



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2022 – 04:21 am BST

PDB ID : 7OD5
Title : F(M197)H mutant structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV LSP crystallization
Authors : Gabdulkhakov, A.G.; Selikhanov, G.K.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on : 2021-04-28
Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

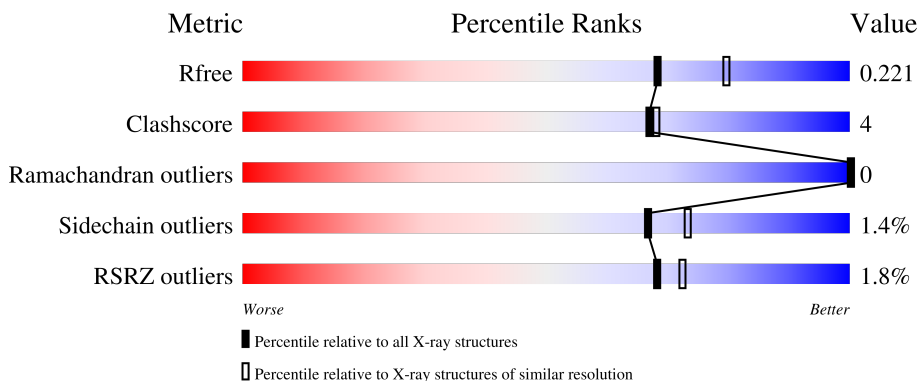
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	H	241	 2% 87% 13%
2	L	281	 2% 94% 5%
3	M	303	 % 89% 11%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7703 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	241	1880	1201	323	346	10	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2436	1650	388	390	8	0	22	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP P0C0Y8

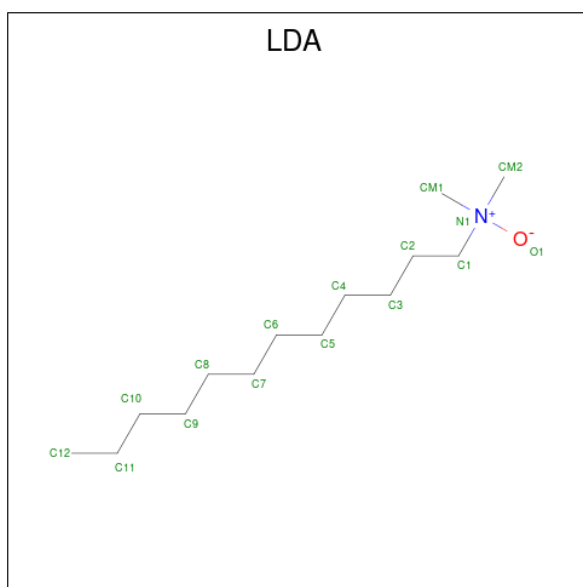
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2460	1639	404	405	12	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).

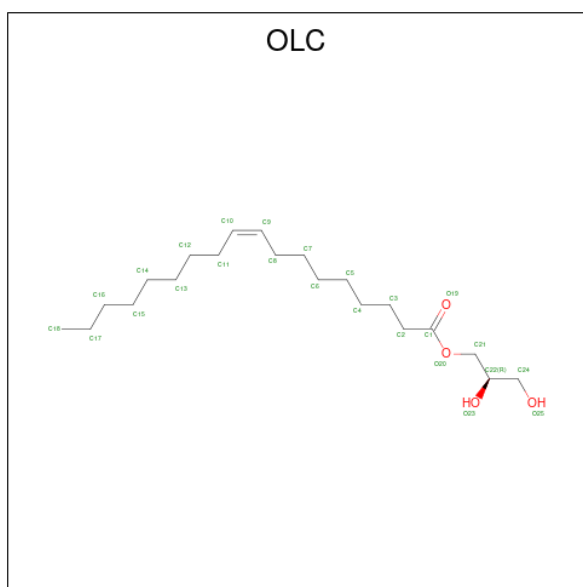


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

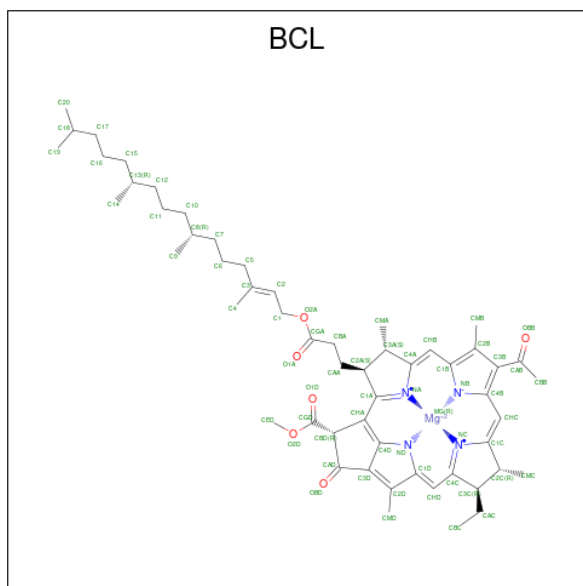
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	C	0	0
			15	15		
5	L	2	Total	C	0	0
			30	30		
5	M	1	Total	C	0	0
			15	15		

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	O			
			25	21	4	0	0	

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



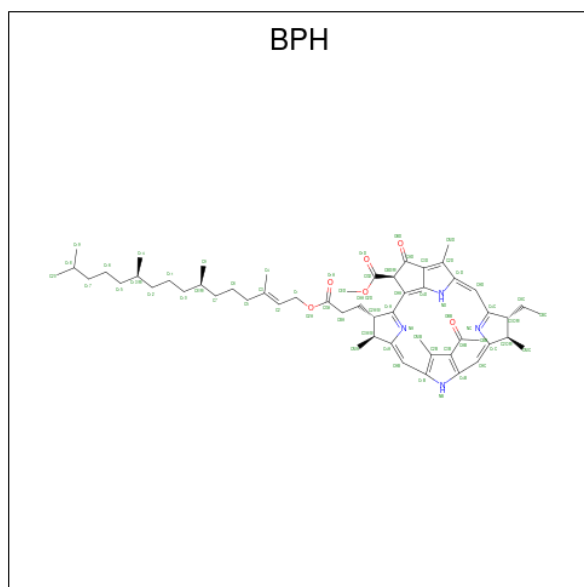
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O		
			66	55	1	4	6	0	0
7	L	1	Total	C	Mg	N	O		
			66	55	1	4	6	0	0

Continued on next page...

Continued from previous page...

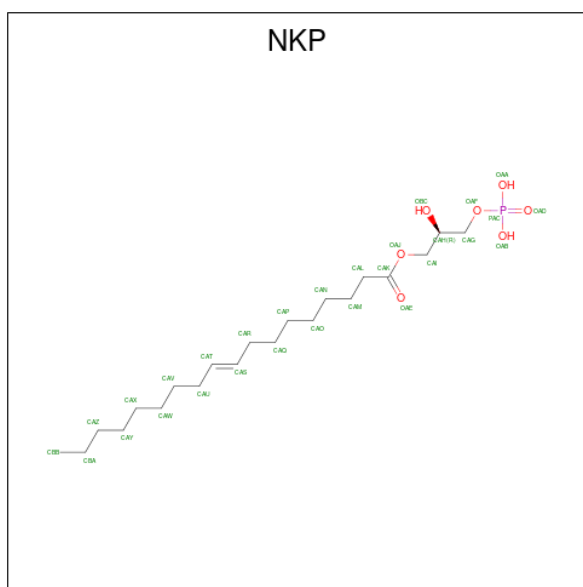
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 9 is (2R)-2-hydroxy-3-(phosphonoxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: $C_{21}H_{41}O_7P$).

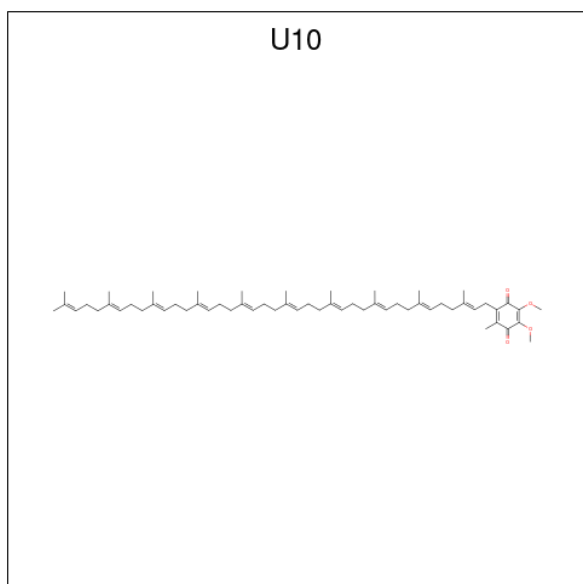


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
9	M	1	Total	C	O	P	0	0
			29	21	7	1		
9	M	1	Total	C	O	P	0	0
			29	21	7	1		

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

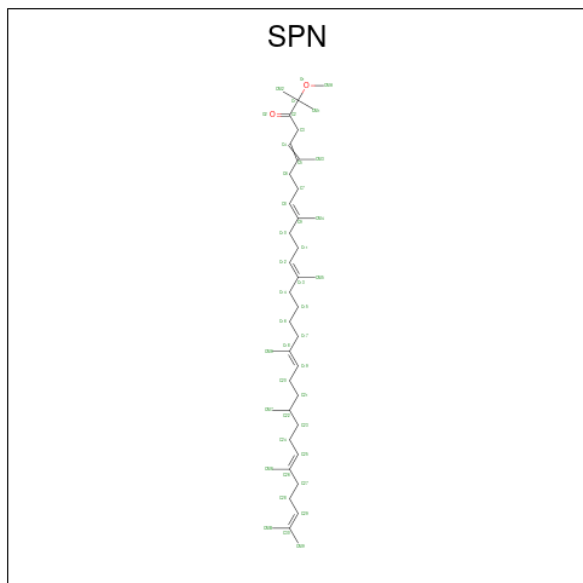
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



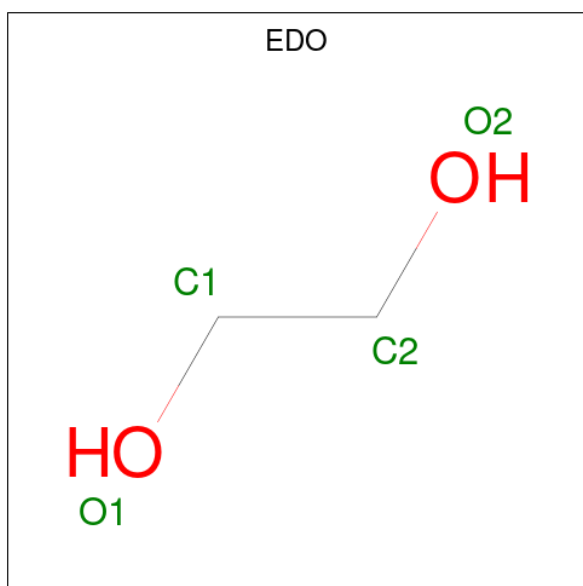
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	C O	0	0
			48	44 4		

- Molecule 12 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			4	2	2		

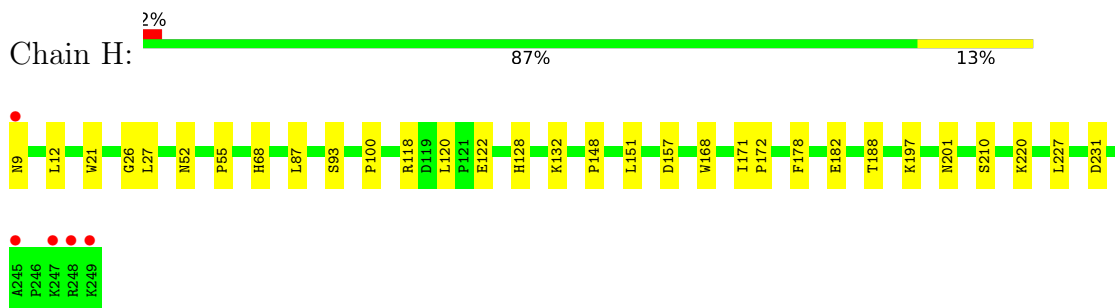
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	101	Total	O	0	0
			101	101		
14	L	65	Total	O	0	0
			65	65		
14	M	64	Total	O	0	0
			64	64		

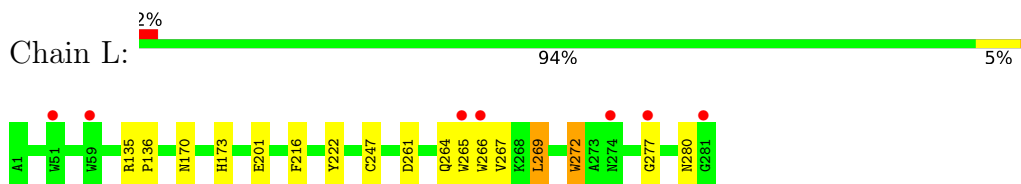
3 Residue-property plots [i](#)

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

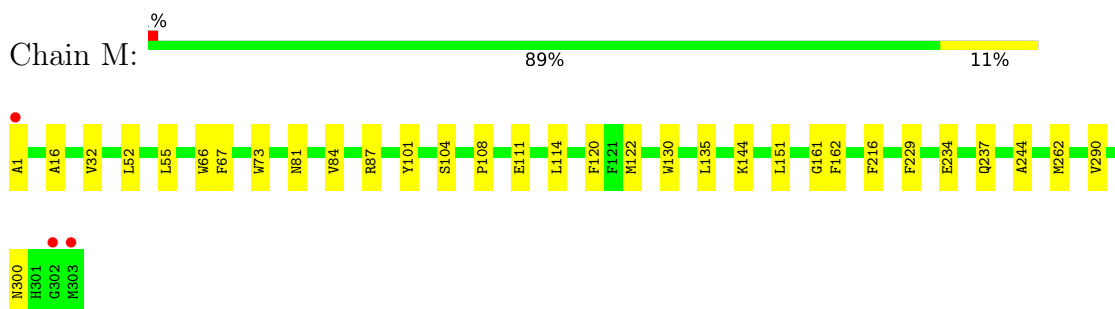
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.98Å 99.98Å 238.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 2.10 48.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.09-2.10) 100.0 (48.93-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 1.18_3861, PHENIX 1.18_3861	Depositor
R, R_{free}	0.179 , 0.221 0.181 , 0.221	Depositor DCC
R_{free} test set	2101 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, UNL, OLC, SPN, FE, LDA, EDO, U10, NKP, BPH

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	H	0.37	0/1932	0.55	0/2627
2	L	0.38	0/2539	0.49	0/3480
3	M	0.42	0/2552	0.50	0/3483
All	All	0.39	0/7023	0.51	0/9590

There are no bond length outliers.

There are no bond angle outliers.

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	H	1880	0	1883	22	0
2	L	2436	0	2365	14	0
3	M	2460	0	2376	23	0
4	H	32	0	62	4	0
4	M	32	0	62	2	0
5	H	15	0	0	0	0
5	L	30	0	0	0	0
5	M	15	0	0	0	0
6	L	25	0	40	1	0
7	L	132	0	148	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	132	0	148	1	0
8	L	65	0	76	0	0
8	M	65	0	76	0	0
9	M	58	0	78	2	0
10	M	1	0	0	0	0
11	M	48	0	63	0	0
12	M	43	0	70	6	0
13	M	4	0	6	0	0
14	H	101	0	0	5	0
14	L	65	0	0	1	0
14	M	64	0	0	0	0
All	All	7703	0	7453	58	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 (58) 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:L:267[A]:VAL:HG13	2:L:280[A]:ASN:HB3	1.63	0.80
2:L:277[B]:GLY:O	3:M:87:ARG:NH2	2.17	0.77
1:H:118[A]:ARG:HD3	1:H:120:LEU:HD12	1.64	0.77
3:M:161:GLY:HA3	12:M:409:SPN:H201	1.76	0.68
1:H:197:LYS:HD3	3:M:1:ALA:O	1.94	0.67
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.77	0.66
1:H:68:HIS:HD2	14:H:600:HOH:O	1.82	0.61
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.85	0.59
1:H:26:GLY:HA3	9:M:401:NKP:HAS	1.86	0.57
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.88	0.56
4:H:403:LDA:H121	4:M:410:LDA:H91	1.90	0.54
3:M:73:TRP:HB2	3:M:114[A]:LEU:HD23	1.89	0.53
1:H:182:GLU:HA	1:H:188:THR:HG22	1.92	0.52
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.92	0.52
7:M:404:BCL:HMB1	7:M:404:BCL:HBB3	1.92	0.52
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.92	0.52
3:M:81:ASN:HB3	3:M:84:VAL:HB	1.90	0.52
1:H:21:TRP:HZ2	4:M:410:LDA:HM13	1.74	0.52
1:H:220:LYS:HE3	14:H:502:HOH:O	2.10	0.51
1:H:132:LYS:HG2	14:H:505:HOH:O	2.12	0.50
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.93	0.50
1:H:55:PRO:HD3	4:H:401:LDA:H32	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:504:BCL:CAB	12:M:409:SPN:H162	2.44	0.48
7:L:504:BCL:C2B	12:M:409:SPN:H141	2.44	0.48
2:L:201:GLU:HG3	3:M:144:LYS:NZ	2.29	0.47
1:H:12:LEU:HD23	3:M:290:VAL:HG21	1.96	0.47
3:M:55:LEU:HD12	3:M:135:LEU:HD12	1.96	0.47
3:M:67:PHE:CE2	12:M:409:SPN:H61	2.49	0.47
1:H:201:ASN:OD1	1:H:201:ASN:N	2.44	0.46
1:H:128:HIS:HD2	14:H:510:HOH:O	1.98	0.46
1:H:68:HIS:HE1	14:H:536:HOH:O	1.97	0.46
2:L:272[A]:TRP:O	3:M:87:ARG:NH1	2.44	0.46
3:M:101:TYR:O	3:M:104:SER:HB3	2.16	0.46
2:L:264[A]:GLN:HG2	14:L:659:HOH:O	2.16	0.45
2:L:267[A]:VAL:HG13	2:L:280[A]:ASN:CB	2.41	0.45
1:H:157:ASP:OD1	1:H:210:SER:OG	2.32	0.45
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.98	0.45
1:H:9:ASN:ND2	3:M:300:ASN:O	2.50	0.44
1:H:52:ASN:ND2	4:H:401:LDA:O1	2.50	0.44
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.99	0.44
2:L:261[A]:ASP:O	2:L:264[A]:GLN:HB2	2.18	0.43
2:L:266[A]:TRP:HA	2:L:269[A]:LEU:HD22	2.00	0.43
3:M:237:GLN:HB3	3:M:262[B]:MET:HG3	1.98	0.43
1:H:27:LEU:HD13	9:M:401:NKP:HAOA	1.99	0.43
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.53	0.43
3:M:130:TRP:NE1	3:M:151[B]:LEU:HG	2.34	0.43
3:M:120:PHE:CD1	12:M:409:SPN:HMB2	2.54	0.43
2:L:170:ASN:O	2:L:173:HIS:HB3	2.19	0.42
4:H:403:LDA:HM11	4:H:403:LDA:H22	1.63	0.42
2:L:135:ARG:HB3	2:L:136:PRO:HD3	2.02	0.42
2:L:267[A]:VAL:HG22	2:L:280[A]:ASN:ND2	2.35	0.42
2:L:222:TYR:HB3	6:L:501:OLC:H11	2.02	0.41
7:L:505:BCL:CBB	7:L:505:BCL:HMB1	2.51	0.41
3:M:162:PHE:HD2	12:M:409:SPN:H242	1.86	0.41
2:L:201:GLU:HG3	3:M:144:LYS:HZ1	1.85	0.41
2:L:269[A]:LEU:HD12	2:L:269[A]:LEU:HA	1.93	0.41
3:M:234:GLU:HG2	3:M:262[A]:MET:SD	2.60	0.41
3:M:130:TRP:HE1	3:M:151[B]:LEU:HG	1.87	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	H	244/241 (101%)	240 (98%)	4 (2%)	0	100	100
2	L	300/281 (107%)	294 (98%)	6 (2%)	0	100	100
3	M	307/303 (101%)	297 (97%)	10 (3%)	0	100	100
All	All	851/825 (103%)	831 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	H	201/196 (103%)	199 (99%)	2 (1%)	76	82
2	L	238/220 (108%)	230 (97%)	8 (3%)	37	39
3	M	242/237 (102%)	239 (99%)	3 (1%)	71	77
All	All	681/653 (104%)	668 (98%)	13 (2%)	67	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	93	SER
1	H	231	ASP
2	L	216	PHE
2	L	247	CYS
2	L	265[A]	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	265[B]	TRP
2	L	269[A]	LEU
2	L	269[B]	LEU
2	L	272[A]	TRP
2	L	272[B]	TRP
3	M	52[A]	LEU
3	M	52[B]	LEU
3	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are unknown and 1 is monoatomic - leaving 16 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	$\# Z > 2$
8	BPH	L	506	-	64,70,70	0.96	4 (6%)	76,101,101	1.04	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	H	401	-	12,15,15	2.05	1 (8%)	14,17,17	0.57	0
12	SPN	M	409	-	40,42,42	0.58	1 (2%)	50,52,52	1.50	8 (16%)
13	EDO	M	412	-	3,3,3	0.37	0	2,2,2	1.15	0
7	BCL	L	504	-	58,74,74	1.32	5 (8%)	69,115,115	1.42	11 (15%)
11	U10	M	408	-	48,48,63	2.60	12 (25%)	58,61,79	1.83	17 (29%)
7	BCL	M	405	-	58,74,74	1.23	5 (8%)	69,115,115	1.29	9 (13%)
9	NKP	M	402	-	28,28,28	0.53	0	31,32,32	0.47	0
4	LDA	H	403	-	12,15,15	2.05	1 (8%)	14,17,17	0.63	0
6	OLC	L	501	-	24,24,24	0.94	1 (4%)	25,25,25	0.83	1 (4%)
7	BCL	M	404	-	58,74,74	1.24	4 (6%)	69,115,115	1.40	9 (13%)
7	BCL	L	505	-	58,74,74	1.32	4 (6%)	69,115,115	1.31	10 (14%)
8	BPH	M	406	-	64,70,70	0.98	3 (4%)	76,101,101	1.14	6 (7%)
4	LDA	M	410	-	12,15,15	2.00	1 (8%)	14,17,17	0.39	0
9	NKP	M	401	-	28,28,28	0.33	0	31,32,32	0.47	0
4	LDA	M	411	-	12,15,15	2.05	1 (8%)	14,17,17	0.50	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
8	BPH	L	506	-	-	5/54/105/105	0/5/6/6
4	LDA	H	401	-	-	7/13/13/13	-
12	SPN	M	409	-	-	12/50/51/51	-
13	EDO	M	412	-	-	1/1/1/1	-
7	BCL	L	504	-	-	1/37/137/137	-
11	U10	M	408	-	-	6/45/69/87	0/1/1/1
7	BCL	M	405	-	-	4/37/137/137	-
9	NKP	M	402	-	-	10/28/28/28	-
4	LDA	H	403	-	-	5/13/13/13	-
6	OLC	L	501	-	-	9/24/24/24	-
7	BCL	M	404	-	-	1/37/137/137	-
7	BCL	L	505	-	-	1/37/137/137	-
8	BPH	M	406	-	-	14/54/105/105	0/5/6/6
4	LDA	M	410	-	-	6/13/13/13	-
9	NKP	M	401	-	-	6/28/28/28	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	411	-	-	4/13/13/13	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	403	LDA	O1-N1	-7.06	1.25	1.42
4	H	401	LDA	O1-N1	-7.06	1.25	1.42
4	M	411	LDA	O1-N1	-7.00	1.25	1.42
4	M	410	LDA	O1-N1	-6.74	1.26	1.42
11	M	408	U10	C8-C9	6.10	1.47	1.33
11	M	408	U10	C33-C34	6.02	1.47	1.33
11	M	408	U10	C28-C29	5.97	1.47	1.33
11	M	408	U10	C18-C19	5.93	1.47	1.33
11	M	408	U10	C23-C24	5.74	1.46	1.33
11	M	408	U10	C13-C14	5.60	1.46	1.33
11	M	408	U10	C38-C39	5.18	1.47	1.32
7	L	504	BCL	C1B-NB	5.14	1.39	1.35
7	M	404	BCL	C1B-NB	4.91	1.39	1.35
7	L	505	BCL	MG-NA	4.85	2.17	2.06
7	M	405	BCL	C1B-NB	4.84	1.39	1.35
11	M	408	U10	O3-C3	-4.83	1.25	1.36
7	L	505	BCL	C1B-NB	4.78	1.39	1.35
11	M	408	U10	O4-C4	-4.64	1.25	1.36
7	M	404	BCL	MG-NA	4.53	2.17	2.06
7	M	405	BCL	MG-NA	4.42	2.16	2.06
7	L	504	BCL	MG-NA	4.10	2.16	2.06
6	L	501	OLC	O20-C1	4.03	1.45	1.33
7	L	504	BCL	MG-NC	3.45	2.14	2.06
7	L	505	BCL	MG-NC	3.43	2.14	2.06
11	M	408	U10	C6-C1	3.14	1.40	1.35
7	L	504	BCL	OBD-CAD	3.13	1.26	1.22
11	M	408	U10	C3-C2	-2.90	1.40	1.48
7	M	404	BCL	MG-NC	2.89	2.13	2.06
8	M	406	BPH	C3D-CAD	-2.76	1.41	1.47
7	M	405	BCL	OBD-CAD	2.73	1.26	1.22
8	L	506	BPH	CHC-C1C	2.67	1.42	1.36
8	M	406	BPH	CHC-C1C	2.62	1.41	1.36
8	L	506	BPH	C3D-CAD	-2.60	1.42	1.47
8	L	506	BPH	C1B-C2B	-2.55	1.40	1.45
11	M	408	U10	C4-C5	-2.52	1.41	1.48
7	M	405	BCL	MG-NC	2.50	2.12	2.06
8	M	406	BPH	C1B-C2B	-2.33	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	505	BCL	C4B-NB	2.31	1.37	1.35
7	M	405	BCL	C4B-NB	2.30	1.37	1.35
12	M	409	SPN	C1-C2	-2.26	1.51	1.53
7	L	504	BCL	C4B-NB	2.23	1.37	1.35
8	L	506	BPH	C1-C2	2.11	1.55	1.49
7	M	404	BCL	C4B-NB	2.08	1.37	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	409	SPN	CM6-C18-C17	4.45	122.76	115.27
7	M	404	BCL	C4A-NA-C1A	4.42	108.69	106.71
7	L	504	BCL	CMB-C2B-C1B	-4.21	121.99	128.46
7	L	505	BCL	CMB-C2B-C1B	-4.20	122.01	128.46
11	M	408	U10	C32-C33-C34	-4.06	117.89	127.66
11	M	408	U10	C30-C29-C31	4.04	122.06	115.27
7	M	405	BCL	CMB-C2B-C1B	-3.95	122.40	128.46
7	M	404	BCL	CMB-C2B-C1B	-3.84	122.57	128.46
12	M	409	SPN	CM3-C5-C6	3.59	121.31	115.27
11	M	408	U10	C15-C14-C16	3.56	121.27	115.27
7	M	405	BCL	OBD-CAD-CBD	-3.45	120.96	125.89
11	M	408	U10	C22-C23-C24	-3.42	119.42	127.66
8	L	506	BPH	C1C-NC-C4C	-3.41	107.54	110.54
12	M	409	SPN	CM5-C13-C14	3.36	120.92	115.27
11	M	408	U10	C35-C34-C36	3.27	120.78	115.27
11	M	408	U10	C17-C18-C19	-3.27	119.80	127.66
7	M	404	BCL	CAD-C3D-C4D	-3.25	106.66	108.47
8	L	506	BPH	OBD-CAD-CBD	-3.25	121.26	125.89
7	M	404	BCL	CHA-C1A-NA	-3.24	118.98	126.40
7	M	404	BCL	C1-C2-C3	-3.11	120.67	126.04
7	M	405	BCL	CAD-C3D-C4D	-3.10	106.74	108.47
7	M	405	BCL	CHA-C1A-NA	-3.07	119.36	126.40
8	M	406	BPH	OBD-CAD-CBD	-3.06	121.52	125.89
7	L	504	BCL	CMB-C2B-C3B	3.06	130.41	124.68
7	L	505	BCL	CMB-C2B-C3B	3.05	130.38	124.68
7	L	505	BCL	OBD-CAD-CBD	-3.04	121.55	125.89
11	M	408	U10	C37-C38-C39	-3.03	117.39	127.75
7	L	504	BCL	OBD-CAD-CBD	-3.01	121.59	125.89
7	L	505	BCL	CAD-C3D-C4D	-2.95	106.83	108.47
7	M	404	BCL	OBD-CAD-CBD	-2.91	121.74	125.89
7	L	504	BCL	CHA-C1A-NA	-2.90	119.75	126.40
7	M	404	BCL	C2A-C1A-CHA	2.90	128.93	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	405	BCL	CMB-C2B-C3B	2.88	130.06	124.68
6	L	501	OLC	O20-C1-O19	-2.88	116.33	123.59
7	L	505	BCL	CHA-C1A-NA	-2.88	119.81	126.40
7	L	505	BCL	C2A-C1A-CHA	2.84	128.83	123.86
11	M	408	U10	C27-C28-C29	-2.82	120.88	127.66
7	M	404	BCL	CMB-C2B-C3B	2.78	129.87	124.68
7	L	504	BCL	CMD-C2D-C3D	2.74	129.80	124.68
7	L	504	BCL	C2A-C1A-CHA	2.71	128.59	123.86
7	M	405	BCL	C2A-C1A-CHA	2.67	128.53	123.86
8	M	406	BPH	CHC-C1C-NC	-2.63	122.08	125.20
11	M	408	U10	C25-C24-C26	2.62	119.67	115.27
7	L	504	BCL	C4A-NA-C1A	2.59	107.87	106.71
7	L	505	BCL	C4A-NA-C1A	2.57	107.86	106.71
8	M	406	BPH	C1C-NC-C4C	-2.49	108.35	110.54
12	M	409	SPN	CM4-C9-C10	2.48	119.44	115.27
7	L	504	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
7	L	504	BCL	CAD-C3D-C4D	-2.47	107.09	108.47
7	M	404	BCL	CMD-C2D-C3D	2.43	129.23	124.68
11	M	408	U10	C41-C39-C40	2.38	119.87	114.60
11	M	408	U10	C12-C13-C14	-2.37	121.95	127.66
7	M	405	BCL	CMD-C2D-C3D	2.34	129.06	124.68
8	M	406	BPH	C3A-C4A-CHB	2.34	125.87	121.83
8	L	506	BPH	CMD-C2D-C3D	2.29	128.97	124.68
8	M	406	BPH	CMD-C2D-C3D	2.28	128.94	124.68
7	L	505	BCL	CMD-C2D-C3D	2.26	128.90	124.68
8	M	406	BPH	C11-C12-C13	2.26	123.21	115.92
11	M	408	U10	C26-C27-C28	-2.24	104.52	111.88
11	M	408	U10	C10-C9-C11	2.22	119.00	115.27
7	L	505	BCL	C1C-NC-C4C	2.20	107.69	106.71
11	M	408	U10	C1M-C1-C6	-2.18	120.85	124.40
7	M	405	BCL	OBB-CAB-CBB	-2.16	115.30	120.17
11	M	408	U10	C32-C31-C29	-2.14	105.94	112.98
12	M	409	SPN	C24-C25-C26	-2.14	122.51	127.66
12	M	409	SPN	C24-C23-C22	-2.13	108.39	115.76
7	L	505	BCL	OBB-CAB-CBB	-2.12	115.41	120.17
11	M	408	U10	C22-C21-C19	-2.11	106.03	112.98
7	L	504	BCL	C6-C7-C8	2.08	122.65	115.92
11	M	408	U10	C4M-O4-C4	2.08	123.82	116.47
12	M	409	SPN	CM8-C26-C27	2.07	118.76	115.27
7	M	405	BCL	C4B-C3B-CAB	-2.07	123.13	127.13
12	M	409	SPN	CMB-C30-CM9	2.03	119.10	114.60
7	L	504	BCL	C4B-C3B-CAB	-2.03	123.22	127.13

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	403	LDA	C2-C1-N1-O1
4	H	403	LDA	C2-C1-N1-CM1
4	M	410	LDA	C2-C1-N1-CM1
4	M	410	LDA	C2-C1-N1-CM2
6	L	501	OLC	O20-C21-C22-O23
8	M	406	BPH	C4B-C3B-CAB-CBB
8	M	406	BPH	C4B-C3B-CAB-OBB
8	M	406	BPH	C2B-C3B-CAB-CBB
12	M	409	SPN	CM1-C1-O1-CMA
12	M	409	SPN	CM2-C1-O1-CMA
12	M	409	SPN	C2-C1-O1-CMA
12	M	409	SPN	C4-C5-C6-C7
12	M	409	SPN	CM3-C5-C6-C7
9	M	402	NKP	OAE-CAK-OAJ-CAI
9	M	402	NKP	CAL-CAK-OAJ-CAI
12	M	409	SPN	C11-C10-C9-CM4
12	M	409	SPN	C16-C17-C18-CM6
12	M	409	SPN	C11-C10-C9-C8
12	M	409	SPN	C16-C17-C18-C19
11	M	408	U10	C24-C26-C27-C28
6	L	501	OLC	O20-C21-C22-C24
8	M	406	BPH	C11-C12-C13-C14
11	M	408	U10	C32-C33-C34-C35
12	M	409	SPN	C26-C27-C28-C29
9	M	401	NKP	OAF-CAG-CAH-OBC
8	M	406	BPH	C5-C6-C7-C8
9	M	402	NKP	CAT-CAU-CAV-CAW
4	H	401	LDA	C6-C7-C8-C9
8	M	406	BPH	C2B-C3B-CAB-OBB
9	M	401	NKP	CAU-CAV-CAW-CAX
4	H	401	LDA	C5-C6-C7-C8
9	M	402	NKP	CAN-CAO-CAP-CAQ
6	L	501	OLC	C14-C15-C16-C17
9	M	401	NKP	CAK-CAL-CAM-CAN
4	H	401	LDA	C2-C3-C4-C5
9	M	401	NKP	CAR-CAS-CAT-CAU
4	M	411	LDA	C7-C8-C9-C10
4	H	403	LDA	C1-C2-C3-C4
9	M	401	NKP	OAF-CAG-CAH-CAI
11	M	408	U10	C32-C33-C34-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	M	406	BPH	C8-C10-C11-C12
4	M	411	LDA	C5-C6-C7-C8
8	M	406	BPH	C11-C12-C13-C15
4	H	401	LDA	C1-C2-C3-C4
9	M	402	NKP	CAP-CAQ-CAR-CAS
6	L	501	OLC	C6-C7-C8-C9
4	H	401	LDA	C7-C8-C9-C10
4	H	401	LDA	C9-C10-C11-C12
6	L	501	OLC	C15-C16-C17-C18
4	M	410	LDA	C1-C2-C3-C4
9	M	402	NKP	CAY-CAZ-CBA-CBB
9	M	402	NKP	CAW-CAX-CAY-CAZ
12	M	409	SPN	C21-C22-C23-C24
4	H	403	LDA	C9-C10-C11-C12
7	M	405	BCL	C13-C15-C16-C17
4	M	411	LDA	C1-C2-C3-C4
8	L	506	BPH	C4-C3-C5-C6
4	M	410	LDA	C3-C4-C5-C6
7	M	405	BCL	C14-C13-C15-C16
7	L	505	BCL	CAD-CBD-CGD-O2D
7	M	405	BCL	CAD-CBD-CGD-O2D
8	M	406	BPH	C16-C17-C18-C19
4	H	403	LDA	C7-C8-C9-C10
8	M	406	BPH	C16-C17-C18-C20
4	M	410	LDA	C2-C1-N1-O1
7	L	504	BCL	C11-C12-C13-C15
8	L	506	BPH	C2-C3-C5-C6
6	L	501	OLC	C12-C13-C14-C15
13	M	412	EDO	O1-C1-C2-O2
7	M	405	BCL	C12-C13-C15-C16
12	M	409	SPN	CM7-C22-C23-C24
9	M	402	NKP	CAQ-CAR-CAS-CAT
4	H	401	LDA	N1-C1-C2-C3
9	M	402	NKP	CAG-CAH-CAI-OAJ
9	M	402	NKP	CAR-CAS-CAT-CAU
8	L	506	BPH	O2A-C1-C2-C3
8	M	406	BPH	C10-C11-C12-C13
11	M	408	U10	C34-C36-C37-C38
4	M	411	LDA	C9-C10-C11-C12
8	M	406	BPH	C11-C10-C8-C9
7	M	404	BCL	CAA-CBA-CGA-O2A
8	L	506	BPH	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

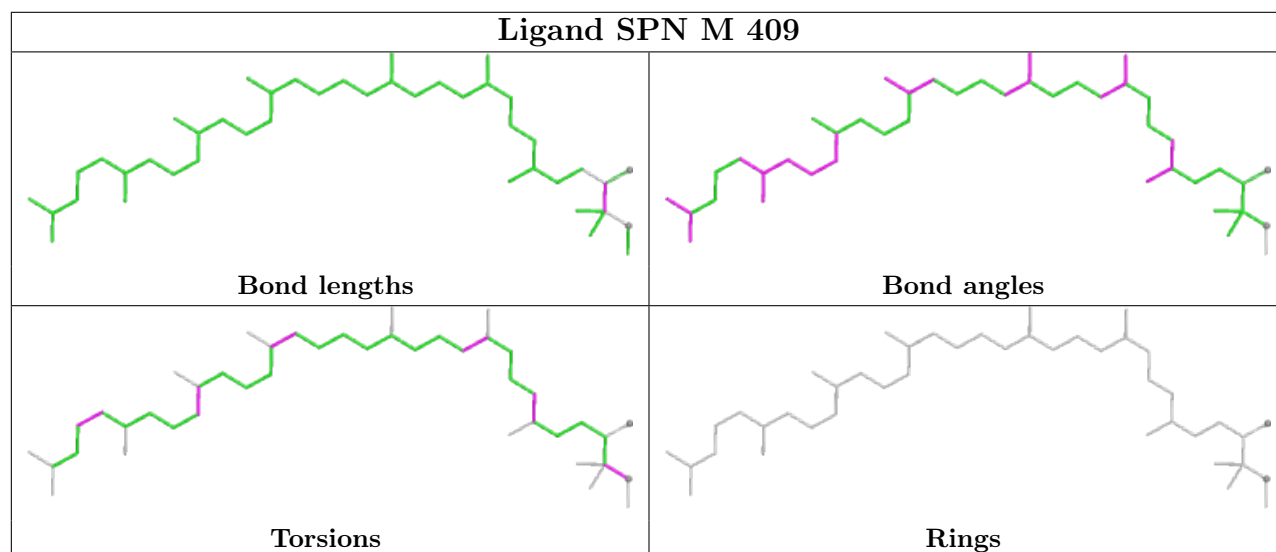
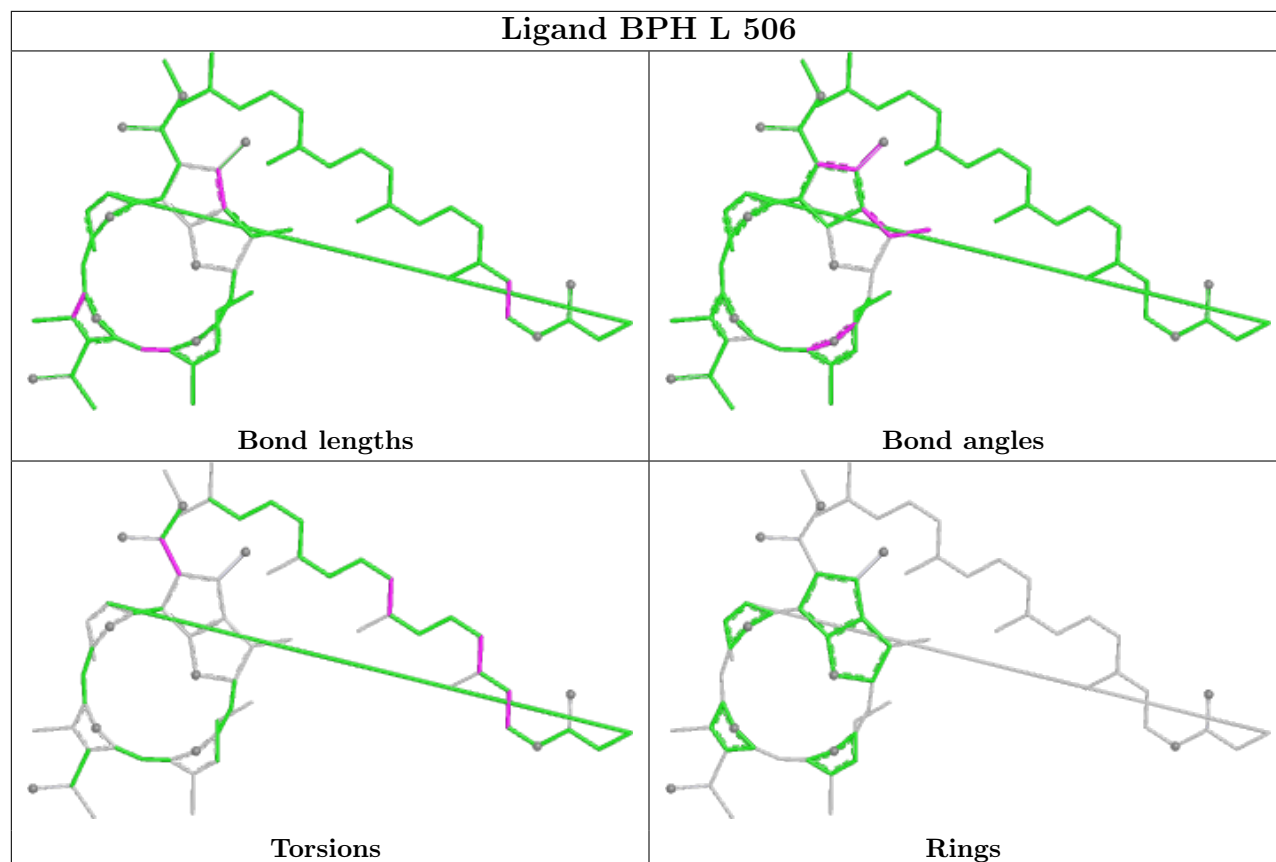
Mol	Chain	Res	Type	Atoms
8	M	406	BPH	CAD-CBD-CGD-O2D
11	M	408	U10	C29-C31-C32-C33
8	M	406	BPH	O2A-C1-C2-C3
6	L	501	OLC	C7-C8-C9-C10
11	M	408	U10	C5-C4-O4-C4M
6	L	501	OLC	C9-C10-C11-C12
9	M	401	NKP	CAL-CAM-CAN-CAO
8	L	506	BPH	C11-C10-C8-C9
4	M	410	LDA	C9-C10-C11-C12
6	L	501	OLC	O20-C1-C2-C3

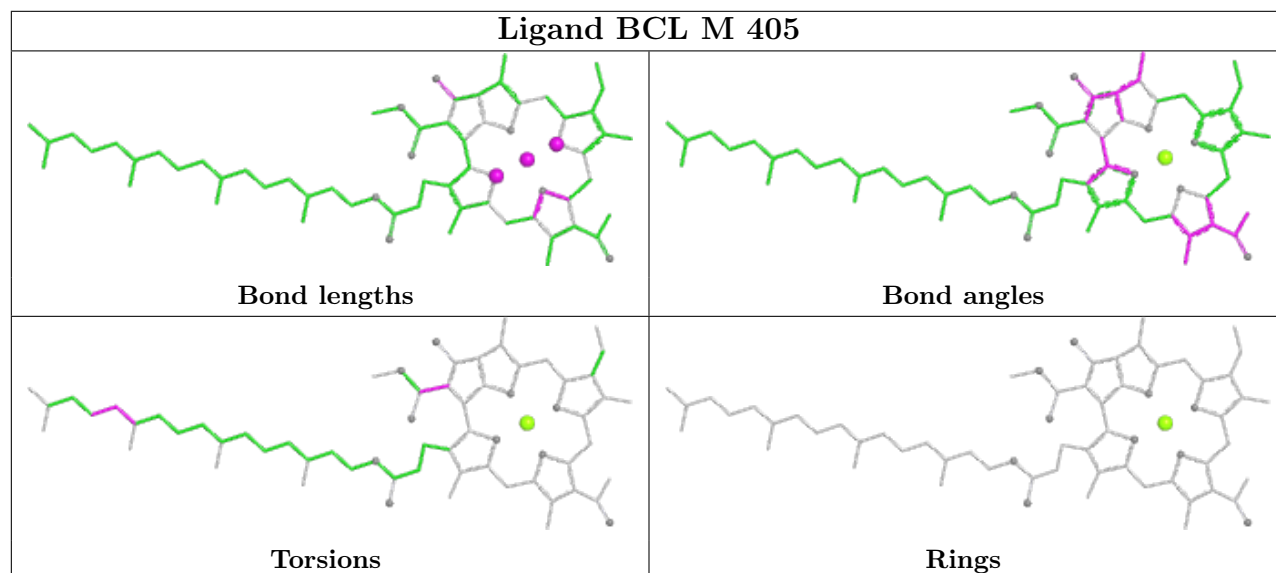
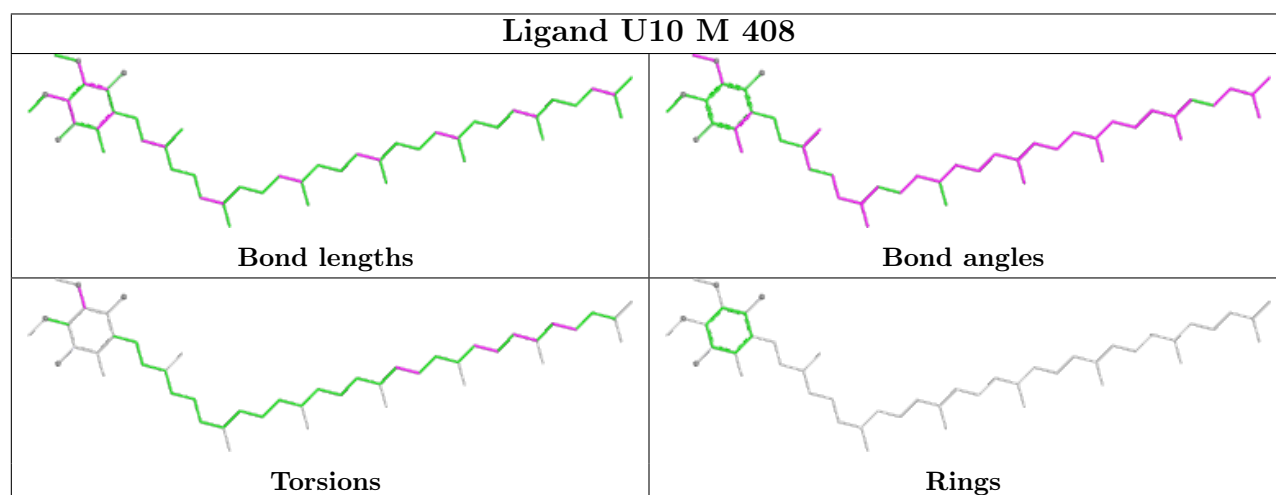
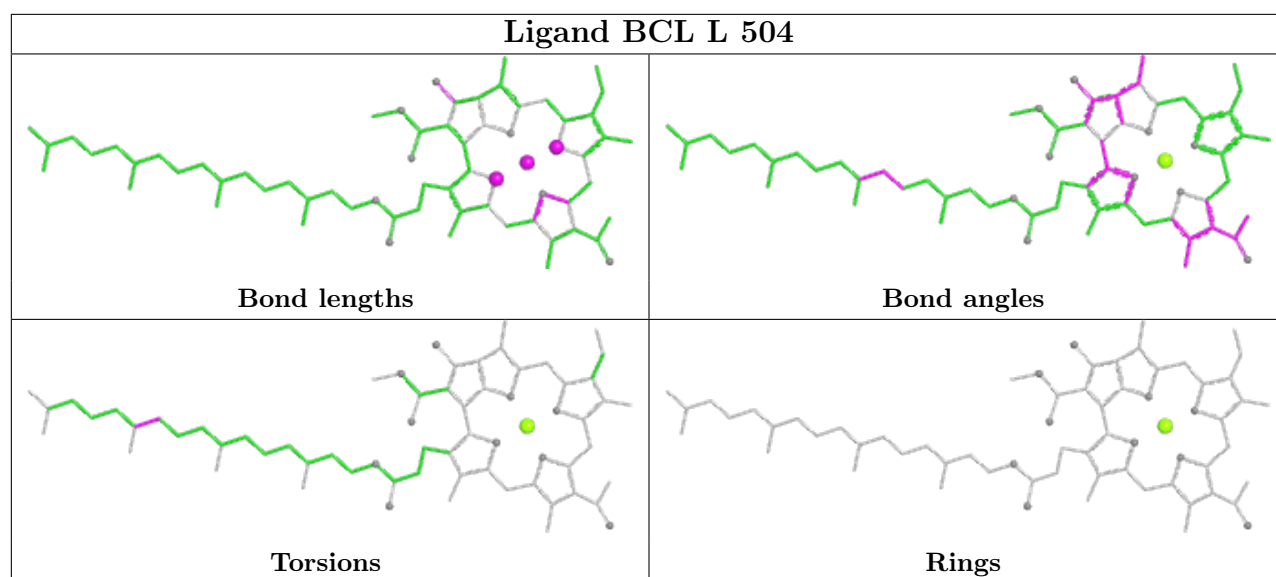
There are no ring outliers.

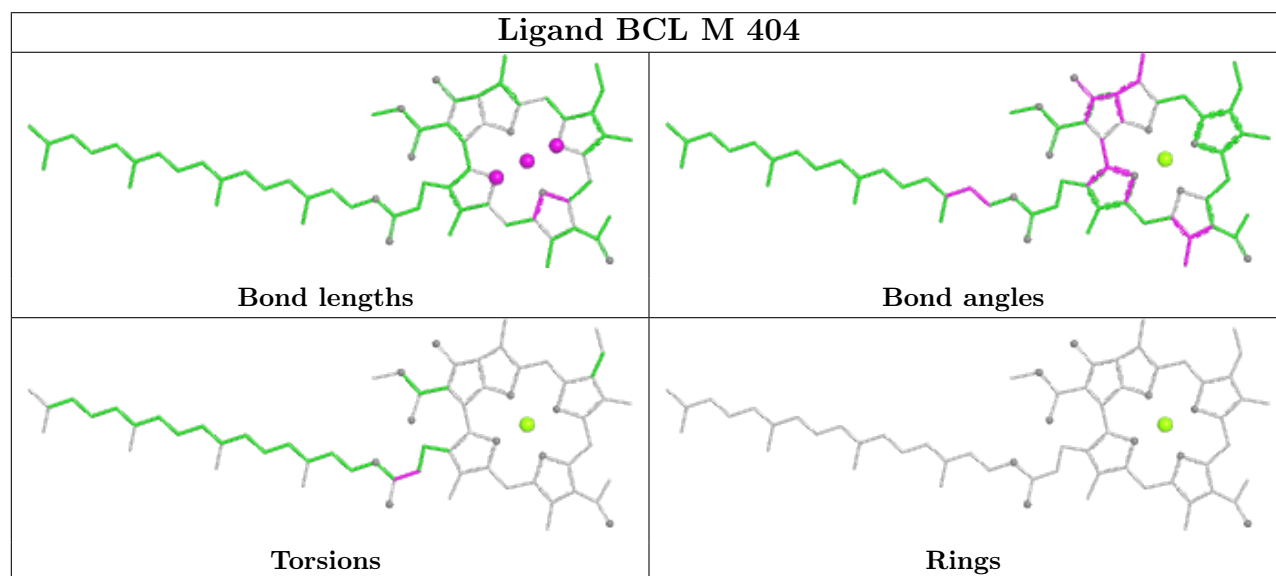
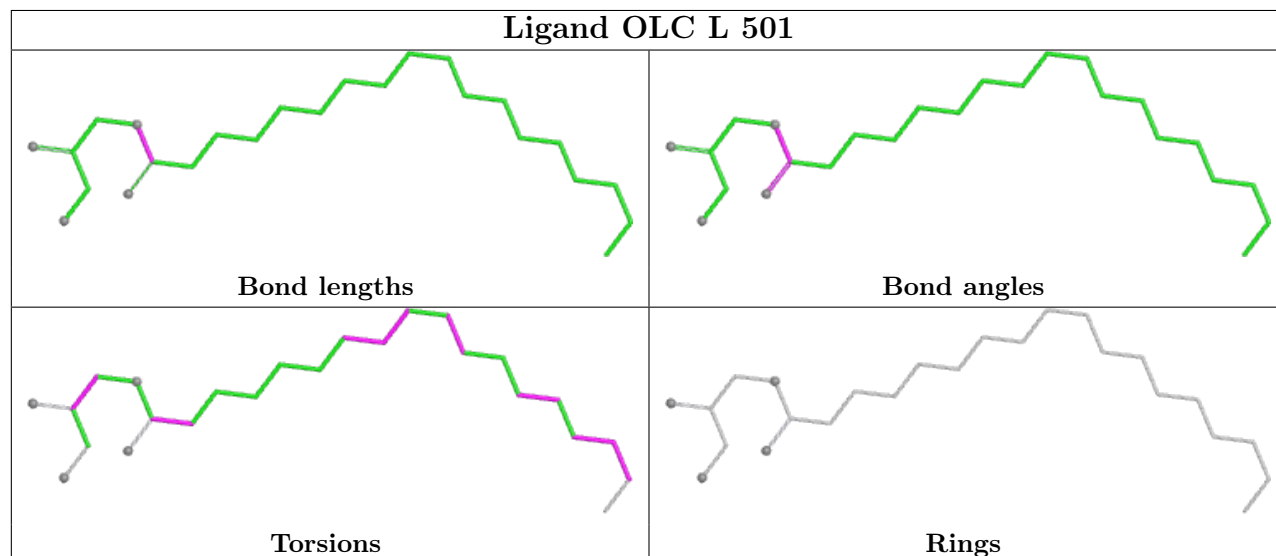
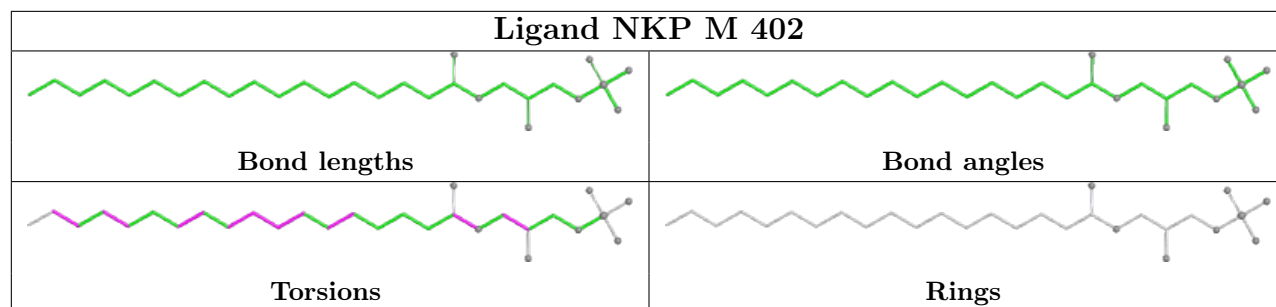
9 monomers are involved in 16 short contacts:

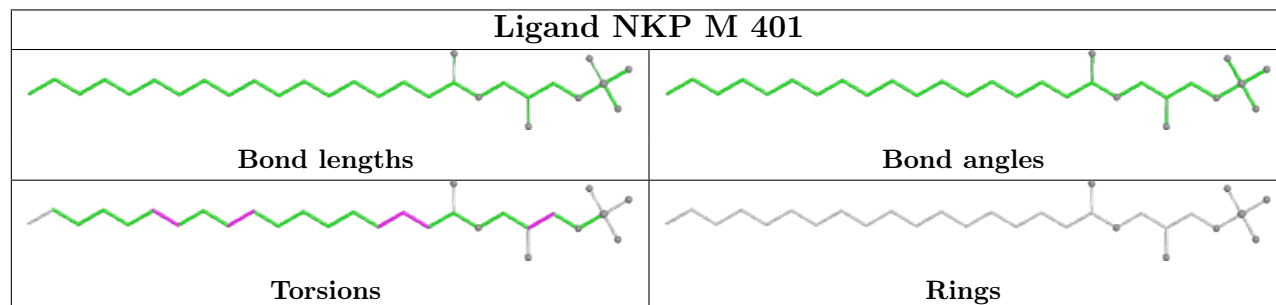
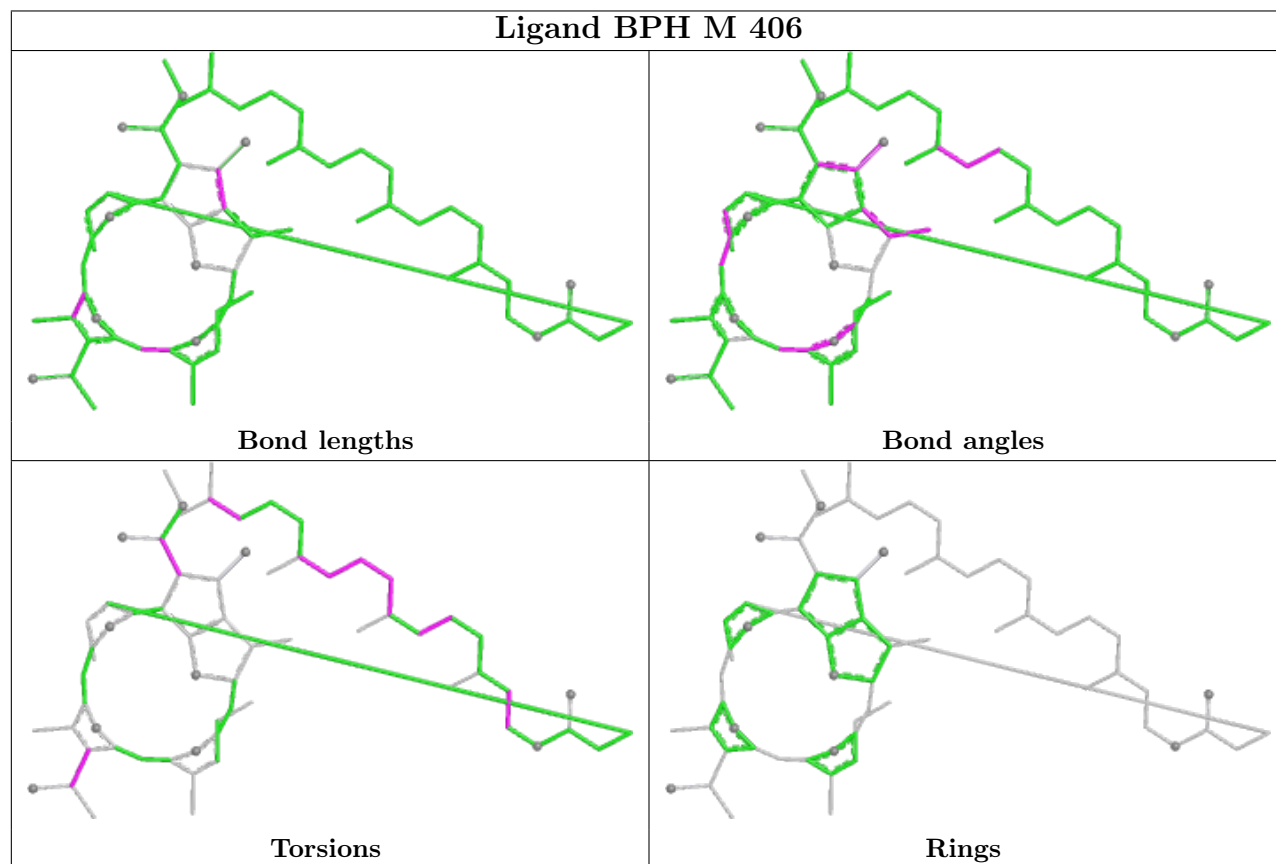
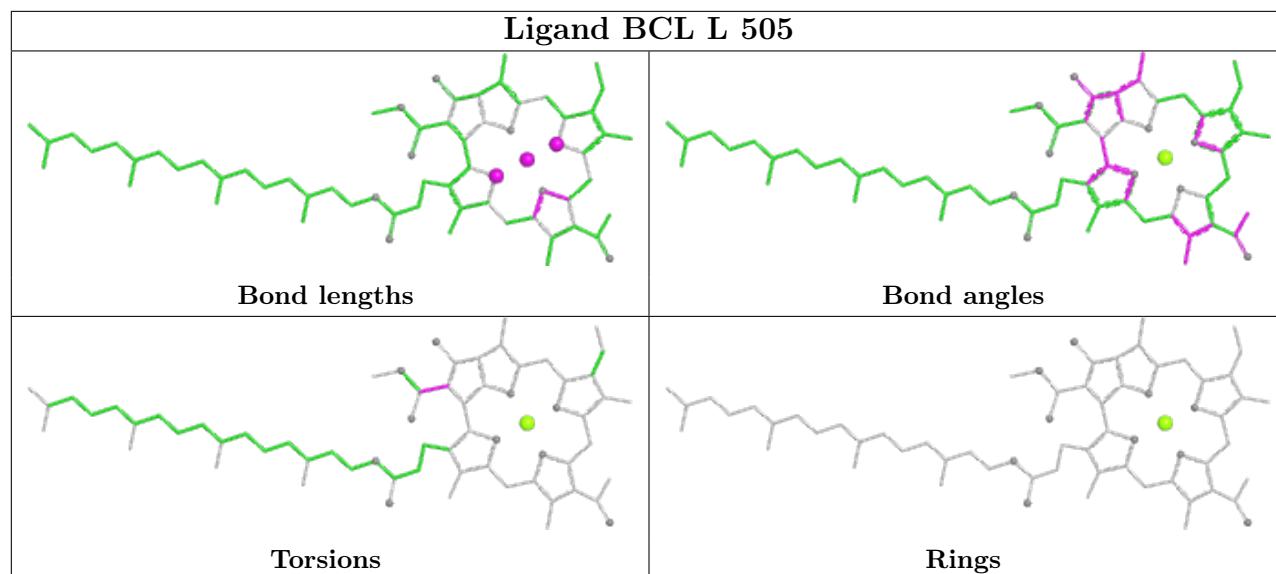
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	401	LDA	2	0
12	M	409	SPN	6	0
7	L	504	BCL	2	0
4	H	403	LDA	2	0
6	L	501	OLC	1	0
7	M	404	BCL	1	0
7	L	505	BCL	1	0
4	M	410	LDA	2	0
9	M	401	NKP	2	0

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.









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	H	241/241 (100%)	-0.35	5 (2%) 63 68	29, 41, 57, 120	0
2	L	281/281 (100%)	-0.38	7 (2%) 57 62	27, 36, 49, 68	0
3	M	303/303 (100%)	-0.31	3 (0%) 82 85	26, 36, 58, 98	0
All	All	825/825 (100%)	-0.35	15 (1%) 68 72	26, 38, 56, 120	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	245	ALA	6.6
2	L	59[A]	TRP	4.4
2	L	277[A]	GLY	4.3
3	M	302	GLY	4.1
3	M	1	ALA	4.0
1	H	249	LYS	3.5
2	L	281[A]	GLY	3.4
2	L	51	TRP	3.2
1	H	9	ASN	2.7
2	L	266[A]	TRP	2.7
2	L	265[A]	TRP	2.6
1	H	248	ARG	2.4
2	L	274[A]	ASN	2.3
1	H	247	LYS	2.3
3	M	303	MET	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

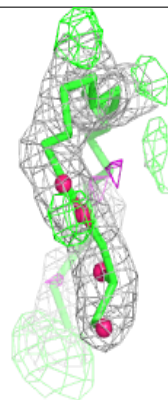
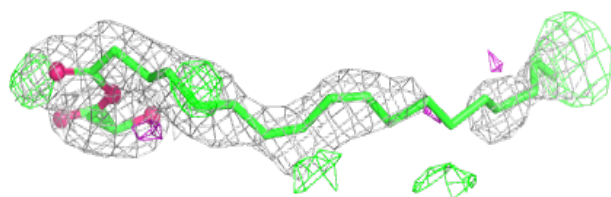
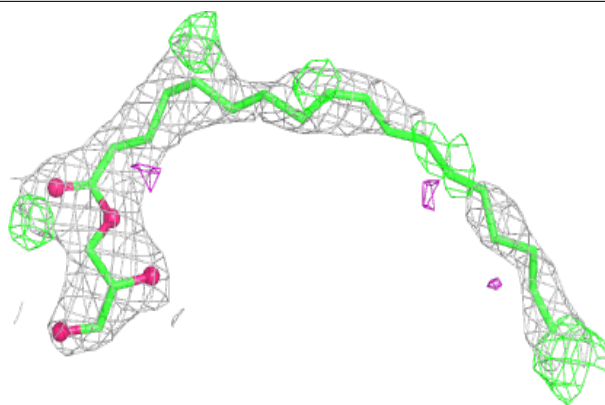
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LDA	M	410	16/16	0.59	0.31	30,55,73,76	0
4	LDA	H	401	16/16	0.77	0.23	54,71,85,86	0
4	LDA	M	411	16/16	0.77	0.34	59,66,93,93	0
6	OLC	L	501	25/25	0.78	0.23	38,52,64,67	0
5	UNL	L	502	15/-	0.80	0.17	42,49,66,68	0
5	UNL	L	503	15/-	0.82	0.22	54,60,73,74	0
5	UNL	H	402	15/-	0.82	0.15	52,59,71,71	0
9	NKP	M	402	29/29	0.82	0.21	38,68,79,88	0
12	SPN	M	409	43/43	0.84	0.22	36,53,71,76	0
5	UNL	M	403	15/-	0.90	0.18	41,51,62,65	0
4	LDA	H	403	16/16	0.91	0.16	36,51,63,67	0
11	U10	M	408	48/63	0.92	0.17	22,34,58,67	0
9	NKP	M	401	29/29	0.93	0.15	39,58,82,95	0
8	BPH	M	406	65/65	0.93	0.13	26,33,85,99	0
13	EDO	M	412	4/4	0.93	0.09	46,49,54,61	0
7	BCL	L	505	66/66	0.95	0.12	25,32,38,44	0
7	BCL	L	504	66/66	0.96	0.11	25,35,67,75	0
7	BCL	M	404	66/66	0.96	0.11	25,31,49,68	0
7	BCL	M	405	66/66	0.97	0.14	23,31,44,57	0
8	BPH	L	506	65/65	0.97	0.15	24,30,36,38	0
10	FE	M	407	1/1	1.00	0.11	29,29,29,29	0

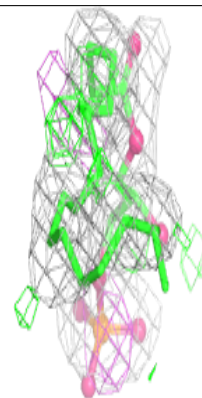
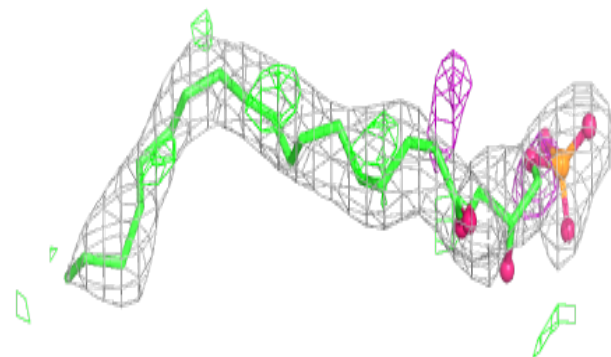
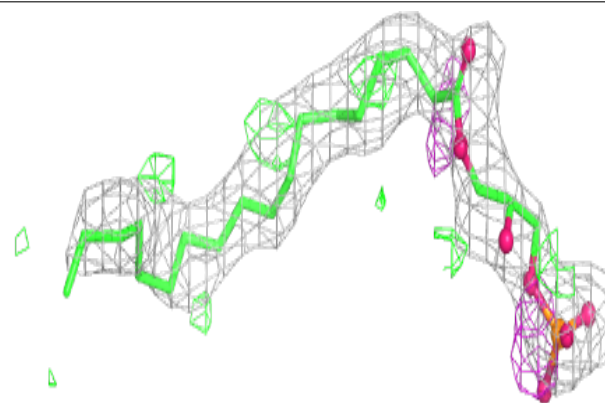
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

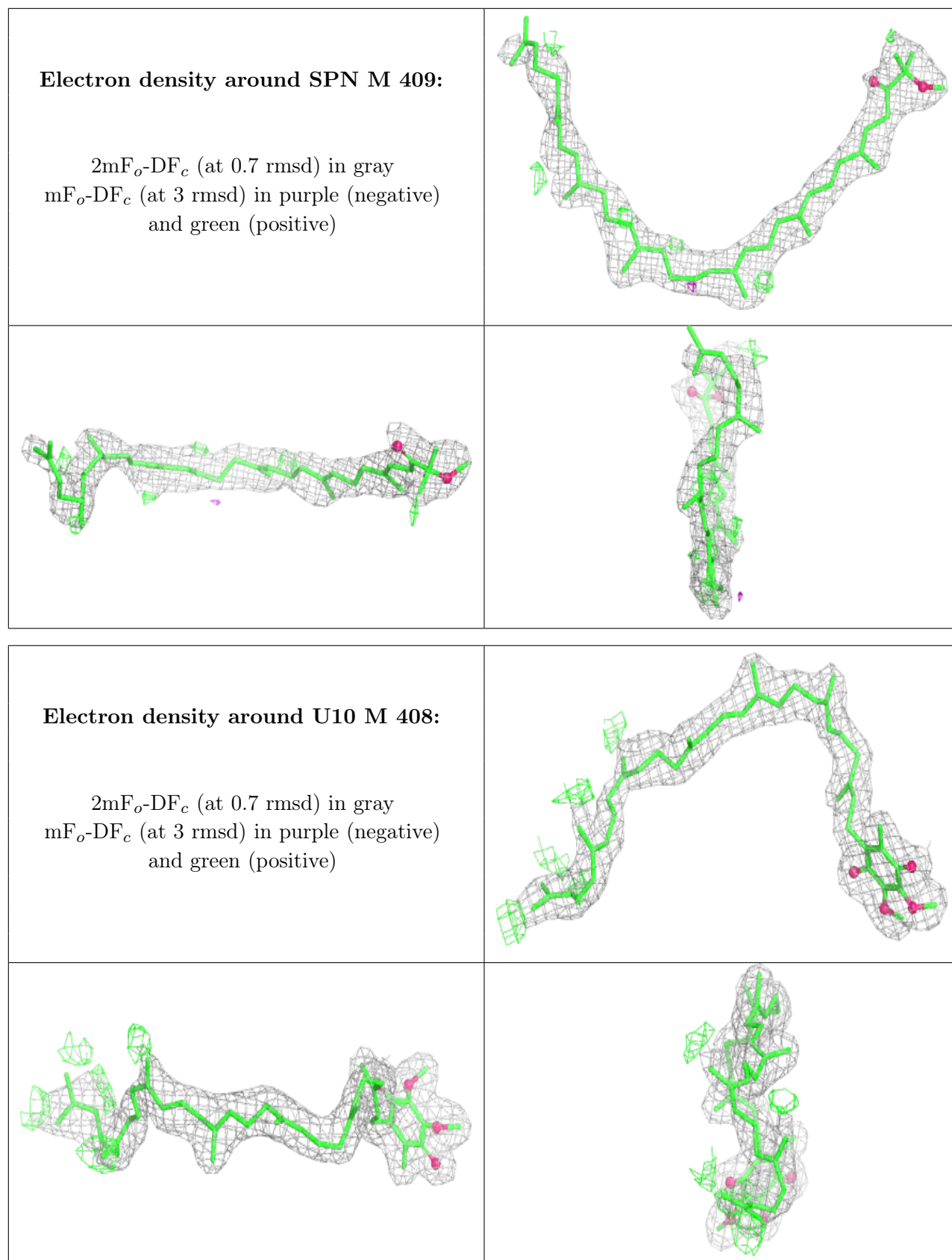
Electron density around OLC L 501:

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

**Electron density around NKP M 402:**

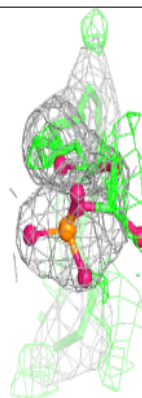
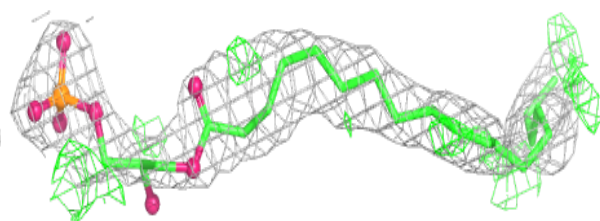
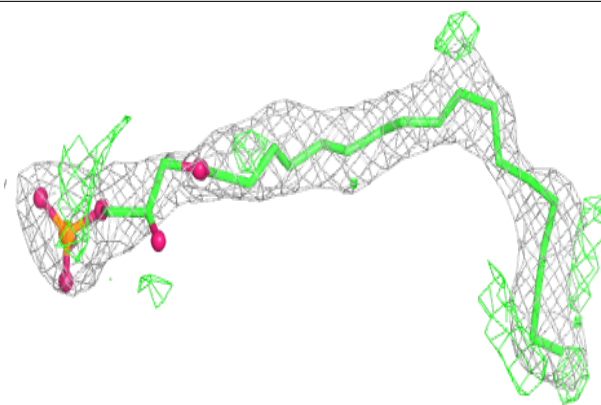
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



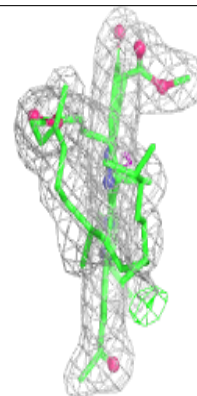
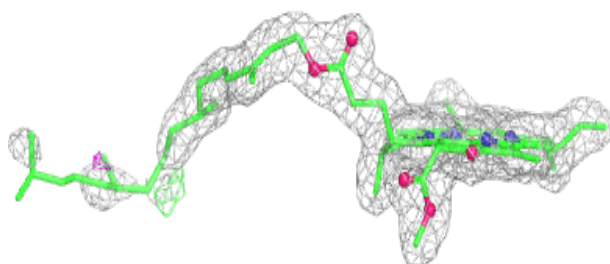
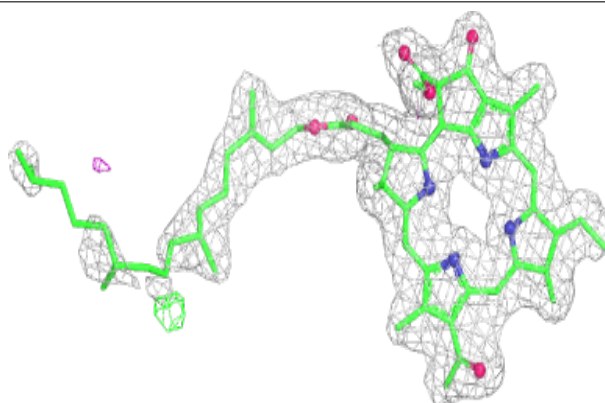


Electron density around NKP M 401:

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

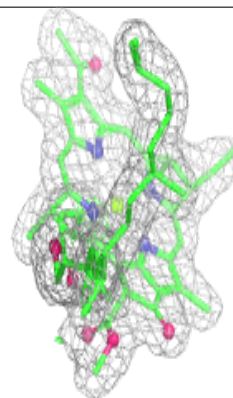
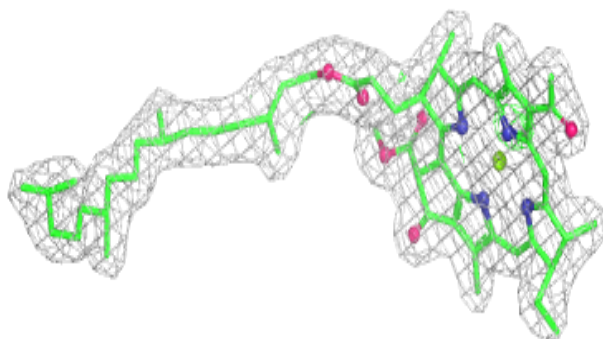
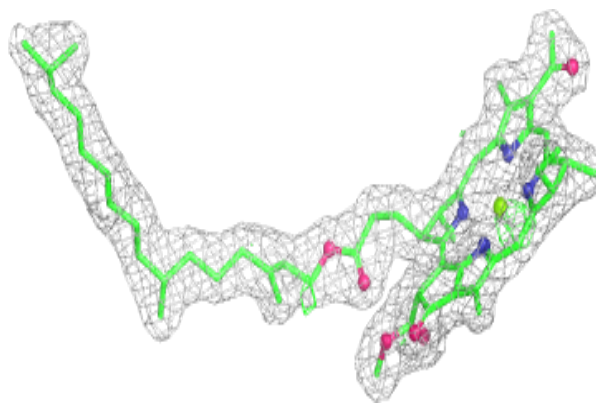
**Electron density around BPH M 406:**

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

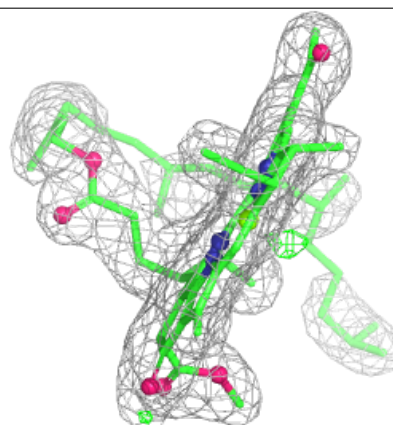
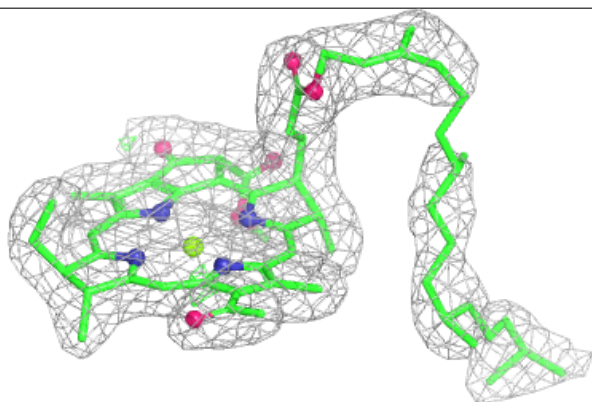
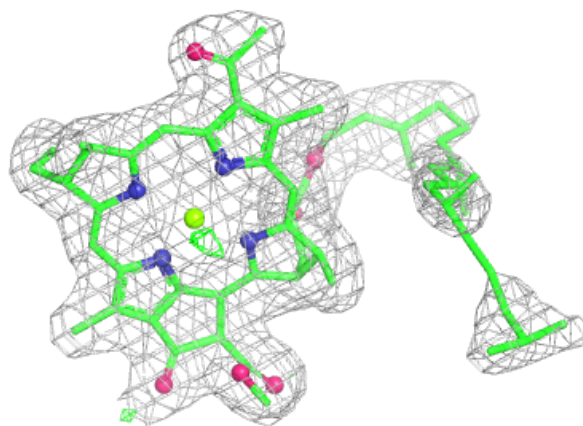


Electron density around BCL L 505:

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

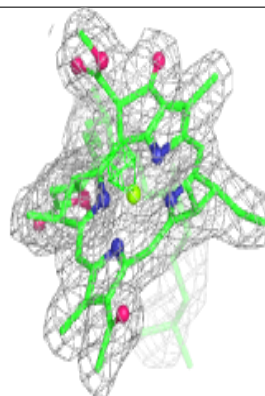
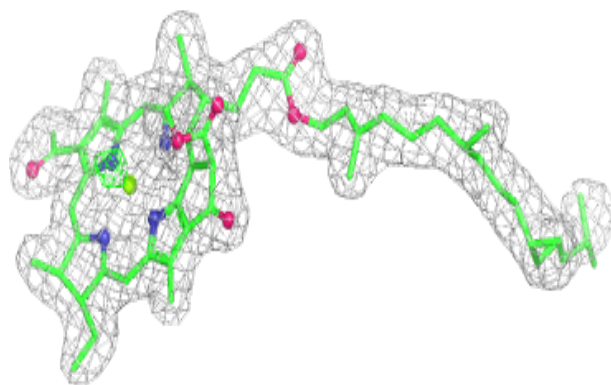
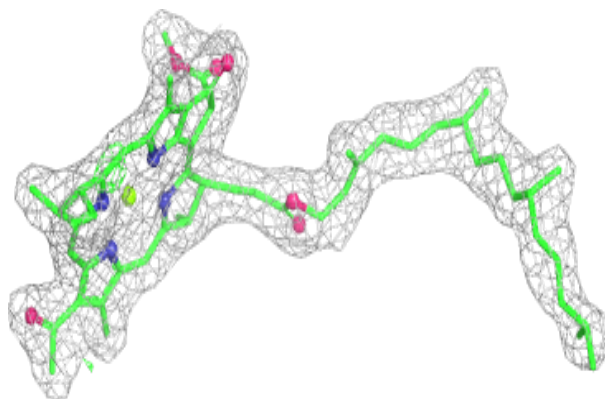
**Electron density around BCL L 504:**

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

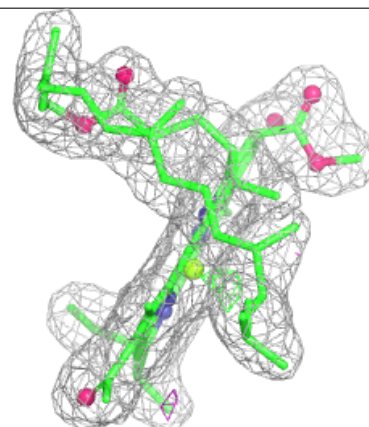
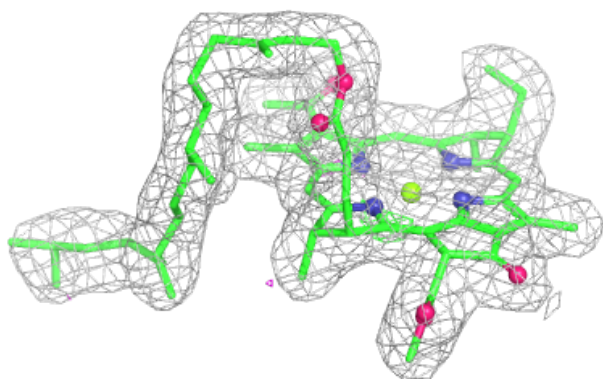
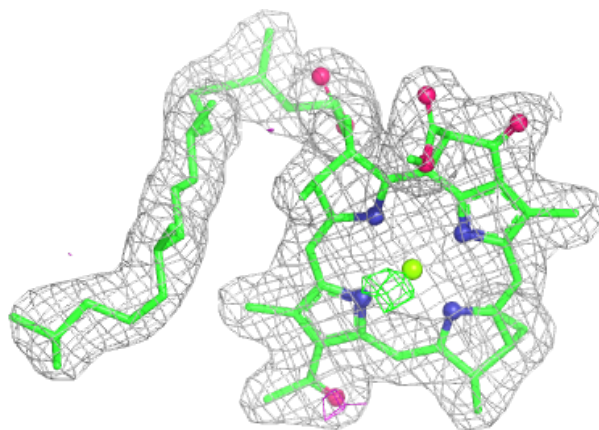


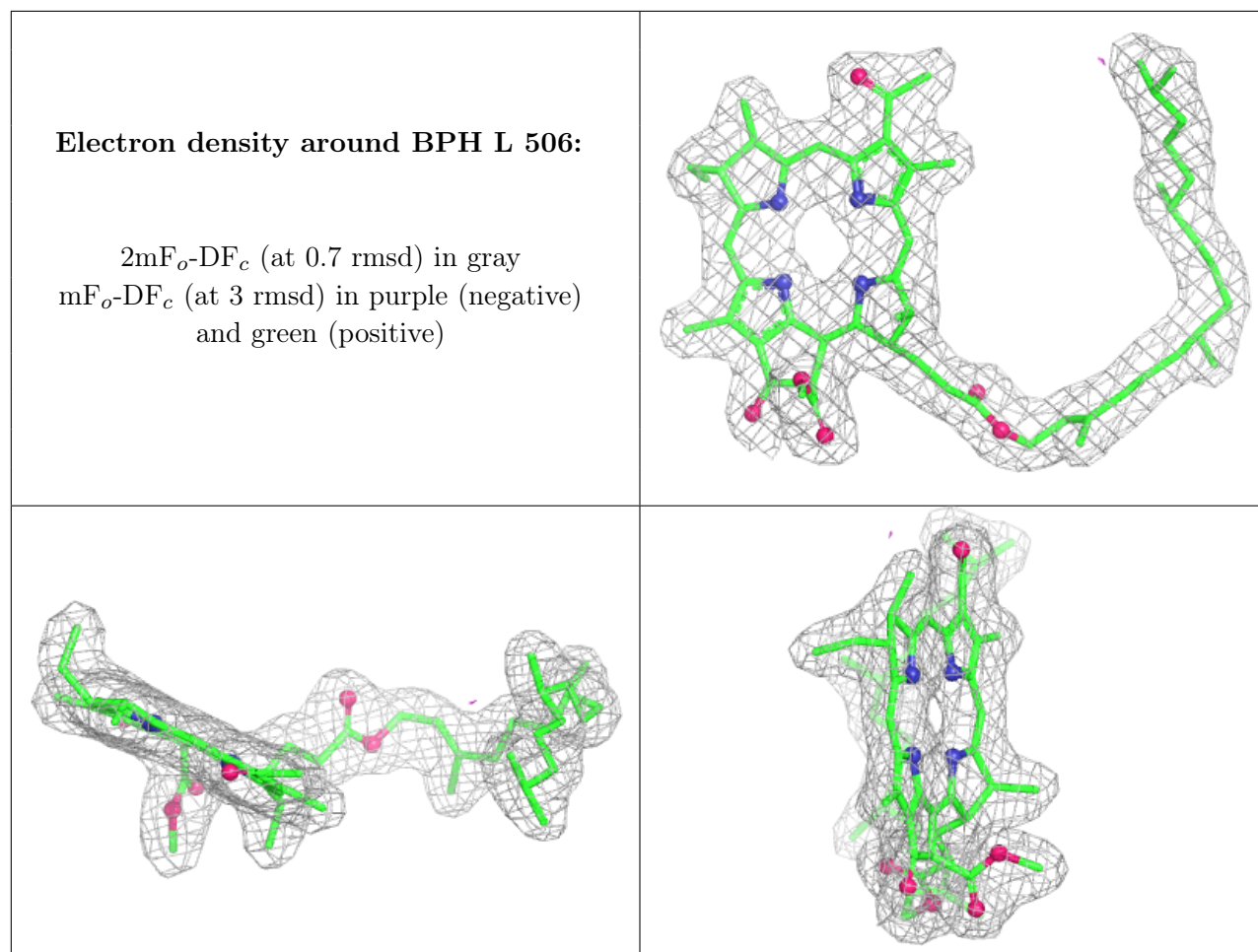
Electron density around BCL M 404:

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

**Electron density around BCL M 405:**

$2mF_o-DF_c$ (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.