



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:57 am BST

PDB ID : 5LRI
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH GLUL212
REPLACED WITH TRP (CHAIN L, EL212W)
Authors : Fyfe, P.K.; Jones, M.R.
Deposited on : 2016-08-19
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

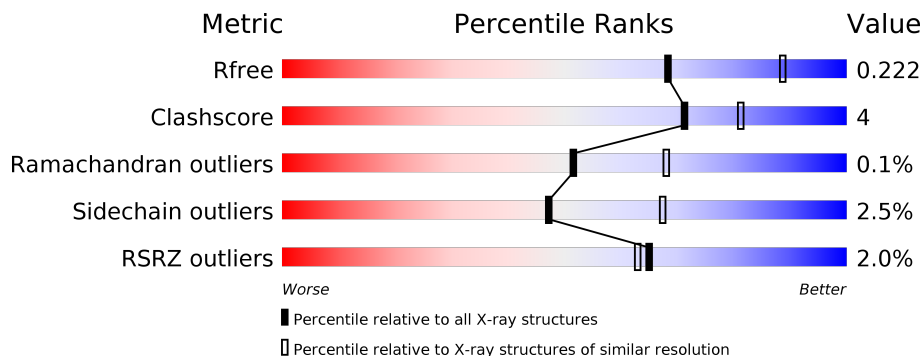
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	 3% 93% 6% 8%
2	M	307	 % 89% 8% 3%
3	H	260	 2% 83% 8% 8%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7494 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2249	1522	357	362	8	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	TRP	GLU	engineered mutation	UNP Q3J1A5

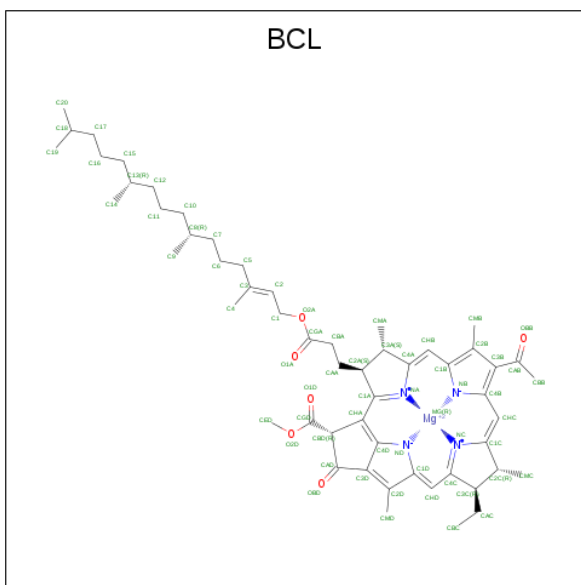
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	300	2400	1602	395	393	10	0	1	0

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

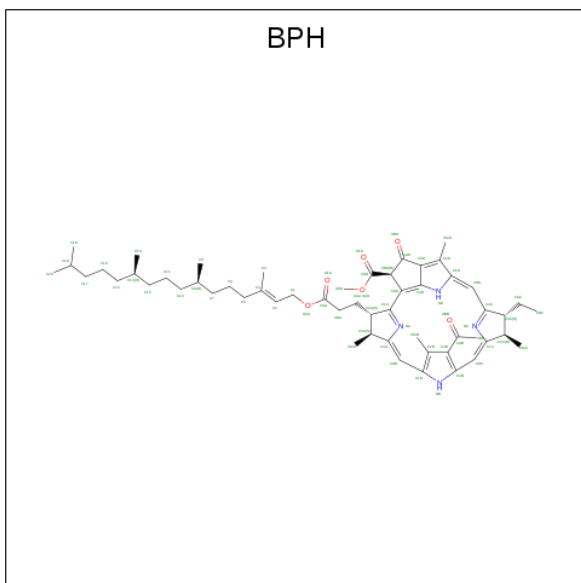
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	239	1837	1174	314	340	9	0	2	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



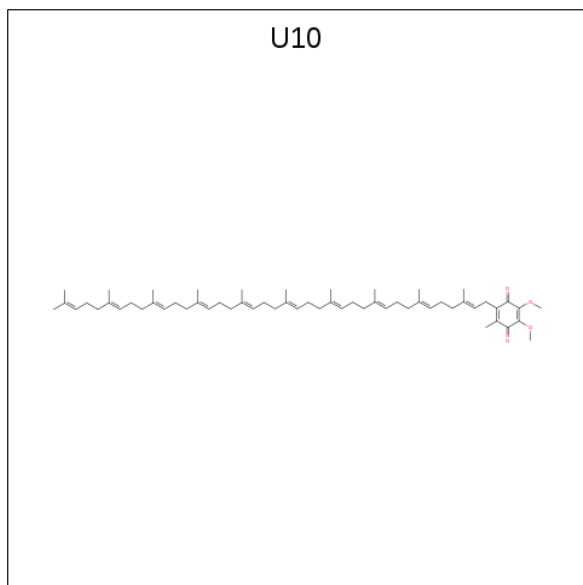
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



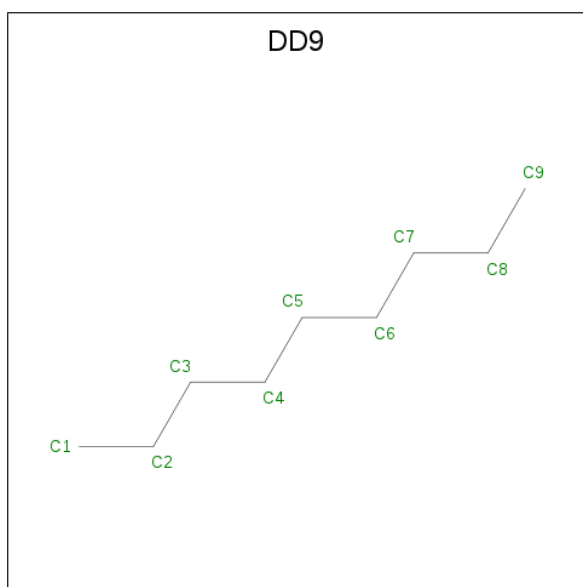
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is nonane (three-letter code: DD9) (formula: C₉H₂₀).

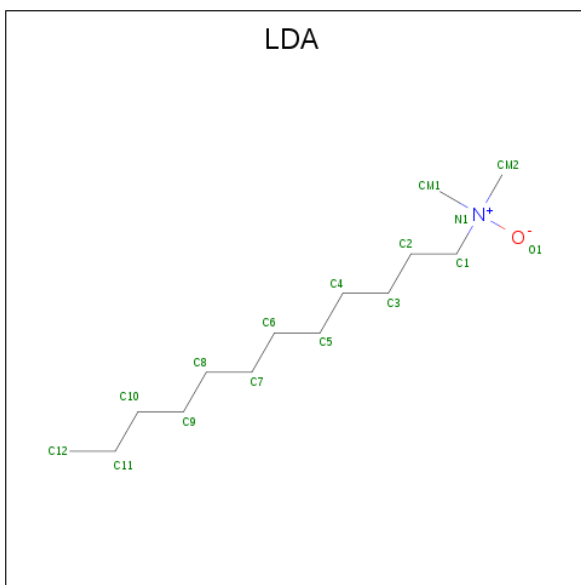


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C 8 8	0	0
7	H	1	Total C 9 9	0	0
7	H	1	Total C 7 7	0	0

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

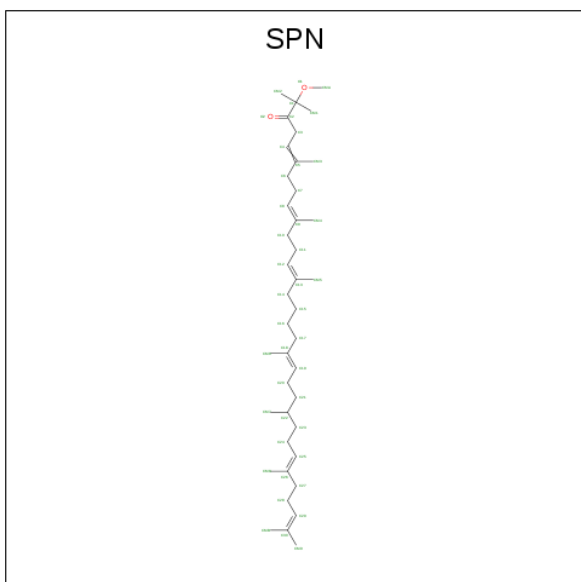
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total Fe 1 1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



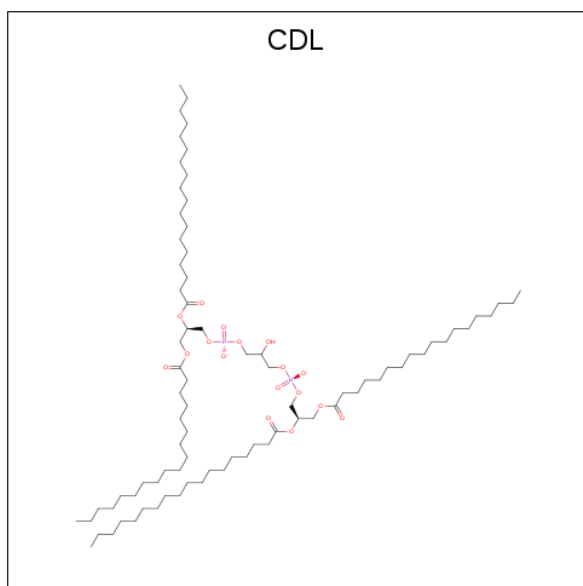
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	M	1	Total 16	C 14	N 1	O 1	0	0
9	M	1	Total 16	C 14	N 1	O 1	0	0
9	M	1	Total 16	C 14	N 1	O 1	0	0
9	M	1	Total 16	C 14	N 1	O 1	0	0
9	H	1	Total 16	C 14	N 1	O 1	0	0

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	M	1	43	41	2	0	0

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
11	M	1	78	59	17	2	0	0

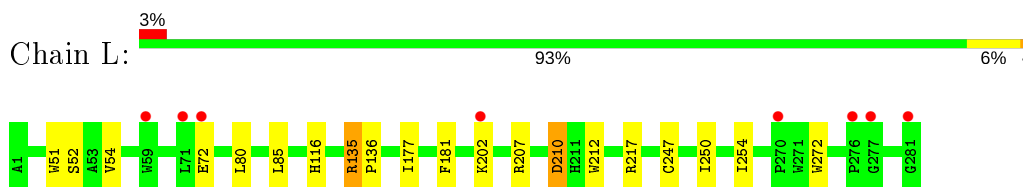
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	L	60	60	60	0	0
12	M	75	75	75	0	0
12	H	157	157	157	0	0

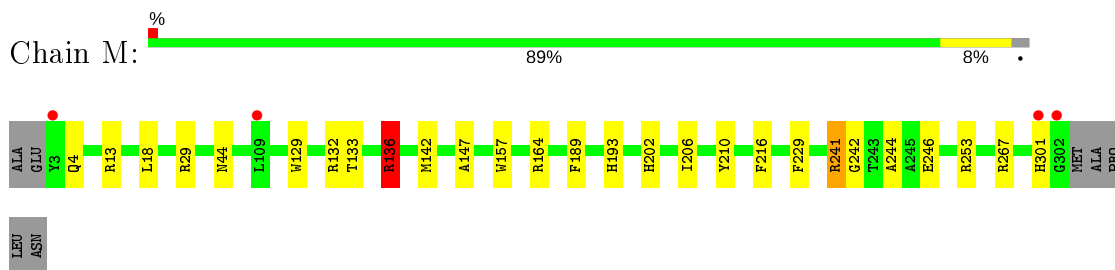
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

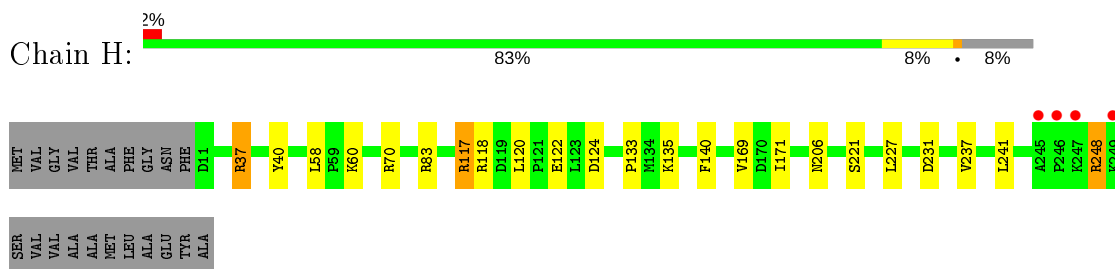
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.82Å 139.82Å 185.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.91 – 2.40 17.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.6 (17.91-2.40) 94.9 (17.89-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.189 , 0.217 0.195 , 0.222	Depositor DCC
R_{free} test set	3863 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, DD9, CDL, BPH, LDA, FE, SPN, U10

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	L	0.75	0/2340	0.77	3/3205 (0.1%)
2	M	0.74	0/2497	0.83	8/3408 (0.2%)
3	H	0.75	0/1889	0.97	11/2569 (0.4%)
All	All	0.75	0/6726	0.85	22/9182 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	37	ARG	NE-CZ-NH2	-12.78	113.91	120.30
3	H	37	ARG	NE-CZ-NH1	11.50	126.05	120.30
2	M	241	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	H	83	ARG	NE-CZ-NH2	-9.37	115.61	120.30
2	M	241	ARG	NE-CZ-NH1	8.45	124.52	120.30
3	H	83	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	L	135	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	L	135	ARG	NE-CZ-NH2	-7.57	116.52	120.30
3	H	248	ARG	NE-CZ-NH1	7.34	123.97	120.30
3	H	117	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	L	210	ASP	CB-CG-OD1	6.73	124.35	118.30
3	H	117	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	M	29	ARG	NE-CZ-NH2	-6.35	117.13	120.30
2	M	136	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	M	29	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	H	248	ARG	NE-CZ-NH2	-5.83	117.38	120.30
3	H	37	ARG	CG-CD-NE	-5.83	99.55	111.80
3	H	124	ASP	CB-CG-OD1	5.81	123.53	118.30
2	M	136	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	M	267	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	M	164	ARG	NE-CZ-NH1	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	37	ARG	CD-NE-CZ	5.09	130.72	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2249	0	2200	9	0
2	M	2400	0	2316	18	0
3	H	1837	0	1838	10	0
4	L	66	0	74	3	0
4	M	198	0	222	10	0
5	L	65	0	76	3	0
5	M	65	0	76	3	0
6	L	48	0	63	0	0
6	M	48	0	63	0	0
7	H	16	0	33	0	0
7	L	8	0	15	0	0
8	L	1	0	0	0	0
9	H	16	0	31	1	0
9	M	64	0	124	3	0
10	M	43	0	69	5	0
11	M	78	0	100	0	0
12	H	157	0	0	0	0
12	L	60	0	0	1	0
12	M	75	0	0	2	0
All	All	7494	0	7300	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) 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)
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.72	0.72
5:L:302:BPH:HHC	5:L:302:BPH:HBB3	1.72	0.71
2:M:157:TRP:CD1	10:M:709:SPN:H202	2.35	0.62
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.29	0.62
1:L:177:ILE:HG12	4:L:301:BCL:HMB3	1.81	0.61
3:H:118:ARG:HD2	3:H:120:LEU:HD12	1.82	0.60
4:M:705:BCL:HBB3	4:M:706:BCL:HMD2	1.82	0.60
5:L:302:BPH:HBB2	2:M:210:TYR:HB3	1.88	0.56
4:M:706:BCL:HMB1	4:M:706:BCL:HBB2	1.88	0.56
1:L:181:PHE:CD2	5:M:707:BPH:HBB1	2.41	0.55
4:M:704:BCL:C3B	10:M:709:SPN:H152	2.37	0.55
4:M:704:BCL:H141	10:M:709:SPN:H101	1.87	0.55
4:M:704:BCL:CAB	10:M:709:SPN:H162	2.36	0.55
4:M:704:BCL:H71	4:M:705:BCL:H202	1.89	0.54
1:L:217:ARG:NH1	12:L:401:HOH:O	2.41	0.53
1:L:250:ILE:HG22	1:L:254:ILE:HD12	1.91	0.53
1:L:116:HIS:HE1	2:M:4:GLN:O	1.92	0.52
2:M:253[B]:ARG:NH2	9:M:702:LDA:HM23	2.25	0.52
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.94	0.50
1:L:207:ARG:HG3	2:M:142:MET:HG2	1.94	0.50
2:M:157:TRP:NE1	10:M:709:SPN:H202	2.26	0.49
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.43	0.48
5:M:707:BPH:HHC	5:M:707:BPH:HBB3	1.95	0.48
2:M:13:ARG:O	3:H:140:PHE:HA	2.14	0.47
3:H:40:TYR:HB3	3:H:58:LEU:HD21	1.97	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.97	0.46
5:M:707:BPH:HBC3	5:M:707:BPH:HHD	1.97	0.46
4:M:706:BCL:HMB1	4:M:706:BCL:CBB	2.46	0.46
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.98	0.45
2:M:136:ARG:HA	2:M:136:ARG:NE	2.31	0.45
9:M:703:LDA:HM13	9:M:703:LDA:H21	1.87	0.45
1:L:51:TRP:CH2	1:L:80:LEU:HD23	2.52	0.45
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.99	0.44
9:H:301:LDA:H21	9:H:301:LDA:HM13	1.85	0.44
2:M:253[A]:ARG:NH2	12:M:803:HOH:O	2.49	0.44
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.82	0.43
5:L:302:BPH:CBB	5:L:302:BPH:HHC	2.45	0.43
2:M:129:TRP:CH2	2:M:132:ARG:NH1	2.85	0.43
4:M:704:BCL:HBB2	4:M:704:BCL:HMB1	2.00	0.43
3:H:169:VAL:HG23	3:H:171:ILE:HD12	2.00	0.43
2:M:189:PHE:O	2:M:193:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:704:BCL:CBB	4:M:704:BCL:HMB1	2.50	0.42
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.55	0.41
2:M:44:ASN:ND2	12:M:806:HOH:O	2.53	0.41
9:M:702:LDA:HM22	9:M:702:LDA:H22	1.84	0.41
3:H:37:ARG:NH2	3:H:60:LYS:O	2.47	0.41
3:H:241:LEU:O	3:H:248:ARG:NH2	2.54	0.40
4:L:301:BCL:OBB	4:L:301:BCL:HHC	2.21	0.40
4:M:705:BCL:HBD	4:M:705:BCL:HAA2	2.03	0.40
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.02	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	L	280/281 (100%)	273 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	285 (95%)	13 (4%)	1 (0%)	41	55
3	H	239/260 (92%)	237 (99%)	2 (1%)	0	100	100
All	All	818/848 (96%)	795 (97%)	22 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS

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	L	221/220 (100%)	214 (97%)	7 (3%)	39	59
2	M	236/240 (98%)	233 (99%)	3 (1%)	69	84
3	H	196/208 (94%)	190 (97%)	6 (3%)	40	60
All	All	653/668 (98%)	637 (98%)	16 (2%)	47	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	54	VAL
1	L	72	GLU
1	L	202	LYS
1	L	210	ASP
1	L	212	TRP
1	L	247	CYS
1	L	272	TRP
2	M	18	LEU
2	M	136	ARG
2	M	216	PHE
3	H	70	ARG
3	H	133	PRO
3	H	135	LYS
3	H	221	SER
3	H	231	ASP
3	H	237	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	116	HIS
1	L	183	ASN
2	M	4	GLN
2	M	44	ASN
2	M	193	HIS
3	H	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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
4	BCL	M	704	-	58,74,74	1.15	3 (5%)	69,115,115	1.53	17 (24%)
5	BPH	L	302	-	64,70,70	0.75	1 (1%)	76,101,101	1.37	10 (13%)
7	DD9	H	302	-	8,8,8	0.33	0	7,7,7	0.38	0
11	CDL	M	710	-	77,77,99	1.17	4 (5%)	83,89,111	1.12	4 (4%)
4	BCL	M	705	-	58,74,74	1.25	3 (5%)	69,115,115	1.48	13 (18%)
9	LDA	M	702	-	12,15,15	2.32	1 (8%)	14,17,17	2.63	3 (21%)
9	LDA	H	301	-	12,15,15	2.36	1 (8%)	14,17,17	2.41	3 (21%)
9	LDA	M	703	-	12,15,15	2.20	1 (8%)	14,17,17	2.46	3 (21%)
7	DD9	H	303	-	6,6,8	0.38	0	5,5,7	0.26	0
9	LDA	M	701	-	12,15,15	2.11	1 (8%)	14,17,17	0.89	1 (7%)
10	SPN	M	709	-	40,42,42	3.63	15 (37%)	50,52,52	2.30	20 (40%)
4	BCL	M	706	-	58,74,74	1.11	3 (5%)	69,115,115	1.74	21 (30%)
7	DD9	L	304	-	7,7,8	0.35	0	6,6,7	0.32	0
5	BPH	M	707	-	64,70,70	0.74	2 (3%)	76,101,101	1.27	9 (11%)
6	U10	L	303	-	48,48,63	1.84	3 (6%)	58,61,79	1.50	8 (13%)
4	BCL	L	301	-	58,74,74	1.15	3 (5%)	69,115,115	1.40	13 (18%)
6	U10	M	708	-	48,48,63	1.72	4 (8%)	58,61,79	1.37	7 (12%)
9	LDA	M	711	-	12,15,15	2.10	1 (8%)	14,17,17	0.38	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	BCL	M	704	-	-	9/37/137/137	-
5	BPH	L	302	-	-	6/54/105/105	0/5/6/6
7	DD9	H	302	-	-	2/6/6/6	-
11	CDL	M	710	-	-	30/88/88/110	-
4	BCL	M	705	-	-	1/37/137/137	-
9	LDA	M	702	-	-	3/13/13/13	-
9	LDA	H	301	-	-	5/13/13/13	-
9	LDA	M	703	-	-	2/13/13/13	-
7	DD9	H	303	-	-	0/4/4/6	-
9	LDA	M	701	-	-	8/13/13/13	-
10	SPN	M	709	-	-	19/50/51/51	-
4	BCL	M	706	-	-	1/37/137/137	-
7	DD9	L	304	-	-	3/5/5/6	-
5	BPH	M	707	-	-	12/54/105/105	0/5/6/6
6	U10	L	303	-	-	19/45/69/87	0/1/1/1
4	BCL	L	301	-	-	6/37/137/137	-
6	U10	M	708	-	-	13/45/69/87	0/1/1/1
9	LDA	M	711	-	-	4/13/13/13	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	709	SPN	C3-C4	-9.47	1.37	1.50
6	L	303	U10	C6-C1	8.23	1.50	1.35
9	H	301	LDA	O1-N1	-8.04	1.23	1.42
9	M	702	LDA	O1-N1	-8.00	1.23	1.42
9	M	703	LDA	O1-N1	-7.47	1.24	1.42
6	M	708	U10	C6-C1	7.29	1.48	1.35
6	L	303	U10	C36-C34	-7.27	1.36	1.51
10	M	709	SPN	C17-C18	-7.20	1.36	1.51
9	M	711	LDA	O1-N1	-7.19	1.25	1.42
10	M	709	SPN	C10-C9	-7.11	1.36	1.51
9	M	701	LDA	O1-N1	-6.93	1.25	1.42
10	M	709	SPN	C6-C5	-6.79	1.37	1.51
10	M	709	SPN	C14-C13	-6.77	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	708	U10	C36-C34	-6.76	1.37	1.51
10	M	709	SPN	C4-C5	6.06	1.47	1.33
4	M	705	BCL	MG-NA	6.01	2.20	2.06
10	M	709	SPN	C12-C13	6.00	1.47	1.33
10	M	709	SPN	C8-C9	5.94	1.47	1.33
10	M	709	SPN	C19-C18	5.76	1.46	1.33
4	L	301	BCL	MG-NA	5.06	2.18	2.06
4	M	705	BCL	C4B-NB	4.81	1.39	1.35
11	M	710	CDL	OB6-CB5	4.76	1.47	1.34
10	M	709	SPN	C20-C19	-4.64	1.35	1.50
11	M	710	CDL	OA6-CA5	4.63	1.47	1.34
4	M	704	BCL	MG-NA	4.63	2.17	2.06
11	M	710	CDL	OA8-CA7	4.59	1.46	1.33
11	M	710	CDL	OB8-CB7	4.44	1.46	1.33
10	M	709	SPN	C7-C8	-4.27	1.36	1.50
10	M	709	SPN	C11-C12	-4.27	1.36	1.50
4	M	706	BCL	C4B-NB	4.09	1.38	1.35
4	M	704	BCL	C4B-NB	3.99	1.38	1.35
4	L	301	BCL	C1B-NB	3.68	1.38	1.35
6	M	708	U10	C4-C3	3.42	1.50	1.36
10	M	709	SPN	C21-C22	-3.17	1.35	1.52
6	L	303	U10	C4-C3	3.10	1.48	1.36
4	M	704	BCL	C1B-NB	3.08	1.38	1.35
4	M	706	BCL	MG-NC	-3.00	1.99	2.06
4	L	301	BCL	C4B-NB	2.86	1.37	1.35
10	M	709	SPN	C16-C15	-2.83	1.35	1.51
4	M	705	BCL	C1B-NB	2.46	1.37	1.35
5	M	707	BPH	C1C-NC	-2.31	1.32	1.37
4	M	706	BCL	C3C-C4C	-2.24	1.48	1.51
5	M	707	BPH	CHC-C1C	2.21	1.41	1.36
10	M	709	SPN	C21-C20	-2.08	1.46	1.53
6	M	708	U10	C33-C34	2.05	1.37	1.33
5	L	302	BPH	CHC-C1C	2.00	1.40	1.36

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	702	LDA	CM1-N1-C1	-7.34	94.82	110.23
9	M	703	LDA	O1-N1-C1	-6.20	94.06	109.27
9	H	301	LDA	O1-N1-C1	-6.06	94.40	109.27
10	M	709	SPN	CM5-C13-C14	5.36	124.28	115.27
9	M	702	LDA	O1-N1-C1	-4.96	97.12	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	710	CDL	OA6-CA5-C11	4.92	122.11	111.50
9	H	301	LDA	CM2-N1-C1	-4.83	100.09	110.23
9	M	703	LDA	CM2-N1-C1	-4.73	100.30	110.23
4	M	706	BCL	CMB-C2B-C1B	-4.68	121.27	128.46
4	M	704	BCL	CMB-C2B-C1B	-4.66	121.31	128.46
9	M	703	LDA	CM1-N1-C1	-4.65	100.47	110.23
10	M	709	SPN	CM3-C5-C6	4.61	123.02	115.27
10	M	709	SPN	CM6-C18-C17	4.49	122.82	115.27
4	M	705	BCL	CMB-C2B-C1B	-4.44	121.64	128.46
9	H	301	LDA	CM1-N1-C1	-4.37	101.06	110.23
11	M	710	CDL	OB6-CB5-C51	4.31	120.79	111.50
5	L	302	BPH	C4-C3-C5	-4.11	108.35	115.27
10	M	709	SPN	CM4-C9-C10	4.04	122.07	115.27
10	M	709	SPN	C15-C14-C13	4.02	123.99	113.45
10	M	709	SPN	C16-C17-C18	3.93	123.75	113.45
6	L	303	U10	C25-C24-C26	3.75	121.58	115.27
9	M	702	LDA	CM2-N1-C1	-3.73	102.41	110.23
6	M	708	U10	C37-C36-C34	3.60	124.83	112.98
10	M	709	SPN	C7-C6-C5	3.55	124.66	112.98
4	L	301	BCL	CMB-C2B-C1B	-3.54	123.02	128.46
6	L	303	U10	C37-C36-C34	3.51	124.53	112.98
4	M	705	BCL	CED-O2D-CGD	3.43	123.69	115.94
10	M	709	SPN	C16-C15-C14	3.43	125.50	113.19
4	M	706	BCL	C1-O2A-CGA	3.42	125.41	116.44
4	M	704	BCL	C1-O2A-CGA	3.41	125.39	116.44
10	M	709	SPN	C11-C10-C9	3.40	124.16	112.98
5	M	707	BPH	C1-O2A-CGA	3.35	125.23	116.44
4	M	706	BCL	CAC-C3C-C2C	-3.34	105.92	114.26
4	M	704	BCL	CHA-C1A-NA	-3.33	118.78	126.40
4	M	705	BCL	C1C-NC-C4C	3.30	108.19	106.71
4	M	706	BCL	CMD-C2D-C3D	3.29	130.83	124.68
4	M	704	BCL	CMB-C2B-C3B	3.28	130.82	124.68
4	M	705	BCL	OBB-CAB-CBB	-3.27	112.81	120.17
5	M	707	BPH	C1B-NB-C4B	3.23	112.60	106.51
4	M	705	BCL	CHA-C1A-NA	-3.22	119.02	126.40
4	M	706	BCL	OBB-CAB-C3B	3.21	125.69	119.99
4	L	301	BCL	CHA-C1A-NA	-3.20	119.08	126.40
10	M	709	SPN	CM7-C22-C21	3.19	122.86	111.29
6	L	303	U10	C30-C29-C28	-3.09	115.75	123.68
5	M	707	BPH	CED-O2D-CGD	3.07	122.89	115.94
10	M	709	SPN	C15-C16-C17	3.03	124.09	113.19
4	M	705	BCL	C4B-C3B-CAB	-3.00	121.34	127.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	707	BPH	C4-C3-C5	-2.96	110.29	115.27
4	M	704	BCL	C4D-C3D-CAD	-2.89	106.86	108.47
6	M	708	U10	C15-C14-C16	2.89	120.13	115.27
5	L	302	BPH	C1-C2-C3	-2.86	121.11	126.04
5	L	302	BPH	C1B-NB-C4B	2.83	111.85	106.51
4	L	301	BCL	CAA-C2A-C3A	-2.83	105.02	112.78
4	L	301	BCL	C4B-C3B-CAB	-2.82	121.69	127.13
4	M	706	BCL	C4D-C3D-CAD	-2.82	106.90	108.47
11	M	710	CDL	OA8-CA7-C31	2.81	120.74	111.91
4	M	704	BCL	C4B-C3B-CAB	-2.80	121.72	127.13
5	L	302	BPH	OBB-CAB-C3B	2.77	125.53	120.41
6	M	708	U10	C10-C9-C11	2.74	119.88	115.27
6	L	303	U10	C32-C33-C34	-2.73	121.09	127.66
6	L	303	U10	C7-C8-C9	-2.69	122.32	126.79
4	M	706	BCL	O1D-CGD-CBD	-2.67	119.03	124.48
4	M	706	BCL	C5-C3-C2	-2.66	115.73	121.12
6	L	303	U10	C15-C14-C16	2.65	119.73	115.27
5	M	707	BPH	CHD-C4C-NC	-2.62	122.09	125.20
4	M	705	BCL	CMB-C2B-C3B	2.62	129.57	124.68
10	M	709	SPN	C17-C18-C19	-2.61	115.83	121.12
4	L	301	BCL	CMB-C2B-C3B	2.60	129.54	124.68
4	M	706	BCL	CAA-CBA-CGA	2.59	120.81	113.25
4	M	706	BCL	CMB-C2B-C3B	2.58	129.51	124.68
10	M	709	SPN	C20-C21-C22	2.57	124.67	115.76
5	L	302	BPH	O2D-CGD-CBD	2.57	115.84	111.27
4	M	705	BCL	CAC-C3C-C4C	-2.57	106.88	112.58
6	L	303	U10	C30-C29-C31	2.56	119.58	115.27
4	L	301	BCL	C1C-NC-C4C	2.56	107.86	106.71
4	M	706	BCL	O2D-CGD-CBD	2.54	115.78	111.27
4	M	706	BCL	C4A-NA-C1A	2.50	107.83	106.71
10	M	709	SPN	C6-C7-C8	2.50	120.10	111.88
4	M	706	BCL	CAA-C2A-C3A	-2.48	106.00	112.78
11	M	710	CDL	OA6-CA5-OA7	-2.47	117.73	123.70
4	M	704	BCL	CAA-C2A-C3A	-2.47	106.03	112.78
4	L	301	BCL	CED-O2D-CGD	2.46	121.51	115.94
6	M	708	U10	C17-C18-C19	-2.45	121.75	127.66
4	M	706	BCL	OBD-CAD-CBD	-2.45	122.40	125.89
6	M	708	U10	C30-C29-C28	-2.43	117.45	123.68
4	M	706	BCL	CAC-C3C-C4C	-2.43	107.20	112.58
4	M	704	BCL	C2C-C3C-C4C	2.39	104.92	101.34
4	M	704	BCL	C2A-C1A-CHA	2.37	128.00	123.86
6	M	708	U10	C1M-C1-C6	-2.35	120.56	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	705	BCL	C4D-C3D-CAD	-2.34	107.16	108.47
10	M	709	SPN	CM8-C26-C27	2.33	119.19	115.27
4	M	706	BCL	OBB-CAB-CBB	-2.32	114.95	120.17
5	L	302	BPH	CAC-C3C-C4C	2.31	118.61	112.67
10	M	709	SPN	C10-C9-C8	-2.31	116.44	121.12
4	L	301	BCL	OBD-CAD-CBD	-2.31	122.60	125.89
4	L	301	BCL	CMA-C3A-C4A	-2.30	105.58	111.77
6	L	303	U10	C3M-O3-C3	2.30	124.62	116.47
5	M	707	BPH	C2B-C1B-NB	-2.30	106.32	109.79
4	L	301	BCL	OBB-CAB-CBB	-2.25	115.11	120.17
4	M	705	BCL	CAC-C3C-C2C	-2.24	108.66	114.26
4	M	706	BCL	C4B-C3B-CAB	-2.24	122.80	127.13
4	M	704	BCL	CMA-C3A-C4A	-2.23	105.78	111.77
10	M	709	SPN	C10-C11-C12	2.22	119.17	111.88
4	M	704	BCL	CAA-CBA-CGA	2.19	119.65	113.25
10	M	709	SPN	CM5-C13-C12	-2.18	118.08	123.68
5	L	302	BPH	CED-O2D-CGD	2.17	120.85	115.94
4	L	301	BCL	C4D-C3D-CAD	-2.16	107.26	108.47
4	L	301	BCL	C11-C12-C13	-2.16	108.93	115.92
5	M	707	BPH	CMD-C2D-C3D	2.16	128.72	124.68
5	M	707	BPH	C5-C3-C2	2.14	125.45	121.12
4	M	705	BCL	OBD-CAD-CBD	-2.13	122.85	125.89
9	M	701	LDA	CM2-N1-C1	2.12	114.68	110.23
5	L	302	BPH	O2A-CGA-O1A	-2.11	118.26	123.59
4	M	704	BCL	CMD-C2D-C3D	2.11	128.62	124.68
5	L	302	BPH	C2B-C1B-NB	-2.11	106.61	109.79
4	M	706	BCL	C4B-CHC-C1C	-2.10	125.95	130.12
4	L	301	BCL	C1-O2A-CGA	2.10	121.96	116.44
4	M	704	BCL	OBD-CAD-CBD	-2.10	122.90	125.89
4	M	704	BCL	OBB-CAB-CBB	-2.09	115.46	120.17
4	M	705	BCL	C4A-NA-C1A	2.07	107.64	106.71
6	M	708	U10	C16-C14-C13	-2.07	116.93	121.12
10	M	709	SPN	C21-C20-C19	2.07	117.69	112.23
10	M	709	SPN	CM7-C22-C23	2.07	118.77	111.29
4	M	704	BCL	OBB-CAB-C3B	2.06	123.65	119.99
4	M	704	BCL	C6-C5-C3	-2.06	108.05	113.45
4	M	706	BCL	C2C-C3C-C4C	2.05	104.42	101.34
4	M	705	BCL	C1-O2A-CGA	2.05	121.82	116.44
5	L	302	BPH	C1C-NC-C4C	-2.05	108.74	110.54
4	M	706	BCL	C1B-CHB-C4A	-2.03	126.10	130.12
4	M	704	BCL	C4-C3-C2	-2.03	118.48	123.68
4	M	706	BCL	C6-C5-C3	-2.03	108.14	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	707	BPH	CAA-C2A-C3A	-2.03	107.23	112.78

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	710	CDL	CA2-OA2-PA1-OA4
11	M	710	CDL	CA3-OA5-PA1-OA4
11	M	710	CDL	CB2-OB2-PB2-OB3
9	M	701	LDA	C2-C1-N1-O1
9	M	701	LDA	C2-C1-N1-CM1
9	M	701	LDA	C2-C1-N1-CM2
5	M	707	BPH	C4B-C3B-CAB-CBB
5	M	707	BPH	C4B-C3B-CAB-OBB
10	M	709	SPN	C20-C21-C22-CM7
6	L	303	U10	C23-C24-C26-C27
6	L	303	U10	C25-C24-C26-C27
6	M	708	U10	C32-C33-C34-C35
6	M	708	U10	C32-C33-C34-C36
9	M	711	LDA	C2-C1-N1-CM1
10	M	709	SPN	C14-C15-C16-C17
6	L	303	U10	C27-C28-C29-C30
6	M	708	U10	C27-C28-C29-C30
6	L	303	U10	C27-C28-C29-C31
6	M	708	U10	C37-C38-C39-C40
10	M	709	SPN	CM3-C5-C6-C7
10	M	709	SPN	C11-C10-C9-CM4
10	M	709	SPN	CM5-C13-C14-C15
10	M	709	SPN	C16-C17-C18-CM6
10	M	709	SPN	C4-C5-C6-C7
10	M	709	SPN	C11-C10-C9-C8
10	M	709	SPN	C12-C13-C14-C15
10	M	709	SPN	C16-C17-C18-C19
6	L	303	U10	C34-C36-C37-C38
6	M	708	U10	C24-C26-C27-C28
10	M	709	SPN	C3-C4-C5-CM3
6	L	303	U10	C17-C18-C19-C20
6	M	708	U10	C27-C28-C29-C31
4	M	704	BCL	C13-C15-C16-C17
6	M	708	U10	C37-C38-C39-C41
4	M	704	BCL	C15-C16-C17-C18
4	M	704	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	M	708	U10	C29-C31-C32-C33
11	M	710	CDL	C36-C37-C38-C39
6	L	303	U10	C35-C34-C36-C37
9	H	301	LDA	C5-C6-C7-C8
5	M	707	BPH	C16-C17-C18-C19
5	M	707	BPH	C16-C17-C18-C20
9	M	702	LDA	C2-C3-C4-C5
5	M	707	BPH	C4-C3-C5-C6
5	M	707	BPH	C2-C3-C5-C6
6	L	303	U10	C33-C34-C36-C37
6	M	708	U10	C33-C34-C36-C37
9	H	301	LDA	C4-C5-C6-C7
9	H	301	LDA	C1-C2-C3-C4
6	L	303	U10	C17-C18-C19-C21
9	M	701	LDA	C3-C4-C5-C6
4	L	301	BCL	C13-C15-C16-C17
6	M	708	U10	C35-C34-C36-C37
10	M	709	SPN	C21-C22-C23-C24
11	M	710	CDL	OA7-CA5-OA6-CA4
9	M	703	LDA	C1-C2-C3-C4
4	M	704	BCL	C5-C6-C7-C8
11	M	710	CDL	C11-CA5-OA6-CA4
11	M	710	CDL	C13-C14-C15-C16
9	M	702	LDA	C6-C7-C8-C9
11	M	710	CDL	CA2-OA2-PA1-OA5
11	M	710	CDL	CA3-OA5-PA1-OA2
11	M	710	CDL	CB2-OB2-PB2-OB5
9	M	711	LDA	C2-C3-C4-C5
5	L	302	BPH	C4-C3-C5-C6
9	M	701	LDA	C1-C2-C3-C4
5	M	707	BPH	C12-C13-C15-C16
5	M	707	BPH	C14-C13-C15-C16
11	M	710	CDL	C11-C12-C13-C14
4	L	301	BCL	C15-C16-C17-C18
11	M	710	CDL	C35-C36-C37-C38
11	M	710	CDL	OA5-CA3-CA4-CA6
11	M	710	CDL	C78-C79-C80-C81
6	L	303	U10	C30-C29-C31-C32
11	M	710	CDL	CA5-C11-C12-C13
5	L	302	BPH	C4C-C3C-CAC-CBC
5	L	302	BPH	C2-C3-C5-C6
10	M	709	SPN	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
9	M	701	LDA	C7-C8-C9-C10
5	L	302	BPH	CAD-CBD-CGD-O2D
5	M	707	BPH	CAD-CBD-CGD-O2D
6	M	708	U10	C30-C29-C31-C32
11	M	710	CDL	CA3-CA4-CA6-OA8
9	M	711	LDA	C2-C1-N1-CM2
11	M	710	CDL	C74-C75-C76-C77
9	M	701	LDA	C9-C10-C11-C12
11	M	710	CDL	C40-C41-C42-C43
4	M	704	BCL	C2-C1-O2A-CGA
9	M	702	LDA	C1-C2-C3-C4
6	L	303	U10	C28-C29-C31-C32
6	M	708	U10	C28-C29-C31-C32
11	M	710	CDL	CA2-OA2-PA1-OA3
11	M	710	CDL	CA3-OA5-PA1-OA3
11	M	710	CDL	CB2-OB2-PB2-OB4
4	M	705	BCL	C13-C15-C16-C17
9	H	301	LDA	C9-C10-C11-C12
11	M	710	CDL	CB7-C71-C72-C73
11	M	710	CDL	OA5-CA3-CA4-OA6
4	L	301	BCL	C11-C12-C13-C15
4	L	301	BCL	C11-C10-C8-C9
11	M	710	CDL	C16-C17-C18-C19
6	L	303	U10	C5-C4-O4-C4M
6	L	303	U10	C15-C14-C16-C17
5	L	302	BPH	C8-C10-C11-C12
11	M	710	CDL	C19-C20-C21-C22
7	L	304	DD9	C3-C4-C5-C6
4	M	706	BCL	C15-C16-C17-C18
11	M	710	CDL	C14-C15-C16-C17
6	L	303	U10	C29-C31-C32-C33
7	H	302	DD9	C2-C3-C4-C5
5	M	707	BPH	C15-C16-C17-C18
10	M	709	SPN	C5-C6-C7-C8
9	M	703	LDA	C7-C8-C9-C10
6	M	708	U10	C5-C4-O4-C4M
5	L	302	BPH	O2A-C1-C2-C3
5	M	707	BPH	O2A-C1-C2-C3
11	M	710	CDL	C17-C18-C19-C20
4	M	704	BCL	C12-C13-C15-C16
6	L	303	U10	C7-C8-C9-C10
9	M	701	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	H	301	LDA	C3-C4-C5-C6
4	M	704	BCL	C4-C3-C5-C6
6	L	303	U10	C13-C14-C16-C17
6	L	303	U10	C24-C26-C27-C28
7	L	304	DD9	C5-C6-C7-C8
10	M	709	SPN	CM8-C26-C27-C28
6	L	303	U10	C20-C19-C21-C22
9	M	711	LDA	C11-C10-C9-C8
4	M	704	BCL	CAD-CBD-CGD-O2D
4	L	301	BCL	CAD-CBD-CGD-O2D
11	M	710	CDL	C33-C34-C35-C36
4	M	704	BCL	C14-C13-C15-C16
7	L	304	DD9	C4-C5-C6-C7
10	M	709	SPN	C10-C11-C12-C13
10	M	709	SPN	C18-C19-C20-C21
7	H	302	DD9	C5-C6-C7-C8
5	M	707	BPH	C13-C15-C16-C17
10	M	709	SPN	C6-C7-C8-C9
10	M	709	SPN	CM2-C1-C2-C3
11	M	710	CDL	C32-C31-CA7-OA8
4	L	301	BCL	C11-C10-C8-C7
6	L	303	U10	C3-C4-O4-C4M
11	M	710	CDL	C32-C31-CA7-OA9

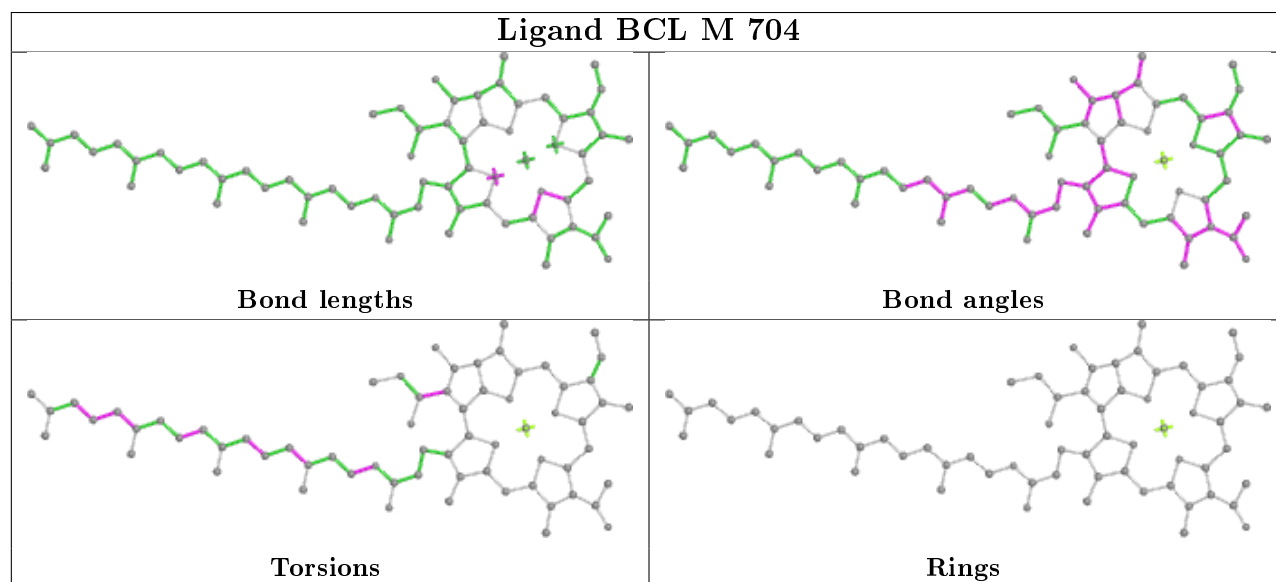
There are no ring outliers.

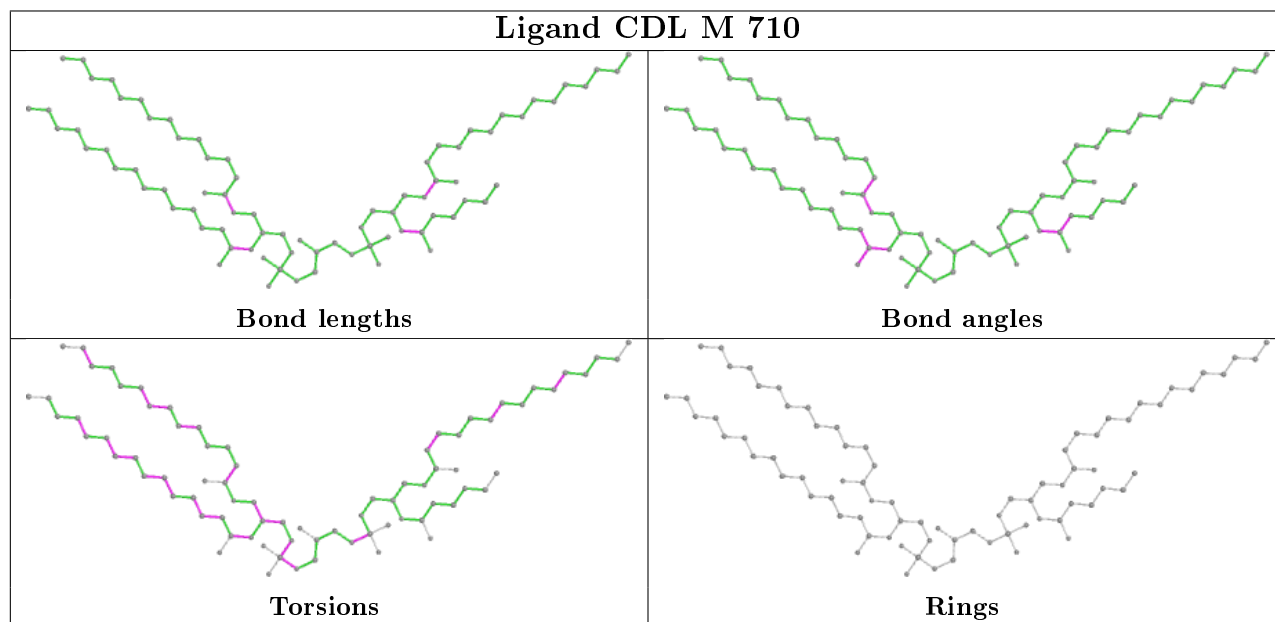
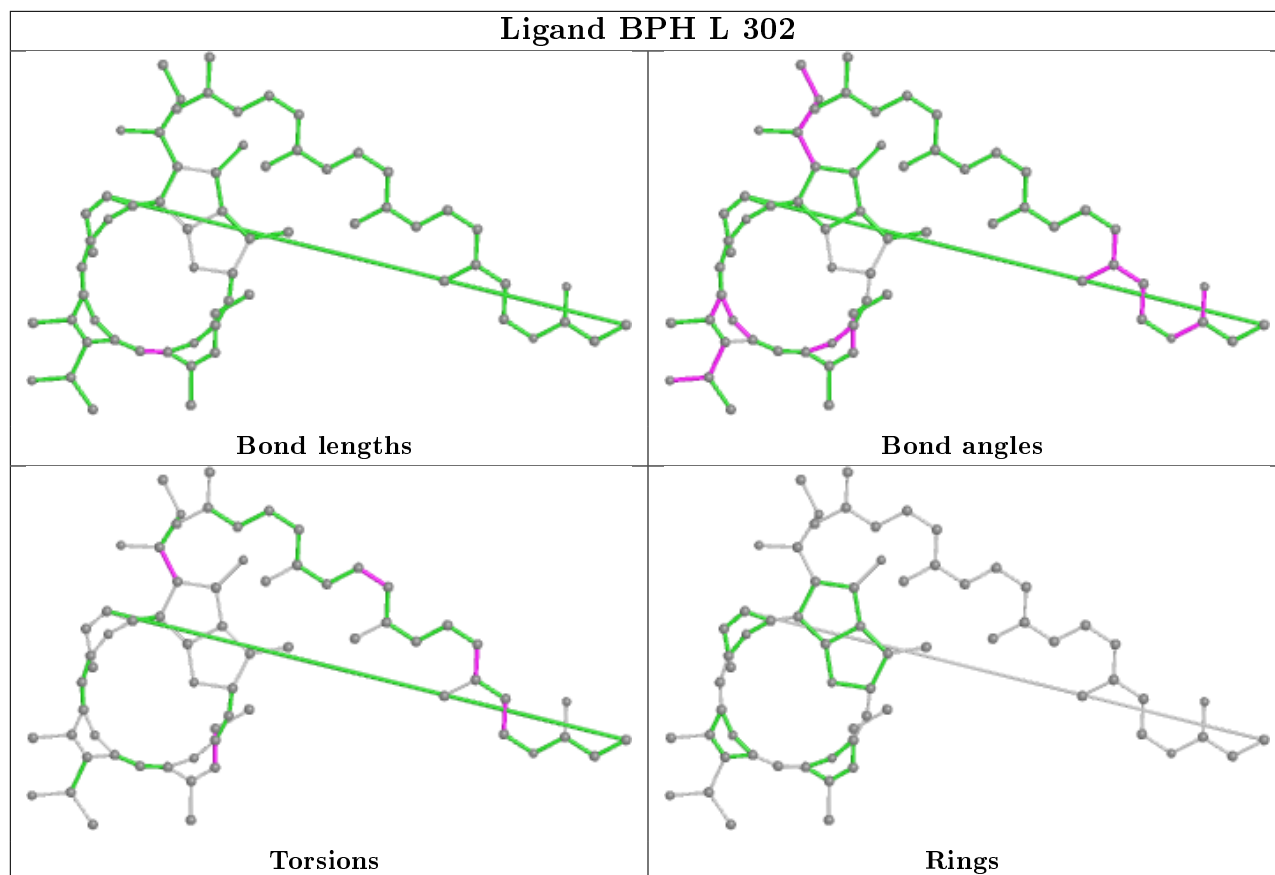
10 monomers are involved in 25 short contacts:

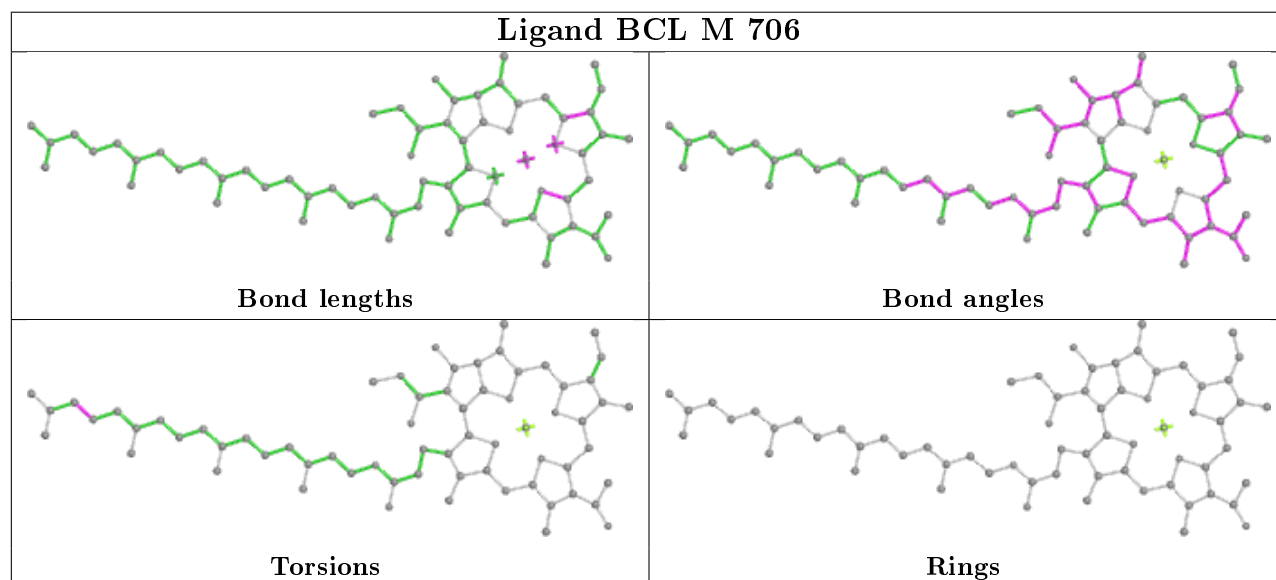
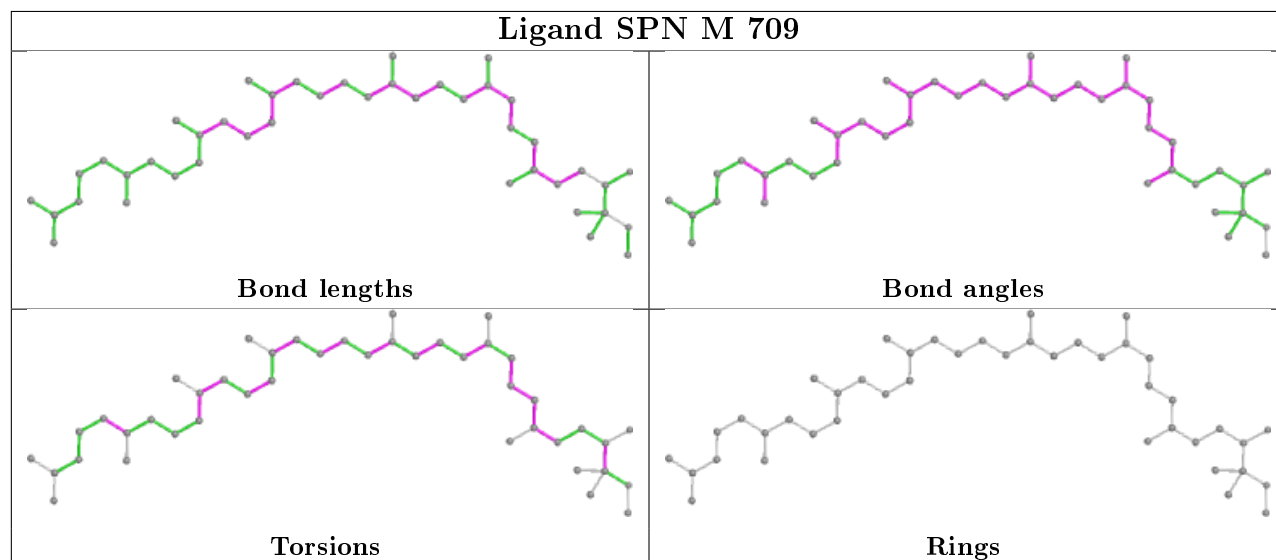
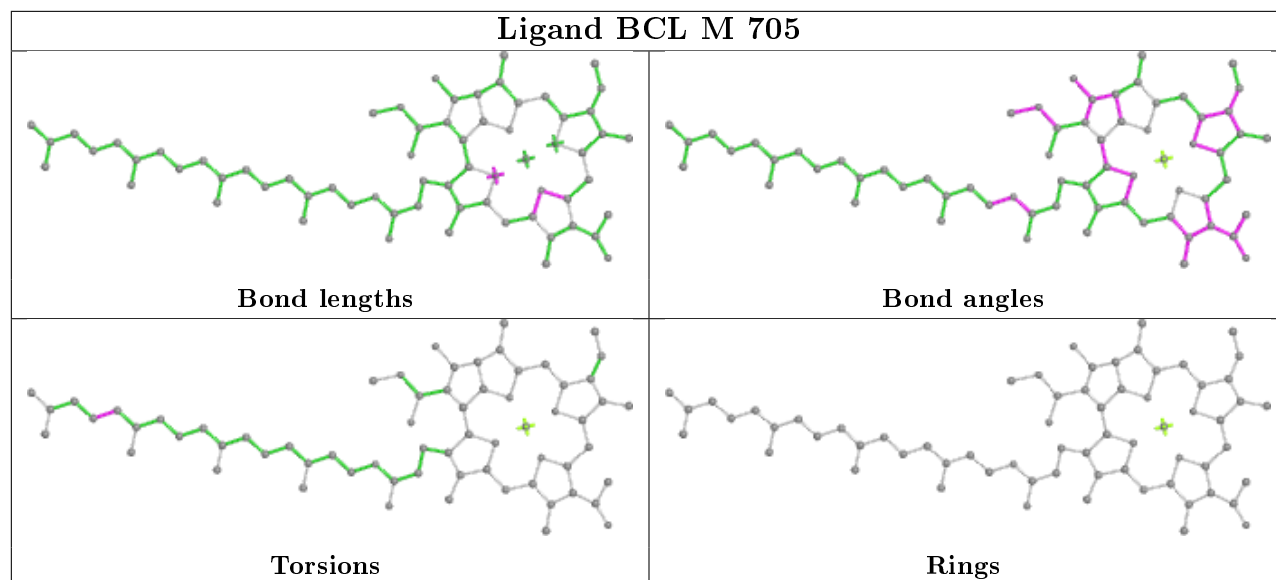
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	704	BCL	6	0
5	L	302	BPH	3	0
4	M	705	BCL	3	0
9	M	702	LDA	2	0
9	H	301	LDA	1	0
9	M	703	LDA	1	0
10	M	709	SPN	5	0
4	M	706	BCL	3	0
5	M	707	BPH	3	0
4	L	301	BCL	3	0

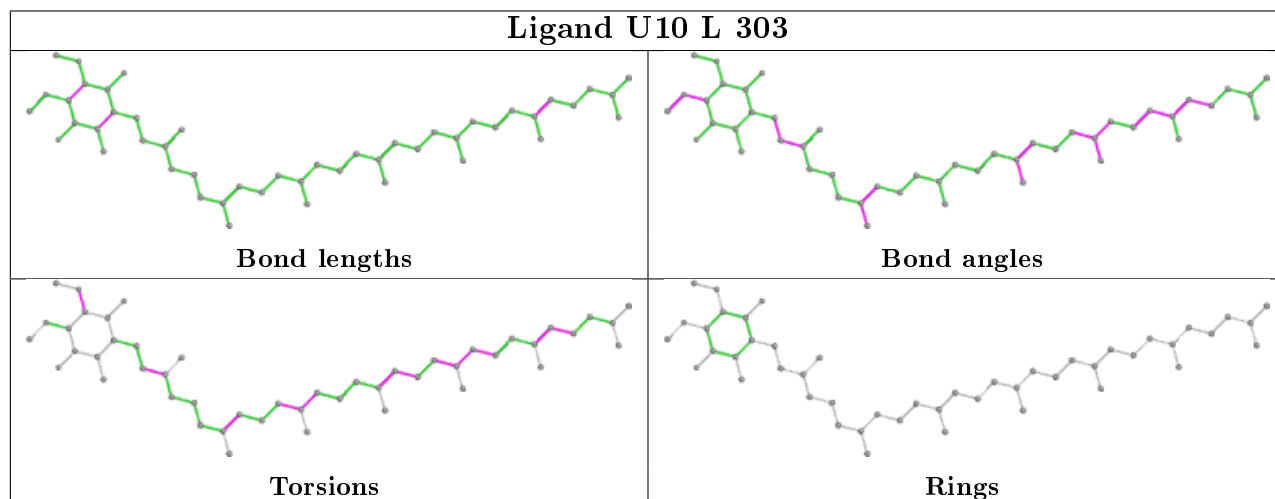
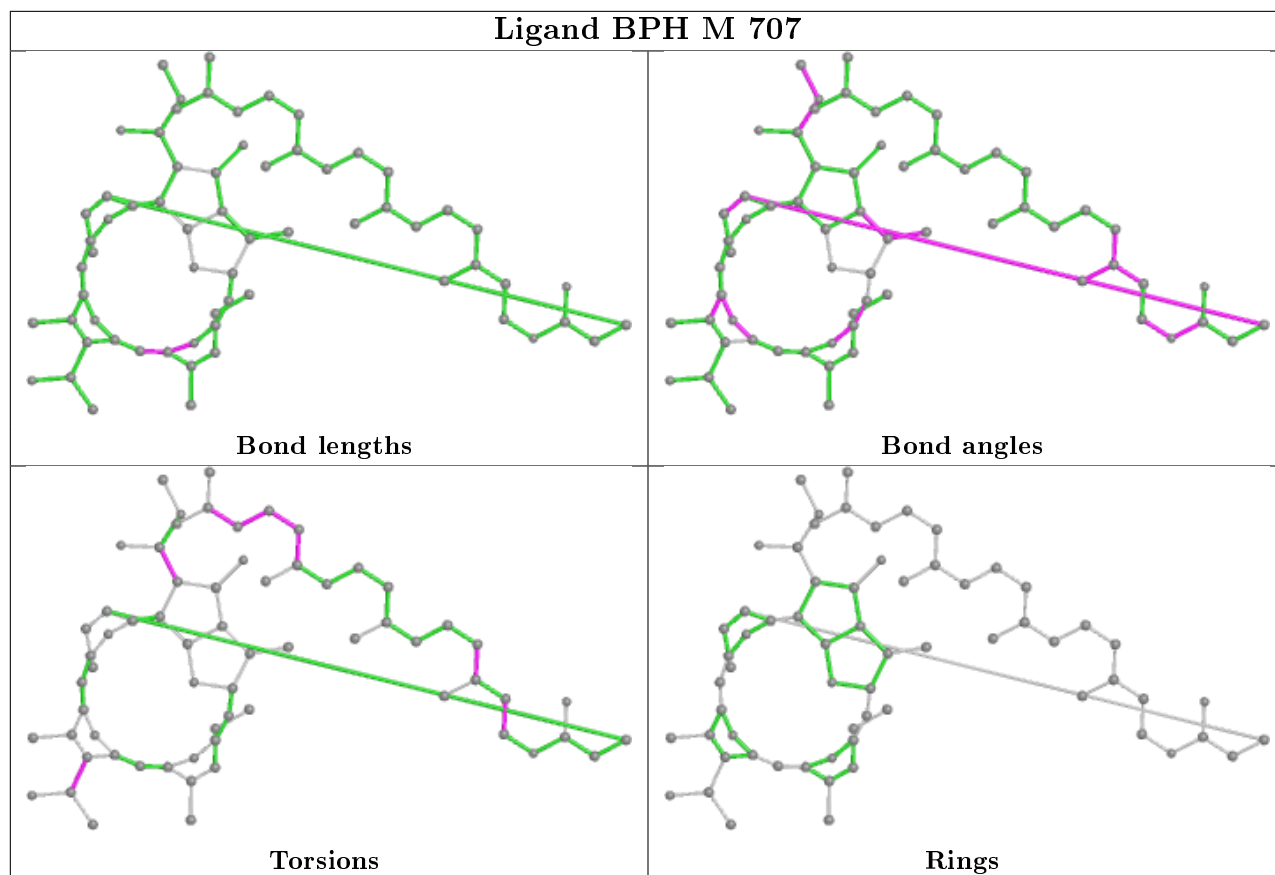
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

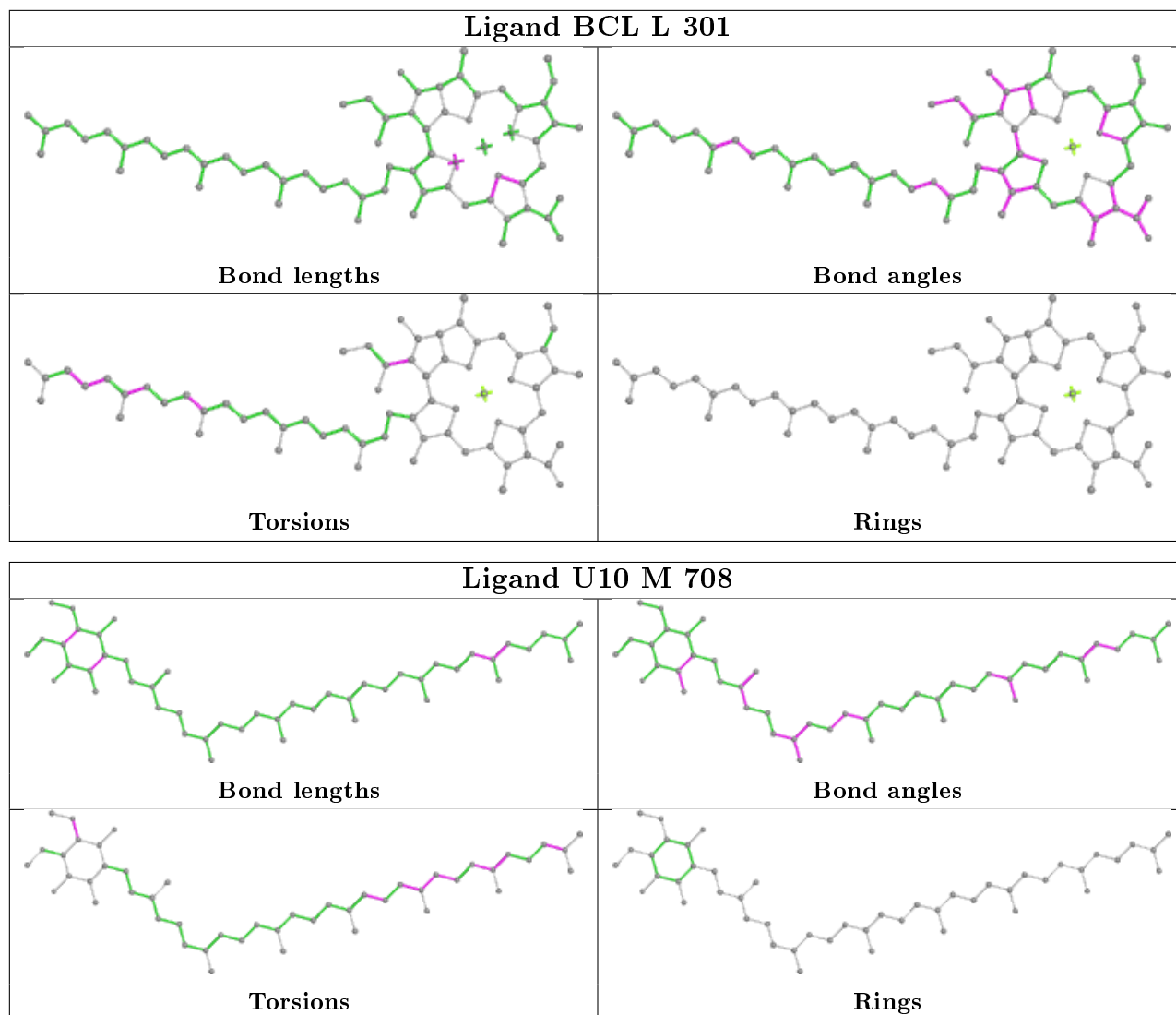
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	-0.43	8 (2%) 53 51	34, 49, 82, 106	0
2	M	300/307 (97%)	-0.58	4 (1%) 77 75	32, 53, 81, 107	0
3	H	239/260 (91%)	-0.54	4 (1%) 70 68	35, 49, 68, 109	0
All	All	820/848 (96%)	-0.52	16 (1%) 65 63	32, 50, 80, 109	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	59	TRP	5.4
3	H	249	LYS	4.4
3	H	245	ALA	3.4
1	L	72	GLU	3.1
2	M	301	HIS	3.1
1	L	281	GLY	3.0
3	H	246	PRO	2.7
1	L	270	PRO	2.6
1	L	277	GLY	2.4
3	H	247	LYS	2.3
1	L	202	LYS	2.3
2	M	3	TYR	2.3
1	L	276	PRO	2.2
2	M	109	LEU	2.1
2	M	302	GLY	2.1
1	L	71	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

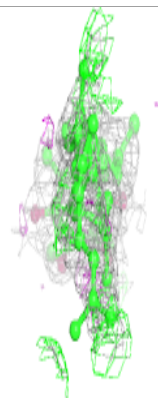
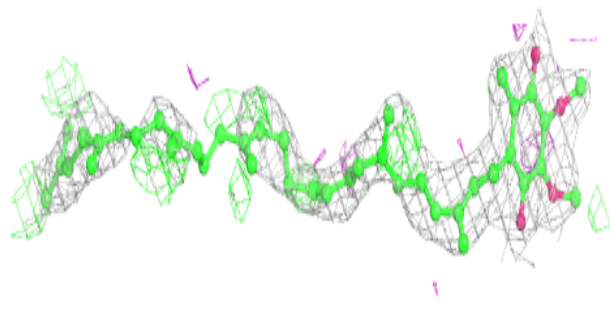
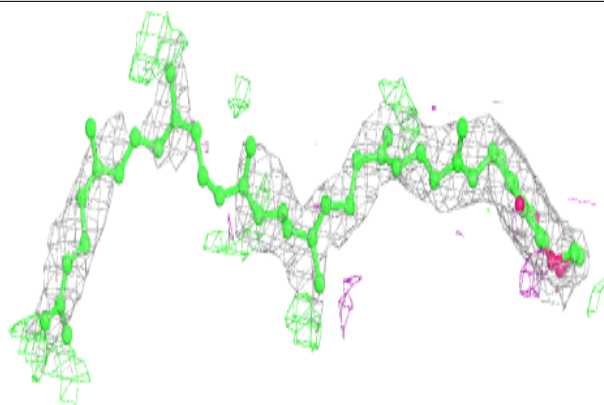
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	DD9	L	304	8/9	0.46	0.36	62,80,90,91	0
9	LDA	M	703	16/16	0.57	0.27	74,84,101,101	0
7	DD9	H	302	9/9	0.67	0.39	77,82,89,89	0
9	LDA	M	711	16/16	0.70	0.28	77,83,106,107	0
7	DD9	H	303	7/9	0.74	0.30	76,80,81,81	0
9	LDA	H	301	16/16	0.79	0.25	99,104,112,112	0
9	LDA	M	701	16/16	0.80	0.23	56,69,79,81	0
6	U10	L	303	48/63	0.81	0.24	55,90,113,120	0
11	CDL	M	710	78/100	0.89	0.20	48,80,97,99	0
5	BPH	M	707	65/65	0.89	0.16	41,52,120,124	0
10	SPN	M	709	43/43	0.89	0.18	46,60,86,93	0
9	LDA	M	702	16/16	0.91	0.18	67,70,77,77	0
6	U10	M	708	48/63	0.92	0.13	30,41,74,81	0
4	BCL	M	704	66/66	0.95	0.12	38,45,90,91	0
4	BCL	M	706	66/66	0.96	0.10	27,34,63,74	0
4	BCL	M	705	66/66	0.96	0.14	33,39,70,84	0
4	BCL	L	301	66/66	0.97	0.13	36,40,55,61	0
5	BPH	L	302	65/65	0.97	0.11	28,39,50,52	0
8	FE	L	305	1/1	0.99	0.07	37,37,37,37	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.

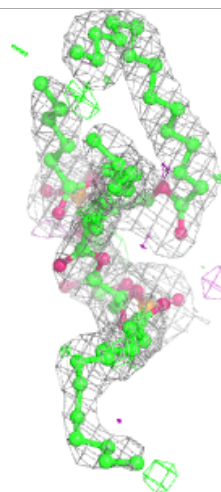
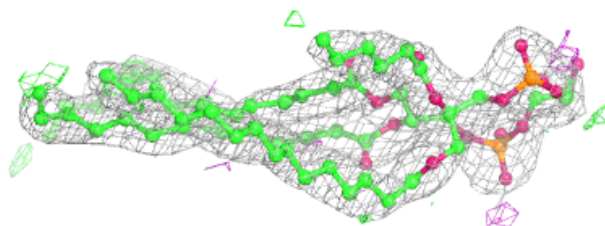
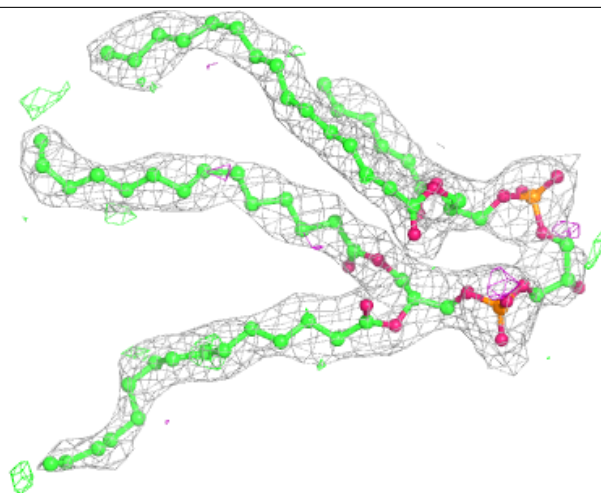
Electron density around U10 L 303:

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



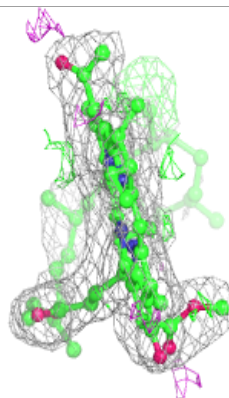
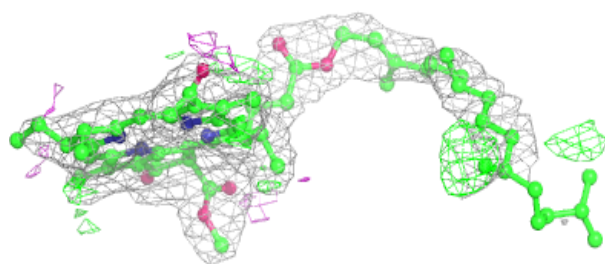
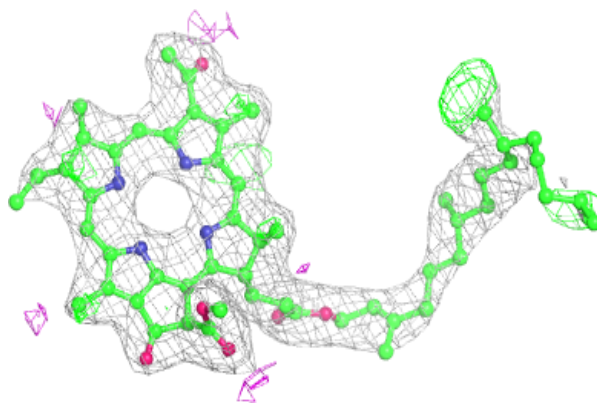
Electron density around CDL M 710:

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

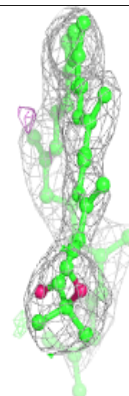
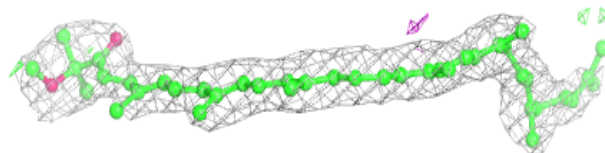
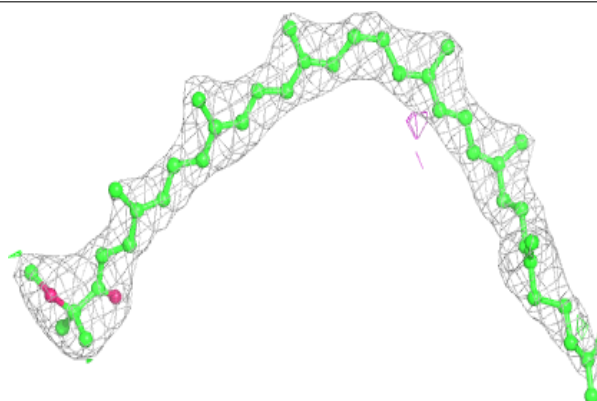


Electron density around BPH M 707:

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

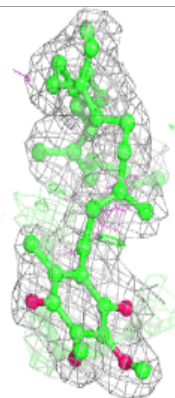
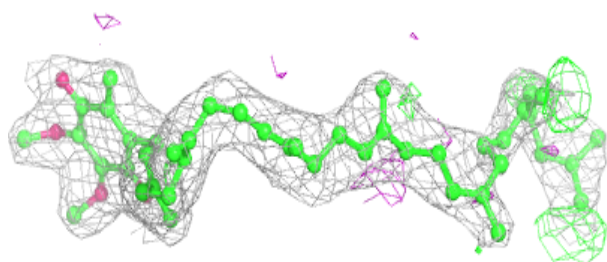
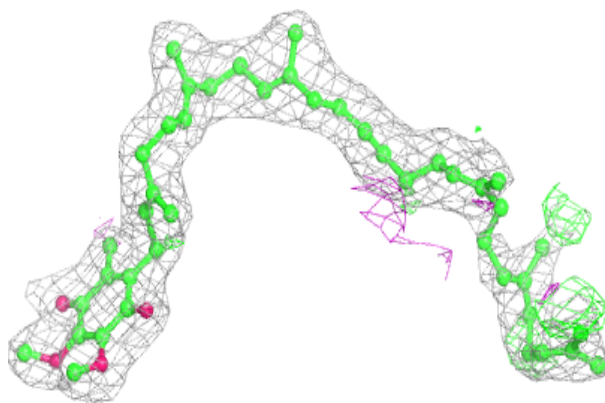
**Electron density around SPN M 709:**

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

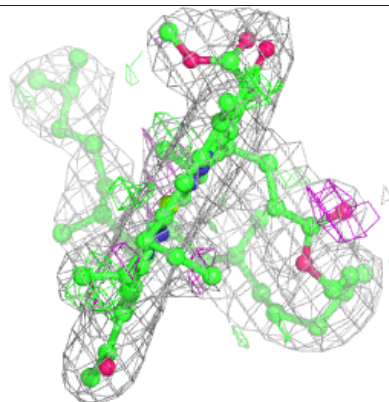
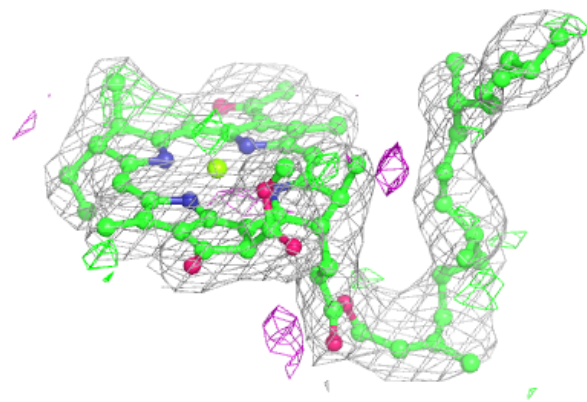
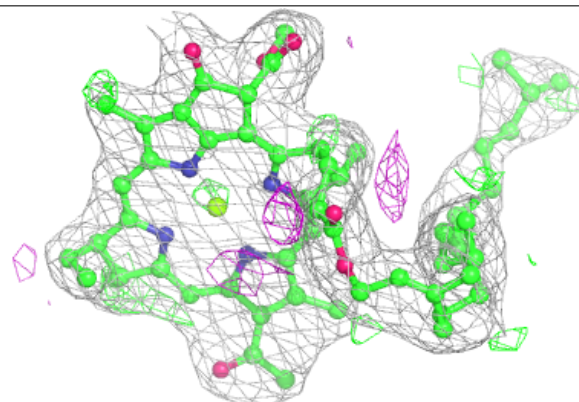


Electron density around U10 M 708:

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

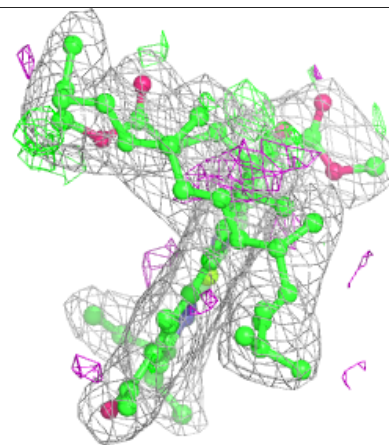
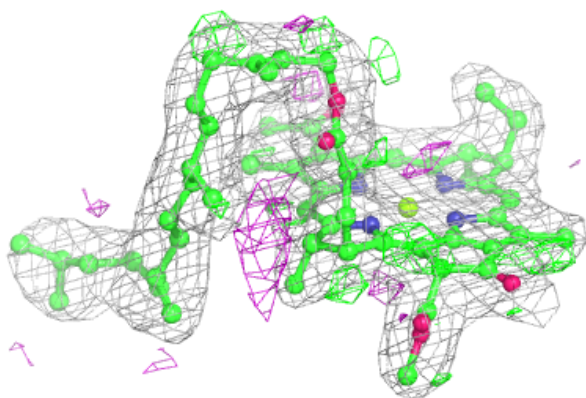
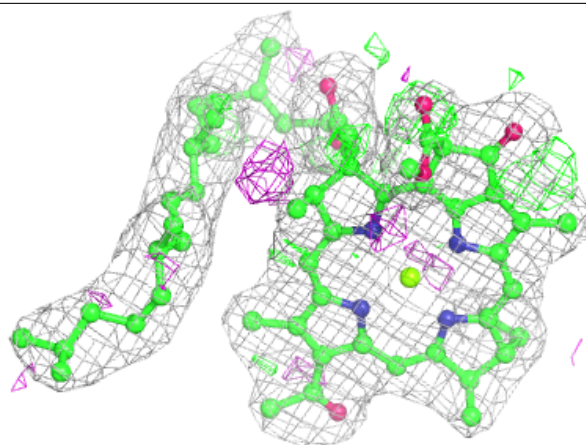
**Electron density around BCL M 704:**

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

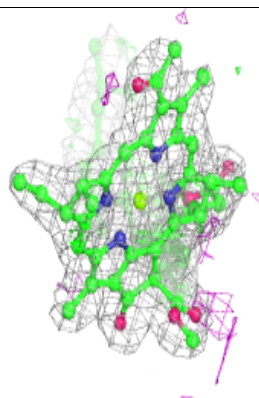
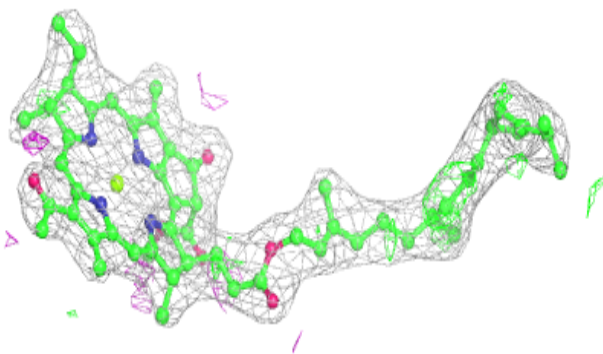
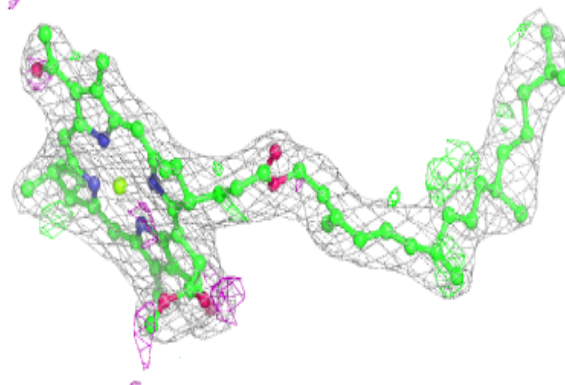


Electron density around BCL M 706:

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

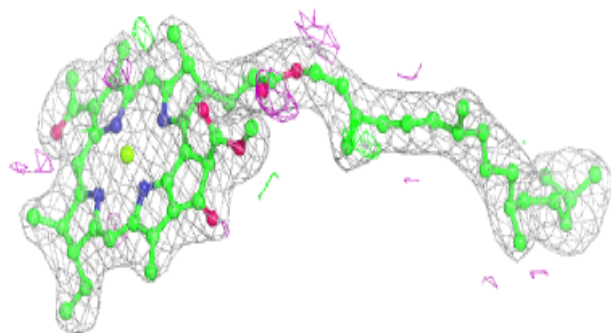
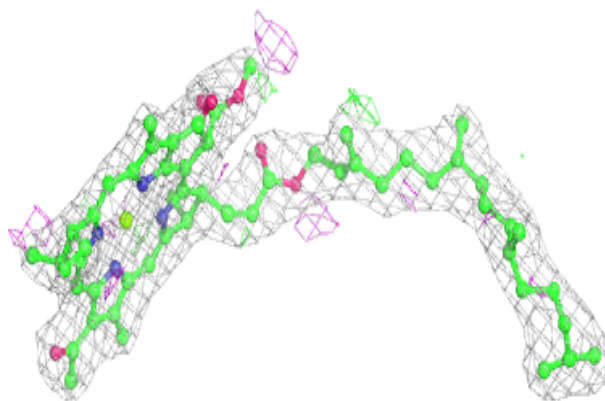
**Electron density around BCL M 705:**

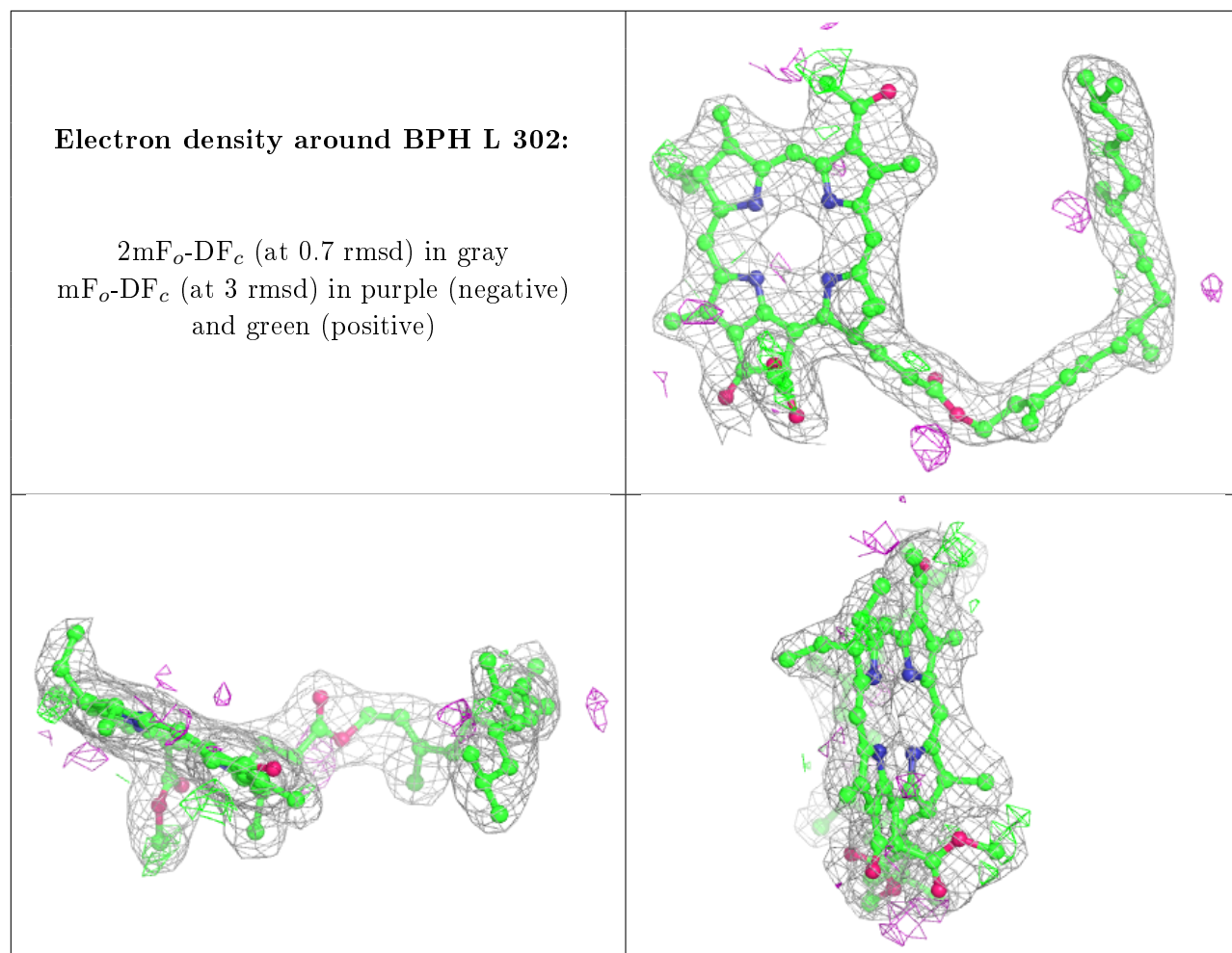
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL L 301:

$2mF_o-DF_c$ (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.