Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 04:22 pm BST

PDB ID	:	8AGP
Title	:	Halogenated product of limonene epoxide turnover by epoxide hydrolase from metagenomic source ch65
Authors	:	Isupov, M.N.; De Rose, S.A.; Mitchell, D.; Littlechild, J.A.
Deposited on	:	2022-07-20
Resolution	:	1.49 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:

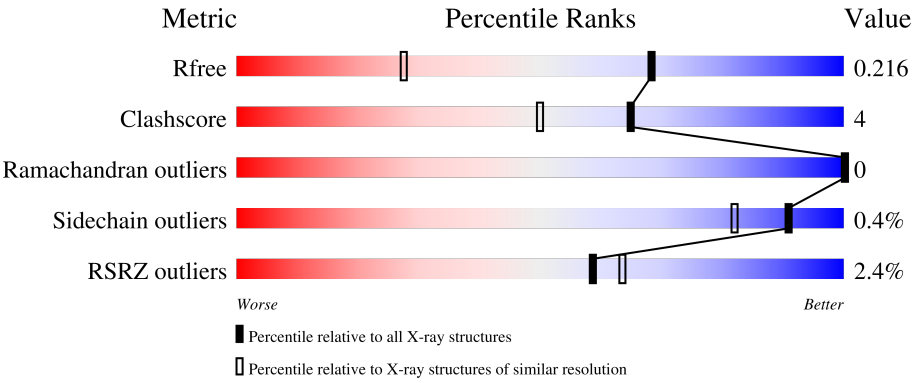
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

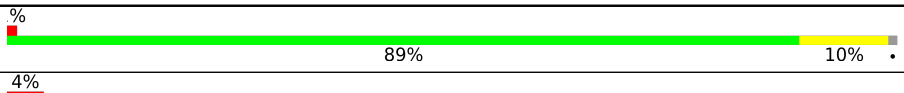
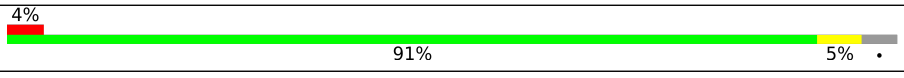
The reported resolution of this entry is 1.49 Å.

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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	AAA	299	
1	BBB	299	

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
4	EDO	AAA	507	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5643 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.

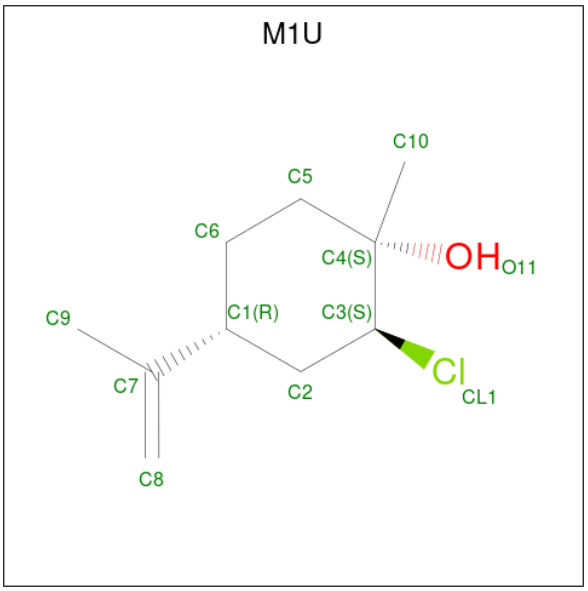
- Molecule 1 is a protein called Alpha/beta epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	297	Total	C	N	O	S	0	34	0
			2649	1758	438	445	8			
1	BBB	287	Total	C	N	O	S	0	19	0
			2483	1639	412	425	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	294	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	295	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	296	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	297	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	298	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	299	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	294	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	295	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	296	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	297	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	298	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	299	HIS	-	expression tag	UNP A0A1U9WZ52

- Molecule 2 is (1 {S},2 {S},4 {R})-2-chloranyl-1-methyl-4-prop-1-en-2-yl-cyclohexan -1-ol (three-letter code: M1U) (formula: $C_{10}H_{17}ClO$) (labeled as "Ligand of Interest" by depositor).

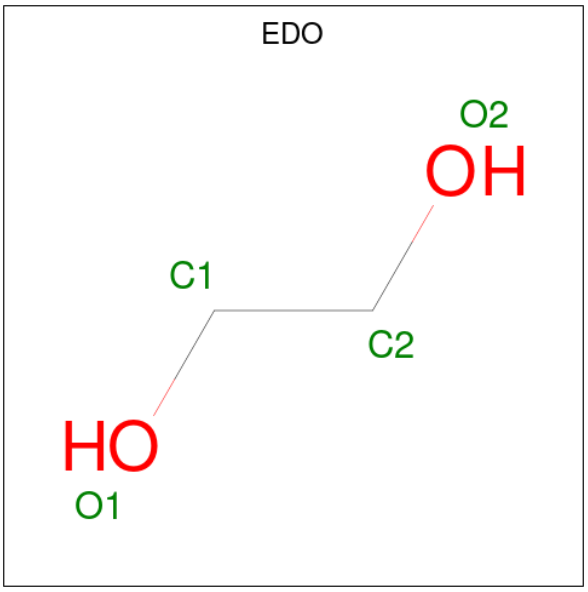


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C Cl O 12 10 1 1	0	0
2	AAA	1	Total C Cl O 12 10 1 1	0	0
2	BBB	1	Total C Cl O 12 10 1 1	0	0
2	BBB	1	Total C Cl O 12 10 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	4	Total Cl 4 4	0	0
3	BBB	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Na 1 1	0	0
5	BBB	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	278	Total O 278 278	0	0

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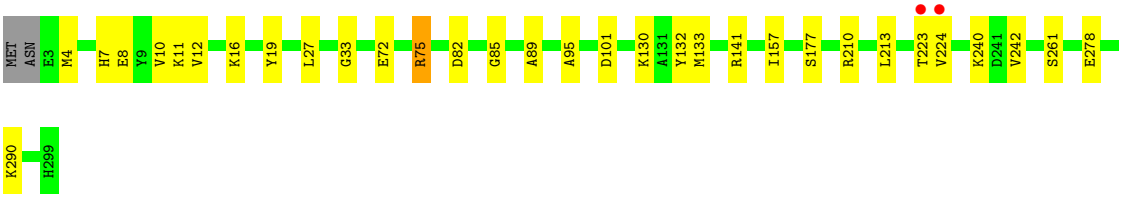
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BBB	154	Total 154	O 154	0	0

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.

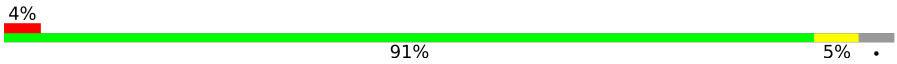
• Molecule 1: Alpha/beta epoxide hydrolase

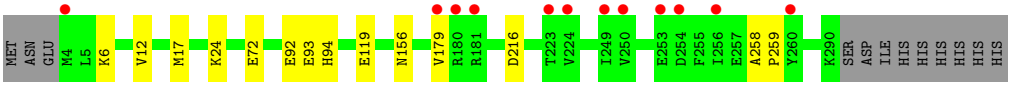
Chain AAA:



• Molecule 1: Alpha/beta epoxide hydrolase

Chain BBB:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.83Å 46.11Å 93.00Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	51.26 – 1.49 51.26 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (51.26-1.49) 99.1 (51.26-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.178 , 0.216 0.178 , 0.216	Depositor DCC
R_{free} test set	4702 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5643	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, EDO, NA, M1U

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	AAA	0.52	0/2823	0.88	4/3812 (0.1%)
1	BBB	0.42	0/2608	0.75	0/3528
All	All	0.48	0/5431	0.82	4/7340 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	75[A]	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	AAA	75[B]	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	AAA	210	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	AAA	261	SER	N-CA-CB	-5.13	102.80	110.50

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	AAA	2649	0	2797	29	0
1	BBB	2483	0	2565	14	0
2	AAA	24	0	0	1	0
2	BBB	24	0	0	1	0
3	AAA	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	1	0	0	0	0
4	AAA	20	0	30	9	0
4	BBB	4	0	6	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
6	AAA	278	0	0	6	0
6	BBB	154	0	0	4	0
All	All	5643	0	5398	43	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 (43) 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:BBB:72[B]:GLU:HG3	6:BBB:548:HOH:O	1.39	1.21
1:AAA:7:HIS:NE2	4:AAA:510:EDO:H12	1.80	0.97
1:AAA:290[A]:LYS:HE2	6:AAA:714:HOH:O	1.72	0.89
1:BBB:12:VAL:HG21	1:BBB:17[B]:MET:SD	2.15	0.86
1:AAA:72[B]:GLU:OE2	1:AAA:75[B]:ARG:NE	2.20	0.74
2:BBB:401:M1U:O11	6:BBB:501:HOH:O	2.05	0.74
1:AAA:278[B]:GLU:OE1	6:AAA:601:HOH:O	2.08	0.71
1:AAA:240[A]:LYS:NZ	6:AAA:602:HOH:O	2.24	0.71
1:AAA:12[B]:VAL:HG11	1:AAA:82:ASP:O	1.91	0.69
1:AAA:11[A]:LYS:HE2	4:AAA:507:EDO:H21	1.73	0.69
1:BBB:12:VAL:HG22	1:BBB:17[B]:MET:HG3	1.74	0.69
1:BBB:6[B]:LYS:HE2	6:BBB:510:HOH:O	1.94	0.67
1:AAA:157[B]:ILE:HD11	1:BBB:216:ASP:OD1	1.96	0.66
1:AAA:132:TYR:HD1	1:AAA:133:MET:HE2	1.61	0.65
1:AAA:12[B]:VAL:HG13	1:AAA:85:GLY:HA3	1.79	0.64
1:AAA:16:LYS:HE3	4:AAA:507:EDO:H11	1.85	0.58
4:AAA:509:EDO:H22	6:AAA:760:HOH:O	2.04	0.58
1:AAA:4[B]:MET:HE3	6:AAA:771:HOH:O	2.06	0.55
1:BBB:12:VAL:CG2	1:BBB:17[B]:MET:SD	2.93	0.54
1:AAA:11[A]:LYS:HG3	4:AAA:507:EDO:H12	1.91	0.52
1:AAA:130[B]:LYS:HE3	1:AAA:224:VAL:O	2.09	0.52
1:BBB:156:ASN:ND2	6:BBB:504:HOH:O	2.39	0.52
1:BBB:93[A]:GLU:OE2	1:BBB:93[A]:GLU:HA	2.09	0.51
1:AAA:8:GLU:HB2	1:AAA:19:TYR:CZ	2.47	0.49
1:BBB:94[A]:HIS:HD2	1:BBB:119[A]:GLU:HB2	1.77	0.49
1:AAA:75[A]:ARG:HG2	4:AAA:509:EDO:H21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:75[B]:ARG:HG2	4:AAA:509:EDO:H21	1.95	0.48
1:BBB:92:GLU:O	1:BBB:93[A]:GLU:OE2	2.33	0.47
1:AAA:10:VAL:HG21	1:AAA:89:ALA:HB1	1.95	0.47
1:BBB:93[B]:GLU:HB3	1:BBB:94[B]:HIS:CE1	2.51	0.46
1:BBB:258:ALA:HB1	1:BBB:259:PRO:HD2	2.00	0.43
1:AAA:33:GLY:HA3	1:AAA:101:ASP:HB3	2.01	0.43
1:BBB:94[A]:HIS:CD2	1:BBB:119[A]:GLU:HB2	2.55	0.42
1:AAA:27:LEU:HD23	1:AAA:95:ALA:HB2	2.02	0.42
1:AAA:213:LEU:HD11	2:AAA:501:M1U:C8	2.50	0.42
1:AAA:132:TYR:HD1	1:AAA:133:MET:CE	2.31	0.41
1:AAA:223:THR:HB	6:AAA:757:HOH:O	2.20	0.41
1:AAA:11[A]:LYS:HE2	4:AAA:507:EDO:H12	2.02	0.41
1:AAA:157[B]:ILE:CD1	1:BBB:216:ASP:OD1	2.67	0.41
1:AAA:7:HIS:CE1	4:AAA:510:EDO:H12	2.53	0.40
1:AAA:12[B]:VAL:HG13	1:AAA:85:GLY:CA	2.50	0.40
1:AAA:141[B]:ARG:H	1:AAA:141[B]:ARG:NE	2.19	0.40
1:AAA:177[A]:SER:HA	1:AAA:242[A]:VAL:HG21	2.04	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	AAA	329/299 (110%)	314 (95%)	15 (5%)	0	100	100
1	BBB	304/299 (102%)	291 (96%)	13 (4%)	0	100	100
All	All	633/598 (106%)	605 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	299/267 (112%)	299 (100%)	0	100 100
1	BBB	274/267 (103%)	272 (99%)	2 (1%)	84 69
All	All	573/534 (107%)	571 (100%)	2 (0%)	91 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	24	LYS
1	BBB	179	VAL

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	M1U	BBB	402	-	11,12,12	0.94	1 (9%)	13,18,18	1.76	3 (23%)
2	M1U	BBB	401	-	11,12,12	1.03	1 (9%)	13,18,18	2.08	4 (30%)
4	EDO	AAA	508	-	3,3,3	0.29	0	2,2,2	0.66	0
4	EDO	AAA	511	-	3,3,3	0.15	0	2,2,2	0.38	0
4	EDO	AAA	507	-	3,3,3	0.66	0	2,2,2	1.56	1 (50%)
2	M1U	AAA	502	-	11,12,12	1.54	2 (18%)	13,18,18	1.11	1 (7%)
4	EDO	AAA	510	-	3,3,3	0.20	0	2,2,2	1.01	0
4	EDO	BBB	404	-	3,3,3	0.10	0	2,2,2	0.23	0
2	M1U	AAA	501	-	11,12,12	1.81	4 (36%)	13,18,18	1.43	1 (7%)
4	EDO	AAA	509	-	3,3,3	0.18	0	2,2,2	0.27	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
2	M1U	BBB	402	-	-	0/4/20/20	0/1/1/1
2	M1U	BBB	401	-	-	4/4/20/20	0/1/1/1
4	EDO	AAA	508	-	-	1/1/1/1	-
4	EDO	AAA	511	-	-	1/1/1/1	-
4	EDO	AAA	507	-	-	1/1/1/1	-
2	M1U	AAA	502	-	-	0/4/20/20	0/1/1/1
4	EDO	AAA	510	-	-	0/1/1/1	-
4	EDO	BBB	404	-	-	1/1/1/1	-
2	M1U	AAA	501	-	-	0/4/20/20	0/1/1/1
4	EDO	AAA	509	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	M1U	O11-C4	3.34	1.50	1.44
2	AAA	502	M1U	C5-C4	3.23	1.57	1.53
2	AAA	501	M1U	C2-C1	3.19	1.60	1.53
2	BBB	401	M1U	C3-CL1	2.76	1.86	1.81
2	BBB	402	M1U	C5-C4	2.64	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	502	M1U	C2-C3	2.57	1.56	1.52
2	AAA	501	M1U	C5-C4	2.40	1.56	1.53
2	AAA	501	M1U	C10-C4	-2.35	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	M1U	O11-C4-C10	-4.89	97.42	108.13
2	BBB	402	M1U	C5-C6-C1	3.48	117.22	111.04
2	AAA	502	M1U	C2-C1-C7	-3.26	107.13	112.65
2	BBB	401	M1U	O11-C4-C5	2.81	113.67	107.69
2	BBB	402	M1U	C10-C4-C5	2.80	114.82	111.03
2	BBB	402	M1U	O11-C4-C10	-2.45	102.75	108.13
2	BBB	401	M1U	C10-C4-C5	-2.35	107.86	111.03
2	BBB	401	M1U	C2-C3-CL1	2.31	111.53	109.20
2	AAA	501	M1U	C2-C3-CL1	-2.24	106.94	109.20
4	AAA	507	EDO	O1-C1-C2	2.00	126.31	111.91

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	401	M1U	C2-C1-C7-C8
2	BBB	401	M1U	C2-C1-C7-C9
4	AAA	507	EDO	O1-C1-C2-O2
4	AAA	508	EDO	O1-C1-C2-O2
4	AAA	511	EDO	O1-C1-C2-O2
4	BBB	404	EDO	O1-C1-C2-O2
4	AAA	509	EDO	O1-C1-C2-O2
2	BBB	401	M1U	C6-C1-C7-C8
2	BBB	401	M1U	C6-C1-C7-C9

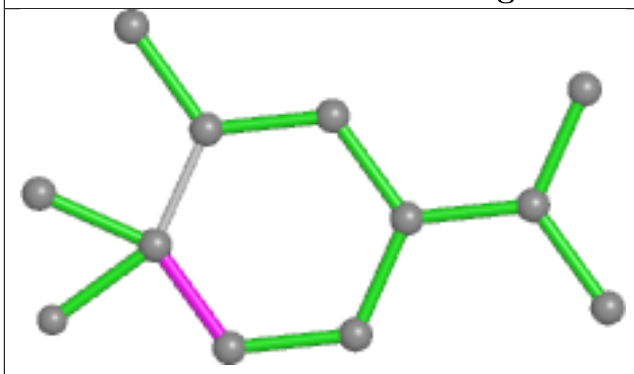
There are no ring outliers.

5 monomers are involved in 11 short contacts:

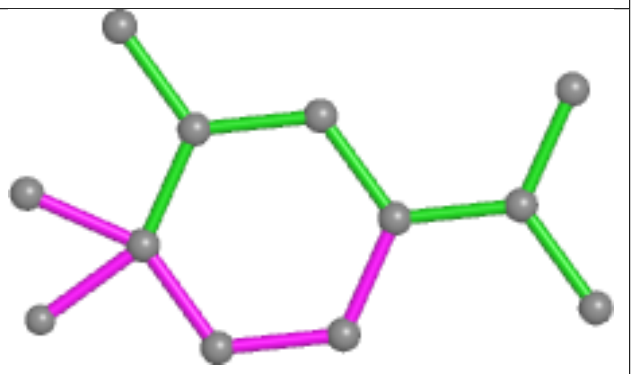
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	401	M1U	1	0
4	AAA	507	EDO	4	0
4	AAA	510	EDO	2	0
2	AAA	501	M1U	1	0
4	AAA	509	EDO	3	0

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 then 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.

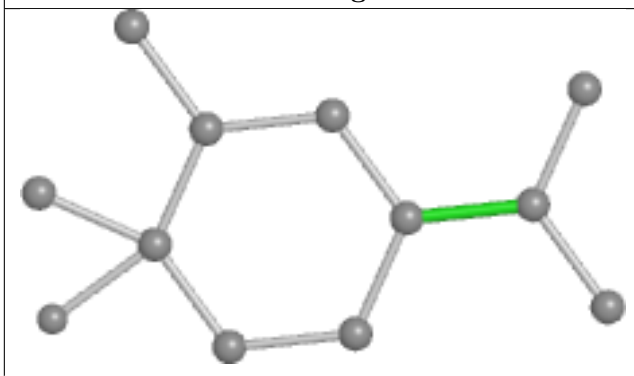
Ligand M1U BBB 402



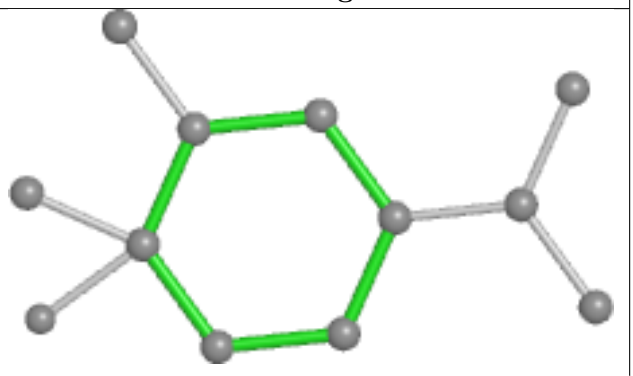
Bond lengths



Bond angles

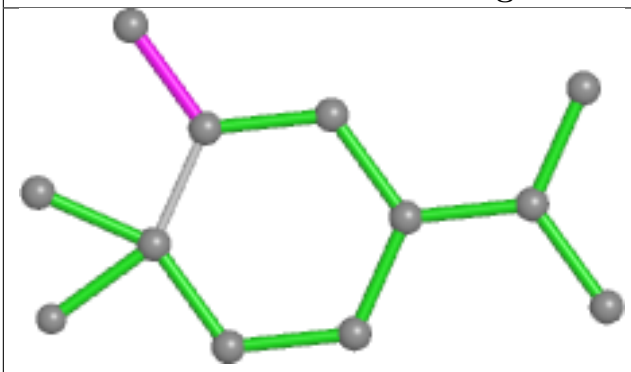


Torsions

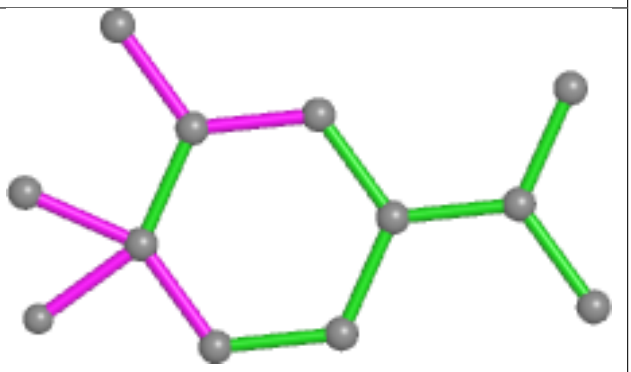


Rings

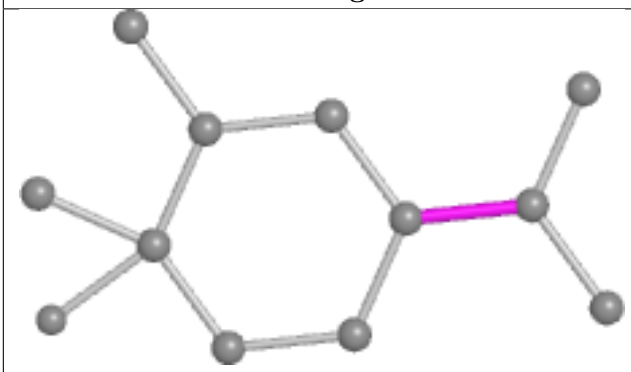
Ligand M1U BBB 401



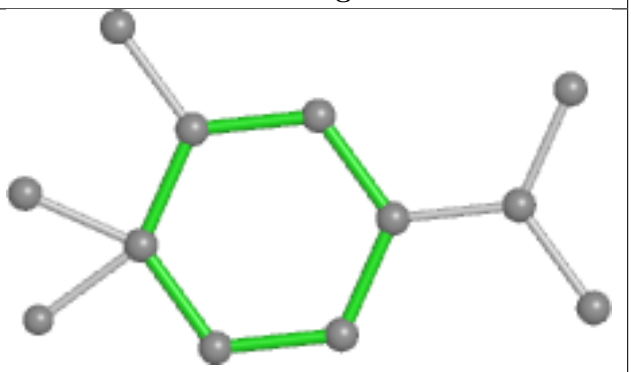
Bond lengths



Bond angles

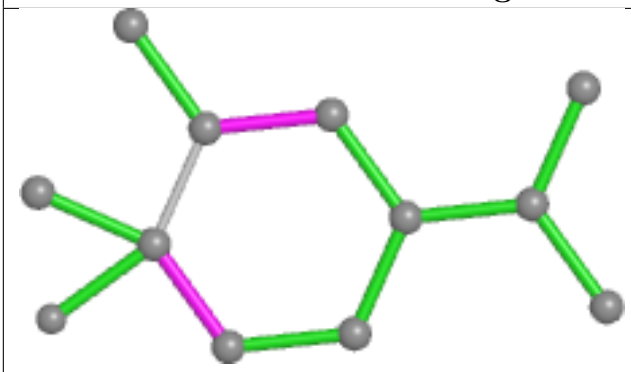


Torsions

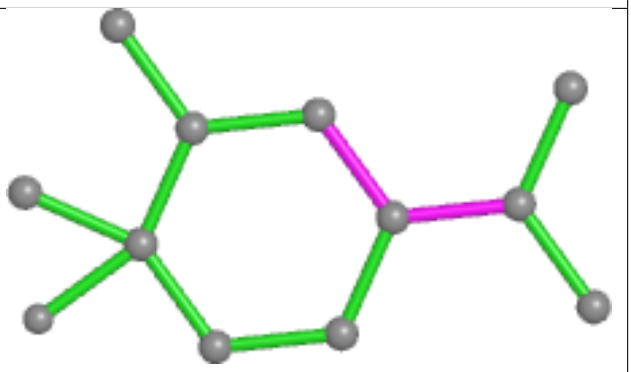


Rings

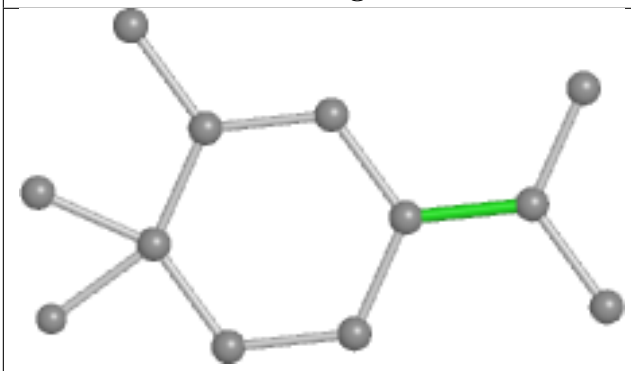
Ligand M1U AAA 502



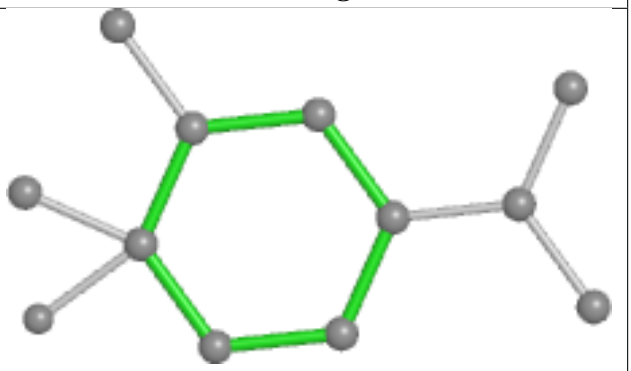
Bond lengths



Bond angles

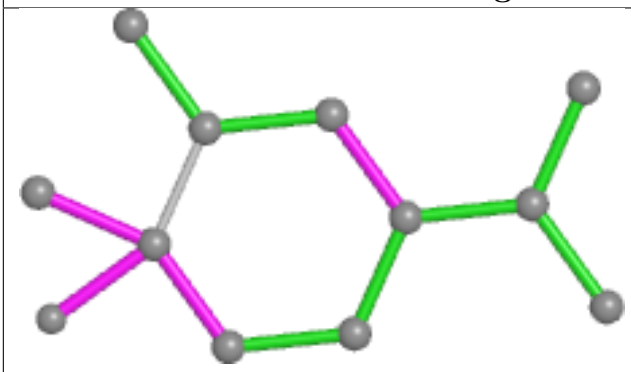


Torsions

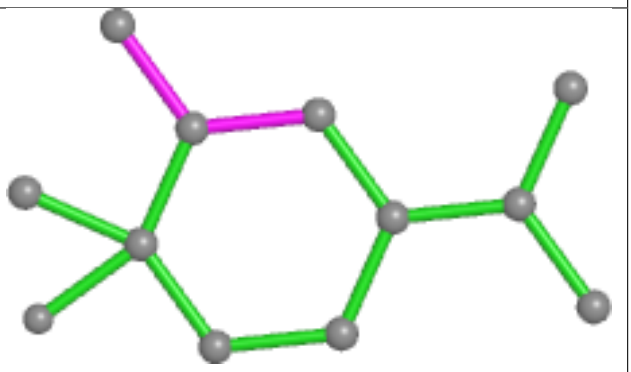


Rings

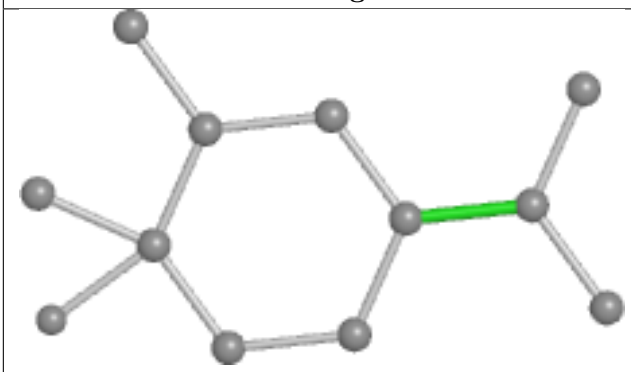
Ligand M1U AAA 501



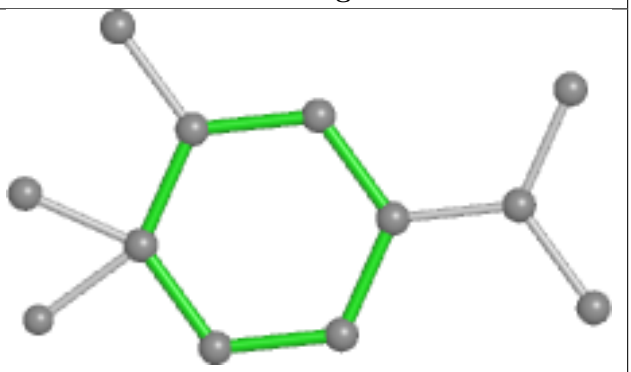
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	AAA	297/299 (99%)	-0.50	2 (0%) 87 90	9, 17, 32, 70	0
1	BBB	287/299 (95%)	-0.01	12 (4%) 36 40	15, 29, 59, 116	0
All	All	584/598 (97%)	-0.26	14 (2%) 59 63	9, 22, 54, 116	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	180	ARG	4.3
1	BBB	179	VAL	3.2
1	BBB	254	ASP	3.2
1	AAA	224	VAL	2.9
1	BBB	223	THR	2.8
1	AAA	223	THR	2.7
1	BBB	260	TYR	2.7
1	BBB	249	ILE	2.6
1	BBB	250	VAL	2.6
1	BBB	181[A]	ARG	2.5
1	BBB	256	ILE	2.4
1	BBB	253	GLU	2.3
1	BBB	224	VAL	2.1
1	BBB	4	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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 (i)

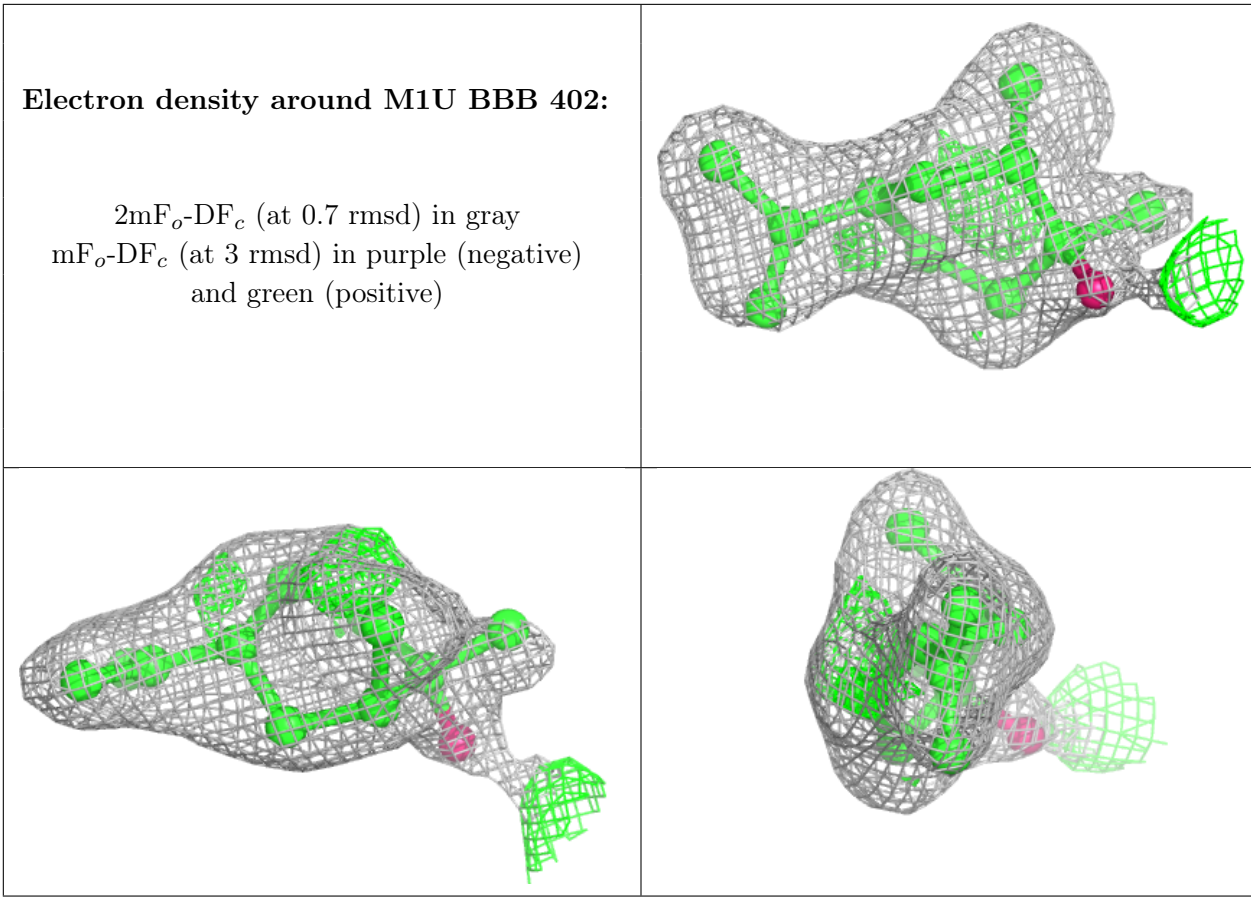
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	NA	AAA	512	1/1	0.67	0.12	56,56,56,56	0
4	EDO	AAA	511	4/4	0.77	0.12	45,47,52,55	0
4	EDO	BBB	404	4/4	0.82	0.13	49,53,62,64	0
2	M1U	BBB	402	12/12	0.83	0.12	28,39,57,72	0
4	EDO	AAA	509	4/4	0.88	0.18	33,38,42,63	0
4	EDO	AAA	507	4/4	0.88	0.12	21,26,38,40	0
4	EDO	AAA	508	4/4	0.90	0.16	30,35,36,70	0
4	EDO	AAA	510	4/4	0.92	0.13	30,33,36,49	0
2	M1U	BBB	401	12/12	0.92	0.09	19,28,38,40	0
5	NA	BBB	405	1/1	0.92	0.23	49,49,49,49	0
2	M1U	AAA	501	12/12	0.97	0.07	12,16,17,20	0
2	M1U	AAA	502	12/12	0.97	0.07	12,16,17,22	0
3	CL	BBB	403	1/1	0.98	0.04	29,29,29,29	0
3	CL	AAA	503	1/1	0.99	0.04	26,26,26,26	0
3	CL	AAA	504	1/1	0.99	0.07	18,18,18,18	0
3	CL	AAA	506	1/1	0.99	0.04	30,30,30,30	0
3	CL	AAA	505	1/1	1.00	0.04	19,19,19,19	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.

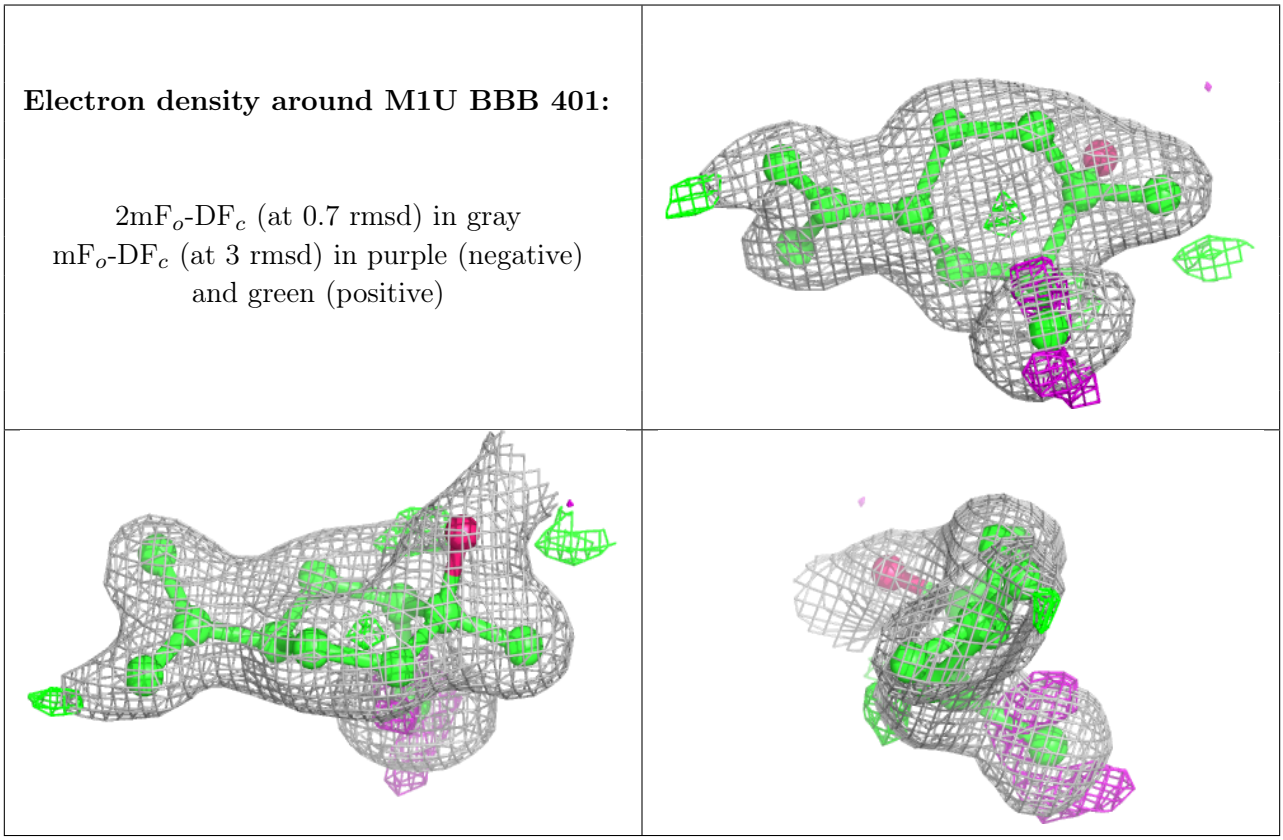
Electron density around M1U BBB 402:

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



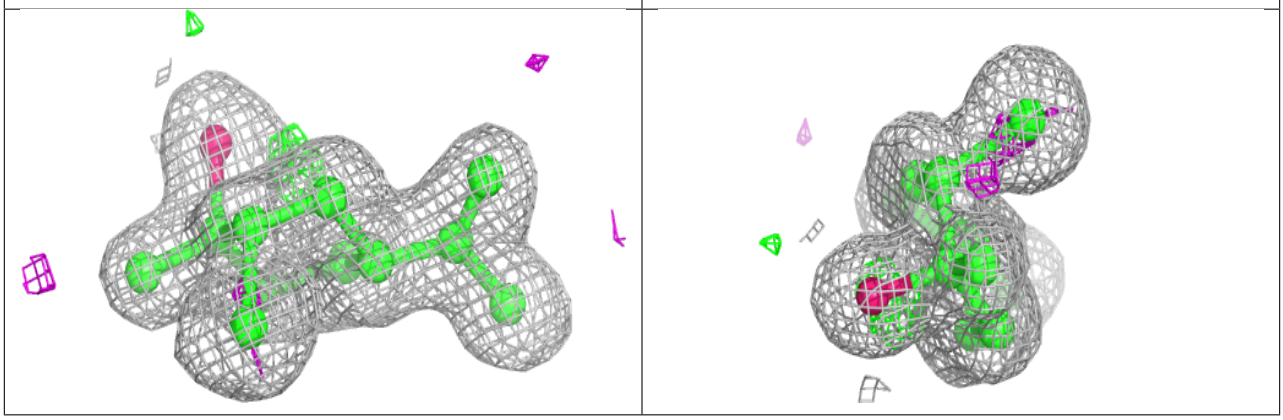
Electron density around M1U BBB 401:

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



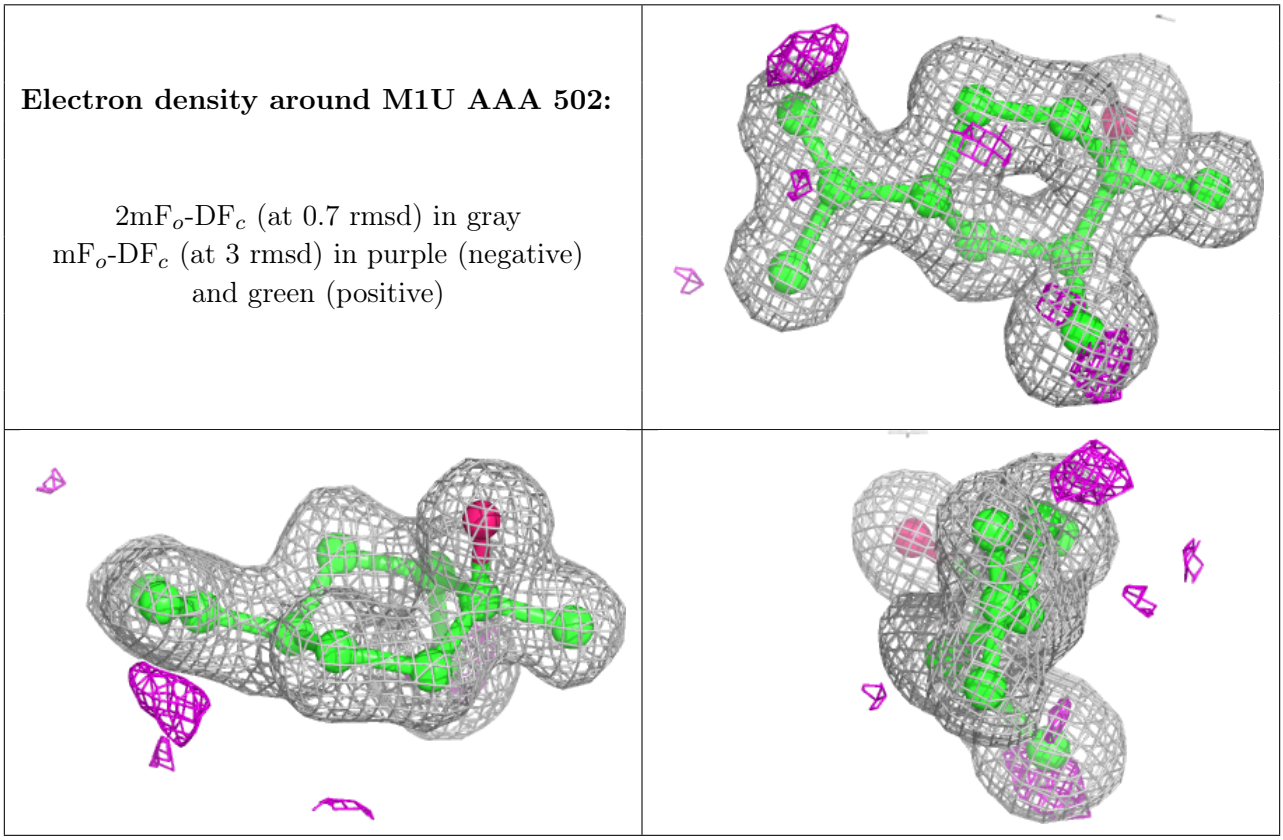
Electron density around M1U AAA 501:

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



Electron density around M1U AAA 502:

$2mF_o$-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.