



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:41 AM UTC

PDB ID : 5NSW / pdb_00005nsw
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 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	:	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

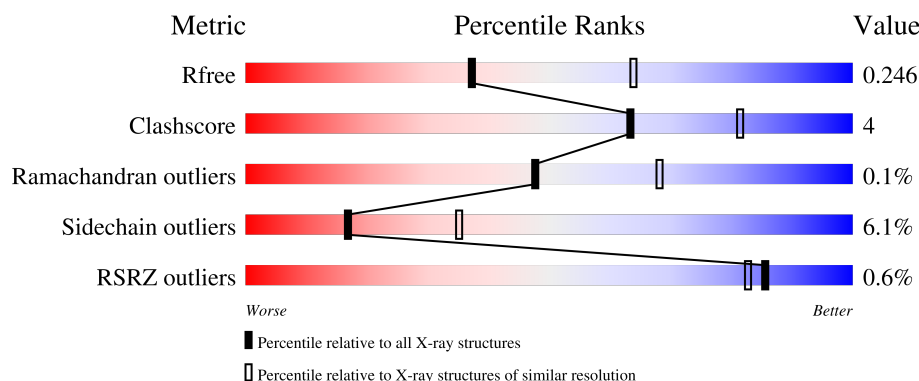
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	A	453	 88% 9% ..
1	B	453	 88% 9% ..
1	C	453	 87% 11% .

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.

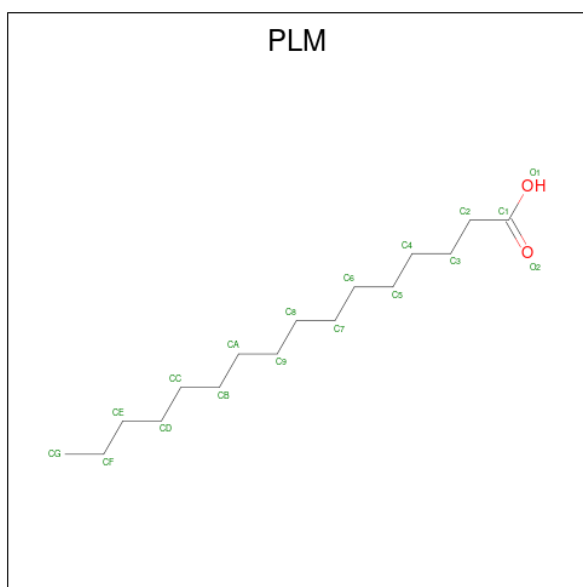
- Molecule 1 is a protein called Multidrug efflux outer membrane protein OprN.

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 (CCD ID: PLM) (formula: C₁₆H₃₂O₂).

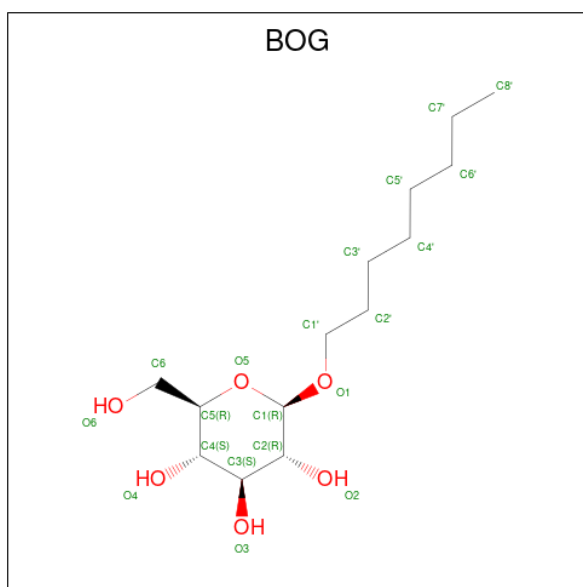


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		
2	A	1	Total	C	O	0	1
			34	32	2		
2	B	1	Total	C	O	0	0
			14	13	1		
2	B	1	Total	C	O	0	0
			17	16	1		
2	C	1	Total	C	O	0	0
			17	16	1		
2	C	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is XENON (CCD ID: XE) (formula: Xe).

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

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: 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 (CCD ID: NA) (formula: Na).

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

- Molecule 6 is NICKEL (II) ION (CCD ID: 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		

Continued on next page...

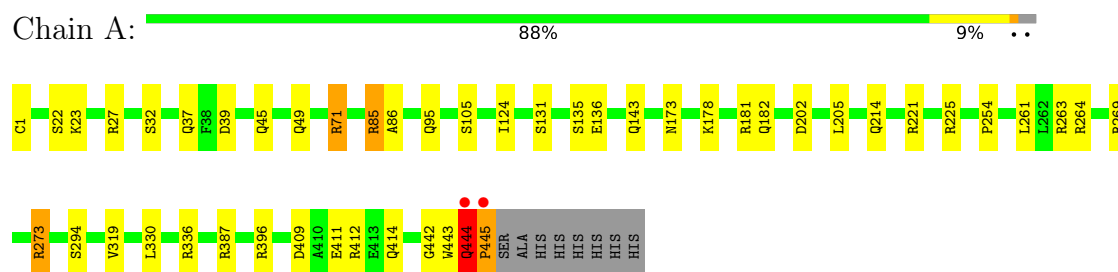
Continued from previous page...

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

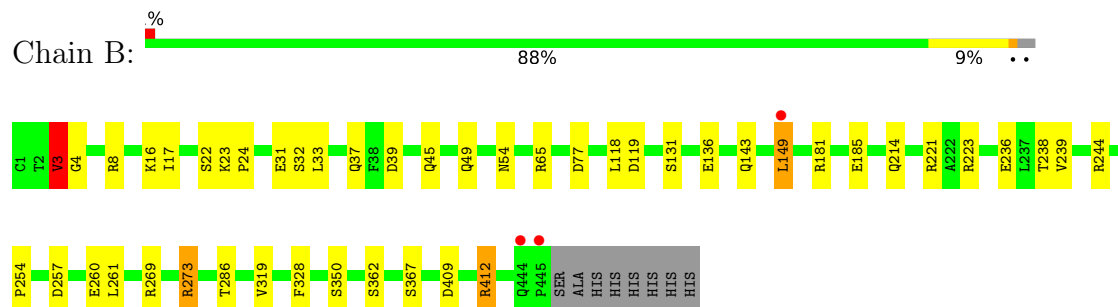
3 Residue-property plots [i](#)

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.

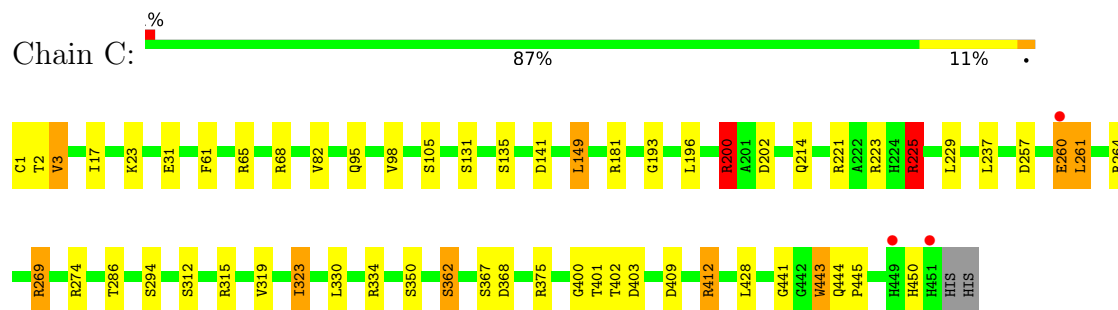
- Molecule 1: Multidrug efflux outer membrane protein OprN



- 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 49.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-2.50) 100.0 (49.42-2.50)	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 0.182 , 0.246	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)	0.33 , 45.1	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	0.93	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, NA, PLM, NI, XE

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	1.18	3/3509 (0.1%)	1.16	6/4752 (0.1%)
1	B	1.19	3/3468 (0.1%)	1.19	4/4697 (0.1%)
1	C	1.21	11/3582 (0.3%)	1.20	6/4848 (0.1%)
All	All	1.19	17/10559 (0.2%)	1.18	16/14297 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CYS	N-CA	8.21	1.61	1.46
1	C	450	HIS	CA-C	7.62	1.62	1.52
1	A	263	ARG	C-O	-6.62	1.15	1.24
1	C	2	THR	C-O	-6.04	1.16	1.24
1	C	264	ARG	C-O	-5.95	1.16	1.24
1	B	350	SER	CB-OG	-5.81	1.30	1.42
1	C	403	ASP	CB-CG	5.50	1.65	1.52
1	B	77	ASP	C-O	-5.38	1.17	1.24
1	C	441	GLY	C-O	-5.26	1.16	1.23
1	C	135	SER	CB-OG	-5.18	1.31	1.42
1	C	200	ARG	CD-NE	-5.15	1.39	1.46
1	C	1	CYS	N-CA	5.15	1.56	1.46
1	A	444	GLN	CA-C	5.14	1.59	1.52
1	C	193	GLY	N-CA	5.04	1.49	1.45
1	C	450	HIS	N-CA	5.04	1.52	1.46
1	B	236	GLU	CD-OE1	5.02	1.34	1.25
1	C	444	GLN	N-CA	5.01	1.51	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	SER	CB-CA-C	-6.40	100.83	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ARG	CG-CD-NE	5.96	125.12	112.00
1	B	65	ARG	CG-CD-NE	-5.80	99.24	112.00
1	C	362	SER	CA-CB-OG	-5.76	99.57	111.10
1	C	412	ARG	CA-CB-CG	5.74	125.58	114.10
1	C	443	TRP	CA-C-O	-5.66	115.17	121.51
1	B	3	VAL	N-CA-CB	-5.58	102.11	111.38
1	A	336	ARG	CG-CD-NE	-5.45	100.02	112.00
1	A	22	SER	CA-C-N	5.30	127.57	120.58
1	A	22	SER	C-N-CA	5.30	127.57	120.58
1	B	119	ASP	N-CA-CB	5.23	119.33	110.49
1	C	261	LEU	CA-CB-CG	5.23	134.61	116.30
1	C	225	ARG	CB-CG-CD	5.07	122.96	111.30
1	A	85	ARG	N-CA-C	5.06	116.10	108.46
1	B	412	ARG	CB-CG-CD	-5.01	99.77	111.30
1	A	330	LEU	N-CA-C	5.01	118.16	111.75

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	2	0
4	C	20	0	28	1	0
5	A	1	0	0	0	0
6	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	84	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 (84) 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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:412:ARG:HH22	1:C:409:ASP:CG	2.13	0.57
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:3:VAL:HG13	1:B:286:THR:HG22	1.90	0.52
1:B:136:GLU:HB2	1:B:273:ARG:HG3	1.92	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:C:412:ARG:HD2	7:C:625:HOH:O	2.09	0.51
1:A:37:GLN:NE2	1:A:254:PRO:CG	2.72	0.51
1:A:136:GLU:HB2	1:A:273:ARG:HG3	1.92	0.51
1:A:409:ASP:CG	1:B:412:ARG:HH22	2.18	0.51
1:B:409:ASP:CG	1:C:412:ARG:HH22	2.18	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
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:O	1:C:401:THR:HG22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:TRP:NE1	1:A:445:PRO:HB3	2.32	0.44
1:A:45[A]:GLN:HE21	1:A:49:GLN:CG	2.30	0.43
1:A:181:ARG:NH1	1:A:202:ASP:OD1	2.47	0.43
1:B:273:ARG:HA	1:B:273:ARG:HD2	1.58	0.43
1:A:173:ASN:HD21	1:A:414:GLN:HE21	1.66	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 [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	A	448/453 (99%)	440 (98%)	7 (2%)	1 (0%)	43	63
1	B	443/453 (98%)	435 (98%)	8 (2%)	0	100	100
1	C	455/453 (100%)	445 (98%)	9 (2%)	1 (0%)	43	63
All	All	1346/1359 (99%)	1320 (98%)	24 (2%)	2 (0%)	48	68

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%)	328 (94%)	22 (6%)	16	34
1	B	345/352 (98%)	324 (94%)	21 (6%)	17	35
1	C	356/352 (101%)	335 (94%)	21 (6%)	18	37
All	All	1051/1056 (100%)	987 (94%)	64 (6%)	17	35

All (64) 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	124	ILE
1	A	131	SER
1	A	135	SER
1	A	178	LYS
1	A	182	GLN
1	A	205	LEU
1	A	225	ARG
1	A	261	LEU
1	A	273	ARG
1	A	294[A]	SER
1	A	294[B]	SER
1	A	319	VAL
1	A	387	ARG
1	A	396	ARG
1	A	445	PRO
1	B	3	VAL
1	B	8	ARG
1	B	16	LYS
1	B	17	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	118	LEU
1	B	131	SER
1	B	149	LEU
1	B	223	ARG
1	B	238	THR
1	B	244	ARG
1	B	261	LEU
1	B	273	ARG
1	B	319	VAL
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	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
1	C	269	ARG
1	C	294	SER
1	C	319	VAL
1	C	323	ILE
1	C	330	LEU
1	C	350	SER
1	C	362	SER
1	C	367	SER
1	C	428	LEU

Sometimes 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	146	GLN
1	A	182	GLN
1	A	308	GLN
1	A	382	GLN
1	A	414	GLN
1	A	444	GLN
1	B	37	GLN
1	B	45	GLN
1	B	76	ASN
1	B	95	GLN
1	B	308	GLN
1	B	353	GLN
1	B	354	GLN
1	B	373	GLN
1	B	382	GLN
1	B	392	GLN
1	B	444	GLN
1	C	146	GLN
1	C	182	GLN
1	C	308	GLN
1	C	382	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	503	1	15,16,17	1.42	0	14,15,17	0.94	0
4	BOG	C	509	-	20,20,20	1.41	3 (15%)	25,25,25	1.52	4 (16%)
2	PLM	B	505	1	15,16,17	0.99	0	14,15,17	0.41	0
2	PLM	B	504	1	12,13,17	1.05	0	11,12,17	1.03	1 (9%)
2	PLM	A	501	1	15,16,17	1.59	1 (6%)	14,15,17	1.35	3 (21%)
2	PLM	A	502[B]	1	15,16,17	1.02	0	14,15,17	0.84	1 (7%)
4	BOG	B	510	-	20,20,20	1.27	4 (20%)	25,25,25	2.09	5 (20%)
2	PLM	C	502	1	15,16,17	1.38	0	14,15,17	1.09	1 (7%)
2	PLM	A	502[A]	1	15,16,17	1.11	0	14,15,17	1.12	1 (7%)
4	BOG	B	509	-	20,20,20	1.46	2 (10%)	25,25,25	1.69	7 (28%)
4	BOG	A	509	-	20,20,20	2.10	6 (30%)	25,25,25	2.91	8 (32%)

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	503	1	-	9/14/14/15	-
4	BOG	C	509	-	-	7/11/31/31	0/1/1/1
2	PLM	B	505	1	-	11/14/14/15	-
2	PLM	B	504	1	-	8/11/11/15	-
2	PLM	A	501	1	-	7/14/14/15	-
2	PLM	A	502[B]	1	-	5/14/14/15	-
4	BOG	B	510	-	-	10/11/31/31	0/1/1/1
2	PLM	C	502	1	-	10/14/14/15	-
2	PLM	A	502[A]	1	-	5/14/14/15	-
4	BOG	B	509	-	-	6/11/31/31	0/1/1/1
4	BOG	A	509	-	-	6/11/31/31	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	509	BOG	O5-C1	4.75	1.54	1.41
4	A	509	BOG	O5-C1	4.58	1.53	1.41
4	A	509	BOG	O1-C1	4.48	1.47	1.40
4	C	509	BOG	O5-C1	3.87	1.51	1.41
4	B	509	BOG	O5-C5	3.12	1.52	1.44
4	A	509	BOG	C1-C2	2.89	1.61	1.52
4	C	509	BOG	C4-C5	2.72	1.58	1.53
4	C	509	BOG	O5-C5	2.68	1.50	1.44
4	B	510	BOG	O5-C1	2.48	1.48	1.41
4	A	509	BOG	O3-C3	2.45	1.49	1.43
4	B	510	BOG	C4-C3	-2.35	1.46	1.52
4	A	509	BOG	O1-C1'	2.35	1.49	1.43
4	B	510	BOG	C3-C2	-2.30	1.46	1.52
4	B	510	BOG	O1-C1	-2.28	1.36	1.40
2	A	501	PLM	O2-C1	2.08	1.31	1.20
4	A	509	BOG	C6'-C5'	2.03	1.61	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	509	BOG	O1-C1-C2	10.42	124.09	108.27
4	A	509	BOG	C1'-O1-C1	5.49	123.05	113.68
4	B	510	BOG	O5-C5-C4	-5.21	100.30	109.70
4	B	510	BOG	O2-C2-C3	-5.00	98.60	110.38
4	B	509	BOG	C1-O5-C5	4.06	121.65	113.72
4	B	510	BOG	O5-C5-C6	3.92	116.16	106.44
4	B	510	BOG	C1-C2-C3	3.58	117.55	110.01
4	A	509	BOG	O3-C3-C2	3.55	118.75	110.38
4	C	509	BOG	O4-C4-C5	3.50	117.94	109.32
4	A	509	BOG	C4-C3-C2	-3.49	104.71	110.83
4	A	509	BOG	O2-C2-C1	3.48	118.36	110.08
4	C	509	BOG	O1-C1-C2	3.29	113.27	108.27
4	B	510	BOG	C1-O5-C5	-3.27	107.33	113.72
4	C	509	BOG	C5'-C4'-C3'	-3.07	98.86	114.37
2	A	502[A]	PLM	O2-C1-C2	-3.06	100.70	126.30
4	B	509	BOG	O5-C5-C4	3.05	115.19	109.70
2	B	504	PLM	O2-C1-C2	-2.80	102.89	126.30
4	A	509	BOG	O5-C1-C2	-2.74	104.75	110.37
2	A	501	PLM	O2-C1-C2	-2.74	103.41	126.30
4	B	509	BOG	O2-C2-C3	2.69	116.72	110.38
2	A	502[B]	PLM	O2-C1-C2	-2.67	103.99	126.30
4	B	509	BOG	C6-C5-C4	-2.59	106.67	113.02
2	A	501	PLM	CC-CB-CA	2.53	127.14	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	509	BOG	O5-C5-C4	2.51	114.23	109.70
2	C	502	PLM	O2-C1-C2	-2.42	106.04	126.30
4	C	509	BOG	C1-O5-C5	2.40	118.41	113.72
4	B	509	BOG	C4-C3-C2	-2.40	106.61	110.83
4	A	509	BOG	O1-C1'-C2'	2.24	116.96	109.37
4	B	509	BOG	O5-C5-C6	2.20	111.89	106.44
2	A	501	PLM	CA-C9-C8	2.19	125.44	114.37
4	B	509	BOG	O5-C1-O1	2.10	115.01	110.04

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	504	PLM	O2-C1-C2-C3
2	B	505	PLM	O2-C1-C2-C3
2	C	502	PLM	O2-C1-C2-C3
4	B	510	BOG	O5-C5-C6-O6
4	C	509	BOG	O5-C5-C6-O6
4	B	510	BOG	C4-C5-C6-O6
2	A	502[A]	PLM	CB-CC-CD-CE
4	B	509	BOG	C2-C1-O1-C1'
4	B	510	BOG	C2-C1-O1-C1'
4	C	509	BOG	C2-C1-O1-C1'
4	B	509	BOG	O5-C1-O1-C1'
4	B	510	BOG	O5-C1-O1-C1'
4	C	509	BOG	O5-C1-O1-C1'
4	C	509	BOG	C4-C5-C6-O6
2	A	501	PLM	C3-C4-C5-C6
2	A	502[A]	PLM	CC-CD-CE-CF
4	B	510	BOG	C2'-C1'-O1-C1
2	B	504	PLM	C7-C8-C9-CA
4	A	509	BOG	C1'-C2'-C3'-C4'
2	B	504	PLM	C6-C7-C8-C9
2	A	502[B]	PLM	C6-C7-C8-C9
2	C	502	PLM	C7-C8-C9-CA
2	C	502	PLM	C4-C5-C6-C7
2	A	502[A]	PLM	C7-C8-C9-CA
4	B	510	BOG	C1'-C2'-C3'-C4'
2	A	502[B]	PLM	C2-C3-C4-C5
2	B	505	PLM	C5-C6-C7-C8
4	A	509	BOG	C2-C1-O1-C1'
2	B	505	PLM	CA-CB-CC-CD

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

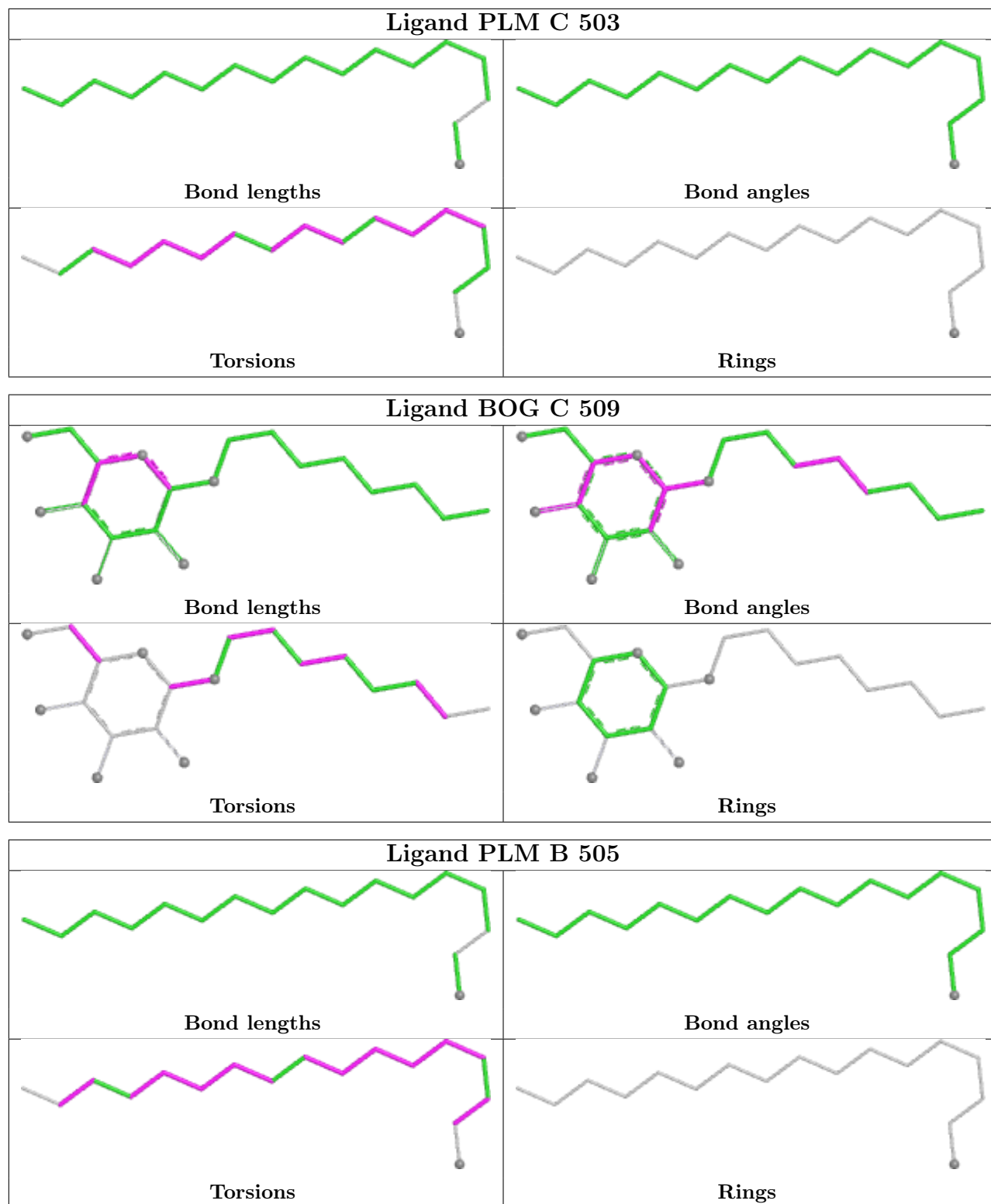
Mol	Chain	Res	Type	Atoms
2	B	505	PLM	CB-CC-CD-CE
2	A	501	PLM	C6-C7-C8-C9
2	C	503	PLM	C7-C8-C9-CA
4	A	509	BOG	C4'-C5'-C6'-C7'
2	B	505	PLM	CD-CE-CF-CG
2	C	502	PLM	CD-CE-CF-CG
4	B	510	BOG	C3'-C4'-C5'-C6'
2	A	502[A]	PLM	C9-CA-CB-CC
4	A	509	BOG	O5-C1-O1-C1'
2	A	501	PLM	C5-C6-C7-C8
2	A	502[A]	PLM	CD-CE-CF-CG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

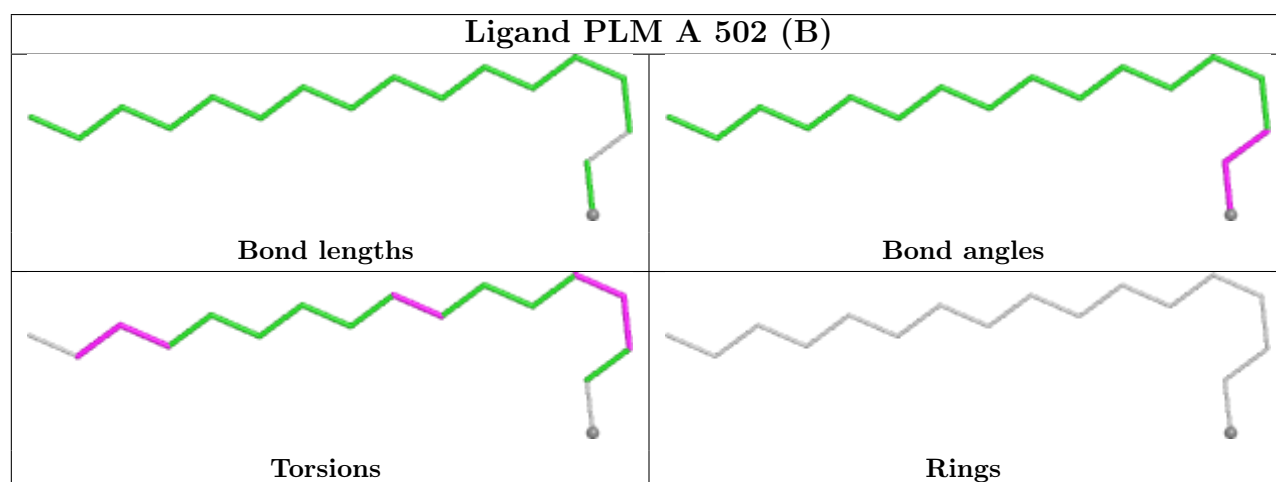
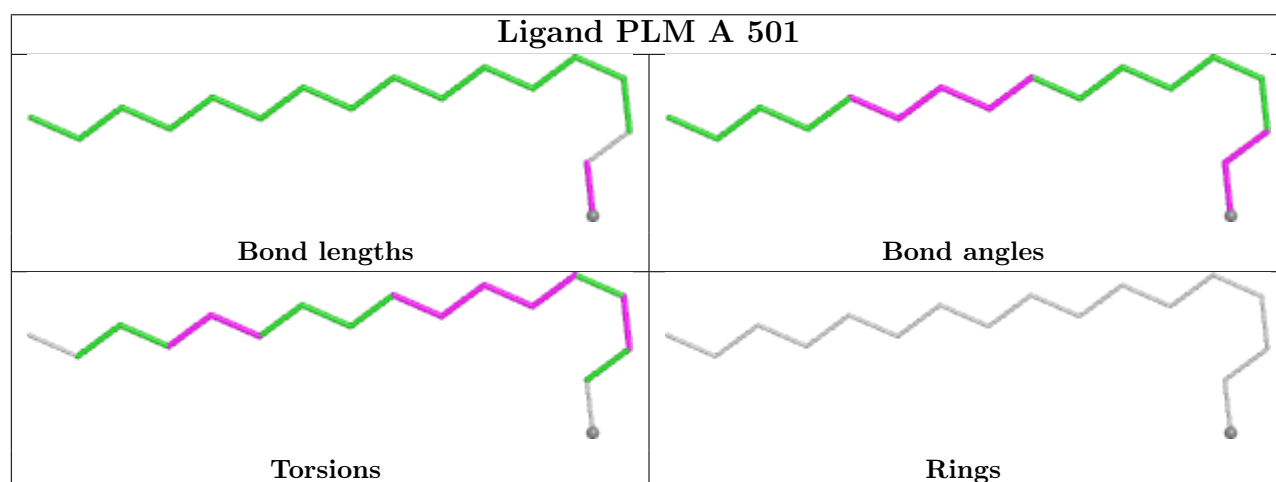
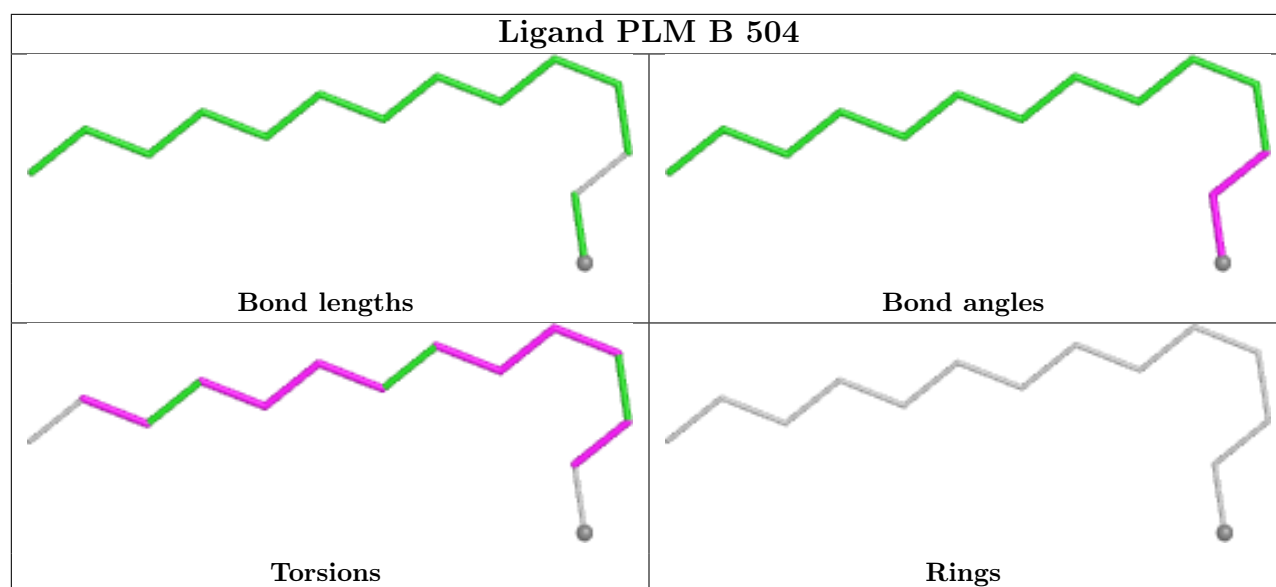
There are no ring outliers.

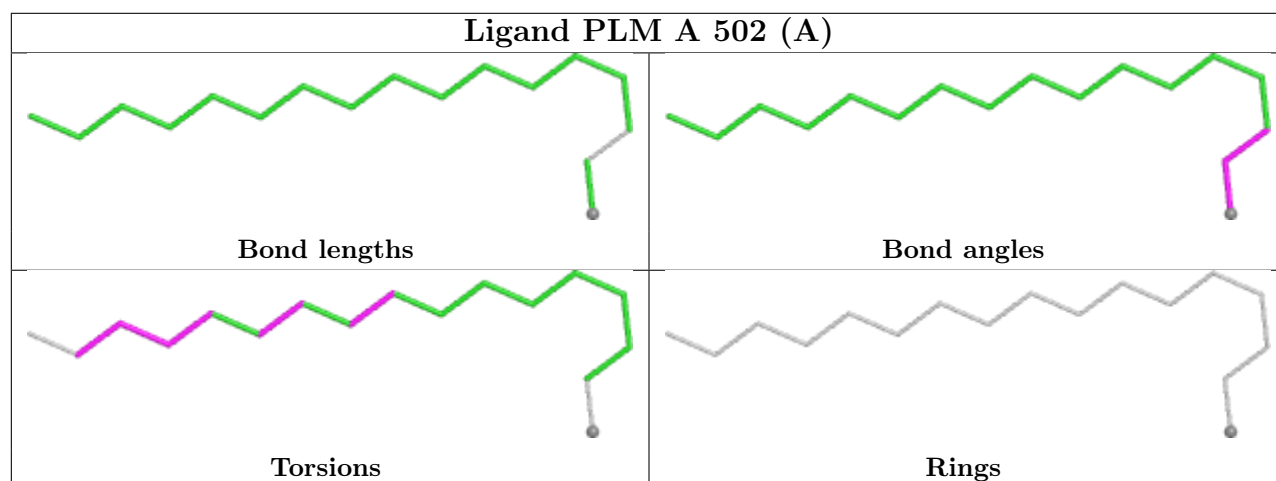
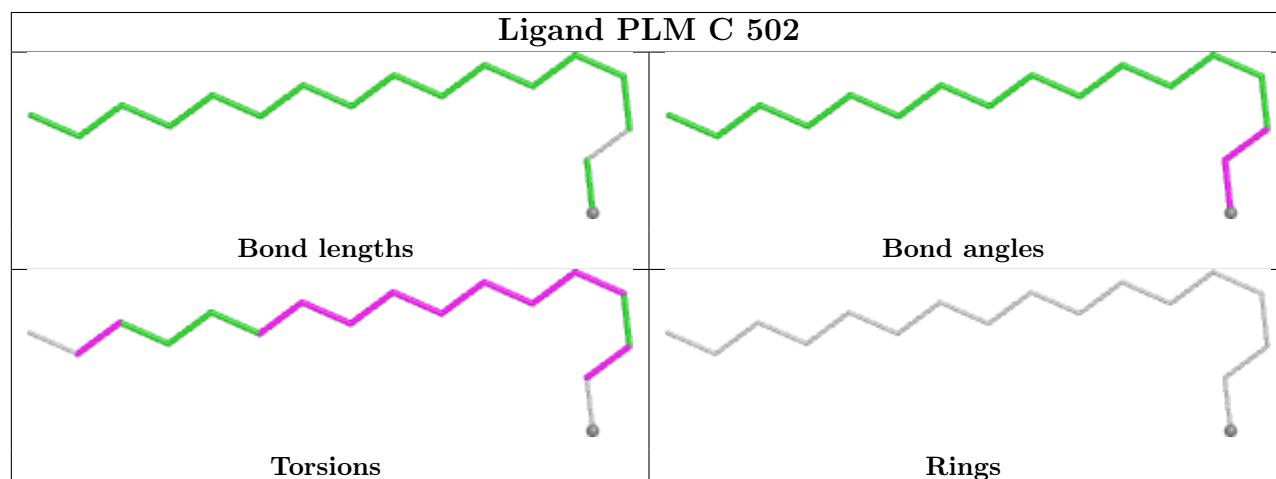
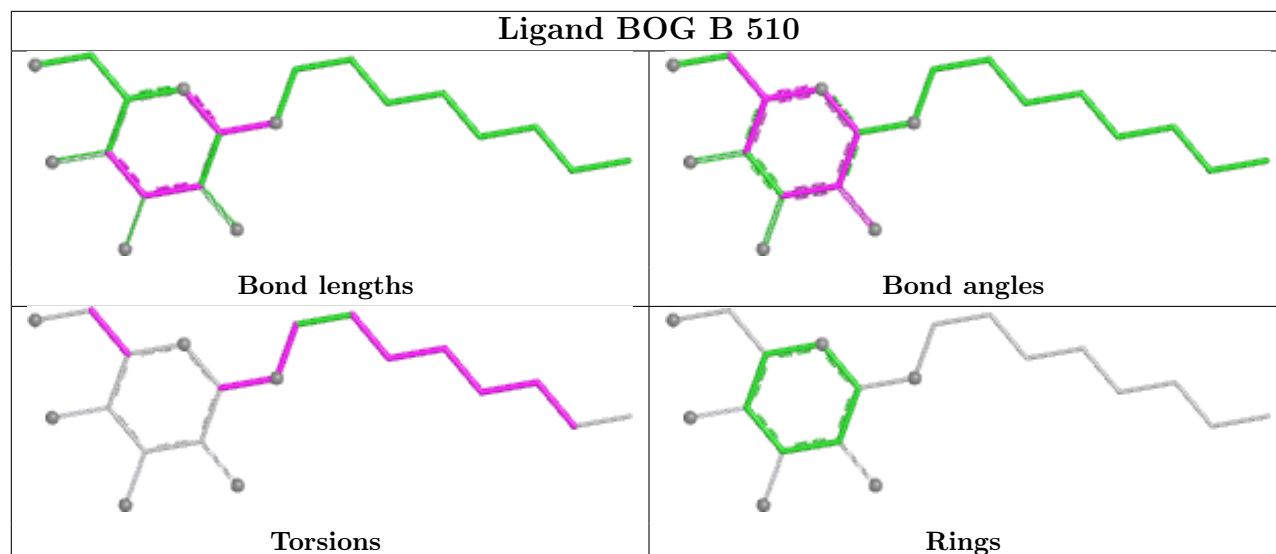
4 monomers are involved in 5 short contacts:

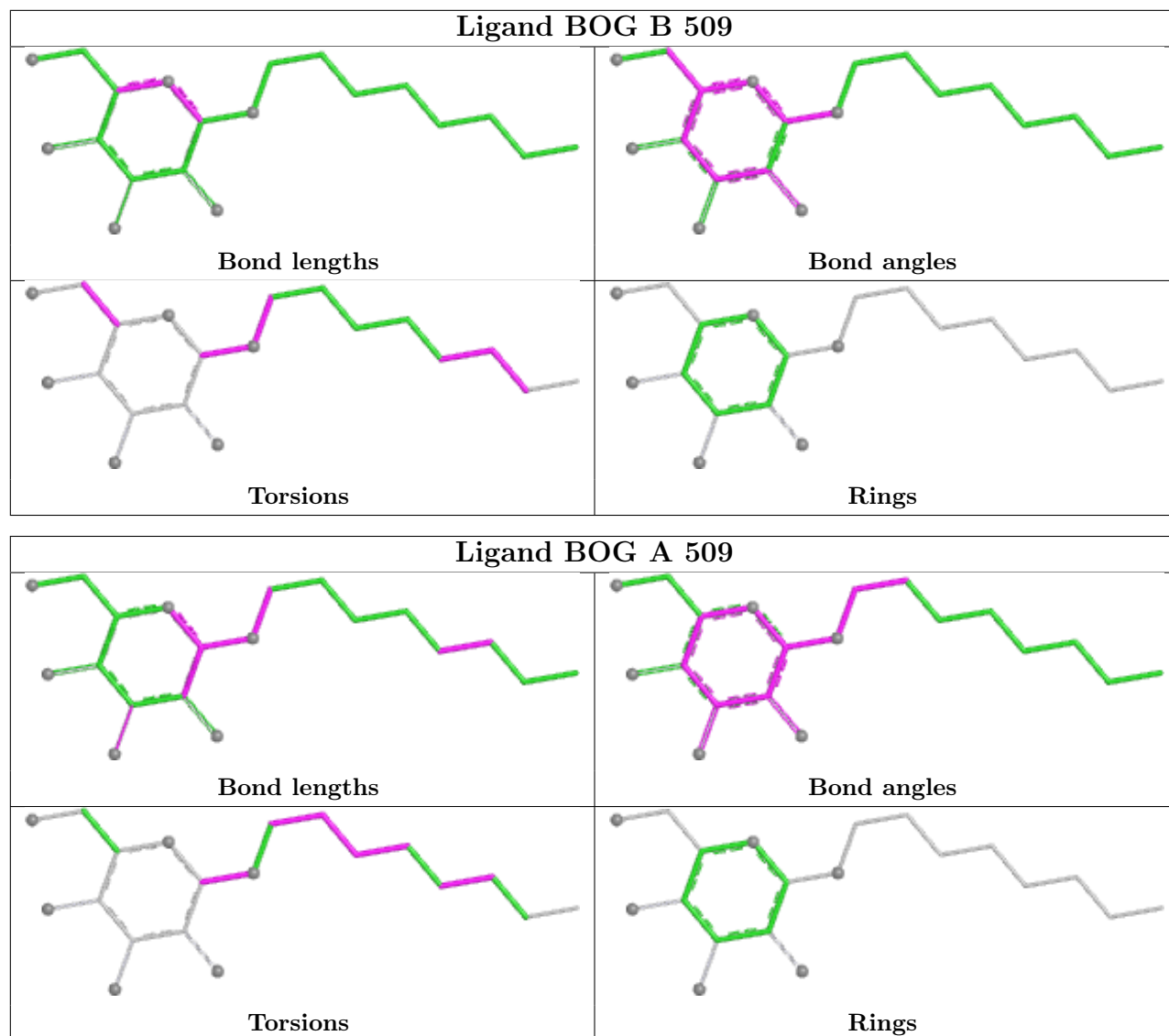
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	509	BOG	1	0
2	C	502	PLM	1	0
2	A	502[A]	PLM	1	0
4	B	509	BOG	2	0

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	A	445/453 (98%)	-0.53	2 (0%)	88 86	17, 37, 64, 112	5 (1%)
1	B	445/453 (98%)	-0.51	3 (0%)	84 81	24, 36, 65, 98	0
1	C	451/453 (99%)	-0.51	3 (0%)	84 81	16, 37, 70, 98	6 (1%)
All	All	1341/1359 (98%)	-0.51	8 (0%)	85 83	16, 37, 67, 112	11 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	451	HIS	4.5
1	B	445	PRO	3.9
1	C	449	HIS	3.2
1	B	444	GLN	2.5
1	A	444	GLN	2.2
1	B	149	LEU	2.2
1	A	445	PRO	2.1
1	C	260	GLU	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,

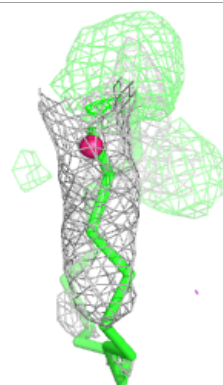
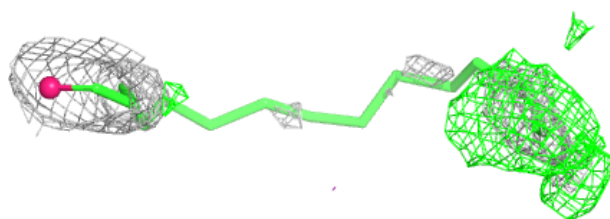
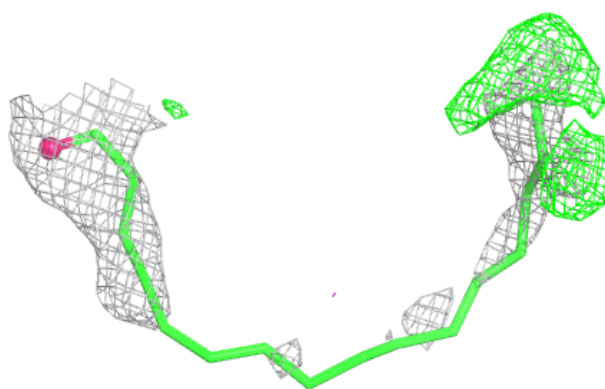
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLM	C	503	17/18	0.78	0.31	71,84,96,96	0
2	PLM	B	505	17/18	0.79	0.34	76,91,103,103	0
2	PLM	A	502[A]	17/18	0.81	0.41	41,52,67,67	17
2	PLM	A	502[B]	17/18	0.81	0.41	40,52,56,56	17
2	PLM	C	502	17/18	0.85	0.24	65,78,88,88	0
4	BOG	A	509	20/20	0.86	0.21	50,77,99,100	0
2	PLM	A	501	17/18	0.88	0.21	49,60,85,97	0
2	PLM	B	504	14/18	0.89	0.24	73,82,98,98	0
4	BOG	B	509	20/20	0.89	0.21	27,43,47,48	20
4	BOG	B	510	20/20	0.92	0.17	32,38,48,50	20
3	XE	B	507	1/1	0.95	0.14	51,51,51,51	1
3	XE	A	507	1/1	0.96	0.11	57,57,57,57	1
3	XE	C	507	1/1	0.97	0.10	54,54,54,54	1
3	XE	C	501	1/1	0.97	0.09	66,66,66,66	1
4	BOG	C	509	20/20	0.97	0.09	44,58,65,65	0
3	XE	B	503	1/1	0.98	0.08	67,67,67,67	1
3	XE	C	508	1/1	0.98	0.19	53,53,53,53	1
3	XE	A	506	1/1	0.98	0.06	60,60,60,60	1
3	XE	A	504	1/1	0.98	0.06	67,67,67,67	1
3	XE	C	505	1/1	0.98	0.06	64,64,64,64	1
3	XE	C	506	1/1	0.98	0.10	56,56,56,56	1
3	XE	B	506	1/1	0.99	0.04	63,63,63,63	1
3	XE	A	508	1/1	0.99	0.15	65,65,65,65	1
3	XE	B	508	1/1	0.99	0.12	58,58,58,58	1
3	XE	B	501	1/1	0.99	0.03	73,73,73,73	1
3	XE	B	502	1/1	0.99	0.09	60,60,60,60	1
3	XE	A	505	1/1	0.99	0.13	63,63,63,63	1
5	NA	A	510	1/1	0.99	0.04	45,45,45,45	0
3	XE	A	503	1/1	1.00	0.11	55,55,55,55	0
6	NI	C	504	1/1	1.00	0.06	57,57,57,57	0

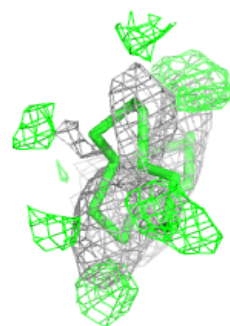
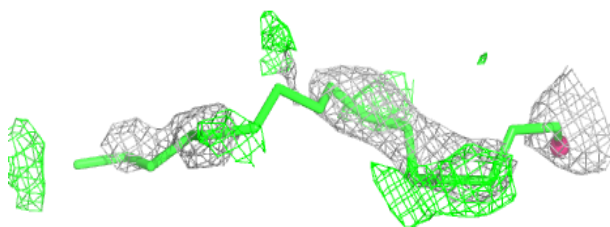
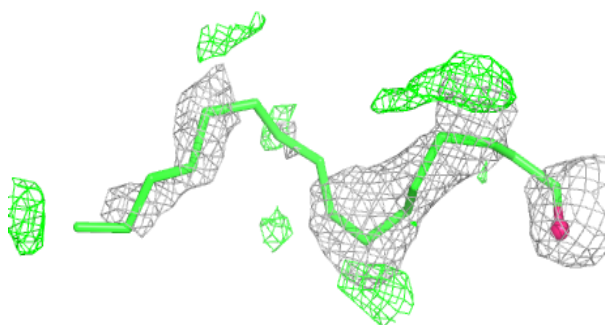
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

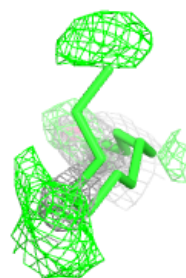
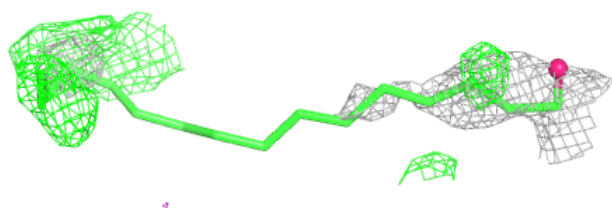
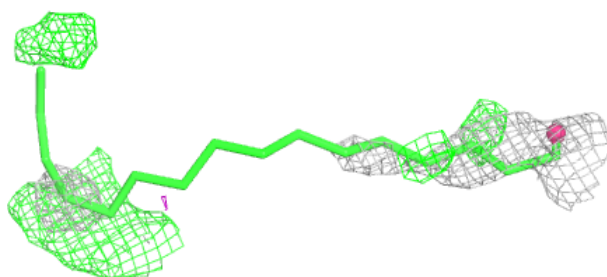
**Electron density around PLM B 505:**

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

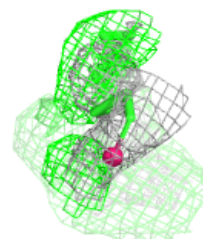
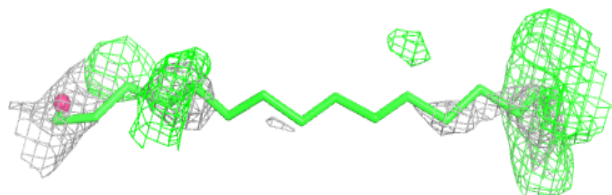
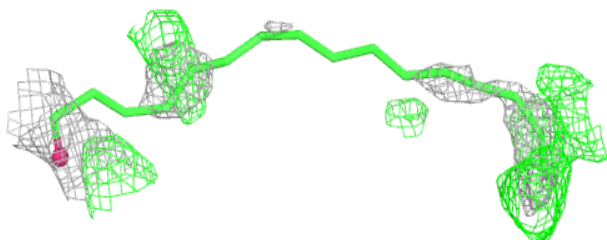


Electron density around PLM A 502 (A):

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

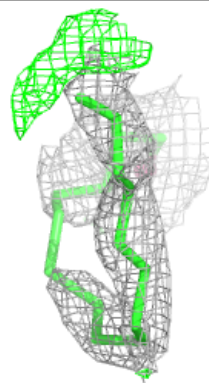
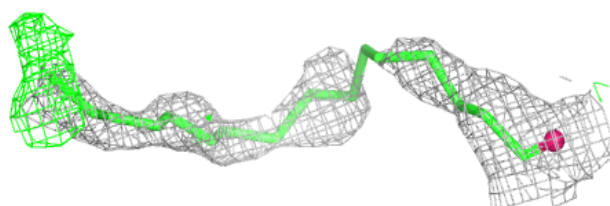
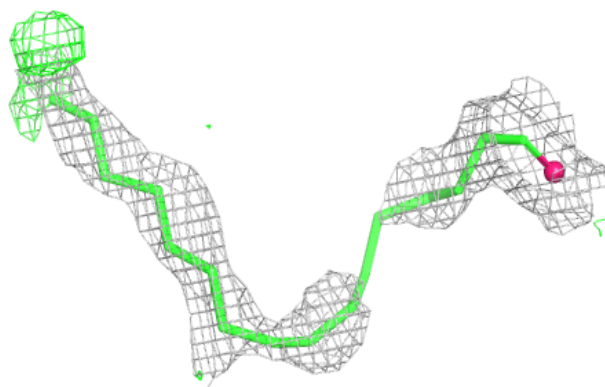
**Electron density around PLM A 502 (B):**

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

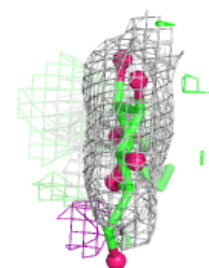
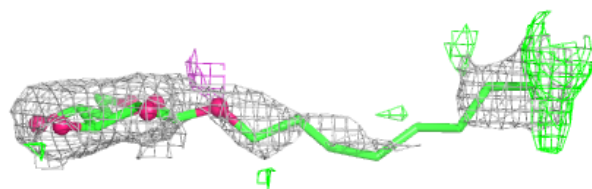
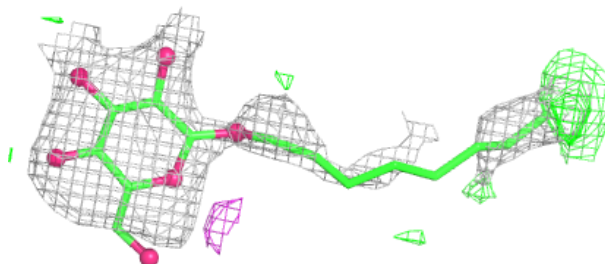


Electron density around PLM C 502:

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

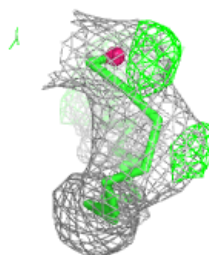
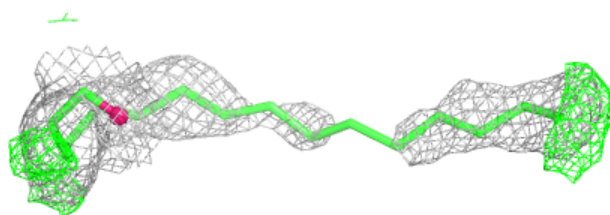
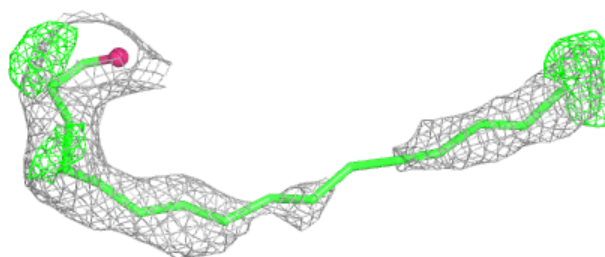
**Electron density around BOG A 509:**

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

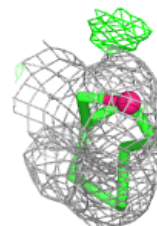
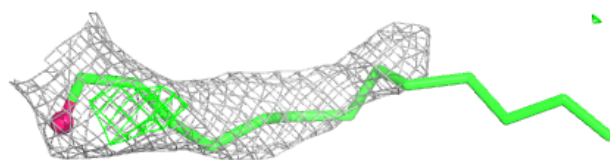
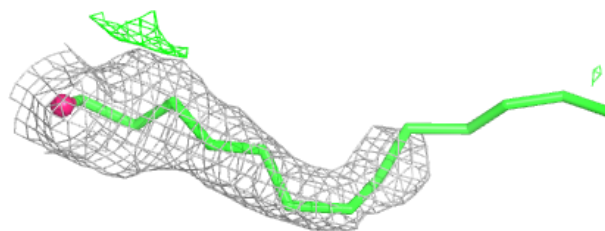


Electron density around PLM A 501:

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

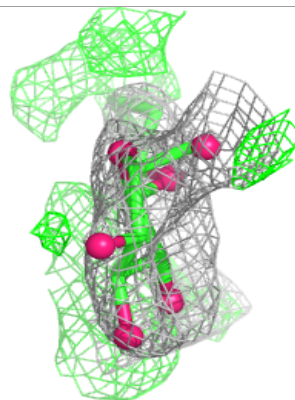
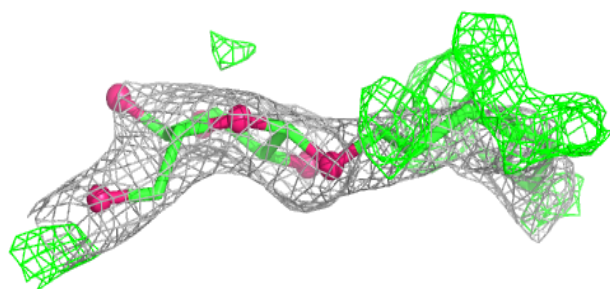
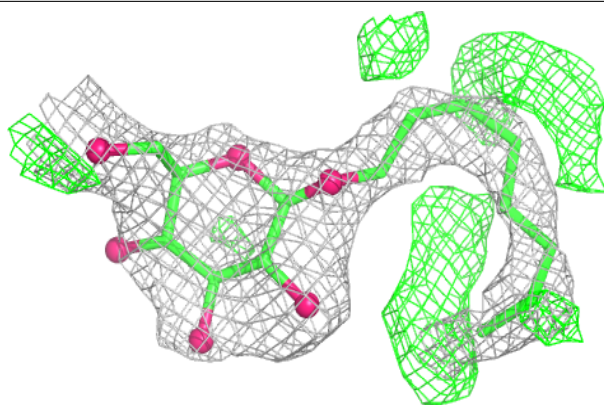
**Electron density around PLM B 504:**

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

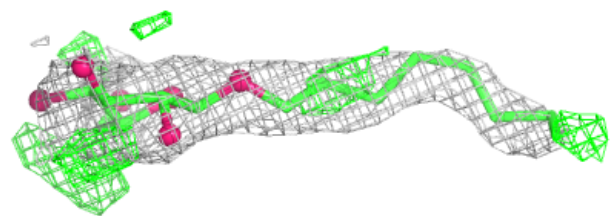
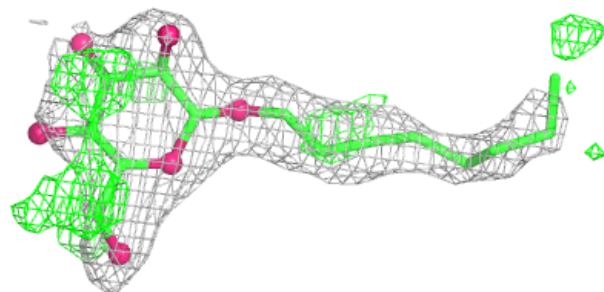


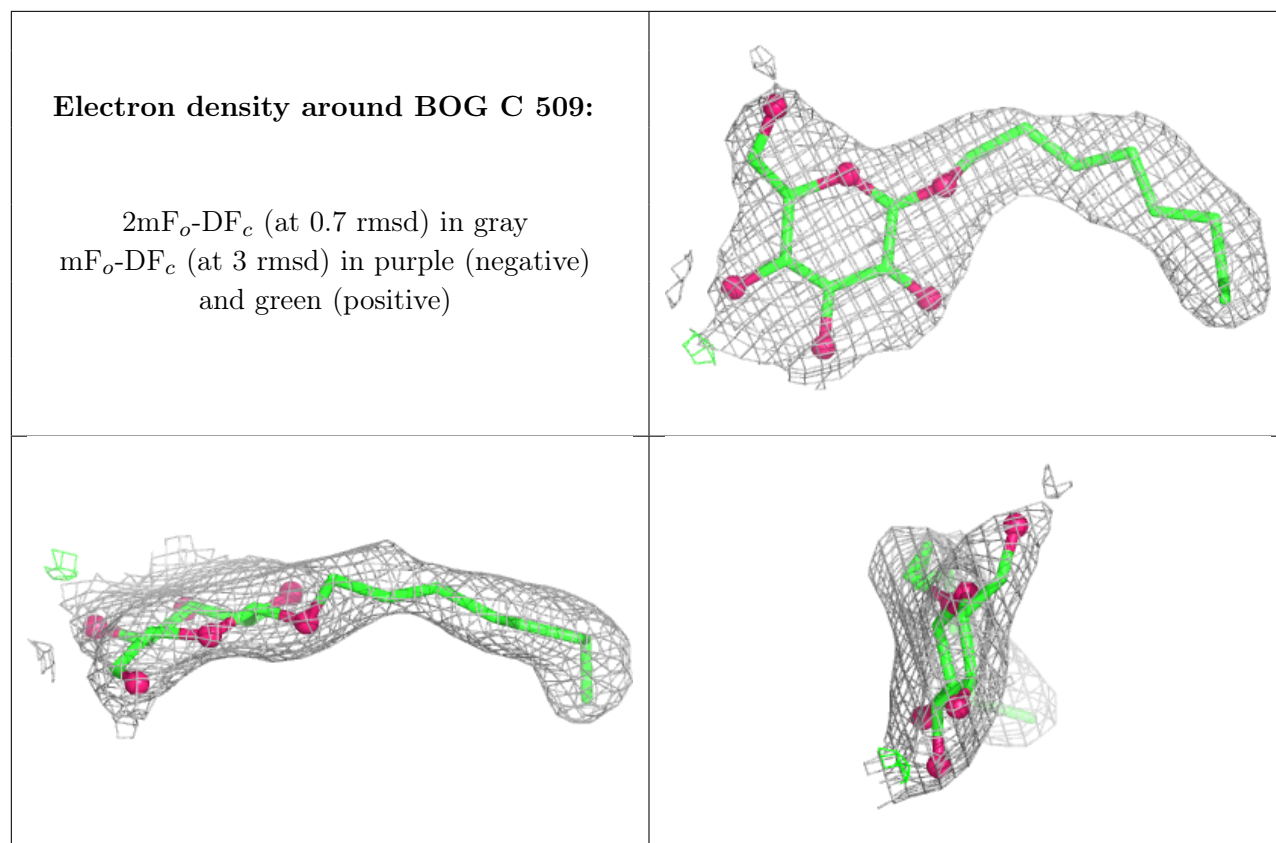
Electron density around BOG B 509:

$2mF_o-DF_c$ (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.