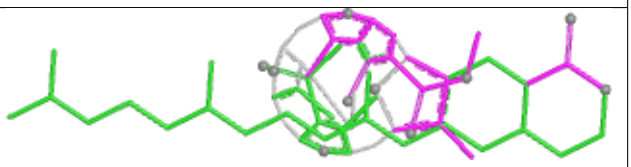


Rings

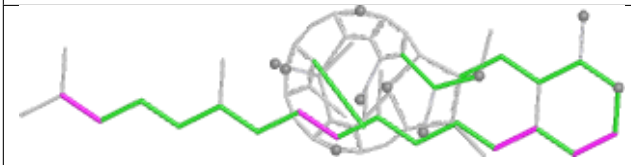
Ligand BPB L 402



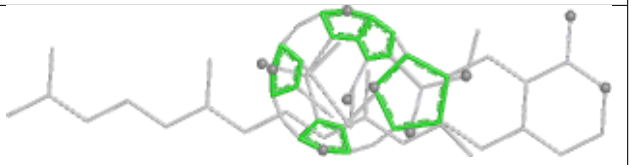
Bond lengths



Bond angles

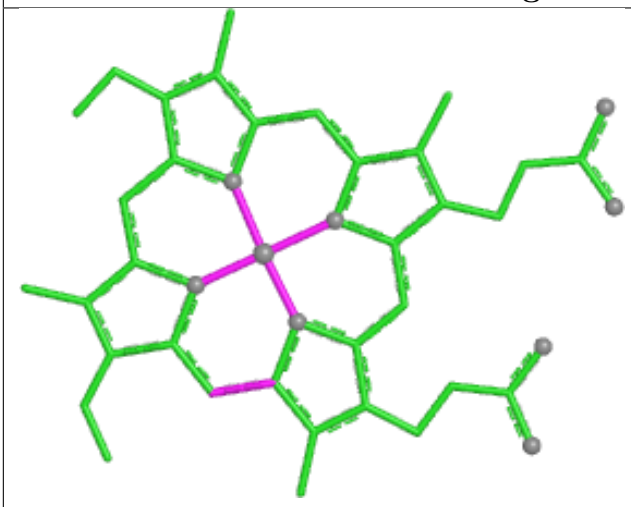


Torsions



Rings

Ligand HEC C 338



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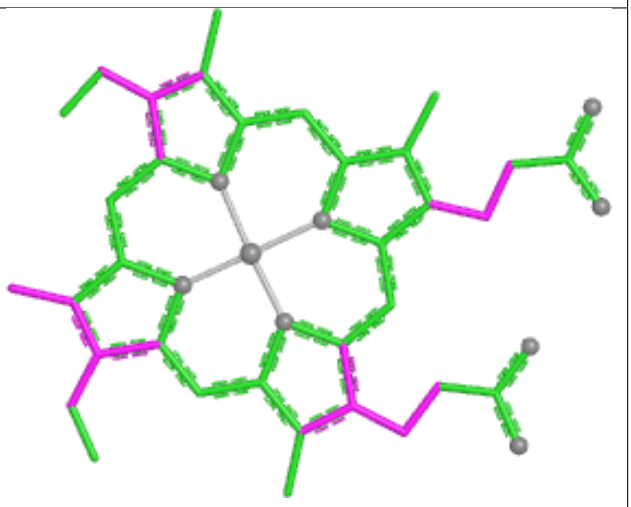
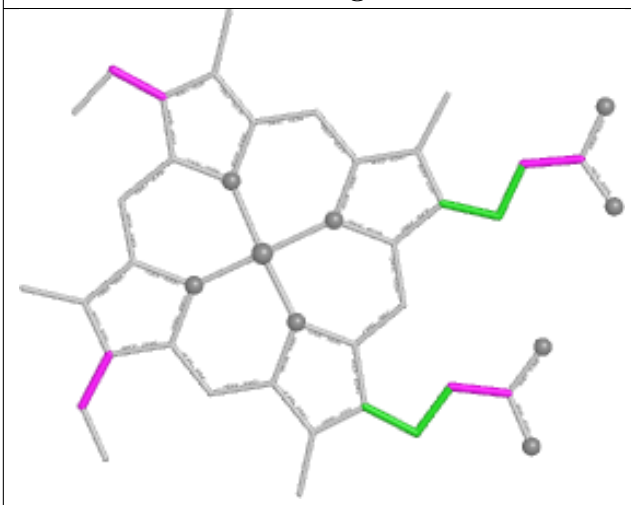


Bond angles



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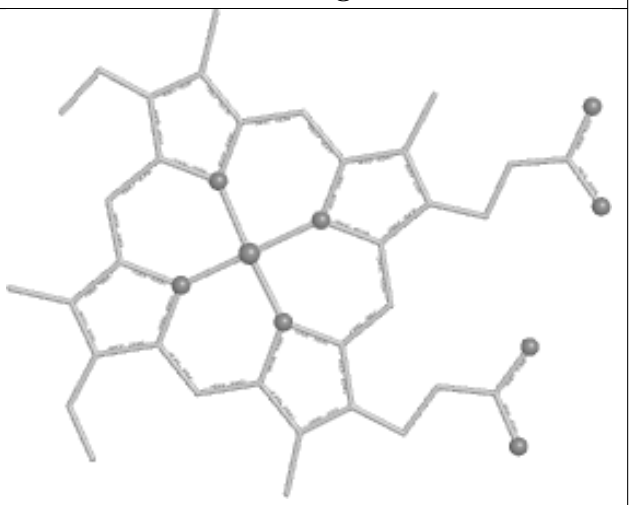


Rings

Ligand MQ7 M 501



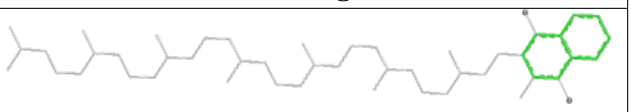
Bond lengths



Bond angles

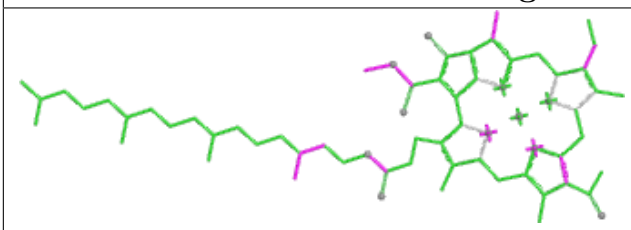


Torsions

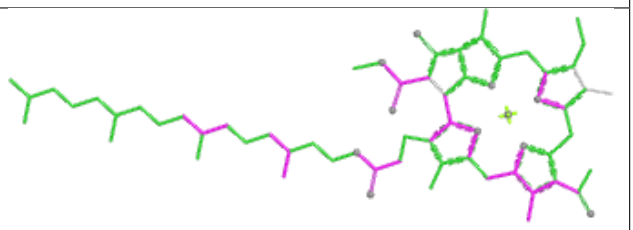


Rings

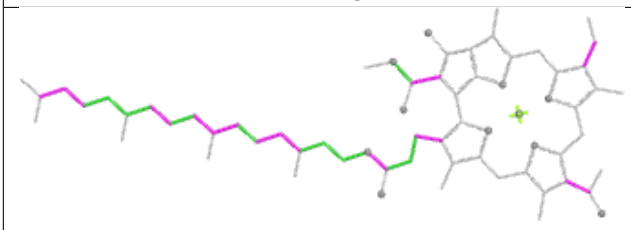
Ligand BCB M 805



Bond lengths



Bond angles



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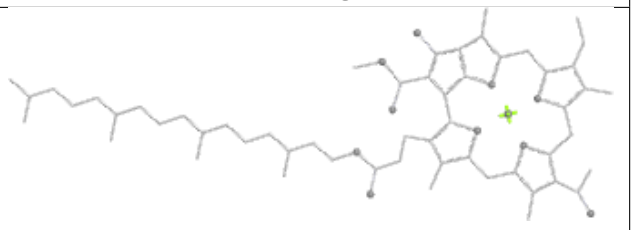
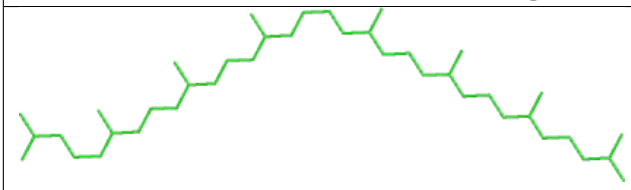


Rings

Ligand NS5 M 600



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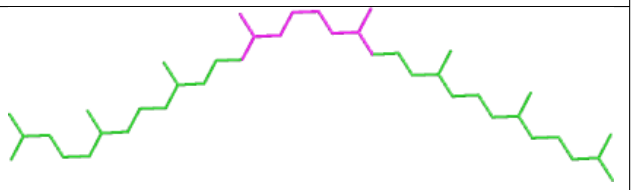
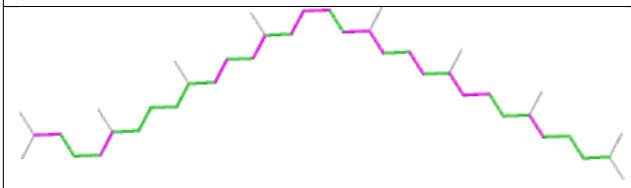


Bond angles



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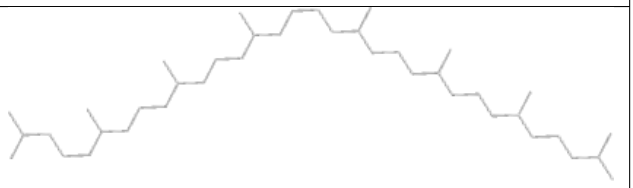
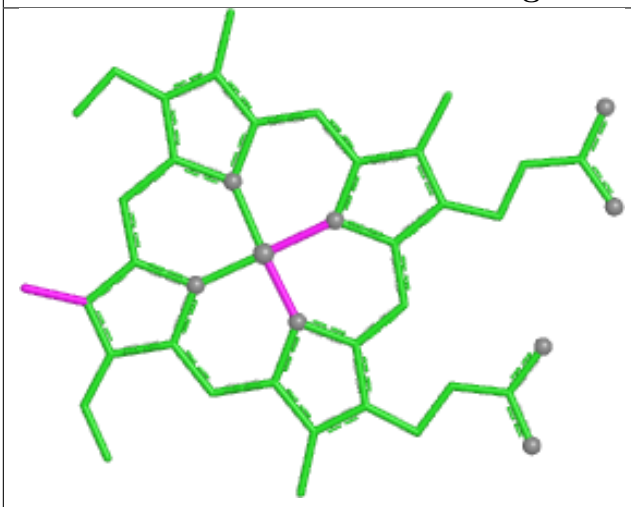
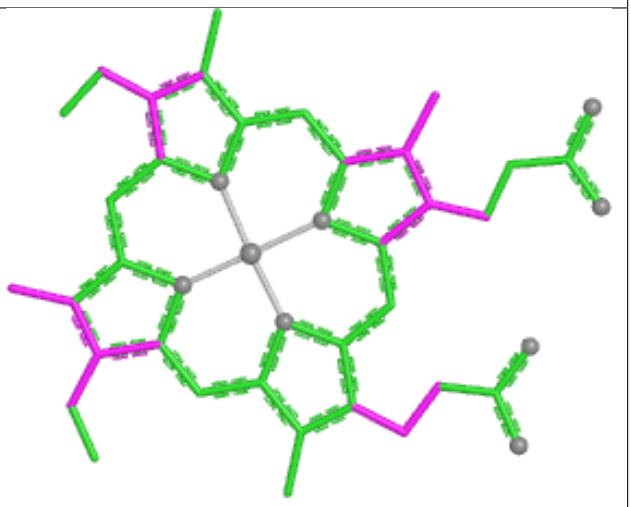


Rings

Ligand HEC C 337



Bond lengths



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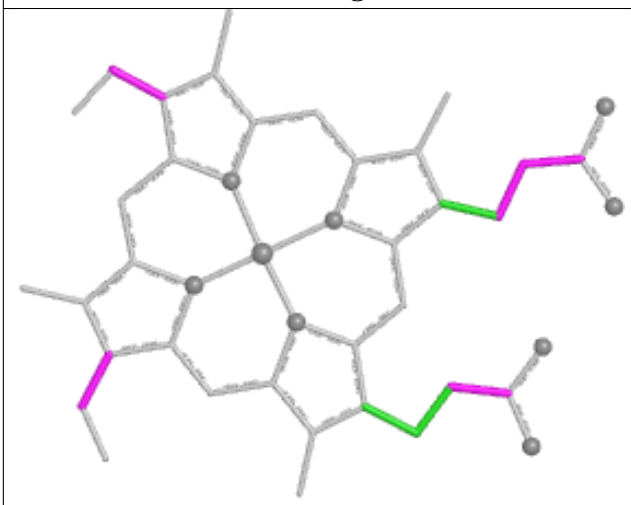
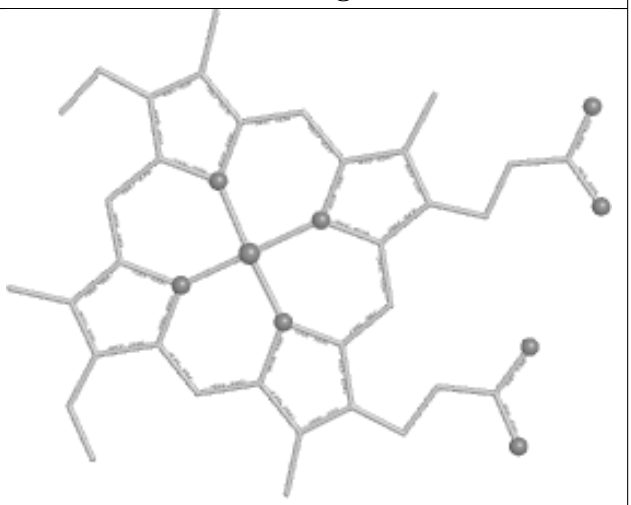
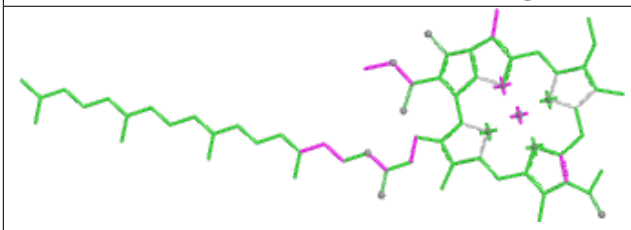


Torsions

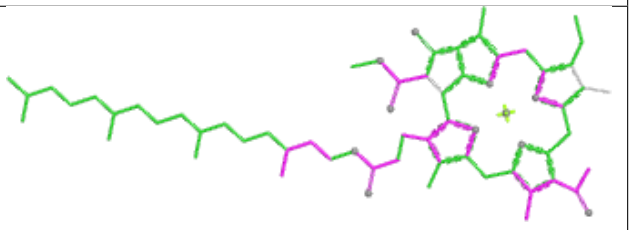


Rings

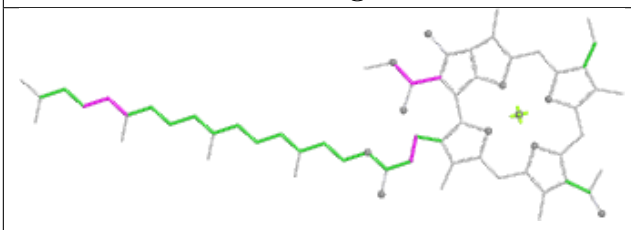
Ligand BCB M 806



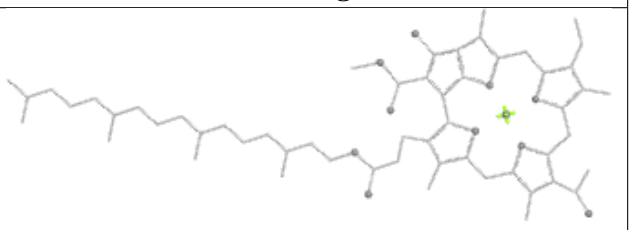
Bond lengths



Bond angles

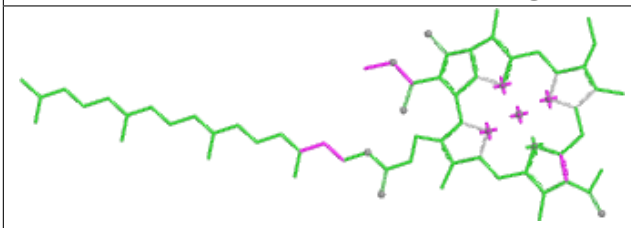


Torsions

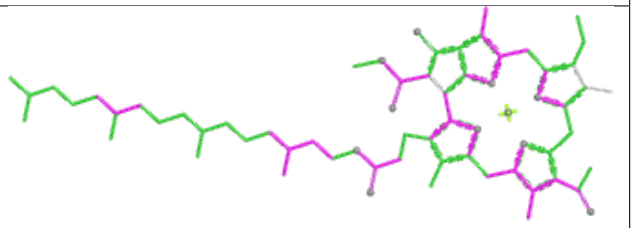


Rings

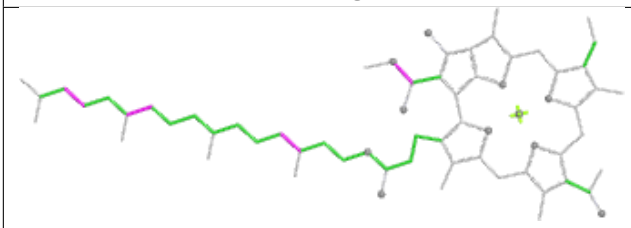
Ligand BCB L 302



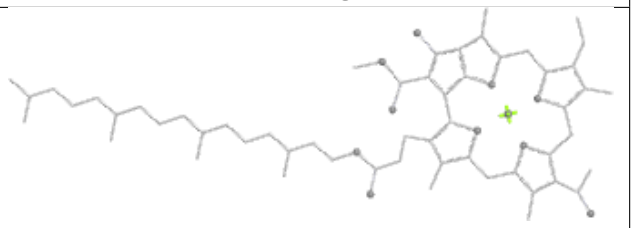
Bond lengths



Bond angles

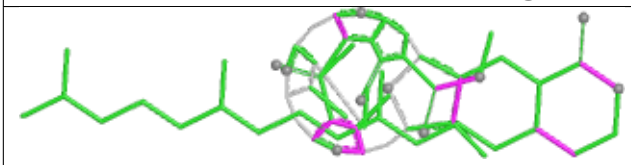


Torsions

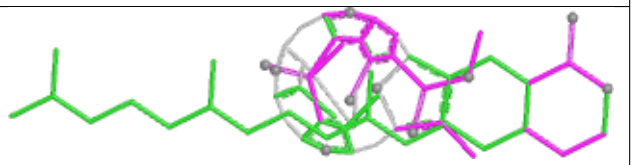


Rings

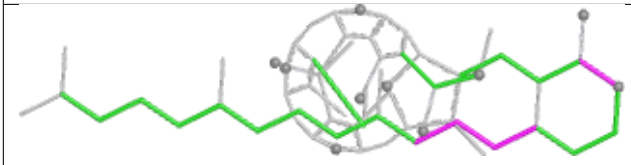
Ligand BPB M 401



Bond lengths



Bond angles



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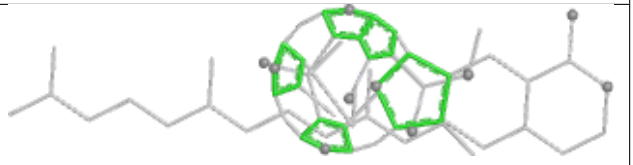
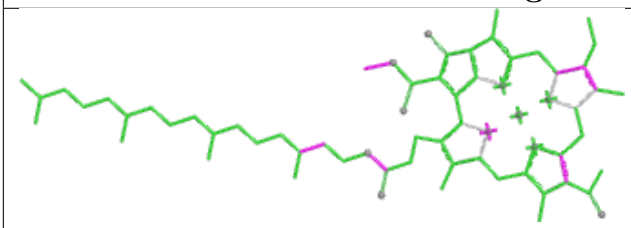
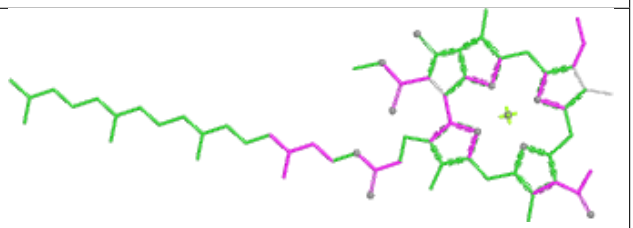


Rings

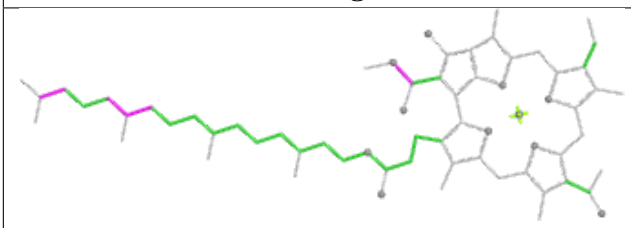
Ligand BCB L 304



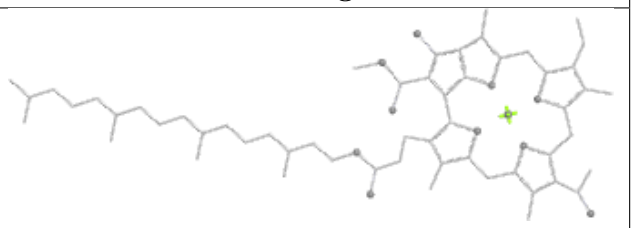
Bond lengths



Bond angles

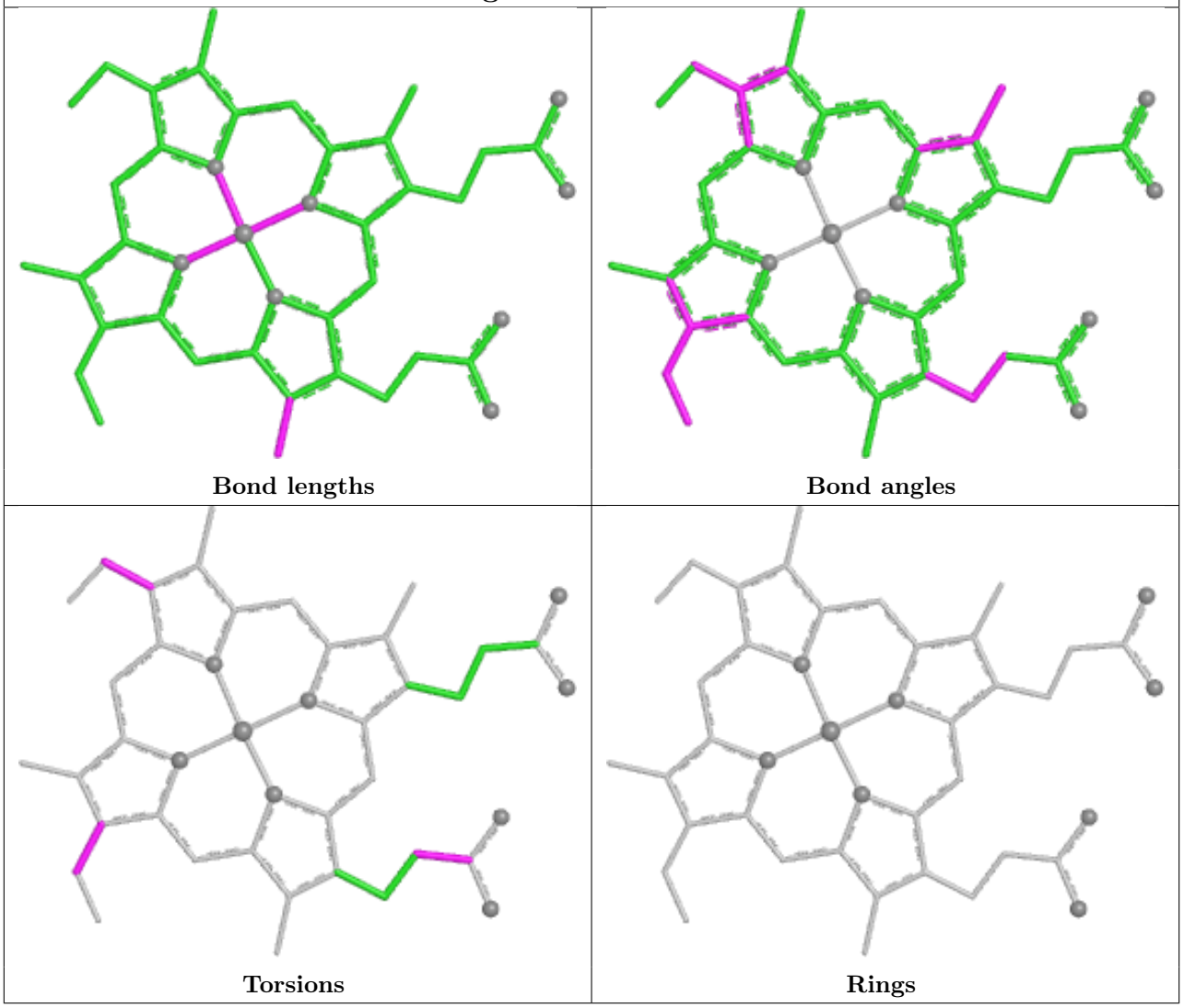


Torsions



Rings

Ligand HEC C 340



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%)	-0.81	1 (0%) 90 91	9, 26, 46, 65	23 (6%)
2	L	273/273 (100%)	-0.93	0 100 100	10, 21, 43, 60	8 (2%)
3	M	323/323 (100%)	-0.82	0 100 100	8, 23, 50, 65	12 (3%)
4	H	249/258 (96%)	-0.56	4 (1%) 70 73	12, 31, 52, 64	21 (8%)
All	All	1177/1190 (98%)	-0.79	5 (0%) 88 89	8, 25, 48, 65	64 (5%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	54	PRO	3.8
4	H	82	ARG	3.3
4	H	55	GLU	2.3
4	H	8	GLN	2.2
1	C	1[A]	CYS	2.1

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(Å^2)	Q<0.9
4	FME	H	1	10/11	0.97	0.05	30,34,36,40	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

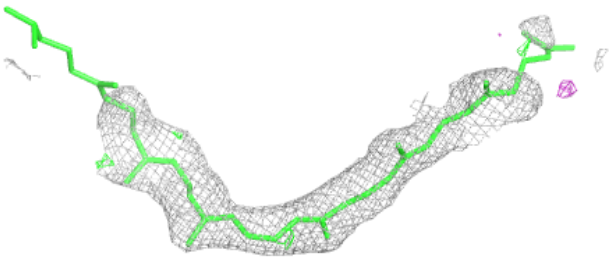
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

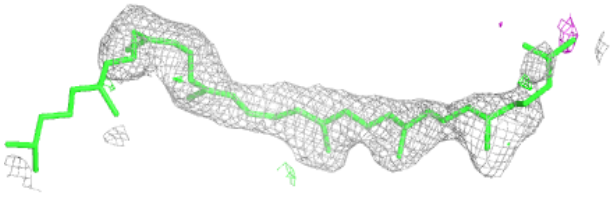
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	LDA	L	705	16/16	0.79	0.11	54,55,60,62	5
9	LDA	M	704	16/16	0.83	0.14	56,60,79,79	0
9	LDA	M	706	16/16	0.86	0.11	60,64,68,68	4
9	LDA	M	702	16/16	0.91	0.10	17,49,67,67	0
9	LDA	H	703	16/16	0.92	0.09	33,39,60,61	0
11	SO4	M	803	5/5	0.92	0.10	77,77,79,79	0
13	NS5	M	600	40/40	0.92	0.08	32,42,52,53	14
8	UQ2	L	502	23/23	0.93	0.06	21,25,38,40	0
11	SO4	H	801	5/5	0.94	0.07	61,62,64,64	0
9	LDA	M	701	16/16	0.95	0.05	26,29,31,31	0
6	BCB	M	805	66/66	0.96	0.06	11,19,48,49	0
12	MQ7	M	501	48/48	0.97	0.05	13,19,39,42	0
7	BPB	M	401	65/65	0.97	0.06	8,24,59,61	7
5	HEC	C	337	43/43	0.98	0.05	23,29,34,41	0
6	BCB	M	806	66/66	0.98	0.04	3,13,30,32	0
11	SO4	M	804	5/5	0.98	0.05	46,48,48,48	0
7	BPB	L	402	65/65	0.98	0.04	2,10,17,20	0
6	BCB	L	302	66/66	0.98	0.04	2,12,17,22	0
6	BCB	L	304	66/66	0.98	0.04	7,14,29,34	0
5	HEC	C	340	43/43	0.99	0.05	13,21,30,39	0
5	HEC	C	338	43/43	0.99	0.04	15,27,31,32	0
11	SO4	M	802	5/5	0.99	0.05	34,34,36,38	0
5	HEC	C	339	43/43	0.99	0.04	10,17,25,30	0
10	FE2	M	500	1/1	1.00	0.01	18,18,18,18	0

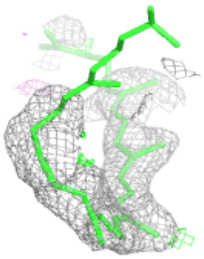
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

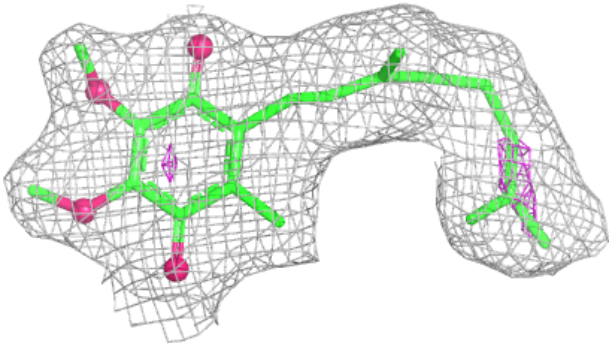


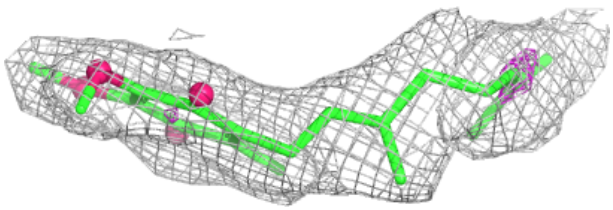


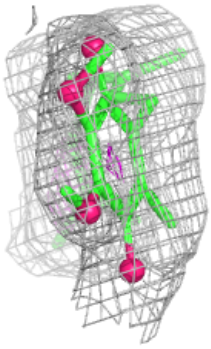


Electron density around UQ2 L 502:

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

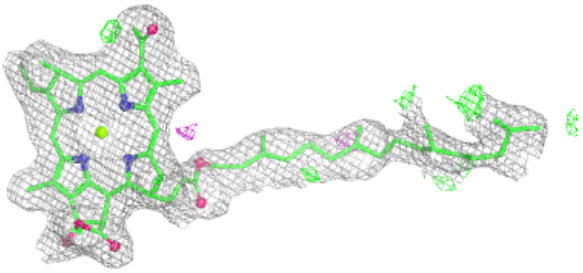


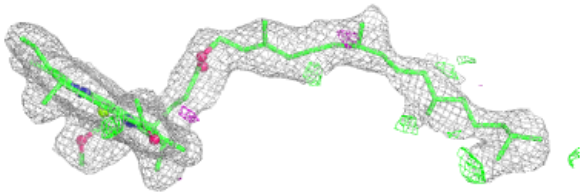


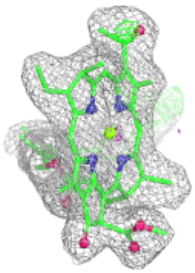


Electron density around BCB M 805:

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

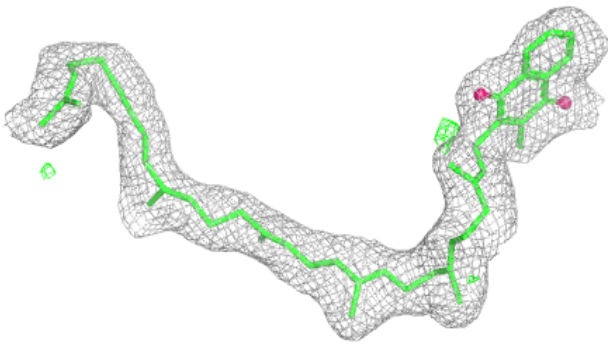


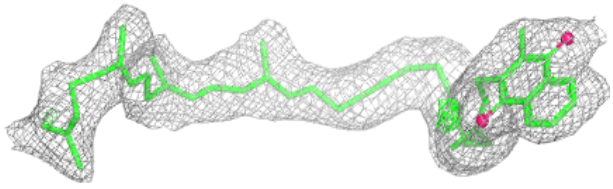


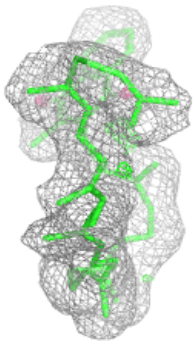


Electron density around MQ7 M 501:

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

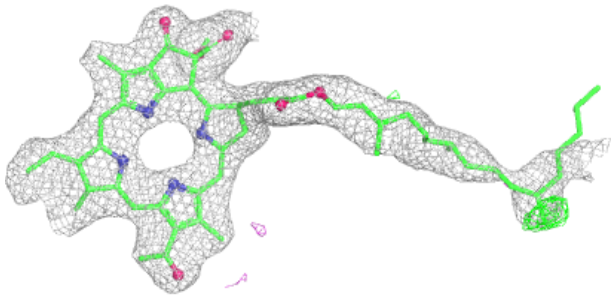


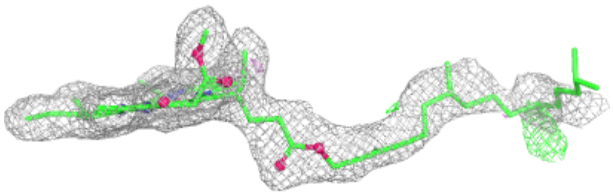




Electron density around BPB M 401:

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

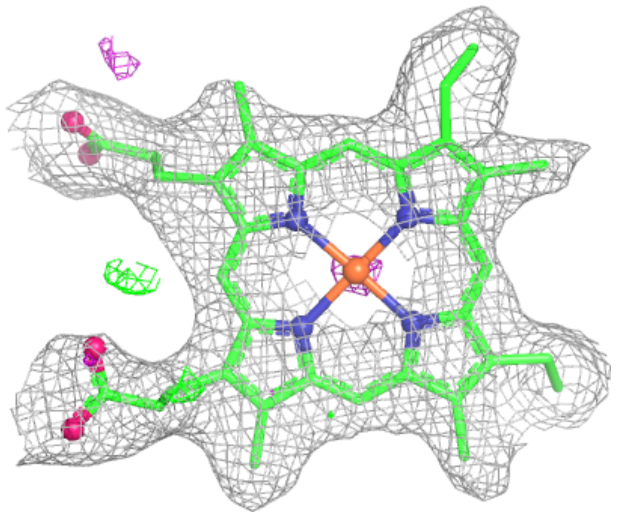


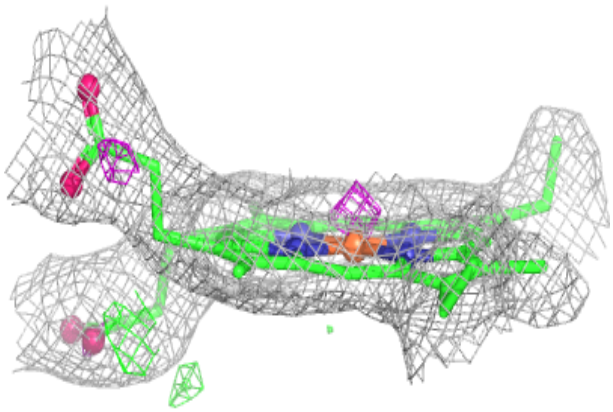


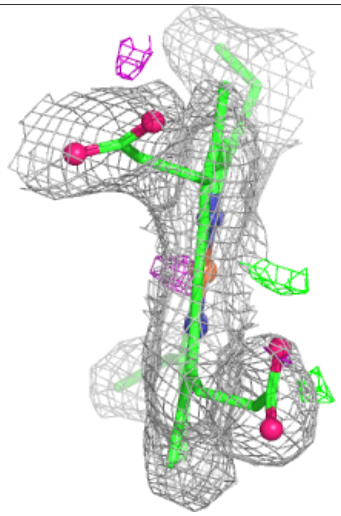


Electron density around HEC C 337:

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

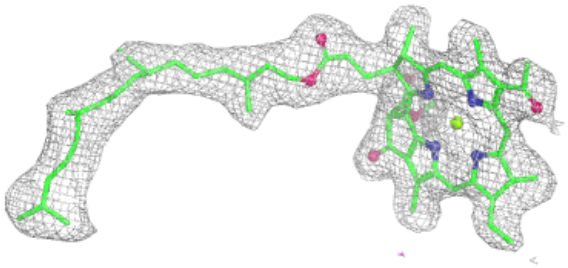


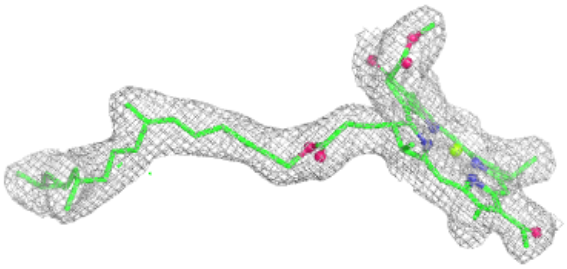


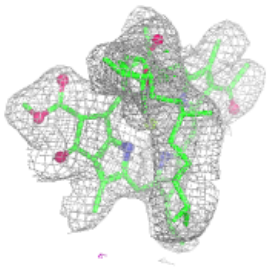


Electron density around BCB M 806:

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

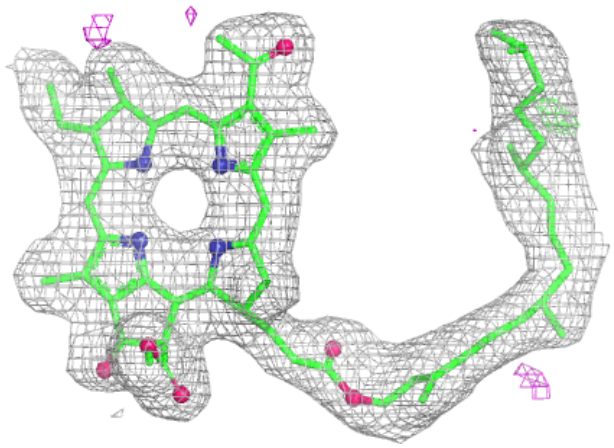


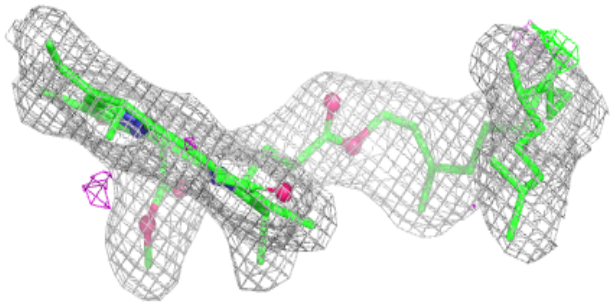


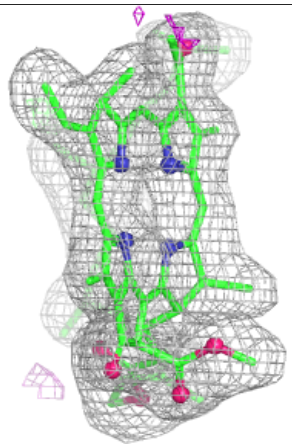


Electron density around BPB L 402:

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

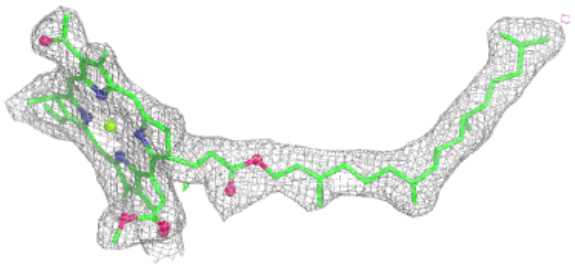


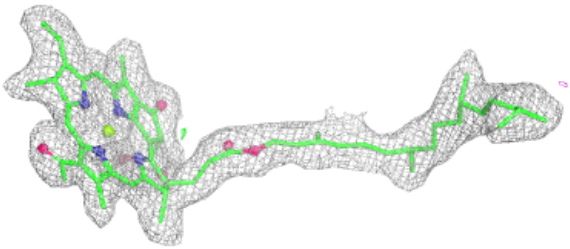


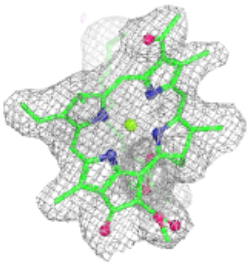


Electron density around BCB L 302:

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

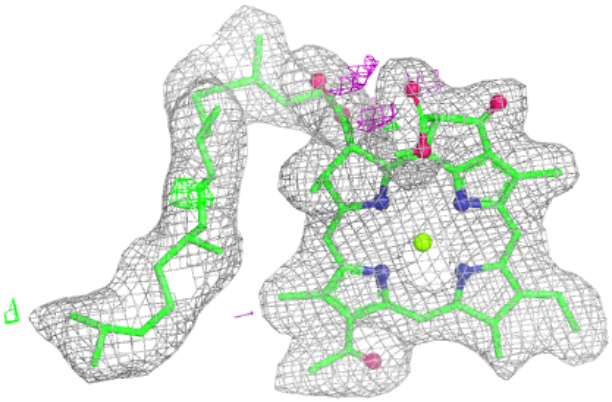


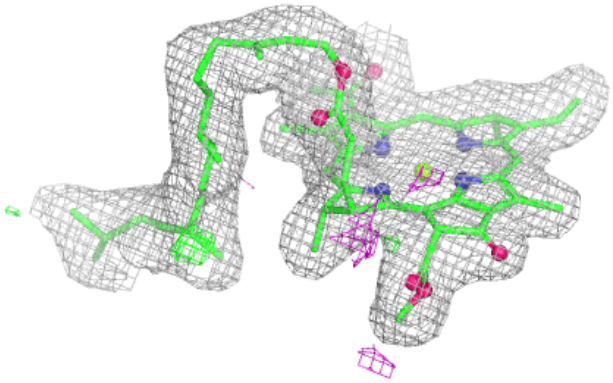


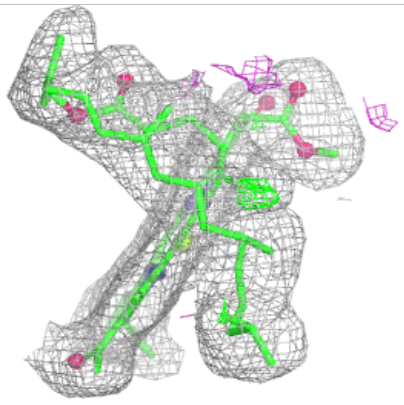


Electron density around BCB L 304:

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

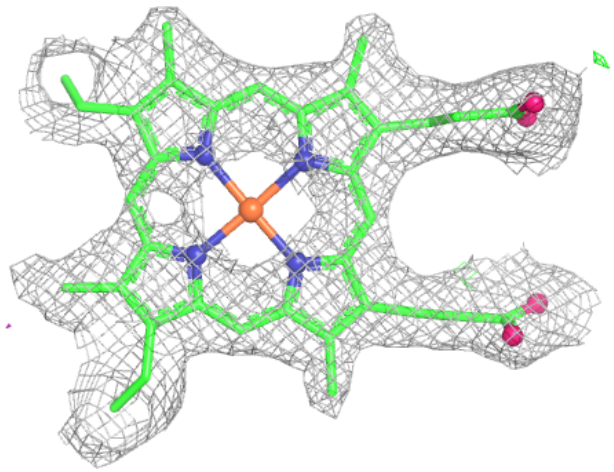


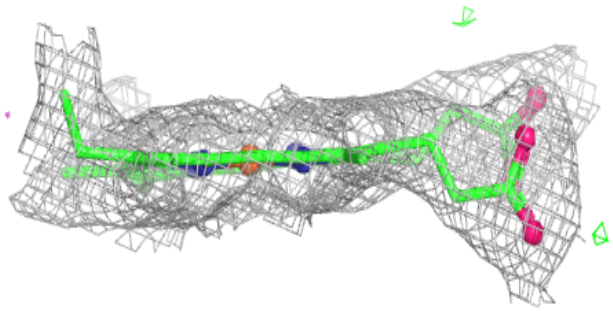


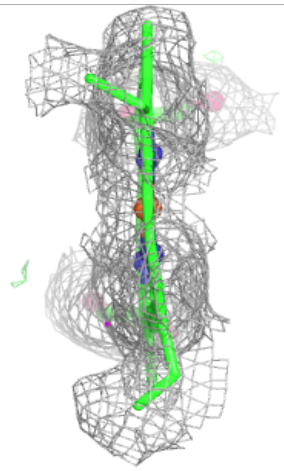


Electron density around HEC C 340:

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

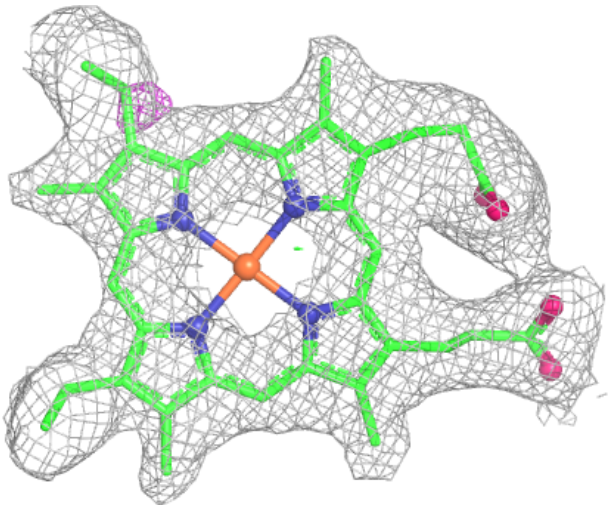


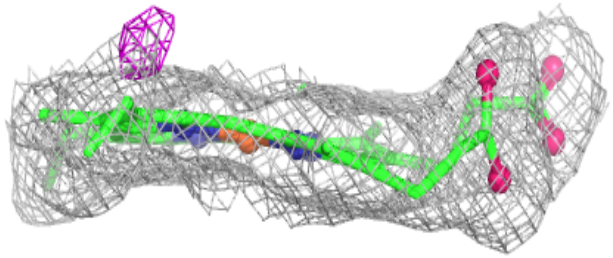


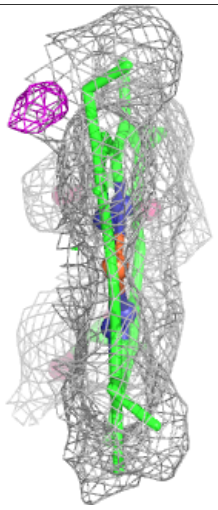


Electron density around HEC C 338:

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

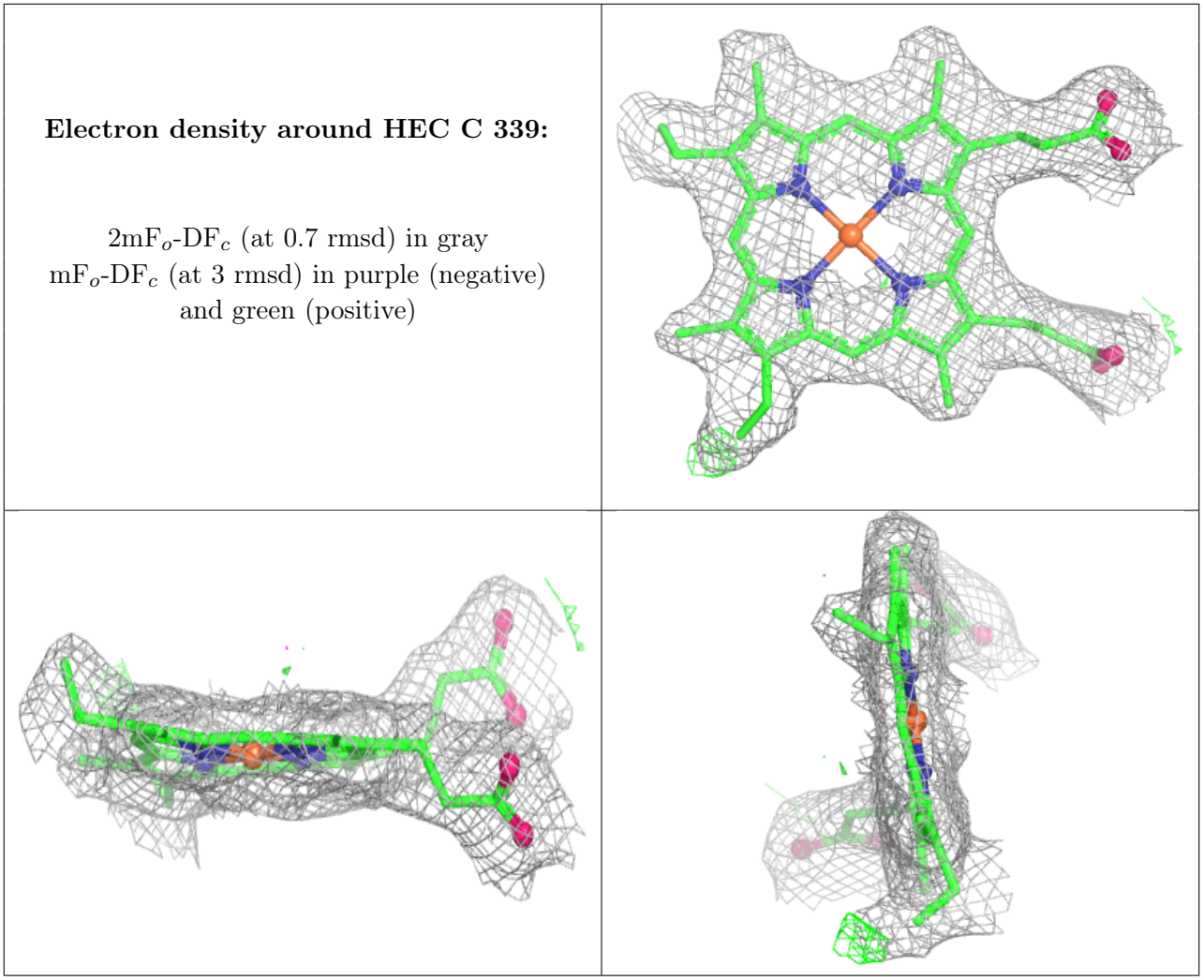






Electron density around HEC C 339:

$2mF_o$-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

There are no such residues in this entry.