



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 AM UTC

PDB ID : 7P2C / pdb_00007p2c
Title : F(M197)H mutant structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV by fixed-target serial synchrotron crystallography (room temperature, 26keV)
Authors : Gabdulkhakov, A.G.; Selikhanov, G.K.; Guenther, S.; Meents, A.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on : 2021-07-05
Resolution : 2.04 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

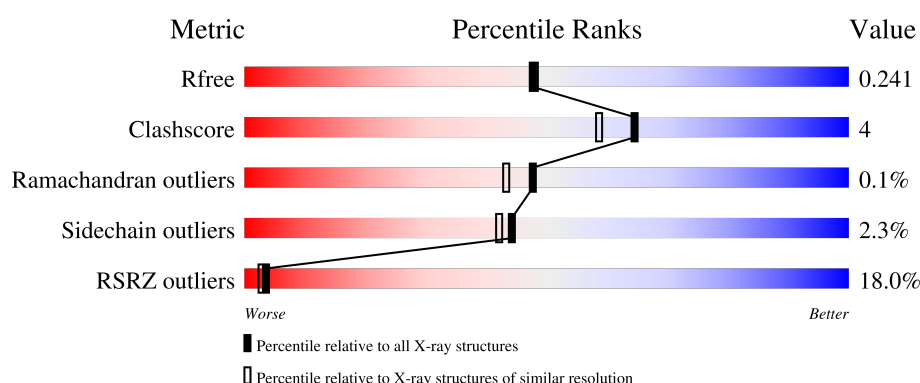
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	242	12% 86% 13% .
2	L	281	23% 92% 7% .
3	M	303	18% 89% 10%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7591 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	239	Total	C	N	O	S	0	5	0
			1862	1191	317	344	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	22	0
			2430	1645	387	390	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP Q3J1A5

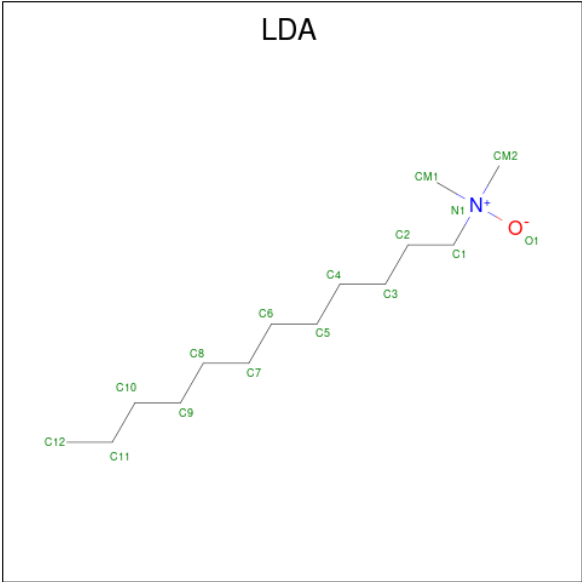
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	6	0
			2455	1636	405	403	11			

There are 2 discrepancies between the modelled and reference sequences:

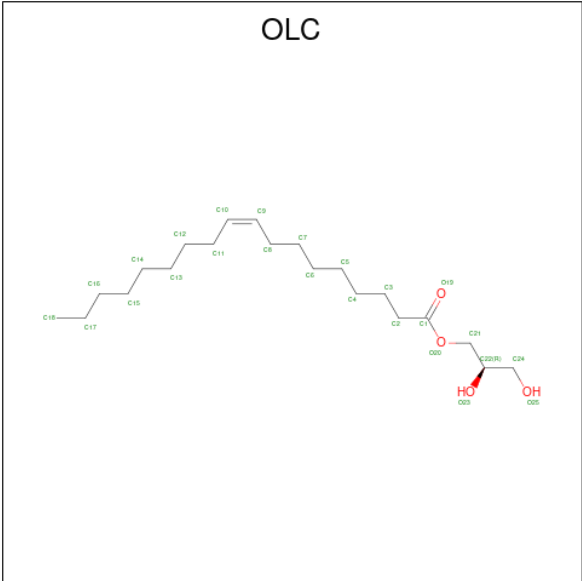
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP Q3J1A6
M	197	HIS	PHE	engineered mutation	UNP Q3J1A6

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



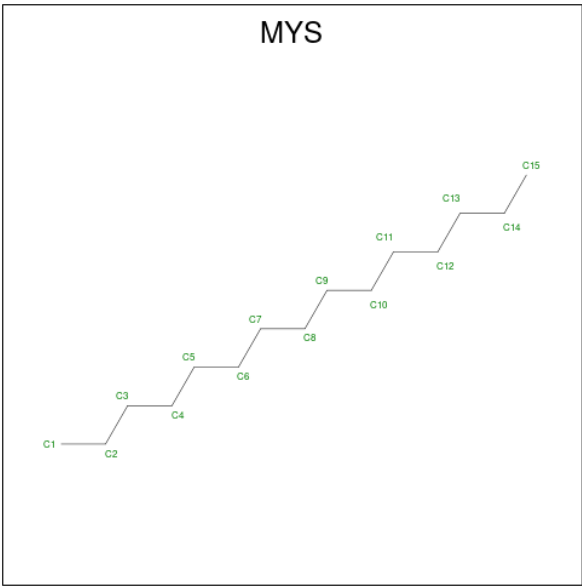
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



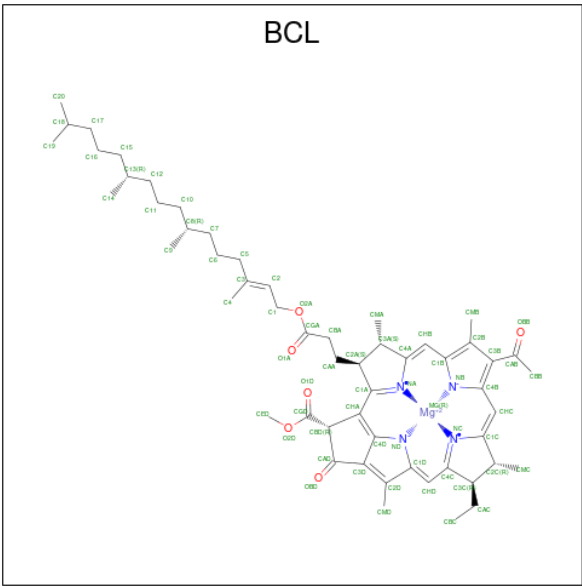
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	O		0	0
			25	21	4			

- Molecule 6 is PENTADECANE (CCD ID: MYS) (formula: C₁₅H₃₂).



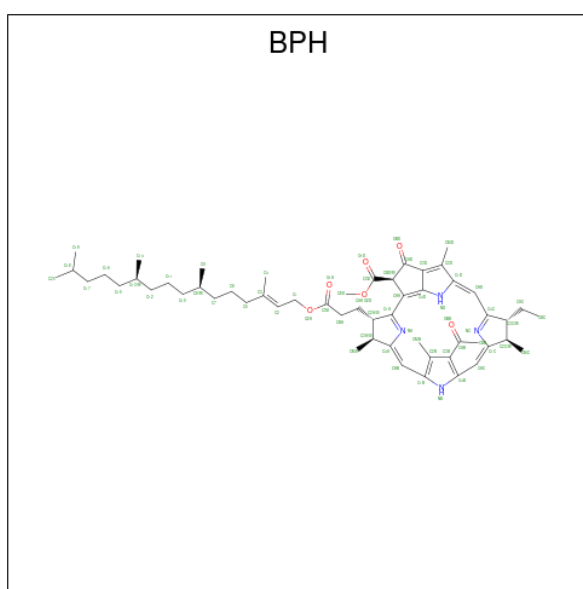
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C 15 15	0	0
6	L	1	Total C 15 15	0	0
6	M	1	Total C 15 15	0	0

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



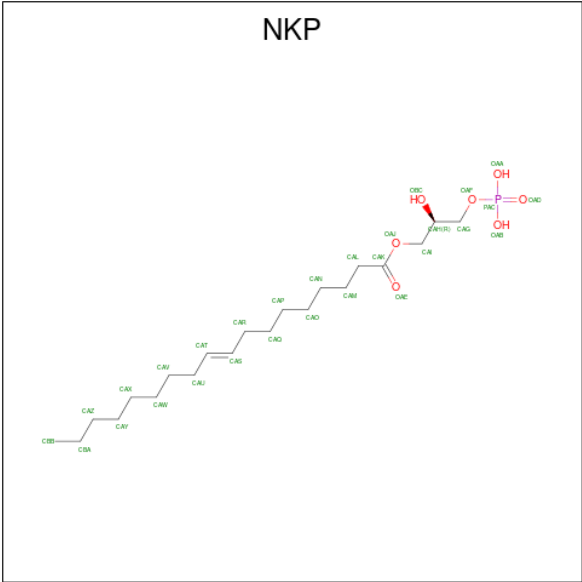
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



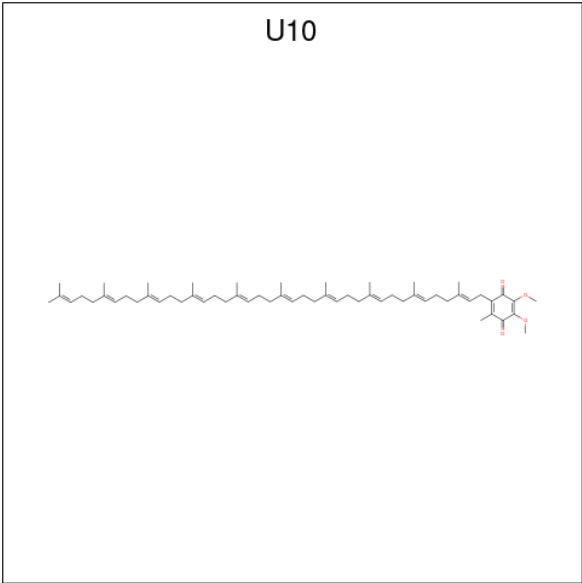
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is (2R)-2-hydroxy-3-(phosphonooxy)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	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 UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).

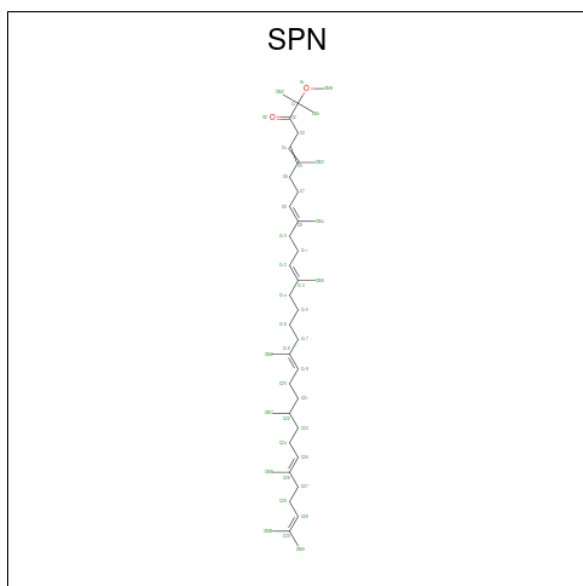


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			63	59	4		

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

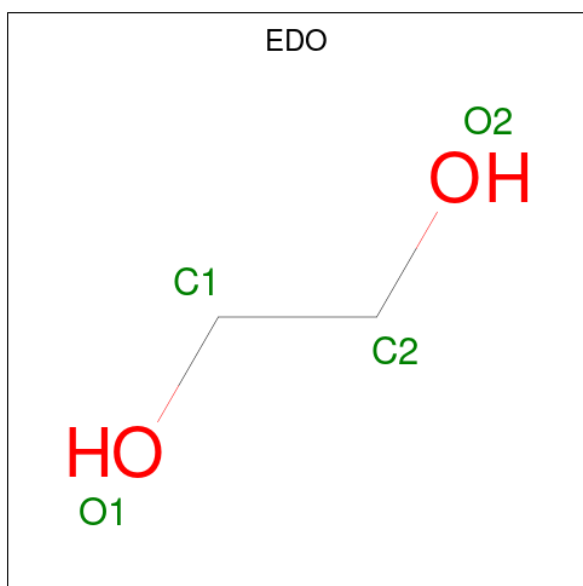
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



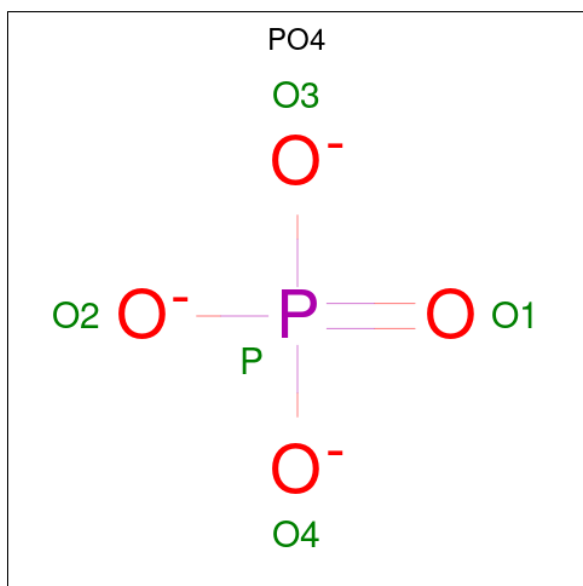
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			43	41	2		

- 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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

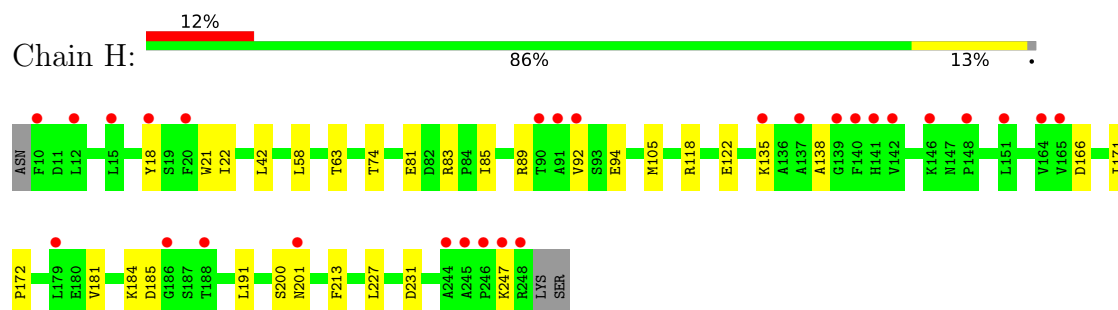
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	78	Total	O	0	0
			78	78		
15	L	53	Total	O	0	0
			53	53		
15	M	43	Total	O	0	0
			43	43		

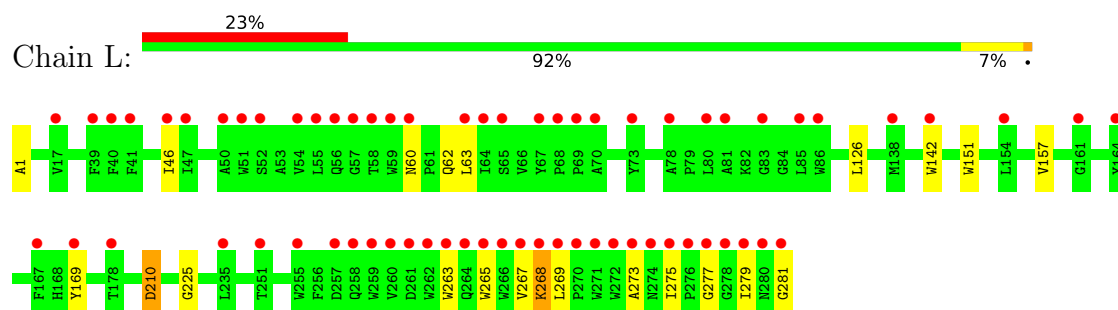
3 Residue-property plots [i](#)

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.

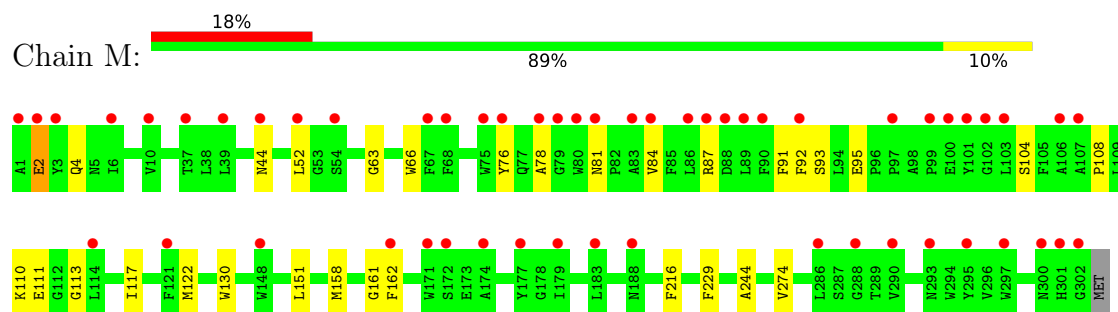
- Molecule 1: Reaction center protein H chain



- 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	102.50Å 102.50Å 237.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.04 47.05 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.04) 99.9 (47.05-2.04)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.201 , 0.229 0.211 , 0.241	Depositor DCC
R_{free} test set	4082 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7591	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MYS, FE, SPN, U10, EDO, BCL, LDA, OLC, NKP, PO4, 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	0.32	0/1911	0.48	0/2601
2	L	0.29	0/2531	0.44	0/3468
3	M	0.32	0/2547	0.48	0/3476
All	All	0.31	0/6989	0.47	0/9545

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	1862	0	1859	17	0
2	L	2430	0	2366	15	0
3	M	2455	0	2374	19	0
4	H	16	0	31	2	0
4	M	16	0	31	2	0
5	L	25	0	40	1	0
6	L	30	0	64	1	0
6	M	15	0	32	0	0
7	L	132	0	148	2	0
7	M	132	0	148	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	65	0	76	0	0
8	M	65	0	76	4	0
9	M	58	0	78	0	0
10	M	63	0	90	2	0
11	M	1	0	0	0	0
12	M	43	0	70	4	0
13	M	4	0	6	0	0
14	M	5	0	0	0	0
15	H	78	0	0	2	0
15	L	53	0	0	0	0
15	M	43	0	0	0	0
All	All	7591	0	7489	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)
7:M:405:BCL:H203	8:M:406:BPH:H8	1.69	0.74
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.76	0.67
1:H:135:LYS:HG2	1:H:166:ASP:OD2	1.98	0.64
1:H:247:LYS:NZ	15:H:402:HOH:O	2.33	0.61
1:H:18:TYR:O	1:H:22:ILE:HD12	2.03	0.58
3:M:161:GLY:HA3	12:M:408:SPN:H201	1.85	0.57
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.36	0.55
3:M:44:ASN:HD22	3:M:44:ASN:N	2.05	0.53
2:L:169:TYR:O	2:L:263[B]:TRP:NE1	2.37	0.51
3:M:63:GLY:HA3	8:M:406:BPH:H5C1	1.92	0.51
3:M:81:ASN:OD1	3:M:84:VAL:HG23	2.12	0.50
4:H:301:LDA:H121	4:M:409:LDA:H91	1.93	0.50
8:M:406:BPH:HBC3	8:M:406:BPH:HHD	1.93	0.50
2:L:277[B]:GLY:O	3:M:87:ARG:NH2	2.45	0.49
3:M:2:GLU:O	3:M:4:GLN:NE2	2.36	0.49
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.28	0.49
3:M:162:PHE:HB2	12:M:408:SPN:HM71	1.93	0.49
4:H:301:LDA:HM11	4:H:301:LDA:H22	1.66	0.47
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.98	0.46
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.46
7:M:404:BCL:H202	12:M:408:SPN:H61	1.96	0.46
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:TRP:HZ2	4:M:409:LDA:HM13	1.80	0.45
7:L:304:BCL:H192	7:L:304:BCL:H161	1.71	0.45
7:M:405:BCL:H172	8:M:406:BPH:H9C2	1.99	0.45
1:H:105[A]:MET:HB3	1:H:105[A]:MET:HE3	1.79	0.45
2:L:275[A]:ILE:O	2:L:281[A]:GLY:HA3	2.17	0.44
2:L:62:GLN:CD	2:L:151:TRP:HE1	2.25	0.44
1:H:201:ASN:OD1	1:H:201:ASN:N	2.50	0.44
2:L:157:VAL:HG12	7:L:304:BCL:HBC2	2.00	0.44
2:L:268[A]:LYS:HD3	2:L:268[A]:LYS:HA	1.75	0.44
2:L:142:TRP:CH2	6:L:302:MYS:H71	2.53	0.44
10:M:402:U10:H371	10:M:402:U10:H412	1.84	0.43
1:H:42:LEU:HB3	2:L:1:ALA:HB1	2.01	0.43
3:M:113:GLY:O	3:M:117:ILE:HD12	2.18	0.43
1:H:181:VAL:HG21	1:H:191:LEU:HD12	2.00	0.42
2:L:60:ASN:OD1	2:L:63:LEU:HG	2.20	0.42
2:L:225:GLY:H	5:L:301:OLC:H22	1.84	0.42
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.55	0.42
3:M:158:MET:HB3	3:M:158:MET:HE3	1.71	0.42
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.00	0.42
3:M:93:SER:OG	3:M:95:GLU:OE2	2.36	0.42
1:H:184:LYS:HG3	1:H:185:ASP:N	2.35	0.42
3:M:130:TRP:NE1	3:M:151[B]:LEU:HG	2.35	0.42
1:H:118:ARG:HD2	15:H:420:HOH:O	2.20	0.41
2:L:279[A]:ILE:HG21	3:M:91:PHE:HB3	2.01	0.41
3:M:76:TYR:OH	3:M:110:LYS:HD3	2.19	0.41
3:M:130:TRP:HE1	3:M:151[B]:LEU:HG	1.84	0.41
7:M:404:BCL:CAB	12:M:408:SPN:H162	2.49	0.41
2:L:268[A]:LYS:HA	2:L:273[A]:ALA:HB2	2.03	0.41
3:M:122:MET:HE1	7:M:404:BCL:HBB3	2.03	0.41
2:L:210:ASP:N	2:L:210:ASP:OD2	2.54	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.03	0.41
10:M:402:U10:H471	10:M:402:U10:H451	1.85	0.41
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.56	0.41
1:H:83:ARG:HE	1:H:83:ARG:HB2	1.73	0.40
1:H:63[B]:THR:HG22	1:H:74:THR:OG1	2.21	0.40
2:L:126:LEU:HD23	2:L:126:LEU:HA	1.97	0.40

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	242/242 (100%)	238 (98%)	3 (1%)	1 (0%)	30	22
2	L	300/281 (107%)	287 (96%)	13 (4%)	0	100	100
3	M	306/303 (101%)	296 (97%)	10 (3%)	0	100	100
All	All	848/826 (103%)	821 (97%)	26 (3%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	ALA

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	199/197 (101%)	195 (98%)	4 (2%)	48	48
2	L	238/220 (108%)	228 (96%)	10 (4%)	26	20
3	M	241/237 (102%)	235 (98%)	6 (2%)	42	39
All	All	678/654 (104%)	658 (97%)	20 (3%)	44	33

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	58	LEU
1	H	92	VAL

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Mol	Chain	Res	Type
1	H	200	SER
1	H	231	ASP
2	L	46	ILE
2	L	210	ASP
2	L	265[A]	TRP
2	L	265[B]	TRP
2	L	267[A]	VAL
2	L	267[B]	VAL
2	L	268[A]	LYS
2	L	268[B]	LYS
2	L	269[A]	LEU
2	L	269[B]	LEU
3	M	2	GLU
3	M	52[A]	LEU
3	M	52[B]	LEU
3	M	104	SER
3	M	216	PHE
3	M	274	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	44	ASN
1	H	126	HIS
3	M	44	ASN
3	M	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
7	BCL	M	405	-	69,74,74	1.28	7 (10%)	79,115,115	1.42	8 (10%)
5	OLC	L	301	-	24,24,24	0.95	1 (4%)	25,25,25	0.90	2 (8%)
7	BCL	L	304	-	69,74,74	1.32	5 (7%)	79,115,115	1.37	8 (10%)
9	NKP	M	401	-	28,28,28	0.34	0	30,32,32	0.64	1 (3%)
6	MYS	M	410	-	14,14,14	0.25	0	13,13,13	0.62	0
7	BCL	L	305	-	69,74,74	1.21	5 (7%)	79,115,115	1.36	7 (8%)
10	U10	M	402	-	63,63,63	2.73	17 (26%)	78,79,79	1.73	21 (26%)
6	MYS	L	302	-	14,14,14	0.26	0	13,13,13	0.55	0
9	NKP	M	403	-	28,28,28	0.54	0	30,32,32	0.47	0
14	PO4	M	412	-	4,4,4	0.97	0	6,6,6	0.37	0
4	LDA	M	409	-	13,15,15	2.29	2 (15%)	14,17,17	0.38	0
8	BPH	M	406	-	59,70,70	1.28	7 (11%)	59,101,101	2.15	10 (16%)
4	LDA	H	301	-	13,15,15	2.46	2 (15%)	14,17,17	0.61	0
7	BCL	M	404	-	69,74,74	1.12	4 (5%)	79,115,115	1.46	11 (13%)
12	SPN	M	408	-	42,42,42	0.57	0	50,52,52	1.41	10 (20%)
13	EDO	M	411	-	3,3,3	0.33	0	2,2,2	1.29	0
8	BPH	L	306	-	59,70,70	1.23	7 (11%)	59,101,101	2.07	12 (20%)
6	MYS	L	303	-	14,14,14	0.28	0	13,13,13	0.51	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
7	BCL	M	405	-	-	1/41/137/137	-
5	OLC	L	301	-	-	7/24/24/24	-
7	BCL	L	304	-	-	1/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NKP	M	401	-	-	7/28/28/28	-
6	MYS	M	410	-	-	2/12/12/12	-
7	BCL	L	305	-	-	2/41/137/137	-
10	U10	M	402	-	-	12/63/87/87	0/1/1/1
6	MYS	L	302	-	-	3/12/12/12	-
9	NKP	M	403	-	-	10/28/28/28	-
4	LDA	M	409	-	-	3/13/13/13	-
8	BPH	M	406	-	-	3/37/105/105	0/5/6/6
4	LDA	H	301	-	-	5/13/13/13	-
7	BCL	M	404	-	-	0/41/137/137	-
12	SPN	M	408	-	-	17/50/51/51	-
13	EDO	M	411	-	-	1/1/1/1	-
8	BPH	L	306	-	-	3/37/105/105	0/5/6/6
6	MYS	L	303	-	-	6/12/12/12	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	409	LDA	O1-N1	-6.70	1.25	1.42
10	M	402	U10	C33-C34	6.59	1.48	1.33
4	H	301	LDA	O1-N1	-6.59	1.26	1.42
10	M	402	U10	C48-C49	6.36	1.47	1.33
10	M	402	U10	C43-C44	6.29	1.47	1.33
10	M	402	U10	C8-C9	6.27	1.47	1.33
10	M	402	U10	C18-C19	6.19	1.47	1.33
10	M	402	U10	C38-C39	6.19	1.47	1.33
10	M	402	U10	C13-C14	6.08	1.47	1.33
10	M	402	U10	C28-C29	6.03	1.46	1.33
10	M	402	U10	C23-C24	5.96	1.46	1.33
4	H	301	LDA	C1-N1	-5.88	1.45	1.51
7	L	304	BCL	MG-NA	5.76	2.19	2.06
7	M	405	BCL	MG-NA	5.54	2.19	2.06
7	L	305	BCL	MG-NA	5.53	2.19	2.06
10	M	402	U10	C53-C54	5.20	1.48	1.32
10	M	402	U10	O3-C3	-4.90	1.25	1.36
10	M	402	U10	O4-C4	-4.79	1.25	1.36
7	M	404	BCL	MG-NA	4.68	2.17	2.06
4	M	409	LDA	C1-N1	-4.63	1.46	1.51
8	M	406	BPH	CBD-CGD	-4.47	1.46	1.52
7	L	304	BCL	MG-NC	4.31	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	301	OLC	O20-C1	4.15	1.45	1.33
8	L	306	BPH	C1D-C2D	3.92	1.43	1.39
7	M	405	BCL	MG-NC	3.71	2.15	2.06
7	L	304	BCL	C3B-C4B	3.38	1.47	1.41
7	M	404	BCL	MG-NC	3.27	2.14	2.06
8	M	406	BPH	C3D-CAD	-3.22	1.41	1.47
8	L	306	BPH	OBD-CAD	3.19	1.26	1.22
8	M	406	BPH	C1B-C2B	3.15	1.43	1.39
7	L	305	BCL	MG-NC	3.13	2.13	2.06
7	M	404	BCL	C3B-C4B	3.04	1.47	1.41
10	M	402	U10	C4-C5	-3.01	1.40	1.48
8	M	406	BPH	CHA-CBD	2.93	1.55	1.51
10	M	402	U10	C3-C2	-2.91	1.40	1.48
8	L	306	BPH	CAC-C3C	2.80	1.59	1.53
7	L	305	BCL	CHD-C1D	2.77	1.43	1.38
7	L	305	BCL	C1D-ND	2.74	1.41	1.37
7	M	405	BCL	C3B-C4B	2.69	1.46	1.41
7	L	304	BCL	C1D-ND	2.62	1.41	1.37
8	L	306	BPH	C3D-CAD	-2.59	1.42	1.47
8	M	406	BPH	C3B-C4B	2.59	1.45	1.41
8	L	306	BPH	CBD-CGD	-2.58	1.49	1.52
8	L	306	BPH	C3B-C4B	2.53	1.45	1.41
10	M	402	U10	C6-C1	2.52	1.39	1.35
7	M	405	BCL	CHD-C1D	2.50	1.43	1.38
10	M	402	U10	C1-C2	-2.42	1.39	1.47
7	L	305	BCL	C3B-C4B	2.33	1.45	1.41
10	M	402	U10	C6-C5	-2.24	1.40	1.46
8	L	306	BPH	CHA-CBD	2.23	1.54	1.51
8	M	406	BPH	OBD-CAD	2.22	1.25	1.22
7	M	405	BCL	C1D-ND	2.15	1.40	1.37
7	M	404	BCL	CHD-C1D	2.15	1.42	1.38
8	M	406	BPH	O2A-CGA	-2.13	1.27	1.33
7	M	405	BCL	C3D-C4D	-2.05	1.39	1.44
7	L	304	BCL	CMB-C2B	2.04	1.55	1.50
7	M	405	BCL	C1-C2	2.04	1.55	1.49

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	406	BPH	C4D-CHA-CBD	-12.23	102.59	108.45
8	L	306	BPH	C4D-CHA-CBD	-10.47	103.43	108.45
7	L	305	BCL	C4D-CHA-C1A	5.81	128.18	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	405	BCL	C4D-CHA-C1A	5.71	128.05	121.24
7	M	404	BCL	C4D-CHA-C1A	4.89	127.08	121.24
7	L	304	BCL	C4D-CHA-C1A	4.70	126.85	121.24
10	M	402	U10	C22-C23-C24	-4.52	117.29	127.62
8	L	306	BPH	C4D-ND-C1D	-4.26	103.77	108.87
7	M	405	BCL	C4A-NA-C1A	4.25	108.62	106.68
8	M	406	BPH	C4D-ND-C1D	-4.24	103.80	108.87
7	L	305	BCL	CHD-C1D-ND	-3.88	119.35	124.80
8	L	306	BPH	O2D-CGD-CBD	3.85	115.18	110.95
10	M	402	U10	C17-C18-C19	-3.84	118.84	127.62
8	L	306	BPH	OBD-CAD-CBD	-3.82	120.22	125.82
10	M	402	U10	C47-C48-C49	-3.81	118.90	127.62
7	M	404	BCL	CHD-C1D-ND	-3.75	119.52	124.80
7	L	304	BCL	CHD-C1D-ND	-3.68	119.62	124.80
7	L	304	BCL	C1D-ND-C4D	-3.67	103.74	106.31
8	L	306	BPH	C3D-C4D-ND	3.59	112.31	107.71
12	M	408	SPN	CM5-C13-C14	3.55	121.39	115.23
8	M	406	BPH	O2D-CGD-CBD	3.50	114.80	110.95
7	L	305	BCL	C1D-ND-C4D	-3.49	103.86	106.31
7	M	404	BCL	C16-C15-C13	3.46	127.48	115.97
7	M	405	BCL	CHD-C1D-ND	-3.44	119.96	124.80
7	M	404	BCL	C1D-ND-C4D	-3.44	103.90	106.31
10	M	402	U10	C30-C29-C31	3.38	121.09	115.23
10	M	402	U10	C45-C44-C46	3.38	121.09	115.23
7	M	405	BCL	C1D-ND-C4D	-3.36	103.95	106.31
7	M	404	BCL	C4A-NA-C1A	3.23	108.15	106.68
8	M	406	BPH	C3D-C4D-ND	3.23	111.85	107.71
7	M	405	BCL	CHA-C1A-NA	-3.23	119.08	126.39
7	L	305	BCL	CHA-C1A-NA	-3.22	119.11	126.39
12	M	408	SPN	CM3-C5-C6	3.21	120.81	115.23
10	M	402	U10	C40-C39-C41	3.14	120.68	115.23
10	M	402	U10	C12-C13-C14	-3.11	120.49	127.62
12	M	408	SPN	CM4-C9-C10	3.05	120.51	115.23
8	M	406	BPH	OBD-CAD-CBD	-3.02	121.39	125.82
7	M	404	BCL	CHA-C1A-NA	-2.98	119.64	126.39
10	M	402	U10	C37-C38-C39	-2.94	120.90	127.62
8	L	306	BPH	C2D-C1D-ND	2.88	111.52	109.43
8	L	306	BPH	CMB-C2B-C3B	2.88	130.44	124.68
10	M	402	U10	C42-C43-C44	-2.88	121.04	127.62
10	M	402	U10	C25-C24-C26	2.84	120.16	115.23
7	L	304	BCL	CHA-C1A-NA	-2.82	120.01	126.39
12	M	408	SPN	CM6-C18-C17	2.81	120.11	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	408	SPN	C3-C4-C5	-2.81	121.99	126.83
8	L	306	BPH	C4C-C3C-C2C	-2.79	100.18	102.84
5	L	301	OLC	O20-C1-C2	2.73	120.17	111.83
7	M	405	BCL	C2A-C1A-CHA	2.70	128.55	123.87
10	M	402	U10	C27-C28-C29	-2.69	121.46	127.62
10	M	402	U10	C10-C9-C11	2.69	119.89	115.23
10	M	402	U10	C50-C49-C51	2.69	119.89	115.23
8	M	406	BPH	C2D-C1D-ND	2.68	111.37	109.43
5	L	301	OLC	O20-C1-O19	-2.67	116.95	123.63
8	M	406	BPH	C11-C10-C8	2.64	124.75	115.97
8	M	406	BPH	C1-C2-C3	-2.62	121.91	126.20
7	L	304	BCL	C2A-C1A-CHA	2.59	128.36	123.87
7	L	305	BCL	C2A-C1A-CHA	2.55	128.29	123.87
12	M	408	SPN	CM8-C26-C27	2.53	119.62	115.23
10	M	402	U10	C15-C14-C16	2.50	119.57	115.23
7	M	404	BCL	C2A-C1A-CHA	2.48	128.17	123.87
7	M	404	BCL	CBC-CAC-C3C	-2.47	108.17	113.41
7	L	304	BCL	CMB-C2B-C1B	-2.44	121.70	125.42
7	M	404	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
7	M	405	BCL	O2D-CGD-CBD	2.40	115.43	111.23
8	L	306	BPH	OBD-CAD-C3D	2.35	131.55	127.89
12	M	408	SPN	C7-C8-C9	-2.35	122.26	127.62
7	M	404	BCL	C1-C2-C3	-2.34	122.37	126.20
10	M	402	U10	C20-C19-C21	2.33	119.27	115.23
10	M	402	U10	C7-C8-C9	-2.31	122.86	126.83
7	M	404	BCL	OBB-CAB-CBB	-2.29	114.65	119.77
10	M	402	U10	C35-C34-C36	2.28	119.18	115.23
10	M	402	U10	C32-C33-C34	-2.26	122.45	127.62
9	M	401	NKP	OAB-PAC-OAF	-2.26	100.79	106.67
10	M	402	U10	C4M-O4-C4	2.25	124.39	116.47
10	M	402	U10	C56-C54-C55	2.23	119.73	114.59
12	M	408	SPN	C20-C19-C18	-2.20	122.59	127.62
7	L	304	BCL	C16-C15-C13	-2.19	108.69	115.97
8	L	306	BPH	O2D-CGD-O1D	-2.16	119.64	123.85
8	M	406	BPH	CMD-C2D-C3D	2.16	129.00	124.68
7	L	304	BCL	OBB-CAB-CBB	-2.16	114.93	119.77
7	L	305	BCL	C11-C10-C8	-2.15	108.81	115.97
8	L	306	BPH	CMD-C2D-C3D	2.14	128.96	124.68
8	L	306	BPH	O2A-CGA-O1A	-2.11	118.35	123.63
12	M	408	SPN	CMB-C30-CM9	2.10	119.43	114.59
7	L	305	BCL	C4A-NA-C1A	2.06	107.62	106.68
10	M	402	U10	C22-C21-C19	-2.06	106.36	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	406	BPH	CMB-C2B-C3B	2.06	128.79	124.68
12	M	408	SPN	C24-C25-C26	-2.05	122.93	127.62
7	M	405	BCL	C4D-C3D-CAD	-2.03	105.90	108.11

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	301	OLC	O20-C21-C22-O23
7	L	305	BCL	CHA-CBD-CGD-O2D
10	M	402	U10	C32-C33-C34-C35
10	M	402	U10	C32-C33-C34-C36
12	M	408	SPN	CM2-C1-C2-O2
12	M	408	SPN	CM2-C1-C2-C3
12	M	408	SPN	CM5-C13-C14-C15
12	M	408	SPN	C26-C27-C28-C29
9	M	403	NKP	OAE-CAK-OAJ-CAI
9	M	403	NKP	CAL-CAK-OAJ-CAI
10	M	402	U10	C45-C44-C46-C47
12	M	408	SPN	C11-C10-C9-CM4
10	M	402	U10	C43-C44-C46-C47
12	M	408	SPN	C12-C13-C14-C15
12	M	408	SPN	C16-C17-C18-CM6
12	M	408	SPN	C16-C17-C18-C19
10	M	402	U10	C24-C26-C27-C28
12	M	408	SPN	C11-C10-C9-C8
10	M	402	U10	C42-C43-C44-C45
12	M	408	SPN	C14-C15-C16-C17
5	L	301	OLC	O20-C21-C22-C24
5	L	301	OLC	C3-C4-C5-C6
6	L	303	MYS	C5-C6-C7-C8
9	M	403	NKP	CAN-CAO-CAP-CAQ
9	M	403	NKP	CAT-CAU-CAV-CAW
6	L	302	MYS	C6-C7-C8-C9
4	H	301	LDA	C1-C2-C3-C4
6	L	303	MYS	C7-C8-C9-C10
8	M	406	BPH	C13-C15-C16-C17
8	L	306	BPH	C4-C3-C5-C6
6	L	302	MYS	C5-C6-C7-C8
12	M	408	SPN	CM3-C5-C6-C7
8	L	306	BPH	C2-C3-C5-C6
12	M	408	SPN	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	M	403	NKP	CAP-CAQ-CAR-CAS
9	M	401	NKP	CAL-CAM-CAN-CAO
4	H	301	LDA	C7-C8-C9-C10
4	H	301	LDA	C9-C10-C11-C12
6	L	303	MYS	C12-C13-C14-C15
9	M	403	NKP	CAY-CAZ-CBA-CBB
9	M	403	NKP	CAW-CAX-CAY-CAZ
5	L	301	OLC	C4-C5-C6-C7
8	M	406	BPH	C4-C3-C5-C6
7	L	304	BCL	C15-C16-C17-C18
6	L	303	MYS	C11-C12-C13-C14
8	M	406	BPH	C2-C3-C5-C6
9	M	401	NKP	CAT-CAU-CAV-CAW
10	M	402	U10	C29-C31-C32-C33
6	L	303	MYS	C11-C10-C9-C8
4	M	409	LDA	C9-C10-C11-C12
12	M	408	SPN	C21-C22-C23-C24
6	M	410	MYS	C11-C10-C9-C8
9	M	401	NKP	CAQ-CAR-CAS-CAT
9	M	401	NKP	CAS-CAT-CAU-CAV
7	L	305	BCL	CHA-CBD-CGD-O1D
12	M	408	SPN	CM2-C1-O1-CMA
9	M	401	NKP	CAU-CAV-CAW-CAX
4	M	409	LDA	C1-C2-C3-C4
9	M	401	NKP	CAG-OAF-PAC-OAD
12	M	408	SPN	CM7-C22-C23-C24
10	M	402	U10	C14-C16-C17-C18
13	M	411	EDO	O1-C1-C2-O2
10	M	402	U10	C5-C4-O4-C4M
6	M	410	MYS	C9-C10-C11-C12
9	M	403	NKP	CAR-CAS-CAT-CAU
4	M	409	LDA	C7-C8-C9-C10
10	M	402	U10	C25-C24-C26-C27
9	M	403	NKP	CAQ-CAR-CAS-CAT
9	M	403	NKP	CAG-CAH-CAI-OAJ
5	L	301	OLC	C2-C3-C4-C5
10	M	402	U10	C23-C24-C26-C27
4	H	301	LDA	C5-C6-C7-C8
10	M	402	U10	C42-C43-C44-C46
5	L	301	OLC	O20-C1-C2-C3
12	M	408	SPN	C9-C10-C11-C12
5	L	301	OLC	C9-C10-C11-C12

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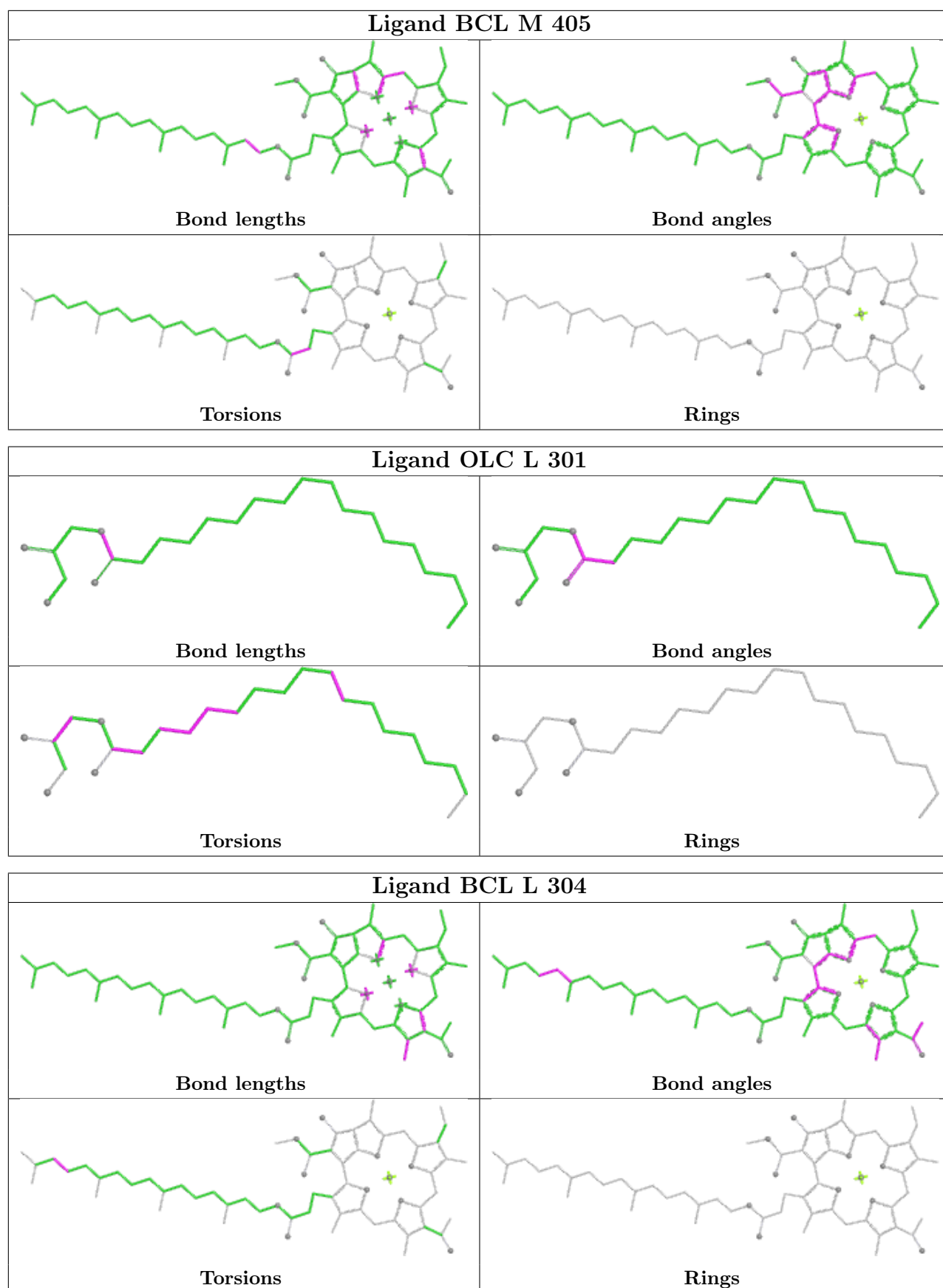
Mol	Chain	Res	Type	Atoms
12	M	408	SPN	C2-C1-O1-CMA
6	L	303	MYS	C4-C5-C6-C7
6	L	302	MYS	C11-C12-C13-C14
4	H	301	LDA	C2-C1-N1-O1
7	M	405	BCL	CAA-CBA-CGA-O2A
8	L	306	BPH	CAD-CBD-CGD-O2D
9	M	401	NKP	OAF-CAG-CAH-OBC

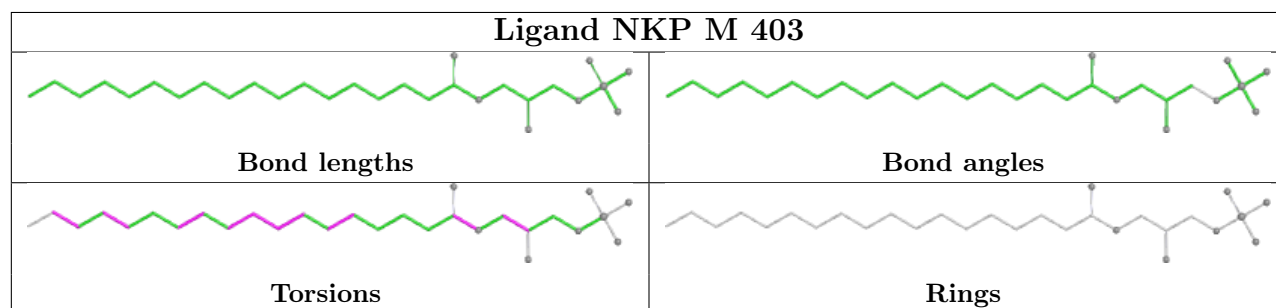
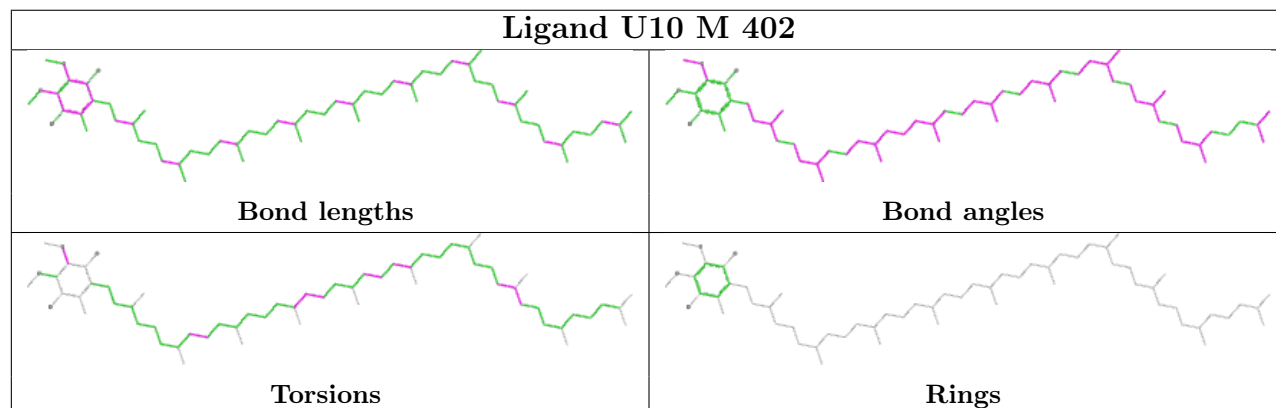
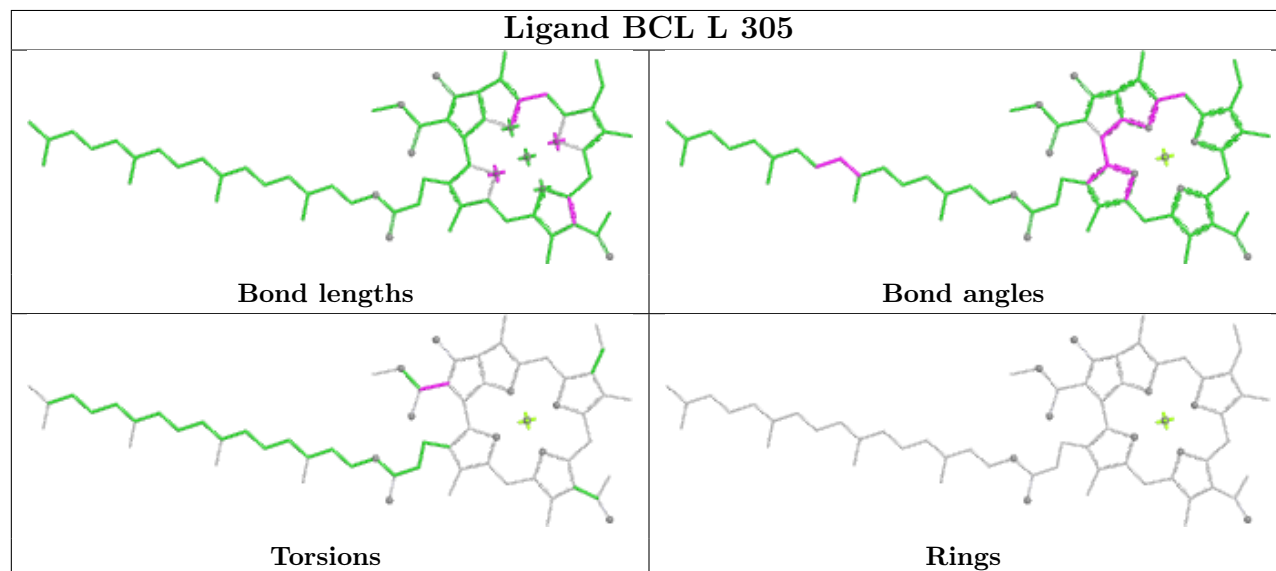
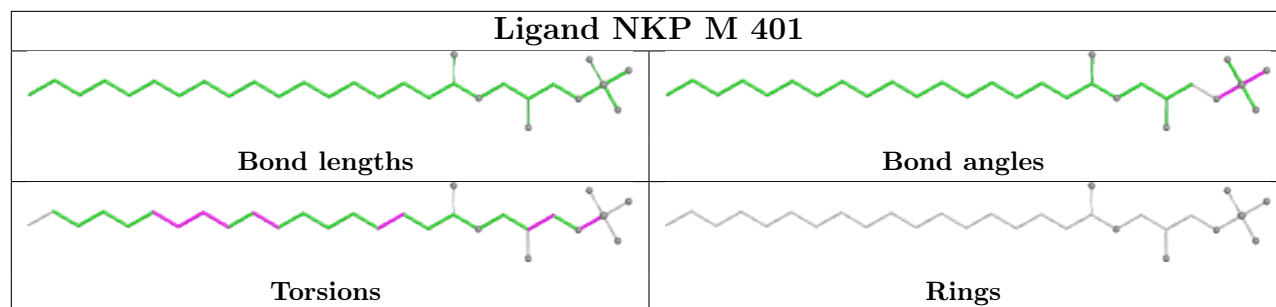
There are no ring outliers.

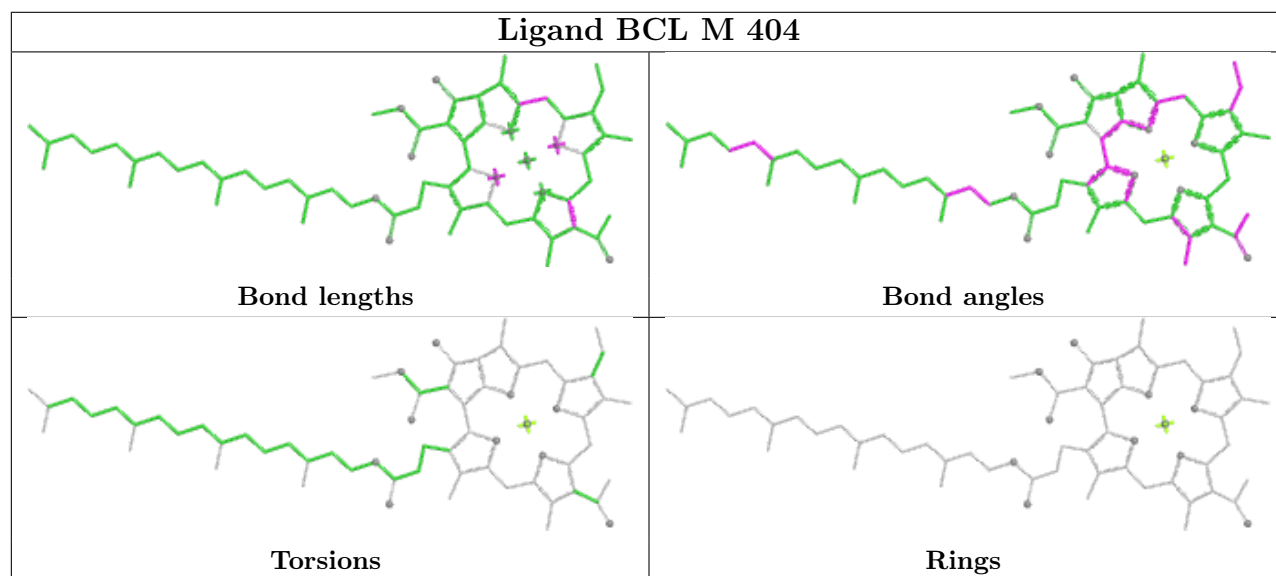
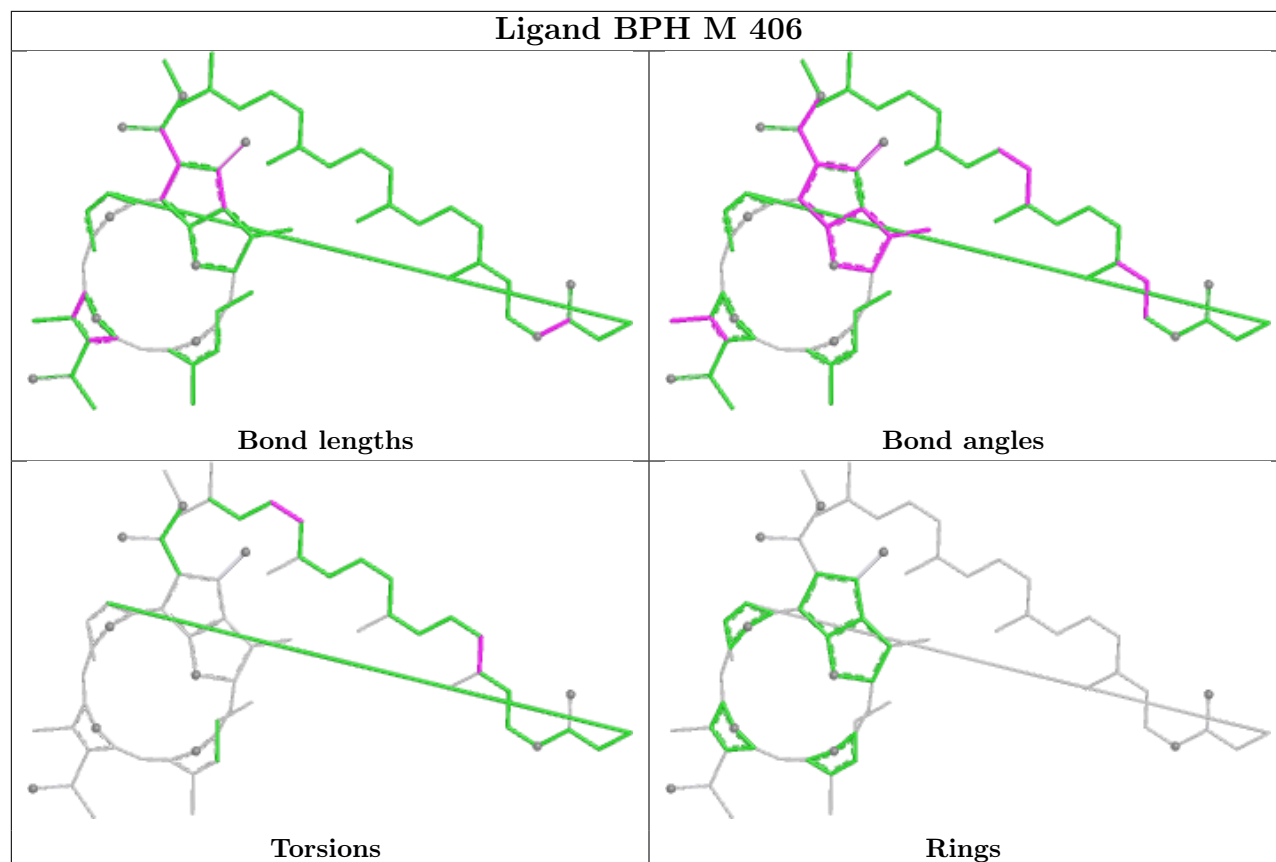
10 monomers are involved in 18 short contacts:

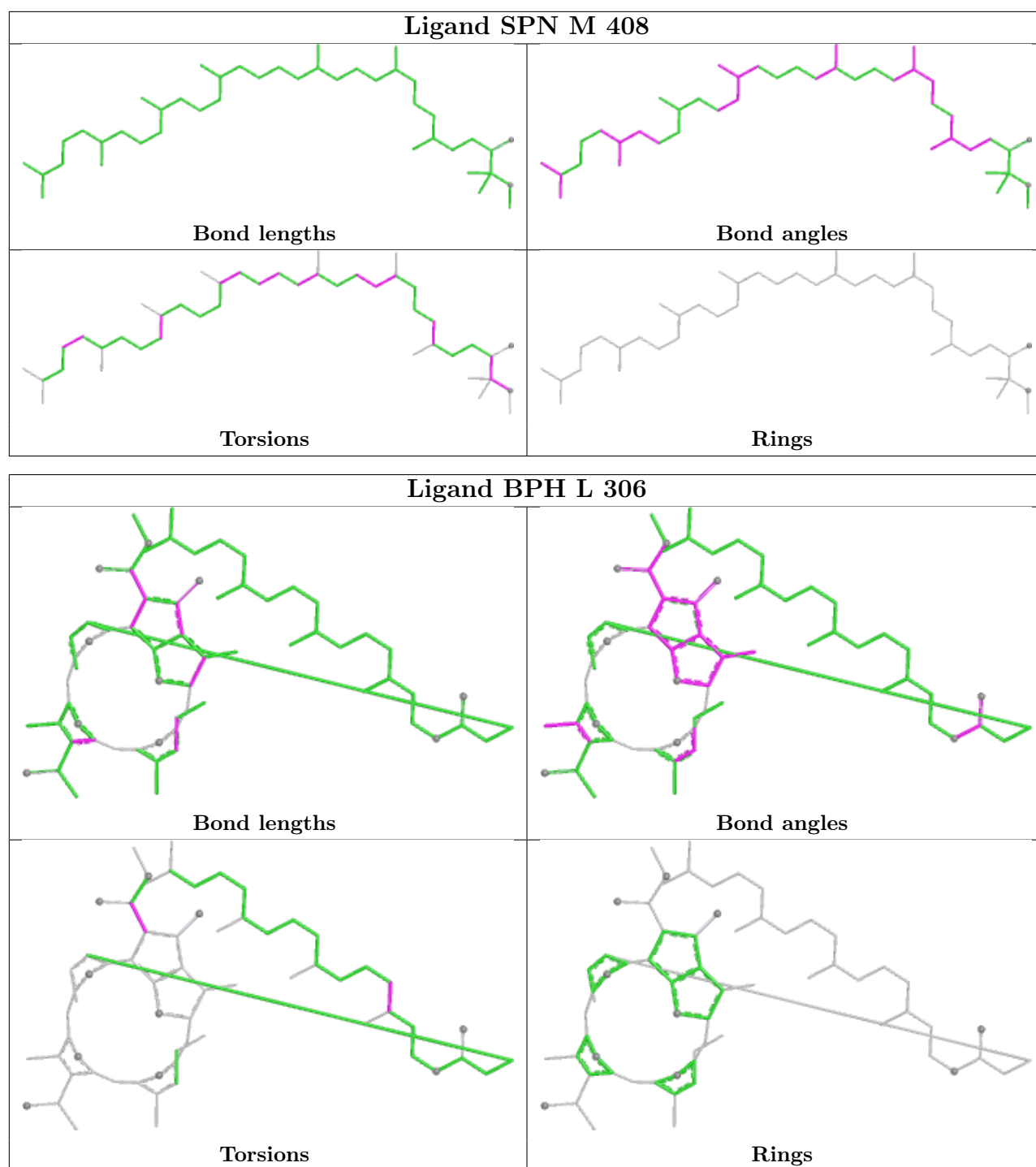
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	405	BCL	2	0
5	L	301	OLC	1	0
7	L	304	BCL	2	0
10	M	402	U10	2	0
6	L	302	MYS	1	0
4	M	409	LDA	2	0
8	M	406	BPH	4	0
4	H	301	LDA	2	0
7	M	404	BCL	3	0
12	M	408	SPN	4	0

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 ⓘ

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	239/242 (98%)	0.72	28 (11%) 9 8	13, 39, 62, 86	5 (2%)
2	L	281/281 (100%)	1.11	66 (23%) 2 1	17, 37, 63, 118	22 (7%)
3	M	302/303 (99%)	0.96	54 (17%) 3 3	11, 37, 67, 98	6 (1%)
All	All	822/826 (99%)	0.94	148 (18%) 3 3	11, 37, 65, 118	33 (4%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	270[A]	PRO	8.0
2	L	277[A]	GLY	7.0
2	L	281[A]	GLY	6.5
2	L	83	GLY	5.6
2	L	273[A]	ALA	5.6
2	L	267[A]	VAL	5.2
1	H	245	ALA	5.1
2	L	63	LEU	5.1
2	L	57	GLY	5.0
2	L	55	LEU	5.0
1	H	90	THR	5.0
2	L	265[A]	TRP	5.0
3	M	297	TRP	5.0
2	L	257	ASP	4.7
3	M	1	ALA	4.7
2	L	59	TRP	4.4
3	M	78	ALA	4.2
2	L	51	TRP	4.2
2	L	268[A]	LYS	3.9
2	L	259	TRP	3.9
3	M	174	ALA	3.8
3	M	302	GLY	3.8
1	H	10	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	262[A]	TRP	3.7
2	L	58	THR	3.7
3	M	84	VAL	3.7
3	M	68	PHE	3.7
2	L	279[A]	ILE	3.7
1	H	18	TYR	3.6
3	M	79	GLY	3.6
2	L	271[A]	TRP	3.5
3	M	92	PHE	3.5
2	L	276[A]	PRO	3.4
2	L	54	VAL	3.4
3	M	106	ALA	3.4
2	L	274[A]	ASN	3.3
2	L	266[A]	TRP	3.3
3	M	101	TYR	3.3
3	M	148	TRP	3.2
3	M	102	GLY	3.2
2	L	69	PRO	3.2
3	M	67	PHE	3.2
1	H	246	PRO	3.2
2	L	80	LEU	3.1
1	H	248	ARG	3.1
2	L	269[A]	LEU	3.1
3	M	80	TRP	3.1
2	L	41	PHE	3.1
3	M	177	TYR	3.1
2	L	64	ILE	3.0
3	M	188	ASN	3.0
3	M	83	ALA	3.0
2	L	67	TYR	3.0
2	L	169	TYR	3.0
2	L	255	TRP	2.9
3	M	286	LEU	2.9
1	H	135	LYS	2.8
2	L	161	GLY	2.8
2	L	263[A]	TRP	2.8
1	H	92	VAL	2.8
3	M	300	ASN	2.8
1	H	142	VAL	2.8
2	L	278[A]	GLY	2.8
2	L	280[A]	ASN	2.7
2	L	56	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
3	M	290	VAL	2.7
2	L	275[A]	ILE	2.7
1	H	247	LYS	2.7
1	H	151	LEU	2.6
2	L	60	ASN	2.6
3	M	76	TYR	2.6
2	L	86	TRP	2.6
3	M	121	PHE	2.6
3	M	3	TYR	2.6
3	M	301	HIS	2.6
1	H	91	ALA	2.6
1	H	141	HIS	2.6
3	M	44	ASN	2.6
1	H	244	ALA	2.6
2	L	154	LEU	2.6
1	H	140	PHE	2.5
1	H	20	PHE	2.5
3	M	54	SER	2.5
3	M	293	ASN	2.5
3	M	107	ALA	2.5
2	L	264[A]	GLN	2.4
3	M	2	GLU	2.4
3	M	88	ASP	2.4
3	M	37	THR	2.4
3	M	172	SER	2.4
1	H	137	ALA	2.4
1	H	146	LYS	2.4
1	H	139	GLY	2.4
3	M	288	GLY	2.4
2	L	142	TRP	2.4
3	M	171	TRP	2.4
2	L	68	PRO	2.4
2	L	78	ALA	2.4
3	M	75	TRP	2.4
2	L	17	VAL	2.3
2	L	260	VAL	2.3
2	L	50	ALA	2.3
2	L	39	PHE	2.3
3	M	6	ILE	2.3
2	L	272[A]	TRP	2.3
3	M	86	LEU	2.3
3	M	183	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	M	295	TYR	2.3
3	M	87	ARG	2.3
3	M	114[A]	LEU	2.3
1	H	201	ASN	2.2
1	H	179	LEU	2.2
2	L	85	LEU	2.2
2	L	251	THR	2.2
2	L	81	ALA	2.2
3	M	89	LEU	2.2
3	M	81	ASN	2.2
1	H	188	THR	2.2
2	L	47	ILE	2.2
2	L	138	MET	2.2
2	L	261[A]	ASP	2.2
2	L	52	SER	2.2
2	L	40	PHE	2.1
2	L	46	ILE	2.1
1	H	15	LEU	2.1
3	M	52[A]	LEU	2.1
2	L	65	SER	2.1
2	L	73	TYR	2.1
3	M	97	PRO	2.1
2	L	167	PHE	2.1
3	M	90	PHE	2.1
1	H	164	VAL	2.1
1	H	165	VAL	2.1
2	L	235[A]	LEU	2.1
3	M	39	LEU	2.1
1	H	12	LEU	2.1
3	M	100	GLU	2.1
1	H	186	GLY	2.1
3	M	10	VAL	2.1
3	M	162	PHE	2.1
3	M	103	LEU	2.0
1	H	148	PRO	2.0
2	L	178	THR	2.0
2	L	164	TYR	2.0
3	M	179	ILE	2.0
2	L	70	ALA	2.0
2	L	258	GLN	2.0
3	M	99	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

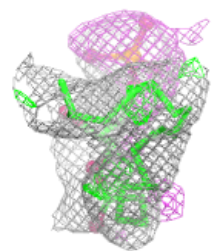
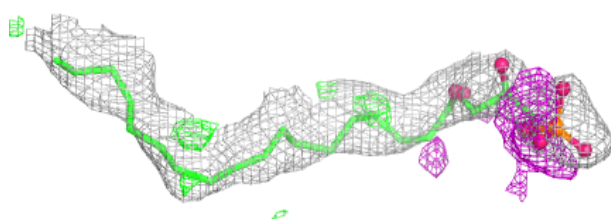
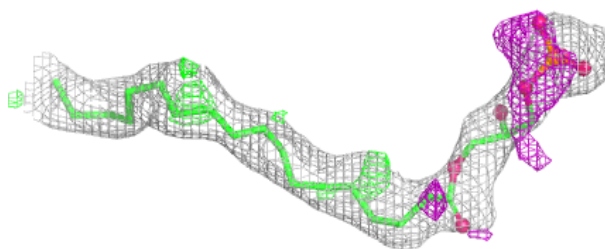
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	M	409	16/16	0.68	0.24	41,62,72,81	0
9	NKP	M	403	29/29	0.73	0.25	36,61,75,81	0
12	SPN	M	408	43/43	0.77	0.21	40,58,81,96	0
6	MYS	L	303	15/15	0.79	0.21	51,58,64,66	0
5	OLC	L	301	25/25	0.80	0.19	35,51,72,74	0
14	PO4	M	412	5/5	0.80	0.12	53,64,72,78	0
9	NKP	M	401	29/29	0.83	0.20	34,71,85,96	0
6	MYS	L	302	15/15	0.84	0.18	56,62,76,80	0
13	EDO	M	411	4/4	0.85	0.15	42,46,53,54	0
6	MYS	M	410	15/15	0.86	0.16	46,62,75,77	0
4	LDA	H	301	16/16	0.87	0.15	34,45,61,70	0
7	BCL	L	304	66/66	0.88	0.13	25,36,50,60	0
7	BCL	L	305	66/66	0.89	0.13	27,35,58,71	0
7	BCL	M	405	66/66	0.90	0.12	25,33,60,78	0
10	U10	M	402	63/63	0.91	0.14	21,48,80,86	0
7	BCL	M	404	66/66	0.91	0.14	28,37,81,85	0
8	BPH	L	306	65/65	0.93	0.10	22,29,45,55	0
8	BPH	M	406	65/65	0.94	0.11	23,34,94,106	0
11	FE	M	407	1/1	1.00	0.02	23,23,23,23	0

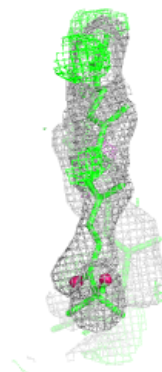
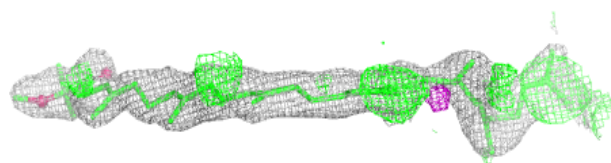
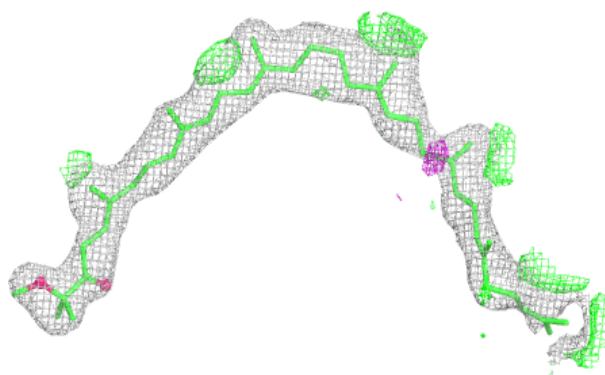
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

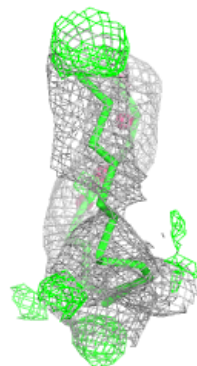
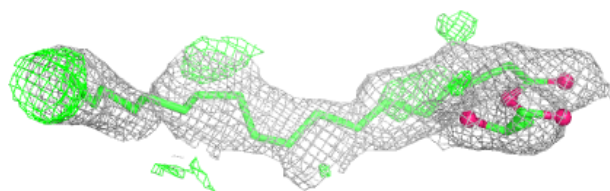
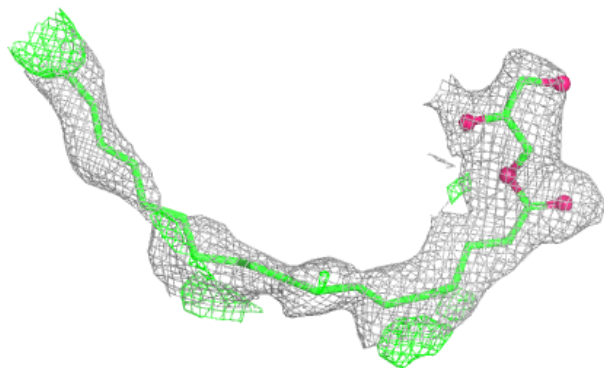
**Electron density around SPN M 408:**

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

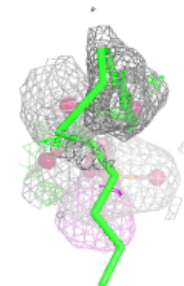
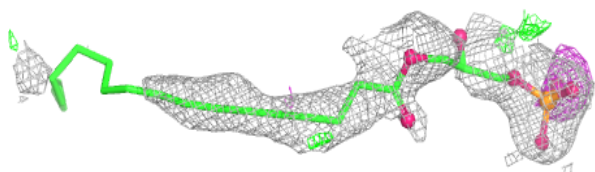
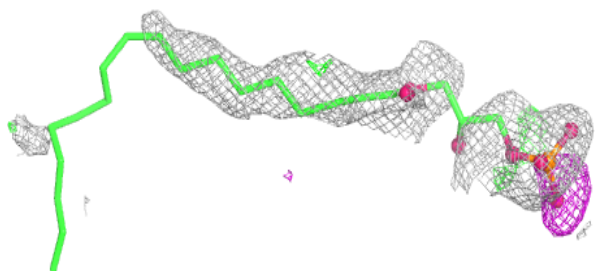


Electron density around OLC L 301:

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

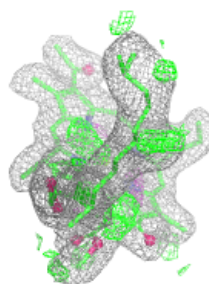
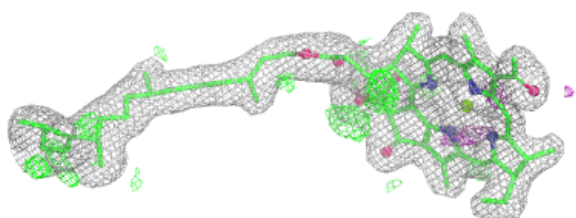
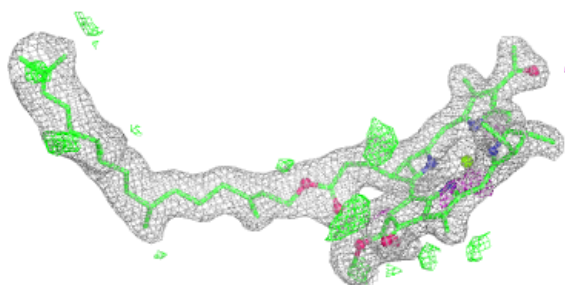
**Electron density around NKP M 401:**

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

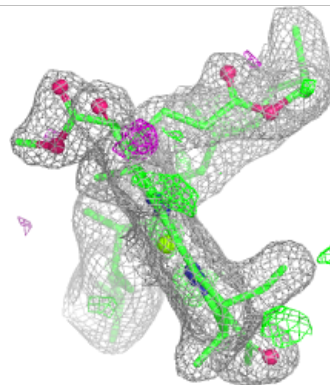
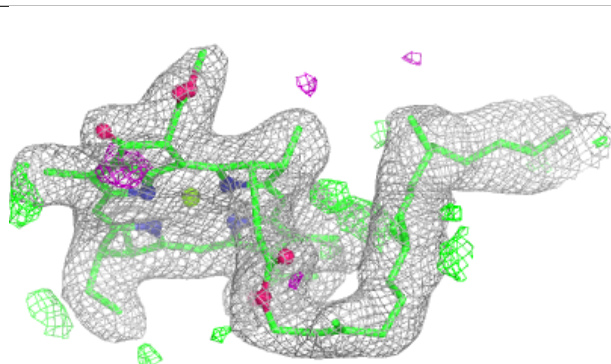
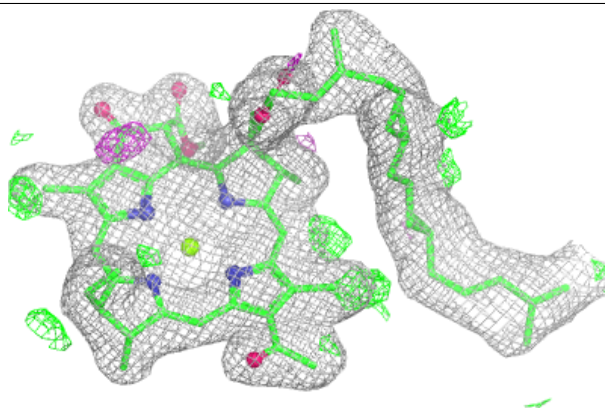


Electron density around BCL L 304:

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

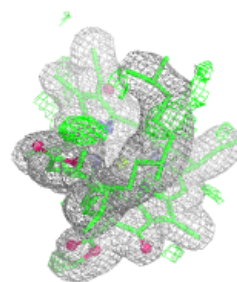
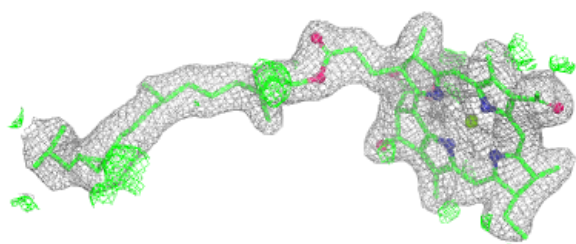
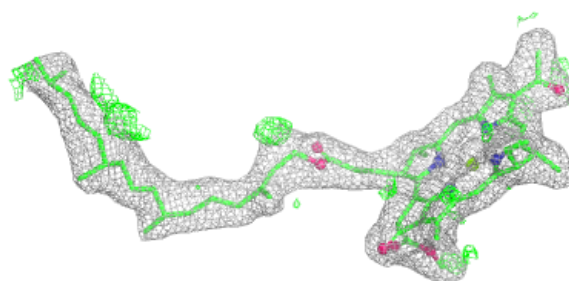
**Electron density around BCL L 305:**

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

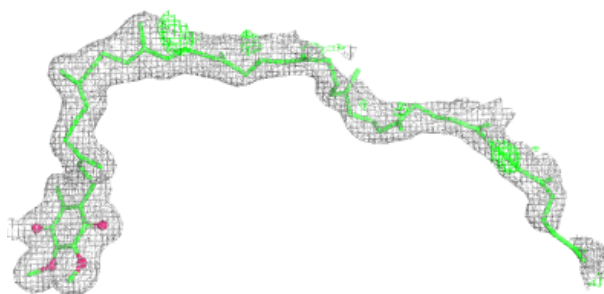


Electron density around BCL M 405:

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

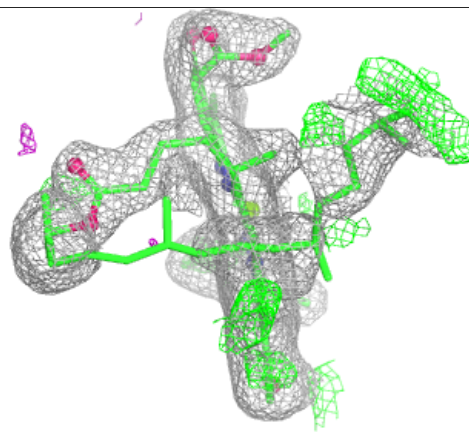
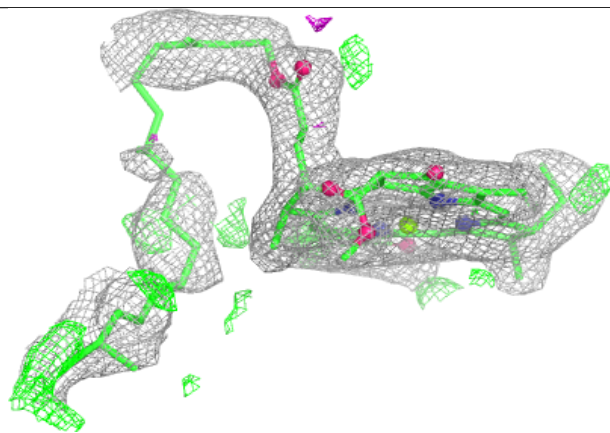
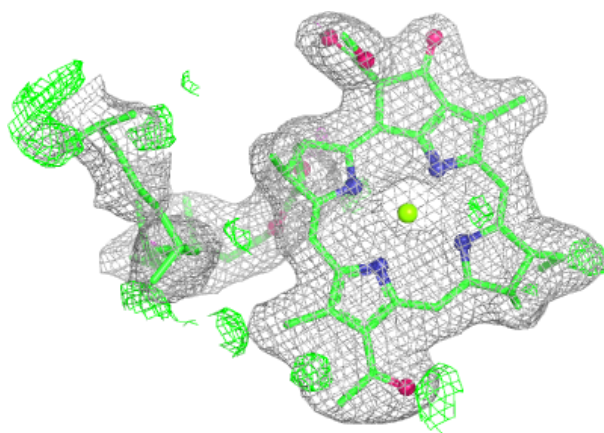
**Electron density around U10 M 402:**

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



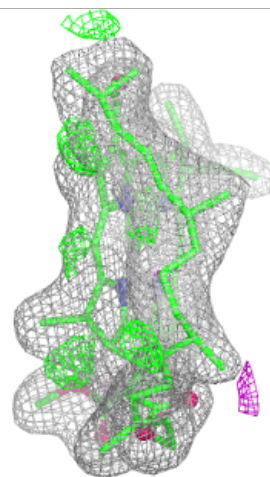
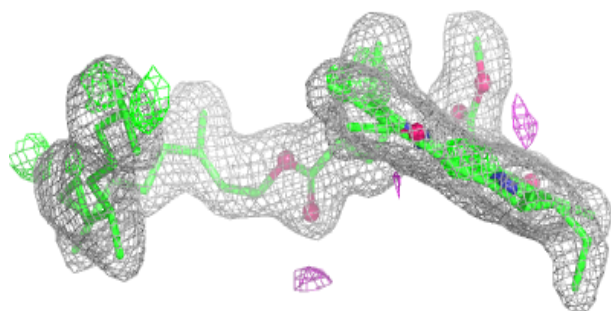
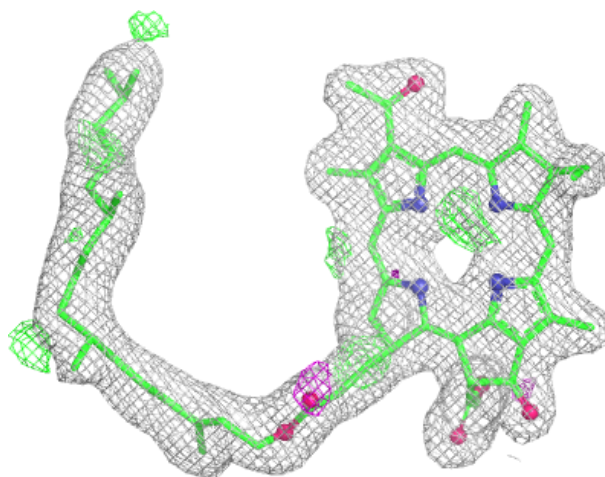
Electron density around BCL M 404:

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



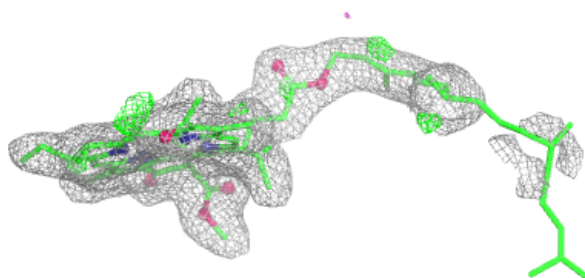
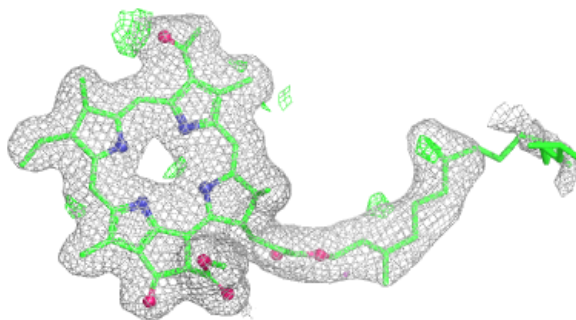
Electron density around BPH L 306:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.