Full wwPDB X-ray Structure Validation Report (i)

Aug 18, 2026 – 12:34 pm BST

PDB ID	:	5M7L / pdb_00005m7l
Title	:	Blastochloris viridis photosynthetic reaction center synchrotron structure
Authors	:	Sharma, A.S.; Johansson, L.; Dunevall, E.; Wahlgren, W.Y.; Neutze, R.; Katona, G.
Deposited on	:	2016-10-28
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

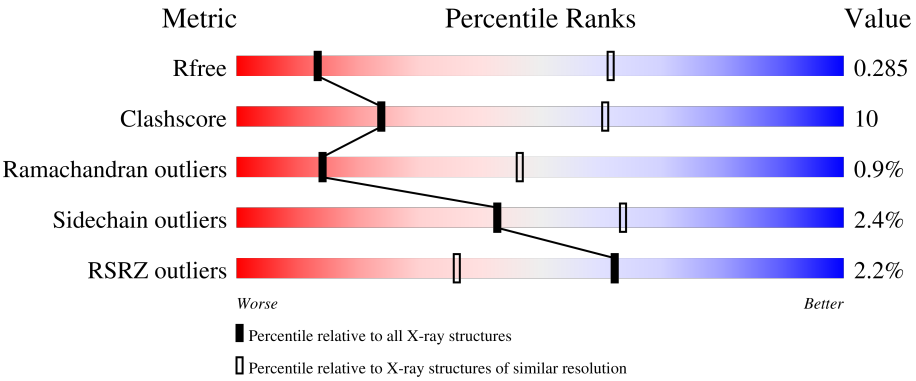
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	A	356	78% 15% · 7%
2	B	274	80% 17% ··
3	C	324	83% 17%
4	D	258	7% 65% 24% 5% 6%

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	A	401	X	-	-	-
5	HEC	A	402	X	-	-	-
5	HEC	A	403	X	-	-	-
5	HEC	A	404	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 9890 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	2	0
			2170	1458	350	355	7			

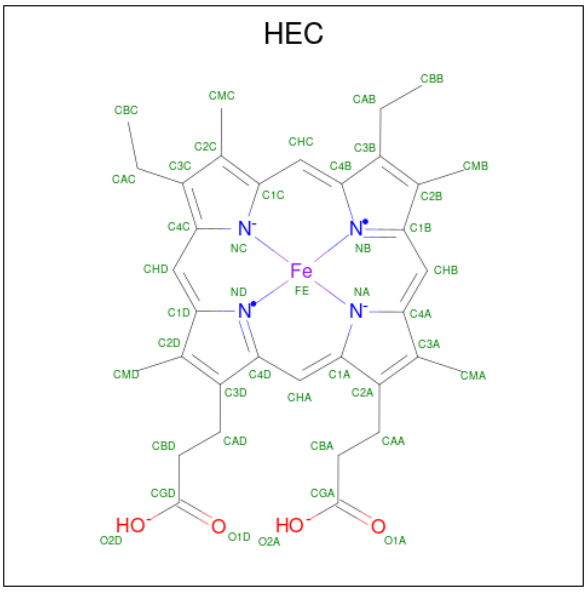
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	323	Total	C	N	O	S	0	0	0
			2546	1696	417	422	11			

- Molecule 4 is a protein called Reaction center protein H chain.

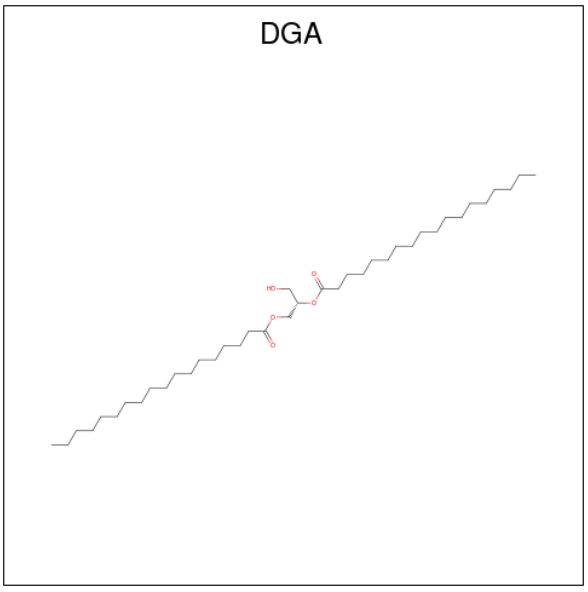
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

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



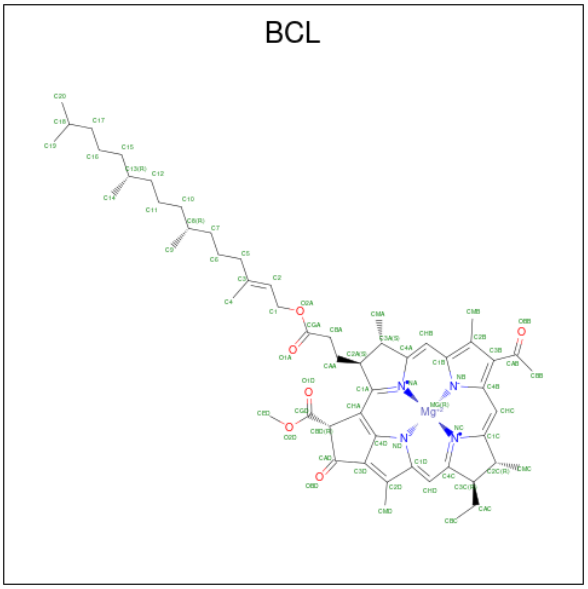
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



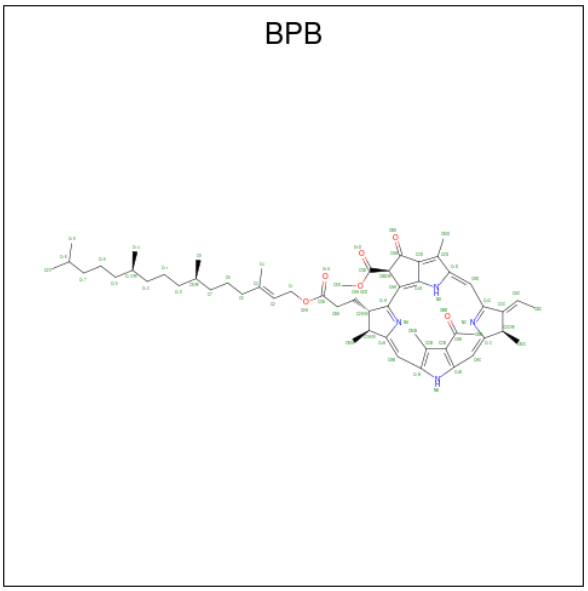
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



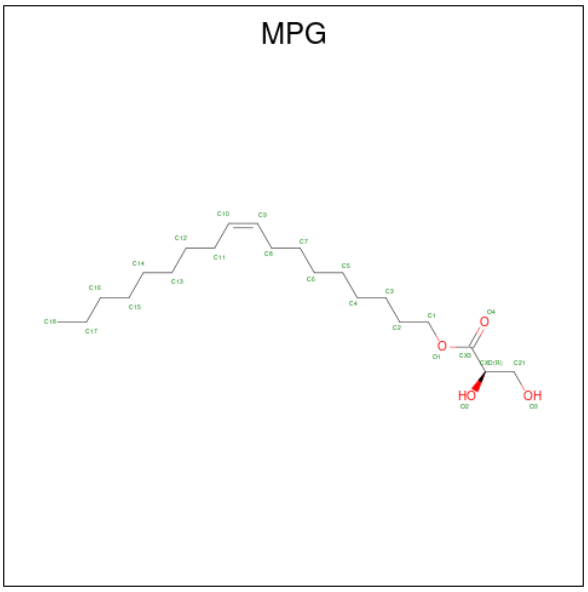
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			65	55	4	6		
8	C	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 9 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			25	21	4		

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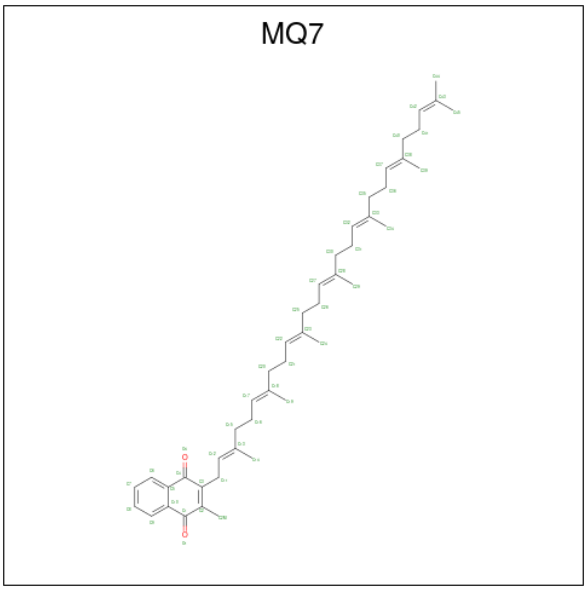
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 25 21 4	0	0
9	C	1	Total C 17 17	0	0

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

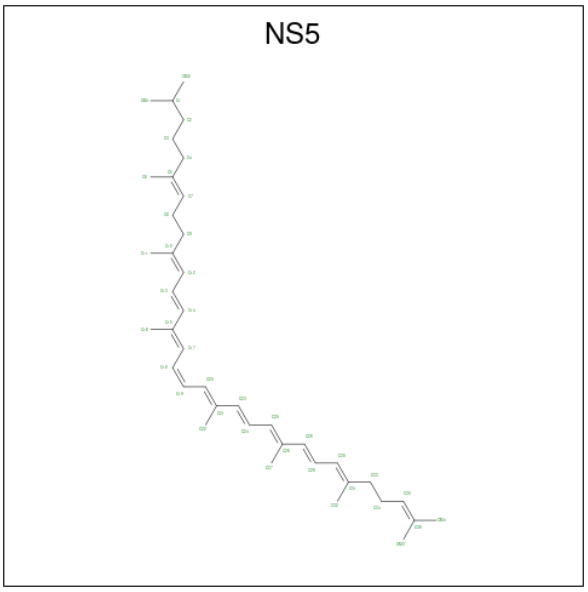
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



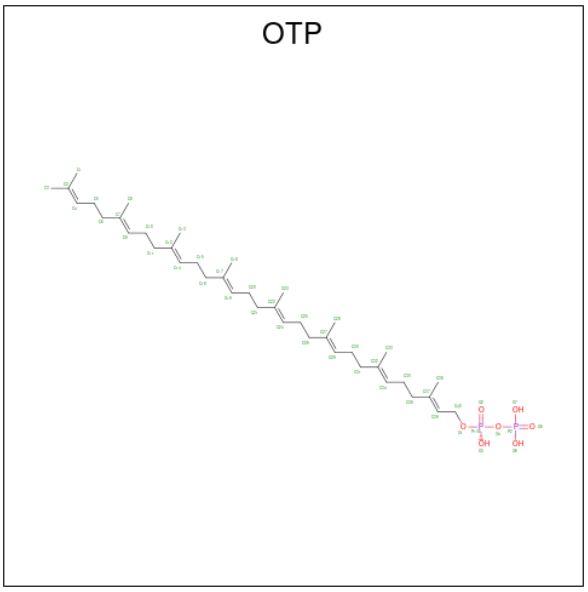
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



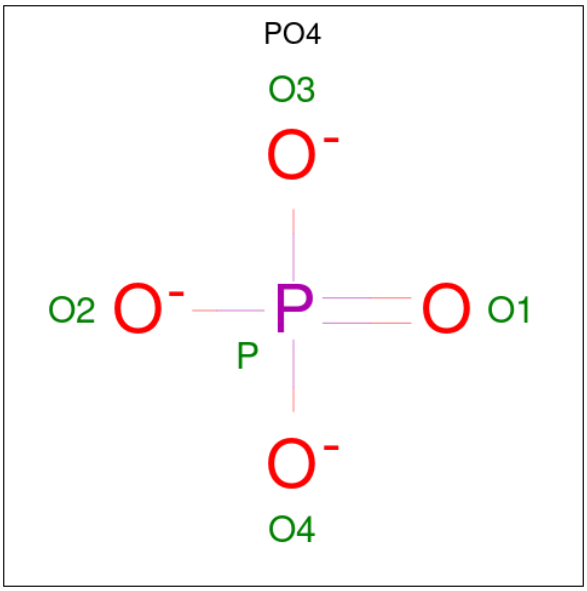
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C 40 40	0	0

- Molecule 13 is (2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLDOTRIACONTA-2,6,10,14,18,22,26,30-OCTAENYL TRIHYDROGEN DIPHOSPHATE (CCD ID: OTP) (formula: $C_{40}H_{68}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 41 40 1	0	0

- Molecule 14 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



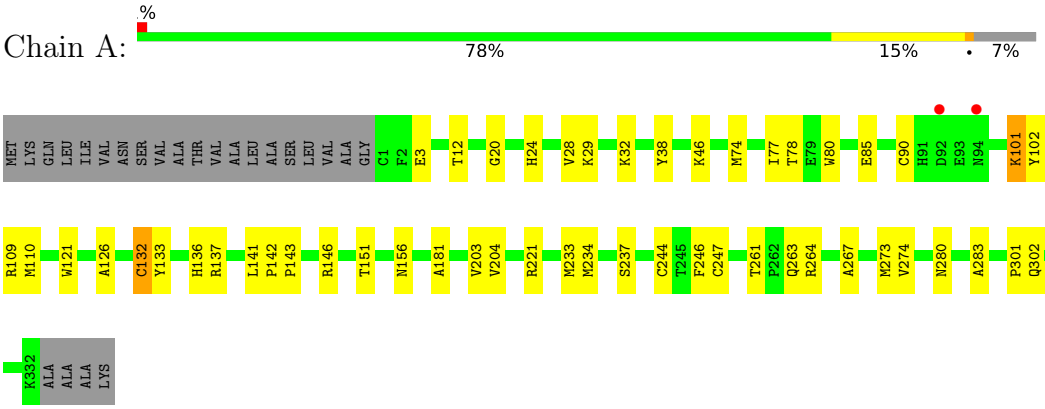
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total O P 5 4 1	0	0
14	C	1	Total O P 5 4 1	0	0

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.

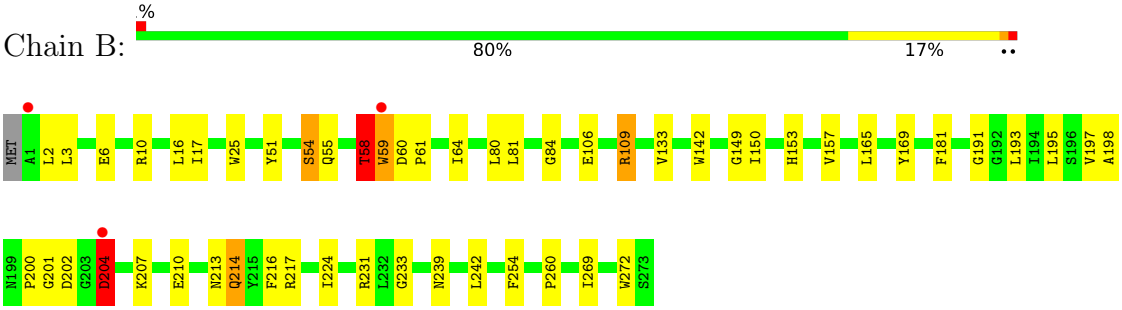
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain A:



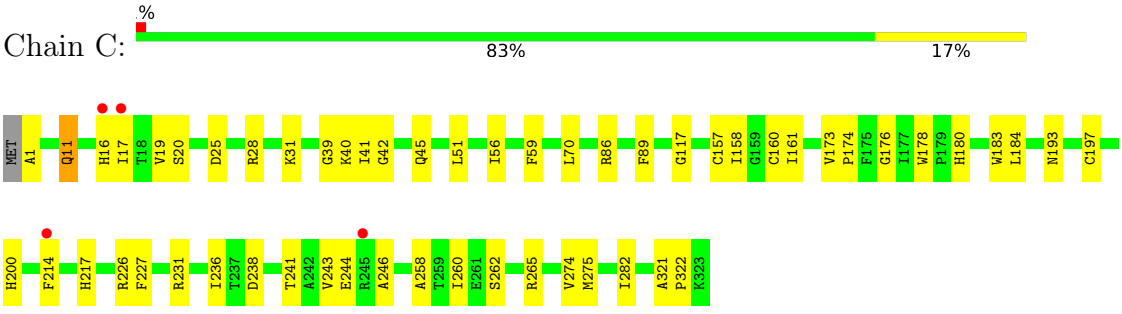
• Molecule 2: Reaction center protein L chain

Chain B:



• Molecule 3: Reaction center protein M chain

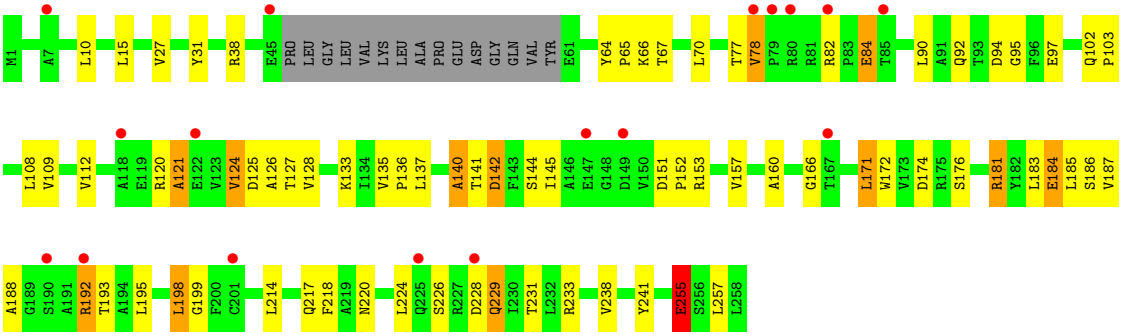
Chain C:



• Molecule 4: Reaction center protein H chain

Chain D:




M1 A7 L10 L15 V27 Y31 R38 E45 PRO LEU GLY LEU VAL LYS LEU ALA PRO GLU ASP GLY GLN VAL TYR E61 Y64 P65 K66 T67 L70 T77 V78 P79 R80 R81 R82 P83 E84 T85 L90 A91 Q92 T93 D94 G95 F96 E97 Q102 P103
L108 V109 V112 A118 E119 R120 A121 E122 V123 V124 D125 A126 T127 V128 K133 I134 V135 P136 L137 A140 T141 D142 F143 S144 I145 A146 E147 G148 D149 V150 D151 P152 R153 V157 A160 G166 T167 L171 W172 V173 D174 R175 S176 R181 Y182 L183 E184 L185 S186 V187
A188 G189 S190 A191 R192 T193 A194 L195 L198 G199 F200 C201 L214 Q217 F218 A219 N220 L224 Q225 S226 R227 D228 Q229 I230 T231 L232 R233 V238 Y241 E255 S256 L257 L258

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.60Å 82.90Å 382.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.50 – 3.60 50.50 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.50-3.60) 99.5 (50.50-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.242 , 0.280 0.247 , 0.285	Depositor DCC
R_{free} test set	1096 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	73.9	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BPB, PO4, FME, FE2, MQ7, DGA, HEC, NS5, BCL, OTP, MPG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/2665	0.83	7/3633 (0.2%)
2	B	0.37	0/2263	0.83	6/3089 (0.2%)
3	C	0.36	0/2650	0.79	2/3629 (0.1%)
4	D	0.59	0/1804	1.12	13/2485 (0.5%)
All	All	0.42	0/9382	0.88	28/12836 (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
2	B	0	1
4	D	0	6
All	All	0	7

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	82	ARG	CA-C-N	10.53	133.00	119.84
4	D	82	ARG	C-N-CA	10.53	133.00	119.84
3	C	31	LYS	CA-C-N	7.82	128.28	119.83
3	C	31	LYS	C-N-CA	7.82	128.28	119.83
4	D	78	VAL	C-N-CD	-7.68	103.70	120.60
4	D	78	VAL	CA-C-N	7.38	144.71	127.00
4	D	78	VAL	C-N-CA	7.38	144.71	127.00
2	B	204	ASP	N-CA-C	6.68	125.03	110.80
1	A	204	VAL	CA-C-N	6.64	126.62	119.78
1	A	204	VAL	C-N-CA	6.64	126.62	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	TYR	CA-C-N	-6.62	112.87	119.56
1	A	102	TYR	C-N-CA	-6.62	112.87	119.56
2	B	201	GLY	N-CA-C	6.52	118.14	111.95
4	D	84	GLU	N-CA-C	-6.08	97.84	110.80
4	D	135	VAL	CA-C-N	5.99	127.33	119.84
4	D	135	VAL	C-N-CA	5.99	127.33	119.84
2	B	58	THR	N-CA-C	5.82	123.19	110.80
2	B	202	ASP	CB-CA-C	-5.62	109.59	117.23
2	B	269	ILE	CA-C-N	5.58	126.81	119.84
2	B	269	ILE	C-N-CA	5.58	126.81	119.84
1	A	126	ALA	CB-CA-C	-5.55	110.16	116.54
4	D	220	ASN	CB-CA-C	-5.26	101.67	110.56
4	D	255	GLU	N-CA-C	5.18	121.84	110.80
4	D	70	LEU	CA-C-N	5.05	125.08	119.32
4	D	70	LEU	C-N-CA	5.05	125.08	119.32
4	D	126	ALA	N-CA-C	5.04	118.37	109.80
1	A	24	HIS	CA-C-N	5.03	126.12	119.84
1	A	24	HIS	C-N-CA	5.03	126.12	119.84

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	58	THR	Peptide
4	D	125	ASP	Peptide
4	D	140	ALA	Peptide
4	D	184	GLU	Peptide
4	D	192	ARG	Peptide
4	D	229	GLN	Peptide
4	D	255	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2576	42	0
2	B	2170	0	2100	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2546	0	2430	43	0
4	D	1771	0	1656	69	0
5	A	172	0	128	19	0
6	A	37	0	58	2	0
7	B	197	0	218	6	0
7	C	66	0	74	1	0
8	B	65	0	74	1	0
8	C	61	0	63	4	0
9	B	50	0	80	3	0
9	C	17	0	31	1	0
10	C	1	0	0	0	0
11	C	48	0	64	0	0
12	C	40	0	60	4	0
13	C	41	0	65	1	0
14	C	10	0	0	0	0
All	All	9890	0	9677	197	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 10.

All (197) 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:D:187:VAL:HB	4:D:192:ARG:HD3	1.49	0.93
4:D:184:GLU:HG2	4:D:195:LEU:HA	1.57	0.86
4:D:187:VAL:HG12	4:D:192:ARG:HB2	1.56	0.85
2:B:214:GLN:NE2	3:C:19:VAL:O	2.15	0.79
4:D:192:ARG:CG	4:D:193:THR:HA	2.12	0.79
1:A:28:VAL:HG12	1:A:32:LYS:HE3	1.68	0.76
4:D:185:LEU:HD11	4:D:192:ARG:NH2	2.03	0.74
3:C:16:HIS:H	3:C:16:HIS:CD2	2.04	0.74
3:C:11:GLN:HE21	3:C:39:GLY:HA3	1.53	0.73
2:B:214:GLN:HG3	3:C:19:VAL:HB	1.70	0.73
4:D:192:ARG:HG2	4:D:193:THR:HA	1.72	0.71
4:D:187:VAL:HB	4:D:192:ARG:HH11	1.55	0.71
4:D:217:GLN:O	4:D:241:TYR:OH	2.06	0.69
3:C:262:SER:HA	3:C:265:ARG:HG3	1.72	0.69
7:B:301:BCL:H3C	3:C:184:LEU:HD21	1.73	0.68
4:D:184:GLU:CG	4:D:195:LEU:HA	2.24	0.68
4:D:136:PRO:HG3	4:D:172:TRP:CE2	2.28	0.67
4:D:226:SER:HB2	4:D:229:GLN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:CYS:C	1:A:101:LYS:HE3	2.20	0.67
3:C:11:GLN:NE2	3:C:39:GLY:HA3	2.10	0.66
4:D:187:VAL:CB	4:D:192:ARG:HD3	2.23	0.66
4:D:192:ARG:HG3	4:D:193:THR:HA	1.75	0.66
4:D:174:ASP:OD2	4:D:181:ARG:NH2	2.29	0.65
3:C:157:CYS:HA	3:C:161:ILE:HB	1.80	0.63
2:B:6:GLU:OE2	2:B:10:ARG:NH1	2.32	0.62
4:D:192:ARG:NH1	4:D:218:PHE:HB3	2.15	0.62
3:C:238:ASP:N	3:C:238:ASP:OD1	2.32	0.62
1:A:181:ALA:HB3	1:A:234:MET:HE3	1.82	0.62
2:B:80:LEU:HA	2:B:84:GLY:HA3	1.80	0.62
4:D:166:GLY:HA3	4:D:186:SER:O	1.99	0.62
7:B:303:BCL:H142	7:B:303:BCL:HMA1	1.82	0.62
2:B:239:ASN:HA	2:B:242:LEU:HB2	1.81	0.61
2:B:55:GLN:HE22	2:B:81:LEU:HB3	1.65	0.61
4:D:187:VAL:HB	4:D:192:ARG:CD	2.27	0.61
4:D:183:LEU:O	4:D:184:GLU:HG3	2.01	0.61
4:D:136:PRO:HG3	4:D:172:TRP:CZ2	2.36	0.60
3:C:243:VAL:HG11	3:C:260:ILE:HB	1.83	0.60
1:A:29:LYS:HA	1:A:32:LYS:HD2	1.83	0.60
3:C:265:ARG:NH1	4:D:31:TYR:OH	2.33	0.60
3:C:241:THR:HA	3:C:244:GLU:HG3	1.84	0.59
3:C:226:ARG:NH1	4:D:199:GLY:O	2.35	0.59
4:D:192:ARG:HH22	4:D:218:PHE:HD1	1.50	0.58
4:D:226:SER:CB	4:D:229:GLN:HB2	2.34	0.58
4:D:133:LYS:HE3	4:D:176:SER:HB2	1.86	0.58
2:B:10:ARG:HH21	2:B:25:TRP:CG	2.22	0.58
2:B:213:ASN:O	2:B:217:ARG:HG2	2.04	0.58
4:D:120:ARG:HD2	4:D:121:ALA:H	1.68	0.57
4:D:124:VAL:HA	4:D:231:THR:HA	1.85	0.57
4:D:137:LEU:HA	4:D:140:ALA:HB3	1.87	0.56
7:B:301:BCL:H193	9:C:407:MPG:H112	1.86	0.56
2:B:55:GLN:HE22	2:B:81:LEU:HD13	1.70	0.56
1:A:233:MET:HB3	5:A:403:HEC:C3B	2.35	0.56
4:D:94:ASP:OD1	4:D:95:GLY:N	2.37	0.56
1:A:274:VAL:HG21	5:A:404:HEC:HAB	1.88	0.55
4:D:66:LYS:HG2	4:D:67:THR:N	2.20	0.55
1:A:80:TRP:HE3	1:A:132:CYS:HG	1.54	0.55
1:A:136:HIS:NE2	5:A:402:HEC:NB	2.55	0.55
4:D:10:LEU:HD21	4:D:15:LEU:HD21	1.88	0.55
2:B:197:VAL:HG13	2:B:207:LYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LEU:HD13	2:B:106:GLU:HG2	1.90	0.54
4:D:152:PRO:HG2	4:D:171:LEU:HD23	1.88	0.54
3:C:117:GLY:HA3	12:C:405:NS5:H92	1.90	0.54
2:B:2:LEU:HG	2:B:10:ARG:NH1	2.23	0.54
4:D:92:GLN:N	4:D:92:GLN:OE1	2.40	0.54
2:B:61:PRO:HA	2:B:64:ILE:HD12	1.90	0.53
1:A:132:CYS:HA	5:A:402:HEC:HHC	1.91	0.53
2:B:224:ILE:HG22	9:B:306:MPG:H212	1.90	0.53
3:C:176:GLY:O	3:C:180:HIS:ND1	2.42	0.53
2:B:193:LEU:HD22	2:B:216:PHE:HE2	1.74	0.53
2:B:272:TRP:HB3	3:C:86:ARG:HD2	1.90	0.53
2:B:55:GLN:OE1	2:B:81:LEU:HD22	2.10	0.52
4:D:108:LEU:HB3	4:D:241:TYR:CE1	2.44	0.52
4:D:160:ALA:HB3	4:D:214:LEU:HD23	1.90	0.52
4:D:90:LEU:HD11	4:D:112:VAL:HB	1.91	0.52
2:B:200:PRO:HG2	2:B:204:ASP:OD1	2.10	0.52
5:A:404:HEC:HHA	5:A:404:HEC:HBD1	1.91	0.52
2:B:2:LEU:HG	2:B:10:ARG:HH11	1.74	0.51
3:C:258:ALA:HB1	3:C:262:SER:OG	2.09	0.51
3:C:160:CYS:HB3	12:C:405:NS5:H82	1.92	0.51
1:A:143:PRO:O	1:A:156:ASN:ND2	2.43	0.51
1:A:301:PRO:HG2	5:A:402:HEC:HBD1	1.91	0.51
3:C:20:SER:OG	3:C:25:ASP:OD2	2.28	0.51
4:D:185:LEU:HD11	4:D:192:ARG:CZ	2.40	0.51
1:A:267:ALA:CB	5:A:403:HEC:HAC	2.41	0.51
2:B:214:GLN:CG	3:C:19:VAL:HB	2.38	0.51
4:D:151:ASP:CG	4:D:153:ARG:HH11	2.19	0.51
4:D:102:GLN:HG3	4:D:103:PRO:HD2	1.93	0.51
4:D:185:LEU:HD12	4:D:185:LEU:C	2.36	0.51
2:B:3:LEU:HB2	2:B:6:GLU:HB2	1.94	0.50
2:B:198:ALA:C	2:B:200:PRO:HD3	2.37	0.50
2:B:210:GLU:OE2	4:D:128:VAL:N	2.45	0.50
3:C:70:LEU:HD21	12:C:405:NS5:H29	1.93	0.50
1:A:247:CYS:HA	1:A:261:THR:OG1	2.12	0.50
7:B:303:BCL:HMD2	7:C:401:BCL:HBB3	1.93	0.50
3:C:39:GLY:HA2	3:C:42:GLY:O	2.12	0.50
2:B:149:GLY:O	2:B:153:HIS:ND1	2.45	0.49
2:B:133:VAL:HA	2:B:142:TRP:HZ3	1.77	0.49
4:D:38:ARG:O	4:D:78:VAL:HG23	2.12	0.49
2:B:233:GLY:HA3	3:C:214:PHE:CE2	2.48	0.49
1:A:247:CYS:HB3	1:A:264:ARG:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ILE:O	7:B:303:BCL:HED1	2.13	0.48
3:C:197:CYS:O	3:C:200:HIS:HB3	2.13	0.48
8:C:402:BPB:HHC	8:C:402:BPB:HBBB	1.95	0.48
4:D:157:VAL:HG21	4:D:185:LEU:HD22	1.94	0.48
4:D:255:GLU:N	4:D:255:GLU:OE1	2.47	0.48
3:C:59:PHE:CD1	8:C:402:BPB:H4	2.49	0.48
3:C:243:VAL:HA	3:C:246:ALA:HB3	1.94	0.48
8:B:304:BPB:HHC	8:B:304:BPB:HBBB	1.95	0.48
9:B:305:MPG:H21C	3:C:1:ALA:HA	1.94	0.48
4:D:187:VAL:H	4:D:192:ARG:HB3	1.79	0.48
1:A:77:ILE:HG22	5:A:401:HEC:HMC2	1.96	0.47
1:A:305:CYS:HA	5:A:404:HEC:HHC	1.96	0.47
2:B:58:THR:O	2:B:59:TRP:HD1	1.97	0.47
3:C:1:ALA:C	3:C:226:ARG:HH22	2.22	0.47
4:D:192:ARG:NH2	4:D:218:PHE:HD1	2.11	0.47
1:A:3:GLU:O	2:B:254:PHE:HA	2.14	0.47
6:A:405:DGA:HA22	6:A:405:DGA:HG11	1.72	0.47
2:B:210:GLU:O	2:B:214:GLN:HB2	2.15	0.47
3:C:227:PHE:HB3	3:C:241:THR:HG23	1.96	0.47
4:D:136:PRO:HA	4:D:172:TRP:CD1	2.49	0.47
1:A:203:VAL:HG12	1:A:221:ARG:NH2	2.30	0.47
2:B:51:TYR:O	2:B:54:SER:HB3	2.15	0.47
1:A:121:TRP:CG	1:A:273:MET:HG3	2.50	0.46
2:B:60:ASP:OD1	2:B:61:PRO:HD2	2.16	0.46
3:C:231:ARG:HH22	4:D:133:LYS:HD3	1.80	0.46
4:D:187:VAL:HG22	4:D:188:ALA:O	2.16	0.46
1:A:80:TRP:CD1	1:A:133:TYR:HB2	2.51	0.46
3:C:158:ILE:HD12	3:C:173:VAL:HG21	1.98	0.46
4:D:187:VAL:N	4:D:192:ARG:HD3	2.30	0.46
3:C:11:GLN:NE2	3:C:39:GLY:CA	2.77	0.45
2:B:181:PHE:HB3	8:C:402:BPB:HBBA	1.97	0.45
2:B:191:GLY:O	2:B:195:LEU:HG	2.16	0.45
9:B:305:MPG:HX32	9:B:305:MPG:H42C	1.54	0.45
12:C:405:NS5:H18	12:C:405:NS5:H161	1.73	0.45
4:D:171:LEU:HD12	4:D:171:LEU:O	2.15	0.45
1:A:74:MET:HB3	5:A:401:HEC:C3B	2.47	0.45
2:B:217:ARG:HH22	3:C:45:GLN:HE21	1.64	0.45
4:D:183:LEU:H	4:D:198:LEU:HD13	1.82	0.45
1:A:38:TYR:HE2	1:A:321:ARG:HG2	1.82	0.45
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.68	0.45
2:B:58:THR:O	2:B:59:TRP:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:PHE:HE1	3:C:217:HIS:HD2	1.65	0.45
1:A:146:ARG:NH2	1:A:151:THR:H	2.14	0.45
4:D:64:TYR:HD1	4:D:65:PRO:O	1.99	0.45
4:D:66:LYS:H	4:D:78:VAL:HG12	1.82	0.45
1:A:109:ARG:NH2	1:A:280:ASN:O	2.47	0.45
3:C:11:GLN:NE2	3:C:39:GLY:C	2.75	0.45
1:A:305:CYS:SG	5:A:404:HEC:CAB	3.06	0.44
4:D:108:LEU:HB3	4:D:241:TYR:HE1	1.82	0.44
1:A:110:MET:HG3	5:A:402:HEC:NA	2.33	0.44
1:A:133:TYR:CE2	1:A:137:ARG:HD3	2.53	0.44
1:A:12:THR:HG23	1:A:20:GLY:HA2	1.98	0.44
1:A:110:MET:HB3	5:A:402:HEC:C3B	2.47	0.43
1:A:132:CYS:SG	5:A:402:HEC:CAB	3.07	0.43
1:A:283:ALA:HB2	1:A:302:GLN:OE1	2.19	0.43
4:D:187:VAL:H	4:D:192:ARG:CB	2.31	0.43
7:B:302:BCL:H61	7:B:302:BCL:H41	1.82	0.43
1:A:305:CYS:SG	5:A:404:HEC:HBB3	2.58	0.43
4:D:27:VAL:O	4:D:31:TYR:HB3	2.19	0.43
1:A:273:MET:HE2	1:A:273:MET:HB3	1.93	0.43
2:B:55:GLN:NE2	2:B:81:LEU:HB3	2.30	0.43
3:C:89:PHE:HB3	3:C:178:TRP:CD1	2.53	0.43
4:D:142:ASP:OD1	4:D:142:ASP:N	2.50	0.43
1:A:244:CYS:SG	5:A:403:HEC:CAB	3.06	0.43
1:A:246:PHE:CZ	1:A:263:GLN:HG2	2.54	0.43
3:C:274:VAL:HG12	3:C:275:MET:HE2	2.01	0.43
4:D:66:LYS:H	4:D:78:VAL:CG1	2.31	0.43
2:B:109:ARG:HH21	4:D:257:LEU:HD11	1.84	0.42
4:D:127:THR:HG22	4:D:128:VAL:N	2.34	0.42
2:B:10:ARG:HH21	2:B:25:TRP:CB	2.32	0.42
4:D:195:LEU:CB	4:D:238:VAL:HG11	2.49	0.42
1:A:90:CYS:SG	1:A:103:PRO:HB2	2.59	0.42
1:A:101:LYS:HB2	1:A:103:PRO:HD2	2.02	0.42
2:B:153:HIS:O	2:B:157:VAL:HG23	2.19	0.42
4:D:198:LEU:HD12	4:D:198:LEU:HA	1.52	0.42
1:A:141:LEU:HD12	1:A:142:PRO:HD2	2.02	0.42
2:B:181:PHE:CD2	8:C:402:BPB:HBB	2.55	0.42
2:B:214:GLN:HE22	3:C:28:ARG:NH2	2.17	0.42
3:C:173:VAL:HA	3:C:174:PRO:HD3	1.86	0.42
4:D:185:LEU:O	4:D:193:THR:OG1	2.32	0.42
1:A:237:SER:HG	5:A:403:HEC:HAB	1.85	0.41
4:D:67:THR:HG23	4:D:77:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:405:DGA:HA31	6:A:405:DGA:HB31	2.02	0.41
3:C:173:VAL:HG22	3:C:183:TRP:CE2	2.55	0.41
4:D:120:ARG:N	4:D:233:ARG:HE	2.17	0.41
4:D:224:LEU:HD12	4:D:224:LEU:HA	1.92	0.41
2:B:169:TYR:CD1	2:B:260:PRO:HG3	2.55	0.41
1:A:107:ALA:CB	5:A:401:HEC:HAC	2.51	0.41
13:C:406:OTP:H51	13:C:406:OTP:H81	1.76	0.41
4:D:120:ARG:HD2	4:D:121:ALA:N	2.35	0.41
2:B:60:ASP:HA	2:B:61:PRO:HD2	1.84	0.41
3:C:282:ILE:HD13	3:C:282:ILE:HA	1.92	0.41
4:D:172:TRP:CZ2	4:D:184:GLU:OE1	2.74	0.41
3:C:321:ALA:HA	3:C:322:PRO:HD3	1.91	0.40
1:A:78:THR:OG1	5:A:401:HEC:HAB	2.21	0.40
4:D:144:SER:OG	4:D:145:ILE:N	2.53	0.40
3:C:236:ILE:HG12	3:C:260:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	330/356 (93%)	313 (95%)	17 (5%)	0	100 100
2	B	273/274 (100%)	257 (94%)	12 (4%)	4 (2%)	8 37
3	C	321/324 (99%)	301 (94%)	18 (6%)	2 (1%)	21 54
4	D	239/258 (93%)	213 (89%)	22 (9%)	4 (2%)	7 35
All	All	1163/1212 (96%)	1084 (93%)	69 (6%)	10 (1%)	14 46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	TRP
2	B	204	ASP
4	D	97	GLU
4	D	141	THR
4	D	84	GLU
4	D	121	ALA
2	B	58	THR
2	B	165	LEU
3	C	193	ASN
3	C	51	LEU

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	A	280/297 (94%)	276 (99%)	4 (1%)	59	71
2	B	218/219 (100%)	213 (98%)	5 (2%)	44	64
3	C	247/250 (99%)	242 (98%)	5 (2%)	48	66
4	D	167/212 (79%)	159 (95%)	8 (5%)	23	50
All	All	912/978 (93%)	890 (98%)	22 (2%)	43	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	85	GLU
1	A	101	LYS
1	A	132	CYS
2	B	17	ILE
2	B	54	SER
2	B	109	ARG
2	B	214	GLN
2	B	231	ARG
3	C	11	GLN
3	C	17	ILE
3	C	40	LYS

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Mol	Chain	Res	Type
3	C	41	ILE
3	C	56	ILE
4	D	109	VAL
4	D	124	VAL
4	D	142	ASP
4	D	171	LEU
4	D	181	ARG
4	D	198	LEU
4	D	228	ASP
4	D	255	GLU

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

Mol	Chain	Res	Type
1	A	24	HIS
1	A	156	ASN
1	A	162	HIS
2	B	166	ASN
3	C	11	GLN
3	C	16	HIS
3	C	45	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	D	1	4	8,9,10	0.91	0	7,9,11	0.97	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
4	FME	D	1	4	-	3/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	FME	N-CA-CB-CG
4	D	1	FME	C-CA-CB-CG
4	D	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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	MPG	C	407	-	16,16,24	0.79	0	15,15,25	0.75	0
7	BCL	B	303	2	69,74,74	1.14	5 (7%)	83,115,115	1.49	11 (13%)
7	BCL	B	302	2	69,74,74	1.18	6 (8%)	83,115,115	1.46	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	MQ7	C	404	-	49,49,49	1.82	10 (20%)	60,63,63	1.64	15 (25%)
7	BCL	C	401	-	69,74,74	1.20	5 (7%)	83,115,115	1.61	14 (16%)
12	NS5	C	405	-	39,39,39	2.32	17 (43%)	44,46,46	2.02	12 (27%)
14	PO4	C	408	-	4,4,4	0.87	0	6,6,6	0.44	0
5	HEC	A	403	1	50,50,50	2.04	7 (14%)	68,82,82	1.61	9 (13%)
5	HEC	A	402	1	50,50,50	2.03	7 (14%)	68,82,82	1.68	10 (14%)
6	DGA	A	405	-	36,36,43	1.24	3 (8%)	38,38,45	3.10	6 (15%)
9	MPG	B	306	-	24,24,24	1.27	1 (4%)	24,25,25	1.28	2 (8%)
8	BPB	C	402	-	53,66,70	1.24	7 (13%)	51,96,101	2.22	11 (21%)
14	PO4	C	409	-	4,4,4	0.91	0	6,6,6	0.42	0
9	MPG	B	305	-	24,24,24	1.25	1 (4%)	24,25,25	1.53	3 (12%)
5	HEC	A	401	1	50,50,50	2.04	6 (12%)	68,82,82	1.64	9 (13%)
13	OTP	C	406	-	40,40,48	0.74	0	47,47,61	1.80	14 (29%)
8	BPB	B	304	-	57,70,70	1.11	6 (10%)	56,101,101	2.04	9 (16%)
7	BCL	B	301	3	68,73,74	1.20	6 (8%)	81,113,115	1.42	8 (9%)
5	HEC	A	404	1	50,50,50	2.07	9 (18%)	68,82,82	1.65	12 (17%)

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	A	401	1	1/1/3/7	8/14/54/54	-
13	OTP	C	406	-	-	13/45/45/55	-
9	MPG	C	407	-	-	8/14/14/25	-
7	BCL	C	401	-	-	5/41/137/137	-
7	BCL	B	303	2	-	6/41/137/137	-
12	NS5	C	405	-	-	16/43/43/43	-
5	HEC	A	403	1	1/1/3/7	4/14/54/54	-
5	HEC	A	402	1	1/1/3/7	9/14/54/54	-
6	DGA	A	405	-	-	14/37/37/45	-
7	BCL	B	302	2	-	5/41/137/137	-
8	BPB	B	304	-	-	3/37/105/105	0/5/6/6
7	BCL	B	301	3	-	9/40/136/137	-
8	BPB	C	402	-	-	8/33/101/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MPG	B	306	-	-	12/25/25/25	-
5	HEC	A	404	1	1/1/3/7	6/14/54/54	-
11	MQ7	C	404	-	-	3/41/61/61	0/2/2/2
9	MPG	B	305	-	-	16/25/25/25	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	HEC	C3D-C2D	8.07	1.53	1.36
5	A	403	HEC	C3D-C2D	7.97	1.53	1.36
5	A	401	HEC	C3D-C2D	7.94	1.53	1.36
5	A	402	HEC	C3D-C2D	7.91	1.53	1.36
11	C	404	MQ7	C3-C2	7.18	1.48	1.35
5	A	401	HEC	FE-ND	5.84	2.13	1.94
5	A	403	HEC	FE-ND	5.58	2.12	1.94
5	A	402	HEC	FE-ND	5.32	2.11	1.94
5	A	404	HEC	FE-NB	5.30	2.11	1.94
5	A	404	HEC	FE-ND	5.05	2.10	1.94
12	C	405	NS5	C30-C31	5.03	1.39	1.34
7	B	301	BCL	MG-NA	4.96	2.18	2.06
9	B	305	MPG	O1-CX3	4.89	1.43	1.33
5	A	401	HEC	FE-NC	4.87	2.11	1.95
9	B	306	MPG	O1-CX3	4.82	1.43	1.33
7	C	401	BCL	MG-NA	4.79	2.17	2.06
5	A	402	HEC	FE-NB	4.70	2.09	1.94
7	B	302	BCL	MG-NA	4.69	2.17	2.06
7	B	303	BCL	MG-NA	4.60	2.17	2.06
5	A	403	HEC	FE-NB	4.48	2.08	1.94
5	A	403	HEC	FE-NC	4.32	2.09	1.95
5	A	404	HEC	FE-NC	4.23	2.09	1.95
12	C	405	NS5	C14-C15	4.21	1.55	1.45
11	C	404	MQ7	C5-C4	4.18	1.56	1.48
11	C	404	MQ7	C10-C1	3.94	1.55	1.48
5	A	401	HEC	CBC-CAC	-3.90	1.34	1.51
5	A	403	HEC	CBC-CAC	-3.89	1.34	1.51
5	A	402	HEC	CBB-CAB	-3.88	1.34	1.51
5	A	401	HEC	CBB-CAB	-3.86	1.34	1.51
5	A	404	HEC	CBC-CAC	-3.85	1.34	1.51
5	A	402	HEC	CBC-CAC	-3.83	1.34	1.51
12	C	405	NS5	C19-C20	3.81	1.55	1.43
5	A	403	HEC	CBB-CAB	-3.80	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	FE-NC	3.75	2.07	1.95
6	A	405	DGA	OG1-CA1	3.72	1.44	1.33
5	A	401	HEC	FE-NB	3.59	2.06	1.94
5	A	404	HEC	CBB-CAB	-3.57	1.35	1.51
8	C	402	BPB	CBD-CGD	-3.55	1.47	1.52
6	A	405	DGA	OG2-CB1	3.54	1.44	1.34
7	C	401	BCL	C3B-C4B	3.54	1.47	1.41
6	A	405	DGA	CG1-CG2	3.50	1.58	1.50
12	C	405	NS5	C23-C21	3.45	1.53	1.45
7	B	302	BCL	MG-NC	3.42	2.14	2.06
8	B	304	BPB	CBD-CGD	-3.41	1.47	1.52
7	B	303	BCL	MG-NC	3.40	2.14	2.06
7	B	301	BCL	MG-NC	3.39	2.14	2.06
12	C	405	NS5	C12-C10	3.38	1.37	1.34
8	C	402	BPB	CAC-C3C	3.37	1.41	1.33
12	C	405	NS5	C18-C17	3.36	1.53	1.43
12	C	405	NS5	C28-C26	3.34	1.53	1.45
12	C	405	NS5	C29-C30	3.27	1.53	1.43
12	C	405	NS5	C24-C25	3.24	1.53	1.43
5	A	402	HEC	FE-NA	3.22	2.06	1.95
8	C	402	BPB	C3B-C4B	3.15	1.47	1.41
7	B	303	BCL	C3B-C4B	3.13	1.46	1.41
12	C	405	NS5	C20-C21	3.05	1.39	1.35
12	C	405	NS5	C4-C5	3.04	1.57	1.51
12	C	405	NS5	C13-C12	2.98	1.52	1.43
7	B	301	BCL	C3B-C4B	2.96	1.46	1.41
8	B	304	BPB	C3B-C4B	2.94	1.46	1.41
7	B	302	BCL	C3B-C4B	2.94	1.46	1.41
8	B	304	BPB	CAC-C3C	2.88	1.40	1.33
11	C	404	MQ7	C20-C18	2.85	1.57	1.51
7	C	401	BCL	MG-NC	2.83	2.13	2.06
8	C	402	BPB	C3D-CAD	-2.65	1.42	1.47
12	C	405	NS5	C7-C5	2.63	1.39	1.33
8	C	402	BPB	C1D-C2D	2.63	1.42	1.39
7	B	301	BCL	CHD-C1D	2.55	1.43	1.38
7	B	302	BCL	CHD-C1D	2.54	1.43	1.38
7	C	401	BCL	CHD-C1D	2.54	1.43	1.38
8	B	304	BPB	C3D-CAD	-2.53	1.42	1.47
7	B	303	BCL	CHD-C1D	2.52	1.43	1.38
12	C	405	NS5	C33-C31	2.48	1.56	1.51
11	C	404	MQ7	C17-C18	2.41	1.38	1.33
11	C	404	MQ7	C27-C28	2.41	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	402	BPB	CHA-CBD	2.39	1.54	1.51
11	C	404	MQ7	C12-C13	2.38	1.38	1.33
5	A	404	HEC	CAB-C3B	2.35	1.57	1.51
12	C	405	NS5	C13-C14	2.32	1.40	1.34
11	C	404	MQ7	C11-C3	2.32	1.55	1.51
8	B	304	BPB	CHA-CBD	2.31	1.54	1.51
11	C	404	MQ7	C22-C23	2.29	1.38	1.33
11	C	404	MQ7	C32-C33	2.28	1.38	1.33
7	B	302	BCL	C1D-C2D	-2.27	1.40	1.45
5	A	404	HEC	FE-NA	2.24	2.02	1.95
7	C	401	BCL	CHC-C1C	2.22	1.42	1.37
7	B	303	BCL	C1D-ND	2.14	1.40	1.37
12	C	405	NS5	C35-C36	2.10	1.38	1.32
5	A	404	HEC	CMA-C3A	2.09	1.55	1.50
7	B	301	BCL	OBD-CAD	2.09	1.26	1.22
8	B	304	BPB	OBD-CAD	2.06	1.25	1.22
7	B	301	BCL	C1D-ND	2.06	1.40	1.37
7	B	302	BCL	OBD-CAD	2.04	1.26	1.22
12	C	405	NS5	C17-C15	2.03	1.38	1.35
8	C	402	BPB	OBD-CAD	2.02	1.25	1.22
5	A	403	HEC	CMA-C3A	2.02	1.55	1.50

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	405	DGA	OG2-CG2-CG3	-13.06	78.07	107.93
8	B	304	BPB	C4D-CHA-CBD	-10.93	103.57	108.52
8	C	402	BPB	C4D-CHA-CBD	-10.12	103.94	108.52
6	A	405	DGA	OG2-CG2-CG1	-9.67	83.73	106.13
6	A	405	DGA	CG3-CG2-CG1	7.06	132.91	112.63
12	C	405	NS5	C18-C17-C15	-6.65	117.81	127.31
7	C	401	BCL	CHD-C1D-ND	-6.36	118.61	124.45
5	A	402	HEC	C1D-ND-C4D	6.27	111.55	105.07
5	A	404	HEC	C1D-ND-C4D	6.19	111.46	105.07
5	A	403	HEC	C1D-ND-C4D	6.07	111.34	105.07
5	A	401	HEC	C1D-ND-C4D	6.02	111.29	105.07
9	B	305	MPG	O1-CX3-CXD	5.67	122.98	111.68
7	B	303	BCL	CHD-C1D-ND	-5.57	119.33	124.45
12	C	405	NS5	C19-C20-C21	-5.50	119.47	127.31
7	B	301	BCL	CHD-C1D-ND	-5.37	119.52	124.45
7	C	401	BCL	C4D-CHA-C1A	5.29	127.68	121.25
7	B	302	BCL	C4D-CHA-C1A	5.24	127.62	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	301	BCL	C4D-CHA-C1A	5.12	127.48	121.25
7	B	302	BCL	CHD-C1D-ND	-5.11	119.76	124.45
5	A	403	HEC	CBC-CAC-C3C	5.04	126.32	112.43
8	C	402	BPB	C1-C2-C3	-5.03	117.34	126.04
8	C	402	BPB	C4D-ND-C1D	-4.90	103.84	108.83
7	B	303	BCL	C4D-CHA-C1A	4.75	127.02	121.25
9	B	306	MPG	O1-CX3-CXD	4.73	121.12	111.68
8	B	304	BPB	C4D-ND-C1D	-4.66	104.08	108.83
5	A	402	HEC	CBC-CAC-C3C	4.62	125.15	112.43
13	C	406	OTP	C33-C32-C31	4.59	122.99	115.27
5	A	404	HEC	CBC-CAC-C3C	4.59	125.08	112.43
5	A	401	HEC	CBB-CAB-C3B	4.57	125.03	112.43
5	A	401	HEC	CBC-CAC-C3C	4.56	125.01	112.43
5	A	402	HEC	CBB-CAB-C3B	4.55	124.97	112.43
5	A	404	HEC	CBB-CAB-C3B	4.46	124.72	112.43
5	A	403	HEC	CBB-CAB-C3B	4.30	124.30	112.43
7	B	303	BCL	C1D-ND-C4D	-4.15	103.39	106.33
7	C	401	BCL	C4A-NA-C1A	4.14	108.57	106.71
12	C	405	NS5	C11-C10-C9	3.81	121.68	115.27
7	B	301	BCL	C1D-ND-C4D	-3.76	103.67	106.33
7	C	401	BCL	CHA-C1A-NA	-3.57	118.22	126.40
7	C	401	BCL	C2A-C1A-CHA	3.57	130.10	123.86
7	C	401	BCL	C1D-ND-C4D	-3.54	103.82	106.33
11	C	404	MQ7	C19-C18-C20	3.50	121.16	115.27
8	C	402	BPB	C3D-C4D-ND	3.47	112.45	107.72
7	B	303	BCL	C4A-NA-C1A	3.38	108.22	106.71
13	C	406	OTP	C28-C27-C26	3.32	120.85	115.27
11	C	404	MQ7	C31-C32-C33	-3.28	119.77	127.66
8	C	402	BPB	OBD-CAD-CBD	-3.25	121.06	125.82
13	C	406	OTP	C15-C14-C12	-3.25	119.84	127.66
12	C	405	NS5	C24-C25-C26	-3.23	122.70	127.31
8	B	304	BPB	C3D-C4D-ND	3.23	112.12	107.72
7	B	302	BCL	CHA-C1A-NA	-3.22	119.02	126.40
11	C	404	MQ7	C11-C12-C13	-3.22	121.44	126.79
6	A	405	DGA	OG1-CA1-CA2	3.19	121.93	111.91
8	B	304	BPB	OBD-CAD-CBD	-3.16	121.19	125.82
11	C	404	MQ7	C26-C27-C28	-3.15	120.06	127.66
6	A	405	DGA	OG2-CB1-CB2	3.15	118.29	111.50
11	C	404	MQ7	C14-C13-C15	3.12	120.52	115.27
13	C	406	OTP	C38-C37-C39	-3.10	115.73	123.68
7	B	301	BCL	CHA-C1A-NA	-3.08	119.35	126.40
11	C	404	MQ7	C16-C17-C18	-3.06	120.29	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	406	OTP	C13-C12-C11	3.06	120.42	115.27
7	B	302	BCL	C2A-C1A-CHA	3.04	129.18	123.86
13	C	406	OTP	C8-C7-C6	3.03	120.36	115.27
11	C	404	MQ7	C39-C38-C40	3.00	120.32	115.27
7	B	302	BCL	C1D-ND-C4D	-2.96	104.23	106.33
7	B	302	BCL	C1-C2-C3	-2.94	120.95	126.04
12	C	405	NS5	C6-C5-C4	2.94	120.21	115.27
7	B	303	BCL	CHA-C1A-NA	-2.89	119.77	126.40
9	B	305	MPG	O1-CX3-O4	-2.89	118.65	124.13
8	B	304	BPB	CBC-CAC-C3C	-2.89	119.03	126.70
7	B	303	BCL	C2A-C1A-CHA	2.88	128.89	123.86
7	C	401	BCL	CHC-C4B-NB	-2.84	121.25	124.26
5	A	404	HEC	C4A-NA-C1A	2.83	108.12	105.35
5	A	404	HEC	C4B-NB-C1B	2.82	107.98	105.07
7	B	302	BCL	C4A-NA-C1A	2.80	107.96	106.71
5	A	402	HEC	C4A-NA-C1A	2.79	108.08	105.35
11	C	404	MQ7	C21-C22-C23	-2.78	120.96	127.66
5	A	402	HEC	CAC-C3C-C2C	2.77	131.30	126.86
13	C	406	OTP	C10-C9-C7	-2.73	121.08	127.66
7	B	302	BCL	CAB-C3B-C2B	2.70	132.39	128.34
8	B	304	BPB	C2D-C1D-ND	2.70	111.39	109.53
7	B	301	BCL	C1-C2-C3	-2.67	121.42	126.04
5	A	401	HEC	C4A-NA-C1A	2.66	107.95	105.35
8	C	402	BPB	C11-C10-C8	2.64	124.45	115.92
7	B	303	BCL	CAB-C3B-C2B	2.64	132.29	128.34
11	C	404	MQ7	C34-C33-C35	2.63	119.69	115.27
13	C	406	OTP	C23-C22-C21	2.62	119.68	115.27
11	C	404	MQ7	C29-C28-C30	2.62	119.68	115.27
5	A	401	HEC	CAA-CBA-CGA	-2.60	108.01	113.60
5	A	401	HEC	C4B-NB-C1B	2.59	107.75	105.07
12	C	405	NS5	C32-C31-C33	2.56	119.58	115.27
5	A	403	HEC	C2A-C1A-NA	-2.56	107.83	110.32
5	A	402	HEC	CAC-C3C-C4C	-2.53	121.40	124.92
5	A	402	HEC	C2A-C1A-NA	-2.53	107.86	110.32
5	A	404	HEC	CAC-C3C-C2C	2.53	130.91	126.86
8	C	402	BPB	C2D-C1D-ND	2.52	111.27	109.53
11	C	404	MQ7	C24-C23-C25	2.51	119.50	115.27
12	C	405	NS5	C13-C14-C15	-2.48	119.45	126.42
7	C	401	BCL	CAB-C3B-C2B	2.48	132.05	128.34
5	A	403	HEC	C4A-NA-C1A	2.48	107.77	105.35
7	B	301	BCL	C2A-C1A-CHA	2.47	128.18	123.86
8	B	304	BPB	CMD-C2D-C3D	2.46	129.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	HEC	CBD-CAD-C3D	-2.45	105.82	112.63
5	A	402	HEC	C4B-NB-C1B	2.45	107.60	105.07
5	A	404	HEC	C2A-C1A-NA	-2.42	107.97	110.32
11	C	404	MQ7	C45-C43-C44	2.39	119.88	114.60
7	B	303	BCL	C4B-C3B-C2B	-2.38	104.53	108.36
11	C	404	MQ7	C36-C37-C38	-2.38	121.94	127.66
13	C	406	OTP	C18-C17-C16	2.36	119.25	115.27
5	A	403	HEC	C4C-NC-C1C	2.36	107.66	105.35
8	C	402	BPB	CMB-C2B-C3B	2.35	129.08	124.68
7	B	303	BCL	CMB-C2B-C1B	-2.34	121.80	125.37
8	C	402	BPB	CMD-C2D-C3D	2.34	129.05	124.68
9	B	306	MPG	O1-CX3-O4	-2.33	119.72	124.13
7	B	303	BCL	CHC-C4B-NB	-2.32	121.80	124.26
5	A	401	HEC	C2A-C1A-NA	-2.32	108.07	110.32
11	C	404	MQ7	C2M-C2-C3	-2.30	120.64	124.40
9	B	305	MPG	O4-CX3-CXD	-2.30	118.36	123.68
12	C	405	NS5	CM4-C36-CM3	2.30	119.68	114.60
7	C	401	BCL	C4B-C3B-C2B	-2.28	104.69	108.36
7	C	401	BCL	CMB-C2B-C1B	-2.27	121.92	125.37
13	C	406	OTP	C1-C2-C3	2.26	119.60	114.60
8	B	304	BPB	CMB-C2B-C3B	2.26	128.91	124.68
12	C	405	NS5	C34-C35-C36	-2.26	120.04	127.75
5	A	404	HEC	CAC-C3C-C4C	-2.25	121.80	124.92
7	B	301	BCL	CHC-C4B-NB	-2.25	121.88	124.26
12	C	405	NS5	C16-C15-C17	-2.24	119.78	122.92
8	C	402	BPB	O2D-CGD-CBD	2.24	113.84	111.00
7	B	303	BCL	OBB-CAB-CBB	-2.24	114.76	119.73
7	B	301	BCL	C4A-NA-C1A	2.24	107.71	106.71
11	C	404	MQ7	C41-C42-C43	-2.21	120.21	127.75
13	C	406	OTP	C18-C17-C19	-2.20	118.04	123.68
5	A	401	HEC	CAC-C3C-C2C	2.18	130.35	126.86
12	C	405	NS5	C24-C23-C21	-2.17	120.32	126.42
8	C	402	BPB	OBB-CAB-C3B	2.17	123.84	119.99
7	B	302	BCL	C4B-C3B-C2B	-2.17	104.87	108.36
7	C	401	BCL	C4D-C3D-CAD	-2.17	105.54	108.10
5	A	404	HEC	CAD-C3D-C4D	2.16	128.43	124.66
13	C	406	OTP	C30-C29-C27	-2.16	122.46	127.66
13	C	406	OTP	C36-C37-C39	2.15	125.46	121.12
5	A	404	HEC	CAD-CBD-CGD	-2.15	108.98	113.60
5	A	403	HEC	C4B-NB-C1B	2.15	107.29	105.07
5	A	403	HEC	CAB-C3B-C4B	-2.13	122.04	124.81
5	A	402	HEC	CBA-CAA-C2A	-2.11	106.77	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	401	BCL	CHD-C1D-C2D	2.11	129.90	125.48
5	A	402	HEC	CAB-C3B-C4B	-2.11	122.08	124.81
7	C	401	BCL	CHC-C1C-NC	-2.10	121.61	124.51
7	C	401	BCL	C1C-NC-C4C	2.10	107.65	106.71
5	A	403	HEC	CAD-C3D-C4D	2.10	128.32	124.66
13	C	406	OTP	C38-C37-C36	2.09	118.78	115.27
7	B	302	BCL	CHC-C4B-NB	-2.07	122.07	124.26
5	A	404	HEC	C3D-C4D-ND	-2.06	108.36	110.36
6	A	405	DGA	OG1-CG1-CG2	2.05	114.28	108.38
8	B	304	BPB	O2D-CGD-CBD	2.04	113.57	111.00
12	C	405	NS5	C25-C24-C23	-2.02	116.92	123.22
5	A	404	HEC	CMC-C2C-C1C	-2.01	122.31	125.37

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	401	HEC	NA
5	A	402	HEC	NA
5	A	403	HEC	NA
5	A	404	HEC	NA

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	405	DGA	CA2-CA1-OG1-CG1
6	A	405	DGA	OA1-CA1-OG1-CG1
6	A	405	DGA	OG1-CG1-CG2-OG2
7	B	301	BCL	C2B-C3B-CAB-OBB
7	B	301	BCL	C2B-C3B-CAB-CBB
7	B	301	BCL	C4B-C3B-CAB-OBB
7	B	301	BCL	C4B-C3B-CAB-CBB
7	C	401	BCL	CAD-CBD-CGD-O1D
7	C	401	BCL	CAD-CBD-CGD-O2D
8	C	402	BPB	C11-C10-C8-C9
9	B	305	MPG	CXD-CX3-O1-C1
9	B	305	MPG	O4-CX3-O1-C1
9	B	305	MPG	O3-C21-CXD-O2
9	B	305	MPG	O3-C21-CXD-CX3
9	B	305	MPG	O1-CX3-CXD-C21
9	B	305	MPG	O4-CX3-CXD-C21
9	B	306	MPG	O3-C21-CXD-O2
9	B	306	MPG	O3-C21-CXD-CX3

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Mol	Chain	Res	Type	Atoms
12	C	405	NS5	C20-C21-C23-C24
12	C	405	NS5	C22-C21-C23-C24
12	C	405	NS5	C25-C26-C28-C29
12	C	405	NS5	C27-C26-C28-C29
13	C	406	OTP	C14-C15-C16-C17
5	A	404	HEC	C4C-C3C-CAC-CBC
5	A	404	HEC	C2B-C3B-CAB-CBB
5	A	404	HEC	C4B-C3B-CAB-CBB
5	A	401	HEC	C4C-C3C-CAC-CBC
5	A	402	HEC	C4C-C3C-CAC-CBC
5	A	403	HEC	C4C-C3C-CAC-CBC
5	A	401	HEC	C2B-C3B-CAB-CBB
5	A	402	HEC	C2B-C3B-CAB-CBB
5	A	403	HEC	C2B-C3B-CAB-CBB
5	A	401	HEC	C4B-C3B-CAB-CBB
5	A	402	HEC	C4B-C3B-CAB-CBB
5	A	403	HEC	C4B-C3B-CAB-CBB
5	A	401	HEC	C2C-C3C-CAC-CBC
5	A	402	HEC	C2C-C3C-CAC-CBC
5	A	403	HEC	C2C-C3C-CAC-CBC
5	A	404	HEC	C2C-C3C-CAC-CBC
8	C	402	BPB	C4-C3-C5-C6
13	C	406	OTP	C15-C16-C17-C18
7	C	401	BCL	C2A-CAA-CBA-CGA
12	C	405	NS5	C2-C3-C4-C5
7	B	302	BCL	C4-C3-C5-C6
12	C	405	NS5	C11-C10-C9-C8
13	C	406	OTP	C30-C31-C32-C33
13	C	406	OTP	C5-C6-C7-C8
7	B	302	BCL	C2-C3-C5-C6
12	C	405	NS5	C12-C10-C9-C8
13	C	406	OTP	C30-C31-C32-C34
13	C	406	OTP	C15-C16-C17-C19
13	C	406	OTP	C5-C6-C7-C9
13	C	406	OTP	C34-C35-C36-C37
12	C	405	NS5	C28-C29-C30-C31
8	C	402	BPB	C2-C3-C5-C6
7	B	302	BCL	C15-C16-C17-C18
9	B	306	MPG	O4-CX3-O1-C1
9	B	305	MPG	C1-C2-C3-C4
12	C	405	NS5	C3-C4-C5-C6
13	C	406	OTP	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
13	C	406	OTP	C19-C20-C21-C22
13	C	406	OTP	C9-C10-C11-C12
9	B	305	MPG	C10-C11-C12-C13
9	B	306	MPG	C3-C4-C5-C6
6	A	405	DGA	CBB-CAB-CB9-CB8
6	A	405	DGA	CA5-CA6-CA7-CA8
9	B	305	MPG	C2-C3-C4-C5
7	B	301	BCL	C4-C3-C5-C6
9	B	305	MPG	C5-C6-C7-C8
9	B	306	MPG	C11-C12-C13-C14
8	B	304	BPB	O2A-C1-C2-C3
8	B	304	BPB	C2-C3-C5-C6
6	A	405	DGA	CA7-CA8-CA9-CAA
8	B	304	BPB	C4-C3-C5-C6
7	B	301	BCL	C2-C3-C5-C6
8	C	402	BPB	C6-C7-C8-C10
9	B	305	MPG	C6-C7-C8-C9
9	B	306	MPG	CXD-CX3-O1-C1
6	A	405	DGA	CCB-CDB-CEB-CFB
6	A	405	DGA	CEB-CFB-CGB-CHB
9	C	407	MPG	C10-C11-C12-C13
12	C	405	NS5	C3-C4-C5-C7
8	C	402	BPB	C6-C7-C8-C9
9	B	306	MPG	C14-C15-C16-C17
12	C	405	NS5	CM2-C1-C2-C3
9	C	407	MPG	C4-C5-C6-C7
12	C	405	NS5	CM1-C1-C2-C3
12	C	405	NS5	C1-C2-C3-C4
9	B	306	MPG	C12-C13-C14-C15
6	A	405	DGA	CB6-CB7-CB8-CB9
11	C	404	MQ7	C38-C40-C41-C42
6	A	405	DGA	CB9-CAB-CBB-CCB
6	A	405	DGA	CA3-CA4-CA5-CA6
5	A	402	HEC	C3D-CAD-CBD-CGD
8	C	402	BPB	C8-C10-C11-C12
9	C	407	MPG	C13-C14-C15-C16
9	C	407	MPG	C2-C3-C4-C5
12	C	405	NS5	C31-C33-C34-C35
5	A	404	HEC	C4D-C3D-CAD-CBD
7	B	301	BCL	C14-C13-C15-C16
7	B	303	BCL	C11-C12-C13-C14
9	B	305	MPG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
9	B	306	MPG	C2-C3-C4-C5
7	B	303	BCL	C11-C12-C13-C15
7	B	303	BCL	CAD-CBD-CGD-O2D
6	A	405	DGA	CB4-CB5-CB6-CB7
9	B	305	MPG	O4-CX3-CXD-O2
5	A	404	HEC	C2D-C3D-CAD-CBD
9	B	305	MPG	C15-C16-C17-C18
13	C	406	OTP	C35-C36-C37-C38
7	B	303	BCL	C16-C17-C18-C19
9	C	407	MPG	C6-C7-C8-C9
8	C	402	BPB	C11-C10-C8-C7
12	C	405	NS5	C26-C28-C29-C30
7	B	303	BCL	C16-C17-C18-C20
11	C	404	MQ7	C39-C38-C40-C41
9	B	305	MPG	C13-C14-C15-C16
9	C	407	MPG	C12-C13-C14-C15
12	C	405	NS5	C10-C12-C13-C14
6	A	405	DGA	CA2-CA3-CA4-CA5
5	A	402	HEC	CAA-CBA-CGA-O2A
5	A	402	HEC	CAA-CBA-CGA-O1A
11	C	404	MQ7	C37-C38-C40-C41
13	C	406	OTP	C35-C36-C37-C39
7	B	301	BCL	C10-C11-C12-C13
5	A	401	HEC	C3A-C2A-CAA-CBA
9	B	306	MPG	O1-CX3-CXD-C21
9	B	306	MPG	O4-CX3-CXD-C21
5	A	402	HEC	CAD-CBD-CGD-O1D
9	C	407	MPG	C7-C8-C9-C10
7	B	301	BCL	CAD-CBD-CGD-O2D
9	B	305	MPG	C7-C8-C9-C10
9	C	407	MPG	C9-C10-C11-C12
7	B	303	BCL	C15-C16-C17-C18
5	A	401	HEC	C1A-C2A-CAA-CBA
9	B	306	MPG	C7-C8-C9-C10
7	B	302	BCL	CHA-CBD-CGD-O1D
7	C	401	BCL	CHA-CBD-CGD-O1D
7	C	401	BCL	CHA-CBD-CGD-O2D
5	A	402	HEC	CAD-CBD-CGD-O2D
5	A	401	HEC	CAA-CBA-CGA-O2A
7	B	302	BCL	CAD-CBD-CGD-O1D
8	C	402	BPB	CAD-CBD-CGD-O1D
6	A	405	DGA	OG2-CB1-CB2-CB3

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Mol	Chain	Res	Type	Atoms
5	A	401	HEC	CAA-CBA-CGA-O1A

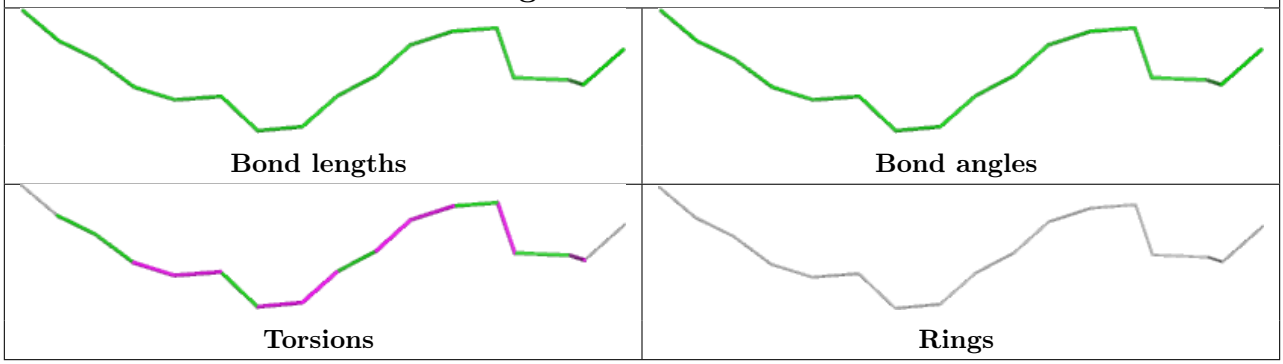
There are no ring outliers.

16 monomers are involved in 40 short contacts:

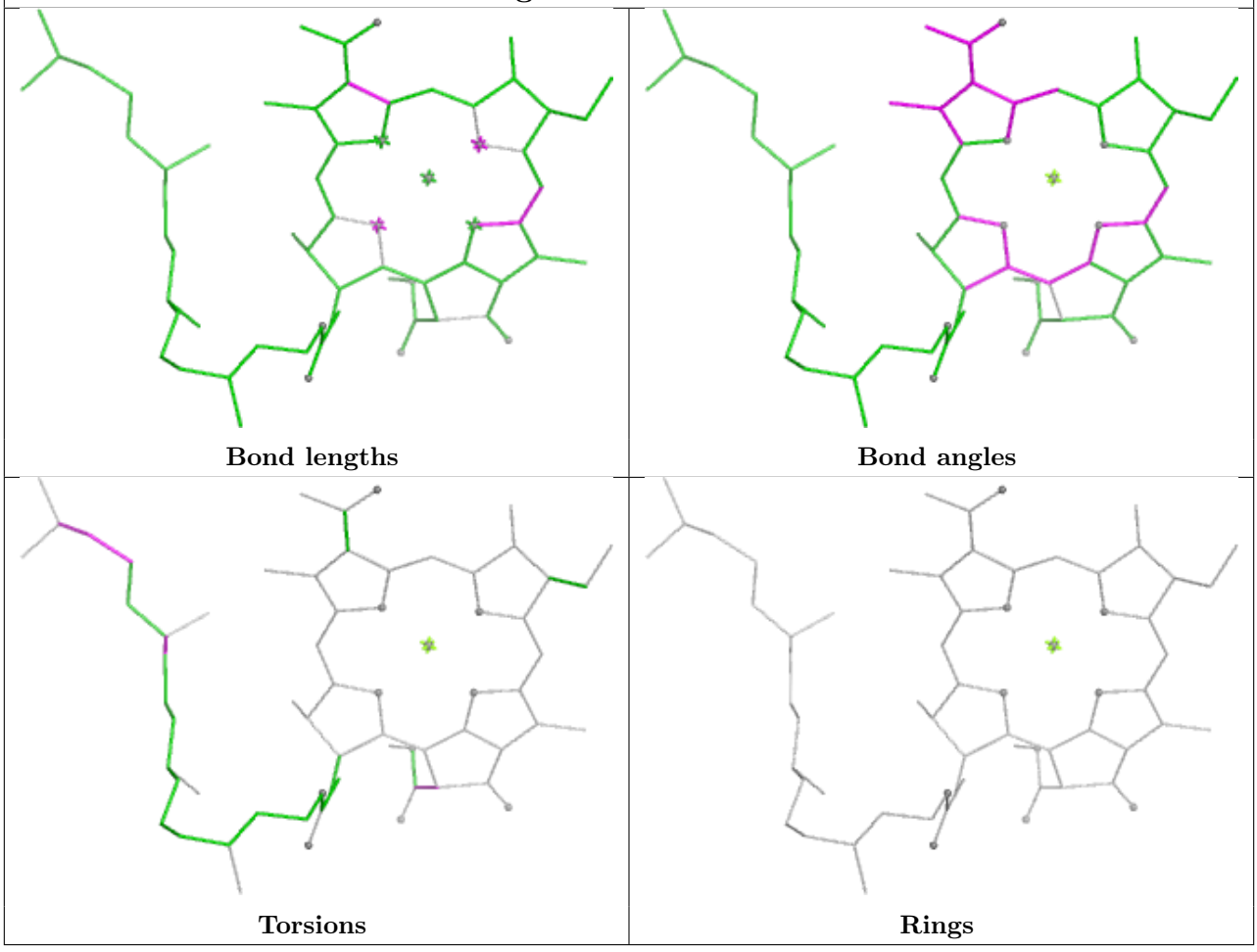
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	407	MPG	1	0
7	B	303	BCL	3	0
7	B	302	BCL	1	0
7	C	401	BCL	1	0
12	C	405	NS5	4	0
5	A	403	HEC	4	0
5	A	402	HEC	6	0
6	A	405	DGA	2	0
9	B	306	MPG	1	0
8	C	402	BPB	4	0
9	B	305	MPG	2	0
5	A	401	HEC	4	0
13	C	406	OTP	1	0
8	B	304	BPB	1	0
7	B	301	BCL	2	0
5	A	404	HEC	5	0

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

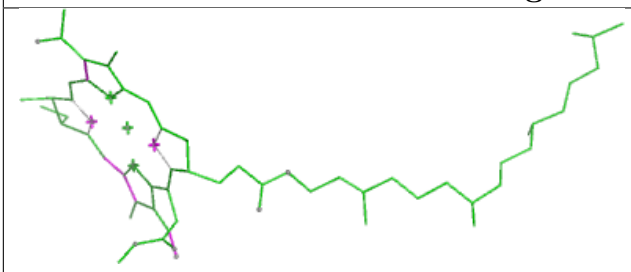
Ligand MPG C 407



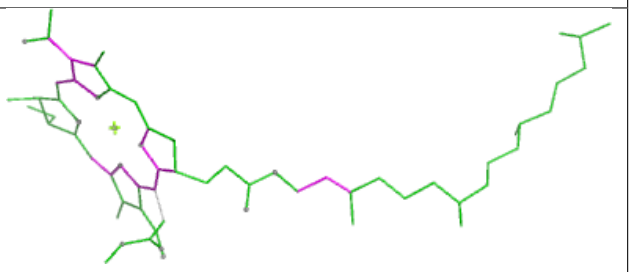
Ligand BCL B 303



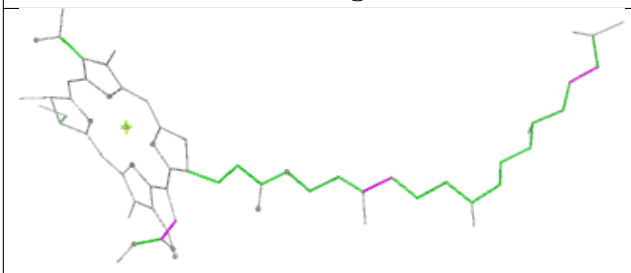
Ligand BCL B 302



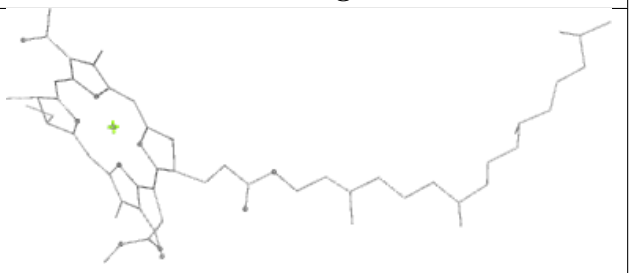
Bond lengths



Bond angles

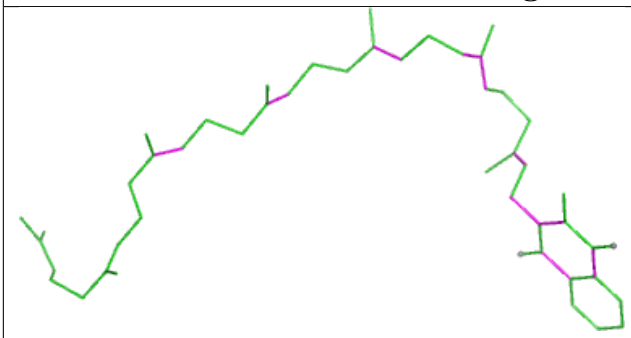


Torsions

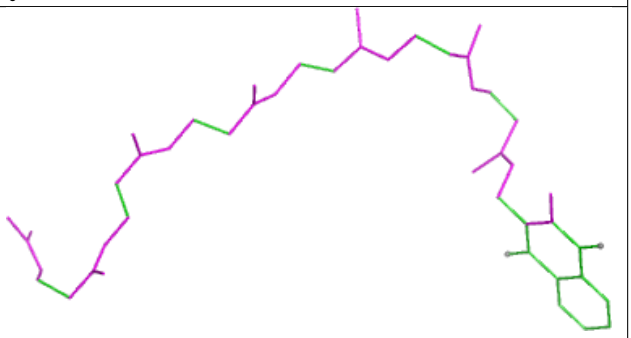


Rings

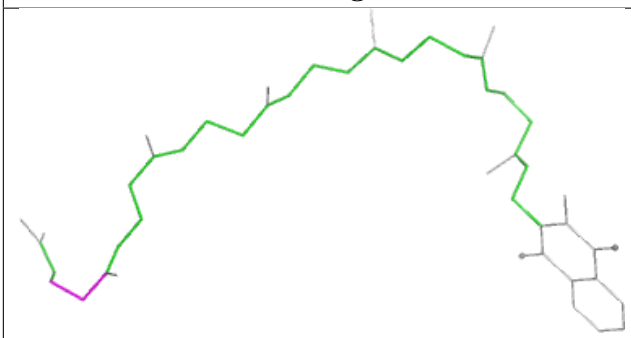
Ligand MQ7 C 404



Bond lengths



Bond angles



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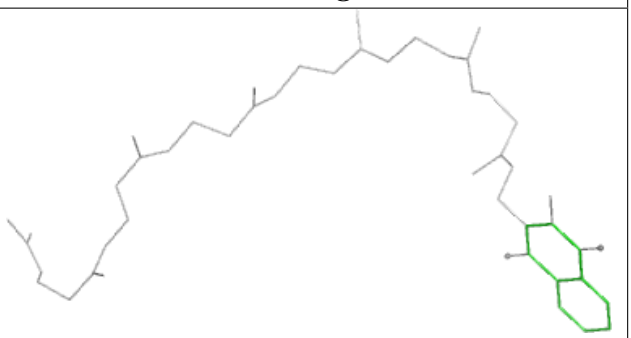
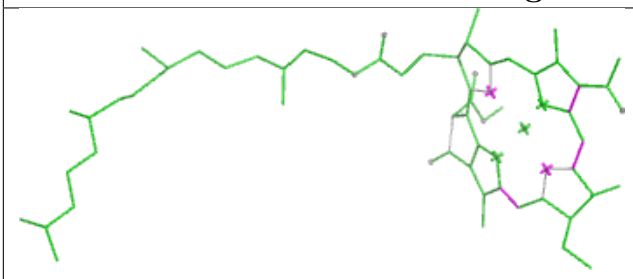
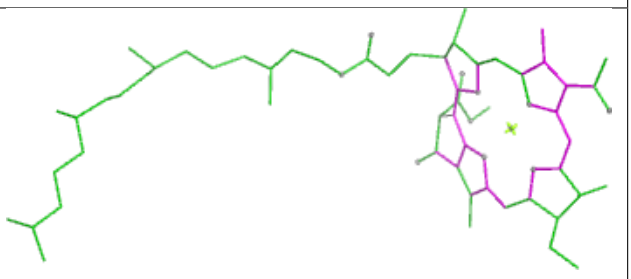


Rings

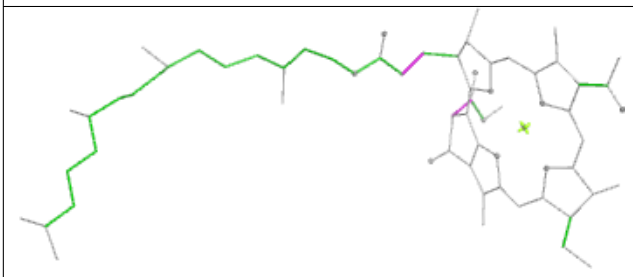
Ligand BCL C 401



Bond lengths



Bond angles



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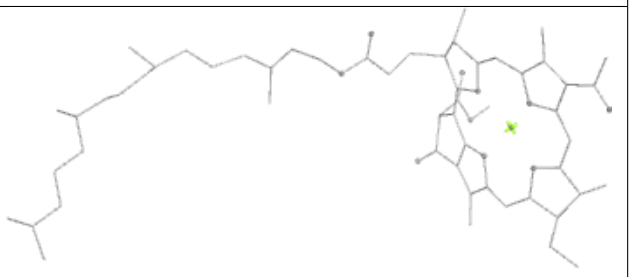
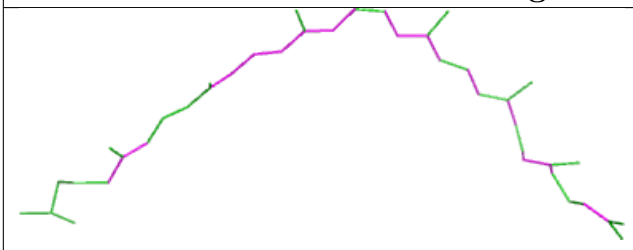
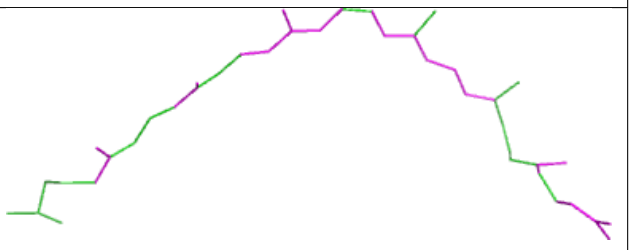


Rings

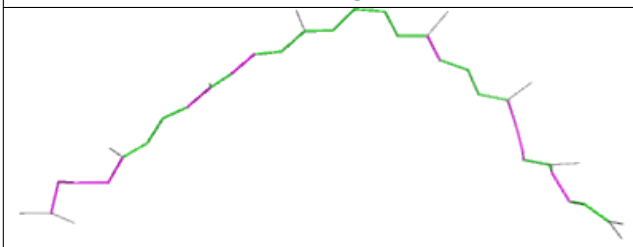
Ligand NS5 C 405



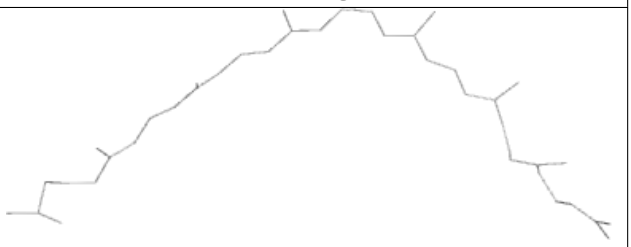
Bond lengths



Bond angles

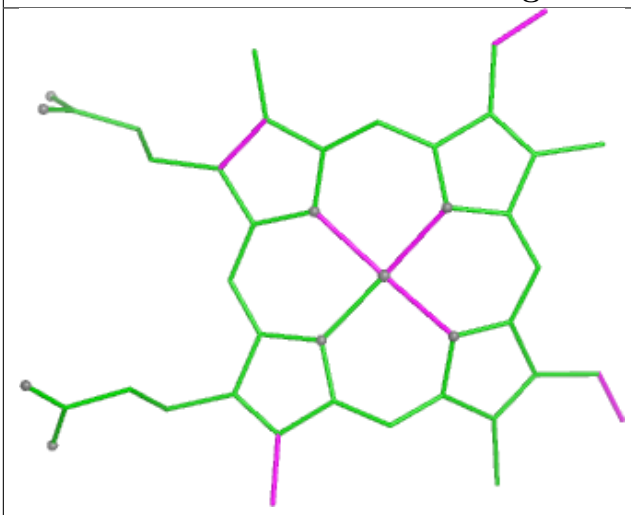


Torsions

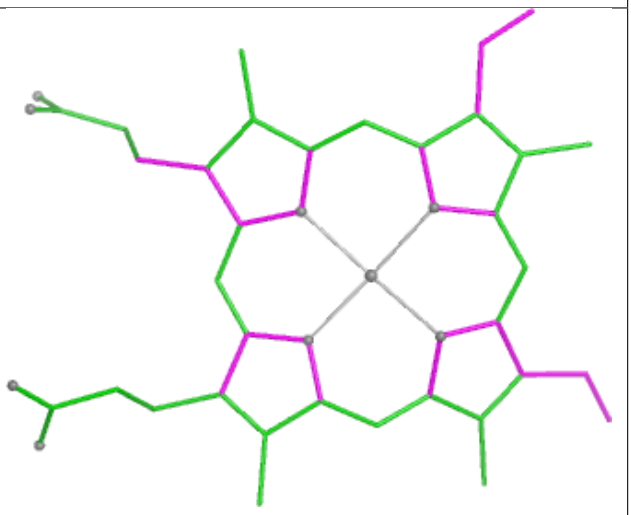


Rings

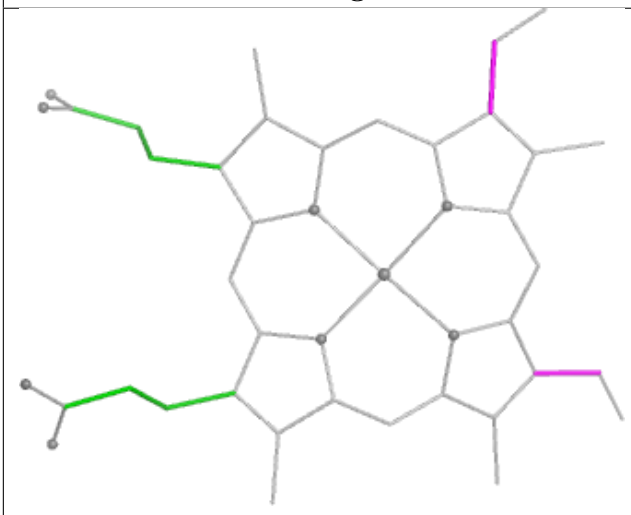
Ligand HEC A 403



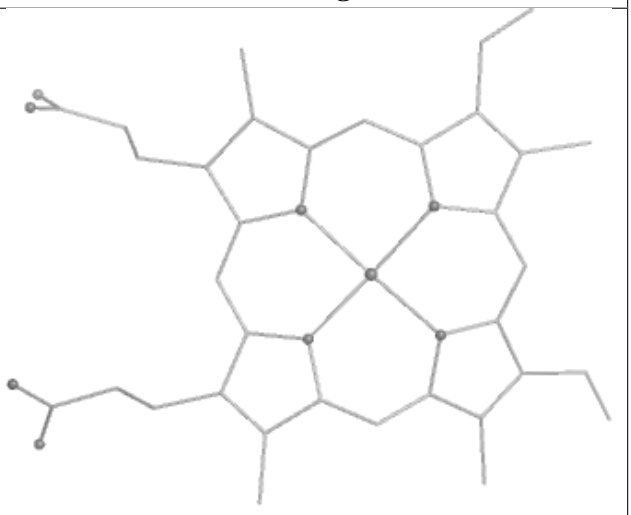
Bond lengths



Bond angles

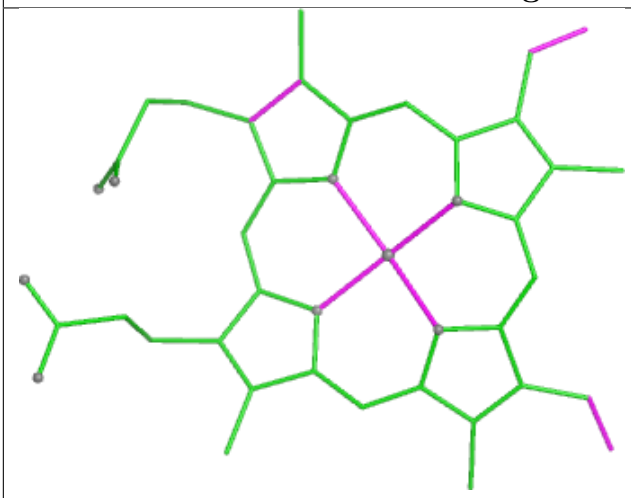


Torsions



Rings

Ligand HEC A 402



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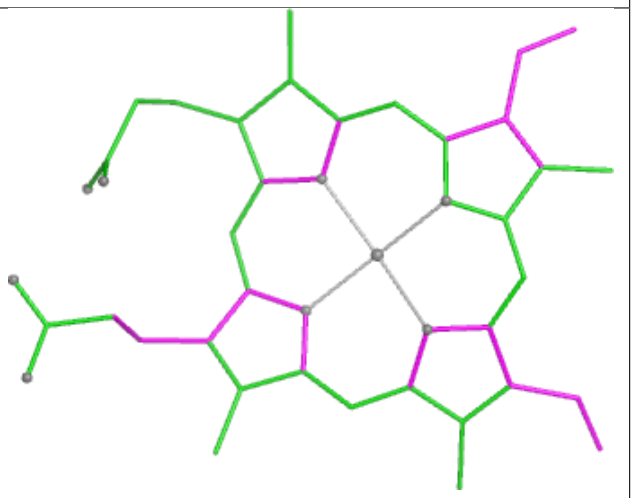
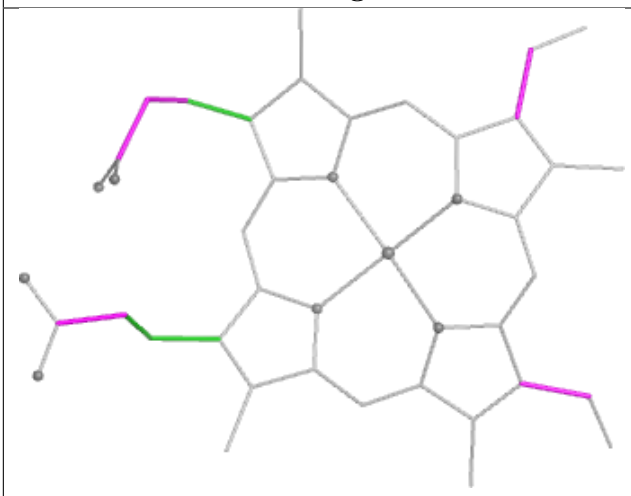
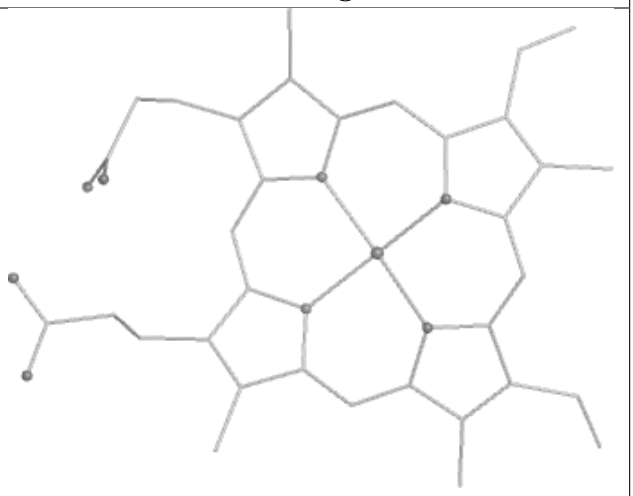


Bond angles

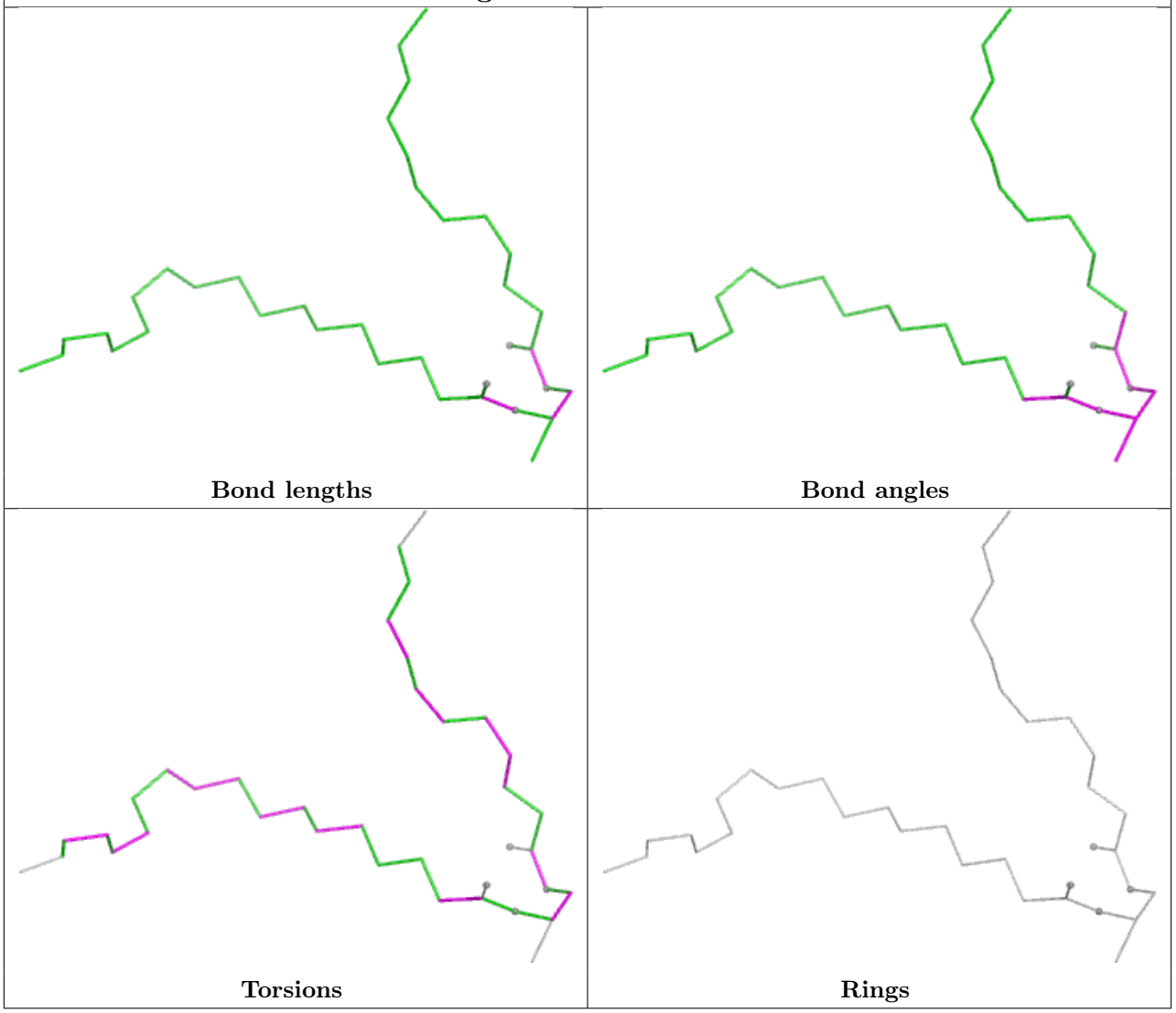


Torsions

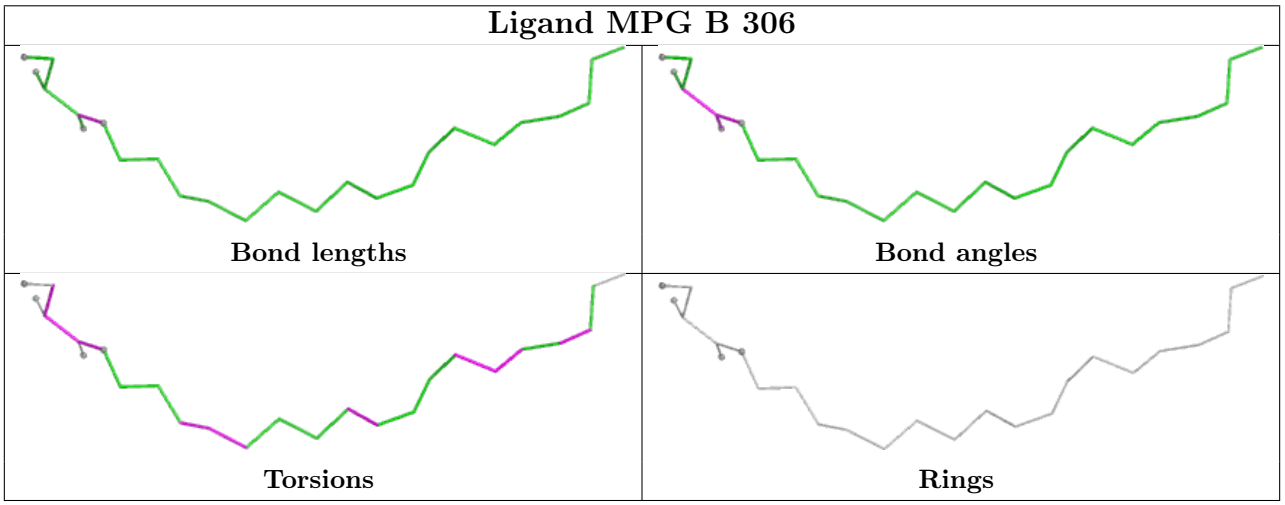


Rings

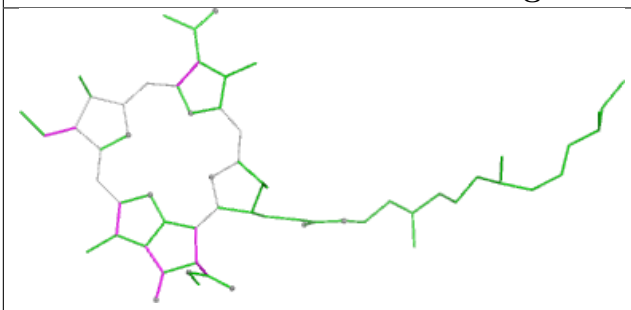
Ligand DGA A 405



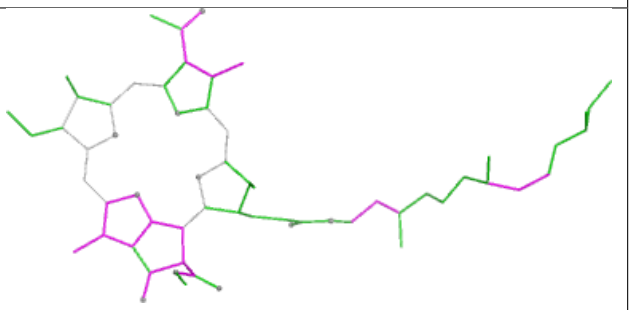
Ligand MPG B 306



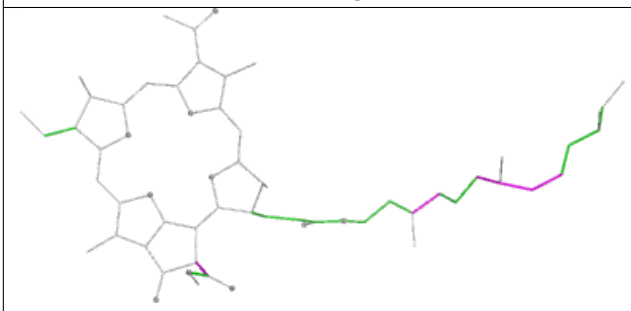
Ligand BPB C 402



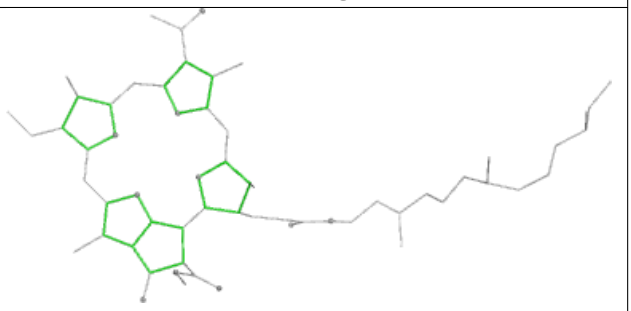
Bond lengths



Bond angles

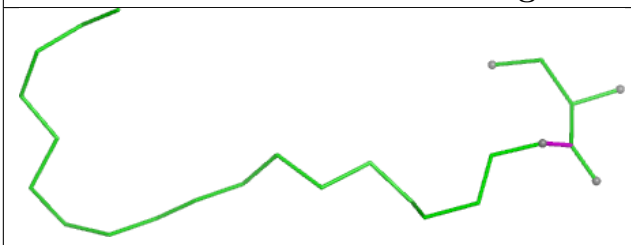


Torsions

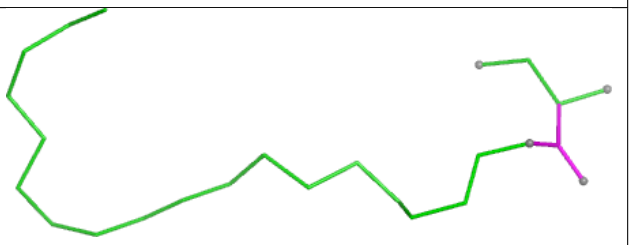


Rings

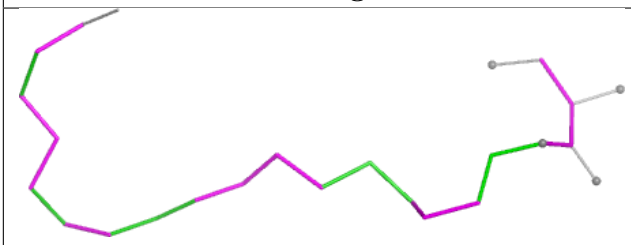
Ligand MPG B 305



Bond lengths



Bond angles



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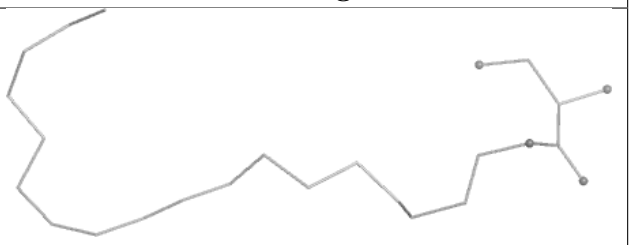
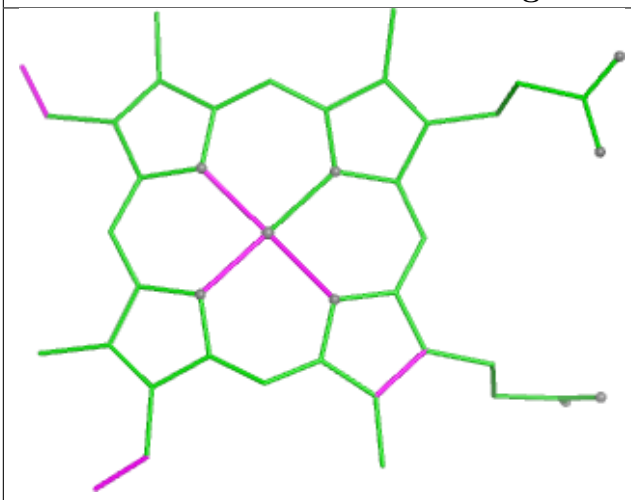
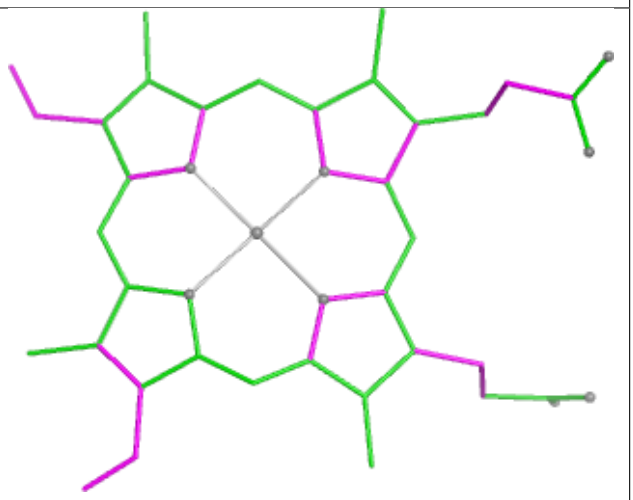


Rings

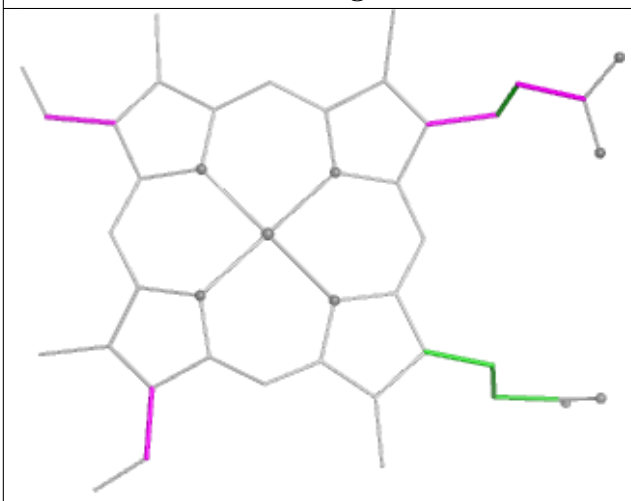
Ligand HEC A 401



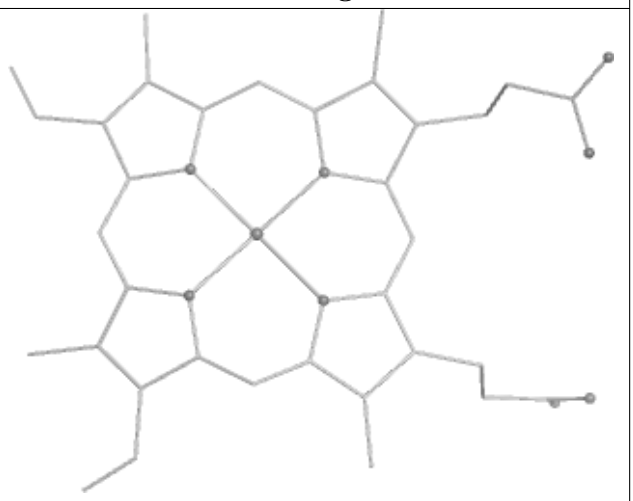
Bond lengths



Bond angles

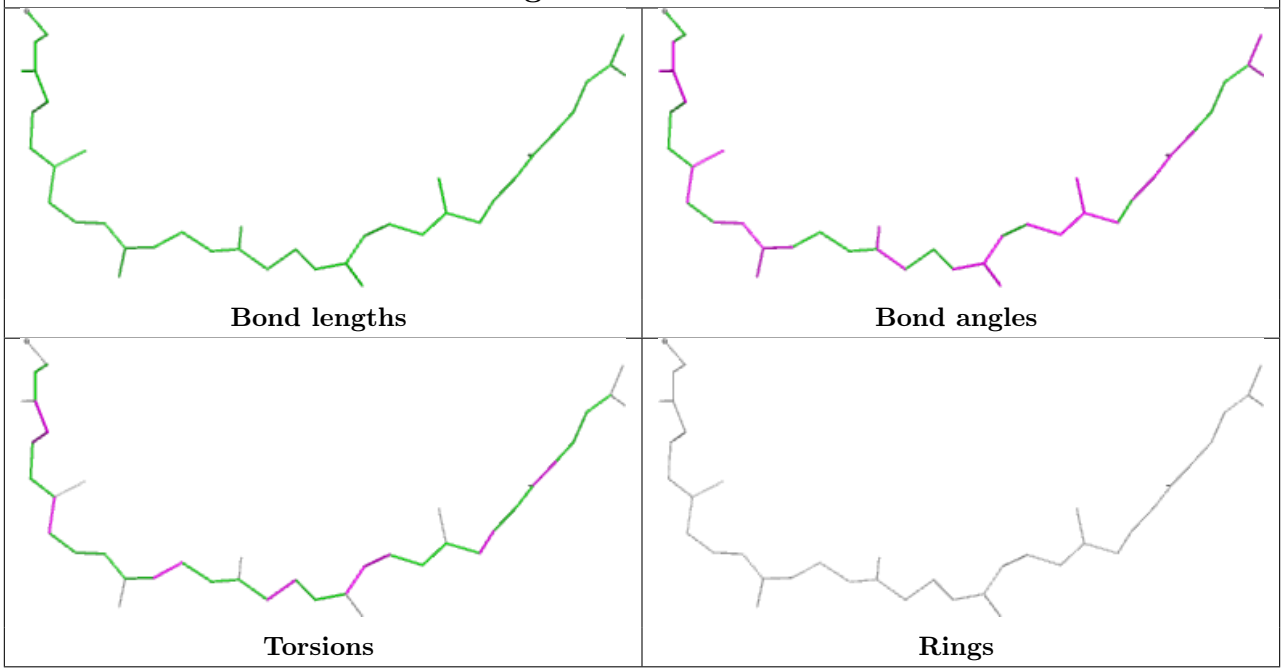


Torsions

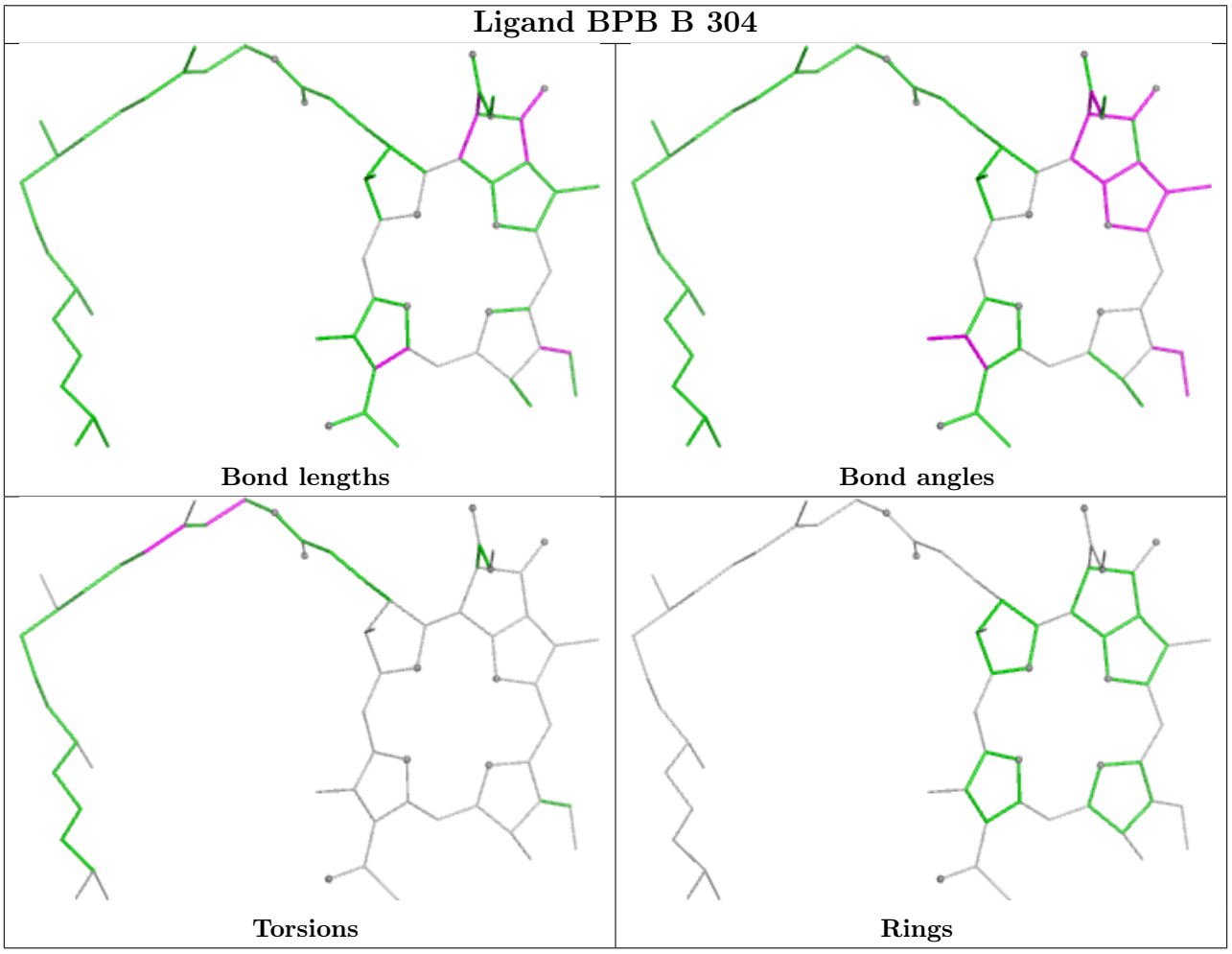


Rings

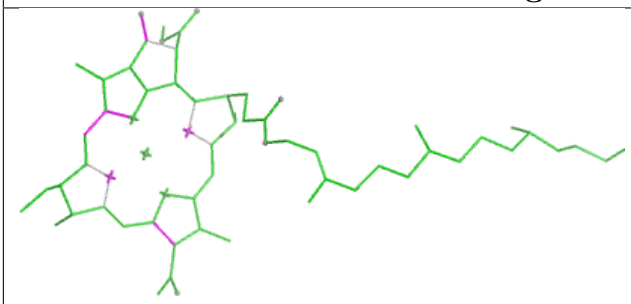
Ligand OTP C 406



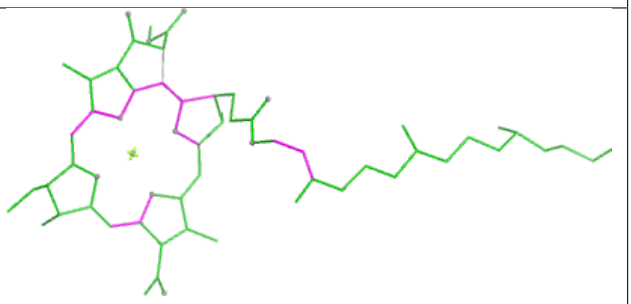
Ligand BPB B 304



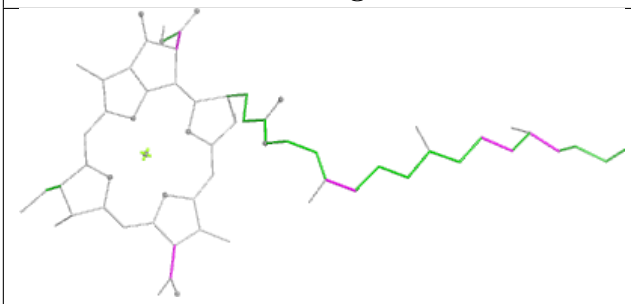
Ligand BCL B 301



Bond lengths



Bond angles



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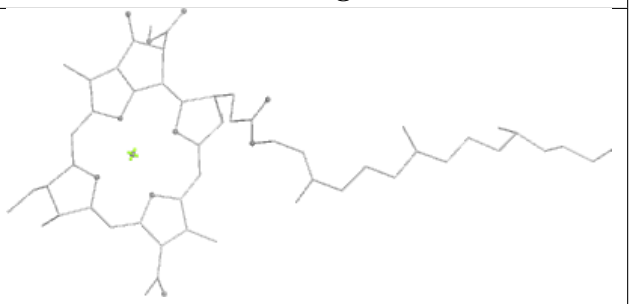
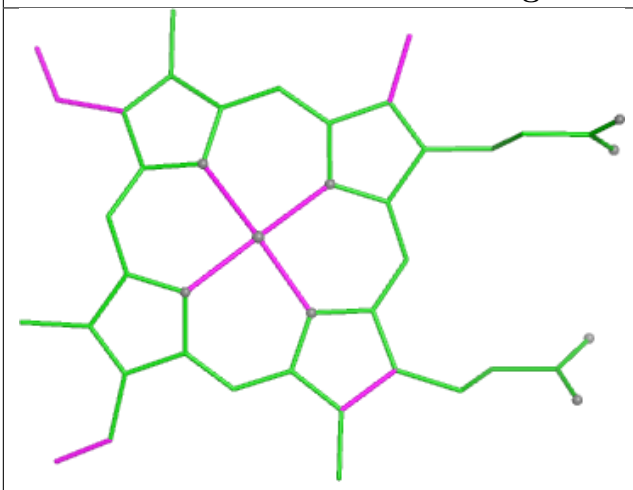
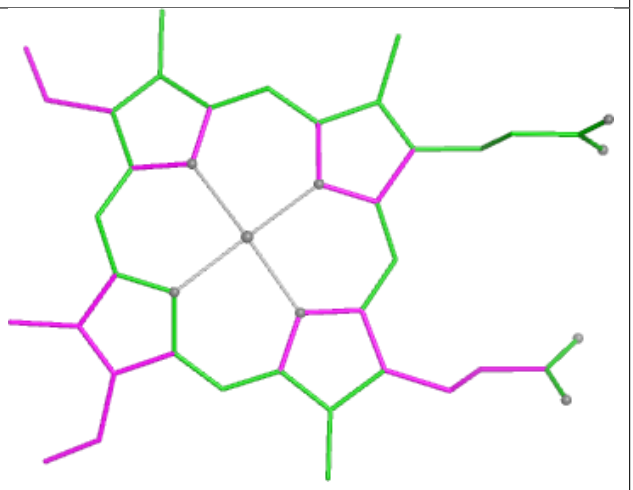


Rings

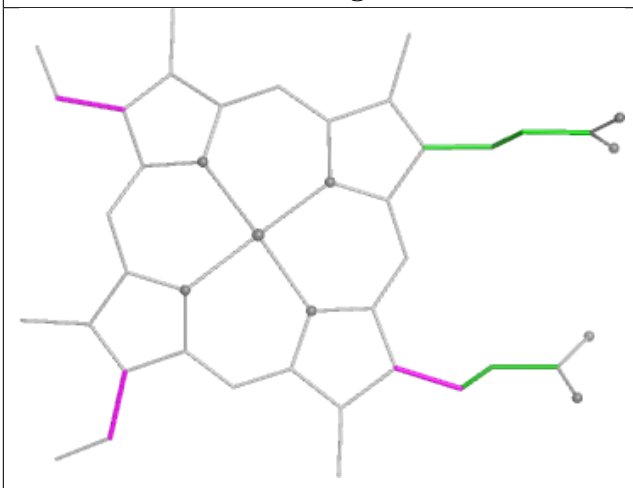
Ligand HEC A 404



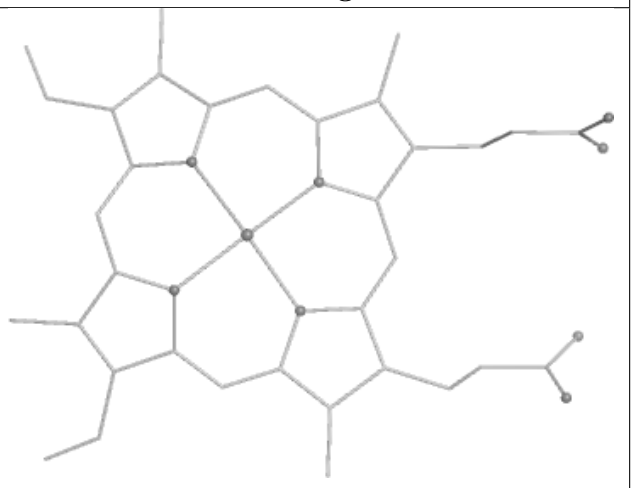
Bond lengths



Bond angles



Torsions



Rings

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	A	332/356 (93%)	0.12	2 (0%)	85	64	48, 63, 86, 116	0
2	B	273/274 (99%)	0.19	3 (1%)	78	52	44, 78, 111, 135	2 (0%)
3	C	323/324 (99%)	0.20	4 (1%)	76	50	51, 77, 116, 141	0
4	D	242/258 (93%)	0.78	17 (7%)	22	15	63, 122, 153, 235	0
All	All	1170/1212 (96%)	0.30	26 (2%)	62	36	44, 76, 134, 235	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	ALA	3.8
4	D	201	CYS	3.4
3	C	214	PHE	3.4
4	D	78	VAL	3.2
1	A	92	ASP	2.8
3	C	17	ILE	2.8
4	D	149	ASP	2.8
4	D	147	GLU	2.8
2	B	59	TRP	2.7
4	D	118	ALA	2.7
4	D	167	THR	2.6
4	D	79	PRO	2.5
4	D	85	THR	2.5
4	D	80	ARG	2.5
4	D	7	ALA	2.4
4	D	82	ARG	2.4
4	D	122	GLU	2.4
1	A	94	ASN	2.3
4	D	45	GLU	2.3
4	D	228	ASP	2.3
3	C	245	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	190	SER	2.1
3	C	16	HIS	2.1
4	D	225	GLN	2.1
2	B	204	ASP	2.1
4	D	192	ARG	2.0

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	D	1	10/11	0.90	0.14	77,81,114,124	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	PO4	C	409	5/5	0.63	0.18	124,125,126,126	0
6	DGA	A	405	37/44	0.68	0.26	68,91,112,114	0
9	MPG	C	407	17/25	0.71	0.39	100,112,133,134	0
9	MPG	B	306	25/25	0.73	0.26	76,94,112,116	0
9	MPG	B	305	25/25	0.78	0.22	61,93,124,125	0
14	PO4	C	408	5/5	0.79	0.16	118,118,119,121	0
13	OTP	C	406	41/49	0.82	0.28	71,78,106,108	0
12	NS5	C	405	40/40	0.83	0.23	65,75,95,96	0
7	BCL	B	301	65/66	0.89	0.18	37,62,166,173	0
11	MQ7	C	404	48/48	0.89	0.19	60,87,93,94	0
8	BPB	C	402	61/65	0.89	0.16	72,80,100,104	0
7	BCL	B	302	66/66	0.93	0.14	48,63,70,71	0

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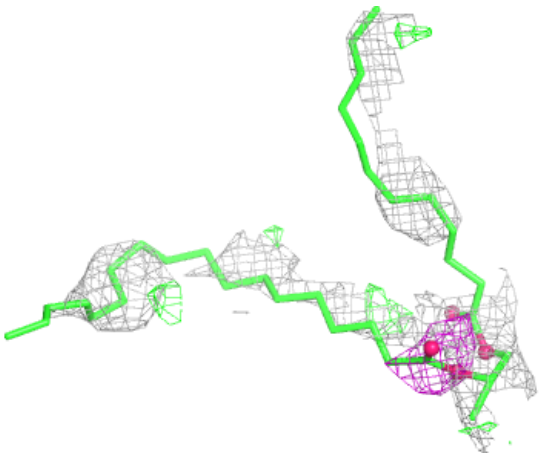
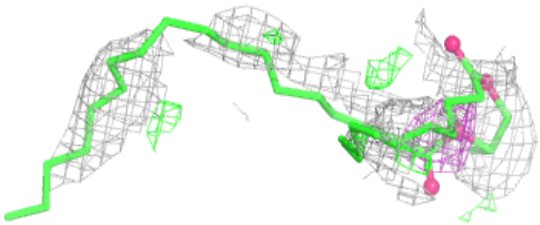
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	BCL	B	303	66/66	0.93	0.14	56,64,74,79	0
7	BCL	C	401	66/66	0.93	0.15	54,64,72,74	0
8	BPB	B	304	65/65	0.94	0.13	57,71,79,80	0
5	HEC	A	403	43/43	0.96	0.14	30,54,56,56	0
5	HEC	A	402	43/43	0.97	0.11	35,54,61,72	0
5	HEC	A	401	43/43	0.97	0.12	45,74,77,80	0
5	HEC	A	404	43/43	0.97	0.11	32,59,62,62	0
10	FE2	C	403	1/1	0.99	0.04	74,74,74,74	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 DGA A 405:

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

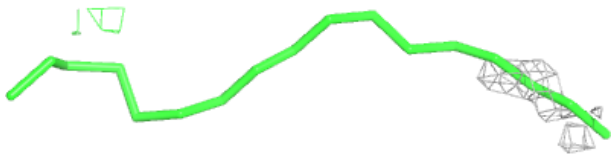


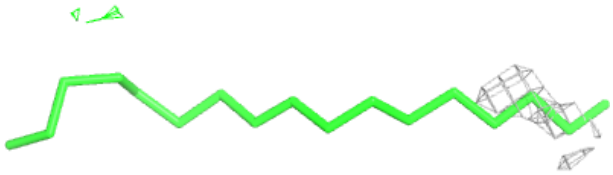


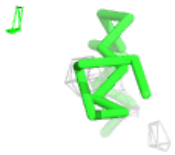


Electron density around MPG C 407:

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

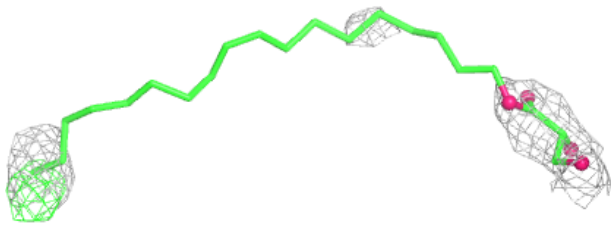


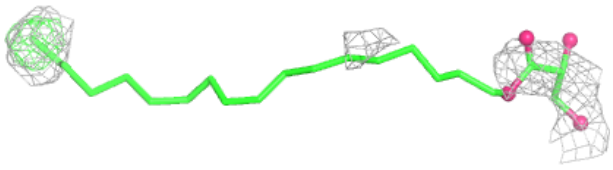


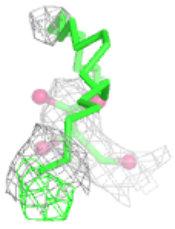


Electron density around MPG B 306:

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

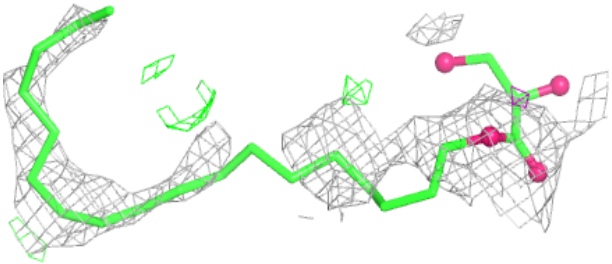


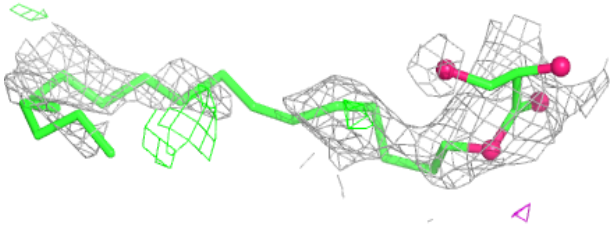


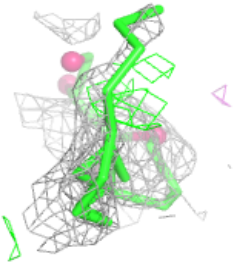


Electron density around MPG B 305:

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



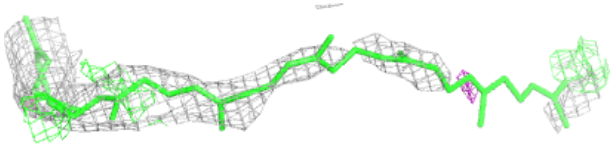


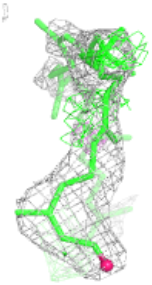


Electron density around OTP C 406:

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

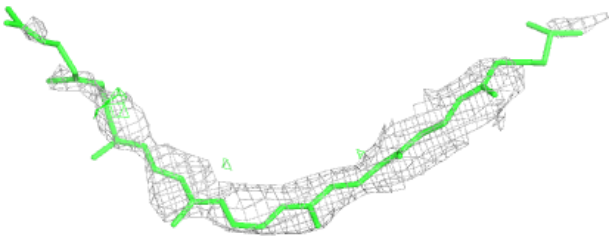


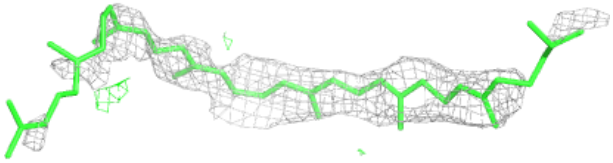




Electron density around NS5 C 405:

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

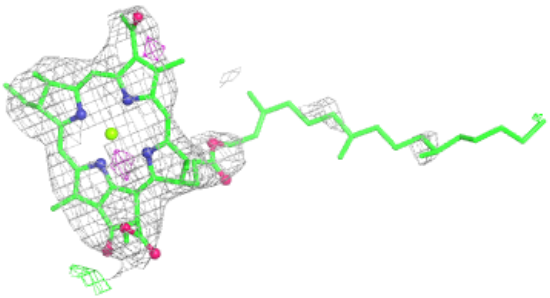


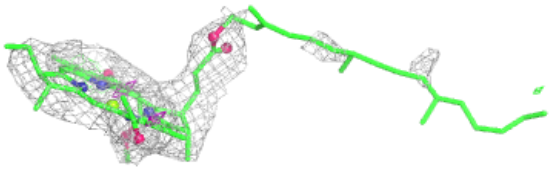


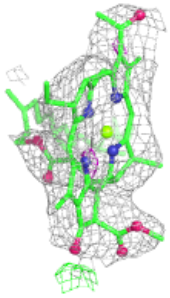


Electron density around BCL B 301:

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

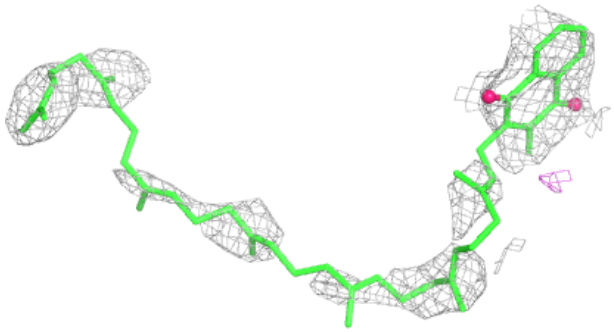


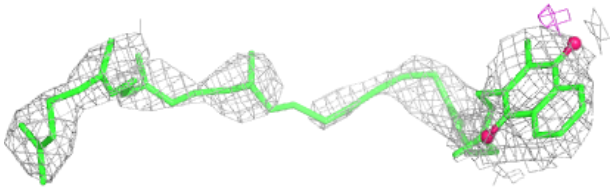




Electron density around MQ7 C 404:

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

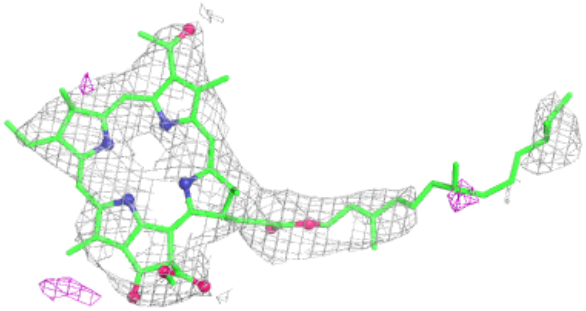




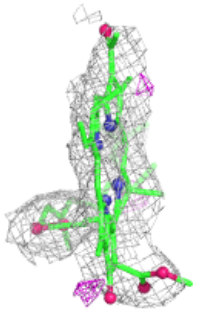


Electron density around BPB C 402:

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

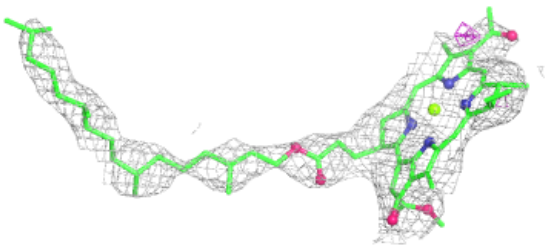


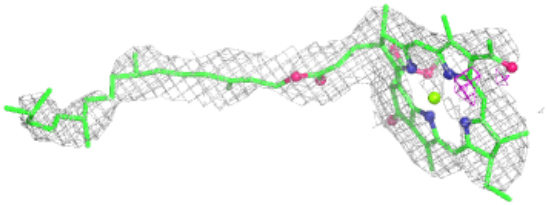


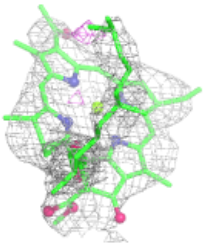


Electron density around BCL B 302:

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

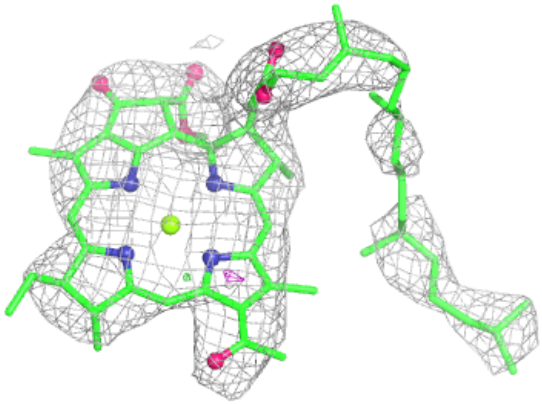


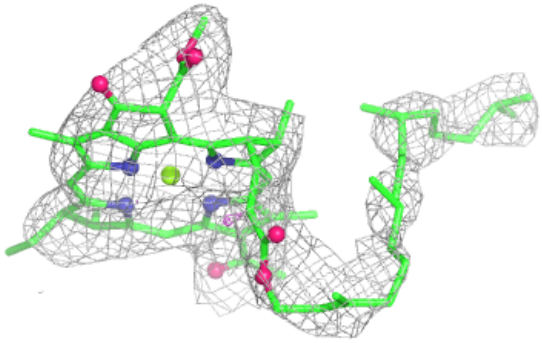


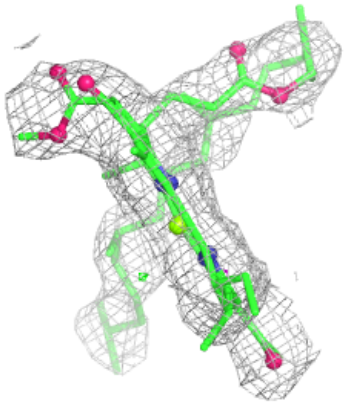


Electron density around BCL B 303:

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

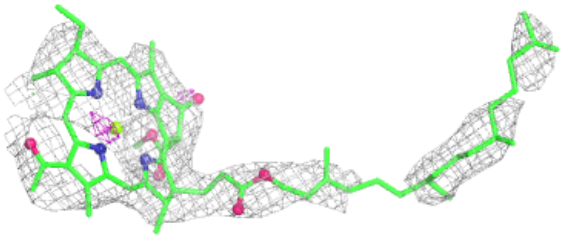


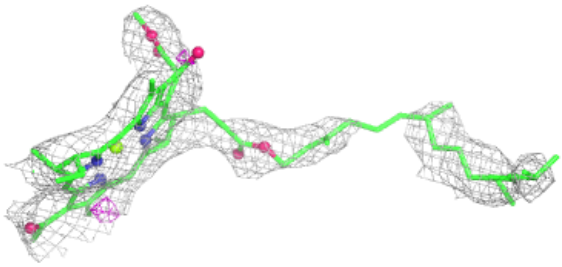


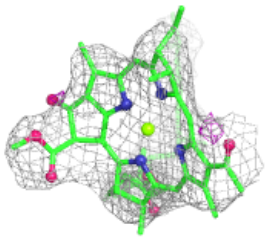


Electron density around BCL C 401:

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

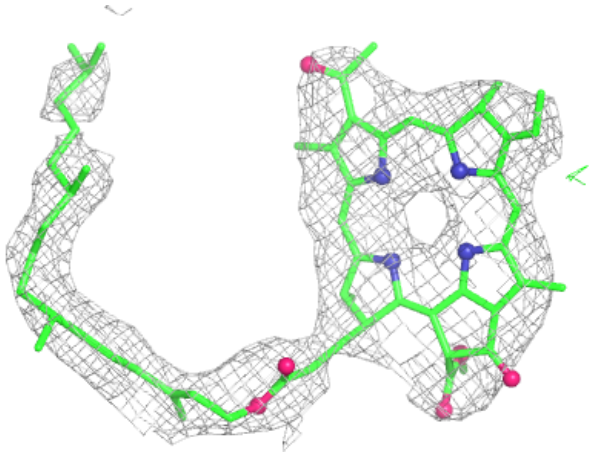


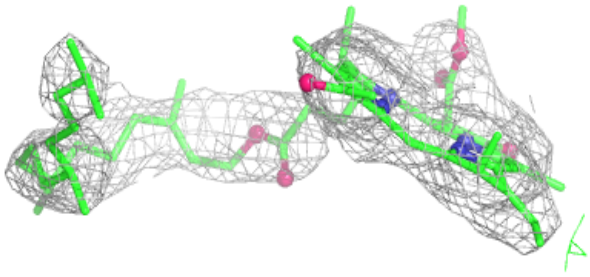


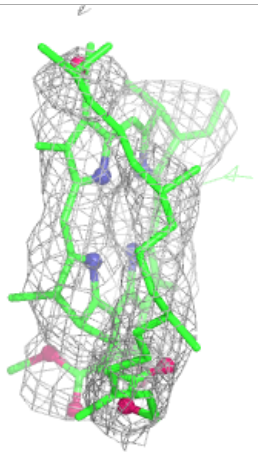


Electron density around BPB B 304:

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

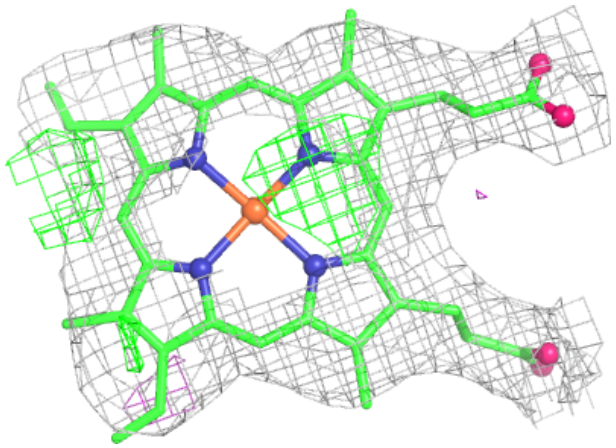


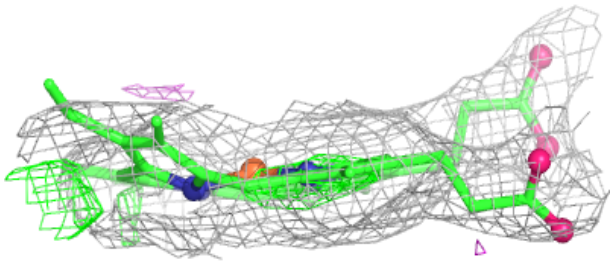


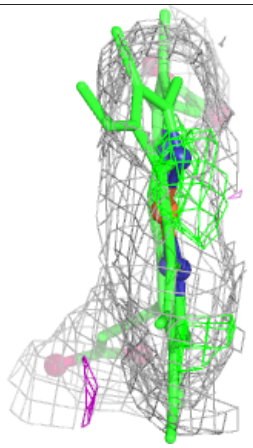


Electron density around HEC A 403:

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

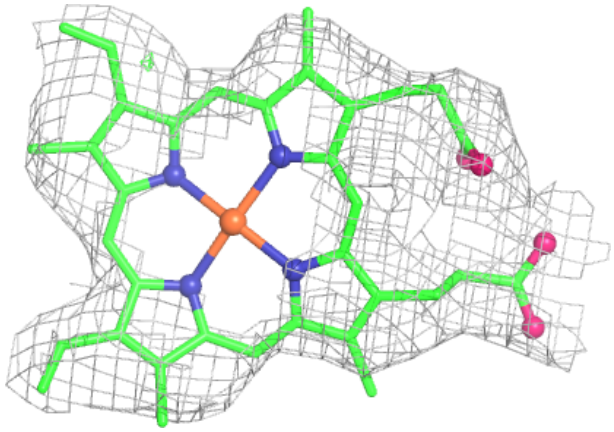


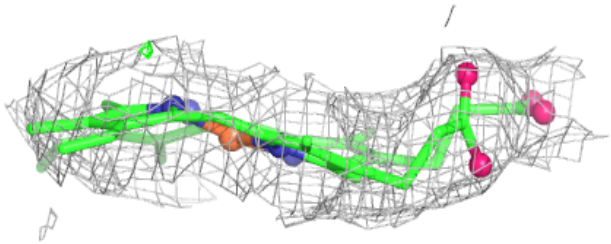


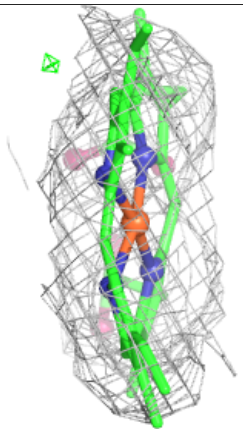


Electron density around HEC A 402:

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

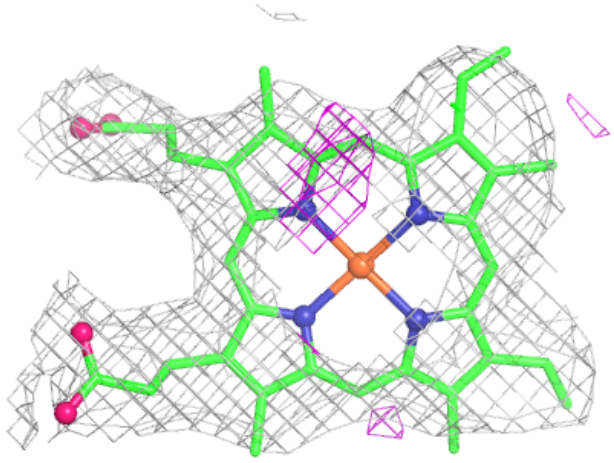


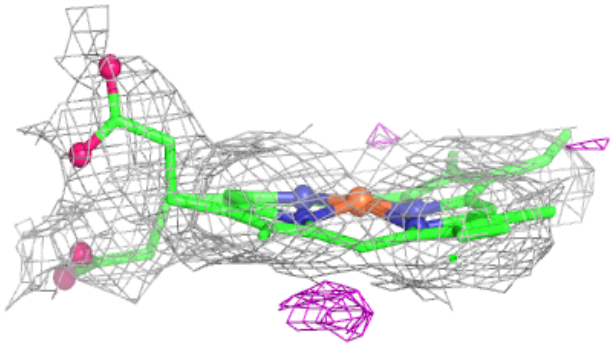




Electron density around HEC A 401:

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

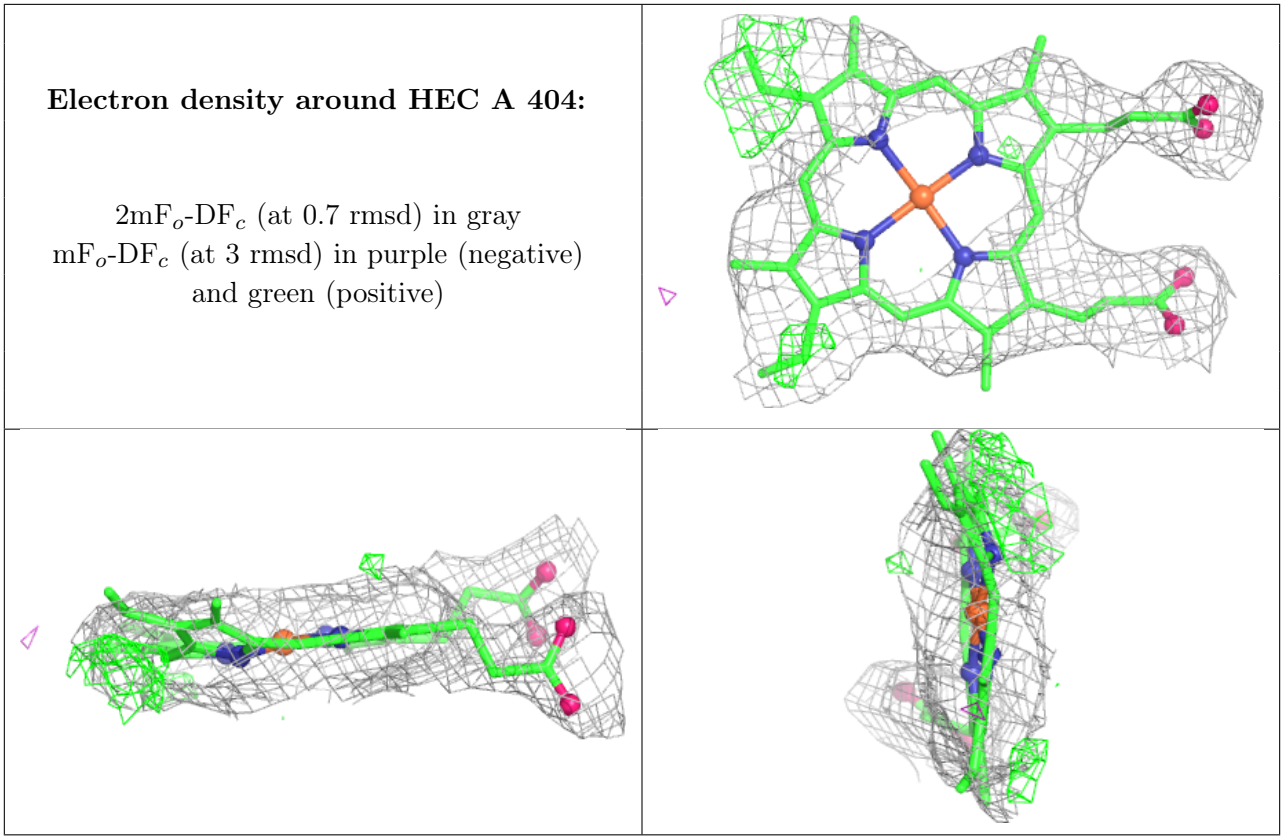






Electron density around HEC A 404:

$2mF_o$-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.