



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:36 PM BST

PDB ID : 5NSW
Title : Xenon for tunnelling analysis of the efflux pump component OprN.
Authors : Phan, G.; Prange, T.; Enguene Ntsogo, Y.V.; Garnier, C.; Ducruix, A.; Broutin, I.
Deposited on : 2017-04-27
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

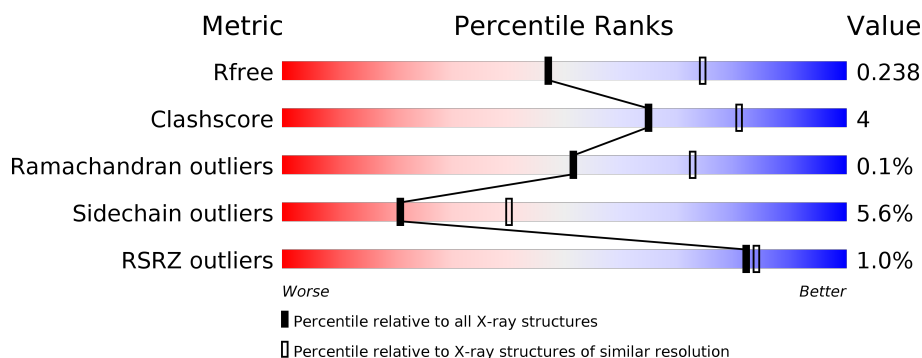
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	453	<div> <div>2%</div> <div>83% 13% . .</div> </div>
1	B	453	<div> <div>83% 14% . .</div> </div>
1	C	453	<div> <div>2%</div> <div>82% 14% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XE	B	507	-	-	X	-
3	XE	C	506	-	-	X	-
3	XE	C	507	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11133 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.

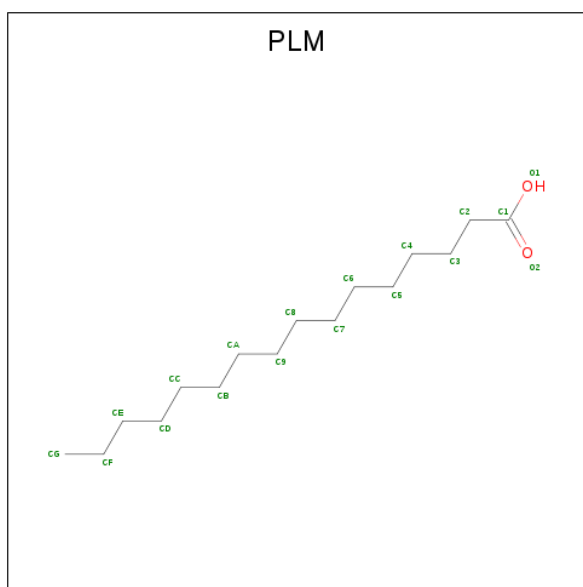
- Molecule 1 is a protein called Multidrug efflux outer membrane protein OprN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	5	0
			3455	2127	648	679	1			
1	B	445	Total	C	N	O	S	0	0	0
			3420	2107	641	671	1			
1	C	451	Total	C	N	O	S	0	6	0
			3515	2164	668	682	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	448	HIS	-	expression tag	UNP Q9I0Y7
A	449	HIS	-	expression tag	UNP Q9I0Y7
A	450	HIS	-	expression tag	UNP Q9I0Y7
A	451	HIS	-	expression tag	UNP Q9I0Y7
A	452	HIS	-	expression tag	UNP Q9I0Y7
A	453	HIS	-	expression tag	UNP Q9I0Y7
B	448	HIS	-	expression tag	UNP Q9I0Y7
B	449	HIS	-	expression tag	UNP Q9I0Y7
B	450	HIS	-	expression tag	UNP Q9I0Y7
B	451	HIS	-	expression tag	UNP Q9I0Y7
B	452	HIS	-	expression tag	UNP Q9I0Y7
B	453	HIS	-	expression tag	UNP Q9I0Y7
C	448	HIS	-	expression tag	UNP Q9I0Y7
C	449	HIS	-	expression tag	UNP Q9I0Y7
C	450	HIS	-	expression tag	UNP Q9I0Y7
C	451	HIS	-	expression tag	UNP Q9I0Y7
C	452	HIS	-	expression tag	UNP Q9I0Y7
C	453	HIS	-	expression tag	UNP Q9I0Y7

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).

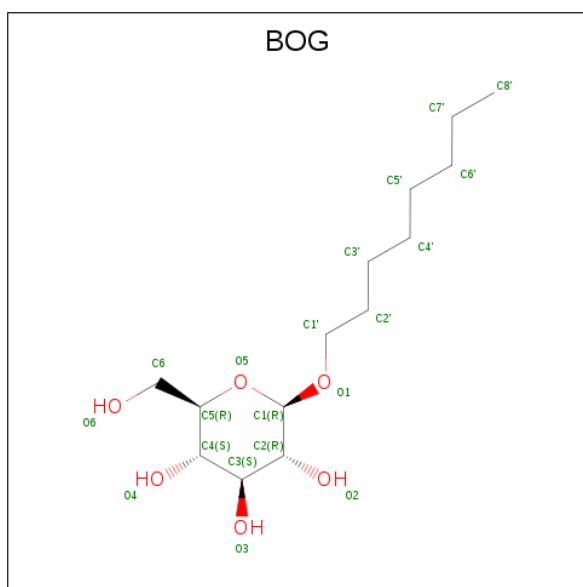


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		
2	A	1	Total	C	O	0	1
			34	32	2		
2	B	1	Total	C	O	0	0
			14	13	1		
2	B	1	Total	C	O	0	0
			17	16	1		
2	C	1	Total	C	O	0	0
			17	16	1		
2	C	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total	Xe	0	0
			6	6		
3	A	6	Total	Xe	0	0
			6	6		
3	C	5	Total	Xe	0	0
			5	5		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ni	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	166	Total	O	0	0
			166	166		

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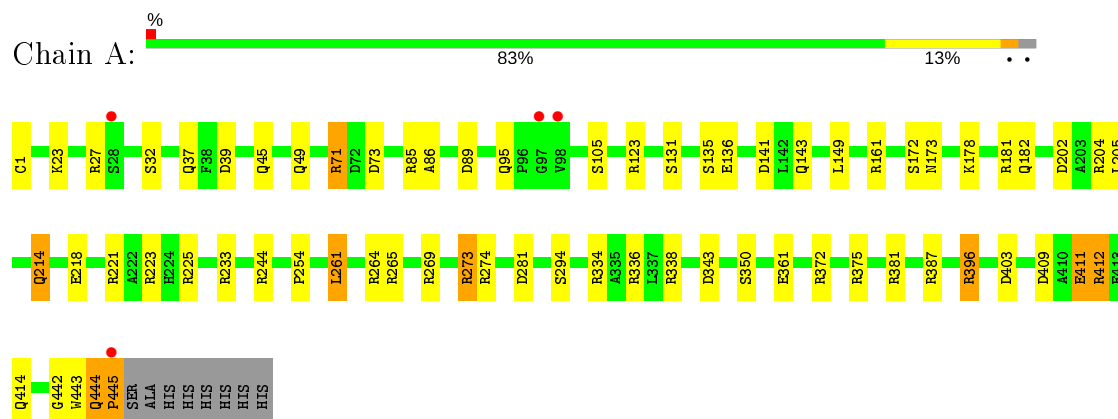
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	188	Total 188	O 188	0	0
7	C	174	Total 174	O 174	0	0

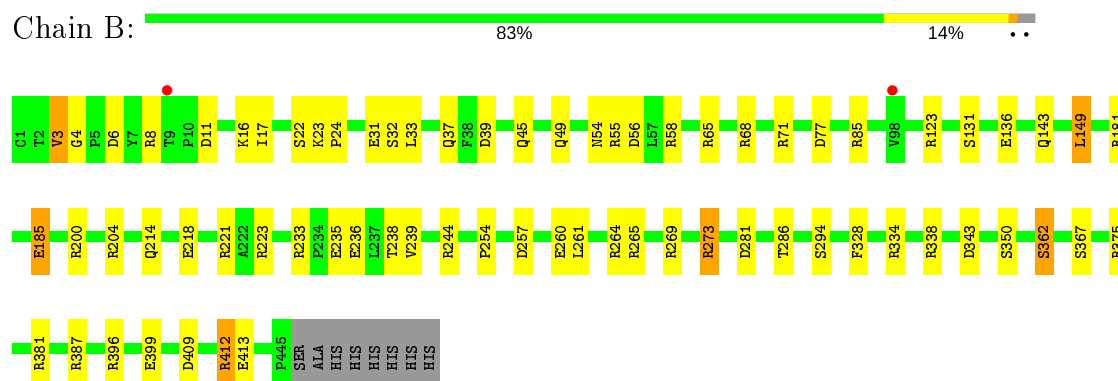
3 Residue-property plots [i](#)

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.

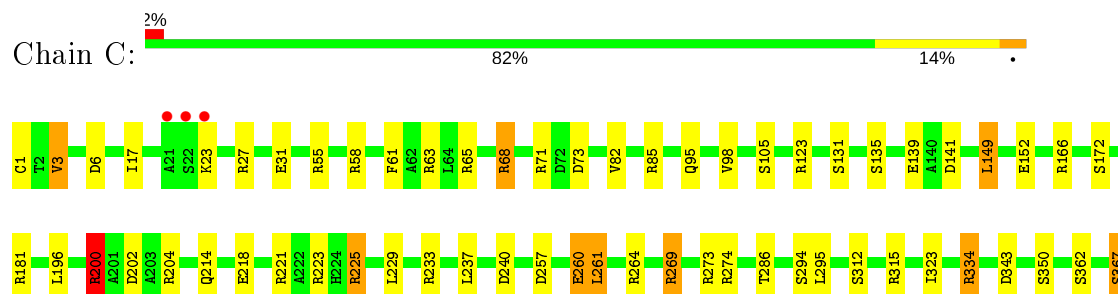
- Molecule 1: Multidrug efflux outer membrane protein OprN

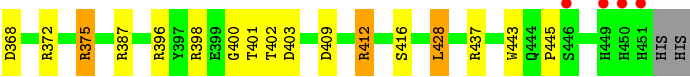


- Molecule 1: Multidrug efflux outer membrane protein OprN



- Molecule 1: Multidrug efflux outer membrane protein OprN





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	256.41 Å 256.41 Å 81.39 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 2.50 45.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-2.50) 100.0 (45.33-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.171 , 0.239 0.175 , 0.238	Depositor DCC
R_{free} test set	4736 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11133	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: BOG, NI, PLM, XE, NA

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	A	0.96	5/3509 (0.1%)	1.14	37/4752 (0.8%)
1	B	1.01	9/3468 (0.3%)	1.16	34/4697 (0.7%)
1	C	1.00	7/3582 (0.2%)	1.20	43/4848 (0.9%)
All	All	0.99	21/10559 (0.2%)	1.17	114/14297 (0.8%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	SER	CB-OG	-9.01	1.30	1.42
1	B	236	GLU	CD-OE1	8.40	1.34	1.25
1	C	135	SER	CB-OG	-8.05	1.31	1.42
1	A	1	CYS	N-CA	7.75	1.61	1.46
1	B	218	GLU	CD-OE1	7.56	1.33	1.25
1	B	235	GLU	CD-OE2	7.28	1.33	1.25
1	C	367	SER	CB-OG	7.05	1.51	1.42
1	A	411	GLU	CD-OE1	7.03	1.33	1.25
1	A	350	SER	CB-OG	-6.82	1.33	1.42
1	B	235	GLU	CD-OE1	6.81	1.33	1.25
1	C	403	ASP	CB-CG	6.69	1.65	1.51
1	C	218	GLU	CD-OE1	6.63	1.32	1.25
1	C	152	GLU	CD-OE2	6.50	1.32	1.25
1	C	172	SER	CB-OG	-6.35	1.33	1.42
1	B	294	SER	CB-OG	-5.86	1.34	1.42
1	A	361	GLU	CD-OE1	5.46	1.31	1.25
1	B	399	GLU	CD-OE1	5.46	1.31	1.25
1	B	185	GLU	CD-OE2	5.42	1.31	1.25
1	A	172	SER	CB-OG	-5.21	1.35	1.42
1	C	416	SER	CB-OG	-5.12	1.35	1.42
1	B	362	SER	CB-OG	-5.00	1.35	1.42

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	B	412	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	C	412	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	C	387	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	375	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	204	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	261	LEU	CA-CB-CG	8.39	134.61	115.30
1	A	233	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	C	343	ASP	CB-CG-OD1	8.23	125.70	118.30
1	A	123	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	396	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	C	166	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	387	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	B	6	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	412	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	B	338	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	372	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	C	412	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	C	58	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	C	139	GLU	OE1-CD-OE2	-7.56	114.23	123.30
1	C	200	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	240	ASP	CB-CG-OD1	7.52	125.06	118.30
1	A	412	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	396	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	204	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	C	123	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	437	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	C	273	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	343	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	274	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	C	403	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	375	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	204	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	244	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	149	LEU	CB-CG-CD2	7.06	123.00	111.00
1	C	343	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	C	123	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	233	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	375	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	387	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	B	11	ASP	CB-CG-OD1	6.74	124.37	118.30
1	C	273	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	89	ASP	CB-CG-OD2	-6.67	112.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	233	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	387	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	B	123	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	85	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	233	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	63	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	338	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	336	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	71	ARG	CG-CD-NE	6.34	125.12	111.80
1	B	265	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	68	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	C	58	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	343	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	412	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	338	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	C	73	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	B	381	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	73	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	396	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	375	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	73	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	336	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	85	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	65	ARG	CG-CD-NE	-5.98	99.24	111.80
1	C	372	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	56	ASP	CB-CG-OD2	5.95	123.65	118.30
1	C	85	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	58	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	C	398	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	89	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	77	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	B	264	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	85	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	6	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	C	396	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	281	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	166	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	223[A]	ARG	CG-CD-NE	-5.72	99.78	111.80
1	A	223[B]	ARG	CG-CD-NE	-5.72	99.78	111.80
1	C	1	CYS	CA-CB-SG	5.72	124.30	114.00
1	A	161	ARG	NE-CZ-NH2	-5.69	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	336	ARG	CG-CD-NE	-5.61	100.02	111.80
1	C	396	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	73	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	218	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	C	412	ARG	CA-CB-CG	5.54	125.58	113.40
1	C	55	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	375	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	1	CYS	CA-CB-SG	5.45	123.81	114.00
1	A	381	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	281	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	244	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	428	LEU	CA-CB-CG	5.33	127.56	115.30
1	C	334	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	141	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	6	ASP	CB-CG-OD1	-5.27	113.55	118.30
1	C	295	LEU	CB-CG-CD2	5.23	119.89	111.00
1	C	27	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	261	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	334	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	265	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	218	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	B	413	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	B	55	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	387	ARG	CG-CD-NE	-5.04	101.21	111.80
1	B	65	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	343	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	200	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	C	264	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	A	3455	0	3423	27	0
1	B	3420	0	3389	27	0
1	C	3515	0	3489	34	0
2	A	51	0	93	1	0
2	B	31	0	53	0	0
2	C	34	0	62	1	0
3	A	6	0	0	3	0
3	B	6	0	0	6	0
3	C	5	0	0	4	0
4	A	20	0	28	0	0
4	B	40	0	56	4	0
4	C	20	0	28	1	0
5	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	166	0	0	2	0
7	B	188	0	0	5	0
7	C	174	0	0	8	0
All	All	11133	0	10621	86	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 (86) 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:B:149:LEU:HD12	3:B:507:XE:XE	2.13	1.27
1:B:149:LEU:HB3	3:B:507:XE:XE	2.18	1.22
1:C:149:LEU:HB3	3:C:506:XE:XE	2.31	1.08
1:A:221:ARG:HD2	7:A:735:HOH:O	1.60	1.01
1:B:37:GLN:HE22	1:B:254:PRO:HG2	1.28	0.95
1:B:149:LEU:CD1	3:B:507:XE:XE	2.95	0.93
1:B:149:LEU:CB	3:B:507:XE:XE	2.94	0.92
4:B:509:BOG:H5'2	4:B:509:BOG:H1'2	1.56	0.85
1:B:37:GLN:NE2	1:B:254:PRO:HG2	1.94	0.82
1:A:444:GLN:H	1:A:445:PRO:HD3	1.45	0.80
1:B:22:SER:HB3	1:B:24:PRO:HD2	1.64	0.79
1:B:37:GLN:HE22	1:B:254:PRO:CG	1.96	0.78
1:C:149:LEU:CB	3:C:506:XE:XE	3.09	0.78
1:A:37:GLN:NE2	1:A:254:PRO:HG2	2.02	0.74
1:A:37:GLN:HE22	1:A:254:PRO:CD	2.01	0.73
1:B:149:LEU:CG	3:B:507:XE:XE	3.17	0.71
1:A:221:ARG:HD3	7:C:716:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:HE22	1:A:254:PRO:HG2	1.57	0.70
3:A:508:XE:XE	1:B:214:GLN:HA	2.70	0.68
1:C:257:ASP:HB3	1:C:260:GLU:HG3	1.75	0.68
1:A:32:SER:HB3	1:A:445:PRO:HD2	1.75	0.67
1:A:37:GLN:HE22	1:A:254:PRO:HD2	1.60	0.66
1:A:37:GLN:HE22	1:A:254:PRO:CG	2.09	0.66
1:C:400:GLY:CA	7:C:723:HOH:O	2.43	0.65
1:A:264:ARG:HD3	1:A:445:PRO:HB2	1.78	0.64
1:C:400:GLY:HA2	7:C:723:HOH:O	1.99	0.62
1:C:196:LEU:O	1:C:200:ARG:HD2	2.00	0.61
3:C:507:XE:XE	7:C:761:HOH:O	2.96	0.61
3:B:508:XE:XE	1:C:214:GLN:HA	2.79	0.60
1:A:214:GLN:HA	3:A:505:XE:XE	2.80	0.60
1:C:181[B]:ARG:HD2	1:C:202:ASP:OD1	2.02	0.60
7:B:761:HOH:O	1:C:221:ARG:CD	2.49	0.59
1:C:223[B]:ARG:HH11	1:C:237:LEU:HD12	1.67	0.59
1:A:444:GLN:H	1:A:445:PRO:CD	2.15	0.58
7:B:761:HOH:O	1:C:221:ARG:HD2	2.05	0.56
1:B:37:GLN:HE22	1:B:254:PRO:CD	2.19	0.56
1:A:221:ARG:CD	7:A:735:HOH:O	2.35	0.54
7:B:761:HOH:O	1:C:221:ARG:HD3	2.08	0.54
1:B:22:SER:CB	1:B:24:PRO:HD2	2.37	0.54
1:B:45:GLN:NE2	7:B:603:HOH:O	2.40	0.53
1:C:312:SER:HB3	1:C:315:ARG:HH21	1.73	0.53
1:B:136:GLU:HB2	1:B:273:ARG:HG3	1.92	0.52
1:B:3:VAL:HG13	1:B:286:THR:HG22	1.90	0.52
1:C:149:LEU:HD13	1:C:229:LEU:HD22	1.91	0.52
1:A:143:GLN:OE1	1:A:269:ARG:NH1	2.41	0.52
1:A:411:GLU:OE1	3:A:504:XE:XE	3.06	0.52
1:A:412:ARG:HH22	1:C:409:ASP:CG	2.13	0.52
1:C:412:ARG:HD2	7:C:625:HOH:O	2.09	0.51
1:A:136:GLU:HB2	1:A:273:ARG:HG3	1.92	0.51
1:A:37:GLN:NE2	1:A:254:PRO:CG	2.72	0.51
1:C:269:ARG:HG2	7:C:733:HOH:O	2.10	0.50
1:B:4:GLY:HA2	4:B:509:BOG:H8'1	1.94	0.50
1:C:257:ASP:HB3	1:C:260:GLU:CG	2.41	0.50
1:B:143:GLN:OE1	1:B:269:ARG:NH1	2.46	0.49
1:C:141:ASP:OD2	1:C:274[A]:ARG:NH2	2.46	0.49
1:C:3:VAL:HG13	1:C:286:THR:HG22	1.95	0.49
1:B:257:ASP:HB3	1:B:260:GLU:HG2	1.95	0.48
1:B:328:PHE:HB2	1:C:82:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:CG	1:B:412:ARG:HH22	2.18	0.47
1:B:409:ASP:CG	1:C:412:ARG:HH22	2.18	0.46
1:C:225:ARG:HG3	3:C:507:XE:XE	2.94	0.46
1:B:45:GLN:NE2	1:B:239:VAL:HG22	2.30	0.46
1:C:375:ARG:NH2	7:C:602:HOH:O	2.47	0.45
1:B:54:ASN:ND2	1:B:149:LEU:HD11	2.31	0.45
1:C:443:TRP:O	1:C:445:PRO:HD3	2.17	0.45
1:A:442:GLY:H	1:A:445:PRO:HG3	1.81	0.45
1:C:223[B]:ARG:NH1	1:C:237:LEU:HD12	2.31	0.45
1:B:181:ARG:HD2	1:B:185:GLU:OE2	2.16	0.45
1:C:401:THR:HG22	1:C:401:THR:O	2.17	0.45
1:A:444:GLN:N	1:A:445:PRO:HD3	2.24	0.44
1:C:61:PHE:CD2	1:C:65[B]:ARG:NH1	2.85	0.44
1:C:68:ARG:HD3	4:C:509:BOG:H6'1	1.99	0.44
1:A:443:TRP:NE1	1:A:445:PRO:HB3	2.32	0.44
1:A:181:ARG:NH1	1:A:202:ASP:OD1	2.47	0.43
1:A:45[A]:GLN:HE21	1:A:49:GLN:CG	2.30	0.43
1:B:273:ARG:HD2	1:B:273:ARG:HA	1.58	0.43
1:A:173:ASN:HD21	1:A:414:GLN:HE21	1.66	0.43
4:B:509:BOG:C1'	4:B:509:BOG:H5'2	2.37	0.43
1:A:86:ALA:HB3	1:C:323:ILE:HG23	2.01	0.42
1:C:334:ARG:HH12	2:C:502:PLM:HG2	1.84	0.42
1:C:400:GLY:HA3	7:C:723:HOH:O	2.12	0.42
1:A:221:ARG:NH1	1:C:368:ASP:OD1	2.53	0.41
1:B:286:THR:OG1	4:B:509:BOG:H7'1	2.21	0.41
2:A:502[A]:PLM:HB2	2:A:502[A]:PLM:HE1	1.83	0.41
1:B:221:ARG:CZ	7:B:684:HOH:O	2.69	0.40
1:C:401:THR:O	1:C:402:THR:HG23	2.21	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	A	448/453 (99%)	440 (98%)	7 (2%)	1 (0%)	47	68
1	B	443/453 (98%)	435 (98%)	8 (2%)	0	100	100
1	C	455/453 (100%)	445 (98%)	9 (2%)	1 (0%)	47	68
All	All	1346/1359 (99%)	1320 (98%)	24 (2%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	C	98	VAL

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	A	350/352 (99%)	329 (94%)	21 (6%)	19	37
1	B	345/352 (98%)	326 (94%)	19 (6%)	21	41
1	C	356/352 (101%)	337 (95%)	19 (5%)	22	43
All	All	1051/1056 (100%)	992 (94%)	59 (6%)	21	40

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	27	ARG
1	A	39	ASP
1	A	71	ARG
1	A	85	ARG
1	A	95	GLN
1	A	105	SER
1	A	131	SER
1	A	135	SER
1	A	178	LYS
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	205	LEU
1	A	214	GLN
1	A	225	ARG
1	A	261	LEU
1	A	273	ARG
1	A	294[A]	SER
1	A	294[B]	SER
1	A	396	ARG
1	A	403	ASP
1	A	445	PRO
1	B	3	VAL
1	B	8	ARG
1	B	16	LYS
1	B	17	ILE
1	B	23	LYS
1	B	31	GLU
1	B	32	SER
1	B	33	LEU
1	B	39	ASP
1	B	49	GLN
1	B	71	ARG
1	B	131	SER
1	B	149	LEU
1	B	223	ARG
1	B	238	THR
1	B	261	LEU
1	B	273	ARG
1	B	362	SER
1	B	367	SER
1	C	3	VAL
1	C	17	ILE
1	C	23	LYS
1	C	31	GLU
1	C	71	ARG
1	C	95	GLN
1	C	105	SER
1	C	131	SER
1	C	149	LEU
1	C	200	ARG
1	C	225	ARG
1	C	260	GLU
1	C	261	LEU

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Mol	Chain	Res	Type
1	C	269	ARG
1	C	294	SER
1	C	350	SER
1	C	362	SER
1	C	367	SER
1	C	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	49	GLN
1	A	146	GLN
1	A	173	ASN
1	A	182	GLN
1	A	414	GLN
1	B	37	GLN
1	B	76	ASN
1	B	144	GLN
1	B	173	ASN
1	B	176	ASN
1	B	353	GLN
1	B	354	GLN
1	B	414	GLN
1	C	146	GLN
1	C	173	ASN
1	C	176	ASN
1	C	182	GLN
1	C	308	GLN
1	C	391	GLN
1	C	414	GLN
1	C	451	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 19 are monoatomic - leaving 11 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	$\# Z > 2$
2	PLM	C	502	1	16,16,17	1.30	0	15,15,17	1.18	1 (6%)
2	PLM	B	505	1	16,16,17	0.98	0	15,15,17	0.58	0
2	PLM	A	501	1	16,16,17	1.46	1 (6%)	15,15,17	1.45	3 (20%)
4	BOG	C	509	-	20,20,20	1.43	3 (15%)	25,25,25	1.51	4 (16%)
2	PLM	A	502[A]	1	16,16,17	1.05	0	15,15,17	1.34	1 (6%)
4	BOG	A	509	-	20,20,20	2.07	5 (25%)	25,25,25	2.86	8 (32%)
4	BOG	B	510	-	20,20,20	1.27	4 (20%)	25,25,25	2.10	5 (20%)
2	PLM	A	502[B]	1	16,16,17	1.01	0	15,15,17	1.04	1 (6%)
2	PLM	C	503	1	16,16,17	1.32	0	15,15,17	0.97	0
2	PLM	B	504	1	13,13,17	0.98	0	12,12,17	1.21	1 (8%)
4	BOG	B	509	-	20,20,20	1.47	2 (10%)	25,25,25	1.70	7 (28%)

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
2	PLM	C	502	1	-	9/13/14/15	-
2	PLM	B	505	1	-	9/13/14/15	-
2	PLM	A	501	1	-	7/13/14/15	-
4	BOG	C	509	-	-	7/11/31/31	0/1/1/1
2	PLM	A	502[A]	1	-	5/13/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BOG	A	509	-	-	6/11/31/31	0/1/1/1
4	BOG	B	510	-	-	10/11/31/31	0/1/1/1
2	PLM	A	502[B]	1	-	5/13/14/15	-
2	PLM	C	503	1	-	9/13/14/15	-
2	PLM	B	504	1	-	7/10/11/15	-
4	BOG	B	509	-	-	6/11/31/31	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	509	BOG	O5-C1	4.79	1.54	1.41
4	A	509	BOG	O5-C1	4.62	1.53	1.41
4	A	509	BOG	O1-C1	4.37	1.47	1.40
4	C	509	BOG	O5-C1	3.91	1.51	1.41
4	B	509	BOG	O5-C5	3.16	1.52	1.44
4	A	509	BOG	C1-C2	2.95	1.61	1.52
4	C	509	BOG	C4-C5	2.75	1.58	1.53
4	C	509	BOG	O5-C5	2.72	1.50	1.44
4	A	509	BOG	O3-C3	2.56	1.49	1.43
4	B	510	BOG	O5-C1	2.50	1.48	1.41
4	B	510	BOG	C4-C3	-2.39	1.46	1.52
4	B	510	BOG	C3-C2	-2.34	1.46	1.52
4	A	509	BOG	O1-C1'	2.31	1.49	1.43
4	B	510	BOG	O1-C1	-2.20	1.36	1.40
2	A	501	PLM	O2-C1	2.11	1.31	1.19

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	509	BOG	O1-C1-C2	10.11	124.09	108.30
4	A	509	BOG	C1'-O1-C1	5.56	123.05	113.84
4	B	510	BOG	O5-C5-C4	-5.17	100.30	109.69
4	B	510	BOG	O2-C2-C3	-5.08	98.60	110.35
4	B	509	BOG	C1-O5-C5	4.06	121.65	113.69
2	A	502[A]	PLM	O2-C1-C2	-3.99	100.70	126.89
4	B	510	BOG	O5-C5-C6	3.91	116.16	106.44
2	B	504	PLM	O2-C1-C2	-3.66	102.89	126.89
4	A	509	BOG	O3-C3-C2	3.63	118.75	110.35
4	B	510	BOG	C1-C2-C3	3.63	117.55	110.00
2	A	501	PLM	O2-C1-C2	-3.58	103.41	126.89
4	A	509	BOG	C4-C3-C2	-3.50	104.71	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502[B]	PLM	O2-C1-C2	-3.49	103.99	126.89
4	C	509	BOG	O4-C4-C5	3.48	117.94	109.30
4	A	509	BOG	O2-C2-C1	3.42	118.36	110.05
4	B	510	BOG	C1-O5-C5	-3.24	107.33	113.69
4	C	509	BOG	O1-C1-C2	3.18	113.27	108.30
2	C	502	PLM	O2-C1-C2	-3.18	106.04	126.89
4	C	509	BOG	C5'-C4'-C3'	-3.07	98.86	114.42
4	B	509	BOG	O5-C5-C4	3.03	115.19	109.69
4	B	509	BOG	O2-C2-C3	2.76	116.72	110.35
4	B	509	BOG	C6-C5-C4	-2.70	106.67	113.00
4	A	509	BOG	O5-C1-C2	-2.65	104.75	110.35
2	A	501	PLM	CC-CB-CA	2.51	127.14	114.42
4	A	509	BOG	O5-C5-C4	2.50	114.23	109.69
4	B	509	BOG	C4-C3-C2	-2.41	106.61	110.82
4	C	509	BOG	C1-O5-C5	2.41	118.41	113.69
4	B	509	BOG	O5-C5-C6	2.19	111.89	106.44
2	A	501	PLM	CA-C9-C8	2.17	125.44	114.42
4	B	509	BOG	O5-C1-O1	2.13	115.01	109.97
4	A	509	BOG	O1-C1'-C2'	2.11	116.96	109.56

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	510	BOG	C2'-C1'-O1-C1
2	A	501	PLM	C1-C2-C3-C4
4	B	510	BOG	O5-C5-C6-O6
4	C	509	BOG	O5-C5-C6-O6
2	A	502[A]	PLM	CB-CC-CD-CE
4	B	510	BOG	C4-C5-C6-O6
4	C	509	BOG	C4-C5-C6-O6
2	A	502[A]	PLM	CC-CD-CE-CF
2	B	504	PLM	C7-C8-C9-CA
2	A	501	PLM	C3-C4-C5-C6
2	C	502	PLM	C7-C8-C9-CA
2	A	502[B]	PLM	C6-C7-C8-C9
4	B	510	BOG	C2-C1-O1-C1'
4	C	509	BOG	C2-C1-O1-C1'
4	B	509	BOG	C2-C1-O1-C1'
2	B	504	PLM	C6-C7-C8-C9
2	A	502[A]	PLM	C7-C8-C9-CA
4	B	510	BOG	O5-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
4	C	509	BOG	O5-C1-O1-C1'
4	B	509	BOG	O5-C1-O1-C1'
2	C	502	PLM	C4-C5-C6-C7
4	B	510	BOG	C4'-C5'-C6'-C7'
2	B	505	PLM	C9-CA-CB-CC
4	B	509	BOG	C2'-C1'-O1-C1
2	C	502	PLM	C2-C3-C4-C5
2	B	505	PLM	C5-C6-C7-C8
2	A	502[B]	PLM	C2-C3-C4-C5
4	B	509	BOG	C4'-C5'-C6'-C7'
2	B	505	PLM	CA-CB-CC-CD
4	A	509	BOG	C1'-C2'-C3'-C4'
2	C	502	PLM	C3-C4-C5-C6
2	C	503	PLM	C9-CA-CB-CC
4	B	510	BOG	C1'-C2'-C3'-C4'
4	B	509	BOG	O5-C5-C6-O6
2	C	503	PLM	C4-C5-C6-C7
4	A	509	BOG	C2-C1-O1-C1'
2	C	502	PLM	C6-C7-C8-C9
2	B	504	PLM	C2-C3-C4-C5
4	A	509	BOG	C2'-C3'-C4'-C5'
2	C	502	PLM	C5-C6-C7-C8
4	B	510	BOG	C2'-C3'-C4'-C5'
4	B	510	BOG	C5'-C6'-C7'-C8'
2	C	502	PLM	C8-C9-CA-CB
2	A	502[B]	PLM	CD-CE-CF-CG
2	B	504	PLM	C8-C9-CA-CB
4	C	509	BOG	C5'-C6'-C7'-C8'
2	A	501	PLM	CA-CB-CC-CD
4	B	509	BOG	C5'-C6'-C7'-C8'
2	C	503	PLM	C2-C3-C4-C5
2	C	503	PLM	CC-CD-CE-CF
4	C	509	BOG	O1-C1'-C2'-C3'
2	C	503	PLM	C6-C7-C8-C9
2	B	504	PLM	CA-CB-CC-CD
2	C	503	PLM	C3-C4-C5-C6
2	A	501	PLM	C4-C5-C6-C7
2	B	505	PLM	C8-C9-CA-CB
2	A	502[B]	PLM	CC-CD-CE-CF
2	B	504	PLM	C3-C4-C5-C6
2	A	502[B]	PLM	C1-C2-C3-C4
2	A	501	PLM	CB-CC-CD-CE

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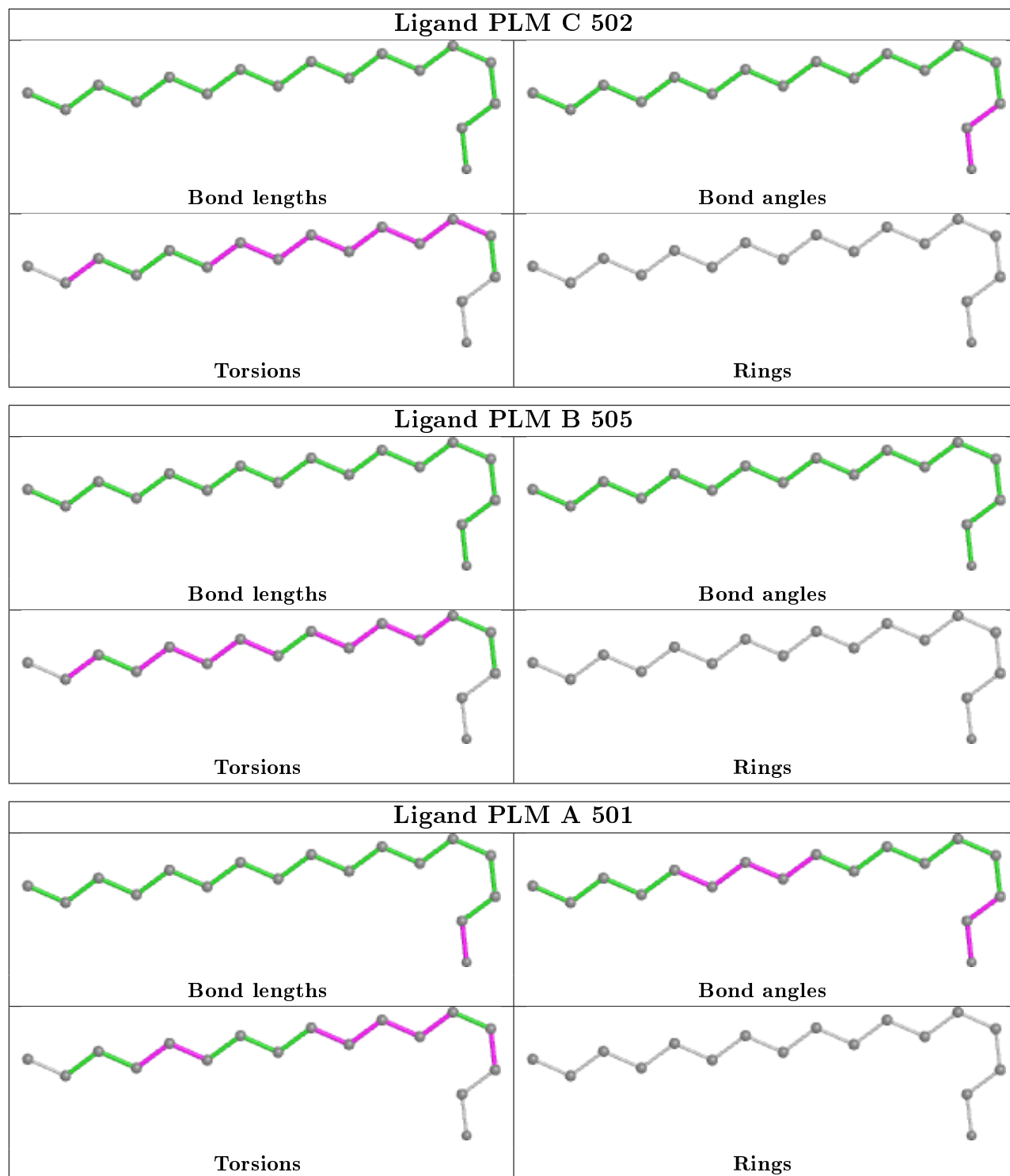
Mol	Chain	Res	Type	Atoms
2	B	505	PLM	C4-C5-C6-C7
4	C	509	BOG	C2'-C3'-C4'-C5'
4	A	509	BOG	O1-C1'-C2'-C3'
2	C	503	PLM	CB-CC-CD-CE
2	B	505	PLM	C3-C4-C5-C6
2	C	503	PLM	CA-CB-CC-CD
2	B	504	PLM	C4-C5-C6-C7
2	B	505	PLM	C6-C7-C8-C9
2	B	505	PLM	CB-CC-CD-CE
4	A	509	BOG	O5-C1-O1-C1'
2	A	501	PLM	C6-C7-C8-C9
4	A	509	BOG	C4'-C5'-C6'-C7'
2	C	503	PLM	C7-C8-C9-CA
2	B	505	PLM	CD-CE-CF-CG
2	C	502	PLM	CD-CE-CF-CG
2	A	502[A]	PLM	C9-CA-CB-CC
4	B	510	BOG	C3'-C4'-C5'-C6'
2	A	501	PLM	C5-C6-C7-C8
2	C	502	PLM	C9-CA-CB-CC
2	A	502[A]	PLM	CD-CE-CF-CG

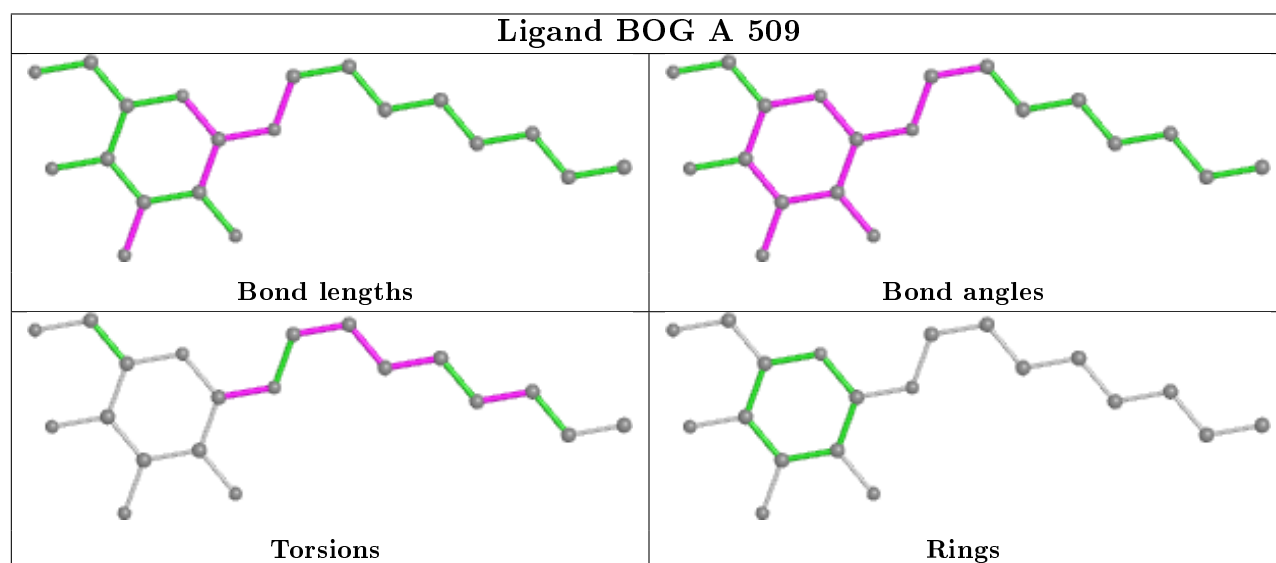
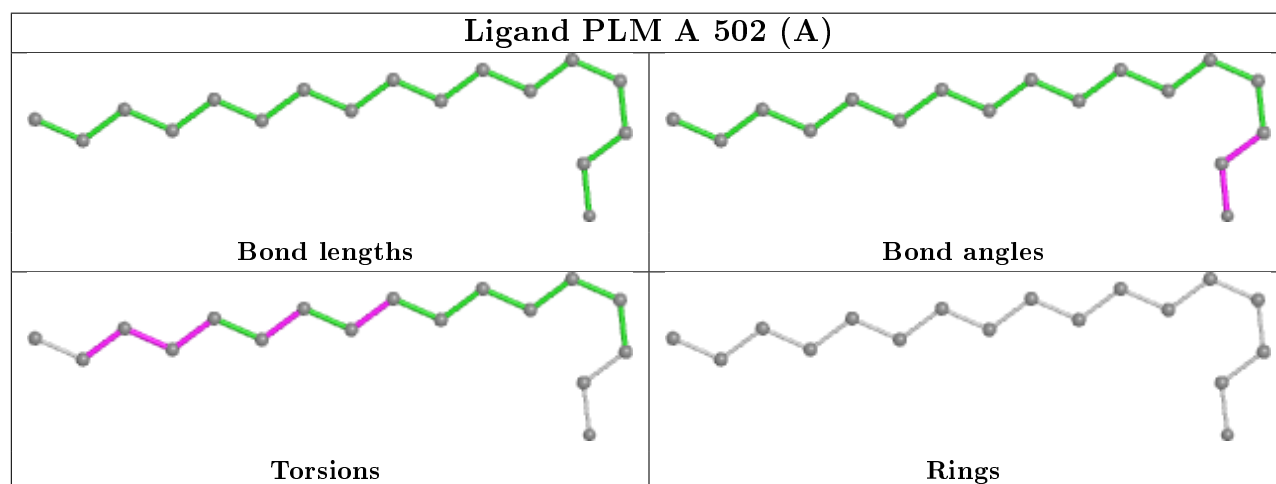
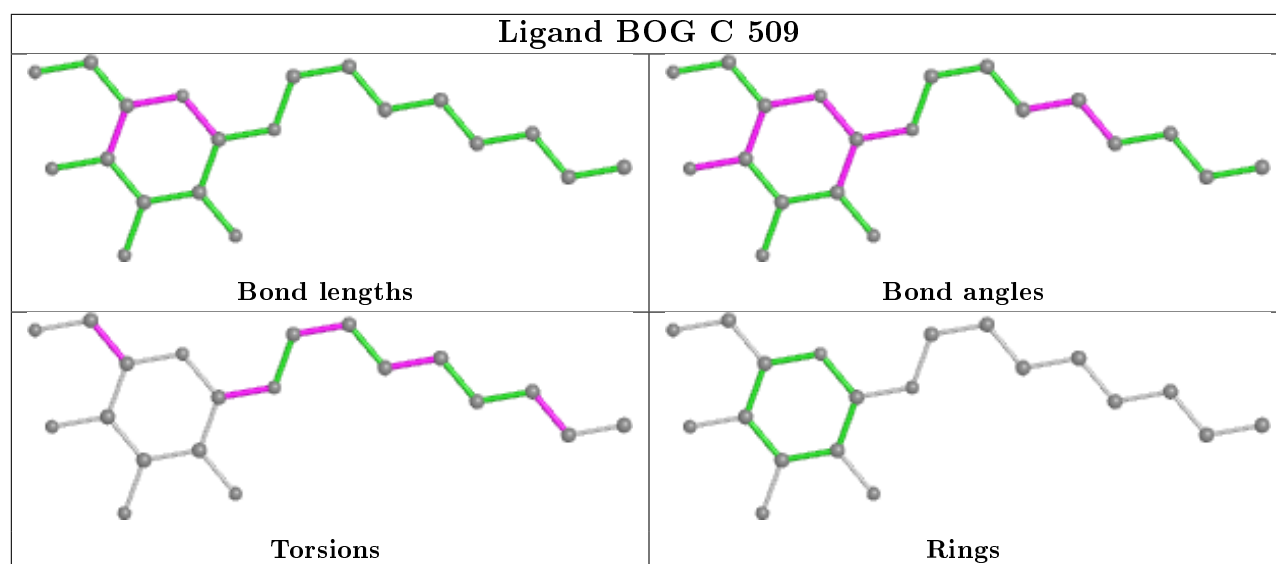
There are no ring outliers.

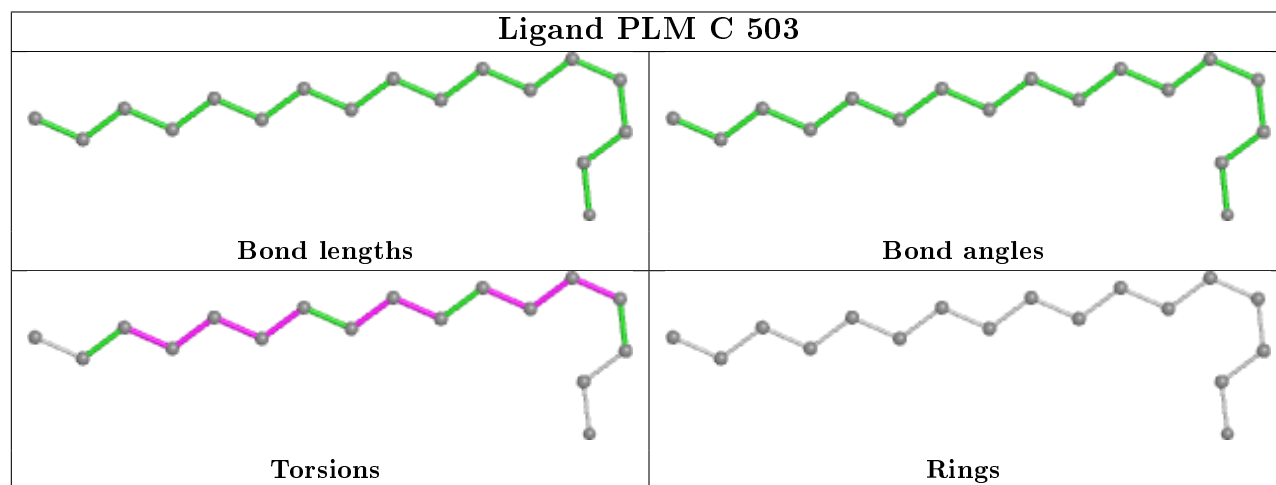
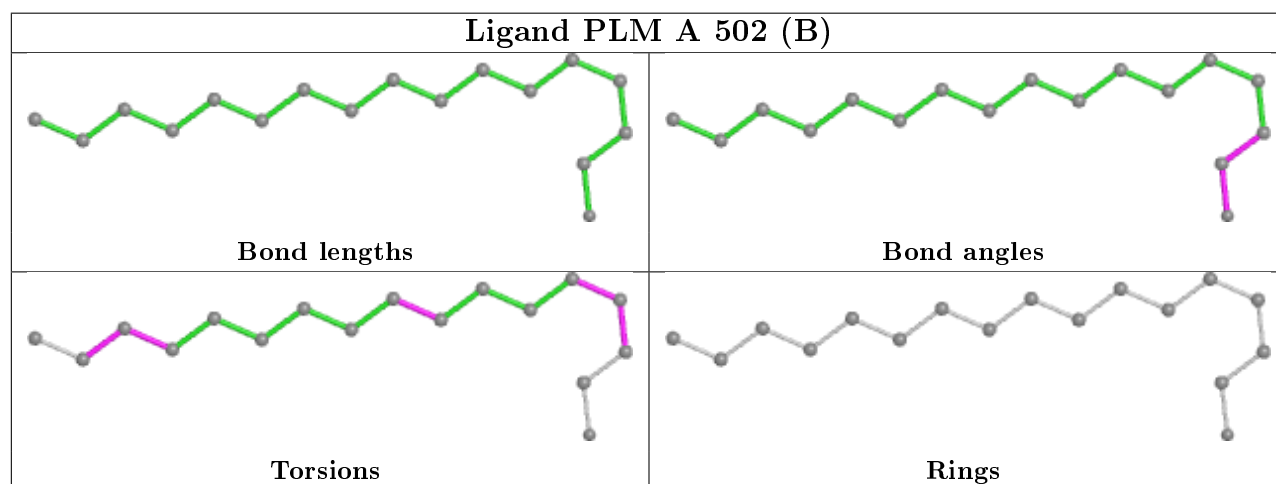
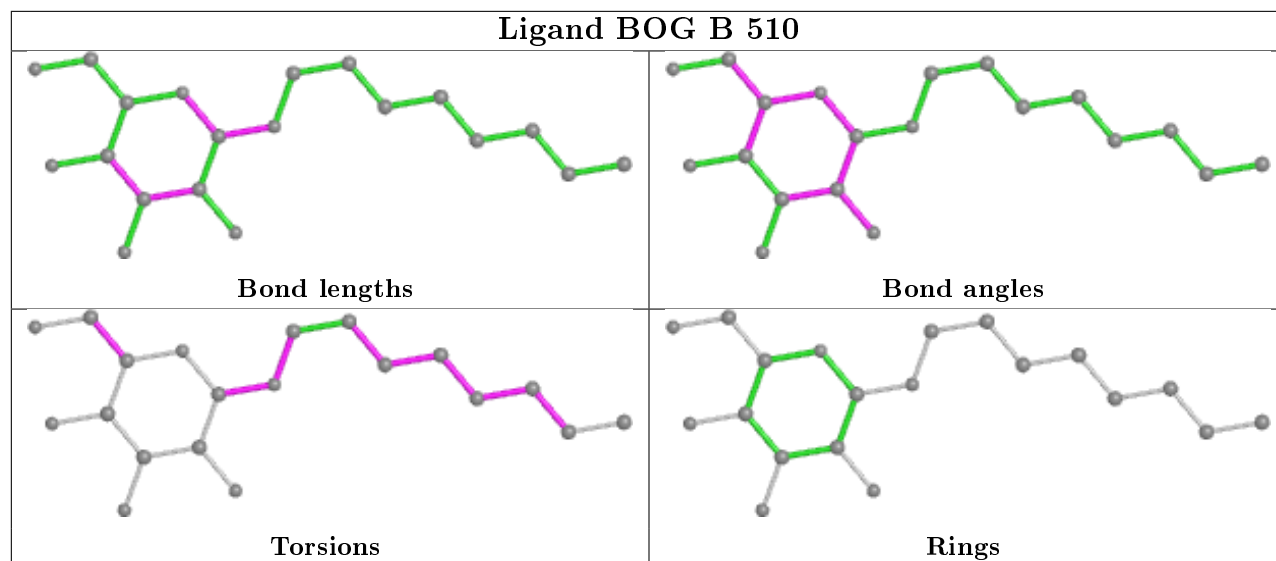
4 monomers are involved in 7 short contacts:

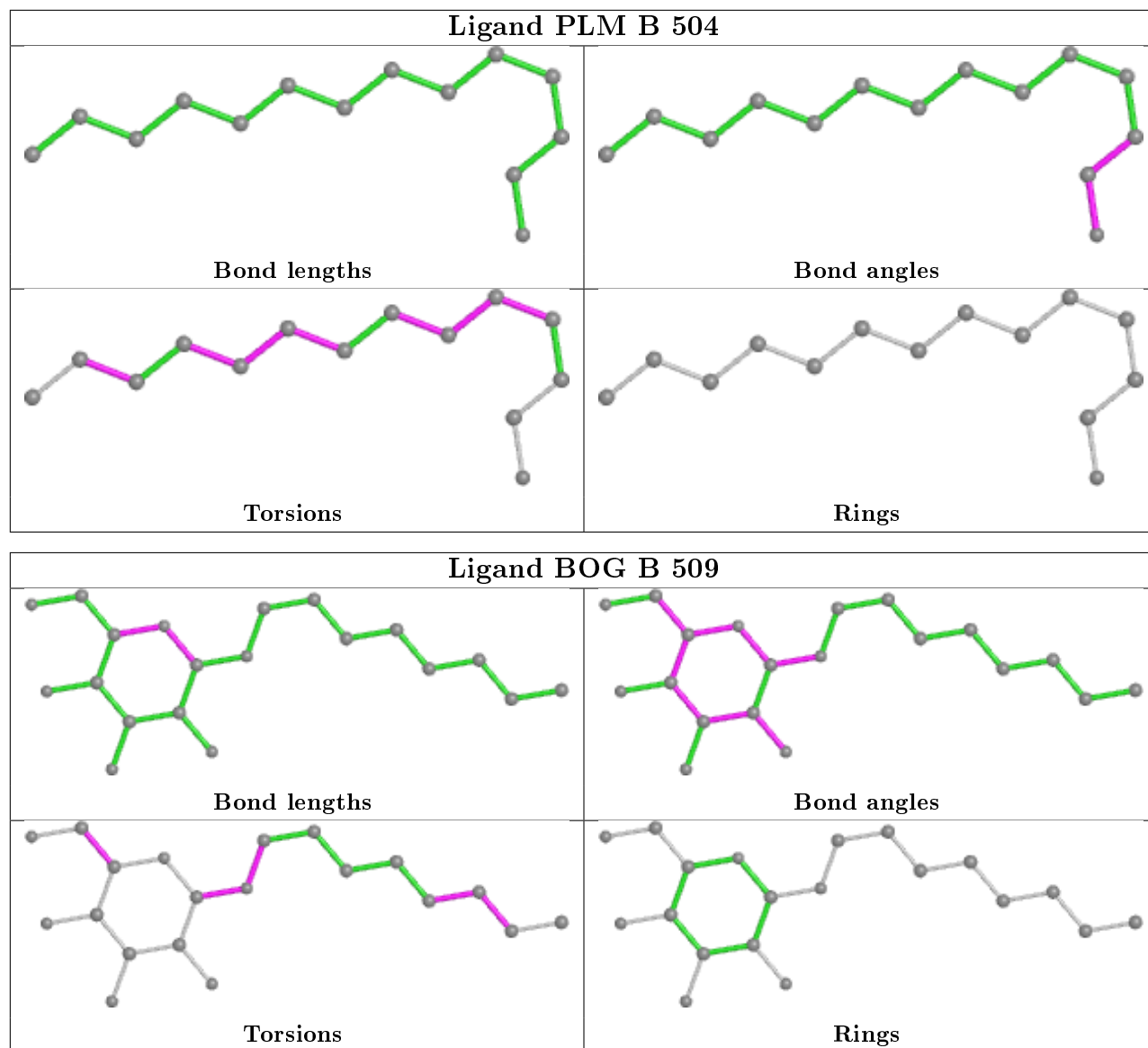
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	PLM	1	0
4	C	509	BOG	1	0
2	A	502[A]	PLM	1	0
4	B	509	BOG	4	0

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 [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	A	445/453 (98%)	-0.24	4 (0%) 84 86	26, 37, 64, 112	0
1	B	445/453 (98%)	-0.28	2 (0%) 92 93	24, 36, 65, 98	0
1	C	451/453 (99%)	-0.16	7 (1%) 72 74	24, 37, 70, 98	0
All	All	1341/1359 (98%)	-0.22	13 (0%) 82 84	24, 37, 67, 112	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	451	HIS	5.2
1	A	98	VAL	4.0
1	C	21	ALA	3.3
1	C	449	HIS	3.3
1	C	446	SER	3.2
1	C	22	SER	2.9
1	A	445	PRO	2.4
1	A	28	SER	2.3
1	B	9	THR	2.3
1	C	23	LYS	2.2
1	B	98	VAL	2.1
1	A	97	GLY	2.1
1	C	450	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

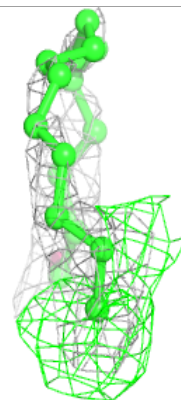
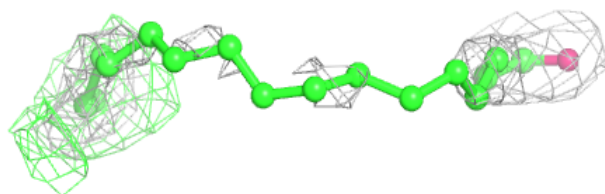
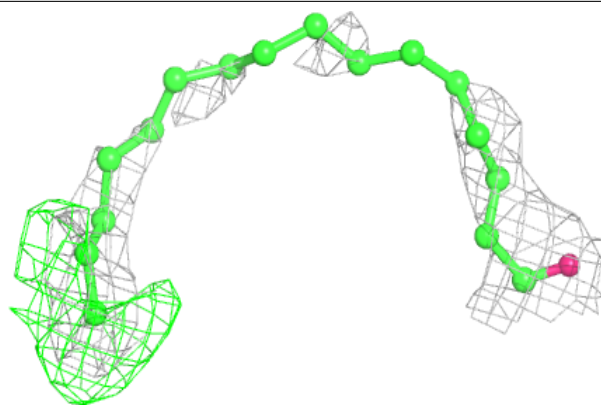
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLM	C	503	17/18	0.73	0.34	71,84,96,96	0
2	PLM	A	502[B]	17/18	0.76	0.38	40,52,56,56	17
2	PLM	A	502[A]	17/18	0.76	0.38	41,52,67,67	17
2	PLM	B	505	17/18	0.80	0.30	76,91,103,103	0
4	BOG	B	509	20/20	0.80	0.20	27,43,47,48	20
4	BOG	A	509	20/20	0.81	0.28	50,77,99,100	0
2	PLM	A	501	17/18	0.82	0.21	49,60,85,97	0
2	PLM	C	502	17/18	0.85	0.20	65,78,88,88	0
2	PLM	B	504	14/18	0.85	0.38	73,82,98,98	0
4	BOG	B	510	20/20	0.88	0.21	32,38,48,50	20
4	BOG	C	509	20/20	0.93	0.18	44,58,65,65	0
3	XE	C	508	1/1	0.94	0.16	53,53,53,53	1
5	NA	A	510	1/1	0.95	0.07	45,45,45,45	0
3	XE	C	507	1/1	0.96	0.18	54,54,54,54	1
3	XE	B	503	1/1	0.96	0.10	67,67,67,67	1
3	XE	C	501	1/1	0.97	0.12	66,66,66,66	1
3	XE	A	507	1/1	0.97	0.14	57,57,57,57	1
3	XE	A	506	1/1	0.98	0.11	60,60,60,60	1
3	XE	C	506	1/1	0.98	0.16	56,56,56,56	1
3	XE	B	507	1/1	0.98	0.12	51,51,51,51	1
3	XE	B	506	1/1	0.98	0.19	63,63,63,63	1
3	XE	C	505	1/1	0.98	0.20	64,64,64,64	1
3	XE	A	504	1/1	0.99	0.16	67,67,67,67	1
3	XE	B	501	1/1	0.99	0.08	73,73,73,73	1
3	XE	A	508	1/1	0.99	0.11	65,65,65,65	1
3	XE	B	502	1/1	0.99	0.14	60,60,60,60	1
3	XE	A	503	1/1	1.00	0.08	55,55,55,55	0
6	NI	C	504	1/1	1.00	0.06	57,57,57,57	0
3	XE	A	505	1/1	1.00	0.08	63,63,63,63	1
3	XE	B	508	1/1	1.00	0.11	58,58,58,58	1

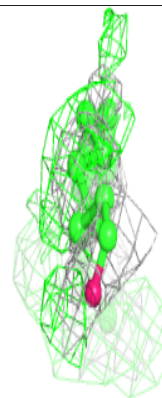
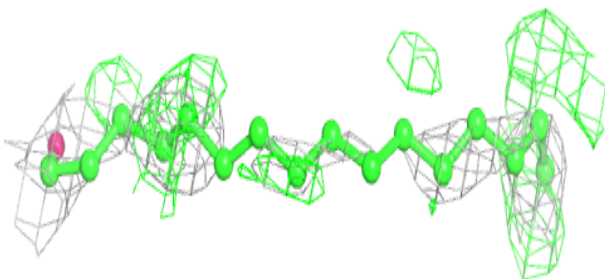
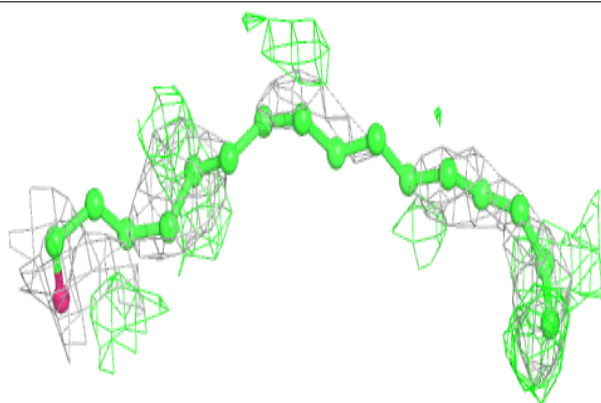
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM C 503:

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

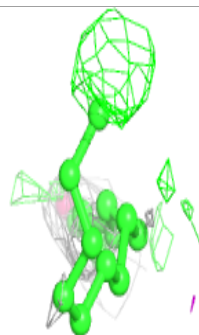
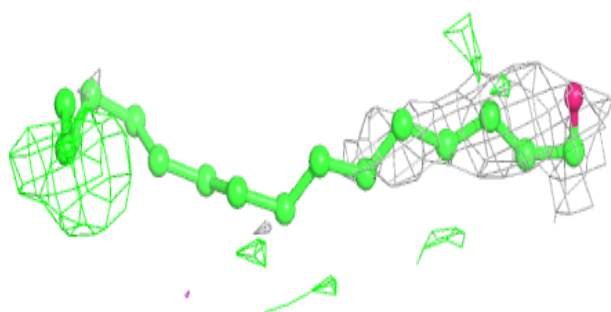
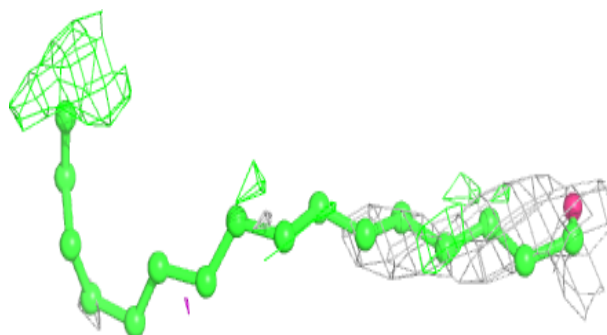
**Electron density around PLM A 502 (B):**

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

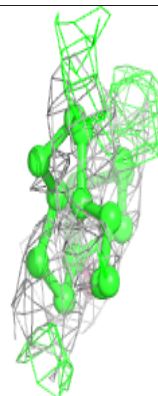
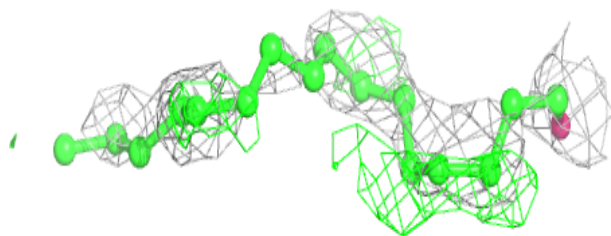
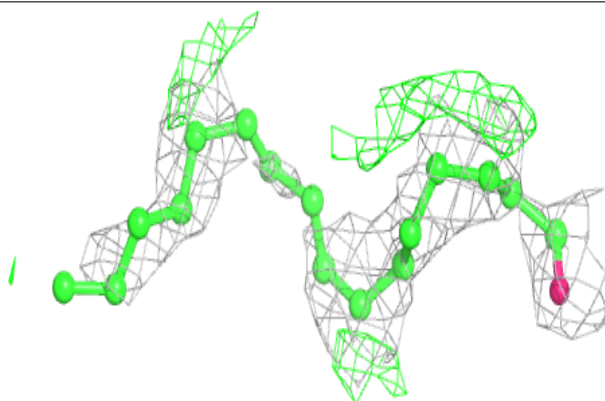


Electron density around PLM A 502 (A):

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

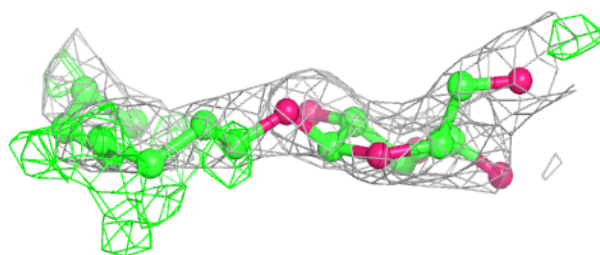
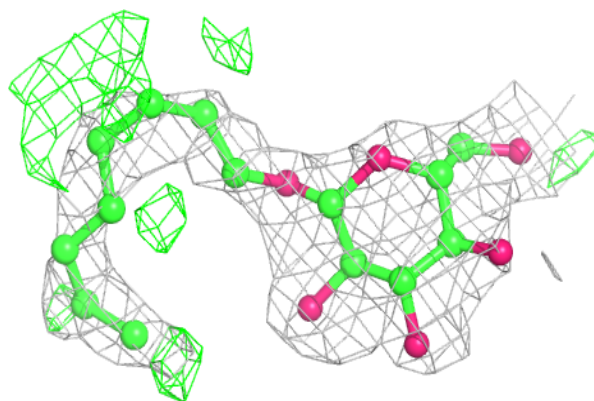
**Electron density around PLM B 505:**

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and green (positive)

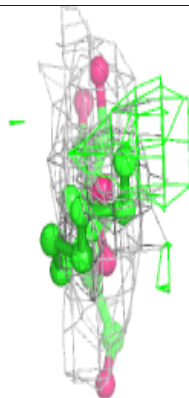
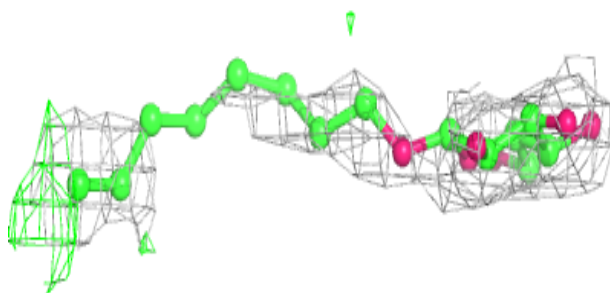
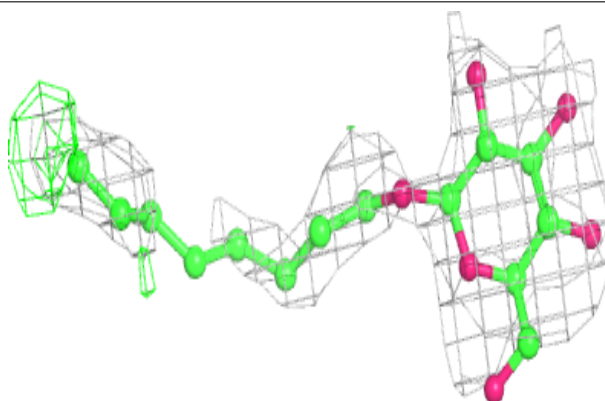


Electron density around BOG B 509:

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

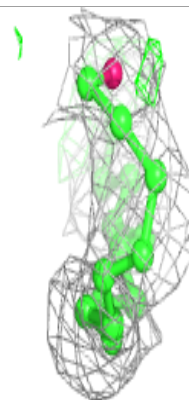
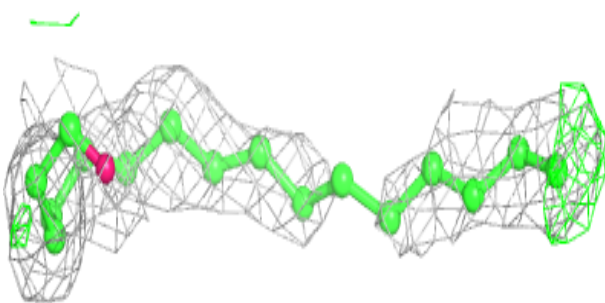
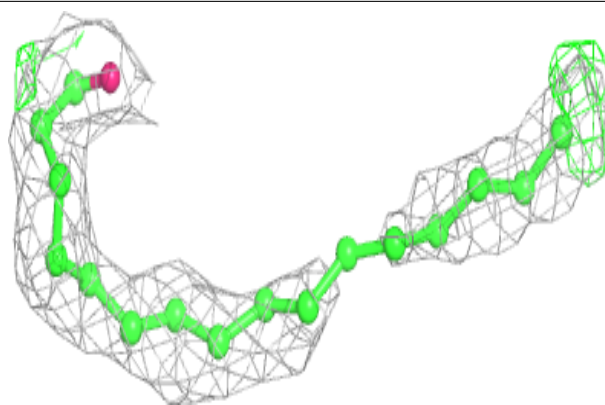
**Electron density around BOG A 509:**

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and green (positive)

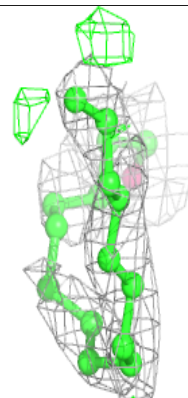
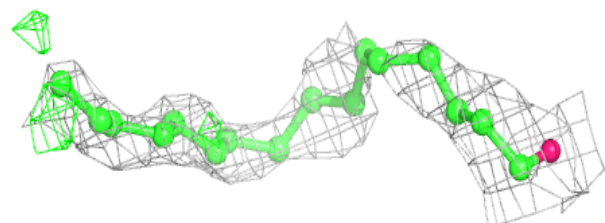
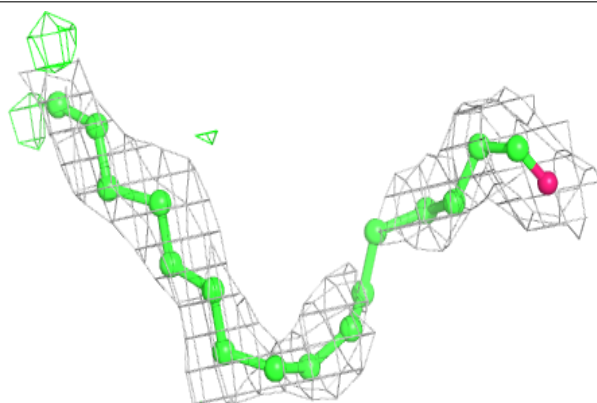


Electron density around PLM A 501:

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

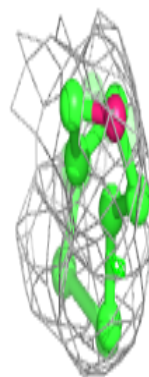
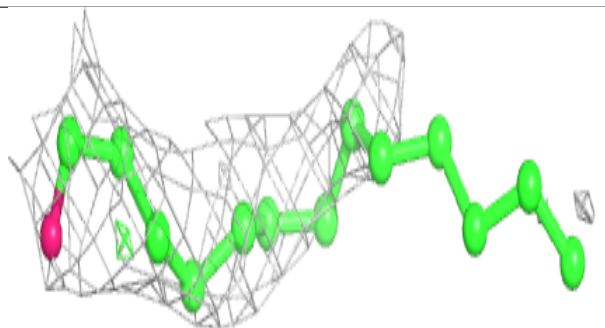
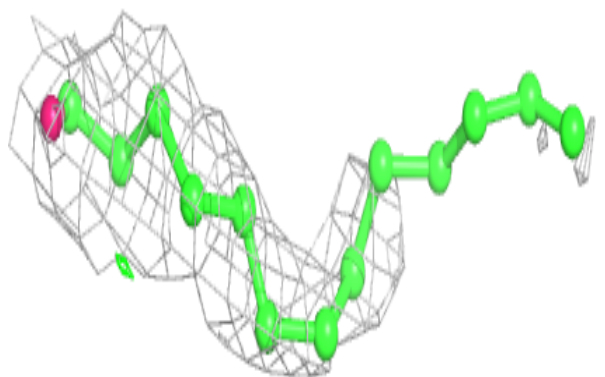
**Electron density around PLM C 502:**

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

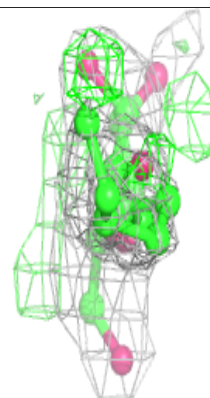
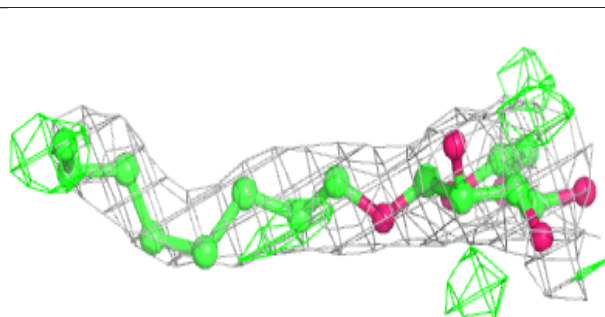
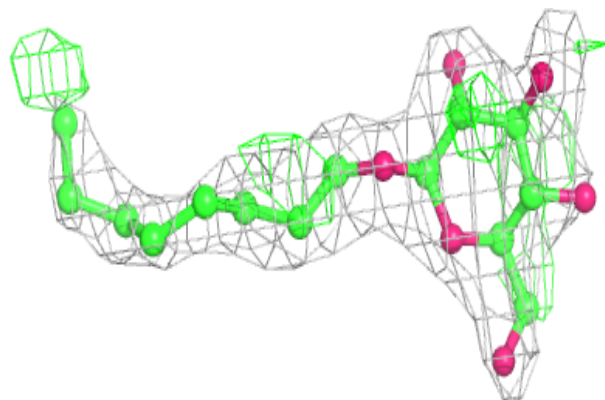


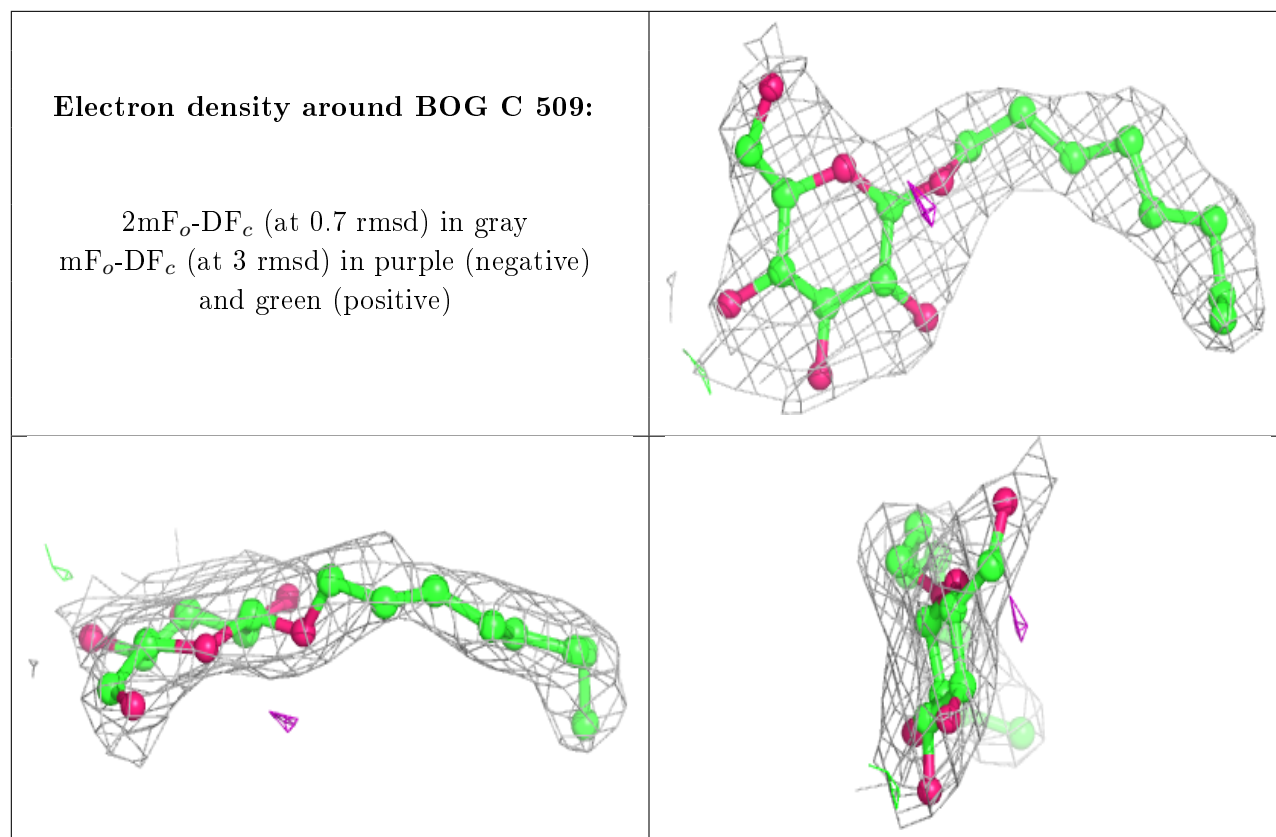
Electron density around PLM B 504:

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

**Electron density around BOG B 510:**

$2mF_o-DF_c$ (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.