



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:09 PM UTC

PDB ID : 7P0Q / pdb_00007p0q
Title : F(M197)H mutant structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV by fixed-target serial synchrotron crystallography (100K, 26keV)
Authors : Gabdulkhakov, A.G.; Selikhanov, G.K.; Guenther, S.; Meents, A.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on : 2021-06-30
Resolution : 1.73 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 ①](#)) 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

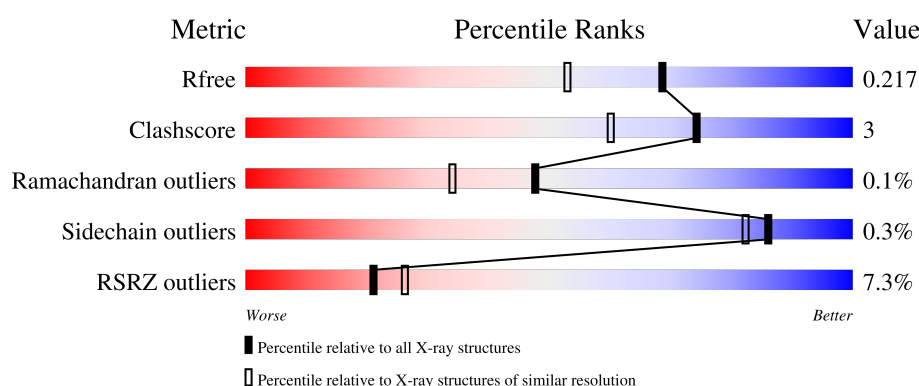
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	6% 91% 9%
2	L	281	8% 96% .
3	M	303	8% 92% 7%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7717 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
1	H	241	Total	C	N	O	S	0	8	0
			1897	1212	325	350	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2247	1519	356	364	8			

There is a discrepancy between the modelled and reference sequences:

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

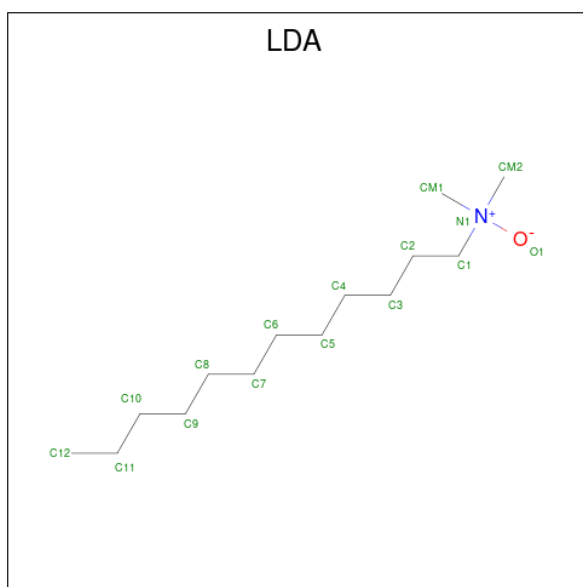
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	3	0
			2432	1622	399	400	11			

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 (CCD ID: LDA) (formula: C₁₄H₃₁NO).

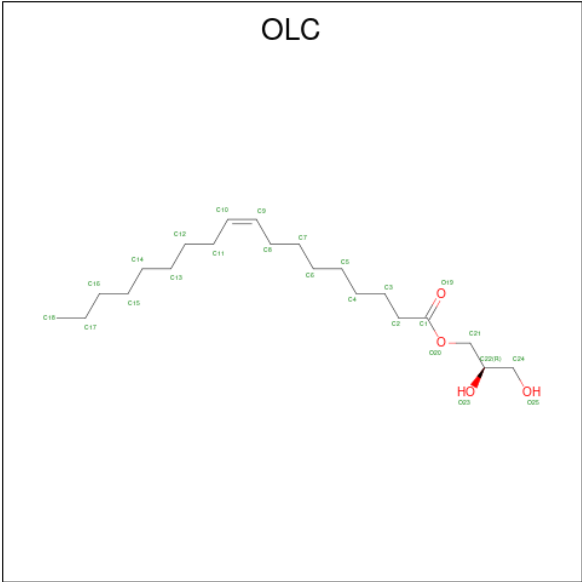


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

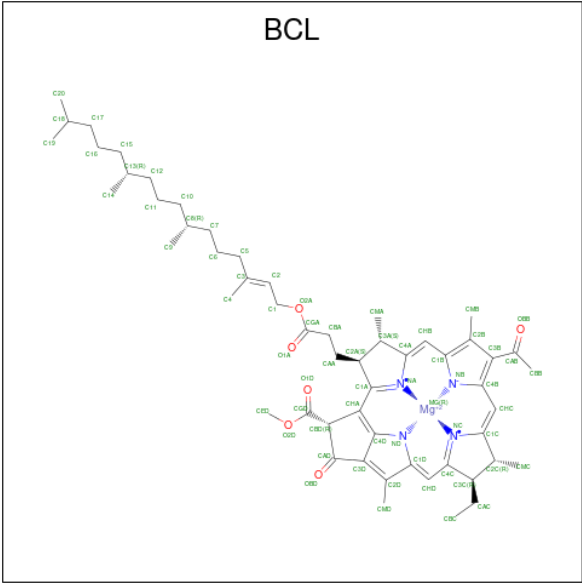
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	C	0	0
			15	15		
5	L	2	Total	C	0	0
			30	30		
5	M	4	Total	C	0	0
			60	60		

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



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

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



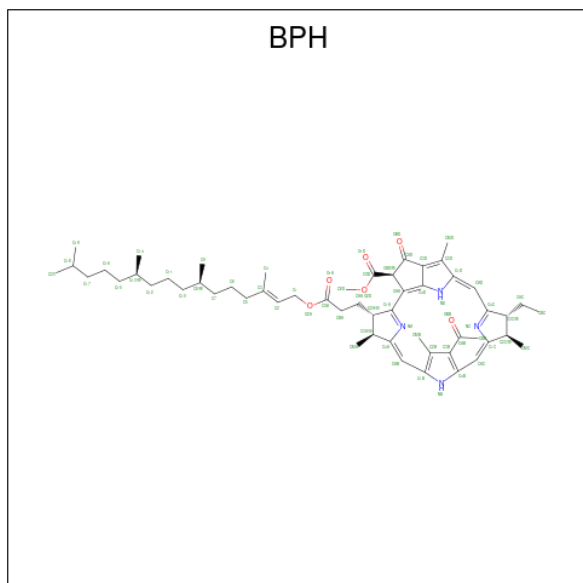
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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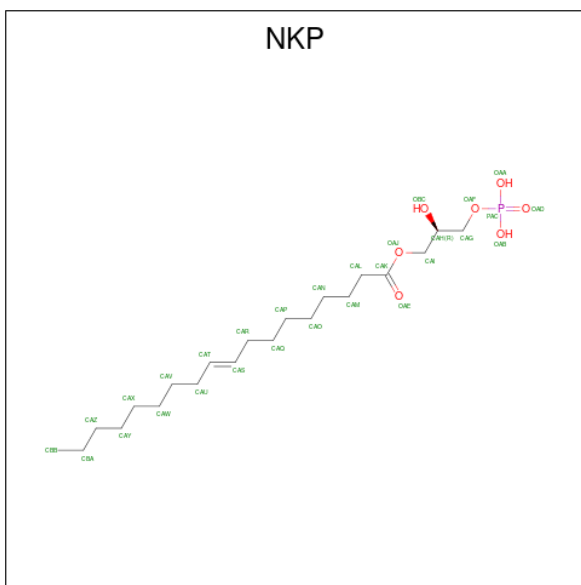
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



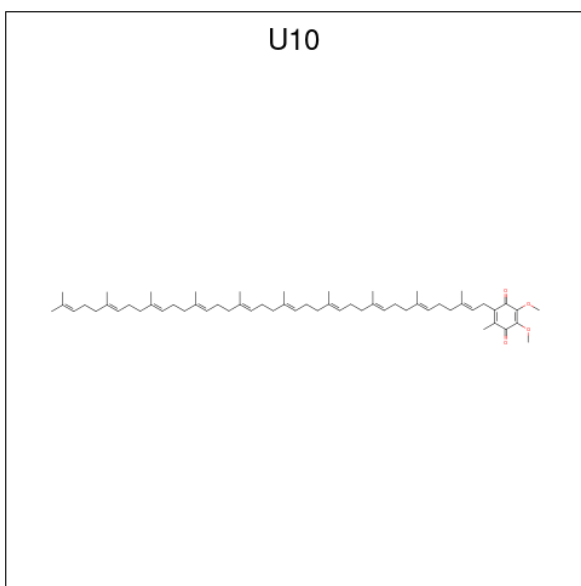
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 10 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

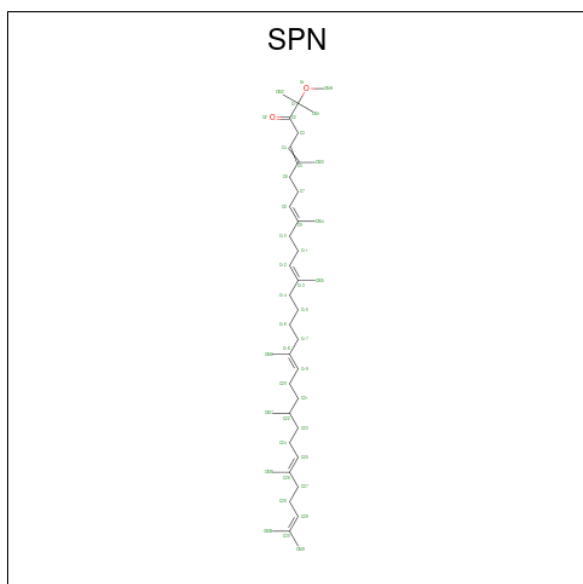


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			63	59	4		

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

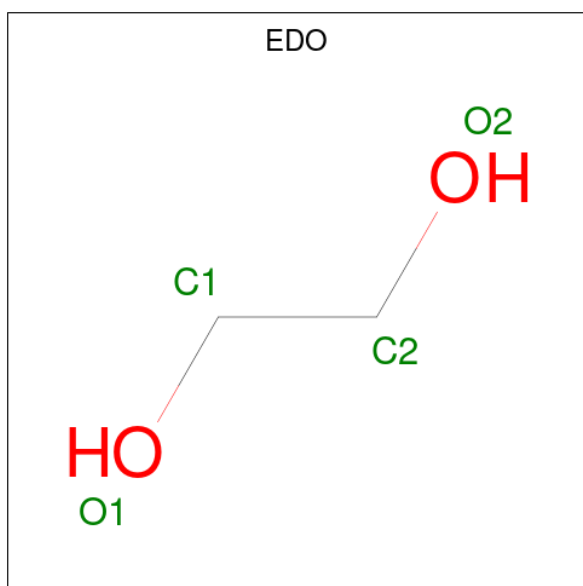
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPEROIDENONE (CCD ID: 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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

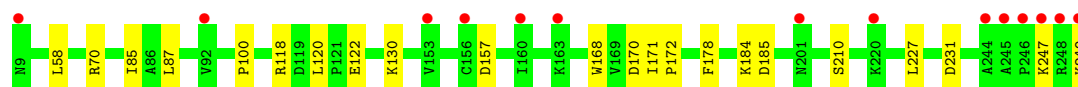
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	186	Total	O	0	0
			186	186		
14	L	96	Total	O	0	0
			96	96		
14	M	102	Total	O	0	0
			102	102		

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.

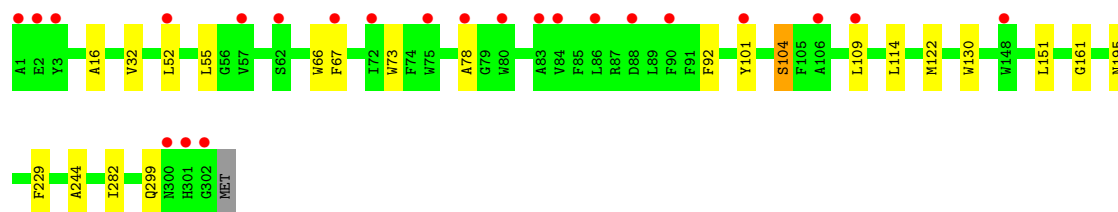
- Molecule 1: Reaction center protein H chain



- 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	99.97Å 99.97Å 239.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 1.73 48.93 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.93-1.73) 100.0 (48.93-1.73)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.203 0.191 , 0.217	Depositor DCC
R_{free} test set	6292 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7717	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, FE, OLC, SPN, U10, NKP, LDA, UNL, EDO, 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	0.48	0/1949	0.62	0/2652
2	L	0.56	1/2339 (0.0%)	0.61	0/3201
3	M	0.52	0/2524	0.60	0/3446
All	All	0.52	1/6812 (0.0%)	0.61	0/9299

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	175	ILE	C-O	-5.63	1.17	1.24

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	1897	0	1898	13	0
2	L	2247	0	2202	9	0
3	M	2432	0	2349	15	0
4	H	32	0	62	1	0
4	M	32	0	62	0	0
5	H	15	0	0	0	0
5	L	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	60	0	0	0	0
6	L	25	0	40	1	0
7	L	132	0	148	0	0
7	M	132	0	148	4	0
8	L	65	0	76	0	0
8	M	65	0	76	1	0
9	M	58	0	78	1	0
10	M	63	0	90	1	0
11	M	1	0	0	0	0
12	M	43	0	70	5	0
13	M	4	0	6	0	0
14	H	186	0	0	1	0
14	L	96	0	0	2	0
14	M	102	0	0	1	0
All	All	7717	0	7305	45	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 3.

All (45) 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)
1:H:118[A]:ARG:HD3	1:H:120:LEU:HD12	1.52	0.92
1:H:70:ARG:O	1:H:118[A]:ARG:NH2	2.29	0.66
3:M:161:GLY:HA3	12:M:411:SPN:H201	1.76	0.66
7:M:407:BCL:CAB	12:M:411:SPN:H162	2.27	0.64
3:M:109:LEU:HG	3:M:114[B]:LEU:HG	1.78	0.64
2:L:268:LYS:HE2	14:L:604:HOH:O	1.99	0.61
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.86	0.58
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.85	0.57
1:H:157:ASP:OD1	1:H:210:SER:OG	2.23	0.56
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.41	0.56
3:M:101:TYR:O	3:M:104:SER:HB3	2.07	0.55
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.88	0.55
2:L:7:ARG:HD2	14:L:602:HOH:O	2.10	0.51
2:L:261:ASP:O	2:L:264:GLN:HB2	2.12	0.50
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.92	0.50
3:M:130:TRP:NE1	3:M:151[B]:LEU:HG	2.27	0.49
3:M:130:TRP:HE1	3:M:151[B]:LEU:HG	1.78	0.48
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.96	0.48
7:M:408:BCL:HMB1	7:M:408:BCL:HBB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:401:LDA:HM11	3:M:282:ILE:HD13	1.95	0.48
8:M:409:BPH:HBC3	8:M:409:BPH:HHD	1.95	0.48
3:M:67:PHE:CE1	12:M:411:SPN:H61	2.49	0.48
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.96	0.47
10:M:405:U10:H501	10:M:405:U10:H521	1.60	0.47
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.98	0.46
2:L:268:LYS:HA	2:L:268:LYS:HD3	1.66	0.46
1:H:85:ILE:O	14:H:501:HOH:O	2.21	0.46
3:M:52:LEU:HA	3:M:52:LEU:HD13	1.68	0.46
3:M:299:GLN:NE2	14:M:503:HOH:O	2.44	0.45
12:M:411:SPN:H111	12:M:411:SPN:HM41	1.84	0.45
1:H:157:ASP:HB3	1:H:247:LYS:HG3	1.98	0.45
2:L:216[B]:PHE:CE2	6:L:501:OLC:H2	2.52	0.45
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.17	0.45
2:L:193:LEU:HD21	2:L:212:GLU:HB3	1.98	0.45
3:M:73:TRP:HB2	3:M:114[A]:LEU:HD23	1.98	0.45
1:H:249:LYS:HD3	1:H:249:LYS:HA	1.71	0.44
9:M:401:NKP:HALA	9:M:401:NKP:HAI	1.64	0.44
3:M:55:LEU:HD23	3:M:55:LEU:HA	1.75	0.43
1:H:58[B]:LEU:HD23	1:H:58[B]:LEU:HA	1.92	0.43
2:L:269:LEU:HD23	2:L:269:LEU:HA	1.81	0.42
2:L:264:GLN:OE1	2:L:264:GLN:HA	2.18	0.42
1:H:184:LYS:HG3	1:H:185:ASP:N	2.34	0.42
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.55	0.41
7:M:407:BCL:OBB	12:M:411:SPN:H162	2.20	0.41
7:M:408:BCL:HAA2	7:M:408:BCL:HBD	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	247/241 (102%)	243 (98%)	4 (2%)	0	100	100
2	L	281/281 (100%)	276 (98%)	5 (2%)	0	100	100
3	M	303/303 (100%)	295 (97%)	7 (2%)	1 (0%)	36	23
All	All	831/825 (101%)	814 (98%)	16 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN

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	H	203/196 (104%)	202 (100%)	1 (0%)	81	75
2	L	222/220 (101%)	222 (100%)	0	100	100
3	M	239/237 (101%)	238 (100%)	1 (0%)	84	79
All	All	664/653 (102%)	662 (100%)	2 (0%)	86	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	231	ASP
3	M	104	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	28	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 7 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
10	U10	M	405	-	63,63,63	2.65	17 (26%)	78,79,79	1.72	22 (28%)
7	BCL	M	408	-	69,74,74	1.44	9 (13%)	79,115,115	1.49	9 (11%)
9	NKP	M	403	-	28,28,28	0.54	0	30,32,32	0.47	0
8	BPH	M	409	-	59,70,70	1.26	6 (10%)	59,101,101	2.54	14 (23%)
12	SPN	M	411	-	42,42,42	0.59	0	50,52,52	1.52	7 (14%)
4	LDA	H	401	-	13,15,15	2.12	2 (15%)	14,17,17	0.76	0
4	LDA	M	412	-	13,15,15	2.07	2 (15%)	14,17,17	0.62	0
7	BCL	L	504	-	69,74,74	1.23	5 (7%)	79,115,115	1.33	7 (8%)
7	BCL	L	503	-	69,74,74	1.37	7 (10%)	79,115,115	1.31	8 (10%)
8	BPH	L	505	-	59,70,70	1.35	9 (15%)	59,101,101	1.78	8 (13%)
13	EDO	M	415	-	3,3,3	0.42	0	2,2,2	1.26	0
4	LDA	H	403	-	13,15,15	2.11	2 (15%)	14,17,17	0.58	0
4	LDA	M	413	-	13,15,15	2.24	2 (15%)	14,17,17	0.60	0
9	NKP	M	401	-	28,28,28	0.39	0	30,32,32	0.62	1 (3%)
6	OLC	L	501	-	24,24,24	0.90	1 (4%)	25,25,25	1.12	2 (8%)
7	BCL	M	407	-	69,74,74	1.28	7 (10%)	79,115,115	1.44	10 (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
10	U10	M	405	-	-	19/63/87/87	0/1/1/1
7	BCL	M	408	-	-	3/41/137/137	-
9	NKP	M	403	-	-	10/28/28/28	-
8	BPH	M	409	-	-	6/37/105/105	0/5/6/6
12	SPN	M	411	-	-	16/50/51/51	-
4	LDA	H	401	-	-	10/13/13/13	-
4	LDA	M	412	-	-	7/13/13/13	-
7	BCL	L	504	-	-	6/41/137/137	-
7	BCL	L	503	-	-	0/41/137/137	-
8	BPH	L	505	-	-	3/37/105/105	0/5/6/6
13	EDO	M	415	-	-	1/1/1/1	-
4	LDA	H	403	-	-	4/13/13/13	-
4	LDA	M	413	-	-	8/13/13/13	-
9	NKP	M	401	-	-	9/28/28/28	-
6	OLC	L	501	-	-	7/24/24/24	-
7	BCL	M	407	-	-	1/41/137/137	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	405	U10	C43-C44	6.81	1.48	1.33
4	M	413	LDA	O1-N1	-6.78	1.25	1.42
4	H	403	LDA	O1-N1	-6.72	1.25	1.42
4	H	401	LDA	O1-N1	-6.58	1.26	1.42
10	M	405	U10	C28-C29	6.40	1.47	1.33
10	M	405	U10	C38-C39	6.40	1.47	1.33
10	M	405	U10	C33-C34	6.38	1.47	1.33
4	M	412	LDA	O1-N1	-6.34	1.26	1.42
10	M	405	U10	C8-C9	6.17	1.47	1.33
10	M	405	U10	C23-C24	6.06	1.47	1.33
10	M	405	U10	C48-C49	5.70	1.46	1.33
10	M	405	U10	C13-C14	5.45	1.45	1.33
7	M	407	BCL	MG-NA	5.18	2.18	2.06
10	M	405	U10	C53-C54	5.13	1.47	1.32
10	M	405	U10	C18-C19	5.13	1.44	1.33
7	M	408	BCL	MG-NA	5.07	2.18	2.06
7	M	408	BCL	MG-NC	4.61	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	408	BCL	C3B-C4B	4.48	1.50	1.41
7	L	503	BCL	MG-NA	4.28	2.16	2.06
4	M	413	LDA	C1-N1	-4.24	1.47	1.51
7	L	503	BCL	MG-NC	4.16	2.16	2.06
7	L	504	BCL	MG-NA	3.99	2.15	2.06
6	L	501	OLC	O20-C1	3.87	1.44	1.33
8	M	409	BPH	C3D-CAD	-3.80	1.40	1.47
10	M	405	U10	O3-C3	-3.74	1.27	1.36
4	H	401	LDA	C1-N1	-3.70	1.47	1.51
10	M	405	U10	O4-C4	-3.69	1.27	1.36
4	M	412	LDA	C1-N1	-3.68	1.47	1.51
7	L	503	BCL	C1D-ND	3.67	1.42	1.37
8	M	409	BPH	CBD-CGD	-3.54	1.48	1.52
8	L	505	BPH	C1-C2	3.49	1.59	1.49
4	H	403	LDA	C1-N1	-3.36	1.48	1.51
7	M	407	BCL	MG-NC	3.33	2.14	2.06
8	L	505	BPH	C4D-CHA	3.24	1.44	1.39
7	L	504	BCL	MG-NC	3.02	2.13	2.06
8	M	409	BPH	CHA-CBD	2.98	1.55	1.51
8	L	505	BPH	CBD-CGD	-2.92	1.48	1.52
10	M	405	U10	C6-C1	2.88	1.40	1.35
10	M	405	U10	C3-C2	-2.86	1.40	1.48
8	M	409	BPH	C1D-C2D	2.83	1.42	1.39
7	L	504	BCL	C3B-C4B	2.81	1.46	1.41
7	M	408	BCL	C1D-ND	2.81	1.41	1.37
10	M	405	U10	C7-C8	2.73	1.54	1.50
7	M	408	BCL	CHD-C1D	2.72	1.43	1.38
7	L	503	BCL	OBD-CAD	2.72	1.27	1.22
7	M	407	BCL	C3B-C4B	2.69	1.46	1.41
7	M	407	BCL	CHD-C1D	2.68	1.43	1.38
8	L	505	BPH	C3D-CAD	-2.60	1.42	1.47
7	L	503	BCL	C3B-C4B	2.58	1.46	1.41
8	L	505	BPH	CAC-C3C	2.54	1.59	1.53
10	M	405	U10	C4-C5	-2.44	1.41	1.48
7	L	503	BCL	C14-C13	2.39	1.60	1.52
7	M	408	BCL	C5-C3	2.38	1.56	1.51
8	L	505	BPH	C3B-C4B	2.36	1.45	1.41
7	M	408	BCL	CAA-CBA	2.35	1.59	1.52
7	L	504	BCL	CHD-C1D	2.34	1.42	1.38
7	M	407	BCL	O1A-CGA	-2.32	1.15	1.22
8	M	409	BPH	C3D-C2D	-2.30	1.35	1.39
7	M	407	BCL	CHC-C1C	2.24	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	505	BPH	OBD-CAD	2.23	1.25	1.22
7	M	408	BCL	C16-C15	-2.18	1.43	1.52
8	M	409	BPH	C1-C2	2.11	1.55	1.49
10	M	405	U10	C6-C5	-2.10	1.40	1.46
7	L	504	BCL	CAA-CBA	2.10	1.59	1.52
8	L	505	BPH	C4-C3	2.09	1.55	1.50
8	L	505	BPH	CHA-CBD	2.05	1.54	1.51
7	M	407	BCL	O2A-C1	2.04	1.51	1.46
7	M	408	BCL	CBD-CGD	-2.03	1.46	1.52
7	L	503	BCL	CHC-C4B	2.02	1.43	1.39

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	409	BPH	C4D-CHA-CBD	-11.50	102.94	108.45
8	L	505	BPH	C4D-CHA-CBD	-9.97	103.67	108.45
8	M	409	BPH	C16-C15-C13	8.04	142.70	115.97
8	M	409	BPH	C11-C10-C8	7.83	141.98	115.97
7	M	408	BCL	C4A-NA-C1A	5.59	109.23	106.68
7	M	408	BCL	C4D-CHA-C1A	5.47	127.77	121.24
7	M	407	BCL	C4D-CHA-C1A	5.38	127.66	121.24
7	L	504	BCL	C4D-CHA-C1A	5.09	127.31	121.24
10	M	405	U10	C47-C48-C49	-4.75	116.75	127.62
12	M	411	SPN	CM6-C18-C17	4.69	123.36	115.23
12	M	411	SPN	CM5-C13-C14	4.41	122.88	115.23
10	M	405	U10	C50-C49-C51	4.23	122.58	115.23
7	L	504	BCL	C1D-ND-C4D	-4.19	103.37	106.31
7	L	503	BCL	C1D-ND-C4D	-4.15	103.40	106.31
8	M	409	BPH	C4D-ND-C1D	-3.99	104.09	108.87
7	L	503	BCL	C4D-CHA-C1A	3.94	125.94	121.24
7	L	504	BCL	CHD-C1D-ND	-3.82	119.43	124.80
7	L	503	BCL	CHD-C1D-ND	-3.58	119.77	124.80
7	M	408	BCL	CHD-C1D-ND	-3.55	119.81	124.80
7	M	407	BCL	CHD-C1D-ND	-3.53	119.84	124.80
8	M	409	BPH	O2D-CGD-CBD	3.48	114.77	110.95
8	L	505	BPH	OBD-CAD-CBD	-3.47	120.73	125.82
8	M	409	BPH	C11-C12-C13	3.46	127.45	115.97
7	L	503	BCL	C4A-NA-C1A	3.45	108.25	106.68
7	M	407	BCL	C1D-ND-C4D	-3.43	103.91	106.31
10	M	405	U10	C20-C19-C21	3.42	121.17	115.23
6	L	501	OLC	O20-C1-O19	-3.31	115.36	123.63
7	M	408	BCL	CHA-C1A-NA	-3.29	118.93	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	405	U10	C27-C28-C29	-3.23	120.24	127.62
8	L	505	BPH	C4D-ND-C1D	-3.21	105.03	108.87
10	M	405	U10	C25-C24-C26	3.14	120.68	115.23
7	L	504	BCL	C2A-C1A-CHA	3.09	129.24	123.87
7	L	504	BCL	CHA-C1A-NA	-3.05	119.49	126.39
10	M	405	U10	C30-C29-C31	3.04	120.51	115.23
7	M	407	BCL	C16-C15-C13	3.04	126.08	115.97
7	M	407	BCL	CHA-C1A-NA	-3.01	119.58	126.39
7	M	407	BCL	C4-C3-C5	-2.96	110.09	115.23
7	M	408	BCL	C1D-ND-C4D	-2.94	104.25	106.31
10	M	405	U10	C56-C54-C55	2.82	121.08	114.59
7	M	408	BCL	C2A-C1A-CHA	2.81	128.74	123.87
8	L	505	BPH	C1-C2-C3	-2.80	121.61	126.20
10	M	405	U10	C35-C34-C36	2.77	120.04	115.23
7	M	407	BCL	CMB-C2B-C1B	-2.71	121.30	125.42
10	M	405	U10	C4M-O4-C4	2.70	125.96	116.47
12	M	411	SPN	CM3-C5-C6	2.69	119.90	115.23
7	M	407	BCL	C2A-C1A-CHA	2.69	128.54	123.87
8	L	505	BPH	C3D-C4D-ND	2.64	111.09	107.71
10	M	405	U10	C32-C33-C34	-2.59	121.70	127.62
7	M	407	BCL	C1-O2A-CGA	2.58	122.89	116.65
10	M	405	U10	C10-C9-C11	2.56	119.68	115.23
10	M	405	U10	C15-C14-C16	2.55	119.65	115.23
8	M	409	BPH	C3D-C4D-ND	2.53	110.95	107.71
12	M	411	SPN	CM4-C9-C10	2.53	119.61	115.23
10	M	405	U10	C37-C38-C39	-2.52	121.85	127.62
12	M	411	SPN	C20-C19-C18	-2.51	121.87	127.62
10	M	405	U10	C12-C13-C14	-2.48	121.94	127.62
7	M	408	BCL	C16-C17-C18	-2.48	104.85	115.94
7	M	408	BCL	CED-O2D-CGD	2.37	121.30	115.92
10	M	405	U10	C1M-C1-C6	-2.36	120.57	124.45
12	M	411	SPN	CM8-C26-C27	2.33	119.27	115.23
7	L	504	BCL	CAB-C3B-C2B	2.31	132.55	127.74
8	M	409	BPH	CMB-C2B-C3B	2.28	129.24	124.68
6	L	501	OLC	O20-C1-C2	2.27	118.77	111.83
12	M	411	SPN	C11-C12-C13	-2.25	122.47	127.62
10	M	405	U10	C45-C44-C46	2.24	119.12	115.23
7	L	503	BCL	CHA-C1A-NA	-2.24	121.32	126.39
8	L	505	BPH	C2D-C1D-ND	2.23	111.04	109.43
10	M	405	U10	C40-C39-C41	2.23	119.09	115.23
7	L	503	BCL	C11-C12-C13	-2.22	108.60	115.97
9	M	401	NKP	OAB-PAC-OAA	2.21	116.09	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	505	BPH	O2D-CGD-CBD	2.19	113.36	110.95
8	M	409	BPH	OBD-CAD-CBD	-2.18	122.63	125.82
8	M	409	BPH	C12-C11-C10	-2.17	103.55	113.28
7	L	503	BCL	C16-C15-C13	-2.16	108.78	115.97
8	L	505	BPH	CMB-C2B-C3B	2.14	128.96	124.68
7	M	407	BCL	OBB-CAB-CBB	-2.12	115.02	119.77
7	M	408	BCL	C1C-NC-C4C	2.08	107.63	106.68
10	M	405	U10	C50-C49-C48	-2.07	118.30	123.63
8	M	409	BPH	CMA-C3A-C4A	-2.07	110.14	114.61
7	L	503	BCL	CMB-C2B-C1B	-2.06	122.28	125.42
10	M	405	U10	C30-C29-C28	-2.06	118.34	123.63
8	M	409	BPH	CMD-C2D-C3D	2.05	128.79	124.68
10	M	405	U10	C52-C53-C54	-2.04	120.84	127.64
8	M	409	BPH	C1-O2A-CGA	2.03	121.57	116.65
7	L	504	BCL	CMB-C2B-C1B	-2.03	122.33	125.42
8	M	409	BPH	C2D-C1D-ND	2.01	110.88	109.43
10	M	405	U10	C6-C1-C2	2.01	120.75	119.17
10	M	405	U10	C3M-O3-C3	2.01	123.52	116.47

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	401	LDA	C2-C1-N1-O1
4	H	401	LDA	C2-C1-N1-CM1
4	H	401	LDA	C2-C1-N1-CM2
4	M	412	LDA	C2-C1-N1-O1
4	M	412	LDA	C2-C1-N1-CM1
4	M	412	LDA	C2-C1-N1-CM2
4	M	413	LDA	C2-C1-N1-O1
4	M	413	LDA	C2-C1-N1-CM1
4	M	413	LDA	C2-C1-N1-CM2
6	L	501	OLC	O20-C21-C22-O23
9	M	401	NKP	CAG-OAF-PAC-OAA
9	M	401	NKP	OAF-CAG-CAH-CAI
10	M	405	U10	C37-C38-C39-C40
10	M	405	U10	C37-C38-C39-C41
12	M	411	SPN	CM1-C1-O1-CMA
12	M	411	SPN	CM2-C1-O1-CMA
12	M	411	SPN	C2-C1-O1-CMA
9	M	401	NKP	OAE-CAK-OAJ-CAI
10	M	405	U10	C52-C53-C54-C56

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Mol	Chain	Res	Type	Atoms
9	M	401	NKP	CAL-CAK-OAJ-CAI
9	M	403	NKP	OAE-CAK-OAJ-CAI
9	M	403	NKP	CAL-CAK-OAJ-CAI
10	M	405	U10	C50-C49-C51-C52
12	M	411	SPN	CM3-C5-C6-C7
12	M	411	SPN	C11-C10-C9-CM4
12	M	411	SPN	CM5-C13-C14-C15
12	M	411	SPN	C4-C5-C6-C7
12	M	411	SPN	C12-C13-C14-C15
10	M	405	U10	C52-C53-C54-C55
9	M	401	NKP	OAF-CAG-CAH-OBC
12	M	411	SPN	C16-C17-C18-CM6
10	M	405	U10	C49-C51-C52-C53
12	M	411	SPN	C26-C27-C28-C29
10	M	405	U10	C48-C49-C51-C52
12	M	411	SPN	C11-C10-C9-C8
12	M	411	SPN	C16-C17-C18-C19
6	L	501	OLC	O20-C21-C22-C24
7	L	504	BCL	C13-C15-C16-C17
8	M	409	BPH	C11-C10-C8-C7
10	M	405	U10	C39-C41-C42-C43
9	M	401	NKP	CAR-CAS-CAT-CAU
7	L	504	BCL	C15-C16-C17-C18
7	M	408	BCL	C16-C17-C18-C20
12	M	411	SPN	C14-C15-C16-C17
7	M	408	BCL	C16-C17-C18-C19
4	M	413	LDA	C7-C8-C9-C10
4	H	401	LDA	C7-C8-C9-C10
9	M	403	NKP	CAN-CAO-CAP-CAQ
9	M	403	NKP	CAT-CAU-CAV-CAW
4	H	401	LDA	C9-C10-C11-C12
8	M	409	BPH	C8-C10-C11-C12
4	H	401	LDA	C2-C3-C4-C5
8	M	409	BPH	C16-C17-C18-C19
8	M	409	BPH	C16-C17-C18-C20
4	M	413	LDA	C1-C2-C3-C4
4	M	412	LDA	C4-C5-C6-C7
4	H	401	LDA	C5-C6-C7-C8
8	M	409	BPH	C5-C6-C7-C8
4	H	401	LDA	C1-C2-C3-C4
9	M	401	NKP	CAG-OAF-PAC-OAD
9	M	403	NKP	CAP-CAQ-CAR-CAS

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Mol	Chain	Res	Type	Atoms
9	M	401	NKP	CAU-CAV-CAW-CAX
10	M	405	U10	C30-C29-C31-C32
10	M	405	U10	C40-C39-C41-C42
9	M	403	NKP	CAY-CAZ-CBA-CBB
9	M	403	NKP	CAW-CAX-CAY-CAZ
10	M	405	U10	C35-C34-C36-C37
4	H	403	LDA	C1-C2-C3-C4
10	M	405	U10	C28-C29-C31-C32
4	H	403	LDA	C9-C10-C11-C12
4	H	401	LDA	C4-C5-C6-C7
10	M	405	U10	C33-C34-C36-C37
10	M	405	U10	C38-C39-C41-C42
10	M	405	U10	C47-C48-C49-C50
6	L	501	OLC	C1-C2-C3-C4
9	M	401	NKP	CAG-OAF-PAC-OAB
4	M	412	LDA	C6-C7-C8-C9
7	L	504	BCL	C16-C17-C18-C19
4	M	412	LDA	C5-C6-C7-C8
7	L	504	BCL	C16-C17-C18-C20
12	M	411	SPN	C21-C22-C23-C24
4	M	413	LDA	C4-C5-C6-C7
6	L	501	OLC	C3-C4-C5-C6
4	M	413	LDA	C2-C3-C4-C5
4	M	412	LDA	C11-C10-C9-C8
7	L	504	BCL	CHA-CBD-CGD-O1D
7	L	504	BCL	CHA-CBD-CGD-O2D
8	M	409	BPH	C11-C10-C8-C9
4	H	401	LDA	C11-C10-C9-C8
13	M	415	EDO	O1-C1-C2-O2
9	M	403	NKP	CAR-CAS-CAT-CAU
12	M	411	SPN	CM2-C1-C2-C3
9	M	403	NKP	CAQ-CAR-CAS-CAT
9	M	403	NKP	CAG-CAH-CAI-OAJ
4	H	403	LDA	C11-C10-C9-C8
10	M	405	U10	C5-C4-O4-C4M
10	M	405	U10	C47-C48-C49-C51
4	H	403	LDA	C7-C8-C9-C10
10	M	405	U10	C45-C44-C46-C47
8	L	505	BPH	C2-C3-C5-C6
10	M	405	U10	C24-C26-C27-C28
7	M	408	BCL	CAA-CBA-CGA-O2A
8	L	505	BPH	CHA-CBD-CGD-O1D

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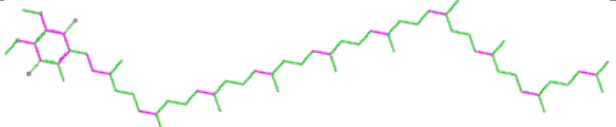
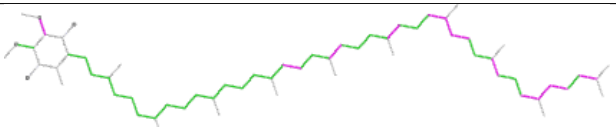
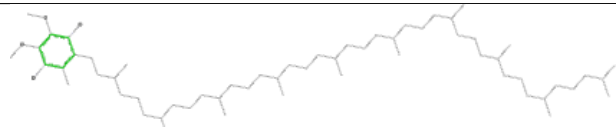
Mol	Chain	Res	Type	Atoms
8	L	505	BPH	C4-C3-C5-C6
6	L	501	OLC	C9-C10-C11-C12
6	L	501	OLC	C5-C6-C7-C8
4	M	413	LDA	C5-C6-C7-C8
6	L	501	OLC	C7-C8-C9-C10
7	M	407	BCL	C2-C1-O2A-CGA
12	M	411	SPN	C10-C11-C12-C13

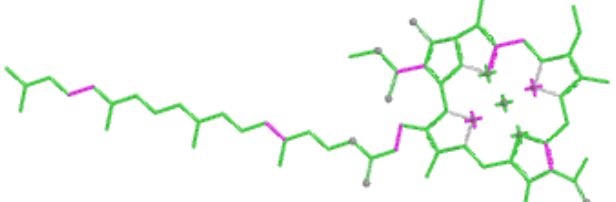
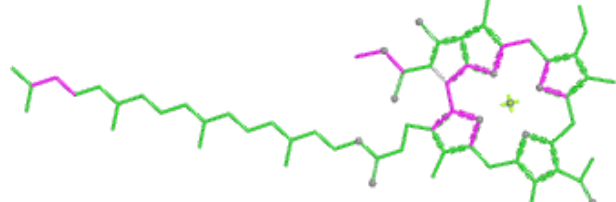
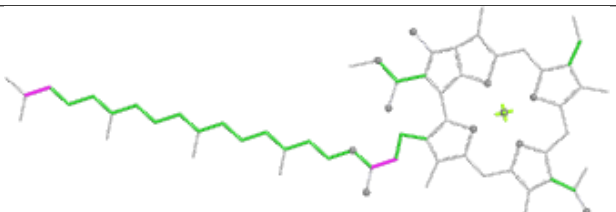
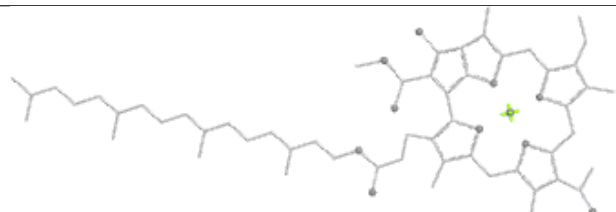
There are no ring outliers.

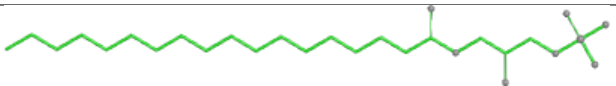
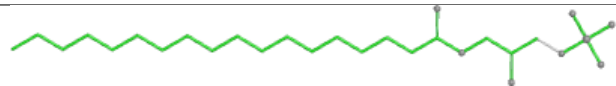
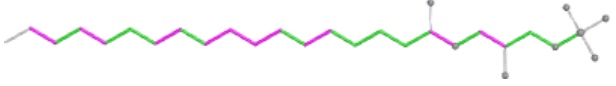
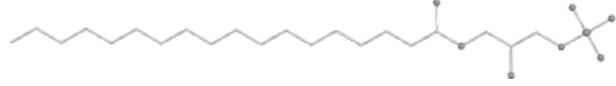
8 monomers are involved in 12 short contacts:

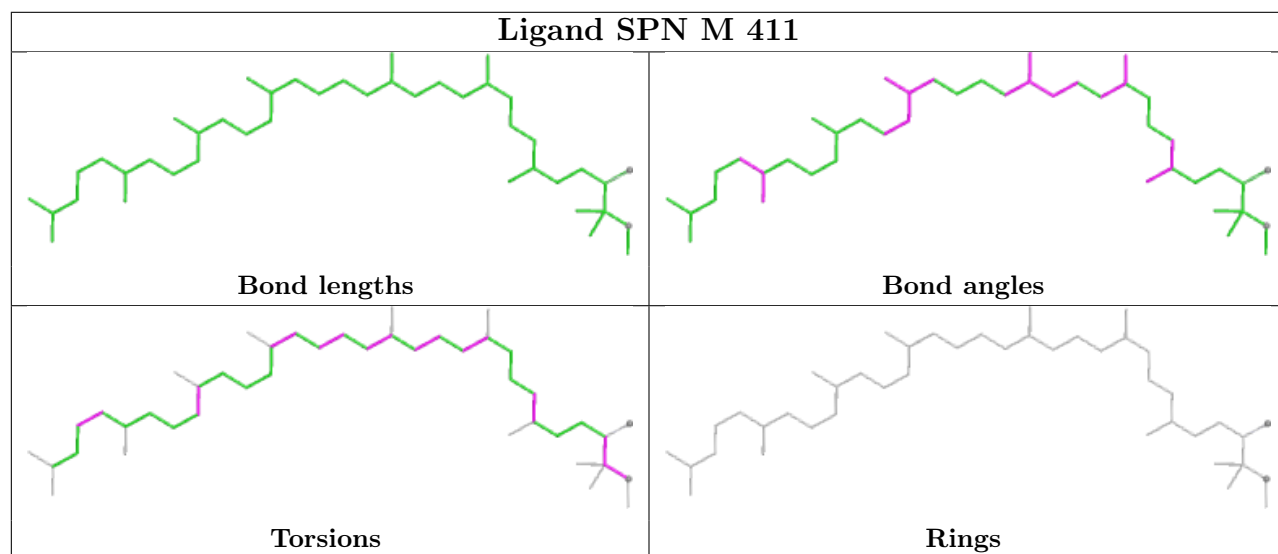
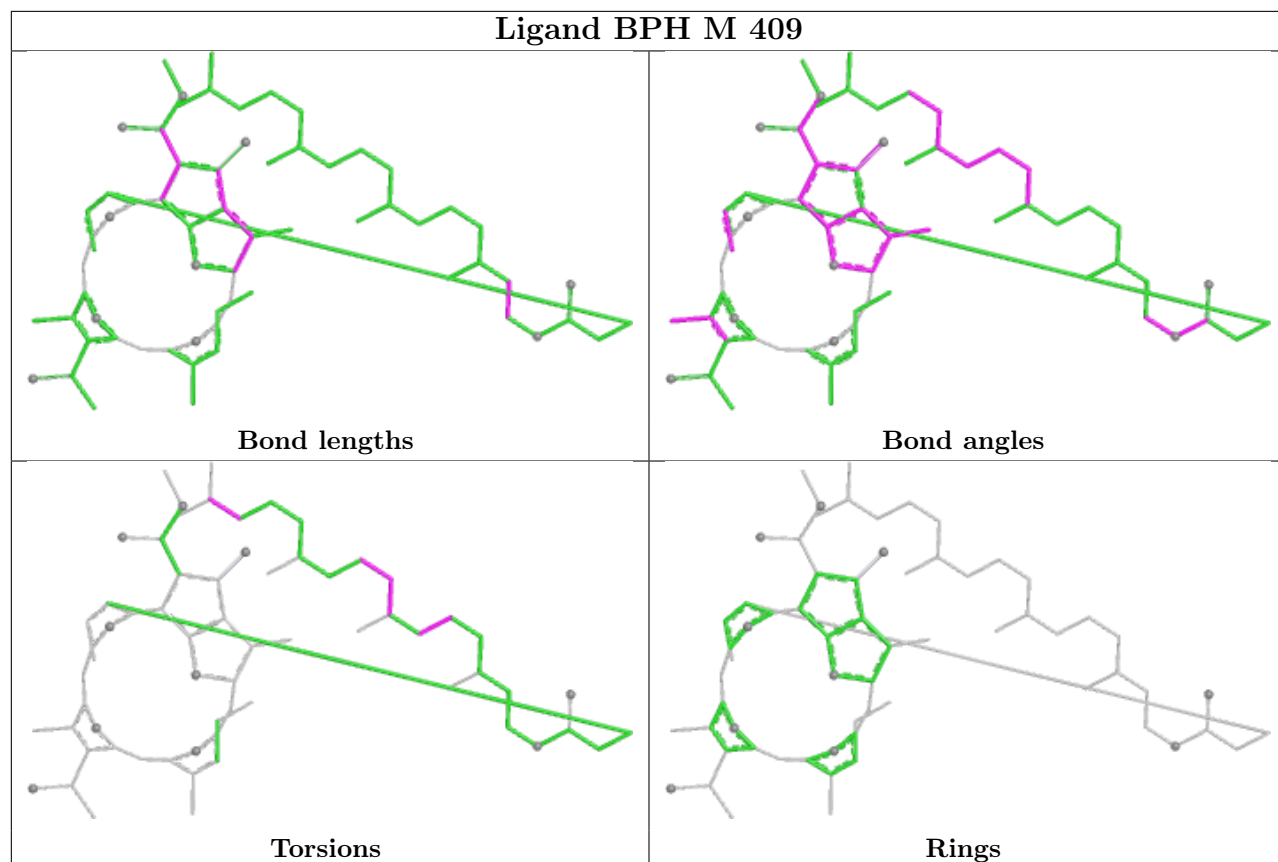
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	405	U10	1	0
7	M	408	BCL	2	0
8	M	409	BPH	1	0
12	M	411	SPN	5	0
4	H	401	LDA	1	0
9	M	401	NKP	1	0
6	L	501	OLC	1	0
7	M	407	BCL	2	0

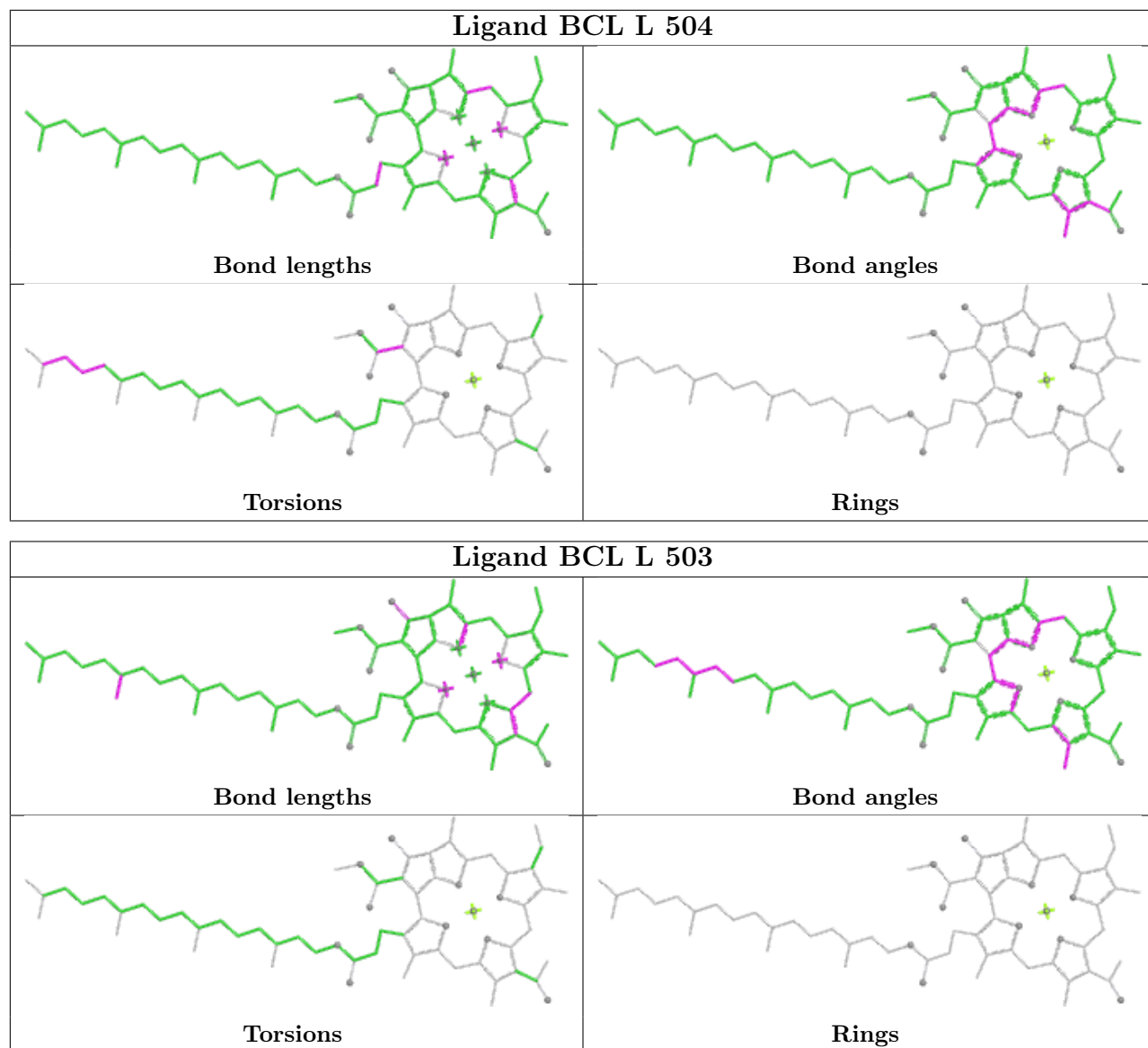
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

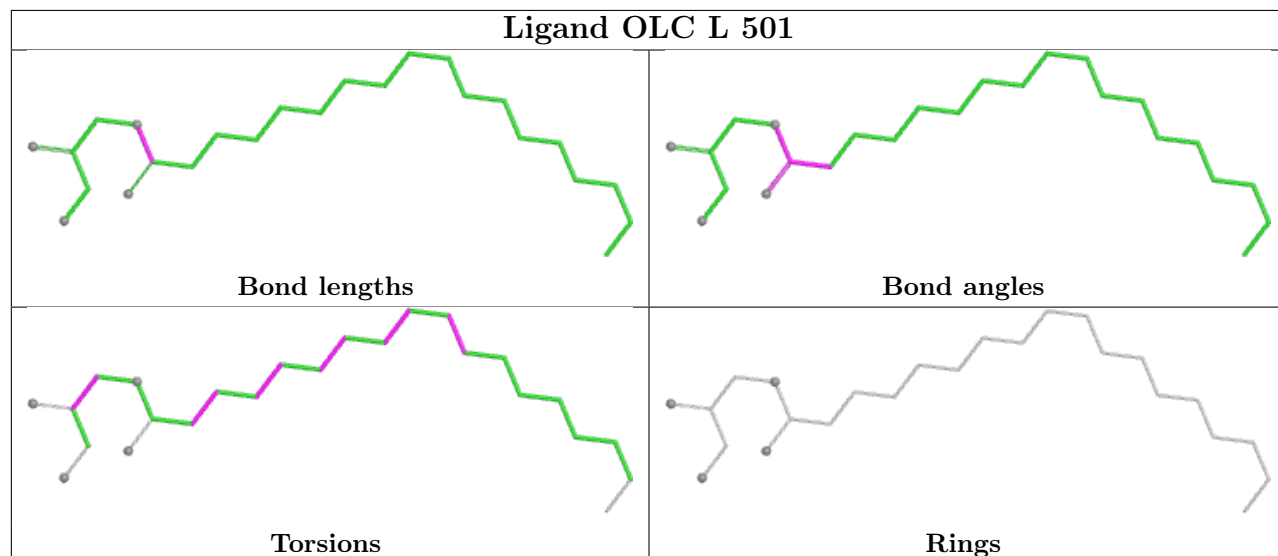
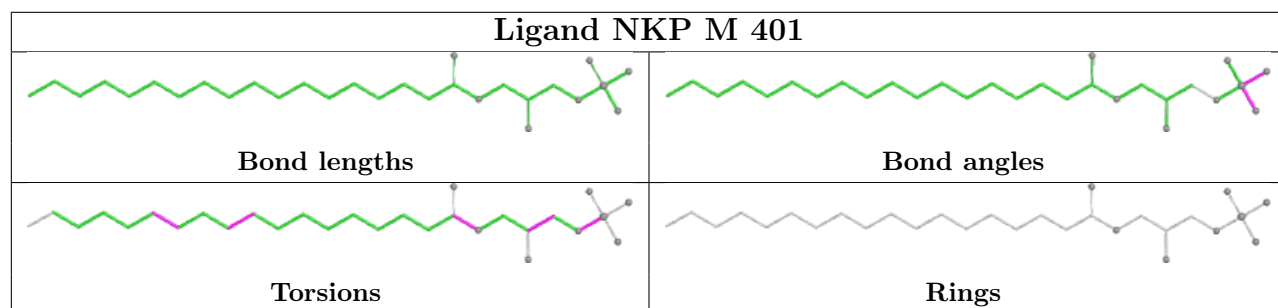
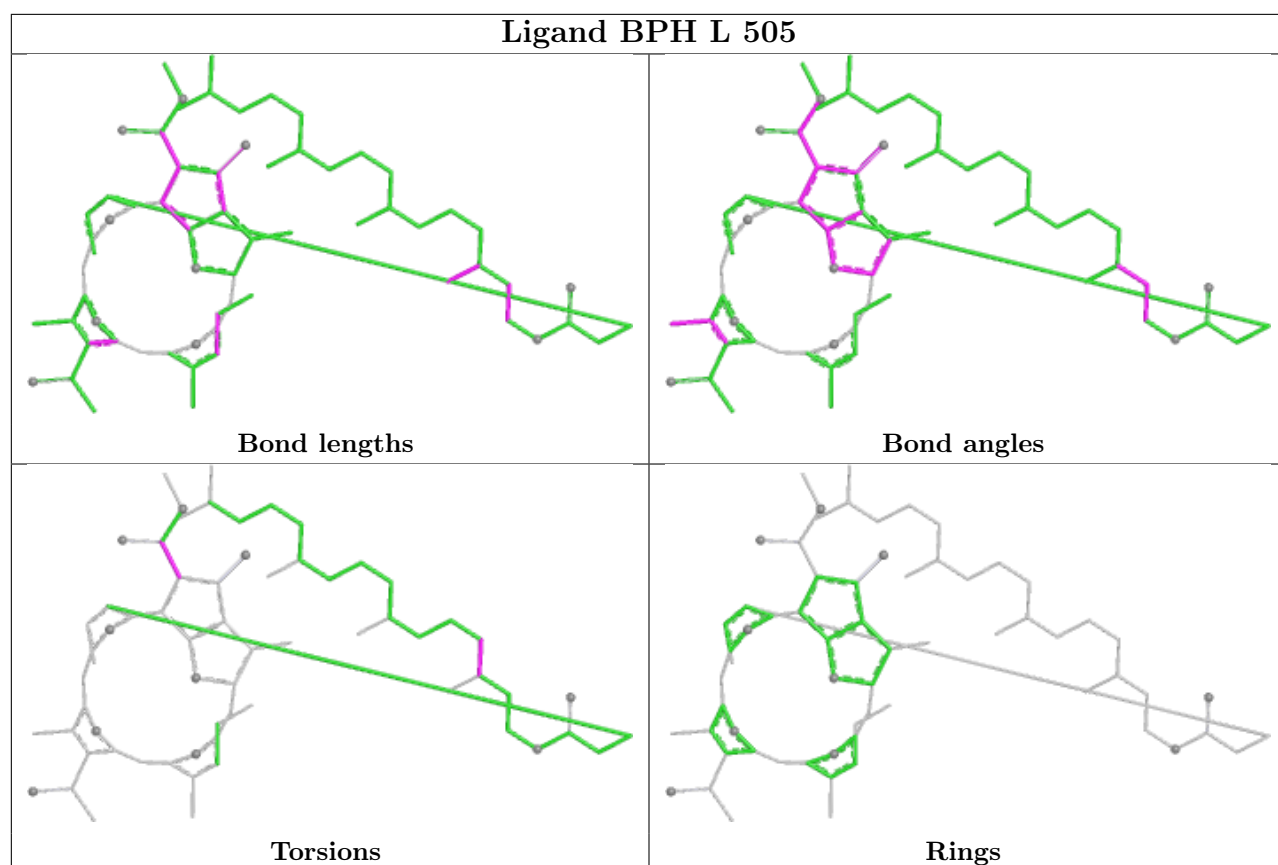
Ligand U10 M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

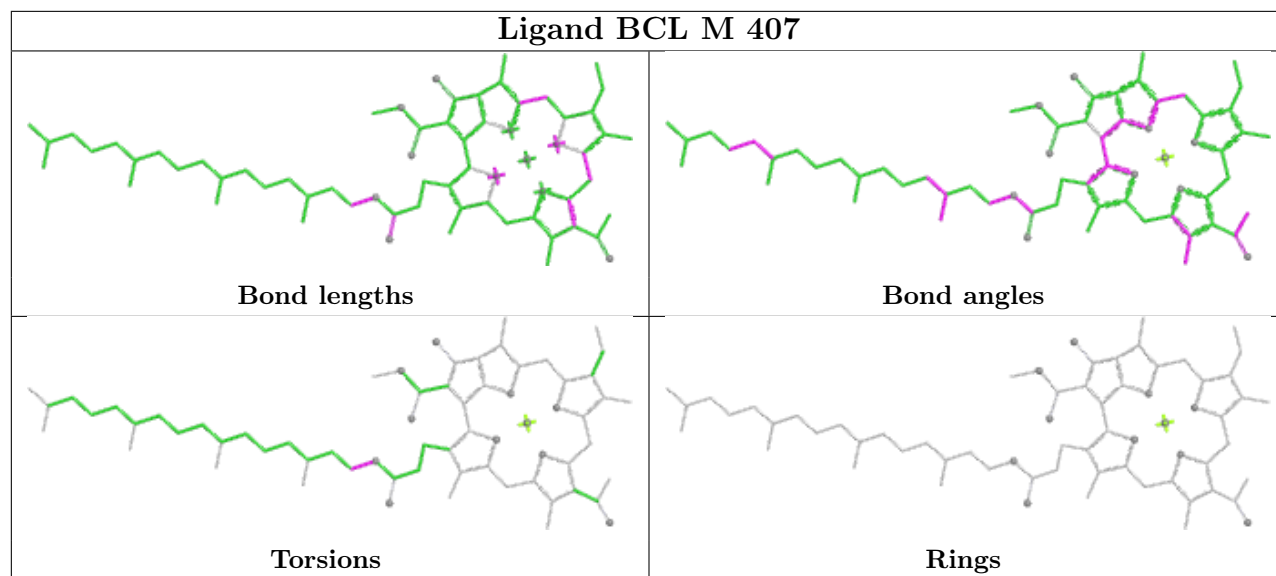
Ligand BCL M 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NKP M 403	
	
Bond lengths	Bond angles
	
Torsions	Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	H	241/241 (100%)	0.49	14 (5%)	29 35	14, 34, 49, 76	8 (3%)
2	L	281/281 (100%)	0.45	23 (8%)	17 23	14, 31, 56, 74	2 (0%)
3	M	302/303 (99%)	0.44	23 (7%)	20 25	12, 32, 54, 80	3 (0%)
All	All	824/825 (99%)	0.46	60 (7%)	21 26	12, 32, 54, 80	13 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	270	PRO	7.2
3	M	84	VAL	6.4
2	L	265	TRP	6.0
3	M	1	ALA	5.6
2	L	271	TRP	5.3
2	L	267	VAL	5.3
1	H	245	ALA	5.1
2	L	272	TRP	5.0
3	M	301	HIS	4.9
2	L	275	ILE	4.7
2	L	269	LEU	4.6
1	H	249	LYS	4.2
2	L	268	LYS	4.2
2	L	276	PRO	4.1
2	L	59	TRP	3.8
1	H	9	ASN	3.7
3	M	148	TRP	3.7
3	M	83	ALA	3.6
2	L	273	ALA	3.5
2	L	40	PHE	3.5
2	L	266	TRP	3.4
2	L	277	GLY	3.3
3	M	3	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	281	GLY	3.2
3	M	302	GLY	3.2
3	M	300	ASN	3.1
1	H	244	ALA	3.0
1	H	156	CYS	3.0
1	H	247	LYS	3.0
3	M	78	ALA	2.9
3	M	86	LEU	2.9
3	M	80	TRP	2.7
1	H	92	VAL	2.6
2	L	254	ILE	2.6
3	M	67	PHE	2.5
2	L	278	GLY	2.5
1	H	160	ILE	2.5
2	L	279	ILE	2.5
1	H	201	ASN	2.4
3	M	2	GLU	2.4
1	H	246	PRO	2.4
1	H	163	LYS	2.4
3	M	75	TRP	2.4
3	M	106	ALA	2.3
1	H	248	ARG	2.3
1	H	220	LYS	2.3
3	M	109	LEU	2.3
3	M	52	LEU	2.2
2	L	46	ILE	2.2
3	M	72	ILE	2.2
1	H	153	VAL	2.2
3	M	57	VAL	2.2
2	L	57	GLY	2.2
3	M	101	TYR	2.2
2	L	264	GLN	2.1
2	L	55	LEU	2.1
3	M	62	SER	2.1
3	M	88	ASP	2.1
2	L	280	ASN	2.0
3	M	90	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

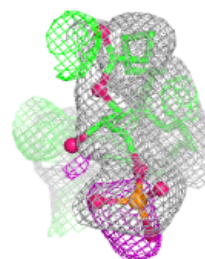
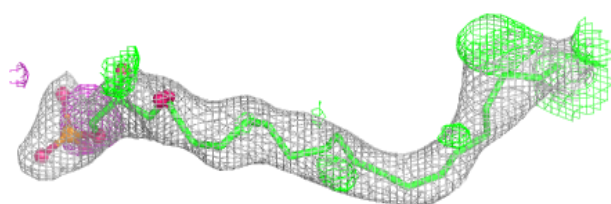
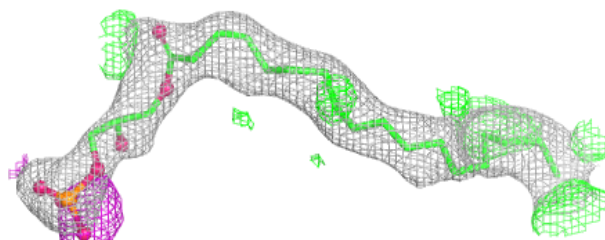
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	M	412	16/16	0.65	0.22	52,57,70,73	0
5	UNL	H	402	15/-	0.70	0.23	49,60,67,67	0
4	LDA	M	413	16/16	0.72	0.23	53,62,82,85	0
5	UNL	M	402	15/-	0.75	0.22	51,62,67,67	0
4	LDA	H	401	16/16	0.76	0.20	49,57,65,66	0
9	NKP	M	403	29/29	0.76	0.22	33,55,69,72	0
5	UNL	L	502	15/-	0.78	0.21	41,48,60,64	0
5	UNL	M	404	15/-	0.82	0.18	31,46,56,57	0
5	UNL	M	414	15/-	0.82	0.17	45,52,61,65	0
4	LDA	H	403	16/16	0.82	0.17	36,44,52,56	0
9	NKP	M	401	29/29	0.84	0.19	32,51,73,78	0
5	UNL	L	506	15/-	0.86	0.16	42,47,54,57	0
12	SPN	M	411	43/43	0.86	0.15	30,43,58,61	0
13	EDO	M	415	4/4	0.86	0.16	44,45,56,58	0
6	OLC	L	501	25/25	0.87	0.15	30,43,54,56	0
5	UNL	M	406	15/-	0.89	0.13	42,47,58,59	0
10	U10	M	405	63/63	0.92	0.13	20,33,64,67	0
8	BPH	M	409	65/65	0.94	0.10	23,30,72,75	0
7	BCL	M	407	66/66	0.95	0.09	23,30,60,63	0
8	BPH	L	505	65/65	0.95	0.07	22,25,31,32	0
7	BCL	L	503	66/66	0.95	0.08	23,26,33,39	0
7	BCL	L	504	66/66	0.95	0.08	22,26,38,48	0
7	BCL	M	408	66/66	0.96	0.08	21,26,47,61	0
11	FE	M	410	1/1	1.00	0.01	25,25,25,25	0

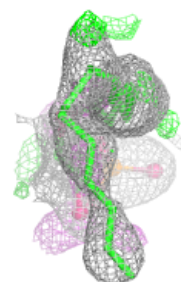
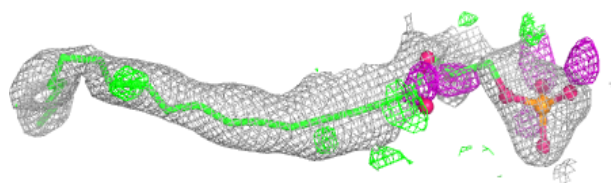
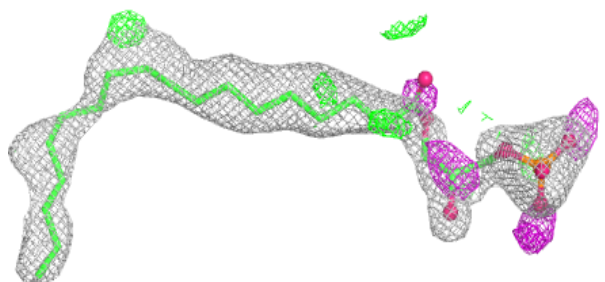
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NKP M 403:

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

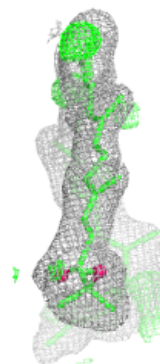
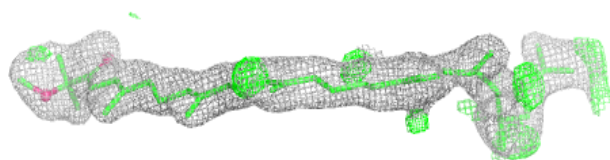
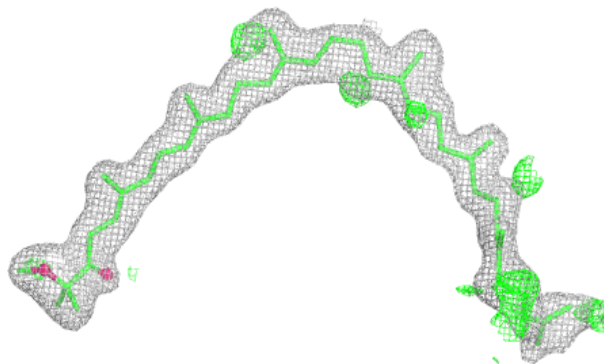
**Electron density around NKP M 401:**

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

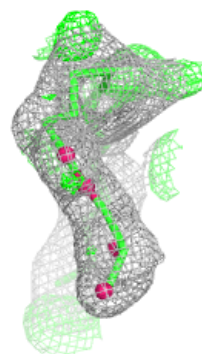
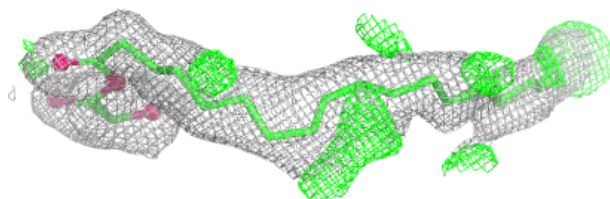
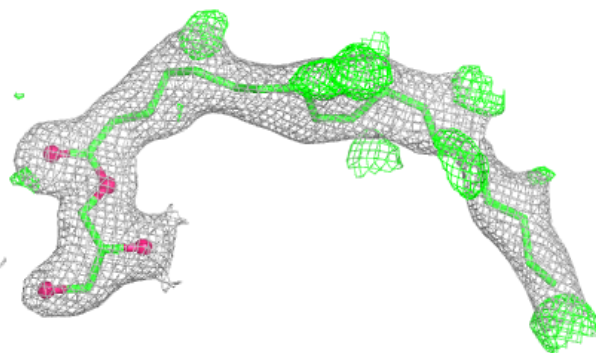


Electron density around SPN M 411:

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

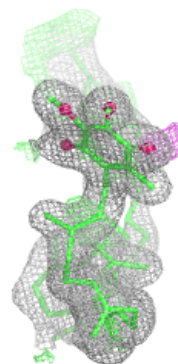
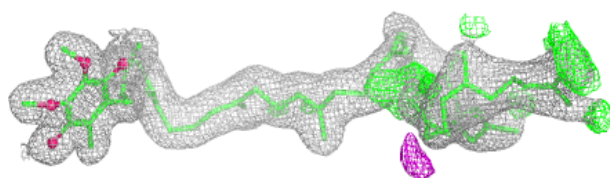
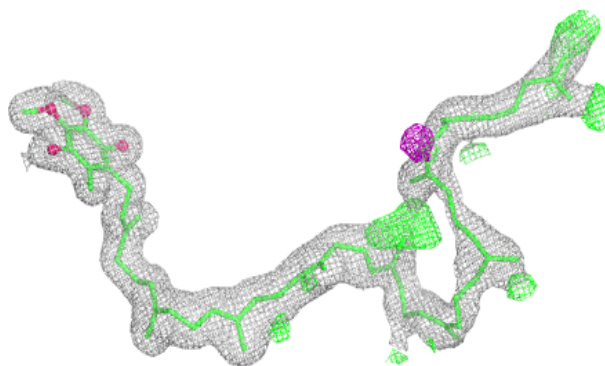
**Electron density around OLC L 501:**

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

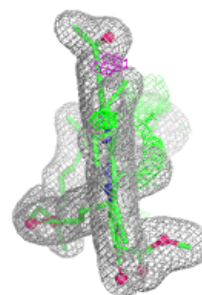
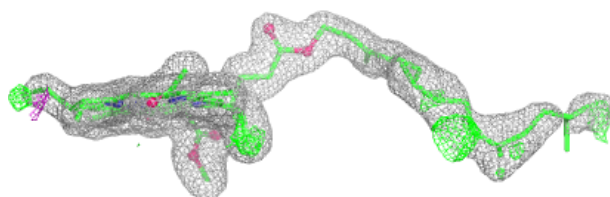
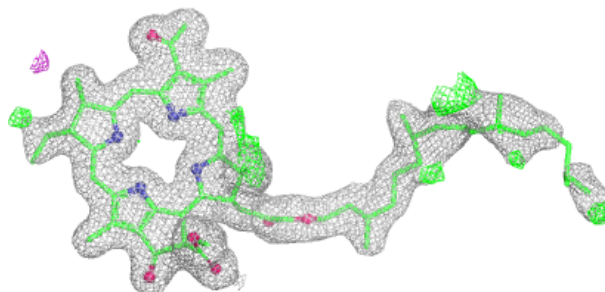


Electron density around U10 M 405:

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

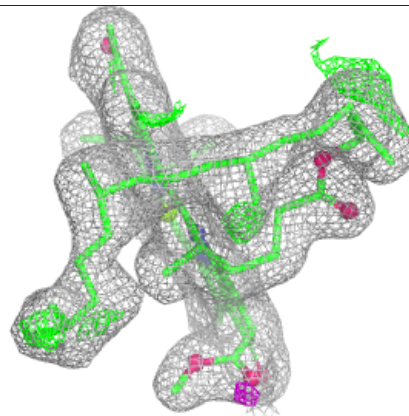
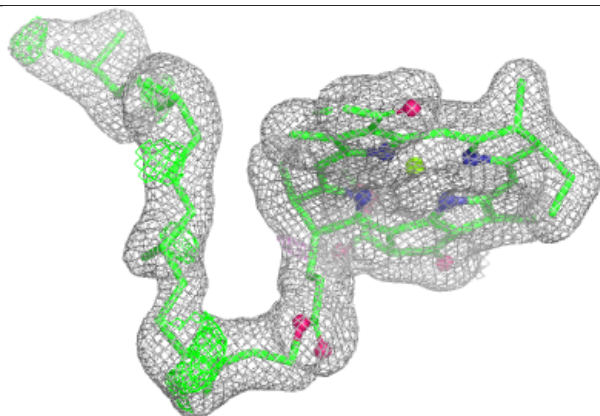
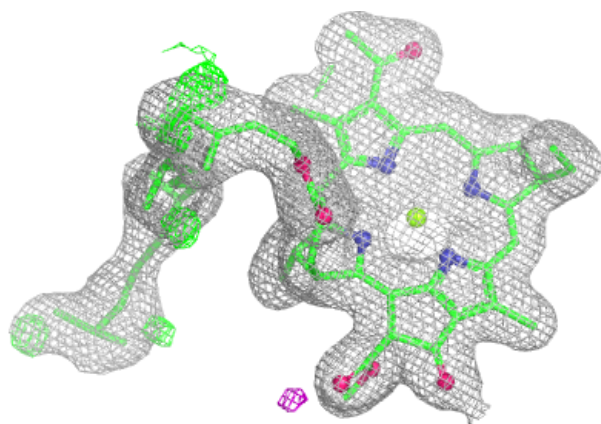
**Electron density around BPH M 409:**

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



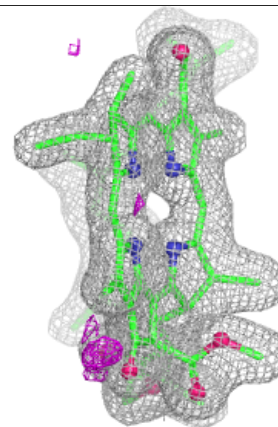
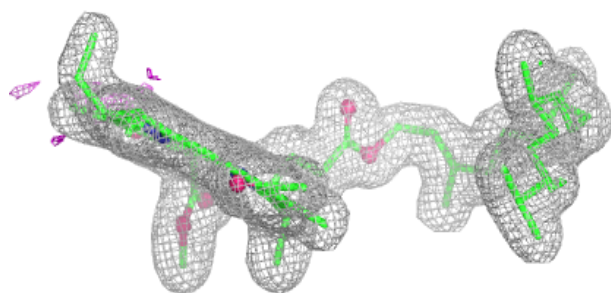
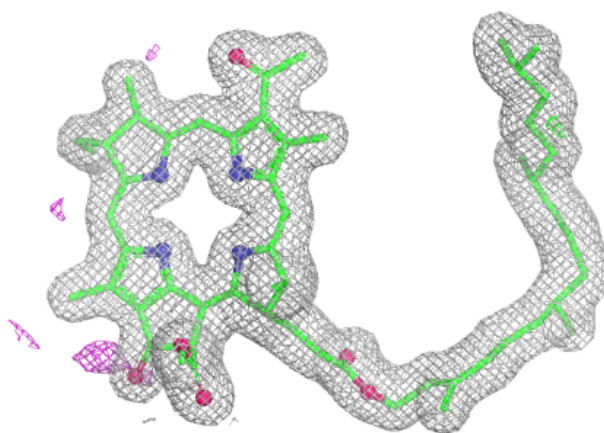
Electron density around BCL M 407:

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

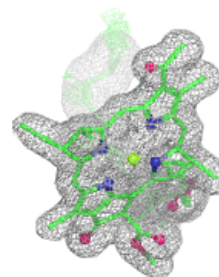
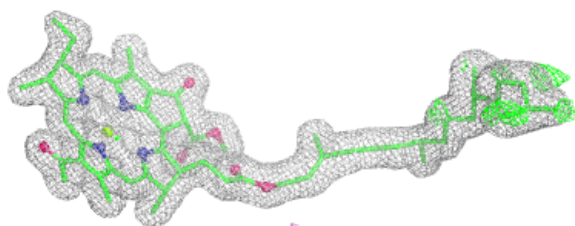
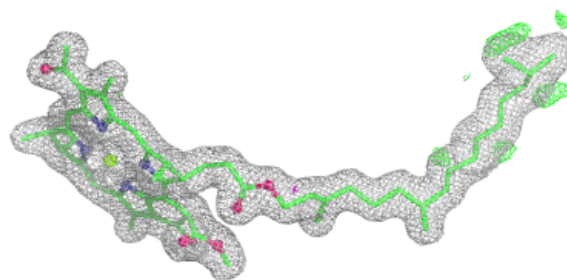


Electron density around BPH L 505:

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

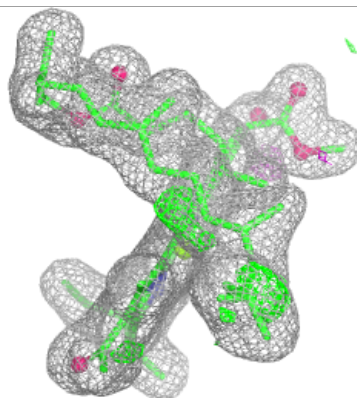
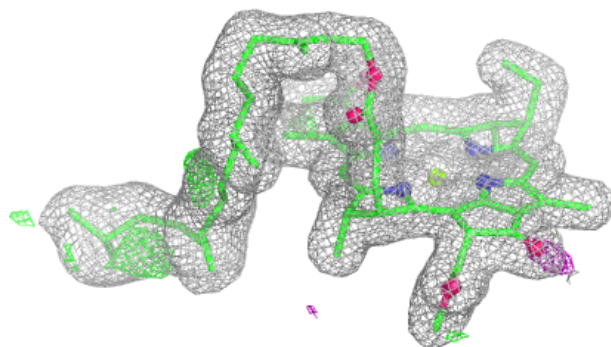
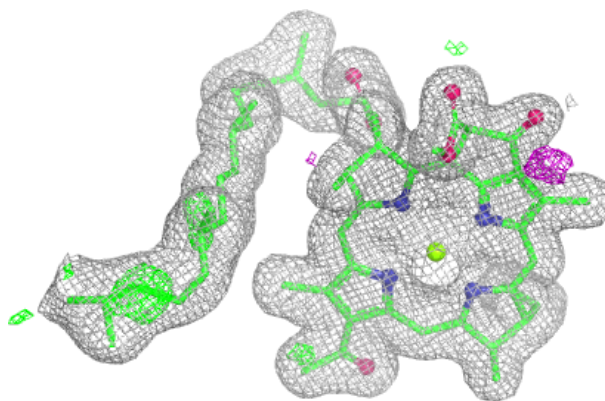
**Electron density around BCL L 503:**

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

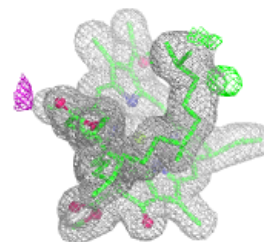
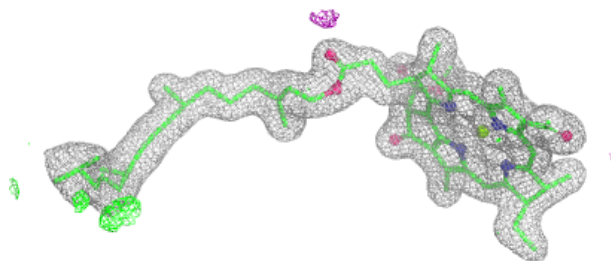
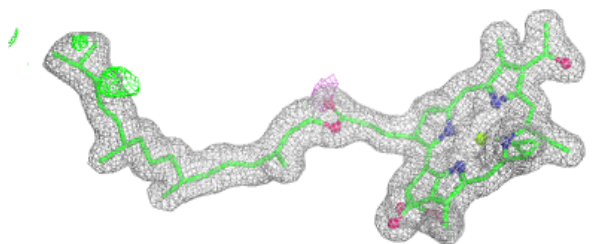


Electron density around BCL L 504:

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

**Electron density around BCL M 408:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.