



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:33 PM UTC

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.; Kato, 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

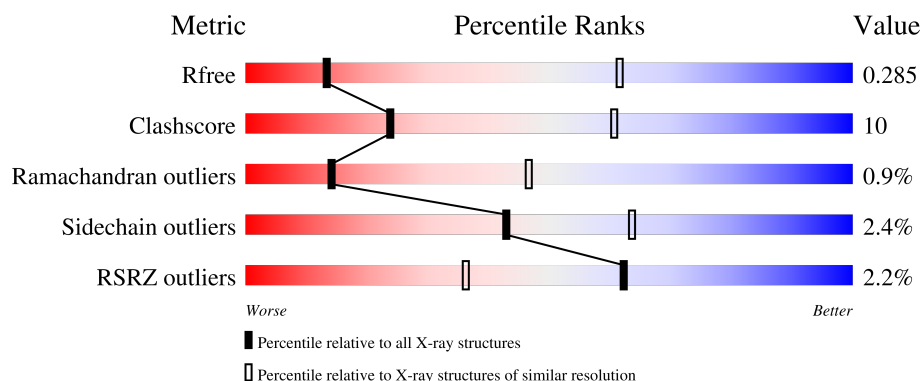
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	356	% 78% 15% 7%
2	B	274	% 80% 17% ..
3	C	324	% 83% 17%
4	D	258	7% 65% 24% 5% 6%

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			

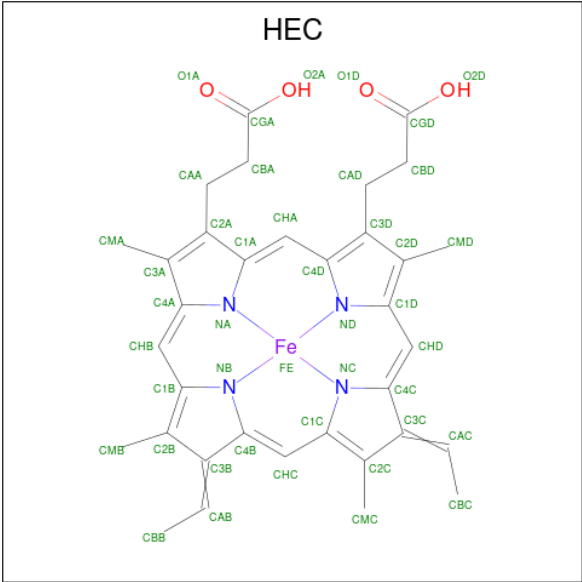
- Molecule 3 is a protein called Reaction center protein M chain.

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.

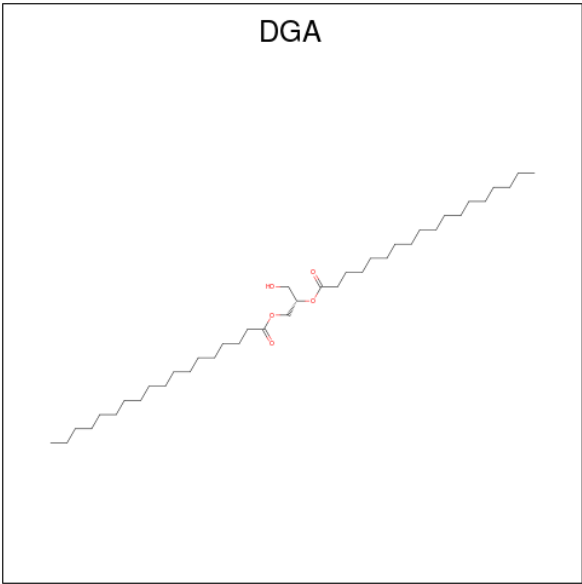
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

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



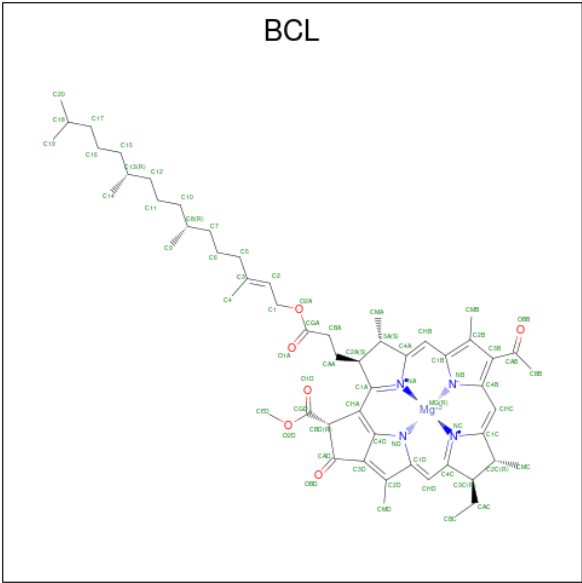
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

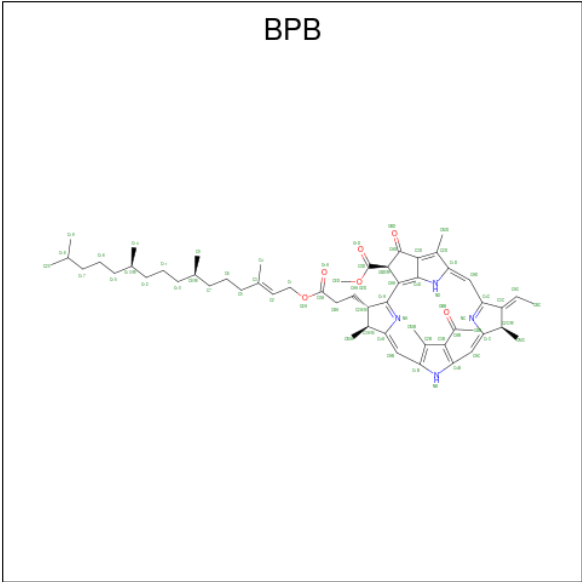
- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



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

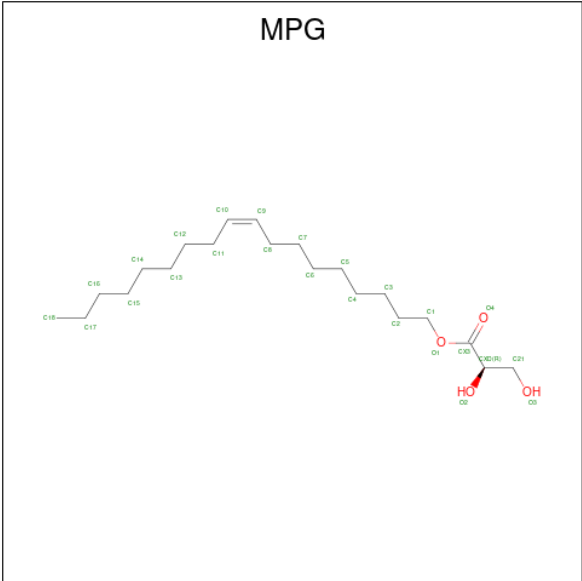
- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).





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: C₂₁H₄₀O₄).



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

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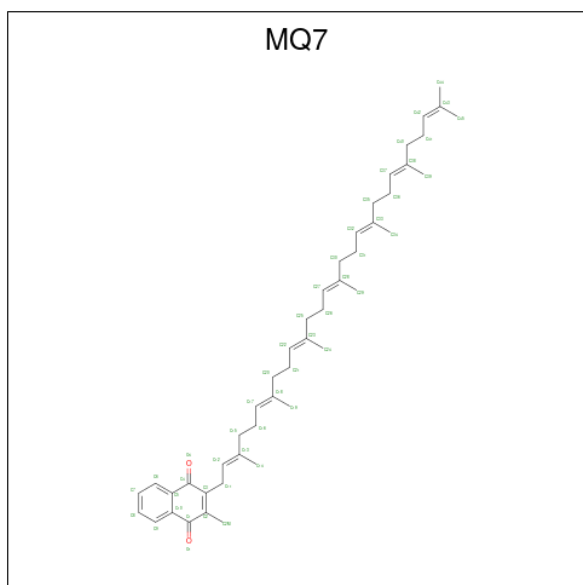
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 25 21 4	0	0
9	C	1	Total C 17 17	0	0

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

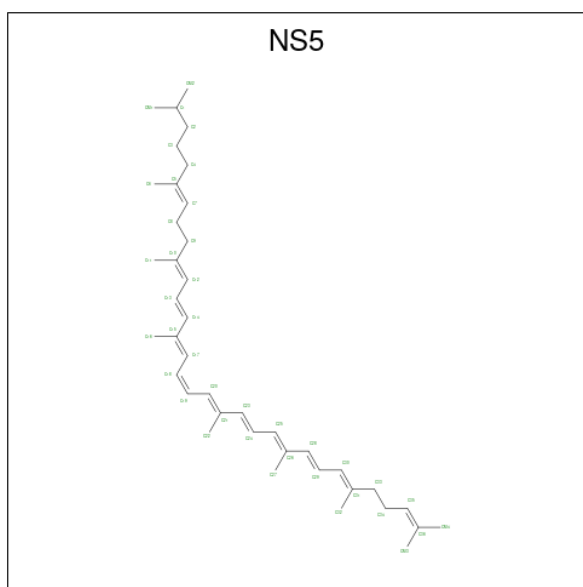
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



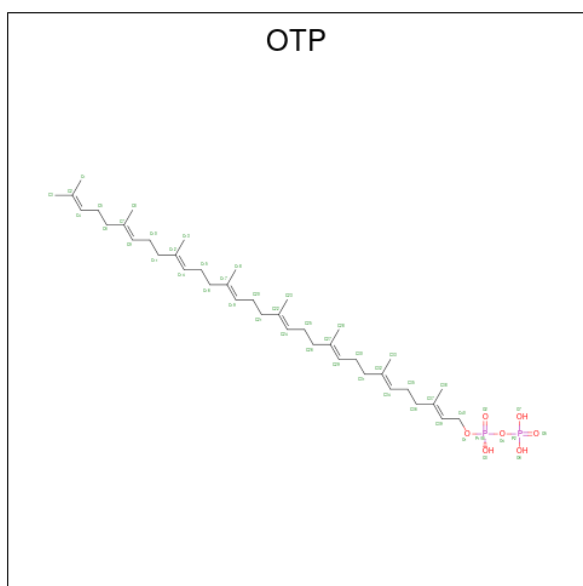
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 48 46 2	0	0

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



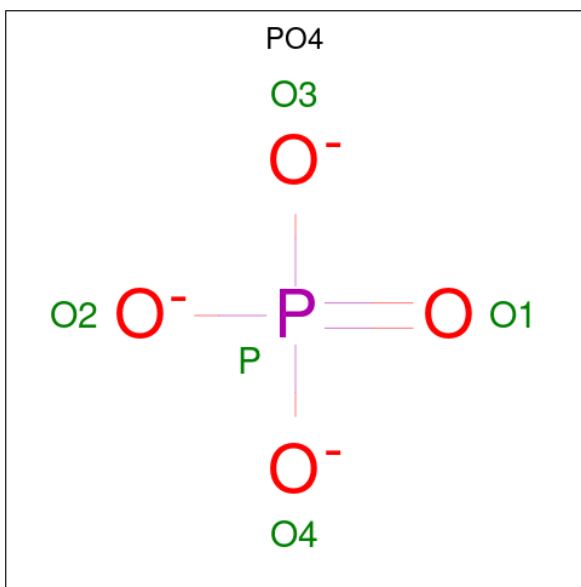
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	C	0	0
			40	40		

- Molecule 13 is (2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLDOT RIACONTA-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	0	0
			41	40	1		

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

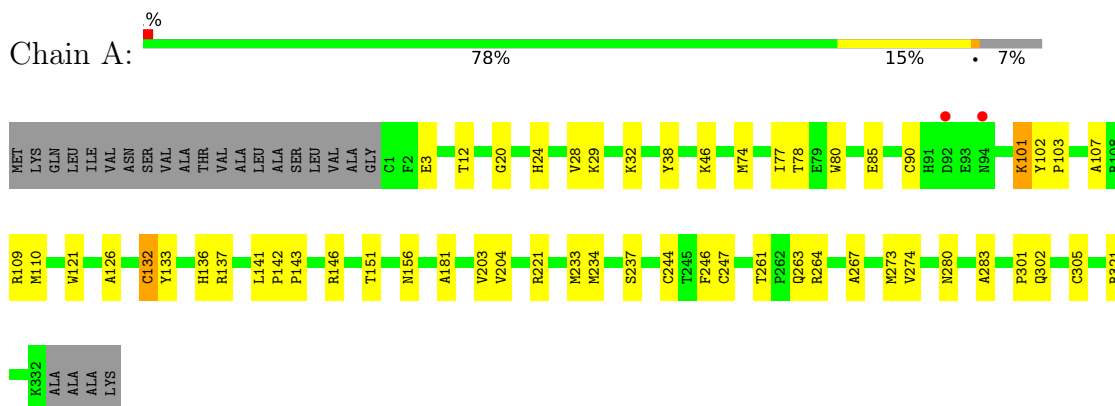


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	O	P	0	0
			5	4	1		
14	C	1	Total	O	P	0	0
			5	4	1		

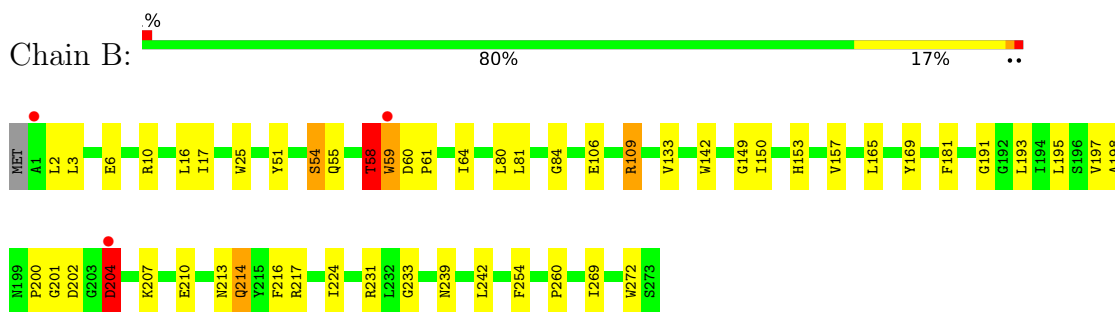
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

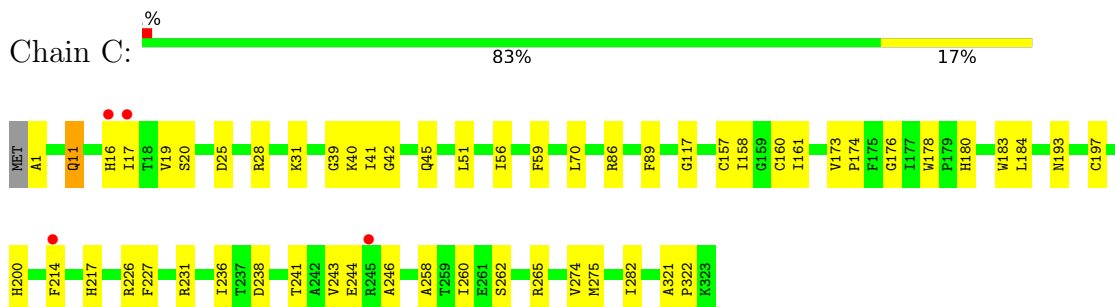
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- Molecule 2: Reaction center protein L chain

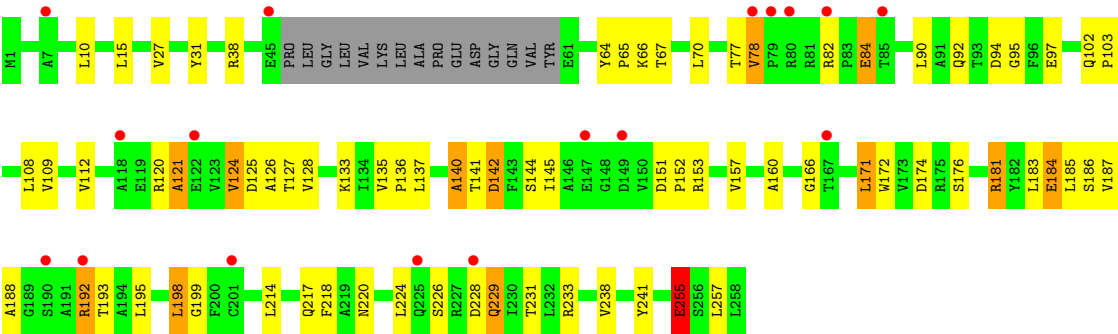


- Molecule 3: Reaction center protein M chain



- Molecule 4: Reaction center protein H chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.60Å 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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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(°)	Ideal(°)
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(°)	Ideal(°)
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 ⓘ

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:HBBB	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 ⓘ

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 ⓘ

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	D	1	4	8,9,10	0.95	0	8,9,11	0.95	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	$\# Z > 2$
7	BCL	B	303	-	69,74,74	1.12	4 (5%)	79,115,115	1.38	9 (11%)
5	HEC	A	404	1	46,50,50	2.05	8 (17%)	58,82,82	1.14	4 (6%)
9	MPG	C	407	-	16,16,24	0.84	0	15,15,25	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MQ7	C	404	-	49,49,49	1.84	10 (20%)	61,63,63	1.66	16 (26%)
14	PO4	C	408	-	4,4,4	0.92	0	6,6,6	0.48	0
7	BCL	B	302	-	69,74,74	1.17	6 (8%)	79,115,115	1.37	8 (10%)
5	HEC	A	403	1	46,50,50	2.02	6 (13%)	58,82,82	1.10	2 (3%)
7	BCL	B	301	-	68,73,74	1.18	5 (7%)	77,113,115	1.33	7 (9%)
8	BPB	C	402	-	53,66,70	1.24	7 (13%)	50,96,101	2.16	12 (24%)
7	BCL	C	401	-	69,74,74	1.18	4 (5%)	79,115,115	1.49	11 (13%)
5	HEC	A	401	1	46,50,50	2.01	7 (15%)	58,82,82	1.18	4 (6%)
5	HEC	A	402	1	46,50,50	2.00	7 (15%)	58,82,82	1.16	3 (5%)
6	DGA	A	405	-	36,36,43	1.26	3 (8%)	38,38,45	3.15	6 (15%)
14	PO4	C	409	-	4,4,4	0.96	0	6,6,6	0.45	0
8	BPB	B	304	-	57,70,70	1.12	5 (8%)	55,101,101	1.93	10 (18%)
9	MPG	B	306	-	24,24,24	1.28	1 (4%)	24,25,25	1.18	2 (8%)
12	NS5	C	405	-	39,39,39	2.07	12 (30%)	46,46,46	2.28	13 (28%)
13	OTP	C	406	-	40,40,48	0.72	0	47,47,61	1.77	14 (29%)
9	MPG	B	305	-	24,24,24	1.26	1 (4%)	24,25,25	1.41	3 (12%)

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
7	BCL	C	401	-	-	3/41/137/137	-
7	BCL	B	303	-	-	6/41/137/137	-
5	HEC	A	404	1	-	2/14/54/54	-
5	HEC	A	401	1	-	4/14/54/54	-
8	BPB	B	304	-	-	3/37/105/105	0/5/6/6
9	MPG	B	306	-	-	10/25/25/25	-
9	MPG	C	407	-	-	8/14/14/25	-
11	MQ7	C	404	-	-	3/41/61/61	0/2/2/2
8	BPB	C	402	-	-	7/33/101/105	0/5/6/6
7	BCL	B	302	-	-	3/41/137/137	-
5	HEC	A	403	1	-	0/14/54/54	-
12	NS5	C	405	-	-	16/43/43/43	-
13	OTP	C	406	-	-	13/45/45/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	402	1	-	5/14/54/54	-
6	DGA	A	405	-	-	13/37/37/45	-
9	MPG	B	305	-	-	16/25/25/25	-
7	BCL	B	301	-	-	8/40/136/137	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	404	MQ7	C3-C2	7.31	1.48	1.35
5	A	404	HEC	CAB-C3B	6.81	1.57	1.35
5	A	403	HEC	CAB-C3B	6.47	1.56	1.35
5	A	402	HEC	CAC-C3C	6.42	1.55	1.35
5	A	401	HEC	CAB-C3B	6.30	1.55	1.35
5	A	403	HEC	CAC-C3C	6.29	1.55	1.35
5	A	404	HEC	CAC-C3C	6.24	1.55	1.35
5	A	401	HEC	CAC-C3C	6.21	1.55	1.35
5	A	402	HEC	CAB-C3B	6.21	1.55	1.35
5	A	404	HEC	C3D-C2D	5.75	1.53	1.38
5	A	403	HEC	C3D-C2D	5.67	1.53	1.38
5	A	401	HEC	C3D-C2D	5.64	1.53	1.38
5	A	402	HEC	C3D-C2D	5.62	1.53	1.38
7	B	301	BCL	MG-NA	4.96	2.18	2.06
9	B	305	MPG	O1-CX3	4.80	1.43	1.33
7	C	401	BCL	MG-NA	4.79	2.17	2.06
9	B	306	MPG	O1-CX3	4.74	1.43	1.33
7	B	302	BCL	MG-NA	4.69	2.17	2.06
7	B	303	BCL	MG-NA	4.60	2.17	2.06
12	C	405	NS5	C14-C15	4.22	1.55	1.46
5	A	401	HEC	CBC-CAC	-4.15	1.34	1.49
5	A	403	HEC	CBC-CAC	-4.14	1.34	1.49
5	A	402	HEC	CBB-CAB	-4.13	1.34	1.49
11	C	404	MQ7	C5-C4	4.11	1.56	1.48
5	A	401	HEC	CBB-CAB	-4.11	1.34	1.49
5	A	404	HEC	CBC-CAC	-4.10	1.34	1.49
5	A	402	HEC	CBC-CAC	-4.07	1.34	1.49
5	A	403	HEC	CBB-CAB	-4.04	1.34	1.49
12	C	405	NS5	C19-C20	3.89	1.55	1.43
11	C	404	MQ7	C10-C1	3.87	1.55	1.48
8	C	402	BPB	CBD-CGD	-3.83	1.47	1.52
5	A	404	HEC	CBB-CAB	-3.76	1.35	1.49
6	A	405	DGA	OG1-CA1	3.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	304	BPB	CBD-CGD	-3.68	1.47	1.52
6	A	405	DGA	CG1-CG2	3.59	1.58	1.50
6	A	405	DGA	OG2-CB1	3.55	1.44	1.34
12	C	405	NS5	C23-C21	3.46	1.53	1.46
12	C	405	NS5	C18-C17	3.44	1.53	1.43
7	B	302	BCL	MG-NC	3.42	2.14	2.06
8	C	402	BPB	C3B-C4B	3.41	1.47	1.41
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	C29-C30	3.35	1.53	1.43
12	C	405	NS5	C28-C26	3.35	1.53	1.46
12	C	405	NS5	C24-C25	3.32	1.53	1.43
7	C	401	BCL	C3B-C4B	3.31	1.47	1.41
8	B	304	BPB	C3B-C4B	3.18	1.46	1.41
12	C	405	NS5	C4-C5	3.06	1.57	1.51
12	C	405	NS5	C13-C12	3.06	1.52	1.43
8	C	402	BPB	C3D-CAD	-3.03	1.42	1.47
7	B	303	BCL	C3B-C4B	2.92	1.46	1.41
8	B	304	BPB	C3D-CAD	-2.91	1.42	1.47
11	C	404	MQ7	C20-C18	2.87	1.57	1.51
7	C	401	BCL	MG-NC	2.83	2.13	2.06
7	B	301	BCL	C3B-C4B	2.76	1.46	1.41
7	B	302	BCL	C3B-C4B	2.74	1.46	1.41
12	C	405	NS5	C7-C5	2.71	1.39	1.33
8	C	402	BPB	C1D-C2D	2.67	1.42	1.39
7	B	301	BCL	CHD-C1D	2.53	1.43	1.38
7	B	302	BCL	CHD-C1D	2.53	1.43	1.38
7	C	401	BCL	CHD-C1D	2.52	1.43	1.38
7	B	303	BCL	CHD-C1D	2.50	1.43	1.38
12	C	405	NS5	C33-C31	2.50	1.56	1.51
11	C	404	MQ7	C17-C18	2.48	1.38	1.33
11	C	404	MQ7	C27-C28	2.48	1.38	1.33
11	C	404	MQ7	C12-C13	2.44	1.38	1.33
11	C	404	MQ7	C22-C23	2.35	1.38	1.33
11	C	404	MQ7	C32-C33	2.34	1.38	1.33
8	C	402	BPB	CHA-CBD	2.32	1.54	1.51
7	B	302	BCL	C1D-C2D	-2.26	1.40	1.45
12	C	405	NS5	C13-C14	2.25	1.40	1.34
8	B	304	BPB	CHA-CBD	2.23	1.54	1.51
8	B	304	BPB	OBD-CAD	2.21	1.25	1.22
5	A	404	HEC	CMA-C3A	2.17	1.55	1.50
8	C	402	BPB	OBD-CAD	2.16	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	402	BPB	C3A-C2A	-2.13	1.52	1.54
5	A	403	HEC	CMA-C3A	2.09	1.55	1.50
7	B	301	BCL	OBD-CAD	2.08	1.26	1.22
5	A	401	HEC	CMB-C2B	2.07	1.55	1.50
11	C	404	MQ7	C11-C3	2.04	1.55	1.51
7	B	302	BCL	OBD-CAD	2.03	1.26	1.22
5	A	401	HEC	CMA-C3A	2.02	1.54	1.50
5	A	404	HEC	CMB-C2B	2.02	1.54	1.50
5	A	402	HEC	CMC-C2C	2.02	1.54	1.50
5	A	404	HEC	CMD-C2D	2.00	1.54	1.50
5	A	402	HEC	CMA-C3A	2.00	1.54	1.50

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	DGA	OG2-CG2-CG3	-13.34	78.07	107.96
8	B	304	BPB	C4D-CHA-CBD	-10.18	103.57	108.45
6	A	405	DGA	OG2-CG2-CG1	-9.77	83.73	106.21
8	C	402	BPB	C4D-CHA-CBD	-9.41	103.94	108.45
6	A	405	DGA	CG3-CG2-CG1	7.19	132.91	112.69
12	C	405	NS5	C18-C17-C15	-6.75	117.81	127.28
12	C	405	NS5	C29-C30-C31	-6.59	118.42	127.69
12	C	405	NS5	C19-C20-C21	-5.57	119.47	127.28
8	C	402	BPB	C1-C2-C3	-5.41	117.34	126.20
7	C	401	BCL	C4D-CHA-C1A	5.40	127.68	121.24
7	B	302	BCL	C4D-CHA-C1A	5.35	127.62	121.24
7	B	301	BCL	C4D-CHA-C1A	5.23	127.48	121.24
7	B	303	BCL	C4D-CHA-C1A	4.85	127.02	121.24
9	B	305	MPG	O1-CX3-CXD	4.84	122.98	111.78
12	C	405	NS5	C13-C12-C10	-4.50	121.36	127.69
13	C	406	OTP	C33-C32-C31	4.47	122.99	115.23
7	C	401	BCL	CHD-C1D-ND	-4.40	118.61	124.80
8	C	402	BPB	C4D-ND-C1D	-4.20	103.84	108.87
7	B	303	BCL	C1D-ND-C4D	-4.17	103.39	106.31
7	C	401	BCL	C4A-NA-C1A	4.14	108.57	106.68
9	B	306	MPG	O1-CX3-CXD	4.04	121.12	111.78
8	B	304	BPB	C4D-ND-C1D	-4.00	104.08	108.87
7	B	303	BCL	CHD-C1D-ND	-3.89	119.33	124.80
7	B	301	BCL	C1D-ND-C4D	-3.77	103.67	106.31
7	B	301	BCL	CHD-C1D-ND	-3.75	119.52	124.80
12	C	405	NS5	C11-C10-C9	3.72	121.68	115.23
8	C	402	BPB	C3D-C4D-ND	3.70	112.45	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	401	BCL	CHA-C1A-NA	-3.61	118.22	126.39
7	C	401	BCL	C2A-C1A-CHA	3.59	130.10	123.87
7	B	302	BCL	CHD-C1D-ND	-3.58	119.76	124.80
7	C	401	BCL	C1D-ND-C4D	-3.56	103.82	106.31
5	A	402	HEC	C4D-ND-C1D	3.52	111.55	105.82
5	A	404	HEC	C4D-ND-C1D	3.46	111.46	105.82
8	B	304	BPB	C3D-C4D-ND	3.44	112.12	107.71
11	C	404	MQ7	C31-C32-C33	-3.43	119.77	127.62
11	C	404	MQ7	C19-C18-C20	3.42	121.16	115.23
13	C	406	OTP	C15-C14-C12	-3.40	119.84	127.62
7	B	303	BCL	C4A-NA-C1A	3.39	108.22	106.68
5	A	403	HEC	C4D-ND-C1D	3.39	111.34	105.82
5	A	401	HEC	C4D-ND-C1D	3.36	111.29	105.82
6	A	405	DGA	OG1-CA1-CA2	3.31	121.93	111.83
11	C	404	MQ7	C26-C27-C28	-3.30	120.06	127.62
12	C	405	NS5	C24-C25-C26	-3.26	122.70	127.28
7	B	302	BCL	CHA-C1A-NA	-3.26	119.02	126.39
8	C	402	BPB	OBD-CAD-CBD	-3.25	121.06	125.82
13	C	406	OTP	C28-C27-C26	3.24	120.85	115.23
11	C	404	MQ7	C16-C17-C18	-3.20	120.29	127.62
7	B	302	BCL	C1-C2-C3	-3.20	120.95	126.20
8	B	304	BPB	OBD-CAD-CBD	-3.16	121.19	125.82
6	A	405	DGA	OG2-CB1-CB2	3.15	118.29	111.48
11	C	404	MQ7	C11-C12-C13	-3.13	121.44	126.83
7	B	301	BCL	CHA-C1A-NA	-3.11	119.35	126.39
13	C	406	OTP	C38-C37-C39	-3.07	115.73	123.63
7	B	302	BCL	C2A-C1A-CHA	3.06	129.18	123.87
11	C	404	MQ7	C14-C13-C15	3.05	120.52	115.23
9	B	305	MPG	O1-CX3-O4	-3.00	118.65	124.14
13	C	406	OTP	C13-C12-C11	2.99	120.42	115.23
7	B	302	BCL	C1D-ND-C4D	-2.97	104.23	106.31
13	C	406	OTP	C8-C7-C6	2.96	120.36	115.23
11	C	404	MQ7	C39-C38-C40	2.93	120.32	115.23
7	B	303	BCL	CHA-C1A-NA	-2.92	119.77	126.39
7	B	301	BCL	C1-C2-C3	-2.91	121.42	126.20
11	C	404	MQ7	C21-C22-C23	-2.91	120.96	127.62
7	B	303	BCL	C2A-C1A-CHA	2.90	128.89	123.87
12	C	405	NS5	C6-C5-C4	2.87	120.21	115.23
13	C	406	OTP	C10-C9-C7	-2.86	121.08	127.62
11	C	404	MQ7	C11-C3-C2	-2.82	120.06	124.89
7	B	302	BCL	C4A-NA-C1A	2.81	107.96	106.68
8	B	304	BPB	C2D-C1D-ND	2.71	111.39	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	BPB	O2D-CGD-CBD	2.63	113.84	110.95
5	A	403	HEC	C2A-C1A-NA	-2.58	107.83	110.32
11	C	404	MQ7	C34-C33-C35	2.57	119.69	115.23
13	C	406	OTP	C23-C22-C21	2.56	119.68	115.23
11	C	404	MQ7	C29-C28-C30	2.56	119.68	115.23
8	C	402	BPB	C11-C10-C8	2.55	124.45	115.97
5	A	402	HEC	C2A-C1A-NA	-2.55	107.86	110.32
8	C	402	BPB	C2D-C1D-ND	2.54	111.27	109.43
12	C	405	NS5	C13-C14-C15	-2.52	119.45	126.36
12	C	405	NS5	C32-C31-C33	2.51	119.58	115.23
7	B	301	BCL	C2A-C1A-CHA	2.48	128.18	123.87
11	C	404	MQ7	C36-C37-C38	-2.48	121.94	127.62
11	C	404	MQ7	C24-C23-C25	2.46	119.50	115.23
5	A	404	HEC	C2A-C1A-NA	-2.44	107.97	110.32
5	A	401	HEC	CBD-CAD-C3D	-2.43	105.82	112.53
9	B	306	MPG	O1-CX3-O4	-2.42	119.72	124.14
8	B	304	BPB	O2D-CGD-CBD	2.39	113.57	110.95
7	B	303	BCL	CMB-C2B-C1B	-2.38	121.80	125.42
7	C	401	BCL	C4D-C3D-CAD	-2.36	105.54	108.11
5	A	401	HEC	C2A-C1A-NA	-2.34	108.07	110.32
11	C	404	MQ7	C2M-C2-C3	-2.32	120.64	124.45
13	C	406	OTP	C18-C17-C16	2.32	119.25	115.23
8	C	402	BPB	OBB-CAB-C3B	2.30	123.84	119.99
8	B	304	BPB	CMD-C2D-C3D	2.30	129.28	124.68
11	C	404	MQ7	C45-C43-C44	2.30	119.88	114.59
7	C	401	BCL	CMB-C2B-C1B	-2.30	121.92	125.42
12	C	405	NS5	C34-C35-C36	-2.28	120.04	127.64
7	B	301	BCL	C4A-NA-C1A	2.27	107.71	106.68
13	C	406	OTP	C30-C29-C27	-2.26	122.46	127.62
7	B	302	BCL	CAB-C3B-C2B	2.24	132.39	127.74
7	B	303	BCL	OBB-CAB-CBB	-2.24	114.76	119.77
11	C	404	MQ7	C41-C42-C43	-2.23	120.21	127.64
12	C	405	NS5	CM4-C36-CM3	2.21	119.68	114.59
12	C	405	NS5	C24-C23-C21	-2.20	120.32	126.36
8	C	402	BPB	CMB-C2B-C3B	2.20	129.08	124.68
7	B	303	BCL	CAB-C3B-C2B	2.19	132.29	127.74
8	C	402	BPB	CMD-C2D-C3D	2.19	129.05	124.68
13	C	406	OTP	C1-C2-C3	2.18	119.60	114.59
13	C	406	OTP	C18-C17-C19	-2.18	118.04	123.63
12	C	405	NS5	C25-C24-C23	-2.17	116.92	123.20
9	B	305	MPG	O4-CX3-CXD	-2.15	118.36	123.56
5	A	401	HEC	CAA-CBA-CGA	-2.13	108.01	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	401	BCL	C1C-NC-C4C	2.13	107.65	106.68
7	C	401	BCL	CHD-C1D-C2D	2.12	129.90	125.49
8	B	304	BPB	CMB-C2B-C3B	2.12	128.91	124.68
8	B	304	BPB	OBB-CAB-CBB	-2.09	115.73	120.19
5	A	402	HEC	CBA-CAA-C2A	-2.09	106.77	112.53
6	A	405	DGA	OG1-CG1-CG2	2.08	114.28	108.35
5	A	404	HEC	CHD-C4C-NC	2.08	126.72	124.45
8	C	402	BPB	OBB-CAB-CBB	-2.07	115.77	120.19
7	C	401	BCL	CAB-C3B-C2B	2.07	132.05	127.74
13	C	406	OTP	C25-C24-C22	-2.06	122.91	127.62
13	C	406	OTP	C38-C37-C36	2.05	118.78	115.23
5	A	404	HEC	CMC-C2C-C1C	-2.04	122.31	125.42
8	B	304	BPB	C6-C5-C3	2.00	118.34	113.47

There are no chirality outliers.

All (120) 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
12	C	405	NS5	C20-C21-C23-C24
12	C	405	NS5	C25-C26-C28-C29
12	C	405	NS5	C27-C26-C28-C29
13	C	406	OTP	C15-C16-C17-C18
12	C	405	NS5	C2-C3-C4-C5
7	B	302	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	C	402	BPB	C4-C3-C5-C6
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
13	C	406	OTP	C14-C15-C16-C17
12	C	405	NS5	C28-C29-C30-C31
12	C	405	NS5	C11-C10-C9-C8
8	C	402	BPB	C2-C3-C5-C6
12	C	405	NS5	C22-C21-C23-C24
9	B	305	MPG	C1-C2-C3-C4
13	C	406	OTP	C24-C25-C26-C27
13	C	406	OTP	C19-C20-C21-C22
9	B	306	MPG	O4-CX3-O1-C1
7	B	302	BCL	C15-C16-C17-C18
7	C	401	BCL	C2A-CAA-CBA-CGA
12	C	405	NS5	C3-C4-C5-C6
13	C	406	OTP	C9-C10-C11-C12
9	B	306	MPG	C3-C4-C5-C6
6	A	405	DGA	CA5-CA6-CA7-CA8
6	A	405	DGA	CBB-CAB-CB9-CB8
9	B	305	MPG	C2-C3-C4-C5
9	B	306	MPG	C11-C12-C13-C14
9	B	305	MPG	C10-C11-C12-C13
12	C	405	NS5	C3-C4-C5-C7
9	B	305	MPG	C5-C6-C7-C8
12	C	405	NS5	CM2-C1-C2-C3
7	B	301	BCL	C4-C3-C5-C6
9	B	306	MPG	CXD-CX3-O1-C1
6	A	405	DGA	CCB-CDB-CEB-CFB
5	A	404	HEC	C4D-C3D-CAD-CBD
6	A	405	DGA	CA7-CA8-CA9-CAA
9	C	407	MPG	C10-C11-C12-C13
9	B	306	MPG	C14-C15-C16-C17
12	C	405	NS5	CM1-C1-C2-C3
9	B	305	MPG	C6-C7-C8-C9
6	A	405	DGA	CEB-CFB-CGB-CHB
7	B	301	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	C	405	NS5	C1-C2-C3-C4
8	B	304	BPB	O2A-C1-C2-C3
9	C	407	MPG	C4-C5-C6-C7
7	B	303	BCL	C11-C12-C13-C14
9	B	306	MPG	C12-C13-C14-C15
6	A	405	DGA	CB6-CB7-CB8-CB9
7	B	303	BCL	C11-C12-C13-C15
8	B	304	BPB	C4-C3-C5-C6
8	B	304	BPB	C2-C3-C5-C6
8	C	402	BPB	C8-C10-C11-C12
6	A	405	DGA	CA3-CA4-CA5-CA6
6	A	405	DGA	CB9-CAB-CBB-CCB
9	C	407	MPG	C13-C14-C15-C16
11	C	404	MQ7	C38-C40-C41-C42
12	C	405	NS5	C31-C33-C34-C35
9	C	407	MPG	C2-C3-C4-C5
8	C	402	BPB	C11-C10-C8-C7
9	B	305	MPG	C12-C13-C14-C15
5	A	402	HEC	C3D-CAD-CBD-CGD
9	B	306	MPG	C2-C3-C4-C5
7	B	301	BCL	C14-C13-C15-C16
6	A	405	DGA	CB4-CB5-CB6-CB7
7	B	303	BCL	C16-C17-C18-C19
13	C	406	OTP	C35-C36-C37-C38
9	C	407	MPG	C6-C7-C8-C9
9	B	305	MPG	C15-C16-C17-C18
7	B	303	BCL	C16-C17-C18-C20
12	C	405	NS5	C10-C12-C13-C14
11	C	404	MQ7	C39-C38-C40-C41
12	C	405	NS5	C26-C28-C29-C30
9	B	305	MPG	O4-CX3-CXD-O2
11	C	404	MQ7	C37-C38-C40-C41
5	A	402	HEC	CAA-CBA-CGA-O2A
5	A	404	HEC	C2D-C3D-CAD-CBD
9	B	305	MPG	C13-C14-C15-C16
9	C	407	MPG	C12-C13-C14-C15
13	C	406	OTP	C35-C36-C37-C39
5	A	402	HEC	CAA-CBA-CGA-O1A
6	A	405	DGA	CA2-CA3-CA4-CA5
8	C	402	BPB	C6-C7-C8-C9
9	C	407	MPG	C7-C8-C9-C10
7	B	301	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	A	401	HEC	C3A-C2A-CAA-CBA
9	B	305	MPG	C7-C8-C9-C10
7	B	303	BCL	C15-C16-C17-C18
9	C	407	MPG	C9-C10-C11-C12
9	B	306	MPG	C7-C8-C9-C10
8	C	402	BPB	C6-C7-C8-C10
5	A	401	HEC	C1A-C2A-CAA-CBA
5	A	402	HEC	CAD-CBD-CGD-O1D
5	A	402	HEC	CAD-CBD-CGD-O2D
5	A	401	HEC	CAA-CBA-CGA-O2A
7	B	303	BCL	CAD-CBD-CGD-O2D
5	A	401	HEC	CAA-CBA-CGA-O1A

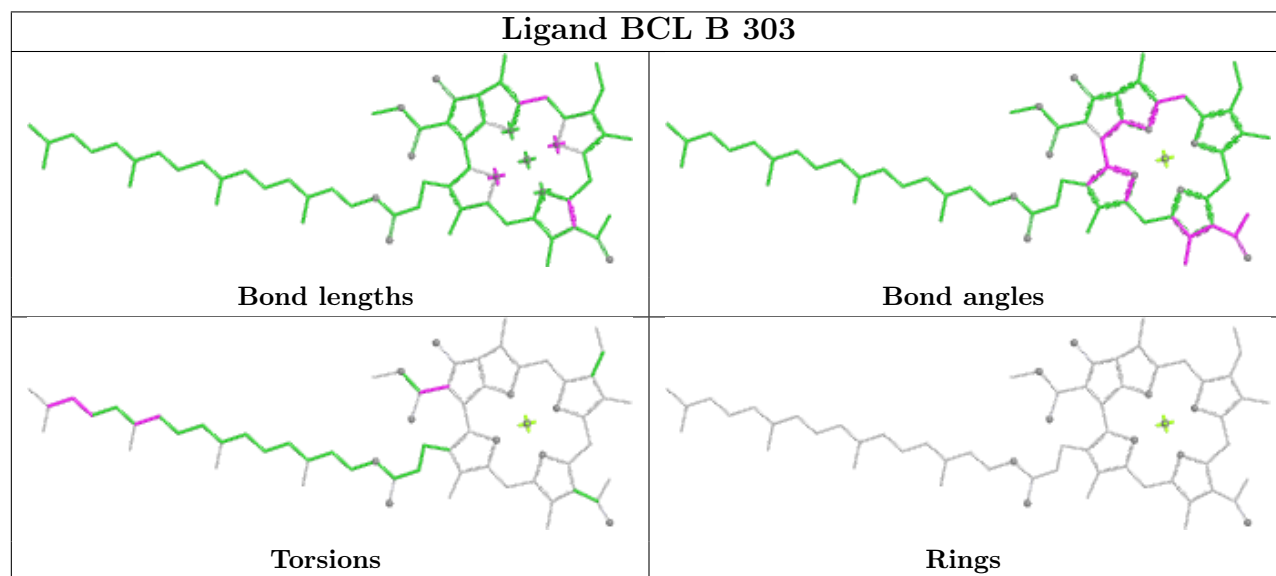
There are no ring outliers.

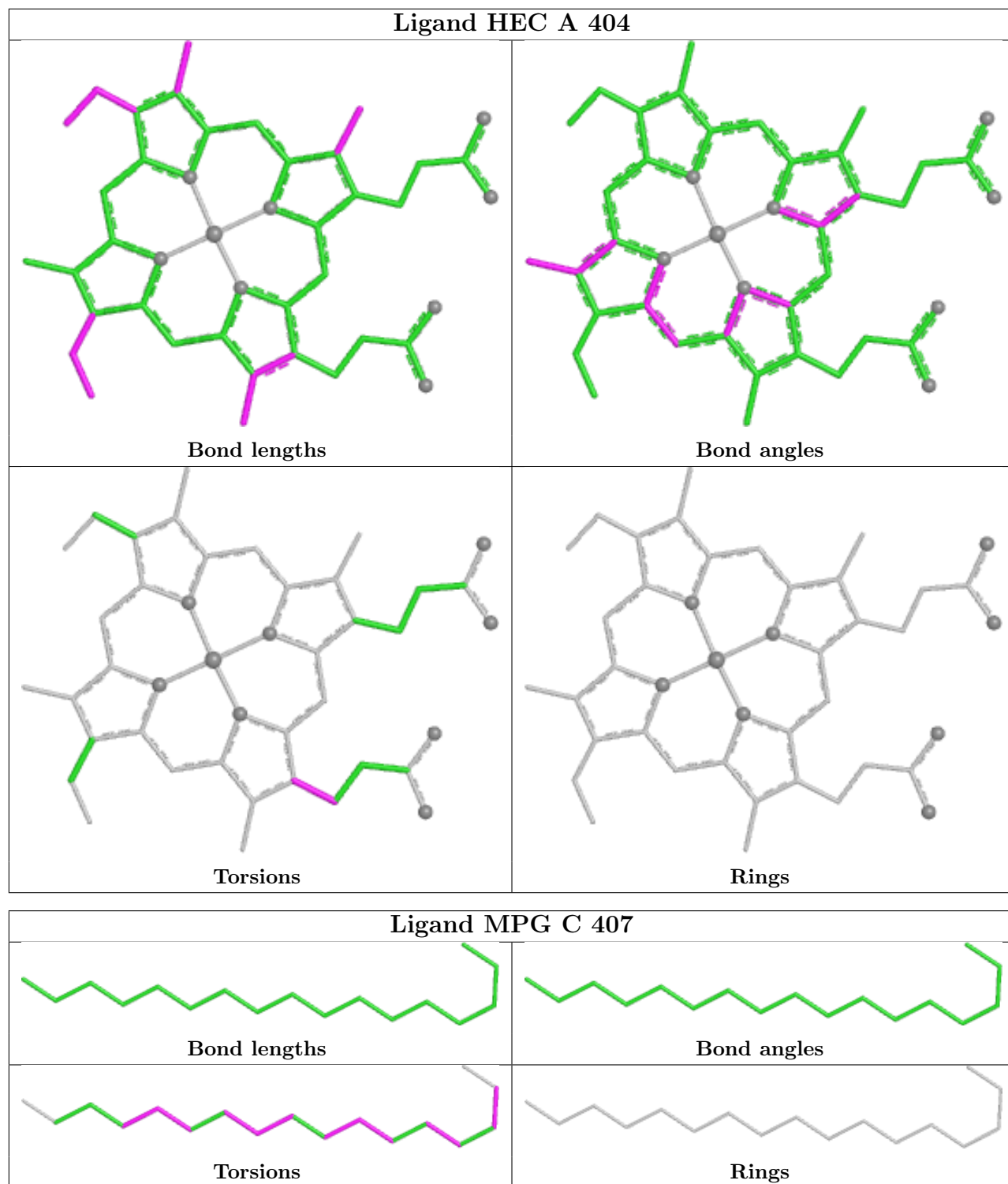
16 monomers are involved in 40 short contacts:

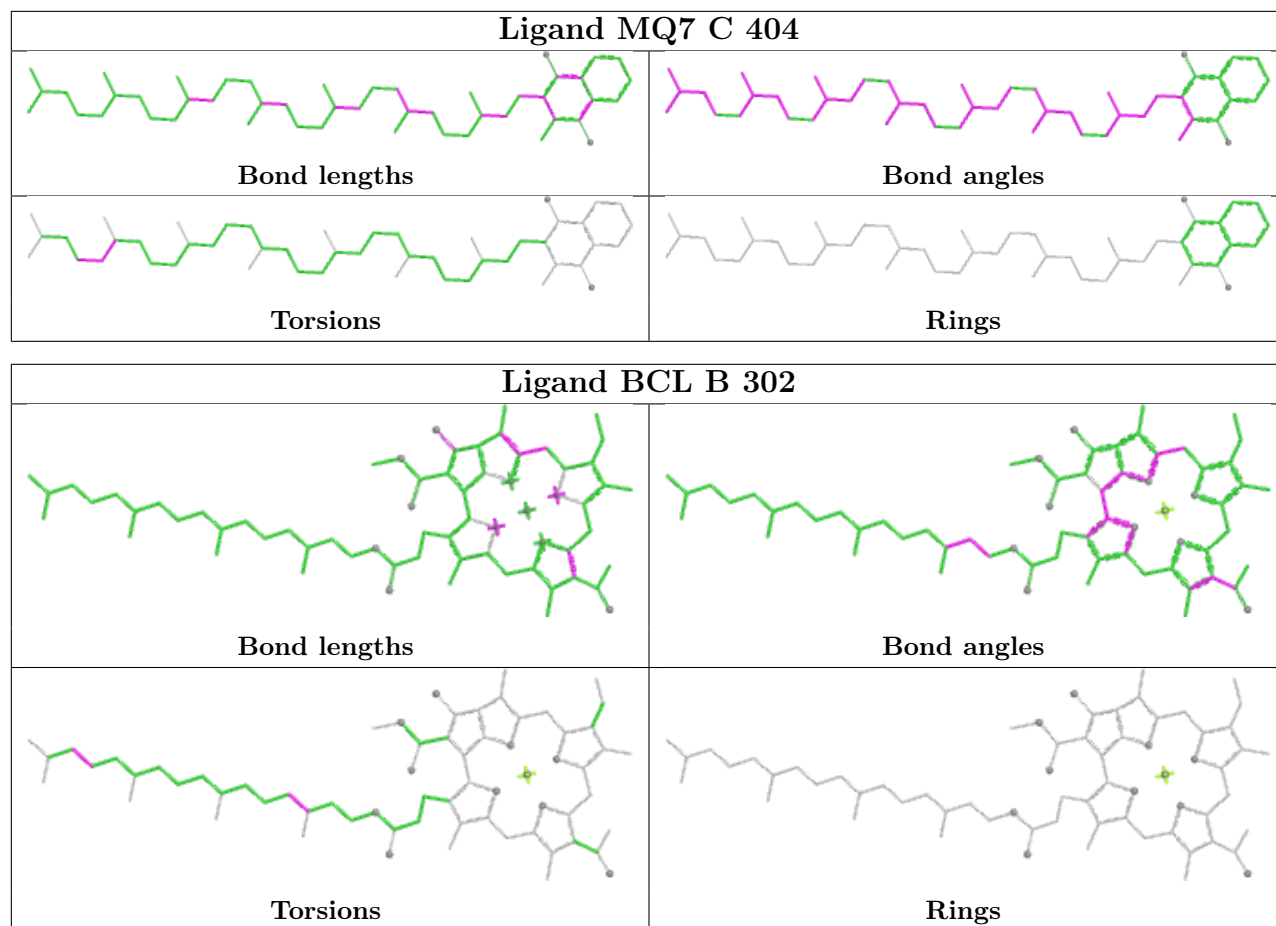
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	303	BCL	3	0
5	A	404	HEC	5	0
9	C	407	MPG	1	0
7	B	302	BCL	1	0
5	A	403	HEC	4	0
7	B	301	BCL	2	0
8	C	402	BPB	4	0
7	C	401	BCL	1	0
5	A	401	HEC	4	0
5	A	402	HEC	6	0
6	A	405	DGA	2	0
8	B	304	BPB	1	0
9	B	306	MPG	1	0
12	C	405	NS5	4	0
13	C	406	OTP	1	0
9	B	305	MPG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

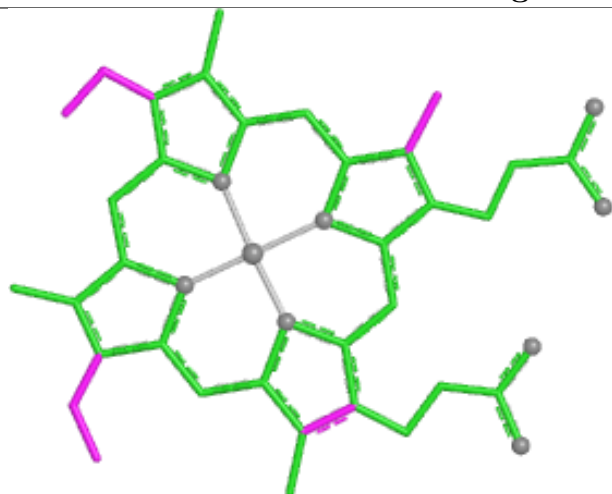
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



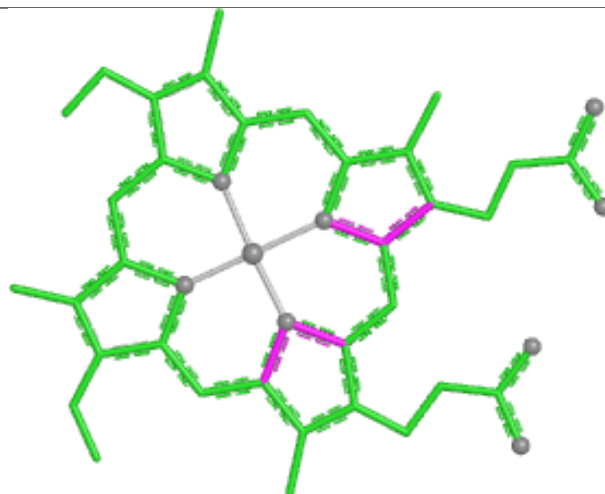




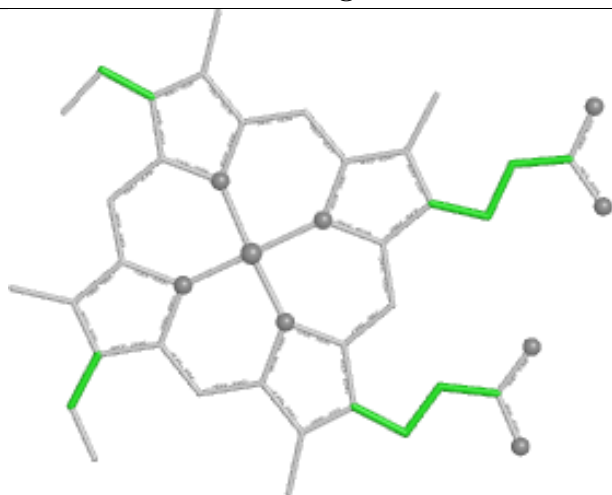
Ligand HEC A 403



Bond lengths



Bond angles

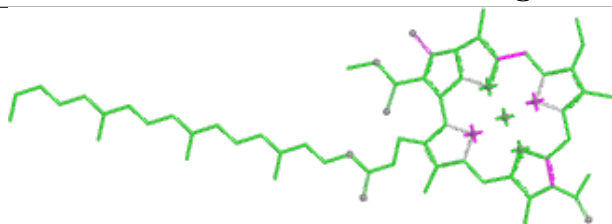


Torsions

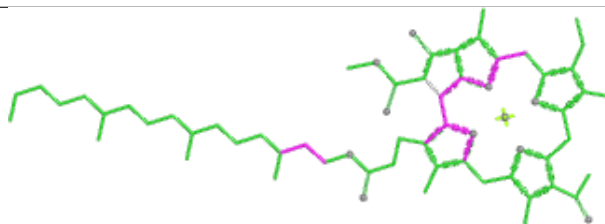


Rings

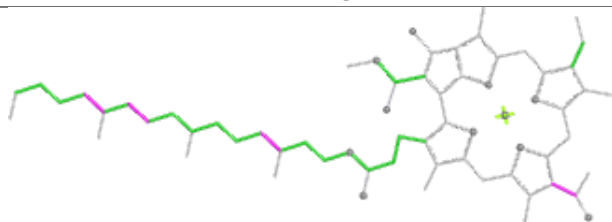
Ligand BCL B 301



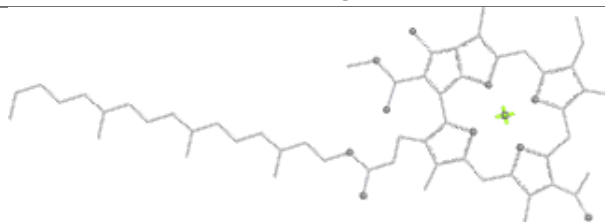
Bond lengths



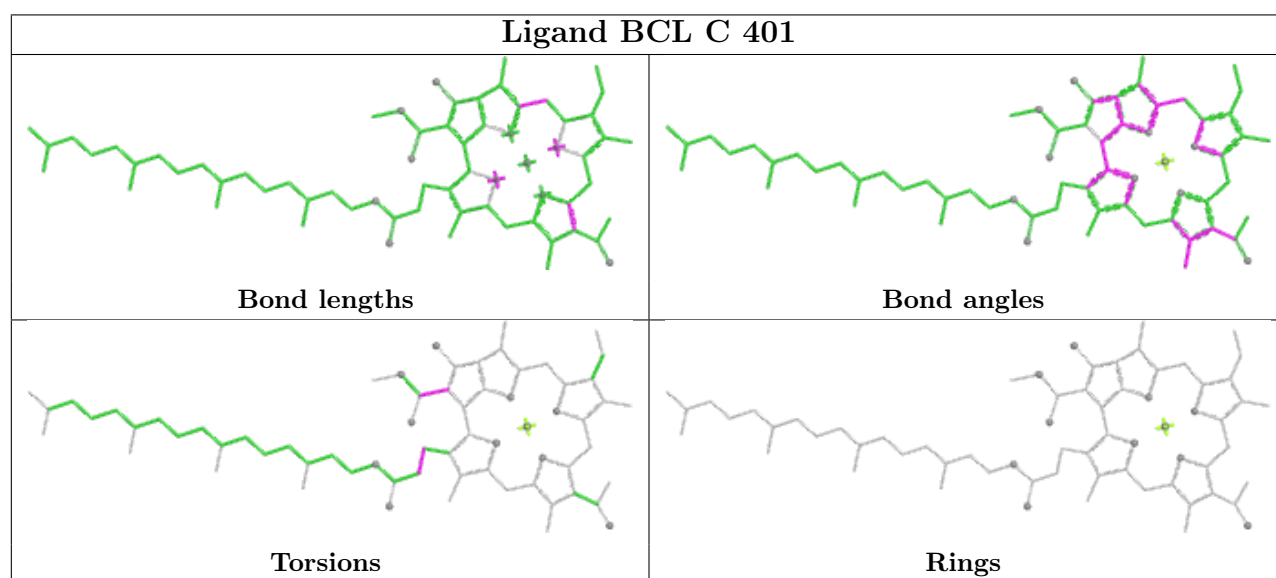
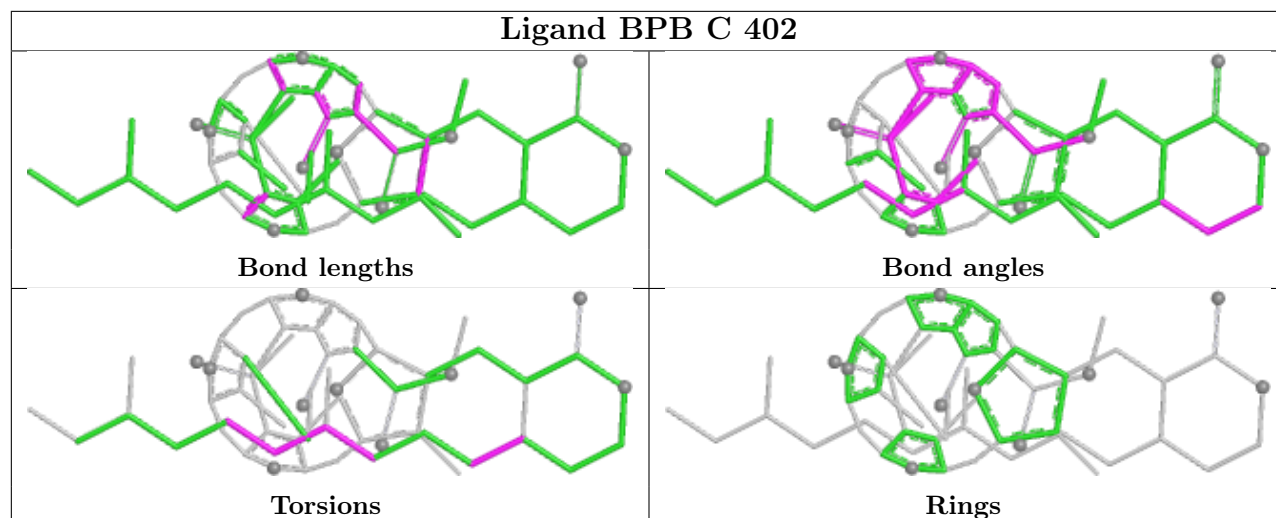
Bond angles



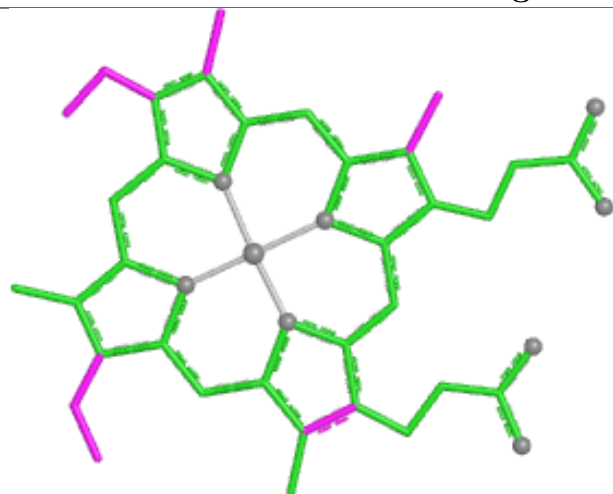
Torsions



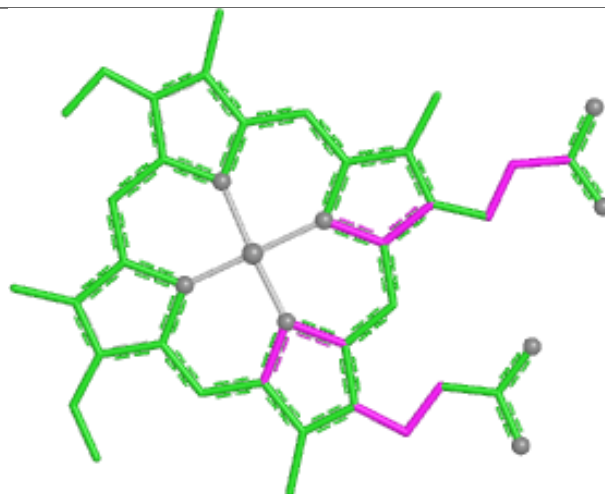
Rings



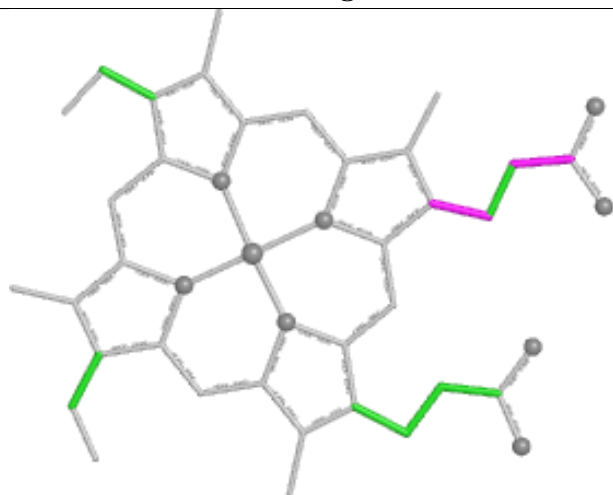
Ligand HEC A 401



Bond lengths



Bond angles

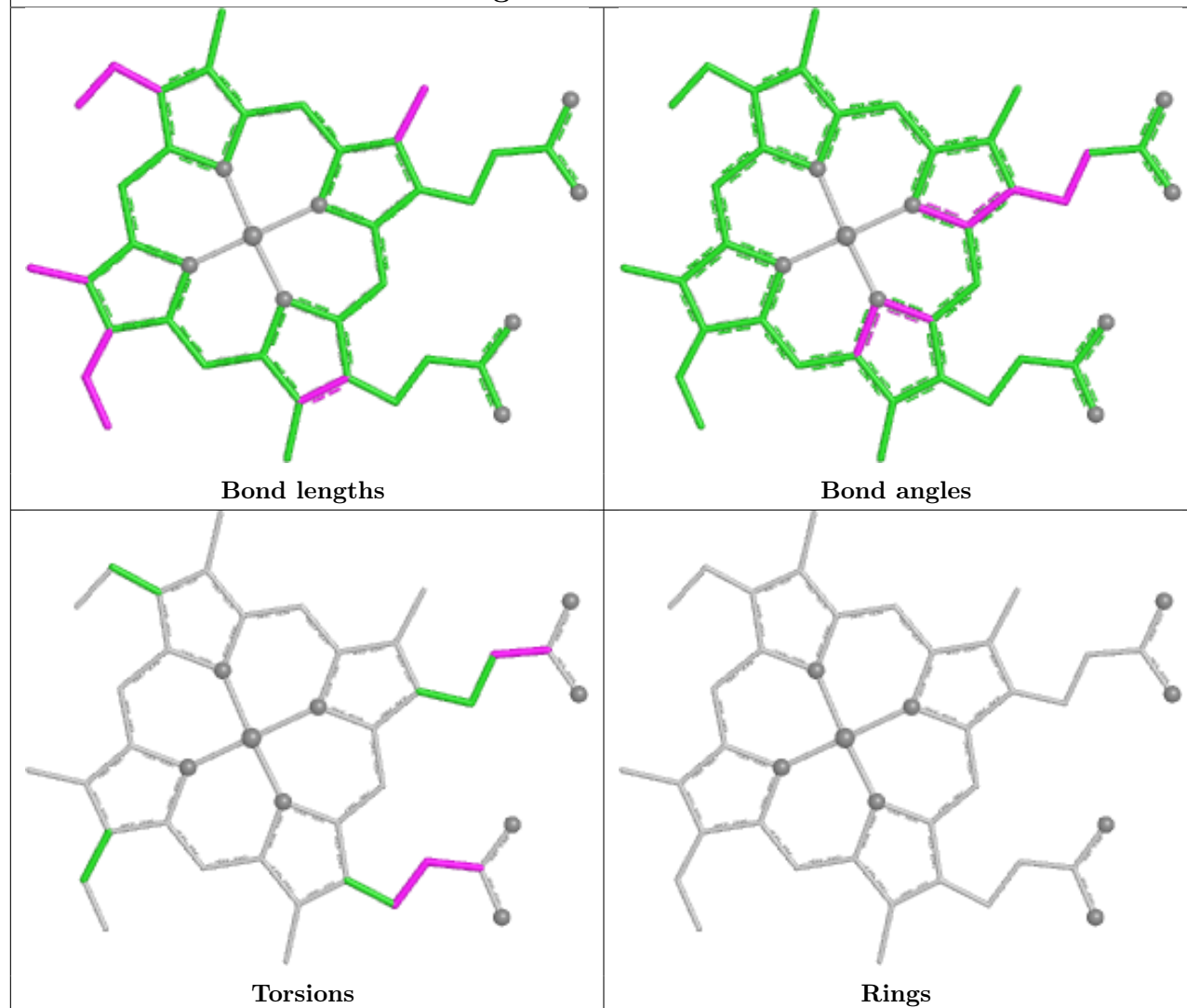


Torsions

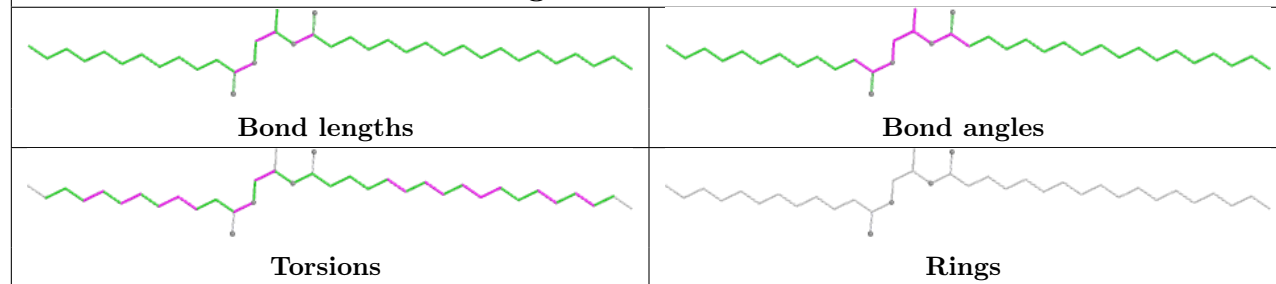


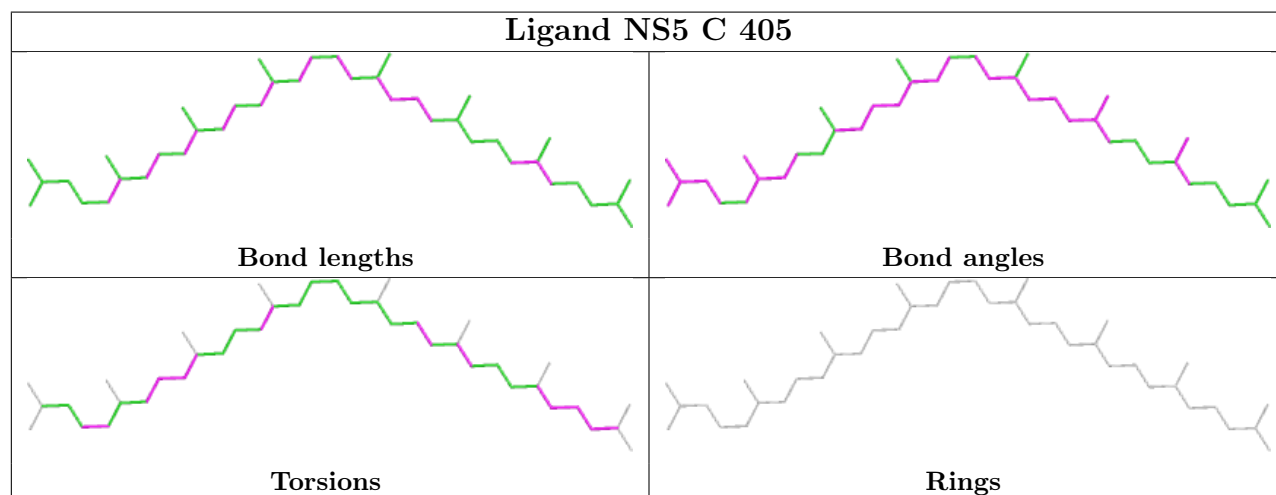
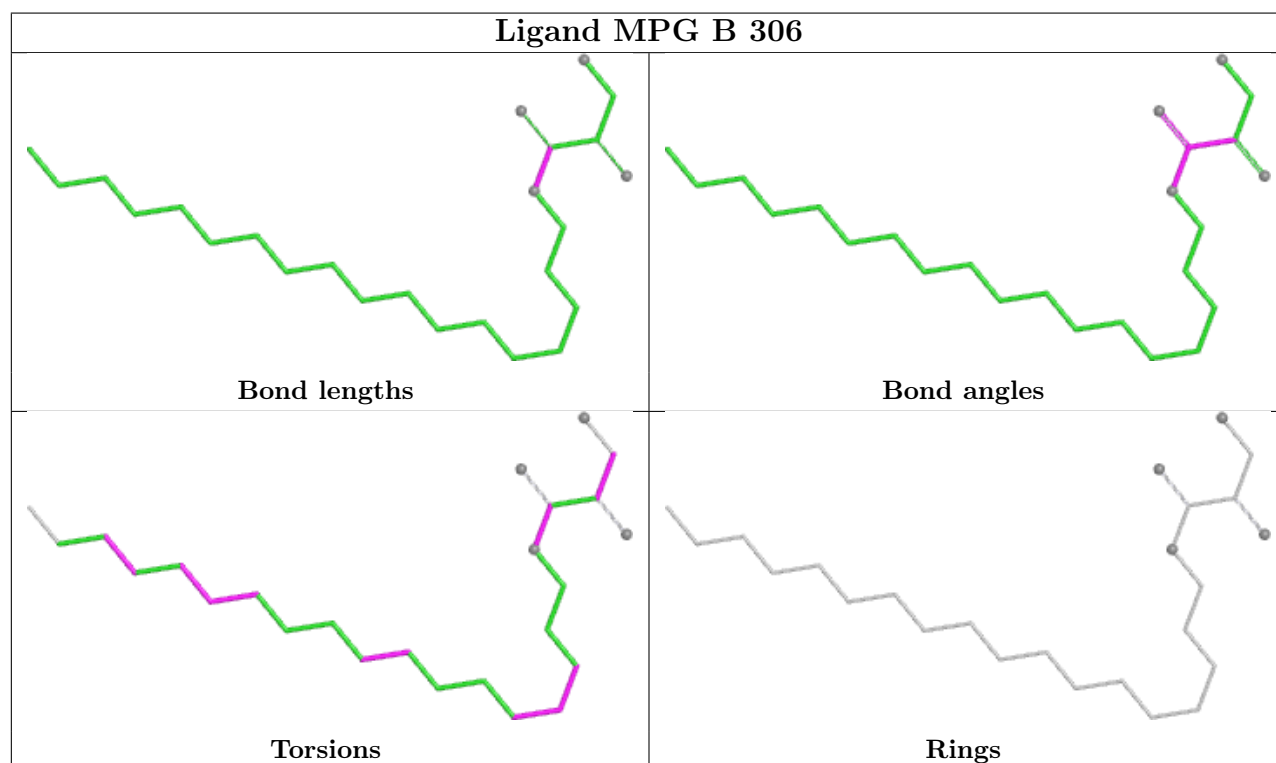
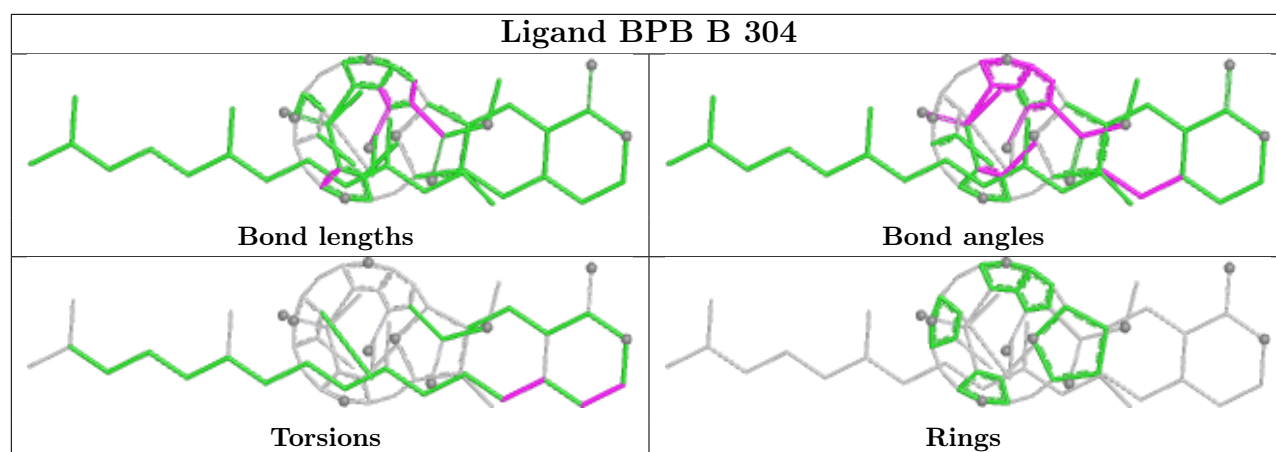
Rings

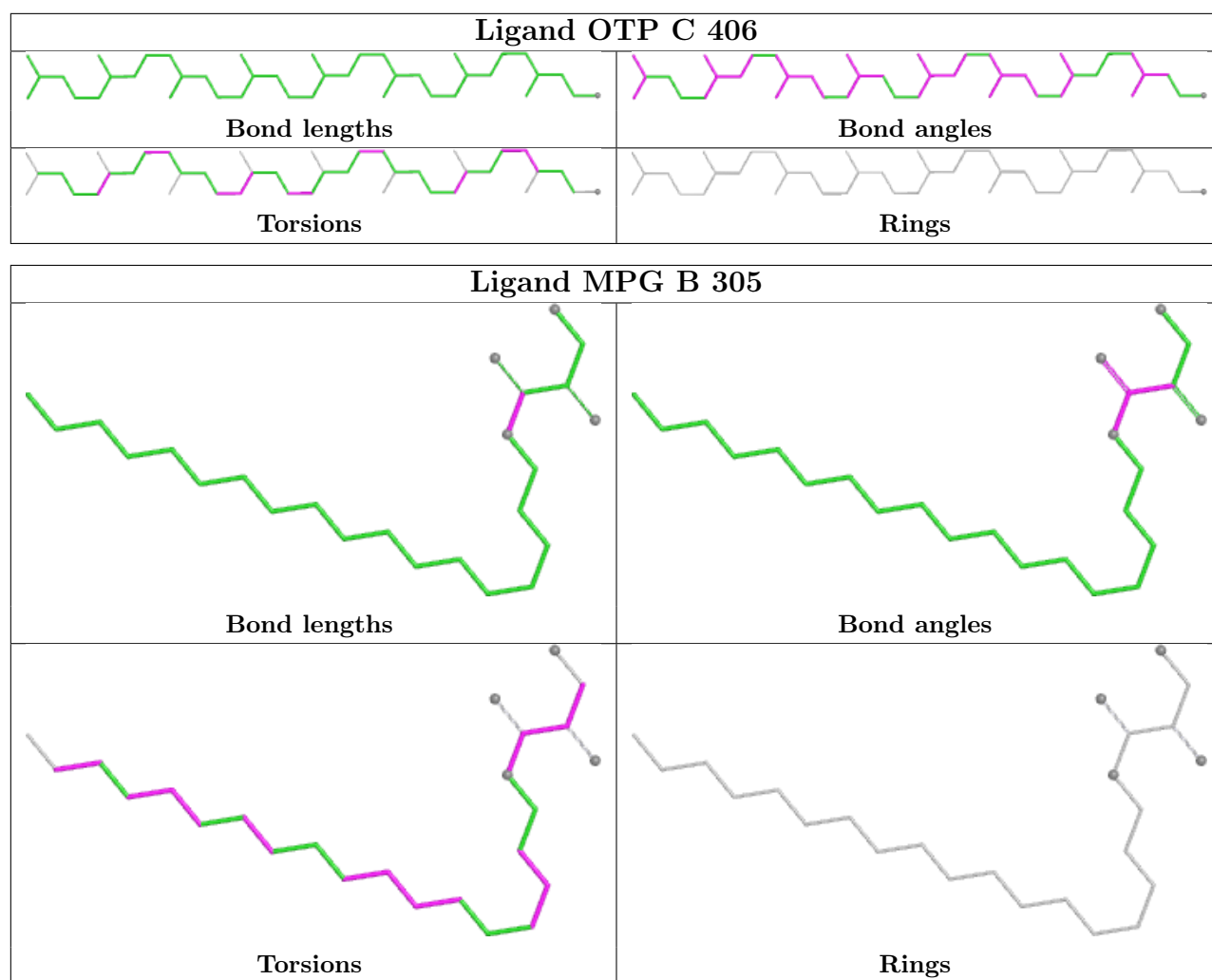
Ligand HEC A 402



Ligand DGA A 405







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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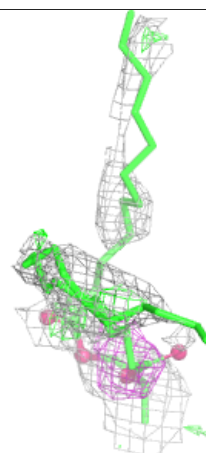
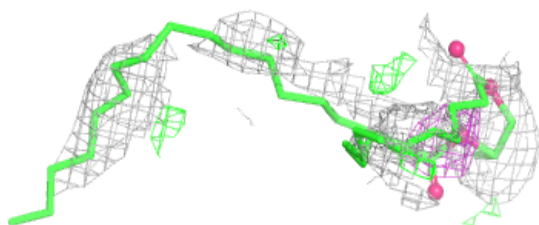
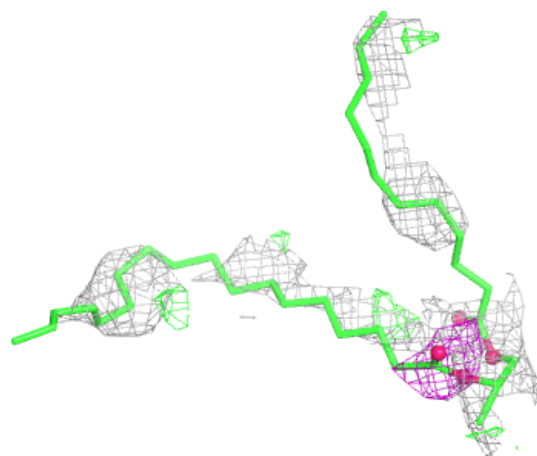
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BCL	B	303	66/66	0.93	0.14	56,64,74,79	0
7	BCL	C	401	66/66	0.93	0.15	54,64,72,74	0
8	BPB	B	304	65/65	0.94	0.13	57,71,79,80	0
5	HEC	A	403	43/43	0.96	0.14	30,54,56,56	0
5	HEC	A	402	43/43	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.

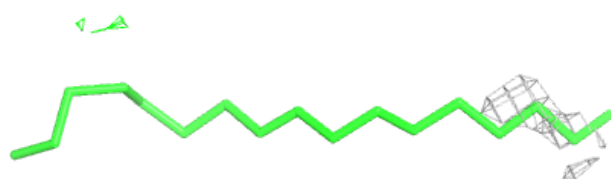
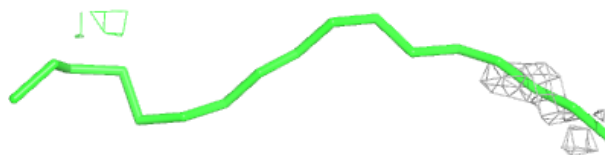
Electron density around DGA A 405:

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

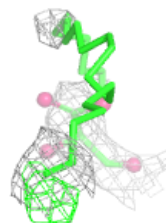
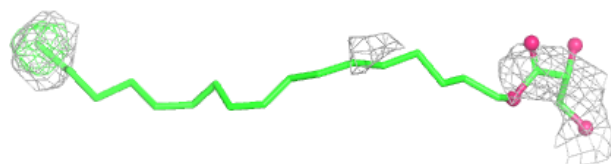
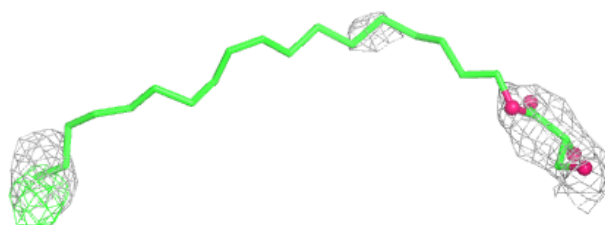


Electron density around MPG C 407:

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

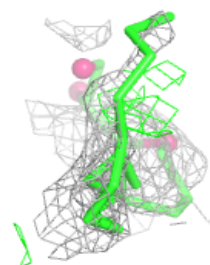
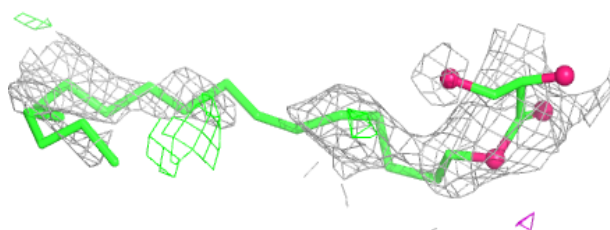
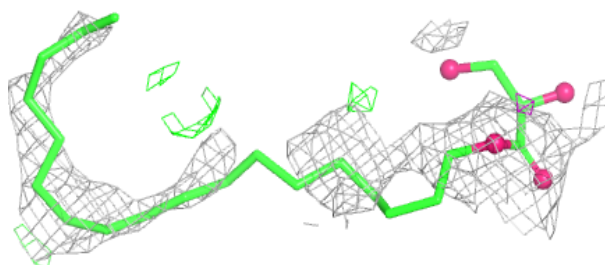
**Electron density around MPG B 306:**

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

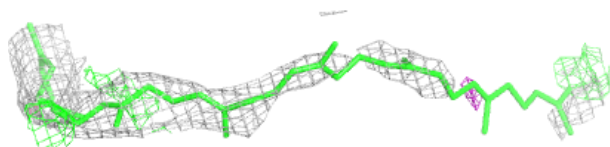
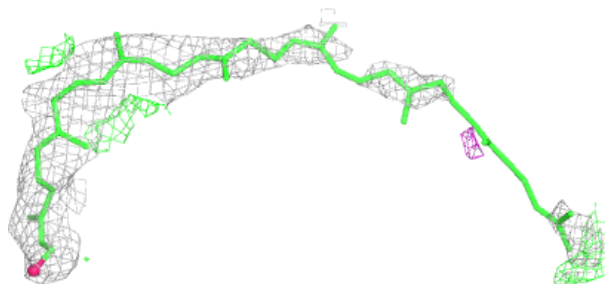


Electron density around MPG B 305:

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

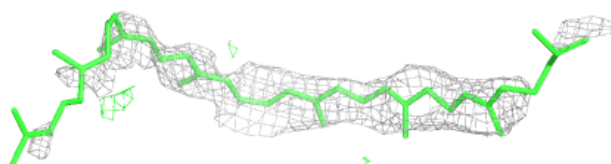
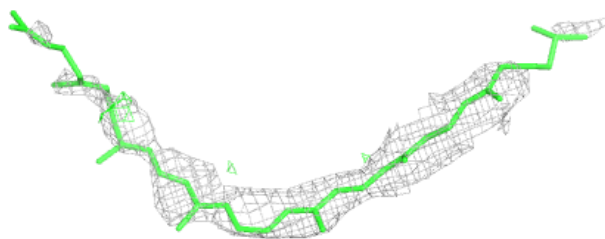
**Electron density around OTP C 406:**

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and green (positive)

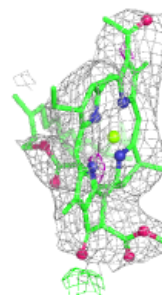
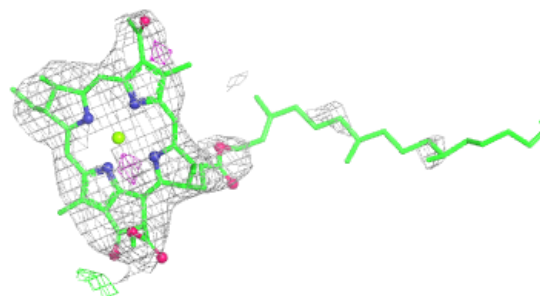


Electron density around NS5 C 405:

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

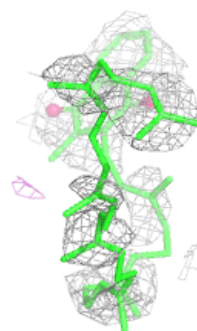
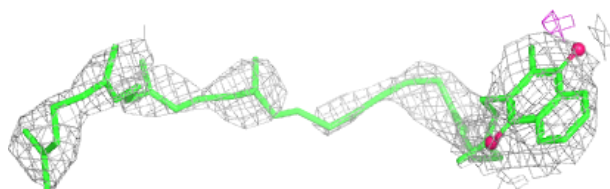
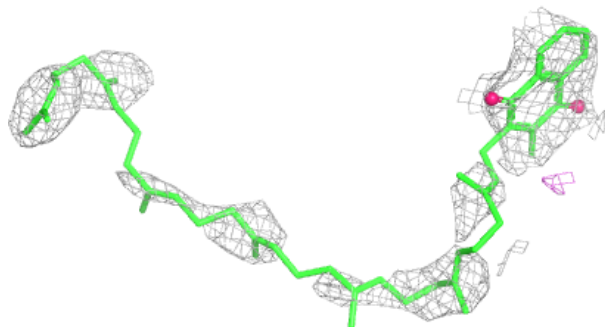
**Electron density around BCL B 301:**

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and green (positive)

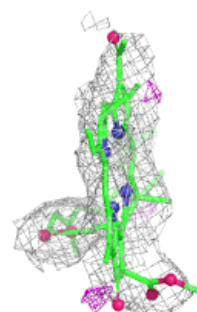
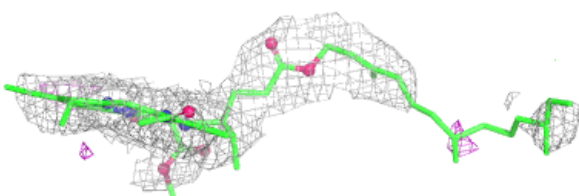
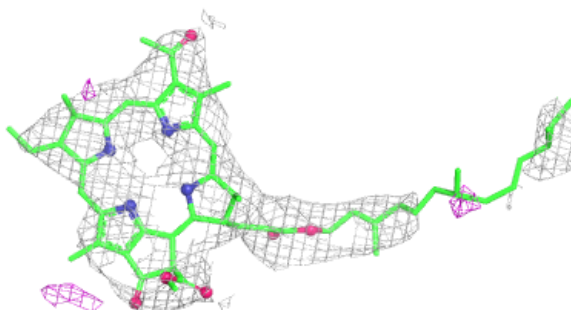


Electron density around MQ7 C 404:

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

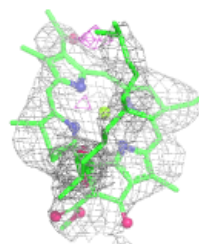
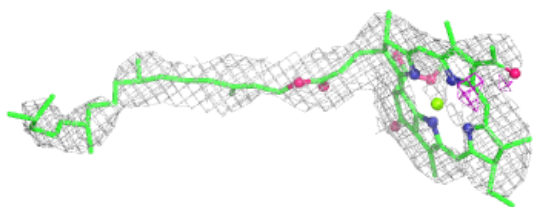
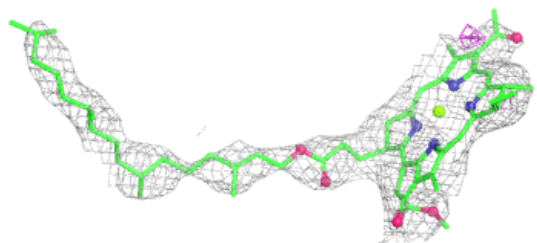
**Electron density around BPB C 402:**

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

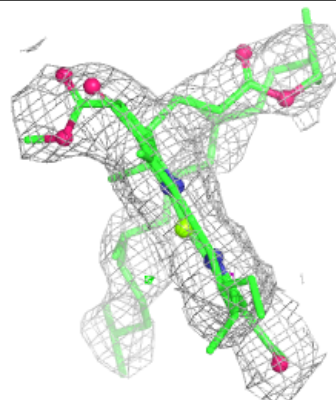
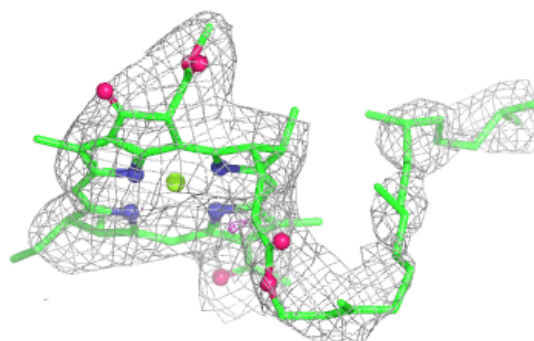
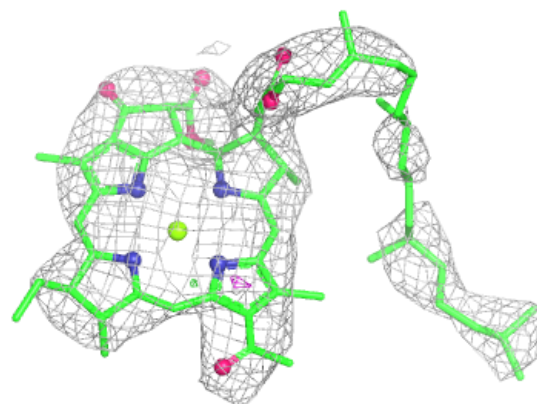


Electron density around BCL B 302:

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

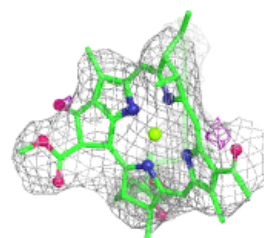
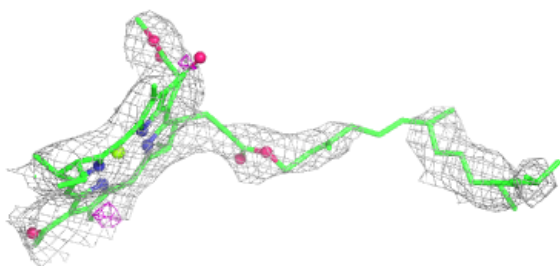
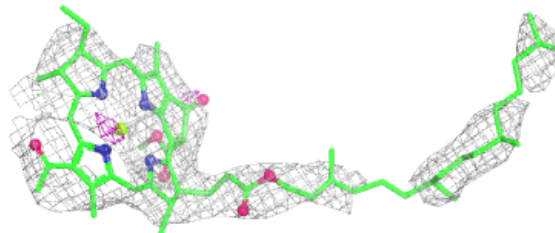
**Electron density around BCL B 303:**

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



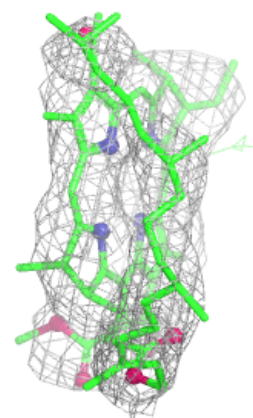
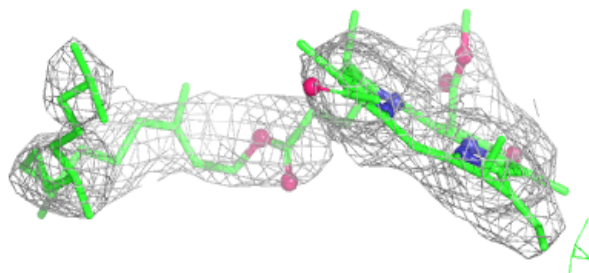
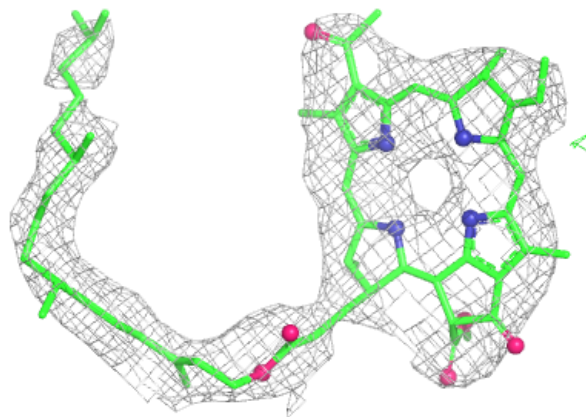
Electron density around BCL C 401:

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



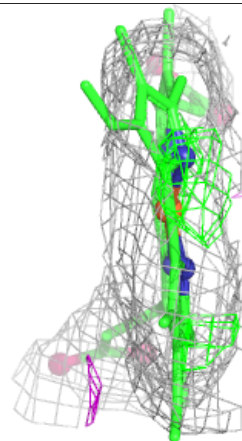
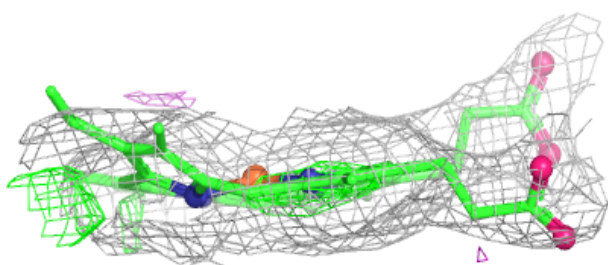
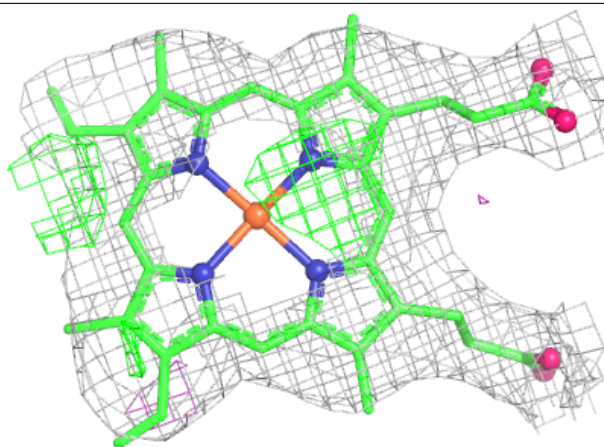
Electron density around BPB B 304:

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



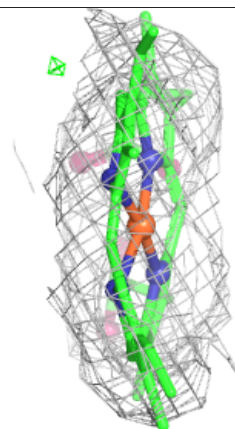
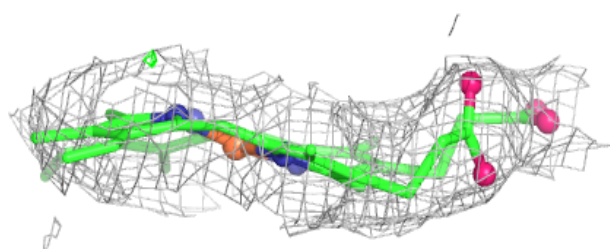
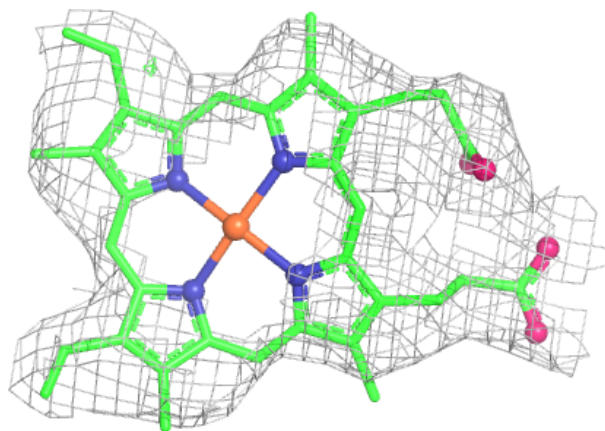
Electron density around HEC A 403:

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



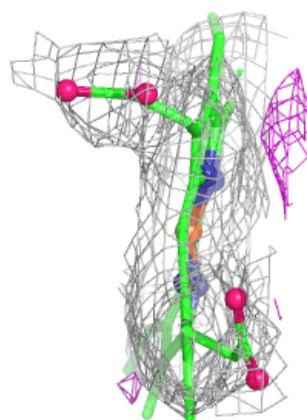
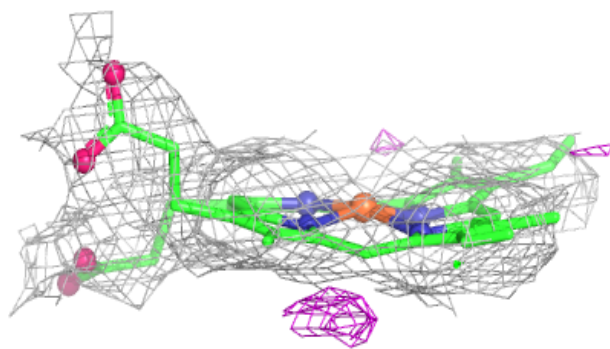
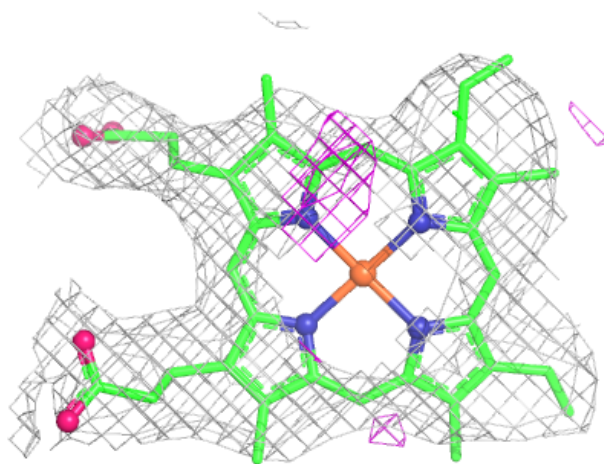
Electron density around HEC A 402:

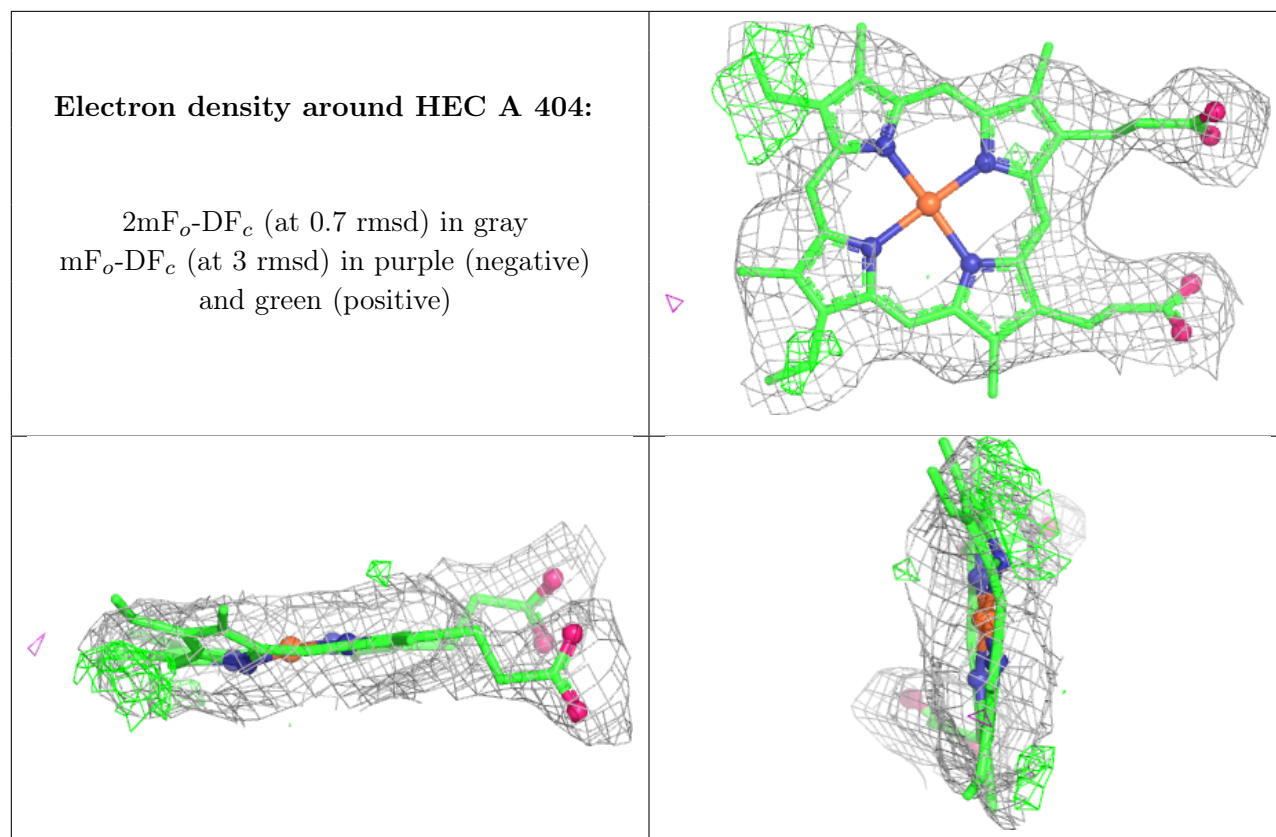
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.