



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 06:12 AM EDT

PDB ID : 5VMA
Title : Structure of *B. pumilus* GH48 in complex with a cellobio-derived isofagomine
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2017-04-27
Resolution : 1.95 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

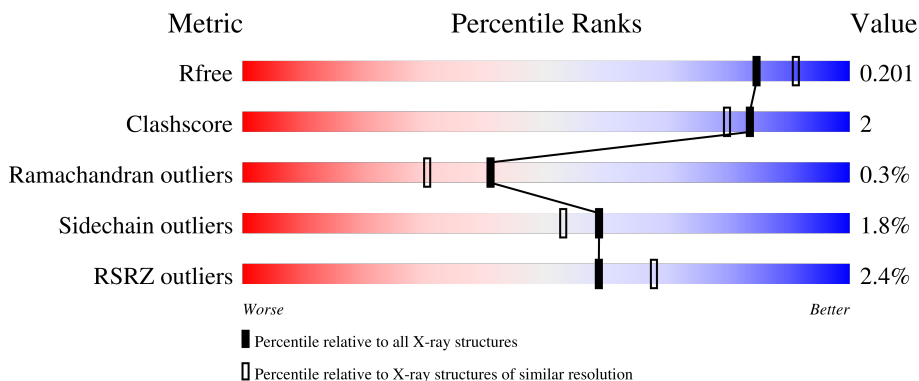
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

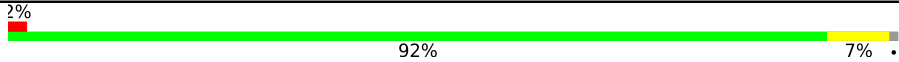
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	709	

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
7	MLI	A	819	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6480 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.

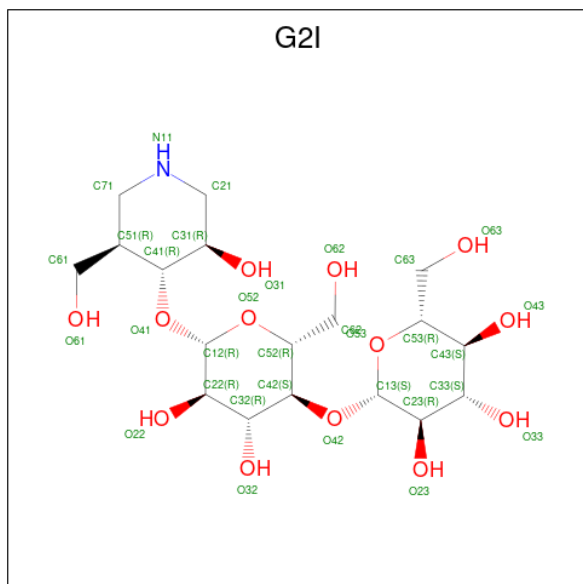
- Molecule 1 is a protein called Glycoside hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	700	5723	3635	961	1108	19	0	22	0

There are 8 discrepancies between the modelled and reference sequences:

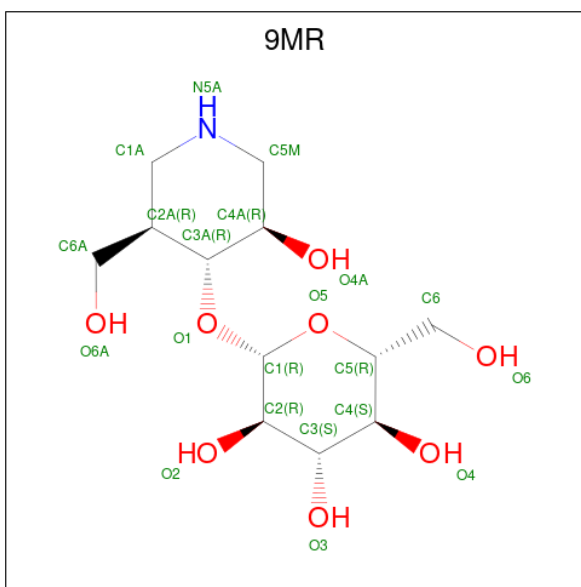
Chain	Residue	Modelled	Actual	Comment	Reference
A	702	LEU	-	expression tag	UNP A8FDC4
A	703	GLU	-	expression tag	UNP A8FDC4
A	704	HIS	-	expression tag	UNP A8FDC4
A	705	HIS	-	expression tag	UNP A8FDC4
A	706	HIS	-	expression tag	UNP A8FDC4
A	707	HIS	-	expression tag	UNP A8FDC4
A	708	HIS	-	expression tag	UNP A8FDC4
A	709	HIS	-	expression tag	UNP A8FDC4

- Molecule 2 is (3R,4R,5R)-3-hydroxy-5-(hydroxymethyl)piperidin-4-yl 4-O-beta-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: G2I) (formula: C₁₈H₃₃NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	18	1	13		
2	A	1	Total	C	N	O	0	0
			32	18	1	13		

- Molecule 3 is (3R,4R,5R)-3-hydroxy-5-(hydroxymethyl)piperidin-4-yl beta-D-glucopyranoside (three-letter code: 9MR) (formula: C₁₂H₂₃NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	12	1	8		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

- 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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



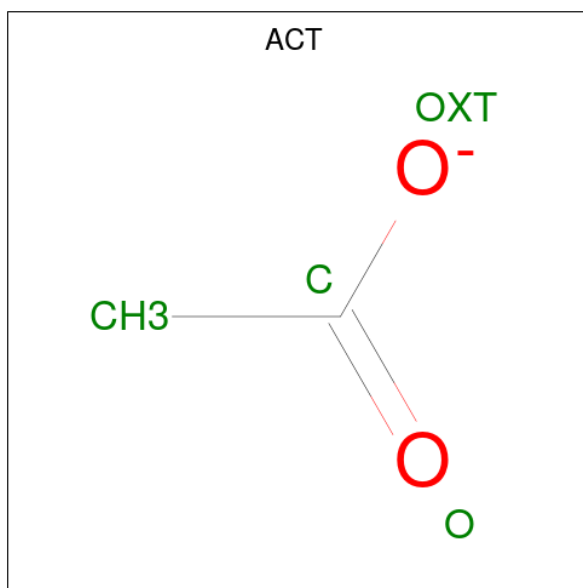
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 8 4 4	0	1
6	A	1	Total C O 8 4 4	0	1
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 8 4 4	0	1
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 8 4 4	0	1
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

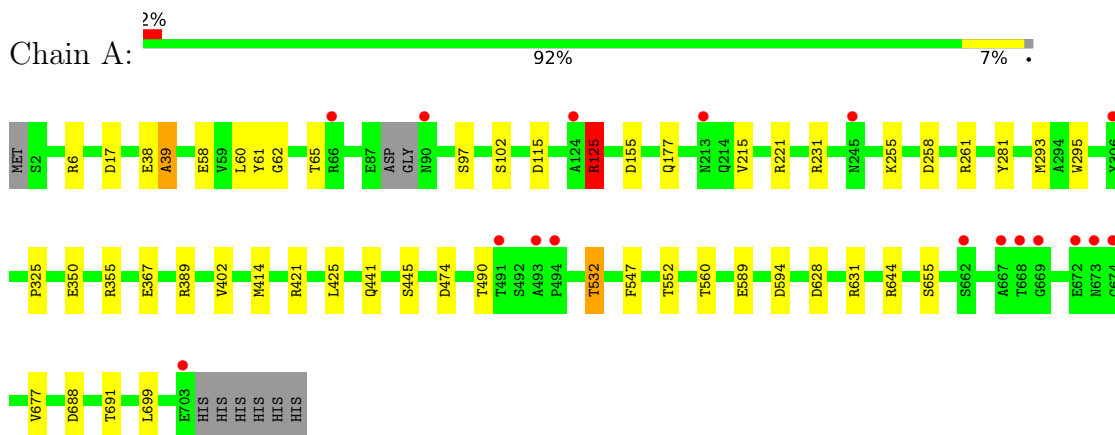
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	579	Total 594	O 594	0	15

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: Glycoside hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.89Å 98.89Å 216.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 58.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-1.95) 97.6 (58.76-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.154 , 0.196 0.166 , 0.201	Depositor DCC
R_{free} test set	3796 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtrriage
Anisotropy	0.576	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6480	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: G2I, EDO, NA, CA, 9MR, ACT, MLI

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	1.09	5/5905 (0.1%)	1.00	20/8044 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	655	SER	CB-OG	-6.00	1.34	1.42
1	A	350	GLU	CD-OE2	-5.93	1.19	1.25
1	A	281	TYR	CE1-CZ	5.72	1.46	1.38
1	A	350	GLU	CD-OE1	-5.23	1.19	1.25
1	A	389	ARG	CD-NE	-5.05	1.37	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	A	628	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	628	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	644	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	355	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	474	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	355	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	261	ARG	NE-CZ-NH2	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	6	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	631	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	231	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	A	389	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	631	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	155	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	17	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	261	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	125[A]	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	A	125[B]	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	A	594	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5723	0	5268	21	0
2	A	64	0	66	4	0
3	A	21	0	11	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	64	0	96	7	0
7	A	7	0	2	2	0
8	A	4	0	3	0	0
9	A	594	0	0	13	0
All	All	6480	0	5446	27	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 2.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:819:MLI:O8	9:A:904:HOH:O	1.65	1.12
6:A:815:EDO:H22	9:A:911:HOH:O	1.49	1.08
7:A:819:MLI:O6	9:A:904:HOH:O	1.98	0.82
6:A:815:EDO:C2	9:A:911:HOH:O	2.13	0.82
1:A:255[B]:LYS:NZ	9:A:909:HOH:O	2.19	0.74
1:A:441[B]:GLN:NE2	9:A:905:HOH:O	1.94	0.74
1:A:97[B]:SER:OG	9:A:1335[B]:HOH:O	2.08	0.70
6:A:813:EDO:H21	9:A:901:HOH:O	1.91	0.69
1:A:125[A]:ARG:NH1	9:A:906:HOH:O	2.01	0.63
1:A:445[B]:SER:OG	9:A:908:HOH:O	2.15	0.63
1:A:414[B]:MET:CE	6:A:817:EDO:H12	2.34	0.56
1:A:58:GLU:OE1	6:A:811:EDO:O1	2.28	0.52
1:A:60:LEU:HD12	1:A:691:THR:HG22	1.91	0.51
1:A:532:THR:HG21	2:A:802:G2I:N11	2.26	0.50
1:A:62:GLY:N	6:A:811:EDO:H12	2.27	0.49
1:A:532:THR:HG21	2:A:802:G2I:HN11	1.78	0.49
1:A:547:PHE:CE1	1:A:699:LEU:HD11	2.50	0.47
1:A:589:GLU:CG	1:A:677:VAL:CG1	2.93	0.47
1:A:532:THR:HG21	2:A:802:G2I:H21A	1.98	0.46
6:A:814[A]:EDO:H11	9:A:1127:HOH:O	2.16	0.45
1:A:295:TRP:CD2	1:A:402:VAL:HG21	2.53	0.44
1:A:61:TYR:CZ	1:A:65:THR:HG21	2.53	0.44
1:A:532:THR:HG21	2:A:802:G2I:C21	2.48	0.43
1:A:552:THR:HB	1:A:560:THR:HG23	1.99	0.43
1:A:325:PRO:HB2	1:A:425:LEU:HD22	2.01	0.43
1:A:293:MET:HG3	9:A:1156:HOH:O	2.18	0.42
1:A:177[B]:GLN:NE2	9:A:907:HOH:O	2.13	0.41

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	717/709 (101%)	699 (98%)	16 (2%)	2 (0%)	41 30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ALA
1	A	38	GLU

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	588/580 (101%)	576 (98%)	12 (2%)	55 48

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102[A]	SER
1	A	102[B]	SER
1	A	115	ASP
1	A	125[A]	ARG
1	A	125[B]	ARG
1	A	215	VAL
1	A	221	ARG
1	A	258	ASP
1	A	367	GLU
1	A	490	THR
1	A	532	THR
1	A	688	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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
3	9MR	A	803	-	21,22,22	1.65	6 (28%)	25,31,31	3.54	15 (60%)
6	EDO	A	812[B]	-	3,3,3	0.60	0	2,2,2	0.08	0
6	EDO	A	808[B]	-	3,3,3	0.52	0	2,2,2	0.32	0
6	EDO	A	813	-	3,3,3	0.50	0	2,2,2	0.50	0
6	EDO	A	814[B]	-	3,3,3	0.94	0	2,2,2	0.41	0
6	EDO	A	809[A]	-	3,3,3	0.88	0	2,2,2	0.85	0
7	MLI	A	819	-	6,6,6	1.32	1 (16%)	7,7,7	0.94	0
6	EDO	A	816	-	3,3,3	0.77	0	2,2,2	0.07	0
2	G2I	A	802	-	33,34,34	1.32	5 (15%)	43,49,49	1.30	5 (11%)
6	EDO	A	818	-	3,3,3	0.36	0	2,2,2	0.70	0
6	EDO	A	812[A]	-	3,3,3	0.58	0	2,2,2	0.44	0
6	EDO	A	817	-	3,3,3	1.45	0	2,2,2	0.57	0
6	EDO	A	811	-	3,3,3	0.47	0	2,2,2	1.36	0
6	EDO	A	815	-	3,3,3	0.48	0	2,2,2	0.43	0
6	EDO	A	809[B]	-	3,3,3	0.94	0	2,2,2	0.46	0
2	G2I	A	801	-	33,34,34	1.57	7 (21%)	43,49,49	2.23	7 (16%)
6	EDO	A	807	-	3,3,3	0.61	0	2,2,2	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	808[A]	-	3,3,3	0.63	0	2,2,2	0.33	0
6	EDO	A	810	-	3,3,3	0.30	0	2,2,2	0.55	0
8	ACT	A	820	-	3,3,3	0.66	0	3,3,3	1.06	0
6	EDO	A	814[A]	-	3,3,3	0.73	0	2,2,2	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	9MR	A	803	-	-	2/8/42/42	0/2/2/2
6	EDO	A	812[B]	-	-	1/1/1/1	-
6	EDO	A	808[B]	-	-	1/1/1/1	-
6	EDO	A	813	-	-	1/1/1/1	-
6	EDO	A	814[B]	-	-	0/1/1/1	-
6	EDO	A	809[A]	-	-	1/1/1/1	-
7	MLI	A	819	-	-	0/4/4/4	-
6	EDO	A	816	-	-	0/1/1/1	-
2	G2I	A	802	-	-	0/14/68/68	0/3/3/3
6	EDO	A	818	-	-	0/1/1/1	-
6	EDO	A	812[A]	-	-	0/1/1/1	-
6	EDO	A	817	-	-	0/1/1/1	-
6	EDO	A	811	-	-	1/1/1/1	-
6	EDO	A	815	-	-	1/1/1/1	-
6	EDO	A	809[B]	-	-	1/1/1/1	-
2	G2I	A	801	-	-	2/14/68/68	0/3/3/3
6	EDO	A	807	-	-	1/1/1/1	-
6	EDO	A	808[A]	-	-	0/1/1/1	-
6	EDO	A	810	-	-	1/1/1/1	-
6	EDO	A	814[A]	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	G2I	C31-C41	4.54	1.62	1.52
3	A	803	9MR	C5M-C4A	4.13	1.56	1.52
2	A	801	G2I	O31-C31	3.28	1.50	1.43
2	A	802	G2I	C21-C31	3.16	1.55	1.52
3	A	803	9MR	C5M-N5A	2.81	1.51	1.46
2	A	801	G2I	C43-C33	-2.72	1.45	1.52
2	A	801	G2I	O42-C42	-2.64	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	G2I	C33-C23	-2.64	1.45	1.52
3	A	803	9MR	O2-C2	2.54	1.49	1.43
2	A	802	G2I	O53-C13	-2.50	1.35	1.41
3	A	803	9MR	O6A-C6A	2.45	1.52	1.42
2	A	801	G2I	C71-N11	2.32	1.50	1.46
2	A	801	G2I	O43-C43	2.23	1.48	1.43
3	A	803	9MR	O5-C5	2.22	1.49	1.44
3	A	803	9MR	O4A-C4A	2.20	1.48	1.43
2	A	801	G2I	O41-C12	-2.18	1.35	1.41
2	A	802	G2I	O41-C12	-2.08	1.35	1.41
2	A	802	G2I	O41-C41	2.07	1.49	1.43
7	A	819	MLI	O9-C3	-2.03	1.23	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	9MR	C1A-N5A-C5M	11.65	124.49	111.70
2	A	801	G2I	C21-N11-C71	10.03	122.71	111.70
3	A	803	9MR	O2-C2-C3	5.92	124.04	110.35
2	A	801	G2I	O53-C53-C63	5.54	120.21	106.44
3	A	803	9MR	O4A-C4A-C5M	5.24	119.87	109.61
2	A	801	G2I	C63-C53-C43	-4.68	102.04	113.00
3	A	803	9MR	O3-C3-C4	-3.81	101.55	110.35
3	A	803	9MR	O2-C2-C1	-3.72	101.01	110.05
3	A	803	9MR	C1-O1-C3A	3.57	126.81	117.96
2	A	801	G2I	C12-O52-C52	-3.16	107.50	113.69
3	A	803	9MR	C3-C4-C5	-3.13	104.66	110.24
2	A	801	G2I	O52-C52-C62	-3.12	98.69	106.44
3	A	803	9MR	O5-C5-C6	3.11	114.17	106.44
2	A	802	G2I	O53-C53-C63	3.05	114.02	106.44
3	A	803	9MR	O4-C4-C3	2.91	117.09	110.35
3	A	803	9MR	C6-C5-C4	-2.75	106.55	113.00
3	A	803	9MR	O3-C3-C2	2.52	116.17	110.35
3	A	803	9MR	C1-O5-C5	-2.48	108.83	113.69
2	A	802	G2I	C21-N11-C71	2.43	114.37	111.70
3	A	803	9MR	O1-C1-O5	2.34	117.20	110.67
2	A	801	G2I	C71-C51-C61	2.27	114.58	110.66
3	A	803	9MR	O4-C4-C5	2.23	114.84	109.30
3	A	803	9MR	O6A-C6A-C2A	2.16	116.32	111.36
2	A	802	G2I	C61-C51-C41	2.15	115.89	112.14
2	A	802	G2I	C13-O42-C42	-2.10	112.77	117.96
2	A	802	G2I	C13-O53-C53	-2.06	109.64	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	G2I	C61-C51-C41	-2.01	108.64	112.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	G2I	O53-C53-C63-O63
2	A	801	G2I	C43-C53-C63-O63
3	A	803	9MR	O5-C5-C6-O6
6	A	810	EDO	O1-C1-C2-O2
6	A	815	EDO	O1-C1-C2-O2
6	A	808[B]	EDO	O1-C1-C2-O2
6	A	813	EDO	O1-C1-C2-O2
3	A	803	9MR	C4-C5-C6-O6
6	A	809[A]	EDO	O1-C1-C2-O2
6	A	809[B]	EDO	O1-C1-C2-O2
6	A	811	EDO	O1-C1-C2-O2
6	A	807	EDO	O1-C1-C2-O2
6	A	812[B]	EDO	O1-C1-C2-O2

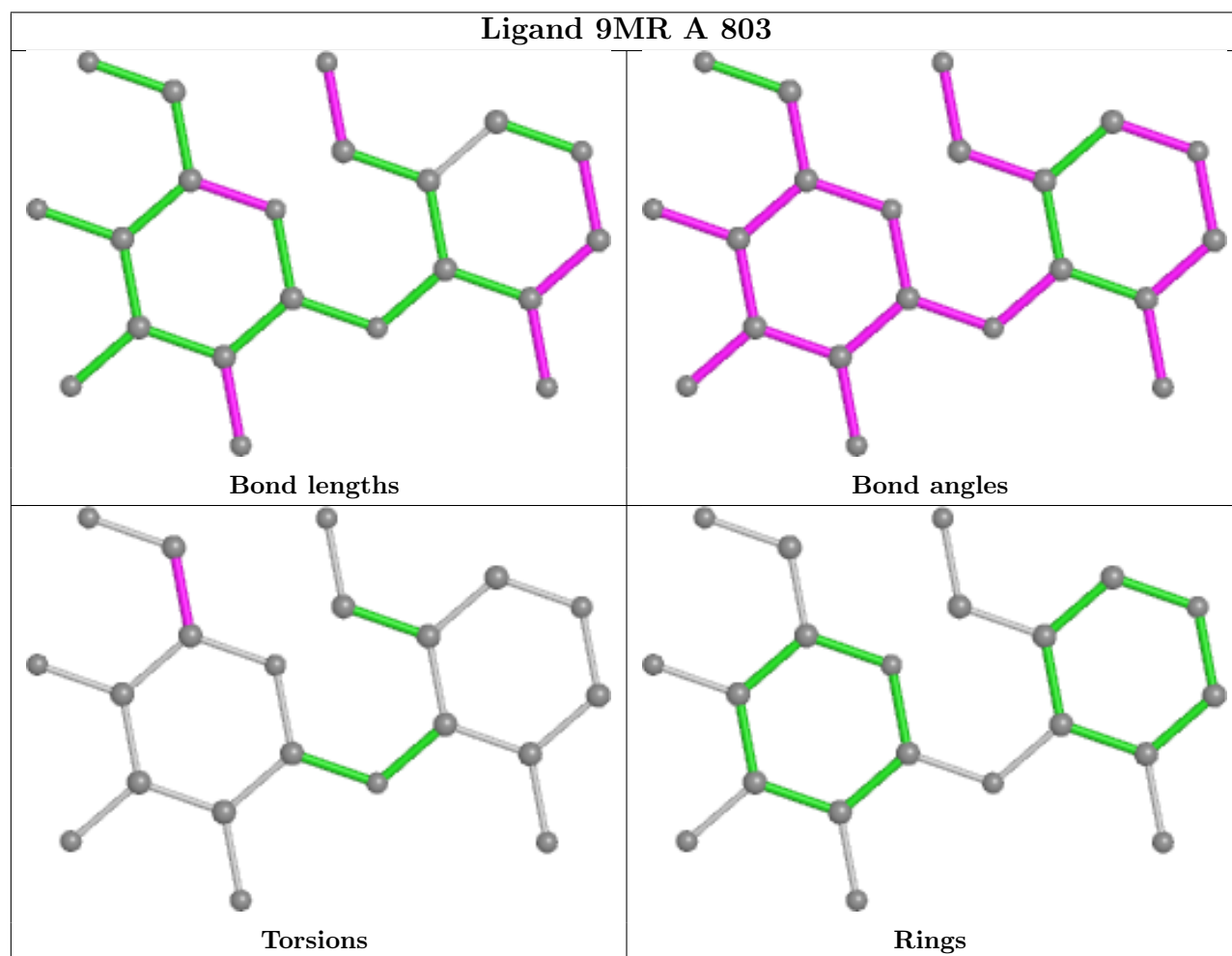
There are no ring outliers.

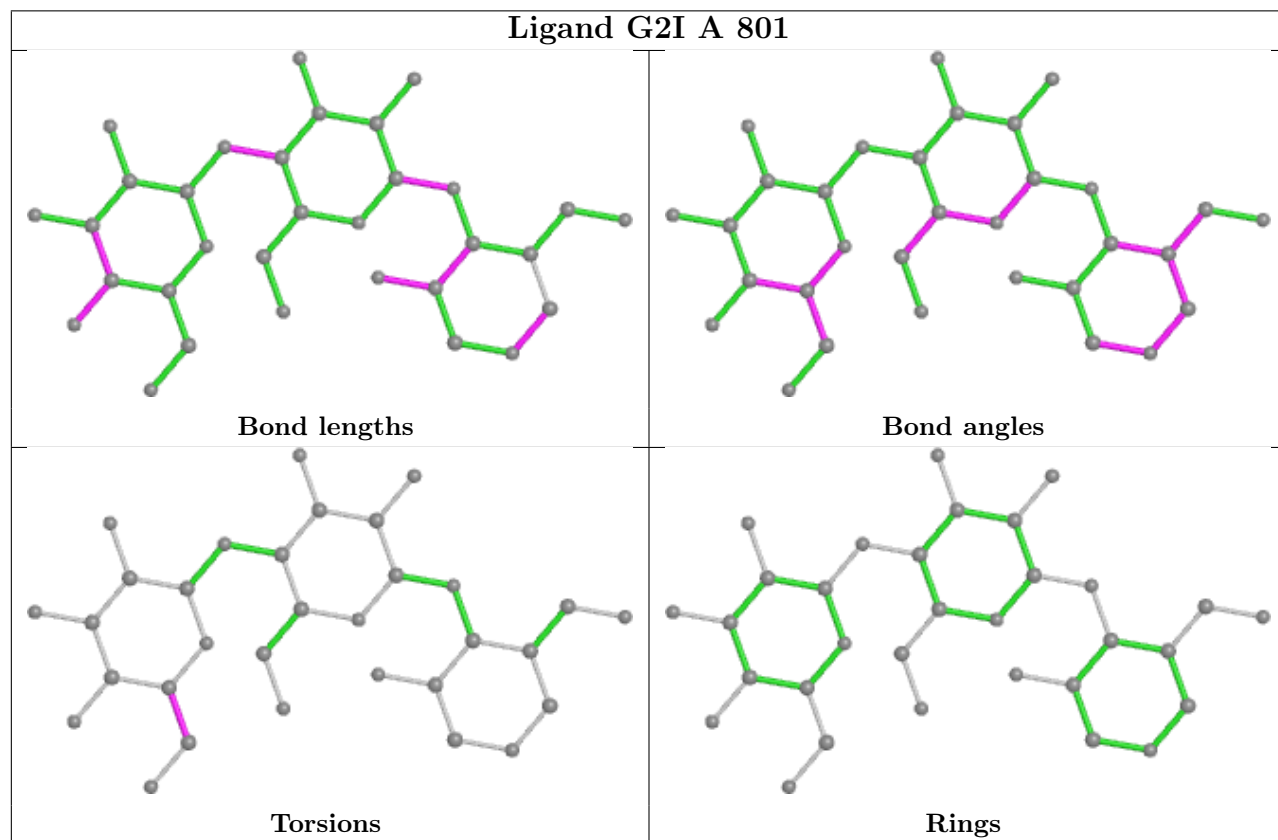
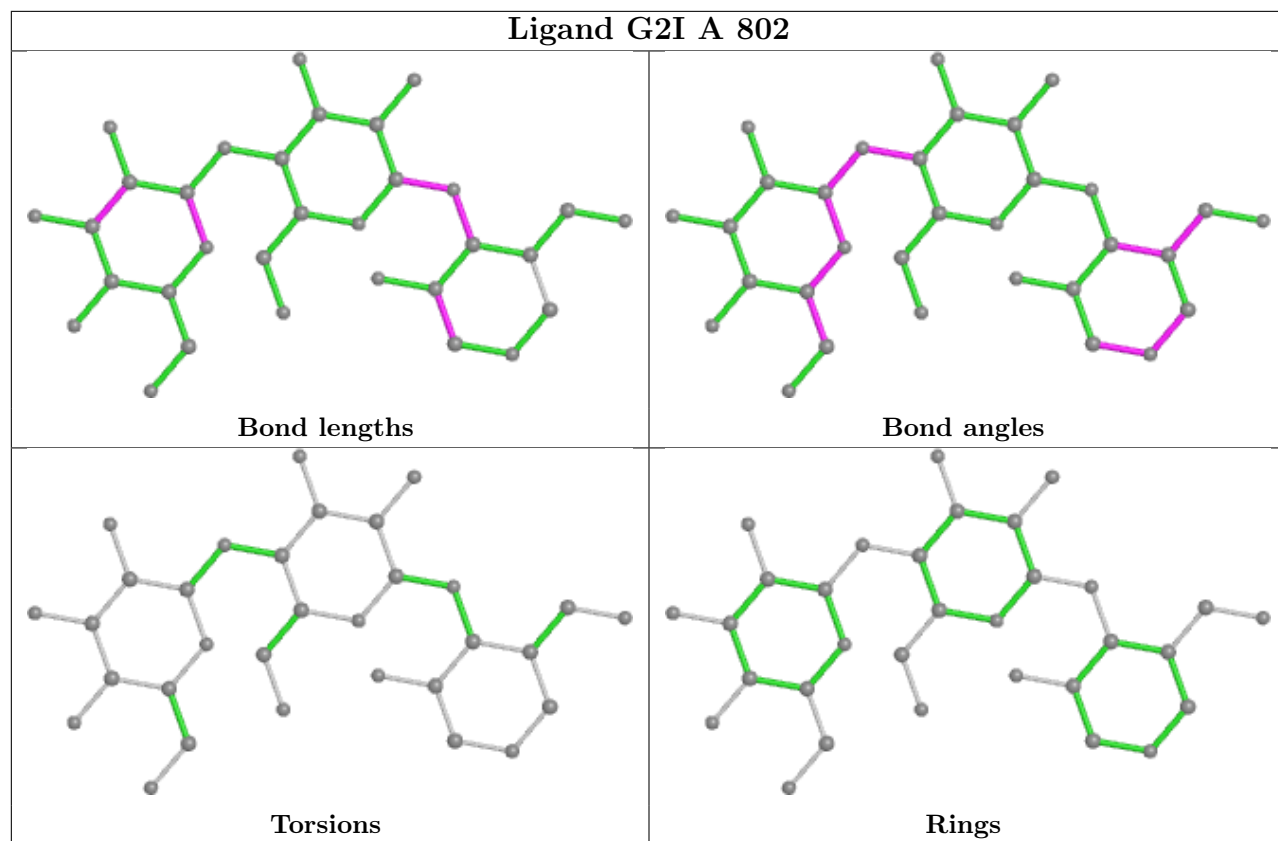
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	813	EDO	1	0
7	A	819	MLI	2	0
2	A	802	G2I	4	0
6	A	817	EDO	1	0
6	A	811	EDO	2	0
6	A	815	EDO	2	0
6	A	814[A]	EDO	1	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	700/709 (98%)	-0.30	17 (2%) 59 68	8, 15, 34, 64	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	TYR	3.8
1	A	245	ASN	3.4
1	A	667	ALA	3.4
1	A	673	ASN	3.3
1	A	674	GLY	2.6
1	A	494	PRO	2.5
1	A	672	GLU	2.5
1	A	124	ALA	2.5
1	A	669	GLY	2.5
1	A	668	THR	2.5
1	A	213	ASN	2.4
1	A	662	SER	2.3
1	A	66	ARG	2.2
1	A	491	THR	2.2
1	A	493	ALA	2.1
1	A	90[A]	ASN	2.0
1	A	703	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 monosaccharides in this entry.

6.4 Ligands

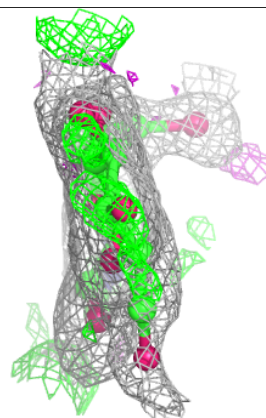
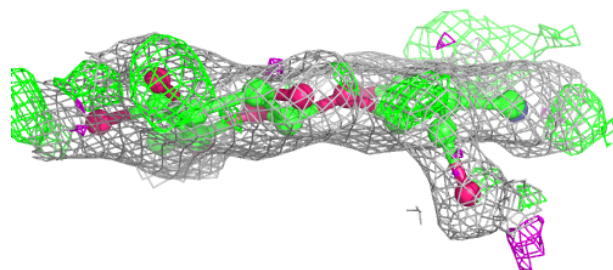
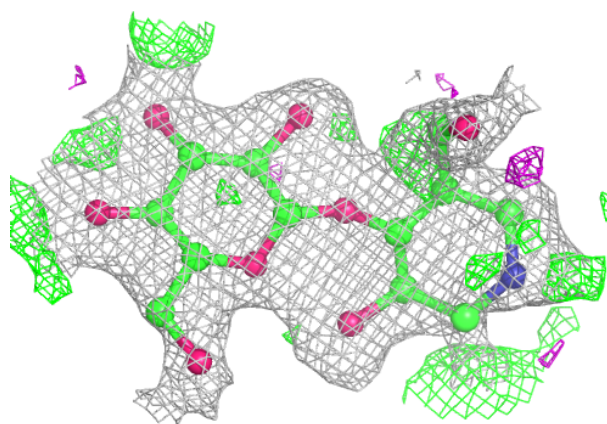
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	817	4/4	0.77	0.31	20,21,21,23	4
3	9MR	A	803	21/21	0.80	0.16	29,37,44,47	0
6	EDO	A	813	4/4	0.81	0.23	23,24,25,27	4
6	EDO	A	809[A]	4/4	0.82	0.27	27,29,31,32	4
6	EDO	A	809[B]	4/4	0.82	0.27	30,30,31,31	4
7	MLI	A	819	7/7	0.82	0.21	35,38,40,46	7
6	EDO	A	815	4/4	0.83	0.19	38,40,42,43	4
6	EDO	A	812[B]	4/4	0.83	0.18	44,48,50,50	4
6	EDO	A	812[A]	4/4	0.83	0.18	43,44,46,46	4
6	EDO	A	814[B]	4/4	0.84	0.18	41,44,46,48	4
6	EDO	A	814[A]	4/4	0.84	0.18	41,43,43,44	4
8	ACT	A	820	4/4	0.85	0.23	42,43,43,47	4
6	EDO	A	816	4/4	0.89	0.23	13,14,14,15	4
6	EDO	A	811	4/4	0.89	0.48	21,21,22,22	4
6	EDO	A	810	4/4	0.90	0.20	32,33,34,41	4
6	EDO	A	818	4/4	0.90	0.14	37,37,39,40	4
6	EDO	A	807	4/4	0.95	0.10	24,24,27,29	0
5	NA	A	806	1/1	0.95	0.10	27,27,27,27	1
6	EDO	A	808[B]	4/4	0.96	0.12	20,24,25,25	4
6	EDO	A	808[A]	4/4	0.96	0.12	22,28,30,31	4
2	G2I	A	801	32/32	0.97	0.08	12,16,19,25	0
4	CA	A	805	1/1	0.98	0.06	24,24,24,24	1
2	G2I	A	802	32/32	0.98	0.08	11,15,26,34	0
4	CA	A	804	1/1	0.99	0.05	17,17,17,17	1

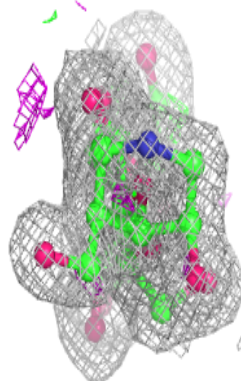
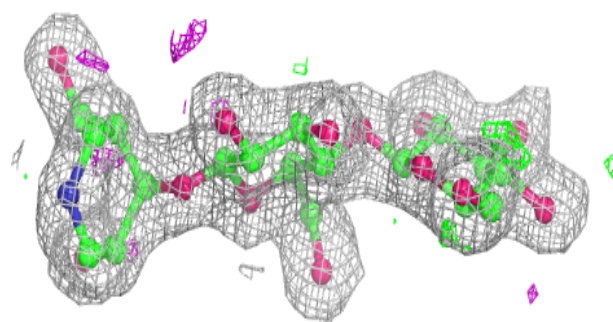
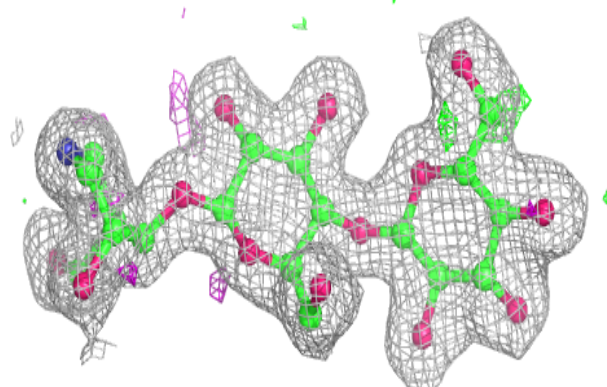
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

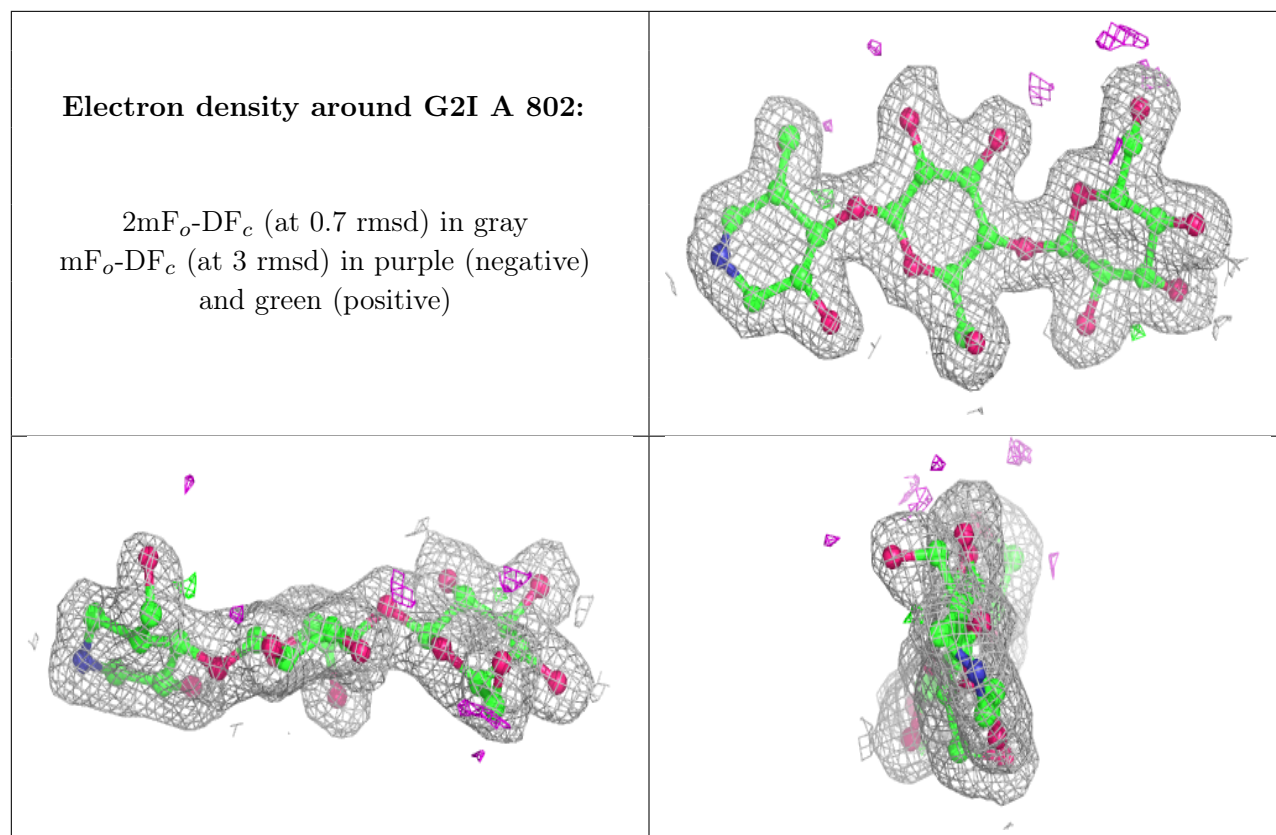
Electron density around 9MR A 803:

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

**Electron density around G2I A 801:**

$2mF_o-DF_c$ (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.