



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2026 – 05:03 am BST

PDB ID : 8C88 / pdb_00008c88
Title : Double mutant G(M19)C/T(L214)C structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors : Gabdulkhakov, A.; Selikhanov, G.; Fufina, T.; Vasilieva, L.; Atamas, A.; Yukhimchuk, D.
Deposited on : 2023-01-19
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

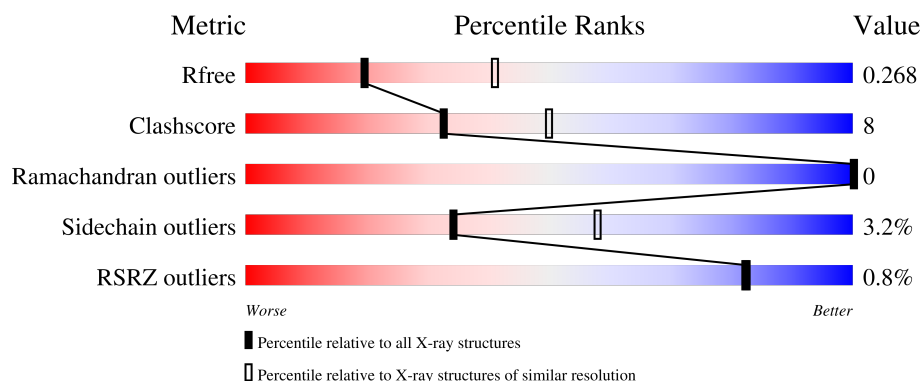
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	2% 79% 20% .
2	L	281	86% 14%
3	M	303	% 80% 19% .

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7341 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	242	Total	C	N	O	S	0	3	0
			1867	1196	320	342	9			

- 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
			2243	1515	356	363	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP P0C0Y8
L	214	CYS	THR	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	1	0
			2427	1619	398	398	12			

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	19	CYS	GLY	engineered mutation	UNP P0C0Y9

- Molecule 4 is (2R)-2-hydroxy-3-(phosphonoxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: C₂₁H₄₁O₇P).



- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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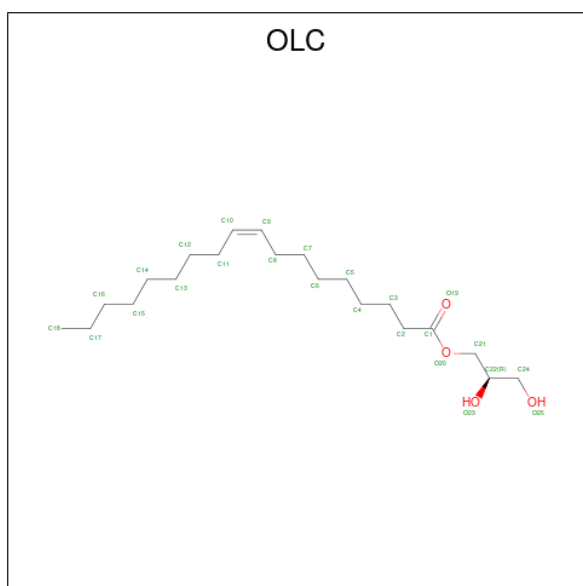
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

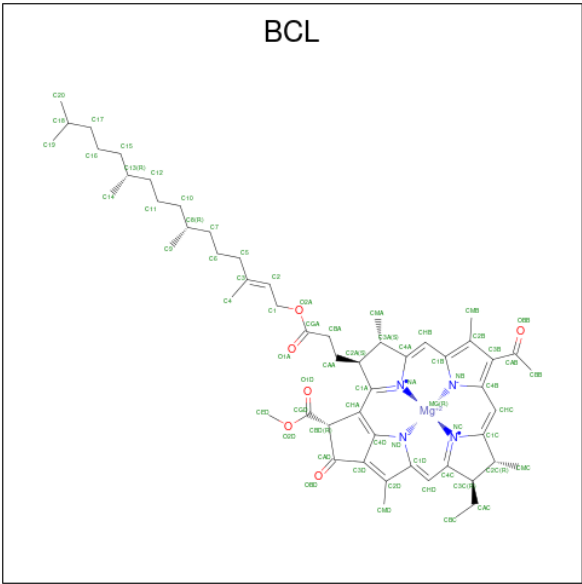
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	3	Total	C	0	0
			39	39		
6	L	3	Total	C	0	0
			37	37		
6	M	1	Total	C	0	0
			12	12		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



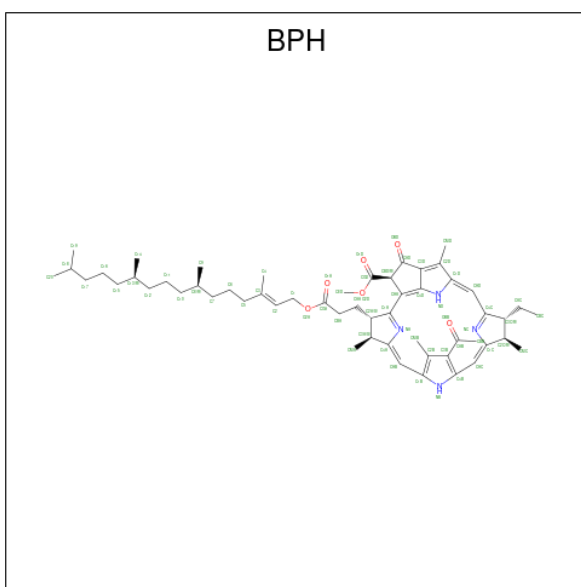
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			25	21	4		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



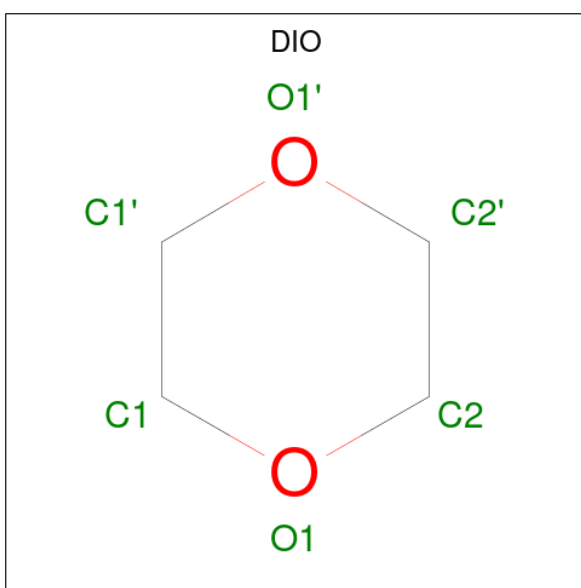
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (la-
beled as "Ligand of Interest" by depositor).



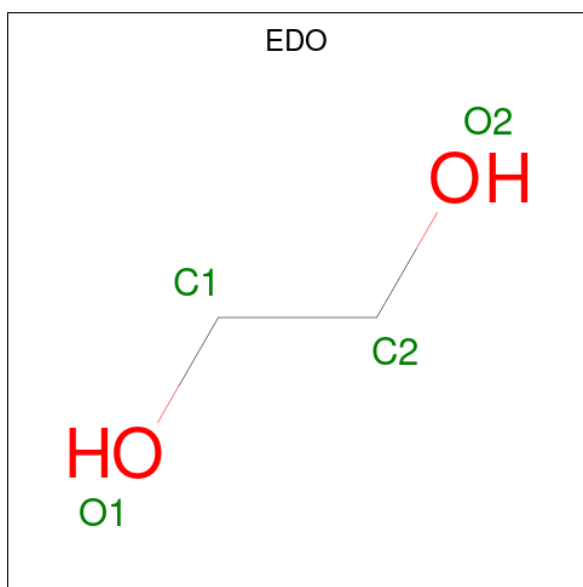
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			65	55	4	6		
9	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 10 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			6	4	2		

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

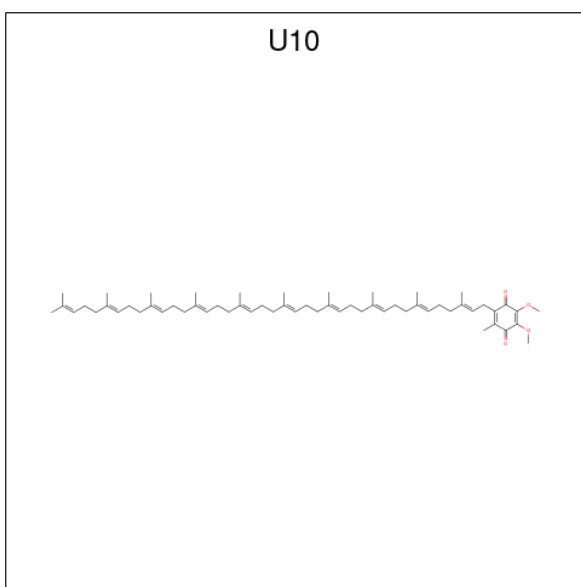


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			4	2	2		
11	L	1	Total	C	O	0	0
			4	2	2		
11	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

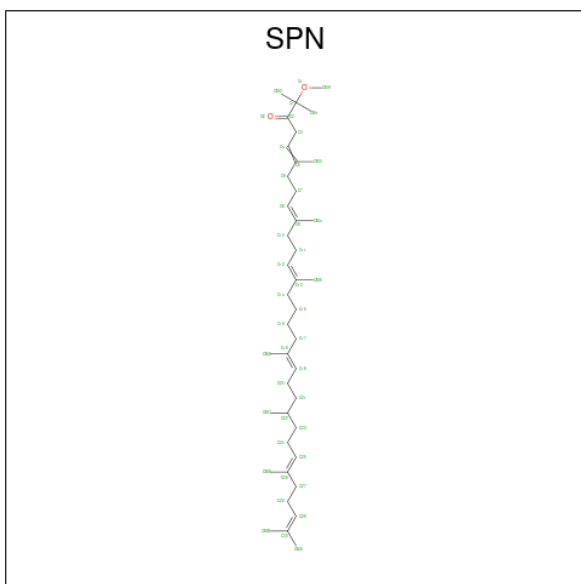
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



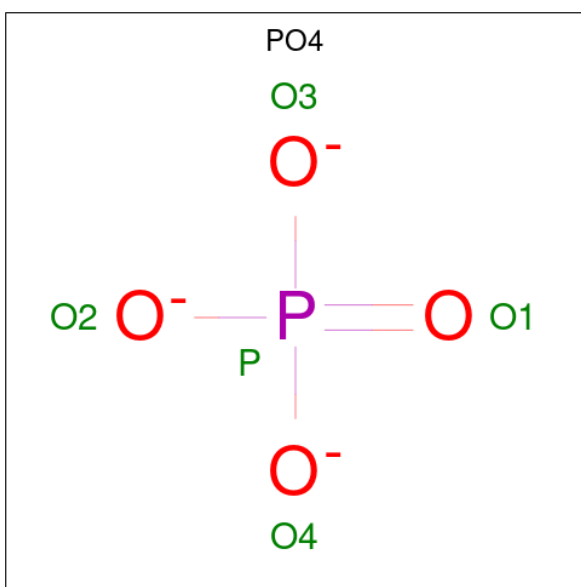
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 14 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

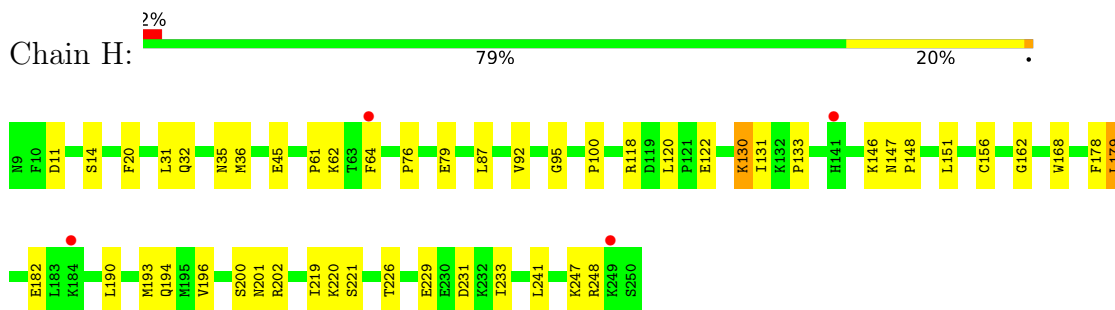
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	3	Total	O	0	0
			3	3		
16	L	8	Total	O	0	0
			8	8		
16	M	12	Total	O	0	0
			12	12		

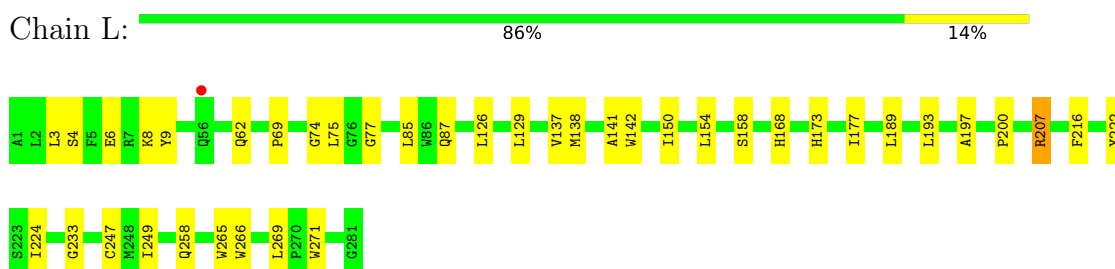
3 Residue-property plots [i](#)

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.

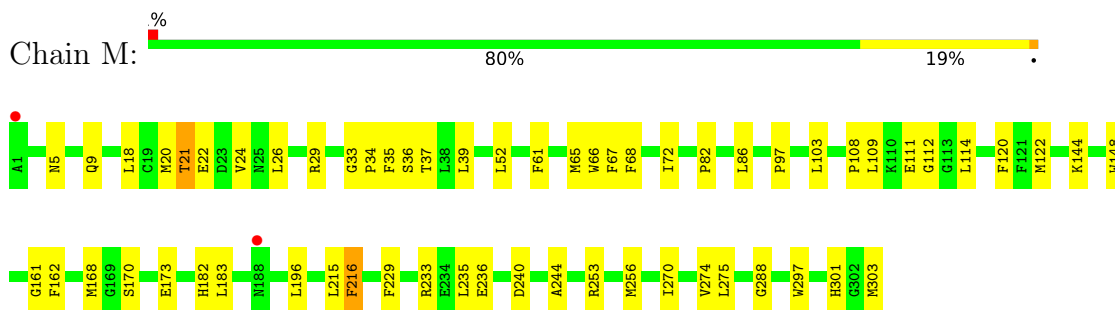
- Molecule 1: Reaction center protein H chain



- 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	100.91Å 100.91Å 237.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.75 46.42 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.42-2.75) 98.1 (46.42-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.271 0.203 , 0.268	Depositor DCC
R_{free} test set	1285 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7341	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NKP, DIO, LDA, OLC, BCL, UNL, U10, FE, PO4, SPN, BPH, EDO

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	0.41	0/1925	0.65	0/2617
2	L	0.39	0/2334	0.57	0/3194
3	M	0.39	0/2522	0.58	0/3442
All	All	0.39	0/6781	0.60	0/9253

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

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	1867	0	1881	40	0
2	L	2243	0	2201	27	0
3	M	2427	0	2346	46	0
4	H	29	0	39	0	0
4	M	29	0	39	0	0
5	H	16	0	31	2	0
5	M	80	0	155	7	0
6	H	39	0	0	0	0
6	L	37	0	0	0	0
6	M	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	25	0	40	2	0
8	L	132	0	148	3	0
8	M	132	0	148	3	0
9	L	65	0	76	2	0
9	M	65	0	76	2	0
10	L	6	0	8	1	0
11	L	12	0	18	2	0
12	M	1	0	0	0	0
13	M	48	0	63	5	0
14	M	43	0	70	7	0
15	M	10	0	0	0	0
16	H	3	0	0	0	0
16	L	8	0	0	0	0
16	M	12	0	0	1	0
All	All	7341	0	7339	116	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 8.

The worst 5 of 116 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)
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.68	0.74
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.54	0.71
1:H:11:ASP:HB3	1:H:14:SER:H	1.55	0.69
1:H:31:LEU:O	1:H:35:ASN:ND2	2.26	0.69
1:H:146:LYS:HD2	1:H:151:LEU:HD11	1.75	0.69

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	243/242 (100%)	235 (97%)	8 (3%)	0	100	100
2	L	281/281 (100%)	270 (96%)	11 (4%)	0	100	100
3	M	302/303 (100%)	287 (95%)	15 (5%)	0	100	100
All	All	826/826 (100%)	792 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	200/197 (102%)	194 (97%)	6 (3%)	36	60
2	L	222/220 (101%)	216 (97%)	6 (3%)	39	62
3	M	239/238 (100%)	230 (96%)	9 (4%)	29	52
All	All	661/655 (101%)	640 (97%)	21 (3%)	34	58

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	21	THR
3	M	196	LEU
3	M	274	VAL
3	M	216	PHE
3	M	182	HIS

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

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 31 ligands modelled in this entry, 7 are unknown and 1 is monoatomic - leaving 23 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	BCL	M	402	3	69,74,74	1.34	7 (10%)	83,115,115	1.59	15 (18%)
14	SPN	M	407	-	40,42,42	0.51	0	50,52,52	0.85	2 (4%)
8	BCL	M	403	3	69,74,74	1.41	6 (8%)	83,115,115	1.50	11 (13%)
8	BCL	L	503	2	69,74,74	1.31	6 (8%)	83,115,115	1.62	15 (18%)
5	LDA	M	411	-	12,15,15	2.00	1 (8%)	14,17,17	0.50	0
5	LDA	M	410	-	12,15,15	2.03	1 (8%)	14,17,17	0.74	0
9	BPH	M	404	-	59,70,70	1.33	6 (10%)	61,101,101	2.21	14 (22%)
10	DIO	L	508	-	6,6,6	0.48	0	6,6,6	0.10	0
11	EDO	L	509	-	3,3,3	0.48	0	2,2,2	0.47	0
15	PO4	M	414	-	4,4,4	0.87	0	6,6,6	0.28	0
5	LDA	H	302	-	12,15,15	2.05	1 (8%)	14,17,17	0.48	0
5	LDA	M	415	-	12,15,15	2.03	1 (8%)	14,17,17	0.56	0
11	EDO	L	510	-	3,3,3	0.47	0	2,2,2	0.47	0
15	PO4	M	413	-	4,4,4	0.73	0	6,6,6	0.48	0
13	U10	M	406	-	48,48,63	2.57	13 (27%)	58,61,79	1.76	13 (22%)
11	EDO	L	511	-	3,3,3	0.55	0	2,2,2	0.17	0
4	NKP	H	301	-	28,28,28	0.32	0	31,32,32	0.61	1 (3%)
7	OLC	L	501	-	24,24,24	1.03	1 (4%)	25,25,25	0.88	2 (8%)
4	NKP	M	401	-	28,28,28	0.35	0	31,32,32	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	L	502	2	69,74,74	1.34	7 (10%)	83,115,115	1.46	11 (13%)
5	LDA	M	408	-	12,15,15	1.97	1 (8%)	14,17,17	0.70	0
9	BPH	L	504	-	59,70,70	1.27	5 (8%)	61,101,101	2.40	14 (22%)
5	LDA	M	409	-	12,15,15	2.03	1 (8%)	14,17,17	0.58	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	BCL	M	402	3	-	5/41/137/137	-
14	SPN	M	407	-	-	15/50/51/51	-
8	BCL	M	403	3	-	6/41/137/137	-
8	BCL	L	503	2	-	9/41/137/137	-
5	LDA	M	411	-	-	12/13/13/13	-
5	LDA	M	410	-	-	6/13/13/13	-
9	BPH	M	404	-	-	4/37/105/105	0/5/6/6
10	DIO	L	508	-	-	-	0/1/1/1
11	EDO	L	509	-	-	0/1/1/1	-
5	LDA	H	302	-	-	4/13/13/13	-
5	LDA	M	415	-	-	9/13/13/13	-
11	EDO	L	510	-	-	0/1/1/1	-
13	U10	M	406	-	-	13/45/69/87	0/1/1/1
11	EDO	L	511	-	-	0/1/1/1	-
4	NKP	H	301	-	-	11/28/28/28	-
7	OLC	L	501	-	-	6/24/24/24	-
4	NKP	M	401	-	-	12/28/28/28	-
8	BCL	L	502	2	-	3/41/137/137	-
5	LDA	M	408	-	-	6/13/13/13	-
9	BPH	L	504	-	-	6/37/105/105	0/5/6/6
5	LDA	M	409	-	-	7/13/13/13	-

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	302	LDA	O1-N1	-7.01	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	410	LDA	O1-N1	-6.98	1.25	1.42
5	M	415	LDA	O1-N1	-6.96	1.25	1.42
5	M	409	LDA	O1-N1	-6.92	1.26	1.42
5	M	411	LDA	O1-N1	-6.83	1.26	1.42

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	504	BPH	C4D-CHA-CBD	-14.21	102.09	108.52
9	M	404	BPH	C4D-CHA-CBD	-10.48	103.77	108.52
9	M	404	BPH	C1-C2-C3	-5.64	116.30	126.04
8	M	402	BCL	CHD-C1D-ND	-5.57	119.34	124.45
8	L	503	BCL	CHD-C1D-ND	-5.45	119.44	124.45

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	NKP	CAG-CAH-CAI-OAJ
4	M	401	NKP	OAF-CAG-CAH-OBC
4	M	401	NKP	OAE-CAK-OAJ-CAI
4	M	401	NKP	CAL-CAK-OAJ-CAI
5	H	302	LDA	C2-C1-N1-O1

There are no ring outliers.

15 monomers are involved in 32 short contacts:

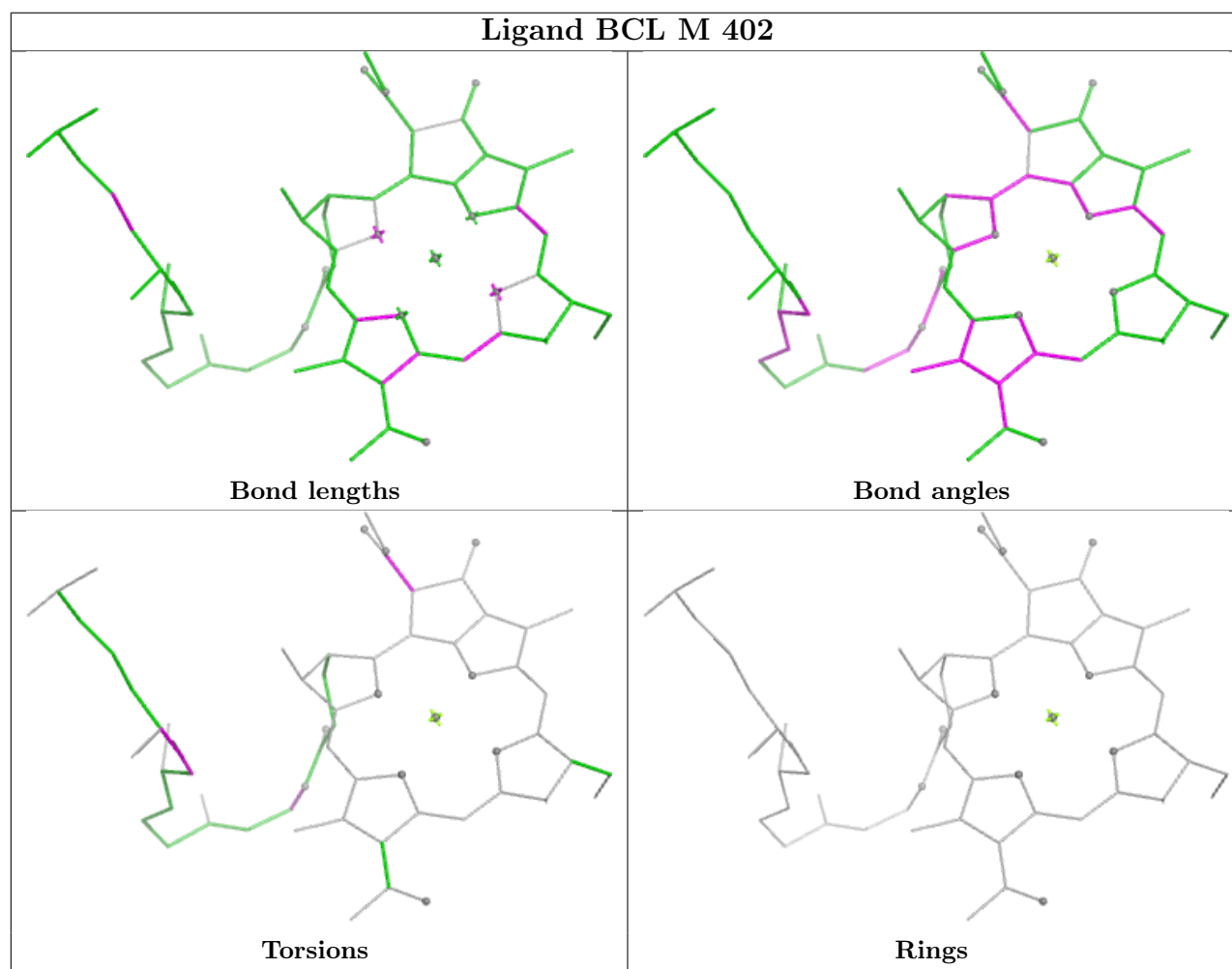
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	402	BCL	2	0
14	M	407	SPN	7	0
8	M	403	BCL	2	0
8	L	503	BCL	2	0
5	M	411	LDA	4	0
9	M	404	BPH	2	0
10	L	508	DIO	1	0
5	H	302	LDA	2	0
5	M	415	LDA	3	0
11	L	510	EDO	1	0
13	M	406	U10	5	0
11	L	511	EDO	1	0
7	L	501	OLC	2	0

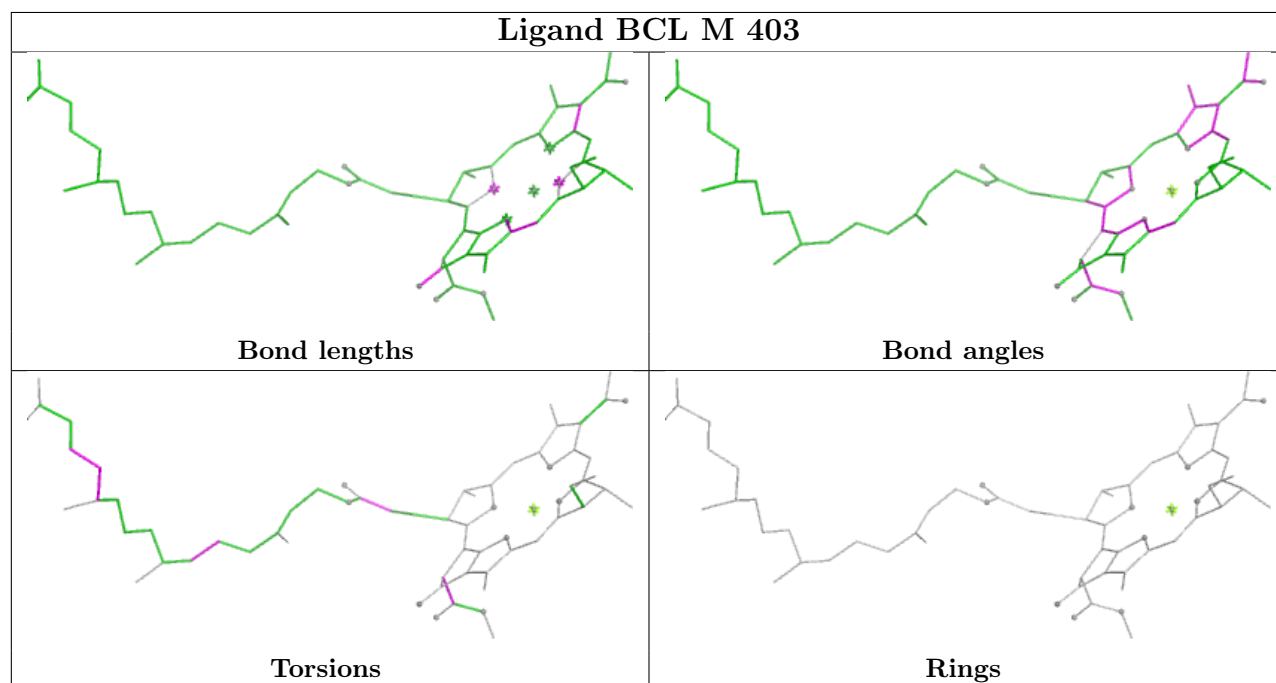
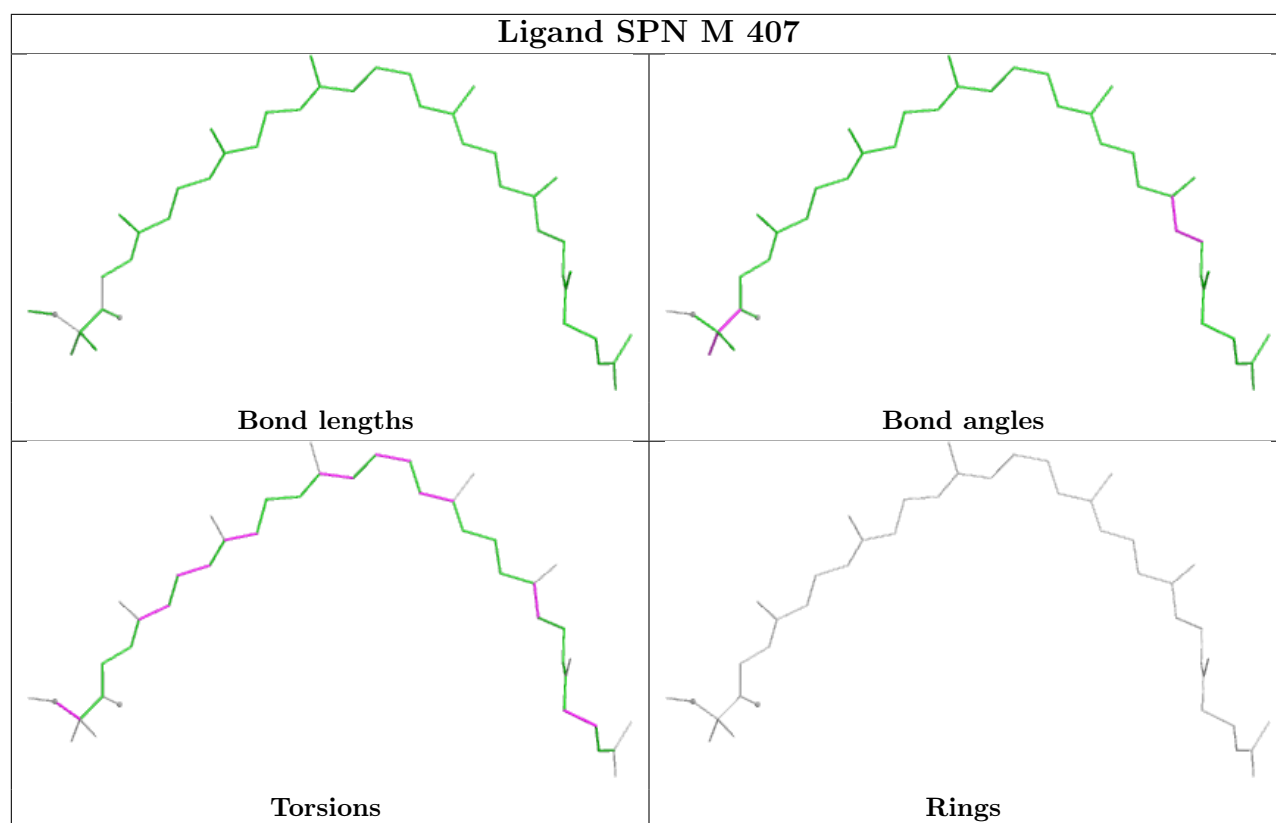
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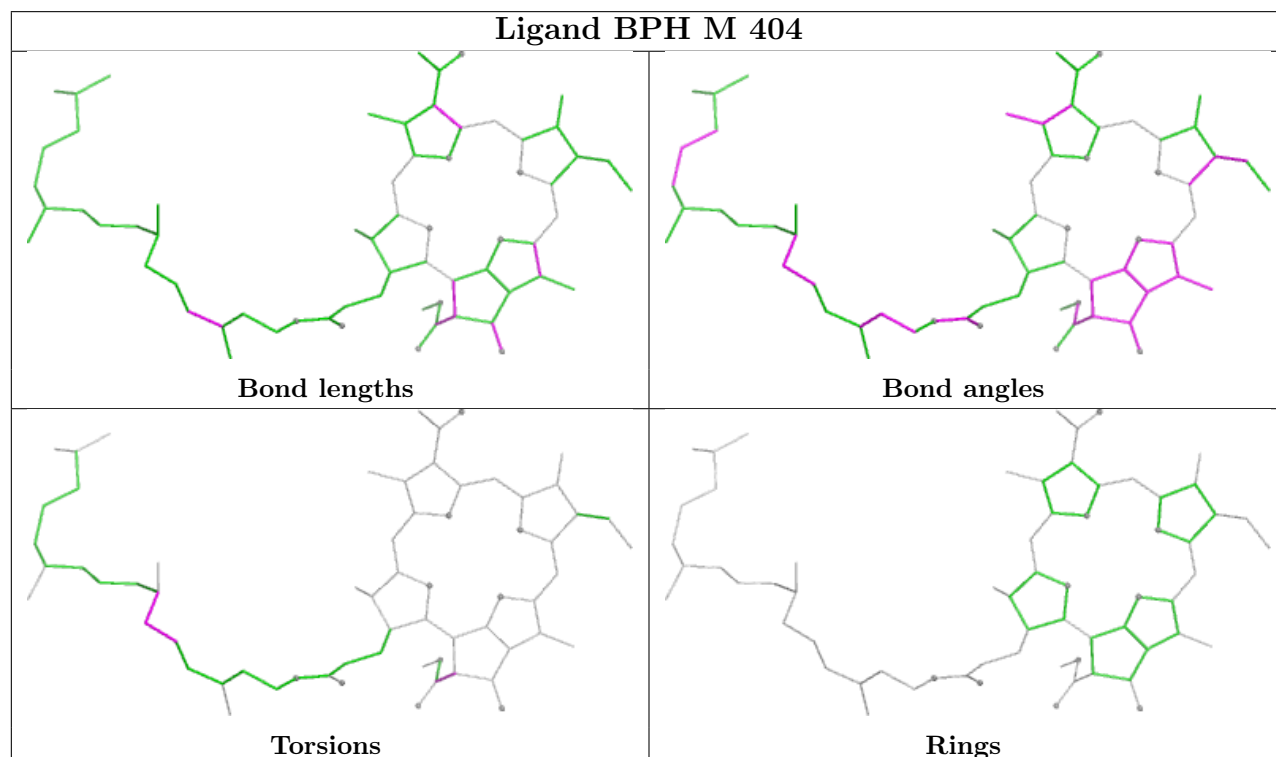
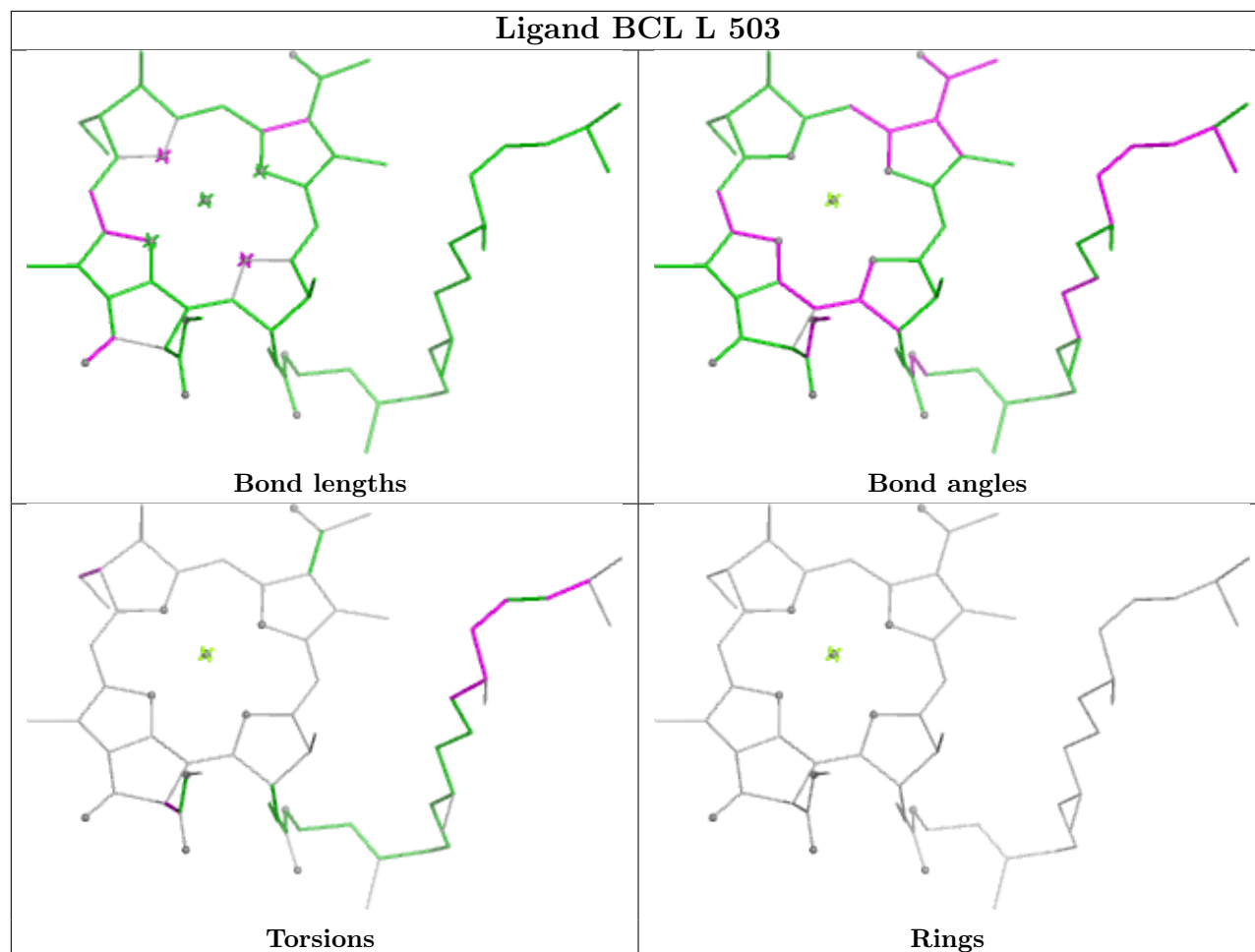
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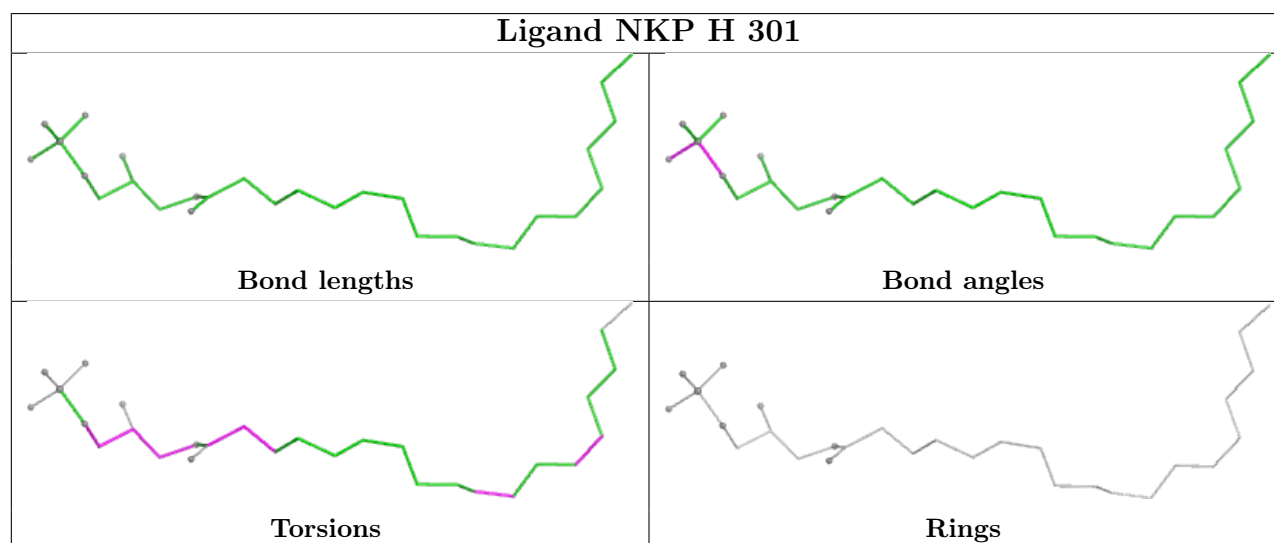
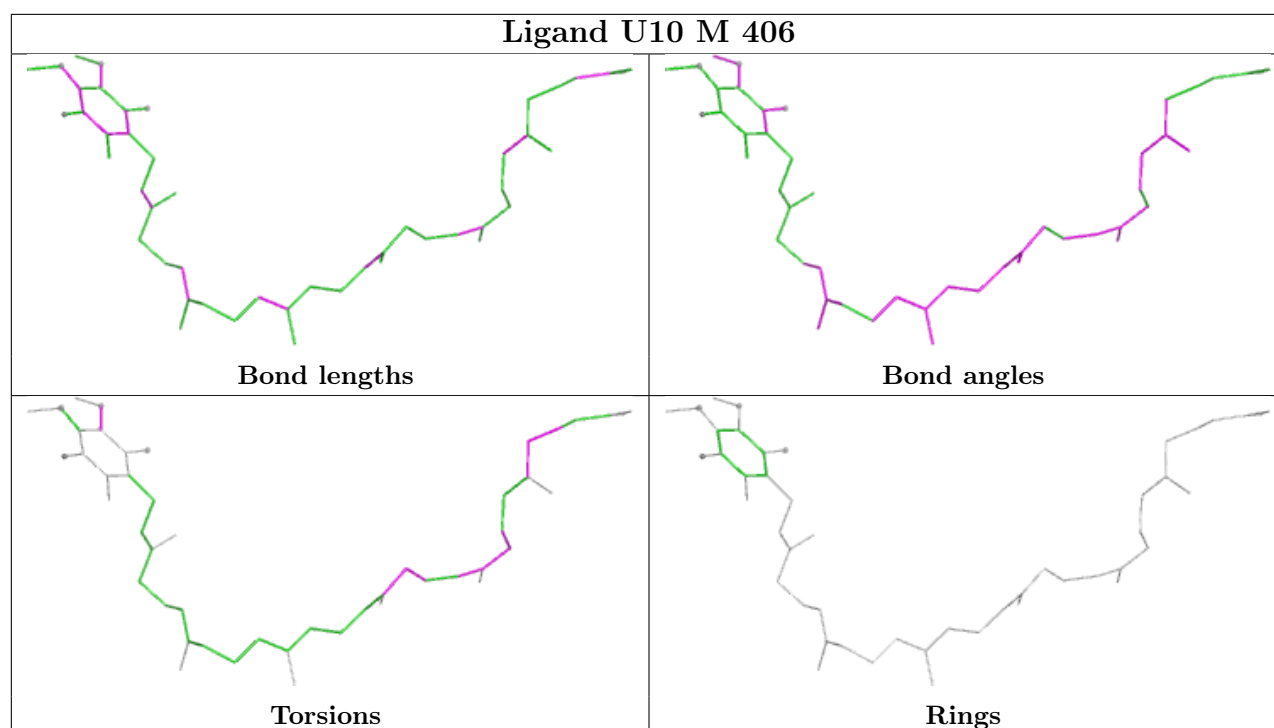
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	502	BCL	3	0
9	L	504	BPH	2	0

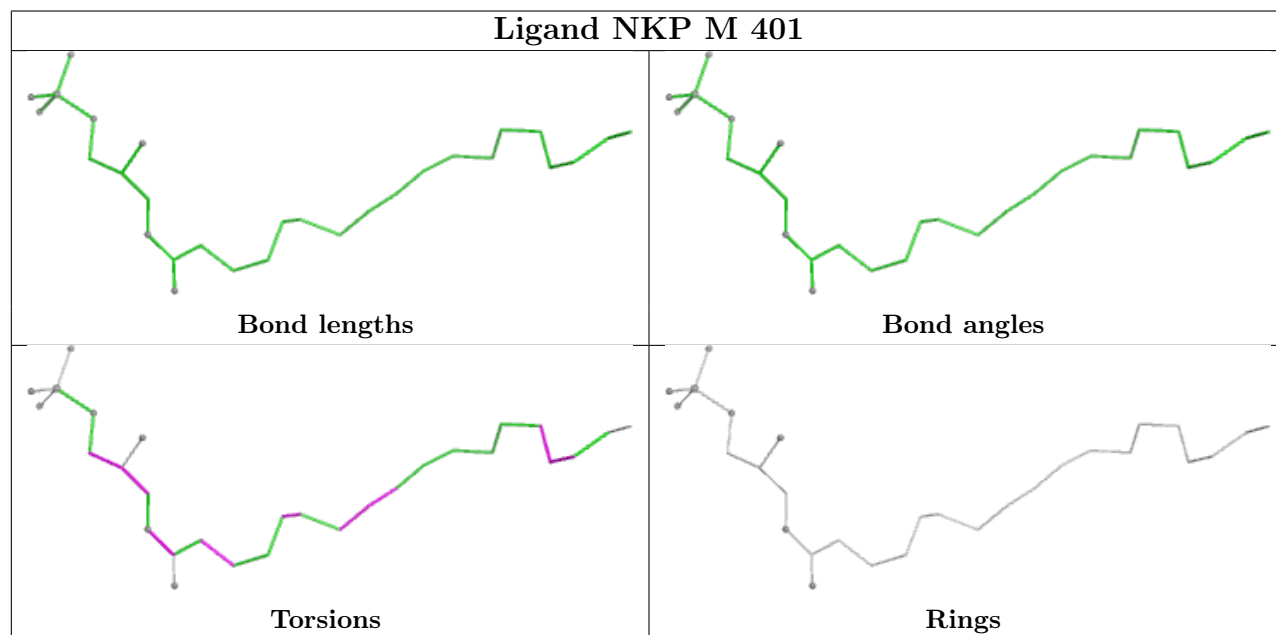
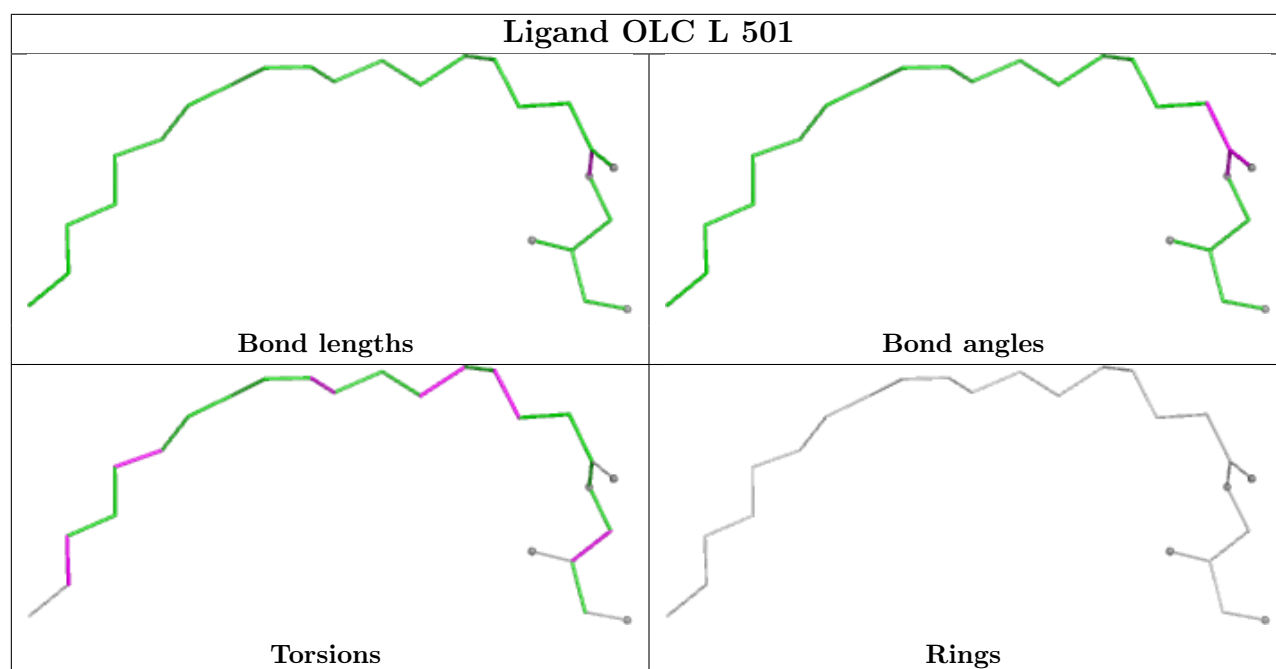
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

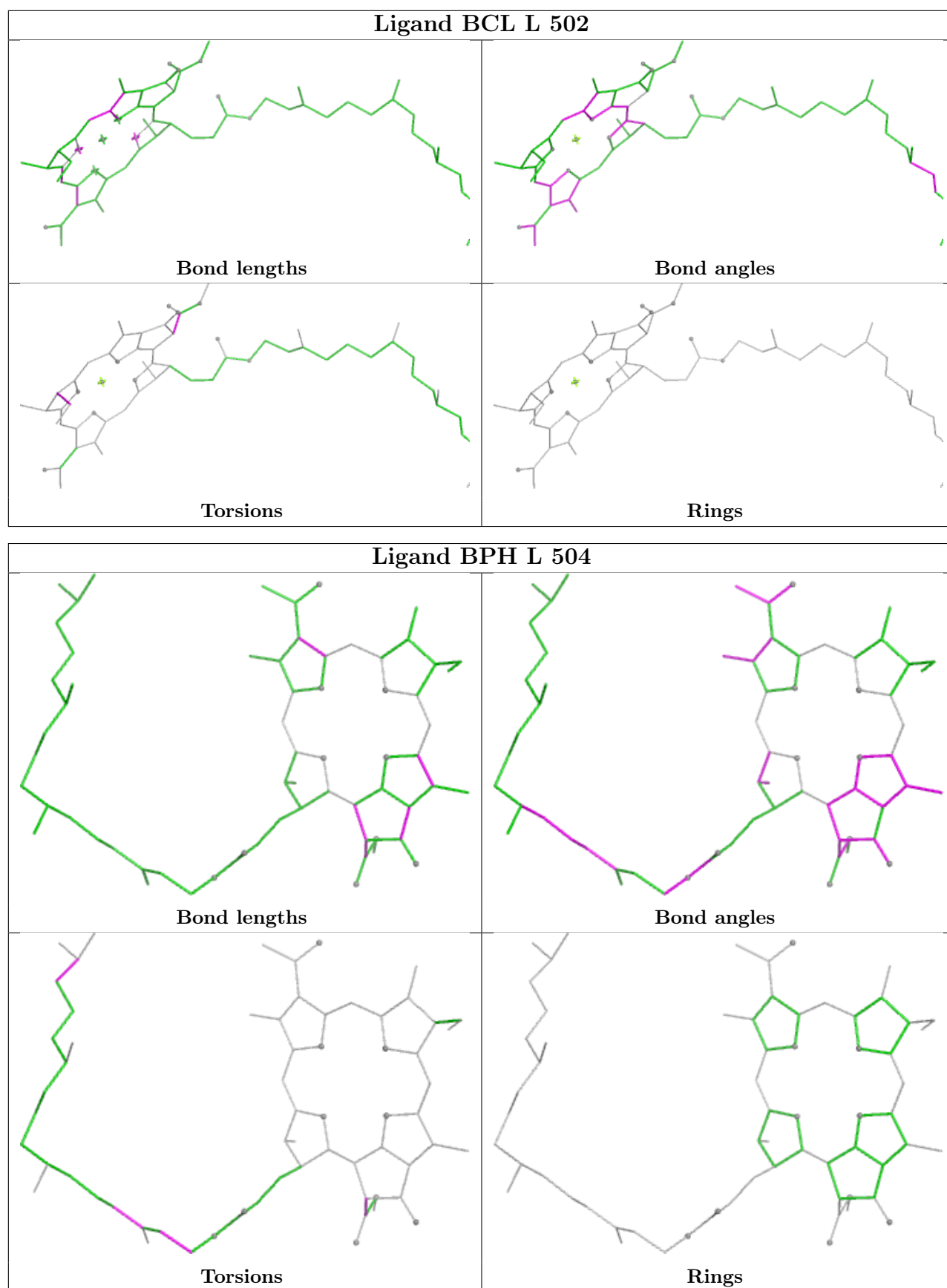












5.7 Other polymers [i](#)

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	242/242 (100%)	-0.10	4 (1%) 69 67	38, 73, 90, 130	3 (1%)
2	L	281/281 (100%)	-0.27	1 (0%) 88 89	37, 64, 108, 123	2 (0%)
3	M	303/303 (100%)	-0.36	2 (0%) 84 84	34, 63, 90, 109	1 (0%)
All	All	826/826 (100%)	-0.25	7 (0%) 82 82	34, 67, 94, 130	6 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	141	HIS	3.4
1	H	249	LYS	2.9
1	H	184	LYS	2.3
3	M	188	ASN	2.3
3	M	1	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

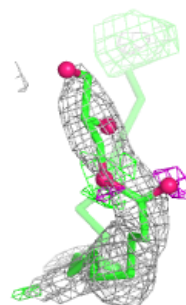
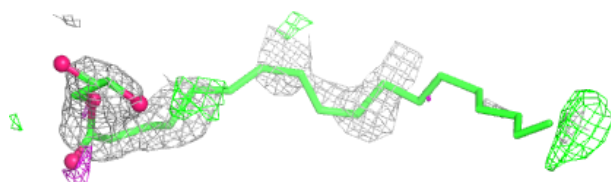
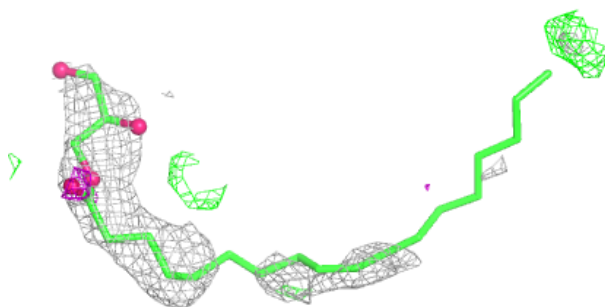
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
6	UNL	H	303	12/-	0.58	0.23	83,93,104,105	0
15	PO4	M	413	5/5	0.71	0.11	107,113,120,141	0
7	OLC	L	501	25/25	0.75	0.21	68,82,89,94	0
6	UNL	H	305	15/-	0.76	0.27	82,91,99,100	0
5	LDA	M	409	16/16	0.79	0.19	71,93,109,114	0
6	UNL	M	412	12/-	0.80	0.23	70,95,109,109	0
5	LDA	M	415	16/16	0.81	0.20	76,89,99,105	0
4	NKP	H	301	29/29	0.81	0.15	60,85,103,107	0
4	NKP	M	401	29/29	0.83	0.15	65,77,103,112	0
15	PO4	M	414	5/5	0.83	0.09	80,86,92,96	5
5	LDA	M	411	16/16	0.84	0.17	86,95,108,109	0
5	LDA	M	410	16/16	0.84	0.17	72,89,124,131	0
6	UNL	H	304	12/-	0.85	0.18	73,84,91,96	0
10	DIO	L	508	6/6	0.86	0.12	94,99,102,109	0
11	EDO	L	509	4/4	0.87	0.17	65,69,74,79	0
6	UNL	L	506	15/-	0.87	0.20	72,88,108,109	0
5	LDA	M	408	16/16	0.87	0.18	40,73,85,86	0
14	SPN	M	407	43/43	0.89	0.15	53,73,88,96	0
6	UNL	L	505	12/-	0.90	0.15	74,76,86,94	0
6	UNL	L	507	10/-	0.90	0.15	74,80,87,91	0
11	EDO	L	510	4/4	0.90	0.17	67,73,82,89	0
11	EDO	L	511	4/4	0.92	0.26	68,73,80,82	0
5	LDA	H	302	16/16	0.92	0.12	67,72,77,78	0
9	BPH	M	404	65/65	0.93	0.11	49,60,101,108	0
13	U10	M	406	48/63	0.94	0.10	45,63,79,84	0
9	BPH	L	504	65/65	0.96	0.08	46,59,64,67	0
8	BCL	M	402	66/66	0.96	0.09	42,60,87,90	0
8	BCL	L	502	66/66	0.97	0.07	50,61,67,74	0
8	BCL	M	403	66/66	0.97	0.08	45,57,66,78	0
8	BCL	L	503	66/66	0.97	0.07	44,55,71,81	0
12	FE	M	405	1/1	1.00	0.04	58,58,58,58	0

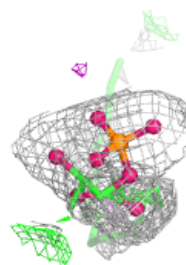
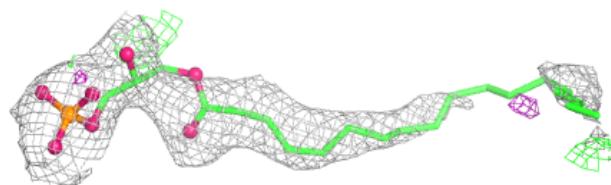
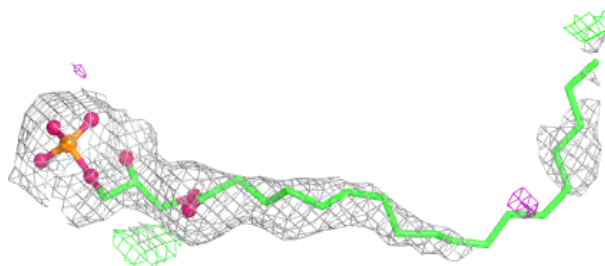
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

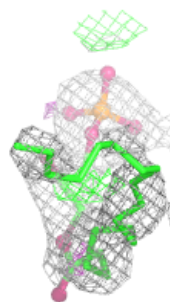
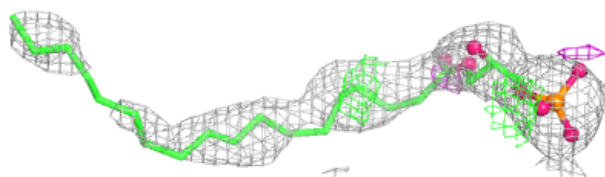
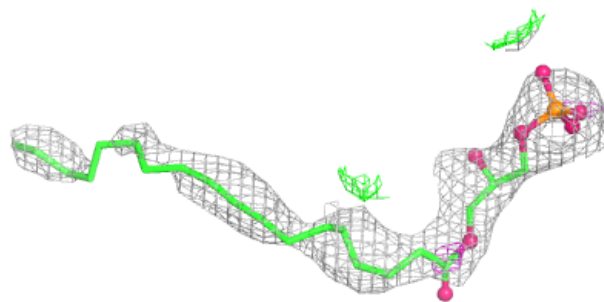
**Electron density around NKP H 301:**

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

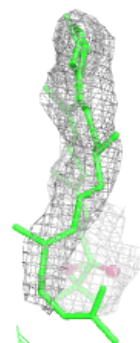
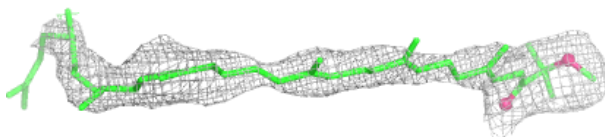
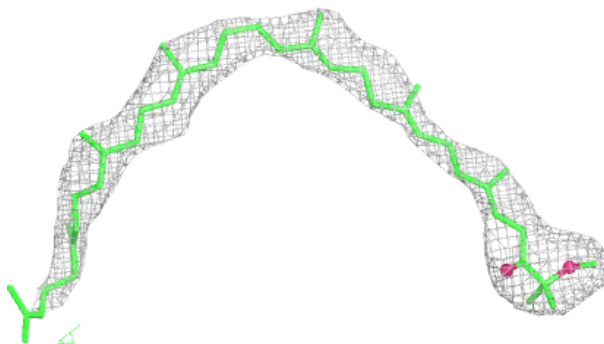


Electron density around NKP M 401:

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

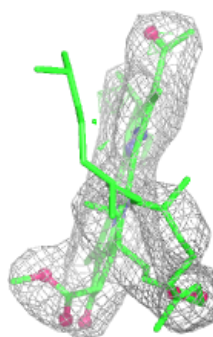
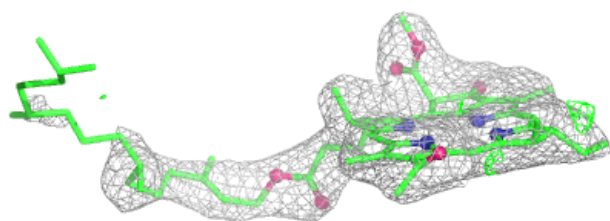
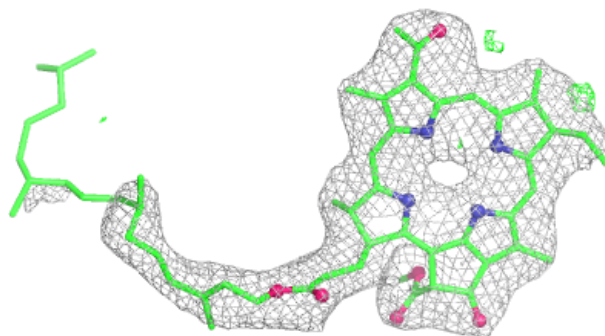
**Electron density around SPN M 407:**

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

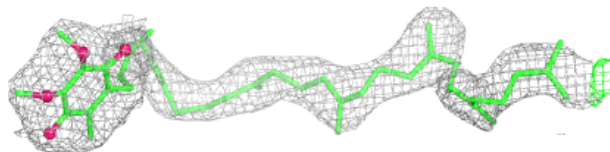
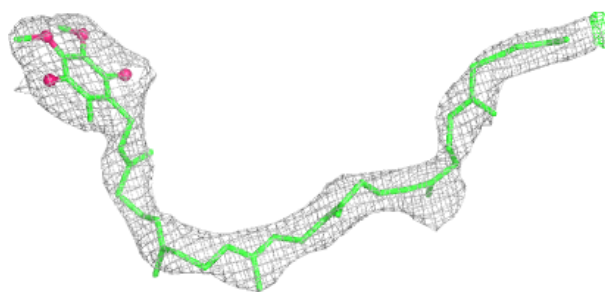


Electron density around BPH M 404:

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

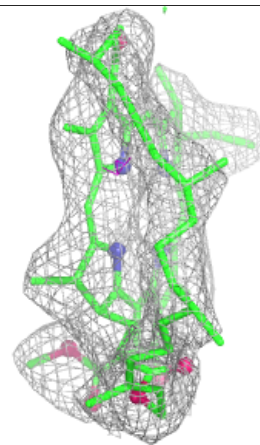
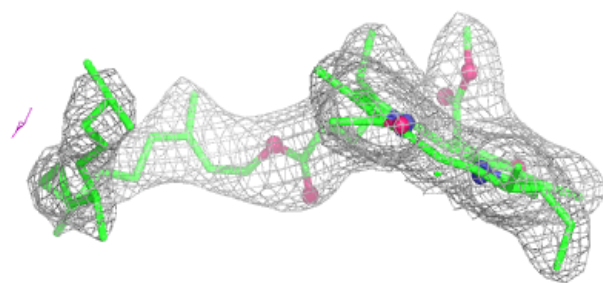
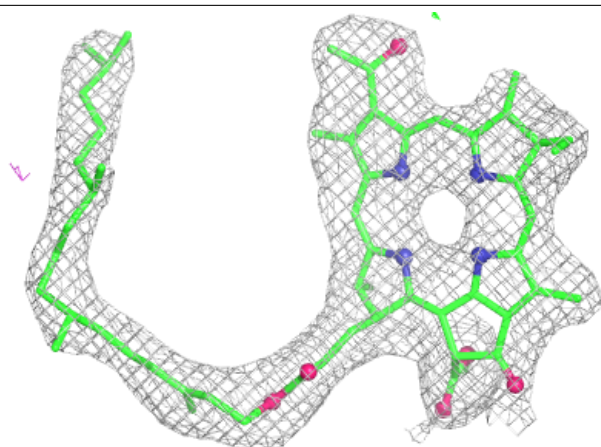
**Electron density around U10 M 406:**

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



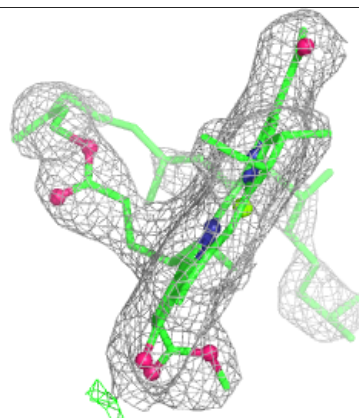
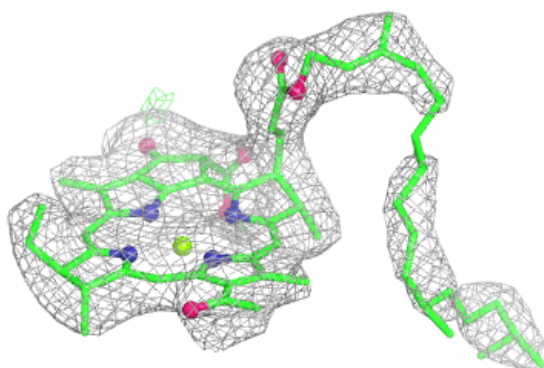
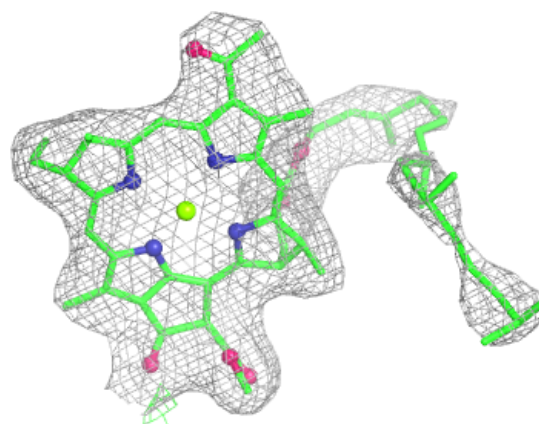
Electron density around BPH L 504:

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

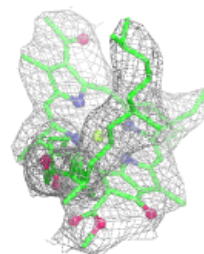
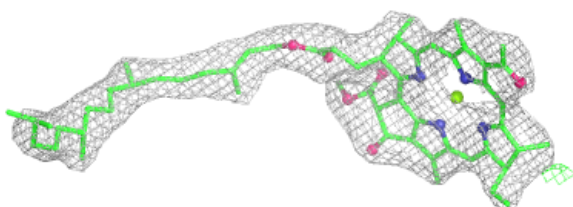
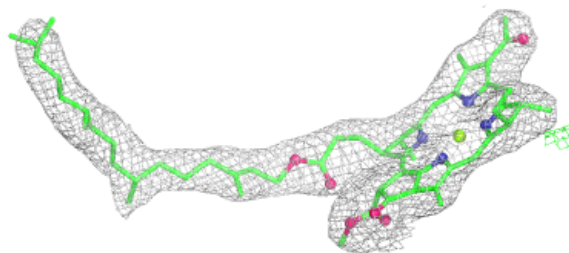


Electron density around BCL M 402:

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

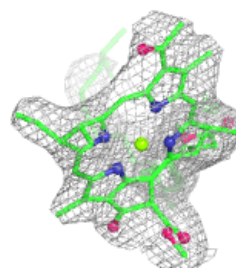
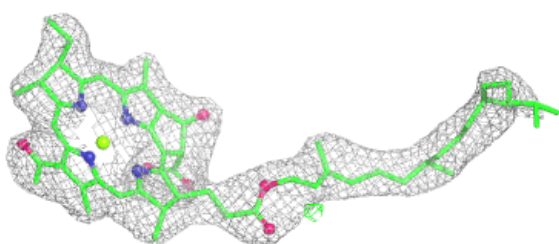
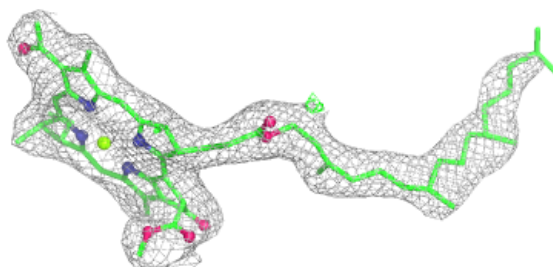
**Electron density around BCL L 502:**

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

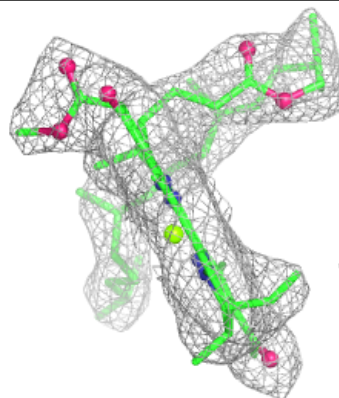
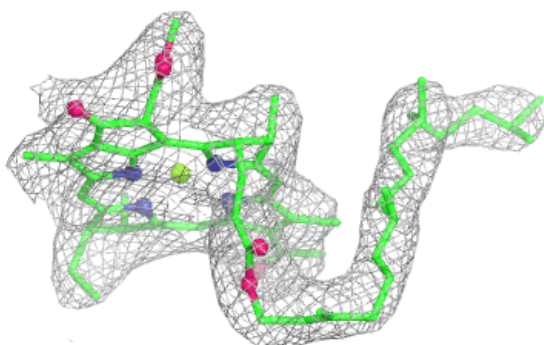
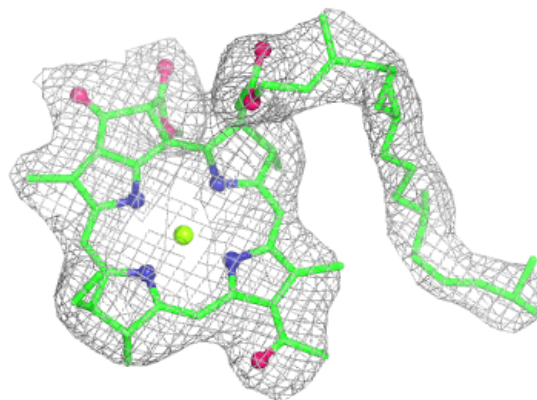


Electron density around BCL M 403:

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

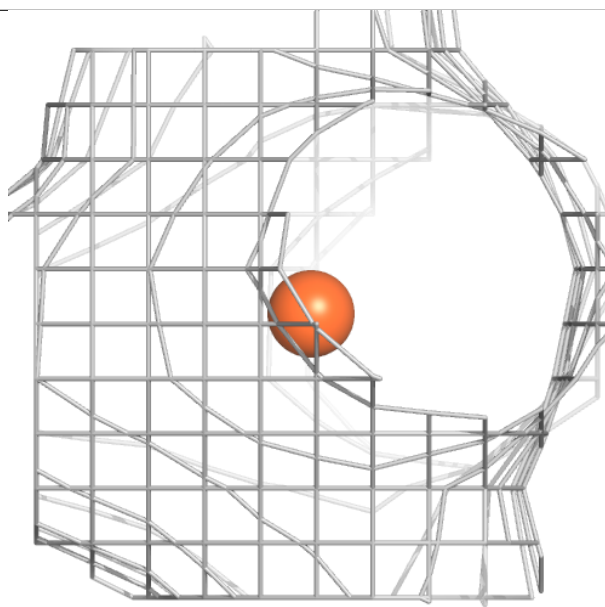
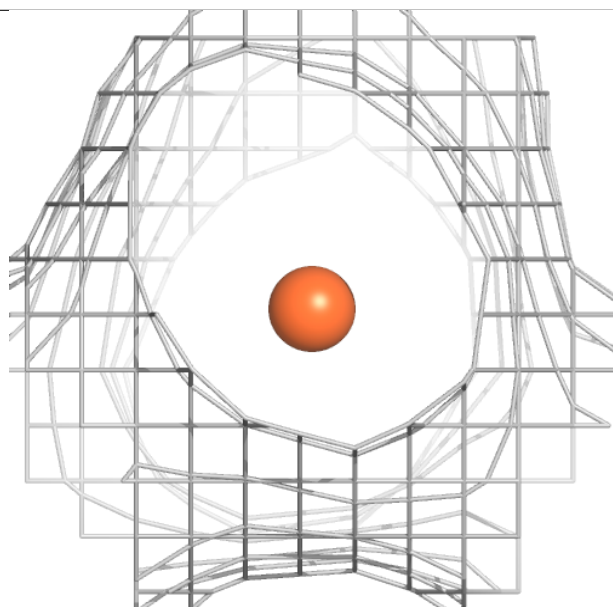
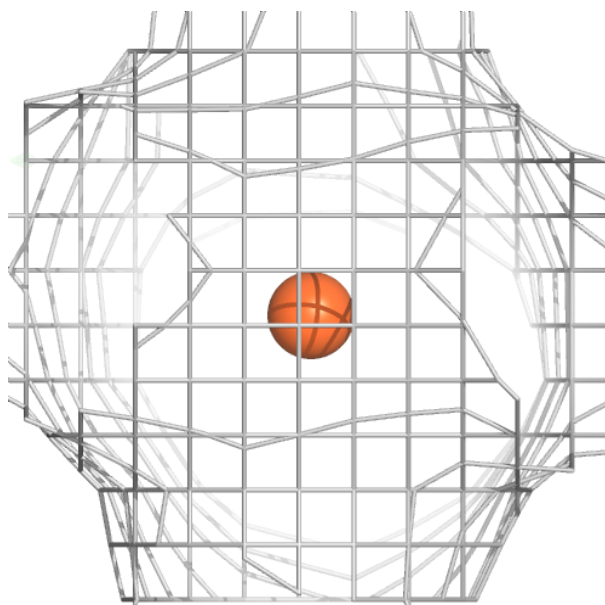
**Electron density around BCL L 503:**

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



Electron density around FE 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.