



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 09:41 PM EDT

PDB ID : 7UZ1
Title : Structure of beta-glycosidase from *Sulfolobus solfataricus* in complex with C5a-bromo-valienide.
Authors : Danby, P.M.; Jeong, A.; Sim, L.; Sweeney, R.P.; Wardman, J.F.; Karimi, R.; Geissner, A.; Worrall, L.J.; Strynadka, N.C.J.; Withers, S.G.
Deposited on : 2022-05-08
Resolution : 1.58 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 : 2.36
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) : 2.36

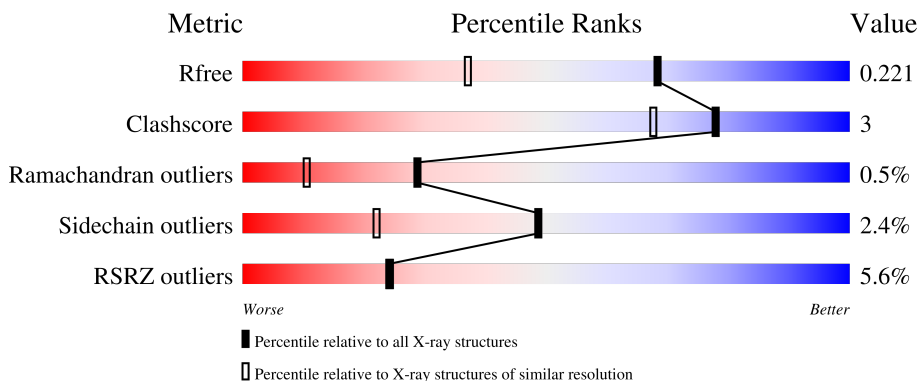
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	489	 4% 91% 9%
1	B	489	 7% 91% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15902 atoms, of which 7541 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.

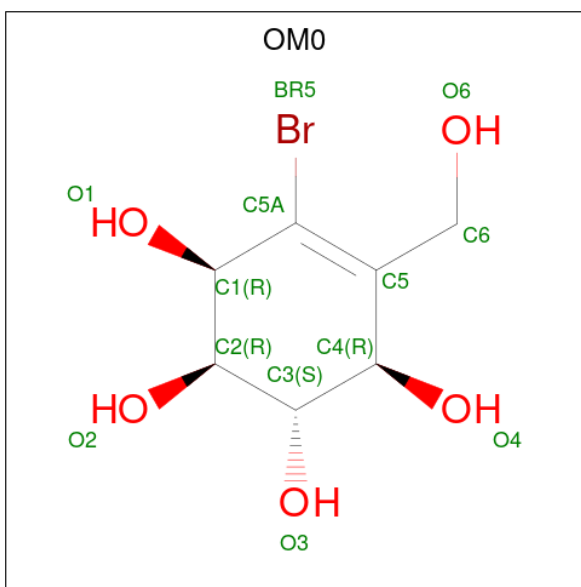
- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	489	7738	2556	3761	681	728	12	120	0	0
1	B	489	7718	2548	3754	682	722	12	118	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	HIS	ALA	engineered mutation	UNP A0A0E3K5E4
B	235	HIS	ALA	engineered mutation	UNP A0A0E3K5E4

- Molecule 2 is (1R,2S,3R,4R)-5-bromo-6-(hydroxymethyl)cyclohex-5-ene-1,2,3,4-tetrol (three-letter code: OM0) (formula: C₇H₁₁BrO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	H	O		
2	A	1	22	1	7	10	4	0	
2	B	1	22	1	7	10	4	0	

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	B	1	10	2	6	2	1	0

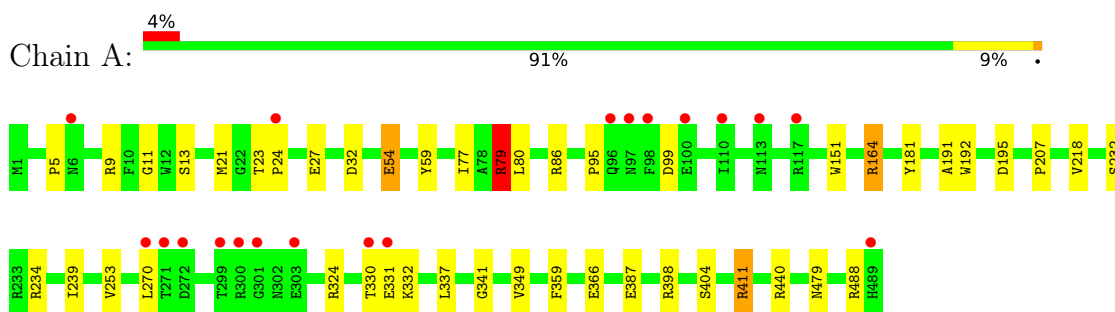
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	209	209	209	0	0
4	B	183	183	183	0	0

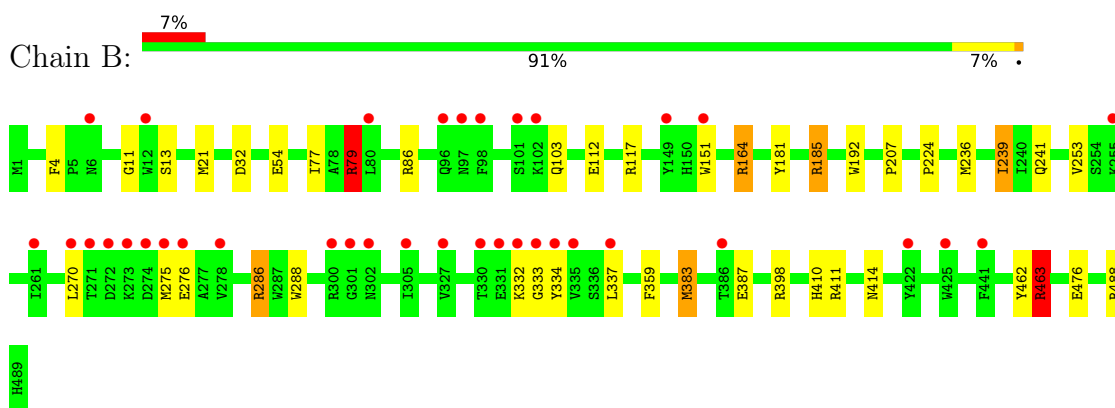
3 Residue-property plots

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: Beta-galactosidase



- Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.09Å 168.09Å 95.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.30 – 1.58 43.26 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.30-1.58) 99.8 (43.26-1.58)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.58Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.212 0.198 , 0.221	Depositor DCC
R_{free} test set	10227 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15902	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: EDO, OM0

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	0.85	4/4107 (0.1%)	1.14	18/5585 (0.3%)
1	B	0.84	1/4094 (0.0%)	1.11	23/5566 (0.4%)
All	All	0.85	5/8201 (0.1%)	1.12	41/11151 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	GLU	CD-OE2	9.94	1.36	1.25
1	A	387	GLU	CD-OE2	9.87	1.36	1.25
1	A	366	GLU	CD-OE1	6.96	1.33	1.25
1	A	79	ARG	CD-NE	-5.49	1.37	1.46
1	A	54	GLU	CD-OE2	5.27	1.31	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NE-CZ-NH2	-18.48	111.06	120.30
1	B	79	ARG	NE-CZ-NH2	-17.16	111.72	120.30
1	A	79	ARG	NE-CZ-NH1	16.90	128.75	120.30
1	A	164	ARG	NE-CZ-NH1	16.58	128.59	120.30
1	B	164	ARG	NE-CZ-NH1	15.74	128.17	120.30
1	B	79	ARG	NE-CZ-NH1	15.25	127.92	120.30
1	B	164	ARG	NE-CZ-NH2	-15.08	112.76	120.30
1	A	164	ARG	NE-CZ-NH2	-14.71	112.94	120.30
1	A	86	ARG	NE-CZ-NH2	-13.85	113.38	120.30
1	A	86	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	B	286	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	B	463	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	164	ARG	CD-NE-CZ	8.96	136.15	123.60
1	B	463	ARG	NE-CZ-NH1	8.70	124.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	79	ARG	CB-CG-CD	-8.49	89.53	111.60
1	B	164	ARG	CD-NE-CZ	8.46	135.44	123.60
1	A	398	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	79	ARG	CD-NE-CZ	7.34	133.87	123.60
1	A	9	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	79	ARG	CG-CD-NE	-6.75	97.62	111.80
1	B	79	ARG	CB-CG-CD	-6.72	94.13	111.60
1	A	79	ARG	CG-CD-NE	-6.71	97.72	111.80
1	B	185	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	79	ARG	CD-NE-CZ	6.42	132.59	123.60
1	B	164	ARG	CG-CD-NE	-6.22	98.73	111.80
1	A	411	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	383	MET	CG-SD-CE	-6.06	90.50	100.20
1	B	241	GLN	CB-CA-C	6.03	122.47	110.40
1	A	86	ARG	CG-CD-NE	-6.01	99.18	111.80
1	B	398	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	462	TYR	CB-CG-CD1	5.76	124.45	121.00
1	B	117	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	440	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	164	ARG	CG-CD-NE	-5.55	100.15	111.80
1	A	411	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	86	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	411	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	117	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	32	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	32	ASP	CB-CG-OD1	5.16	122.95	118.30

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	3977	3761	3728	26	0
1	B	3964	3754	3720	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	10	0	0	0
2	B	12	10	0	0	0
3	B	4	6	6	1	0
4	A	209	0	0	4	0
4	B	183	0	0	5	0
All	All	8361	7541	7454	44	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 (44) 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:13:SER:OG	1:B:79:ARG:HD3	1.73	0.89
1:A:13:SER:OG	1:A:79:ARG:HD3	1.73	0.88
4:A:678:HOH:O	1:B:164:ARG:CD	2.29	0.81
1:A:164:ARG:HD2	4:B:715:HOH:O	1.81	0.80
1:A:23:THR:HB	1:A:24:PRO:CD	2.13	0.79
1:B:270:LEU:HD22	1:B:337:LEU:HD11	1.66	0.78
1:A:164:ARG:CD	4:B:715:HOH:O	2.33	0.76
1:A:270:LEU:HD22	1:A:337:LEU:HD11	1.68	0.75
1:A:488:ARG:NH2	1:B:488:ARG:NH2	2.36	0.72
1:A:23:THR:HB	1:A:24:PRO:HD2	1.72	0.70
4:A:678:HOH:O	1:B:164:ARG:HD3	1.91	0.70
4:A:678:HOH:O	1:B:164:ARG:HD2	1.91	0.69
1:B:286:ARG:HD3	4:B:766:HOH:O	1.95	0.66
1:A:488:ARG:HH22	1:B:488:ARG:NH2	2.01	0.57
1:B:253:VAL:HG12	1:B:253:VAL:O	2.05	0.56
1:A:330:THR:HG22	1:A:332:LYS:H	1.74	0.53
1:A:488:ARG:HH22	1:B:488:ARG:HH22	1.56	0.53
1:B:13:SER:OG	1:B:79:ARG:CD	2.53	0.52
1:B:463:ARG:HD2	4:B:646:HOH:O	2.10	0.52
1:A:207:PRO:HB2	1:A:239:ILE:HG21	1.93	0.51
1:A:270:LEU:HD22	1:A:337:LEU:CD1	2.38	0.51
1:B:270:LEU:HD22	1:B:337:LEU:CD1	2.38	0.50
1:A:13:SER:OG	1:A:79:ARG:CD	2.56	0.49
1:A:164:ARG:HD3	4:B:715:HOH:O	2.08	0.47
1:B:192:TRP:HA	1:B:253:VAL:HG11	1.96	0.47
1:A:21:MET:HB3	1:A:54:GLU:HA	1.97	0.46
1:A:191:ALA:O	1:A:195:ASP:HB2	2.16	0.45
1:A:331:GLU:H	1:A:331:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:TYR:CE1	1:B:185:ARG:HD2	2.52	0.45
1:A:11:GLY:HA3	1:A:77:ILE:O	2.17	0.45
1:B:253:VAL:O	1:B:253:VAL:CG1	2.63	0.45
1:A:95:PRO:HG3	1:A:181:TYR:CE2	2.52	0.44
1:A:330:THR:HG23	1:A:331:GLU:OE2	2.17	0.44
1:A:59:TYR:OH	1:A:80:LEU:HD21	2.18	0.43
1:B:11:GLY:HA3	1:B:77:ILE:O	2.19	0.43
1:A:5:PRO:HD3	4:A:765:HOH:O	2.18	0.43
1:A:404:SER:HA	1:A:479:ASN:HD22	1.83	0.43
1:B:21:MET:HB3	1:B:54:GLU:HA	2.01	0.42
1:B:236:MET:HB3	1:B:288:TRP:HH2	1.84	0.42
1:A:324:ARG:O	1:A:341:GLY:HA3	2.20	0.42
1:B:4:PHE:CZ	1:B:410:HIS:HB2	2.55	0.41
1:B:207:PRO:HB2	1:B:239:ILE:HG21	2.02	0.41
1:A:218:VAL:HG21	3:B:502:EDO:H22	2.02	0.41
1:A:192:TRP:CA	1:A:253:VAL:HG11	2.51	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	487/489 (100%)	473 (97%)	13 (3%)	1 (0%)	47 25
1	B	487/489 (100%)	475 (98%)	8 (2%)	4 (1%)	19 5
All	All	974/978 (100%)	948 (97%)	21 (2%)	5 (0%)	29 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	B	151	TRP

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Mol	Chain	Res	Type
1	B	334	TYR
1	B	332	LYS
1	B	333	GLY

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	410/422 (97%)	402 (98%)	8 (2%)	55	29
1	B	408/422 (97%)	396 (97%)	12 (3%)	42	16
All	All	818/844 (97%)	798 (98%)	20 (2%)	49	22

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	79	ARG
1	A	99	ASP
1	A	232	SER
1	A	234	ARG
1	A	349	VAL
1	A	359	PHE
1	A	411	ARG
1	B	79	ARG
1	B	103	GLN
1	B	112	GLU
1	B	224	PRO
1	B	239	ILE
1	B	275	MET
1	B	276	GLU
1	B	359	PHE
1	B	383	MET
1	B	414	ASN
1	B	463	ARG
1	B	476	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	128	ASN
1	A	235	HIS
1	A	264	ASN
1	A	410	HIS
1	A	477	HIS
1	A	479	ASN
1	B	128	ASN
1	B	410	HIS
1	B	449	ASN
1	B	479	ASN

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](#)

3 ligands are modelled in this entry.

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	OM0	A	501	1	9,12,13	0.99	1 (11%)	8,17,19	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OM0	B	501	1	9,12,13	1.04	0	8,17,19	1.26	1 (12%)
3	EDO	B	502	-	3,3,3	1.86	1 (33%)	2,2,2	0.98	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	OM0	A	501	1	-	0/2/22/26	0/1/1/1
2	OM0	B	501	1	-	0/2/22/26	0/1/1/1
3	EDO	B	502	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	EDO	O1-C1	2.90	1.57	1.42
2	A	501	OM0	BR5-C5A	2.01	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	OM0	O6-C6-C5	-2.56	107.58	112.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	EDO	O1-C1-C2-O2

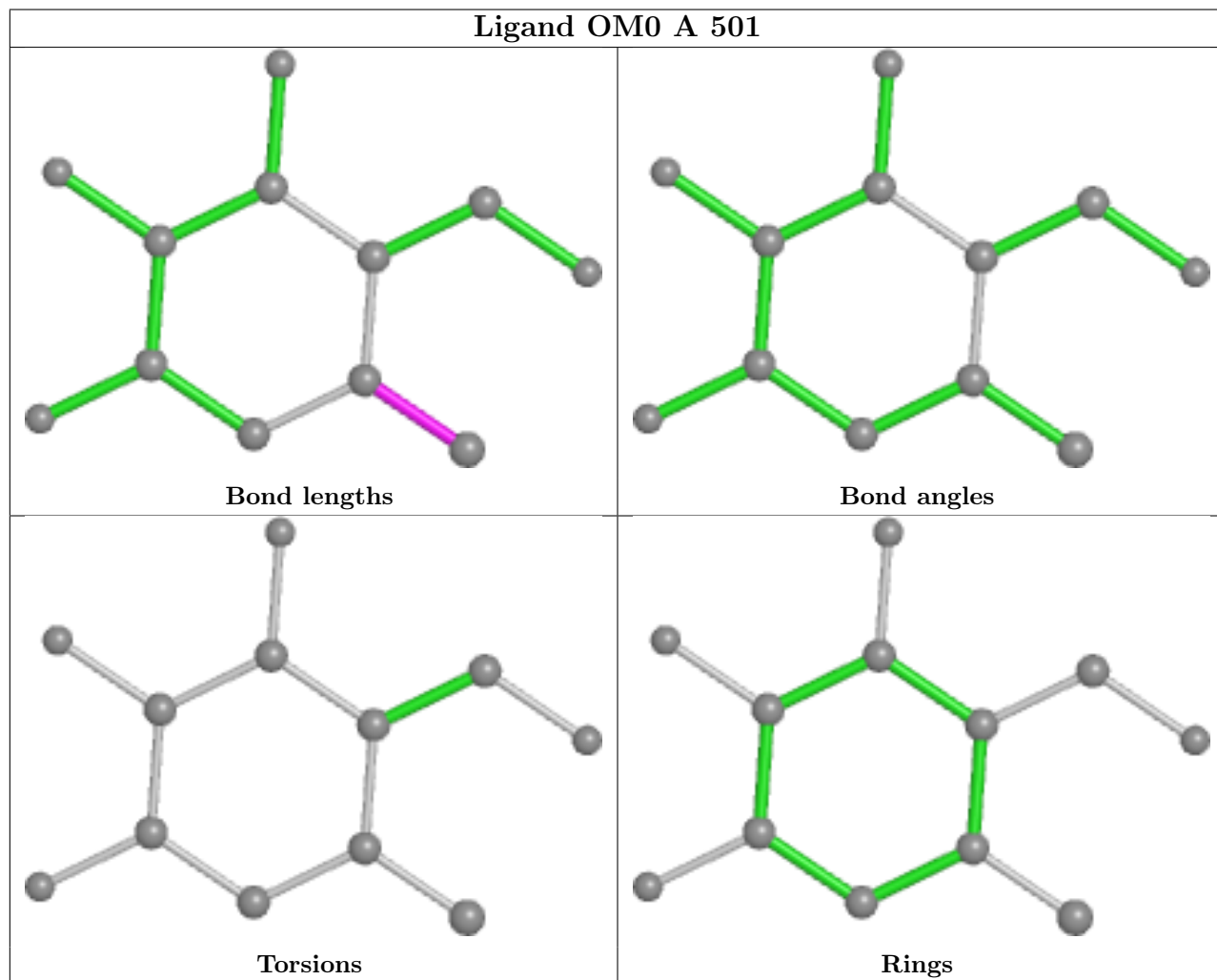
There are no ring outliers.

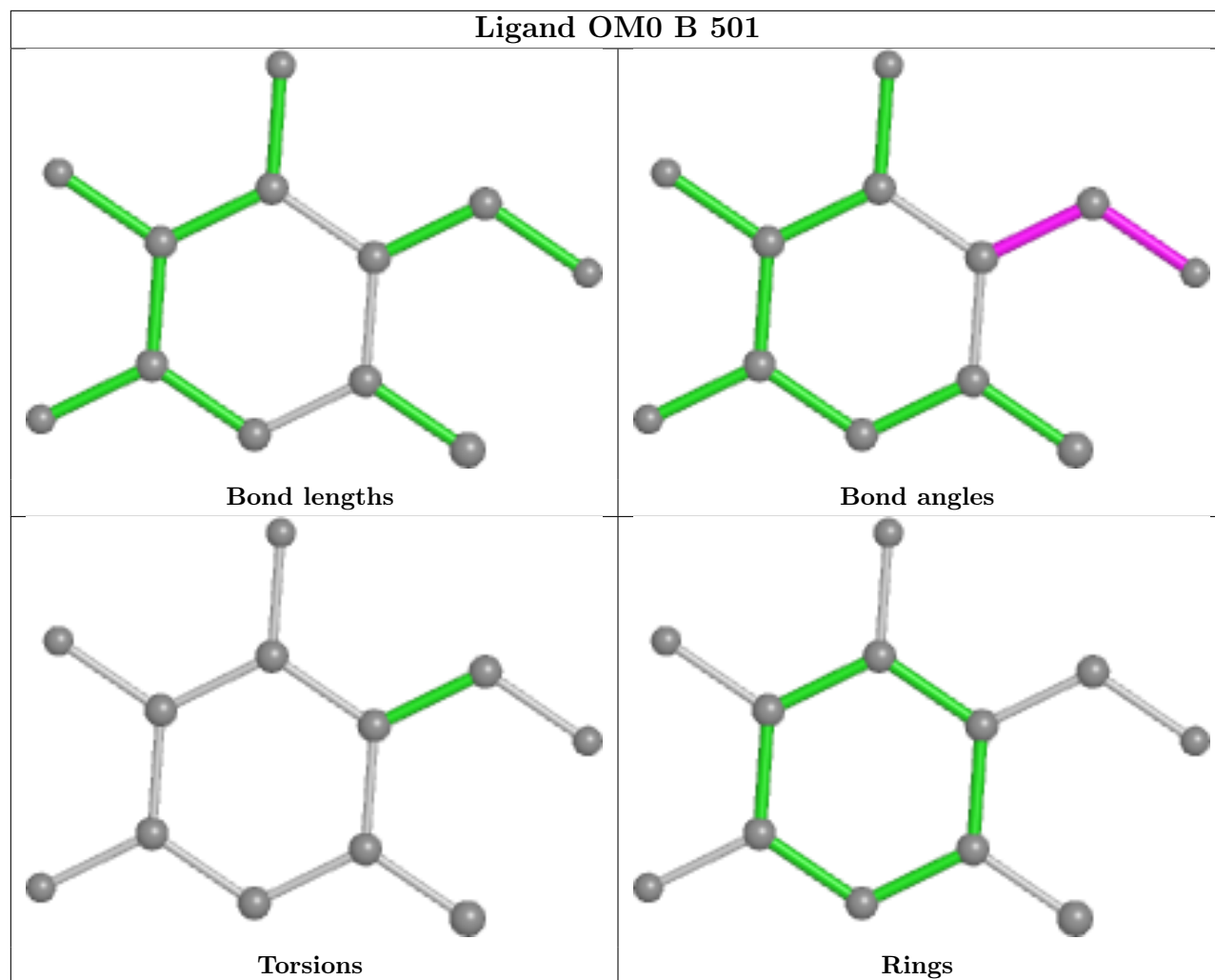
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	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

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, 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	489/489 (100%)	-0.03	19 (3%) 39 40	23, 32, 55, 87	0
1	B	489/489 (100%)	0.28	36 (7%) 14 14	26, 35, 59, 88	0
All	All	978/978 (100%)	0.13	55 (5%) 24 24	23, 33, 57, 88	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	THR	7.9
1	B	333	GLY	7.8
1	B	97	ASN	7.5
1	A	97	ASN	5.6
1	B	335	VAL	5.3
1	B	272	ASP	4.7
1	B	96	GLN	4.6
1	A	301	GLY	4.4
1	B	98	PHE	4.1
1	A	300	ARG	4.0
1	B	6	ASN	3.9
1	B	334	TYR	3.9
1	B	271	THR	3.8
1	A	98	PHE	3.8
1	B	101	SER	3.7
1	B	332	LYS	3.6
1	B	276	GLU	3.5
1	B	261	ILE	3.5
1	B	300	ARG	3.5
1	B	302	ASN	3.3
1	A	303	GLU	3.3
1	A	272	ASP	3.3
1	B	331	GLU	3.3
1	B	275	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	299	THR	3.2
1	B	425	TRP	3.2
1	A	117	ARG	3.1
1	B	270	LEU	3.1
1	A	96	GLN	3.0
1	B	301	GLY	3.0
1	A	271	THR	2.9
1	A	24	PRO	2.9
1	A	331	GLU	2.9
1	B	274	ASP	2.8
1	B	102	LYS	2.7
1	A	6	ASN	2.7
1	B	273	LYS	2.6
1	B	305	ILE	2.6
1	B	337	LEU	2.5
1	B	441	PHE	2.5
1	A	270	LEU	2.5
1	B	80	LEU	2.5
1	B	12	TRP	2.5
1	A	110	ILE	2.4
1	A	100	GLU	2.4
1	B	151	TRP	2.3
1	B	327	VAL	2.3
1	B	386	THR	2.2
1	B	255	LYS	2.2
1	A	489	HIS	2.1
1	A	113	ASN	2.1
1	B	149	TYR	2.1
1	B	422	TYR	2.1
1	B	278	VAL	2.1
1	A	330	THR	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](#)

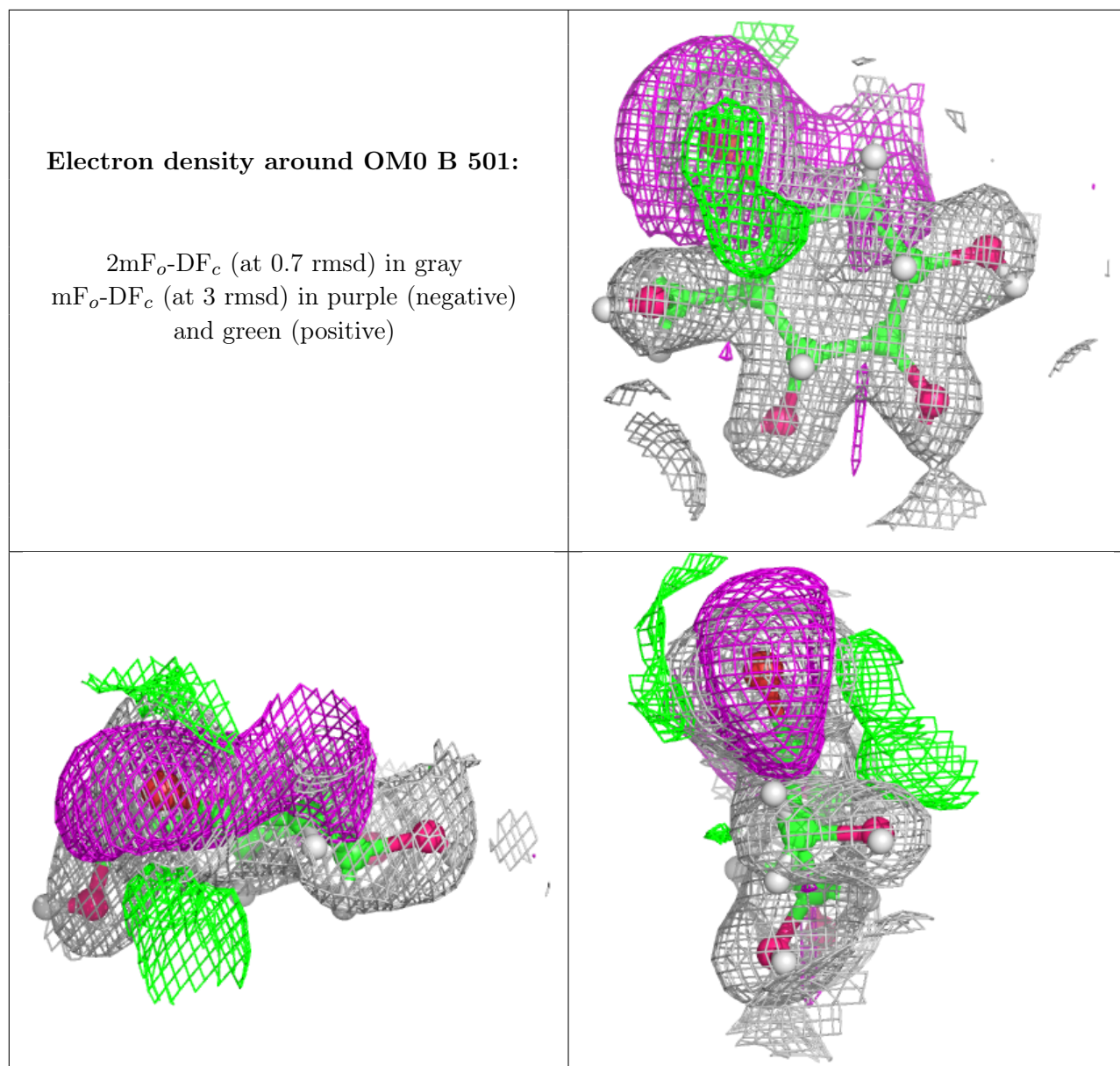
There are no monosaccharides in this entry.

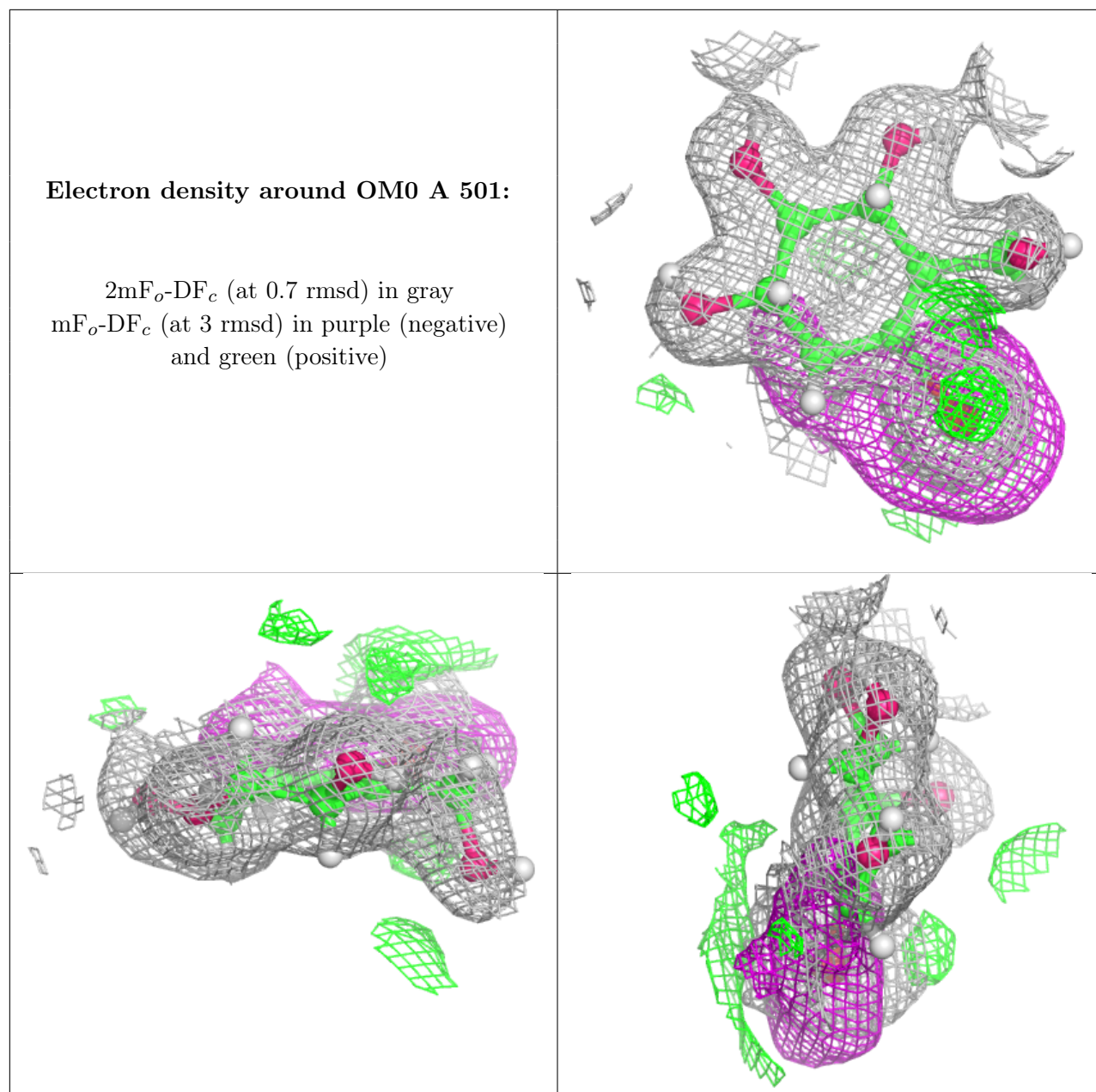
6.4 Ligands

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
3	EDO	B	502	4/4	0.68	0.14	20,41,53,58	1
2	OM0	B	501	12/13	0.95	0.10	26,31,36,43	4
2	OM0	A	501	12/13	0.96	0.09	26,30,34,41	4

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.