



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:50 PM BST

PDB ID : 5IUJ  
Title : Structural insights of the outer-membrane channel OprN  
Authors : Ntsogo, Y.; Garnier, C.; Phan, G.; Monlezun, L.; Benas, P.; Broutin, I.  
Deposited on : 2016-03-18  
Resolution : 2.29 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](mailto: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.

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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

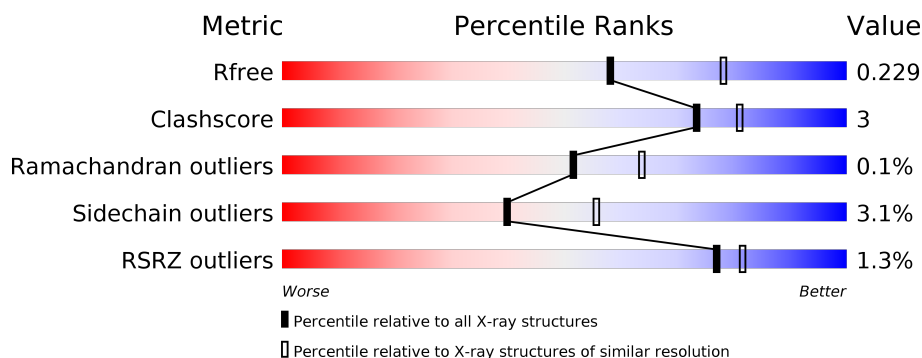
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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>%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	453	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	C	453	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11176 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.

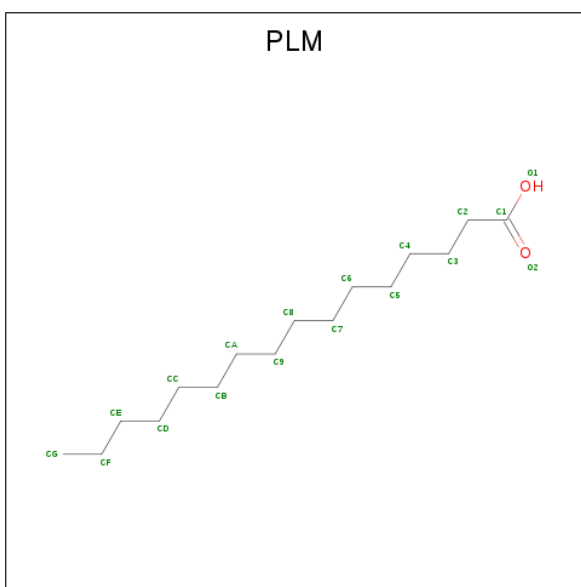
- Molecule 1 is a protein called Multidrug efflux outer membrane protein OprN.

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: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).

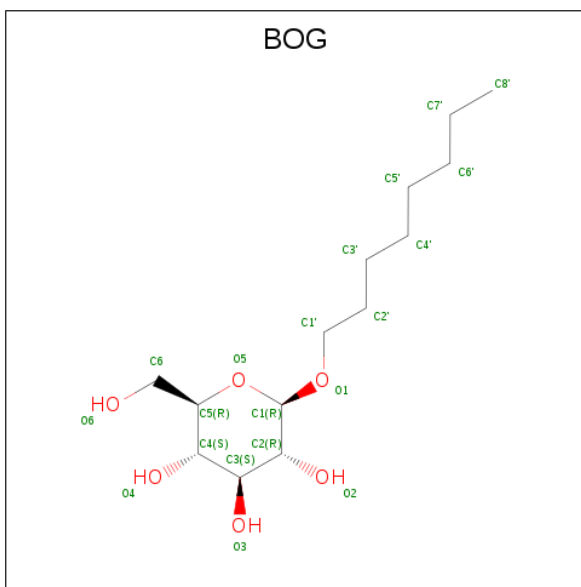


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C	O	0	0
			6	5	1		
2	B	1	Total	C	O	0	0
			8	7	1		
2	C	1	Total	C	O	0	0
			11	10	1		
2	C	1	Total	C	O	0	0
			6	5	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



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	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	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		

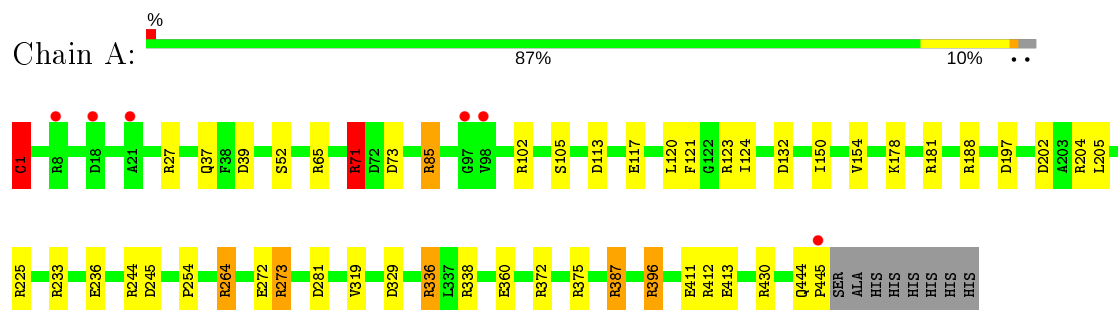
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	208	Total	O	0	0
			208	208		
7	B	240	Total	O	0	0
			240	240		
7	C	233	Total	O	0	0
			233	233		

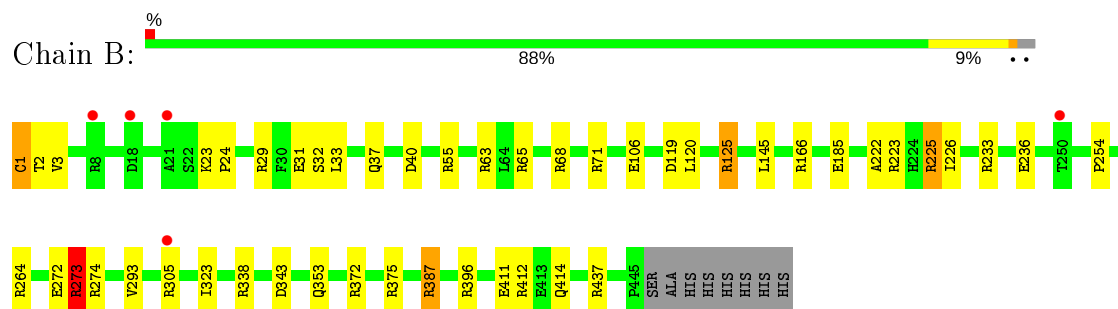
### 3 Residue-property plots [i](#)

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.

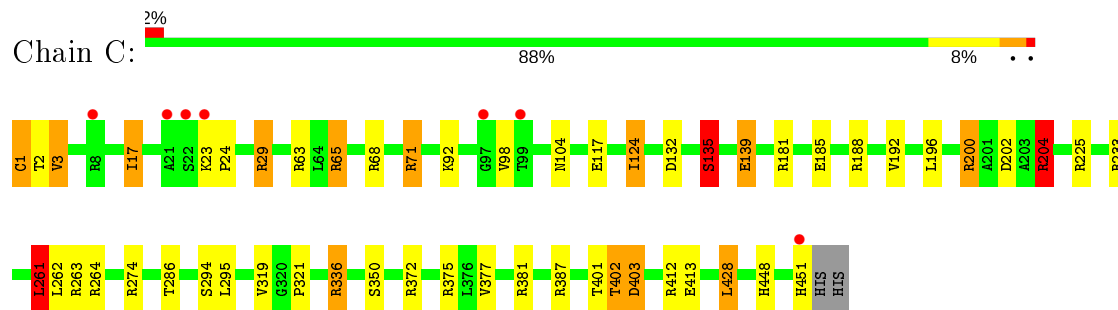
- Molecule 1: Multidrug efflux outer membrane protein OprN



- 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, $\alpha$ , $\beta$ , $\gamma$	257.65Å 257.65Å 81.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.18 – 2.29 49.59 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.4 (182.18-2.29) 99.4 (49.59-2.29)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.188 , 0.225 0.196 , 0.229	Depositor DCC
$R_{free}$ test set	6012 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, FMT, BOG, PLM, CL

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	0.99	6/3509 (0.2%)	1.27	39/4752 (0.8%)
1	B	1.04	4/3468 (0.1%)	1.28	39/4697 (0.8%)
1	C	1.06	7/3582 (0.2%)	1.17	27/4848 (0.6%)
All	All	1.03	17/10559 (0.2%)	1.24	105/14297 (0.7%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	CYS	C-N	18.48	1.76	1.34
1	B	1	CYS	C-N	14.88	1.68	1.34
1	A	1	CYS	C-N	10.84	1.58	1.34
1	B	236	GLU	CD-OE1	10.01	1.36	1.25
1	C	403	ASP	CB-CG	6.84	1.66	1.51
1	C	350	SER	CB-OG	-6.81	1.33	1.42
1	C	135	SER	CB-OG	-6.36	1.33	1.42
1	A	411	GLU	CD-OE1	5.90	1.32	1.25
1	A	1	CYS	CB-SG	-5.90	1.72	1.81
1	B	185	GLU	CD-OE2	5.89	1.32	1.25
1	C	139	GLU	N-CA	5.86	1.58	1.46
1	A	338	ARG	CD-NE	-5.80	1.36	1.46
1	C	413	GLU	CD-OE2	5.72	1.31	1.25
1	C	200	ARG	CD-NE	-5.63	1.36	1.46
1	A	338	ARG	CZ-NH2	-5.41	1.26	1.33
1	B	411	GLU	CD-OE1	5.30	1.31	1.25
1	A	236	GLU	CD-OE1	5.10	1.31	1.25

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ARG	NE-CZ-NH2	-22.05	109.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	CYS	O-C-N	-19.84	90.95	122.70
1	B	225	ARG	NE-CZ-NH2	-18.89	110.86	120.30
1	A	338	ARG	NE-CZ-NH1	16.43	128.51	120.30
1	A	65	ARG	NE-CZ-NH2	-15.03	112.78	120.30
1	B	65	ARG	NE-CZ-NH2	-14.62	112.99	120.30
1	B	387	ARG	NE-CZ-NH2	-14.61	112.99	120.30
1	C	200	ARG	NE-CZ-NH2	-14.31	113.15	120.30
1	B	225	ARG	NE-CZ-NH1	13.39	127.00	120.30
1	B	387	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	B	65	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	A	65	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	B	338	ARG	NE-CZ-NH2	-12.05	114.27	120.30
1	A	336	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	B	338	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	C	387	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	273	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	C	412	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	A	336	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	C	387	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	C	412	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	71	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	B	273	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	412	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	C	372	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	412	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	C	200	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	B	63	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	C	261	LEU	CA-CB-CG	8.45	134.72	115.30
1	C	1	CYS	N-CA-CB	-8.28	95.70	110.60
1	A	387	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	273	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	273	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	387	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	375	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	A	412	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	1	CYS	CA-CB-SG	-7.53	100.45	114.00
1	A	1	CYS	C-N-CA	-7.43	103.11	121.70
1	A	396	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	396	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	B	63	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	375	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	225	ARG	CD-NE-CZ	6.93	133.31	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	233	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	63	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	396	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	336	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	73	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	C	65[A]	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	C	65[B]	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	B	29	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	372	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	274	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	85	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	85	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	123	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	204	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	396	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	336	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	372	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	387	ARG	CD-NE-CZ	6.16	132.22	123.60
1	B	412	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	71	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	166	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	233	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	65	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	264	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	197	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	430	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	338	ARG	CG-CD-NE	-5.88	99.45	111.80
1	B	40	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	245	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	1	CYS	CA-CB-SG	5.78	124.40	114.00
1	B	1	CYS	N-CA-CB	-5.77	100.21	110.60
1	C	188	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	375	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	1	CYS	C-N-CA	5.70	135.94	121.70
1	C	1	CYS	N-CA-C	-5.63	95.79	111.00
1	B	437	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	73	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	233	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	343	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	65	ARG	CG-CD-NE	-5.50	100.24	111.80
1	A	188	ARG	NE-CZ-NH1	5.50	123.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	274	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	263	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	281	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	102	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	55	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	139	GLU	N-CA-C	-5.35	96.55	111.00
1	B	233	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	338	ARG	CD-NE-CZ	5.28	130.99	123.60
1	B	264	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	1	CYS	O-C-N	-5.26	114.28	122.70
1	C	261	LEU	CB-CG-CD2	5.20	119.83	111.00
1	C	71	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	264	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	197	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	329	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	68	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	375	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	65	ARG	CD-NE-CZ	5.09	130.73	123.60
1	C	428	LEU	CA-CB-CG	5.06	126.95	115.30

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	3424	19	0
1	B	3420	0	3392	22	0
1	C	3515	0	3489	29	0
2	A	15	0	18	2	0
2	B	8	0	10	1	0
2	C	17	0	22	0	0
3	A	1	0	0	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	20	0	28	0	0
5	B	1	0	0	0	0
6	B	3	0	1	0	0
7	A	208	0	0	5	0
7	B	240	0	0	2	0
7	C	233	0	0	6	0
All	All	11176	0	10440	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (69) 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:1:CYS:C	1:B:2:THR:N	1.68	1.45
1:C:1:CYS:C	1:C:2:THR:N	1.76	1.37
1:C:181[B]:ARG:NH1	1:C:185:GLU:OE1	2.12	0.83
1:B:1:CYS:O	1:B:2:THR:N	2.12	0.81
1:A:37:GLN:HE22	1:A:254:PRO:HD2	1.48	0.78
1:B:223:ARG:HD3	7:B:779:HOH:O	1.83	0.78
1:C:377:VAL:HG12	1:C:381:ARG:NH1	2.00	0.77
1:B:23:LYS:HG3	1:B:24:PRO:HD3	1.65	0.77
1:A:37:GLN:HE22	1:A:254:PRO:CD	2.01	0.73
1:A:71:ARG:HD2	1:A:132:ASP:OD1	1.89	0.72
1:C:377:VAL:HG12	1:C:381:ARG:HH12	1.58	0.68
1:B:119:ASP:O	1:B:125:ARG:NH2	2.29	0.66
1:B:23:LYS:HG3	1:B:24:PRO:CD	2.27	0.64
1:B:1:CYS:HB3	1:B:120:LEU:O	1.97	0.64
1:C:139:GLU:OE2	1:C:448:HIS:CE1	2.50	0.63
1:C:68:ARG:HD2	1:C:135:SER:OG	2.02	0.60
1:A:244:ARG:NH1	7:A:602:HOH:O	2.35	0.59
1:C:403:ASP:HB2	7:C:699:HOH:O	2.03	0.58
1:B:222:ALA:O	1:B:226:ILE:HG13	2.04	0.57
1:C:196:LEU:O	1:C:200:ARG:HD2	2.04	0.56
1:C:17:ILE:CD1	7:C:694:HOH:O	2.53	0.56
1:B:23:LYS:CG	1:B:24:PRO:HD3	2.33	0.55
1:B:106:GLU:OE1	1:B:305:ARG:NH1	2.39	0.55
1:B:37:GLN:HE22	1:B:254:PRO:HD2	1.73	0.54
1:A:204:ARG:NH1	7:A:603:HOH:O	2.41	0.53
1:A:150:ILE:O	1:A:154:VAL:HG23	2.09	0.50
1:A:360:GLU:OE2	1:B:225:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ASP:O	1:C:135:SER:HB2	2.12	0.50
1:C:3:VAL:HG13	1:C:286:THR:HG22	1.94	0.50
1:A:71:ARG:CD	1:A:132:ASP:OD1	2.59	0.49
1:A:181:ARG:HD3	1:A:202:ASP:OD1	2.11	0.49
1:C:23:LYS:HG3	1:C:24:PRO:HD3	1.94	0.49
1:A:413:GLU:HB3	7:A:625:HOH:O	2.13	0.48
1:B:353:GLN:HA	1:B:353:GLN:NE2	2.29	0.48
1:B:23:LYS:CG	1:B:24:PRO:CD	2.90	0.48
1:B:353:GLN:HA	1:B:353:GLN:HE21	1.79	0.48
1:C:401:THR:HG22	1:C:401:THR:O	2.13	0.48
1:B:387:ARG:NH2	7:B:601:HOH:O	2.42	0.48
1:C:336:ARG:HD2	7:C:710:HOH:O	2.13	0.47
1:C:139:GLU:OE2	1:C:448:HIS:ND1	2.48	0.47
1:C:117[B]:GLU:OE1	1:C:124:ILE:HD11	2.15	0.47
1:B:37:GLN:NE2	1:B:254:PRO:HG2	2.30	0.47
1:C:192:VAL:O	1:C:192:VAL:HG22	2.16	0.45
1:A:120:LEU:O	2:A:502:PLM:H21	2.16	0.45
1:C:274[A]:ARG:NH1	7:C:608:HOH:O	2.49	0.45
1:B:272:GLU:OE1	1:B:273:ARG:HD2	2.18	0.44
1:C:319:VAL:HG12	1:C:321:PRO:HD3	2.00	0.44
1:A:272:GLU:OE1	1:A:273:ARG:HD2	2.18	0.44
1:B:120:LEU:HD12	1:B:293:VAL:HG21	1.99	0.43
1:A:336:ARG:HD2	7:A:636:HOH:O	2.17	0.43
1:A:120:LEU:O	2:A:502:PLM:C2	2.66	0.43
1:B:1:CYS:CB	1:B:120:LEU:O	2.65	0.43
1:C:295:LEU:HD11	1:C:319:VAL:HG13	1.99	0.43
1:A:85:ARG:HD3	1:A:113:ASP:OD2	2.18	0.42
1:A:264:ARG:HD3	1:A:445:PRO:HB2	2.00	0.42
1:C:261:LEU:HD22	1:C:262:LEU:HG	2.01	0.42
1:C:65[A]:ARG:NH2	7:C:602:HOH:O	2.35	0.42
1:C:3:VAL:HG13	1:C:286:THR:CG2	2.49	0.42
1:C:92:LYS:HE2	1:C:104:ASN:OD1	2.20	0.42
1:C:181[B]:ARG:HD2	1:C:202:ASP:OD1	2.20	0.42
1:C:196:LEU:O	1:C:200:ARG:CD	2.67	0.41
1:C:401:THR:O	1:C:402:THR:HG23	2.19	0.41
1:C:204:ARG:NE	7:C:604:HOH:O	2.45	0.41
1:A:1:CYS:HB3	1:A:121:PHE:HA	2.01	0.41
1:C:377:VAL:CG1	1:C:381:ARG:HH12	2.30	0.41
1:A:387:ARG:NH2	7:A:608:HOH:O	2.52	0.41
1:A:117[B]:GLU:OE1	1:A:124:ILE:HD11	2.20	0.41
1:B:387:ARG:HA	1:B:414:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:CYS:HB2	2:B:501:PLM:H22	1.98	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%)	47	58
1	B	443/453 (98%)	435 (98%)	8 (2%)	0	100	100
1	C	455/453 (100%)	445 (98%)	9 (2%)	1 (0%)	47	58
All	All	1346/1359 (99%)	1320 (98%)	24 (2%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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%)	339 (97%)	11 (3%)	40	55
1	B	345/352 (98%)	337 (98%)	8 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	356/352 (101%)	343 (96%)	13 (4%)	34	48
All	All	1051/1056 (100%)	1019 (97%)	32 (3%)	40	57

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	27	ARG
1	A	39	ASP
1	A	52	SER
1	A	71	ARG
1	A	105	SER
1	A	178	LYS
1	A	205	LEU
1	A	225	ARG
1	A	319	VAL
1	A	396	ARG
1	B	3	VAL
1	B	31	GLU
1	B	32	SER
1	B	33	LEU
1	B	71	ARG
1	B	145	LEU
1	B	273	ARG
1	B	323	ILE
1	C	3	VAL
1	C	17	ILE
1	C	29	ARG
1	C	71	ARG
1	C	124	ILE
1	C	135	SER
1	C	204	ARG
1	C	225	ARG
1	C	261	LEU
1	C	294	SER
1	C	402	THR
1	C	428	LEU
1	C	451	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	37	GLN
1	A	49	GLN
1	A	146	GLN
1	A	182	GLN
1	A	308	GLN
1	B	37	GLN
1	B	76	ASN
1	B	173	ASN
1	B	176	ASN
1	B	353	GLN
1	B	414	GLN
1	B	444	GLN
1	C	146	GLN
1	C	173	ASN
1	C	176	ASN
1	C	414	GLN
1	C	450	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
6	FMT	B	504	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PLM	C	502	1	5,5,17	0.60	0	4,4,17	0.75	0
4	BOG	A	504	-	20,20,20	1.57	2 (10%)	25,25,25	1.99	6 (24%)
2	PLM	B	501	1	7,7,17	0.53	0	6,6,17	1.32	1 (16%)
2	PLM	A	501	1	8,8,17	0.48	0	7,7,17	0.81	1 (14%)
2	PLM	C	501	1	10,10,17	0.38	0	9,9,17	0.89	0
4	BOG	C	503	-	20,20,20	0.62	0	25,25,25	1.03	2 (8%)
2	PLM	A	502	1	5,5,17	0.74	0	4,4,17	0.77	0
4	BOG	B	503	-	20,20,20	0.97	1 (5%)	25,25,25	1.48	6 (24%)

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	-	1/2/3/15	-
4	BOG	A	504	-	-	4/11/31/31	0/1/1/1
2	PLM	B	501	1	-	2/4/5/15	-
2	PLM	A	501	1	-	1/5/6/15	-
2	PLM	C	501	1	-	5/7/8/15	-
4	BOG	C	503	-	-	3/11/31/31	0/1/1/1
2	PLM	A	502	1	-	1/2/3/15	-
4	BOG	B	503	-	-	6/11/31/31	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	BOG	O1-C1	5.27	1.49	1.40
4	B	503	BOG	O1-C1	3.32	1.45	1.40
4	A	504	BOG	C1-C2	2.31	1.59	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	BOG	O1-C1-C2	6.56	118.54	108.30
4	A	504	BOG	O2-C2-C1	3.54	118.65	110.05
4	B	503	BOG	O5-C5-C4	3.27	115.64	109.69
4	B	503	BOG	O1-C1-C2	3.07	113.09	108.30
4	C	503	BOG	O4-C4-C3	-2.45	104.67	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	BOG	O4-C4-C5	2.44	115.35	109.30
4	B	503	BOG	O2-C2-C1	2.40	115.87	110.05
2	B	501	PLM	O2-C1-C2	-2.40	111.17	126.89
4	C	503	BOG	O1-C1-C2	-2.37	104.60	108.30
4	A	504	BOG	C4-C3-C2	-2.31	106.79	110.82
4	A	504	BOG	O3-C3-C2	2.27	115.61	110.35
4	A	504	BOG	C1'-O1-C1	2.23	117.54	113.84
4	B	503	BOG	O4-C4-C3	-2.20	105.26	110.35
4	B	503	BOG	C3-C4-C5	2.11	113.99	110.24
2	A	501	PLM	O2-C1-C2	-2.10	113.08	126.89
4	B	503	BOG	O4-C4-C5	2.04	114.37	109.30

There are no chirality outliers.

All (23) torsion outliers are listed below:

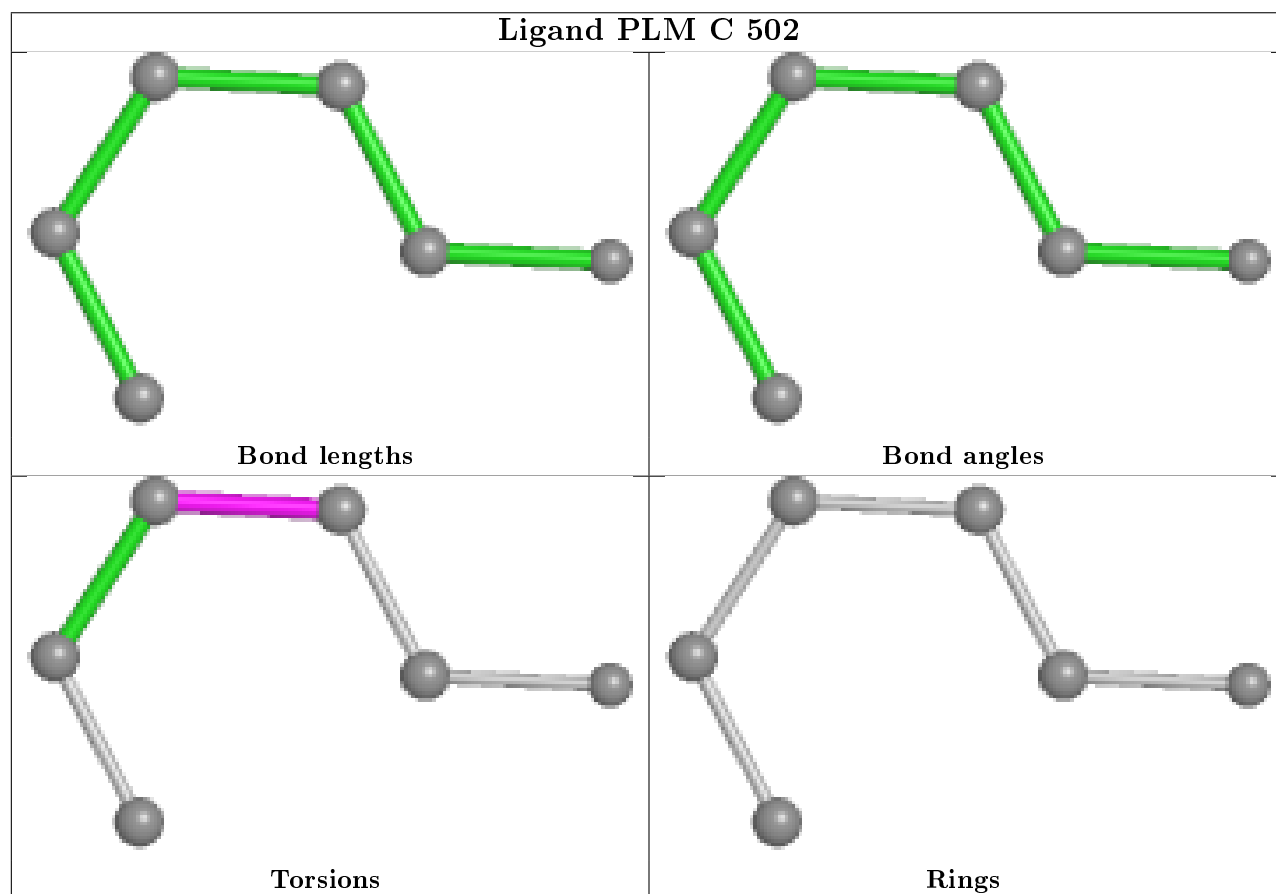
Mol	Chain	Res	Type	Atoms
2	C	502	PLM	C1-C2-C3-C4
4	B	503	BOG	O5-C5-C6-O6
4	B	503	BOG	O5-C1-O1-C1'
2	C	501	PLM	C3-C4-C5-C6
4	B	503	BOG	C4-C5-C6-O6
2	C	501	PLM	C5-C6-C7-C8
4	C	503	BOG	C3'-C4'-C5'-C6'
4	A	504	BOG	C2'-C1'-O1-C1
4	B	503	BOG	C1'-C2'-C3'-C4'
4	B	503	BOG	C5'-C6'-C7'-C8'
2	C	501	PLM	C7-C8-C9-CA
4	B	503	BOG	O1-C1'-C2'-C3'
2	B	501	PLM	C3-C4-C5-C6
4	A	504	BOG	C4'-C5'-C6'-C7'
4	A	504	BOG	C2'-C3'-C4'-C5'
2	B	501	PLM	C1-C2-C3-C4
2	A	501	PLM	C1-C2-C3-C4
2	C	501	PLM	C1-C2-C3-C4
4	A	504	BOG	O1-C1'-C2'-C3'
2	C	501	PLM	C2-C3-C4-C5
2	A	502	PLM	C2-C3-C4-C5
4	C	503	BOG	C5'-C6'-C7'-C8'
4	C	503	BOG	O1-C1'-C2'-C3'

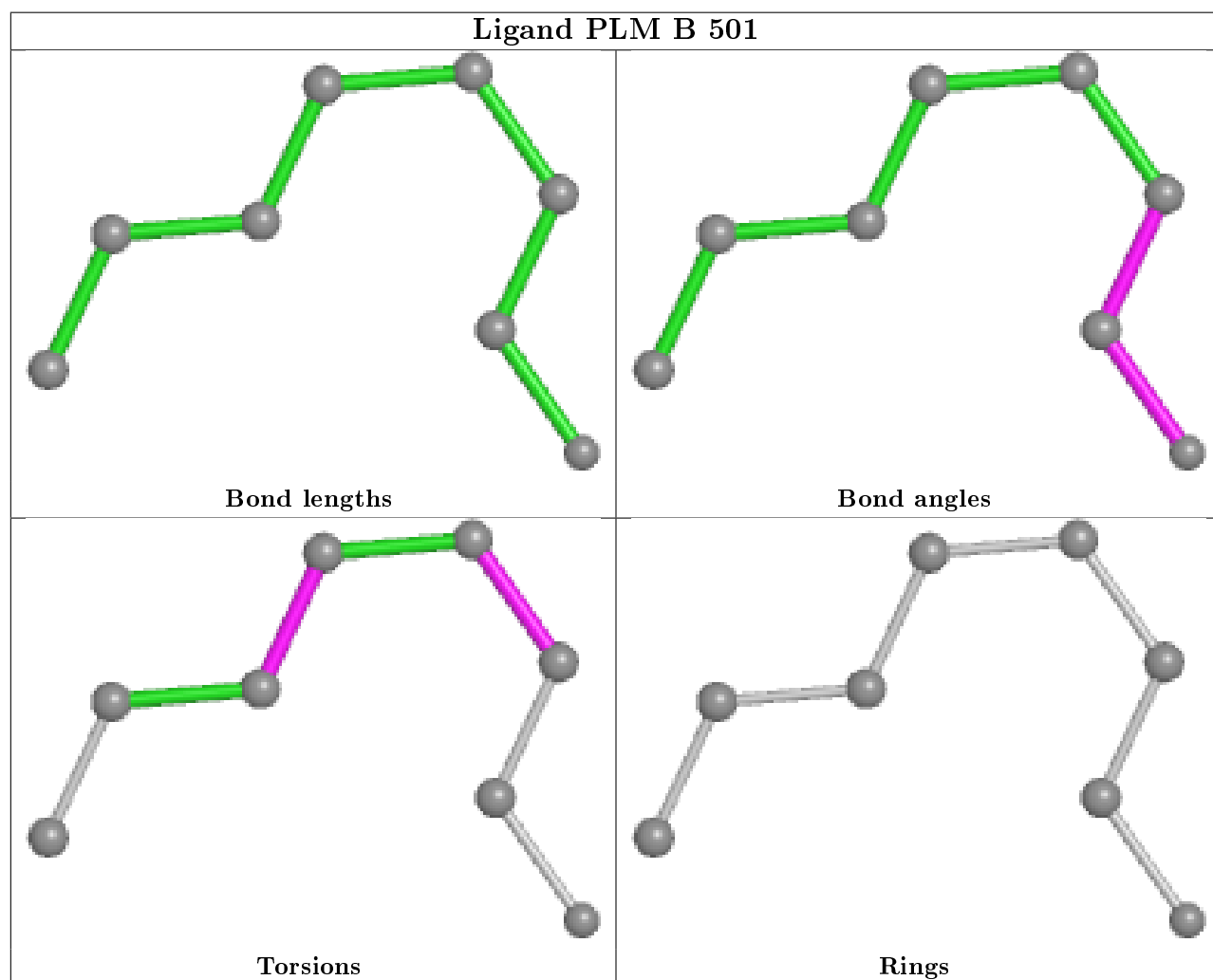
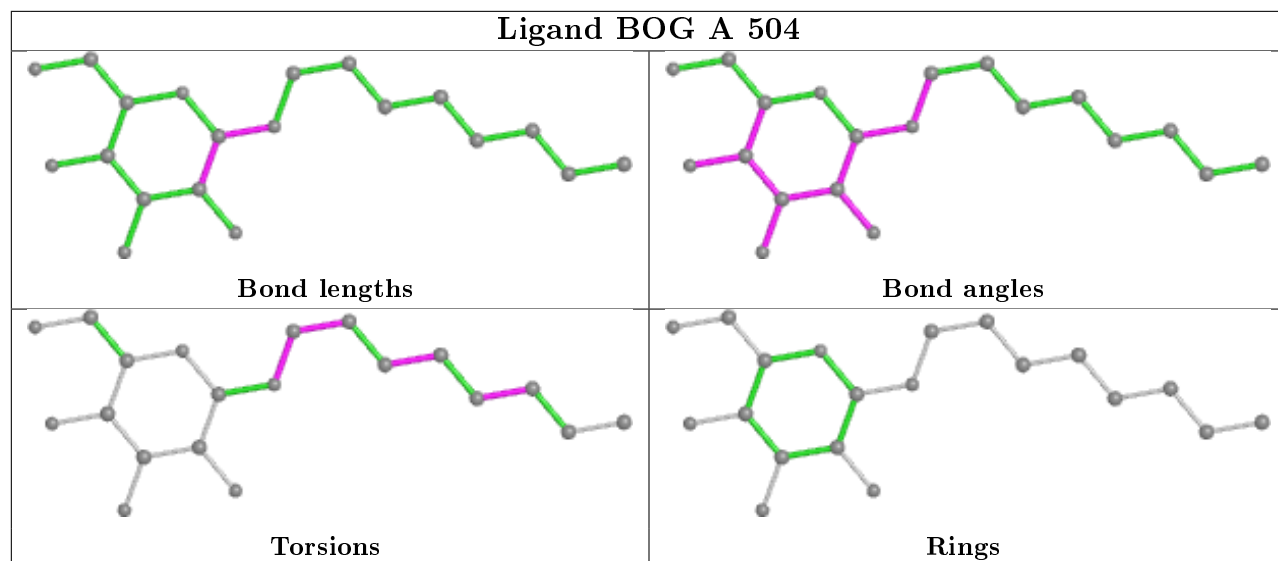
There are no ring outliers.

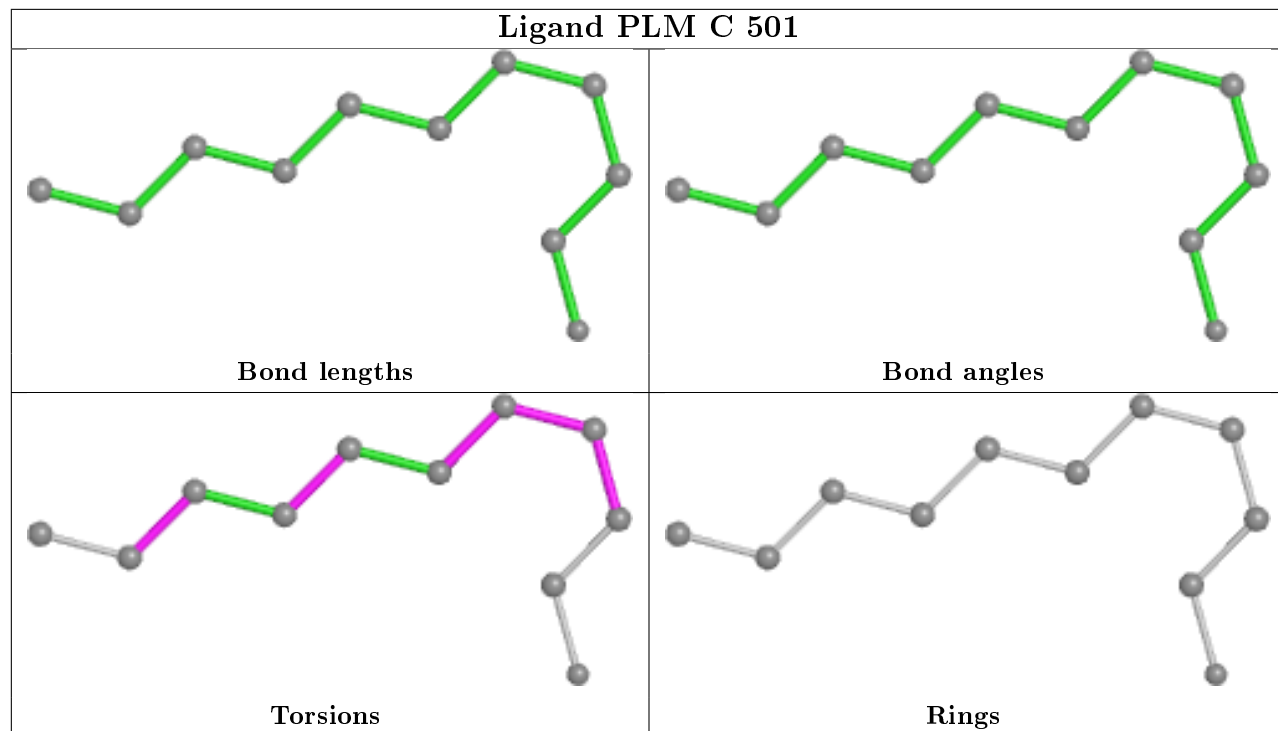
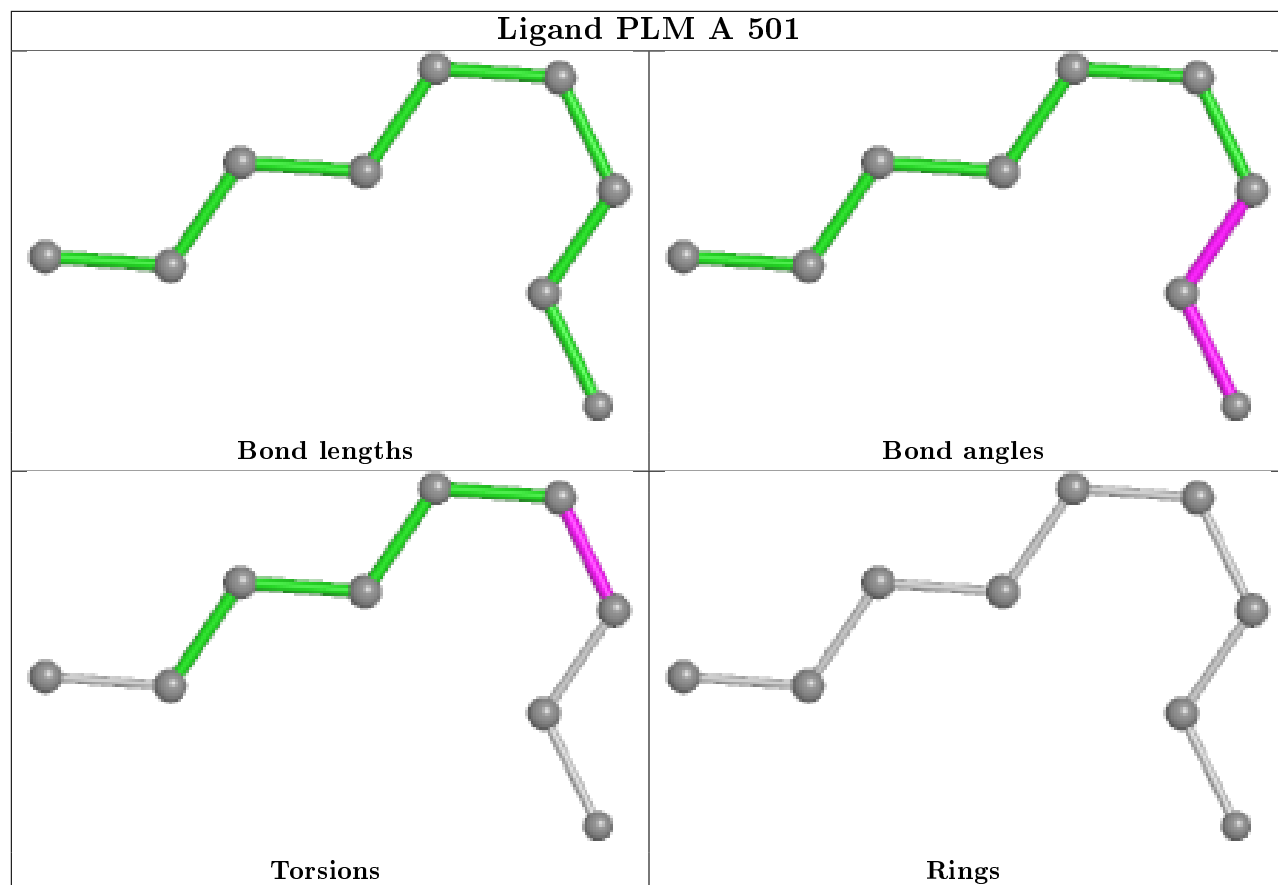
2 monomers are involved in 3 short contacts:

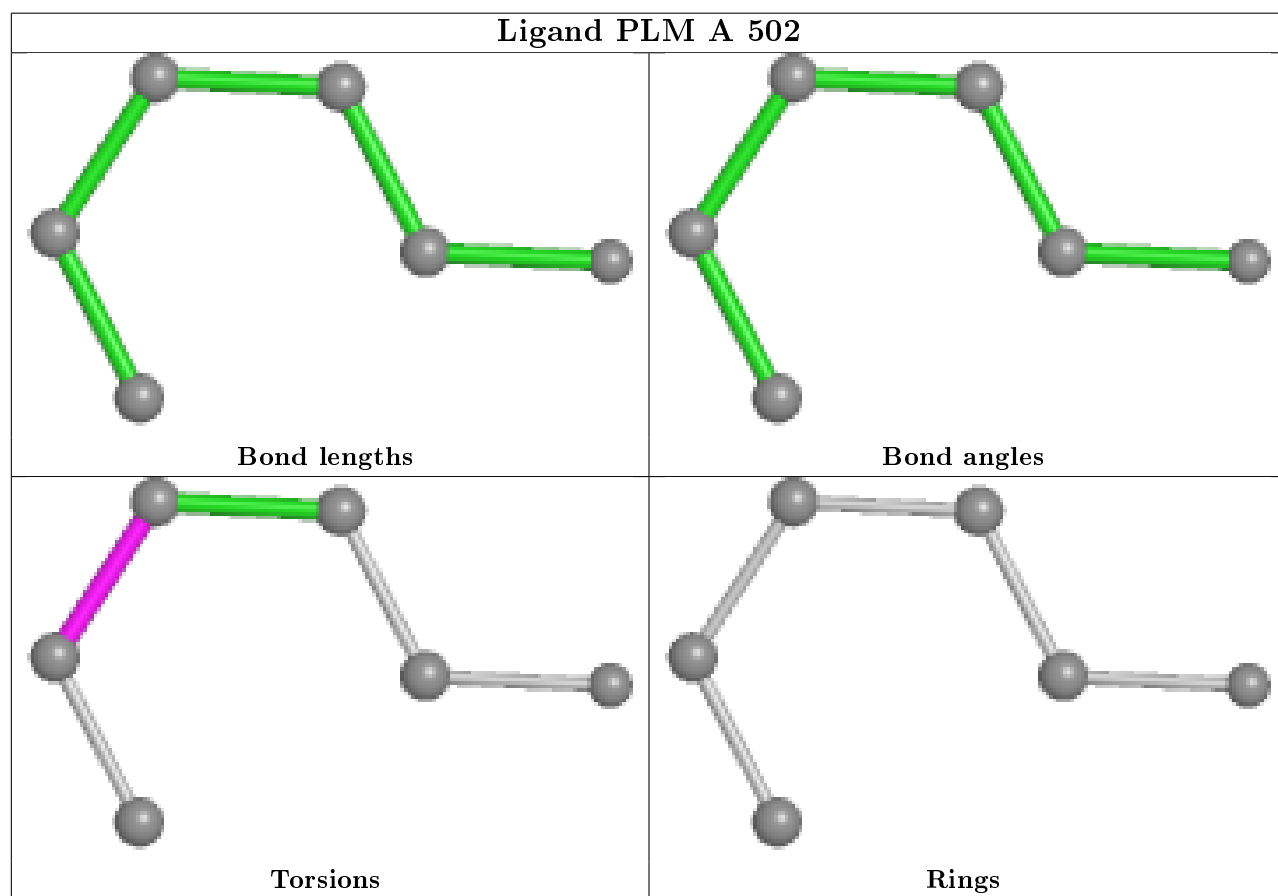
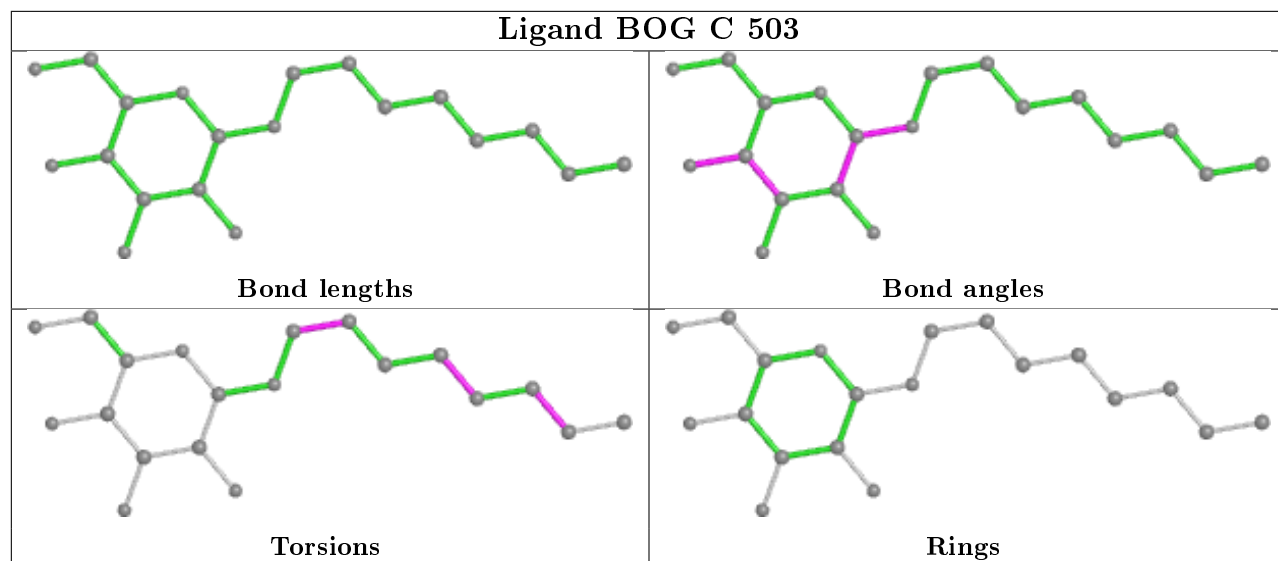
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PLM	1	0
2	A	502	PLM	2	0

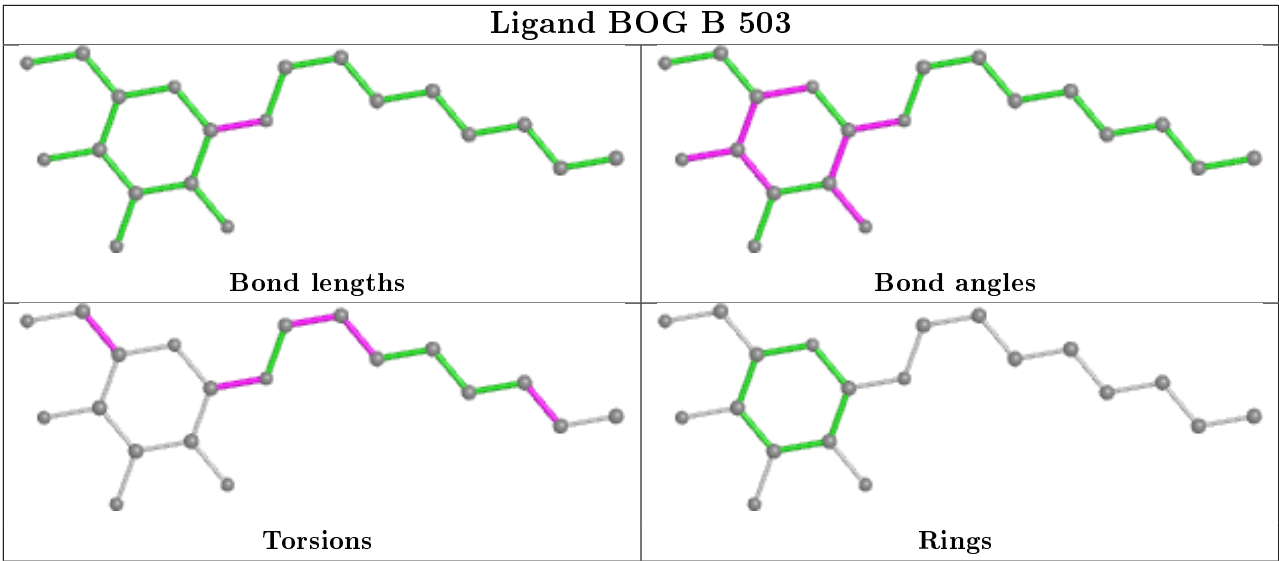
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1:CYS	C	2:THR	N	1.76
1	B	1:CYS	C	2:THR	N	1.68



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	445/453 (98%)	-0.29	6 (1%) 77 81	21, 33, 58, 102	0
1	B	445/453 (98%)	-0.23	5 (1%) 80 85	20, 31, 60, 75	0
1	C	451/453 (99%)	-0.19	7 (1%) 72 77	19, 32, 60, 83	0
All	All	1341/1359 (98%)	-0.23	18 (1%) 77 81	19, 32, 60, 102	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	GLY	4.3
1	C	22	SER	3.7
1	A	98	VAL	3.2
1	C	21	ALA	3.2
1	C	23	LYS	3.1
1	A	445	PRO	2.8
1	A	21	ALA	2.7
1	C	99	THR	2.5
1	C	451	HIS	2.5
1	B	18	ASP	2.5
1	A	8	ARG	2.4
1	B	21	ALA	2.4
1	C	8	ARG	2.3
1	B	250	THR	2.3
1	A	18	ASP	2.1
1	B	8	ARG	2.1
1	B	305	ARG	2.0
1	A	97	GLY	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

There are no monosaccharides in this entry.

### 6.4 Ligands

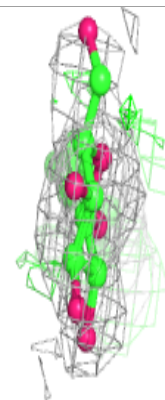
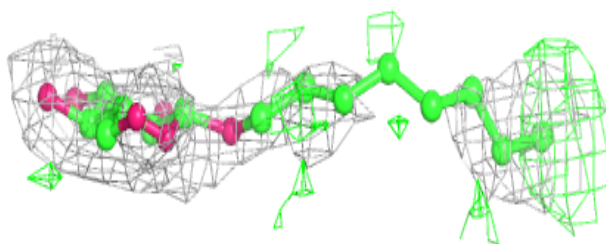
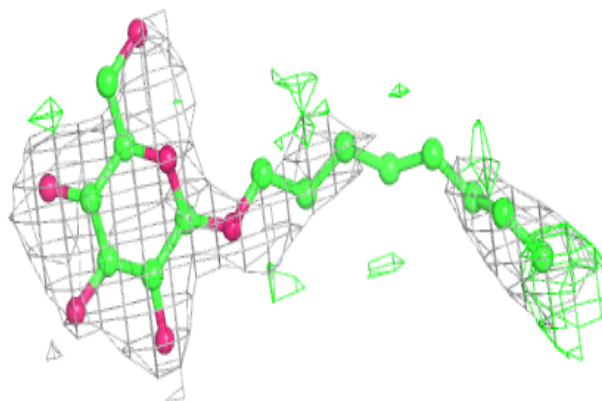
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BOG	A	504	20/20	0.66	0.28	55,84,97,100	0
4	BOG	B	503	20/20	0.69	0.27	63,73,78,79	0
2	PLM	C	501	11/18	0.71	0.17	58,67,98,105	0
2	PLM	C	502	6/18	0.71	0.24	53,58,71,74	0
2	PLM	A	501	9/18	0.75	0.16	52,57,63,67	0
2	PLM	B	501	8/18	0.86	0.11	44,51,66,67	0
2	PLM	A	502	6/18	0.87	0.15	52,56,57,60	0
6	FMT	B	504	3/3	0.92	0.15	50,50,50,55	0
4	BOG	C	503	20/20	0.95	0.12	29,36,40,43	0
5	NA	B	502	1/1	0.96	0.07	34,34,34,34	0
3	CL	A	503	1/1	0.99	0.17	62,62,62,62	0

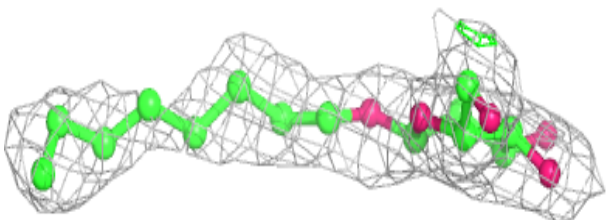
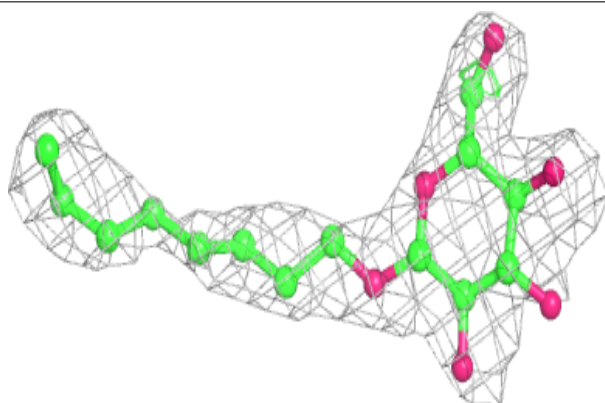
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BOG A 504:**

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

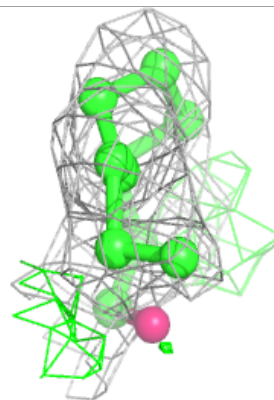
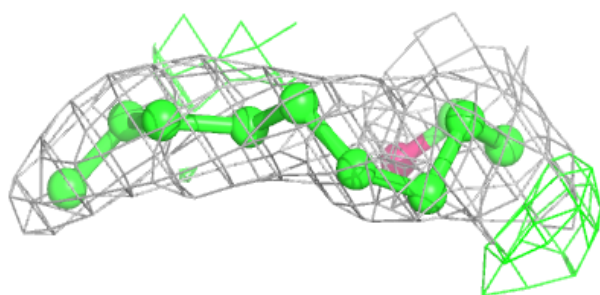
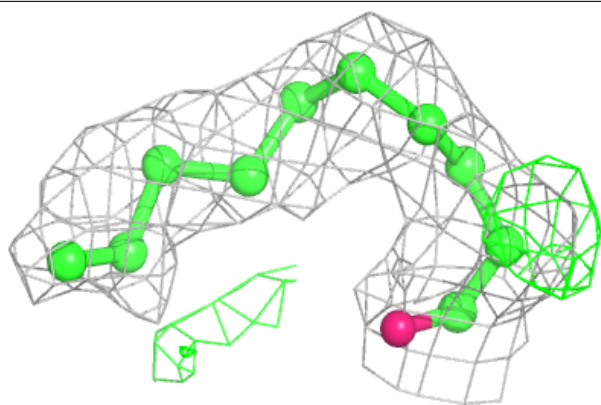
**Electron density around BOG B 503:**

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

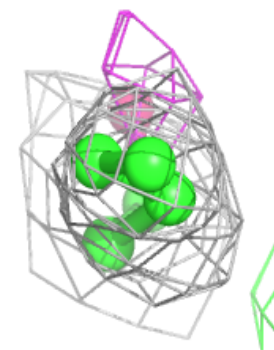
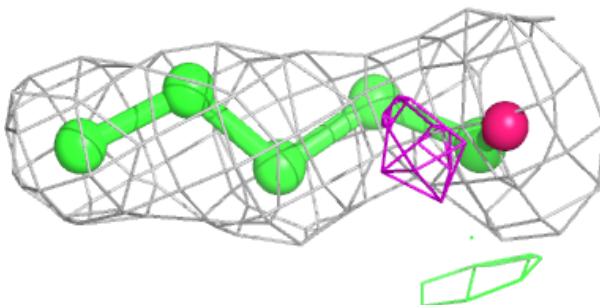
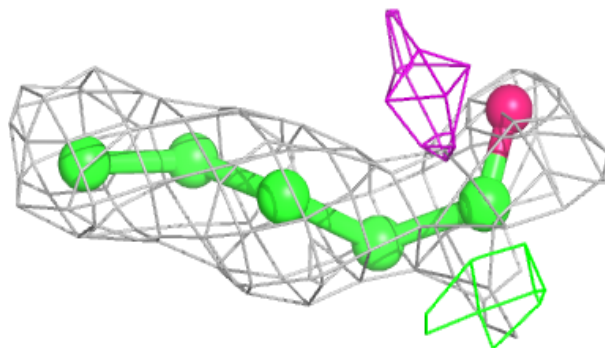


**Electron density around PLM C 501:**

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

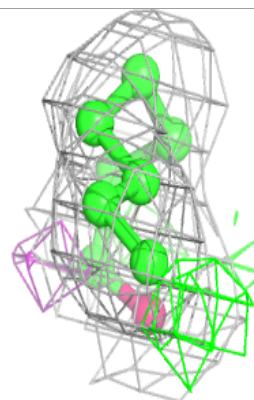
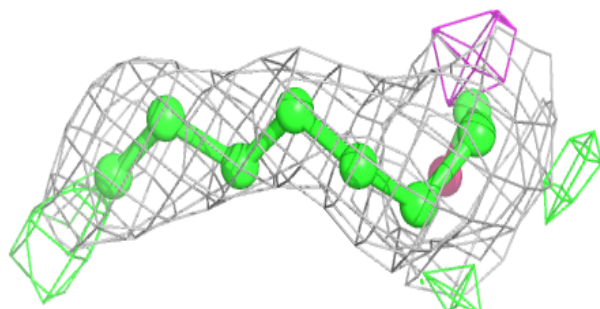
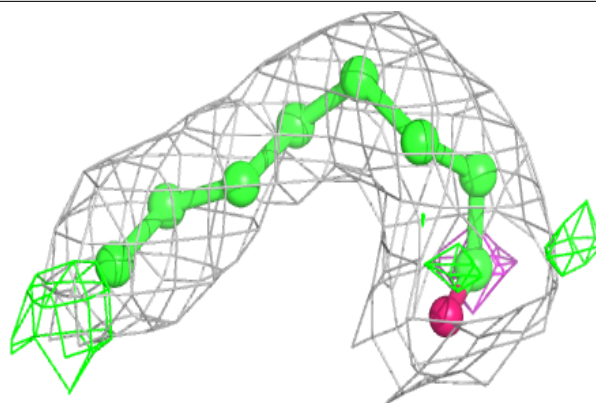
**Electron density around PLM C 502:**

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

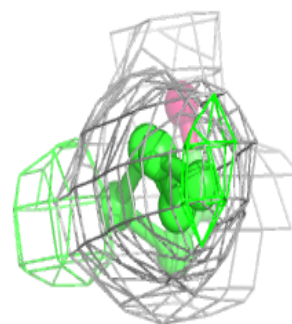
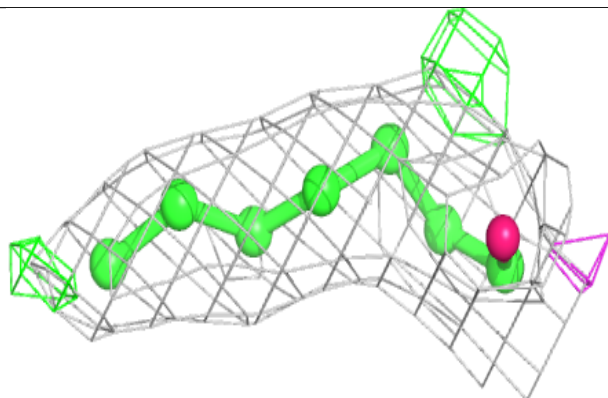
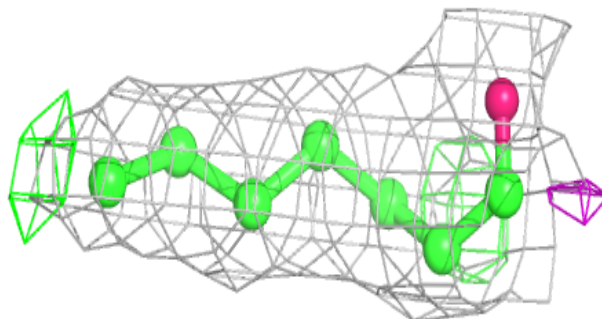


**Electron density around PLM A 501:**

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

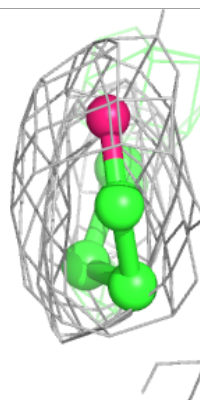
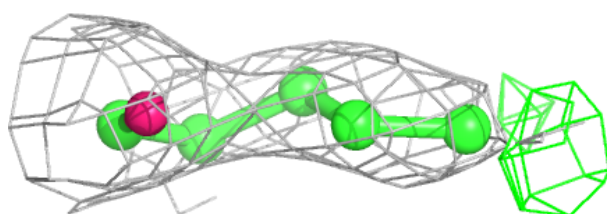
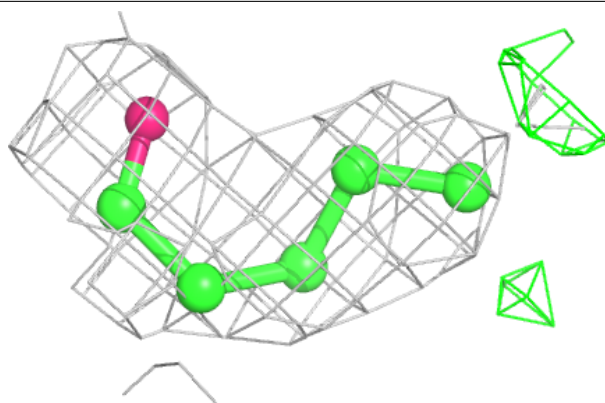
**Electron density around PLM B 501:**

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

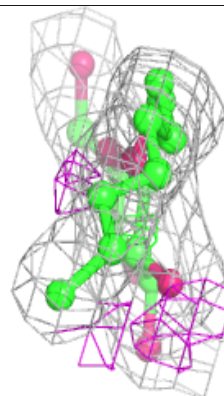
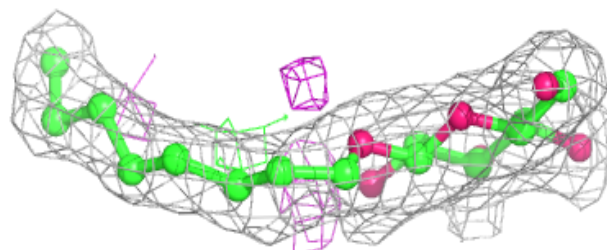
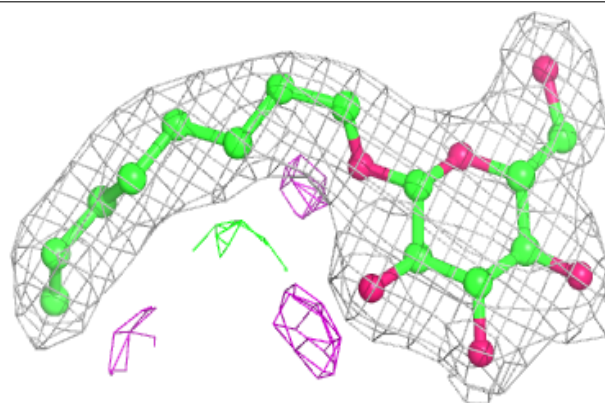


**Electron density around PLM A 502:**

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

**Electron density around BOG 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)



## 6.5 Other polymers

There are no such residues in this entry.