



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:52 AM UTC

PDB ID : 5M1I / pdb_00005m1i
Title : Structure of GH36 alpha-galactosidase from *Thermotoga maritima* in a covalent complex with a cyclopropyl carbasugar.
Authors : Pengelly, R.; Gloster, T.
Deposited on : 2016-10-07
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

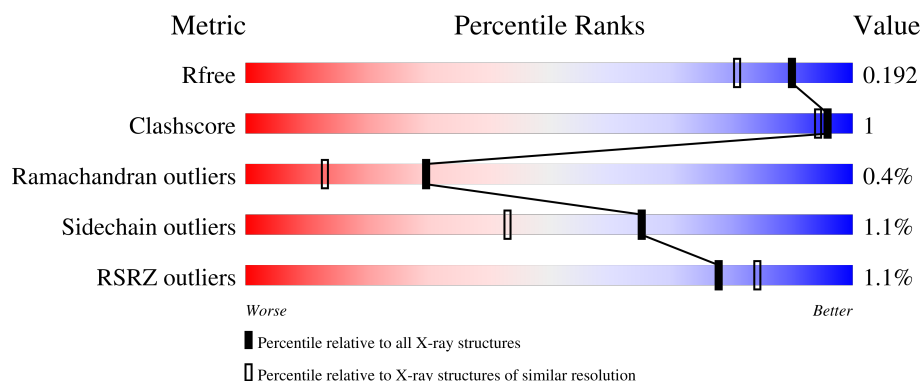
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	575	% 89% . 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4931 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	539	4478	2883	749	827	19	0	16	0

There are 23 discrepancies between the modelled and reference sequences:

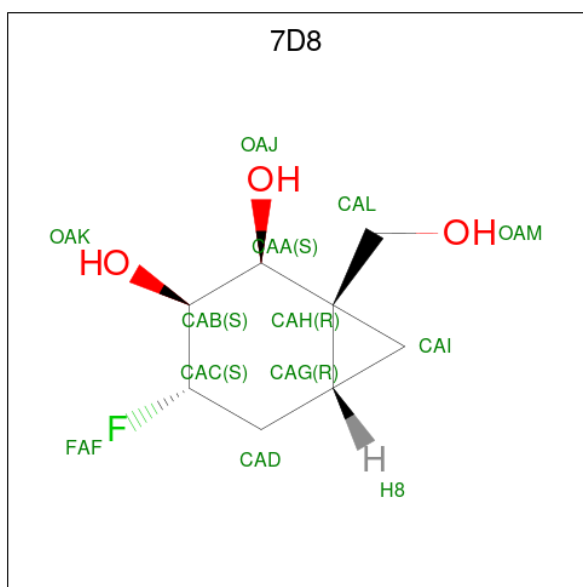
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP O33835
A	-21	GLY	-	expression tag	UNP O33835
A	-20	SER	-	expression tag	UNP O33835
A	-19	SER	-	expression tag	UNP O33835
A	-18	HIS	-	expression tag	UNP O33835
A	-17	HIS	-	expression tag	UNP O33835
A	-16	HIS	-	expression tag	UNP O33835
A	-15	HIS	-	expression tag	UNP O33835
A	-14	HIS	-	expression tag	UNP O33835
A	-13	HIS	-	expression tag	UNP O33835
A	-12	SER	-	expression tag	UNP O33835
A	-11	SER	-	expression tag	UNP O33835
A	-10	GLY	-	expression tag	UNP O33835
A	-9	LEU	-	expression tag	UNP O33835
A	-8	VAL	-	expression tag	UNP O33835
A	-7	PRO	-	expression tag	UNP O33835
A	-6	ARG	-	expression tag	UNP O33835
A	-5	GLY	-	expression tag	UNP O33835
A	-4	SER	-	expression tag	UNP O33835
A	-3	HIS	-	expression tag	UNP O33835
A	-2	MET	-	expression tag	UNP O33835
A	-1	ALA	-	expression tag	UNP O33835
A	0	SER	-	expression tag	UNP O33835

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



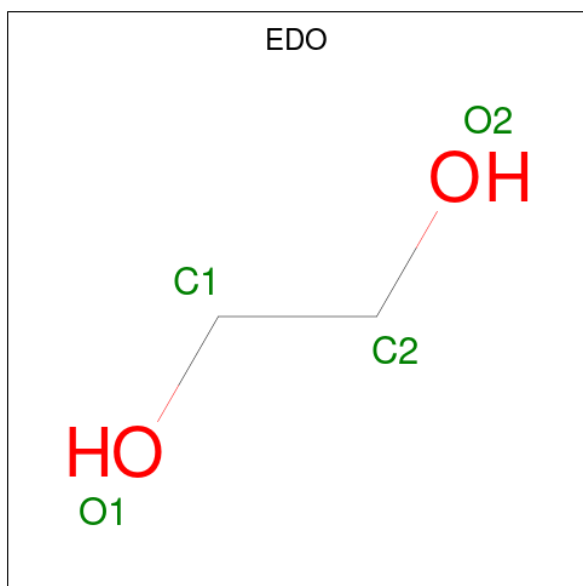
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (1 {R},2 {S},3 {S},4 {S},6 {R})-4-fluoranyl-1-(hydroxymethyl)bicyclo[4.1.0]heptane-2,3-diol (CCD ID: 7D8) (formula: C₈H₁₃FO₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

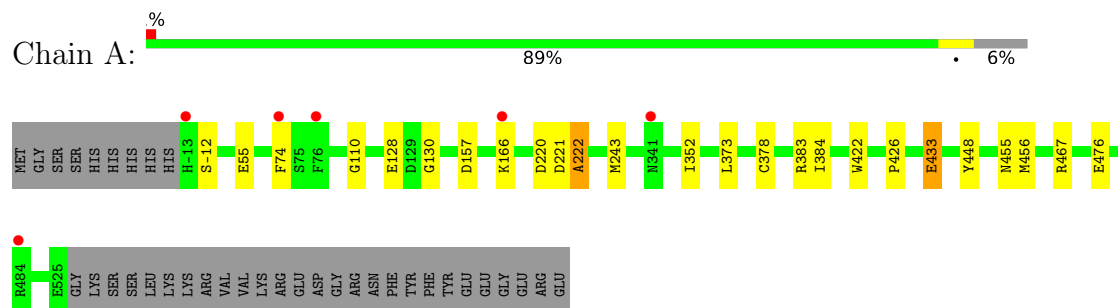
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	360	Total	O	0	3
			363	363		

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: Alpha-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.90Å 96.24Å 97.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.52 – 1.55 68.52 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.52-1.55) 99.9 (68.52-1.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.154 , 0.183 0.168 , 0.192	Depositor DCC
R_{free} test set	4571 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4931	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 7D8, EDO

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	0.94	2/4600 (0.0%)	0.90	1/6235 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	LEU	N-CA	5.25	1.51	1.46
1	A	243	MET	SD-CE	-5.19	1.66	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	MET	CG-SD-CE	-6.86	85.81	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	ARG	Sidechain

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	4478	0	4372	10	0
2	A	30	0	0	0	0
3	A	12	0	0	0	0
4	A	48	0	72	2	0
5	A	363	0	0	0	0
All	All	4931	0	4444	10	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 1.

All (10) 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:A:352[A]:ILE:HG12	1:A:378[A]:CYS:SG	2.48	0.54
1:A:426:PRO:HD3	1:A:455:ASN:HB3	1.93	0.51
1:A:-12:SER:H	4:A:614:EDO:H12	1.79	0.48
1:A:221:ASP:O	1:A:222:ALA:HB2	2.15	0.46
1:A:448:TYR:OH	1:A:476:GLU:OE1	2.26	0.45
1:A:456[B]:MET:HB2	1:A:456[B]:MET:HE2	1.76	0.44
1:A:128:GLU:OE2	4:A:619:EDO:C2	2.67	0.42
1:A:433:GLU:OE1	1:A:467:ARG:HB2	2.18	0.42
1:A:74:PHE:HE1	1:A:130:GLY:HA2	1.85	0.41
1:A:110:GLY:HA2	1:A:157:ASP:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	553/575 (96%)	534 (97%)	17 (3%)	2 (0%)	30	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ALA
1	A	422	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/505 (96%)	479 (99%)	6 (1%)	63	40

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	166[A]	LYS
1	A	166[B]	LYS
1	A	220	ASP
1	A	384	ILE
1	A	433	GLU

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
4	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	A	619	-	3,3,3	0.44	0	2,2,2	0.17	0
2	SO4	A	605	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	603	-	4,4,4	0.53	0	6,6,6	1.53	1 (16%)
4	EDO	A	618	-	3,3,3	0.41	0	2,2,2	0.52	0
2	SO4	A	602	-	4,4,4	0.70	0	6,6,6	0.89	0
2	SO4	A	604	-	4,4,4	0.59	0	6,6,6	1.32	1 (16%)
2	SO4	A	606	-	4,4,4	0.49	0	6,6,6	0.28	0
4	EDO	A	615	-	3,3,3	0.49	0	2,2,2	0.37	0
4	EDO	A	608	-	3,3,3	1.28	0	2,2,2	0.11	0
4	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.36	0
4	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.46	0
2	SO4	A	601	-	4,4,4	0.54	0	6,6,6	1.10	1 (16%)
4	EDO	A	611	-	3,3,3	0.24	0	2,2,2	0.69	0
4	EDO	A	614	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	A	612	-	3,3,3	0.20	0	2,2,2	1.15	0
4	EDO	A	610	-	3,3,3	0.33	0	2,2,2	0.48	0
3	7D8	A	607	1	13,13,13	1.56	1 (7%)	13,21,21	2.22	3 (23%)
4	EDO	A	616	-	3,3,3	0.17	0	2,2,2	0.42	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
4	EDO	A	610	-	-	0/1/1/1	-
4	EDO	A	609	-	-	0/1/1/1	-
4	EDO	A	619	-	-	0/1/1/1	-
4	EDO	A	613	-	-	1/1/1/1	-
4	EDO	A	611	-	-	1/1/1/1	-
3	7D8	A	607	1	-	3/3/29/29	0/2/2/2
4	EDO	A	614	-	-	1/1/1/1	-
4	EDO	A	615	-	-	1/1/1/1	-
4	EDO	A	618	-	-	1/1/1/1	-
4	EDO	A	612	-	-	0/1/1/1	-
4	EDO	A	608	-	-	0/1/1/1	-
4	EDO	A	616	-	-	1/1/1/1	-
4	EDO	A	617	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	7D8	CAH-CAA	-4.25	1.46	1.55

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	607	7D8	CAD-CAC-CAB	6.61	118.83	111.98
3	A	607	7D8	OAJ-CAA-CAB	-2.53	104.31	110.00
2	A	604	SO4	O4-S-O3	2.33	121.41	108.54
2	A	603	SO4	O4-S-O3	2.30	121.22	108.54
2	A	601	SO4	O4-S-O2	-2.17	98.22	109.56
3	A	607	7D8	OAJ-CAA-CAH	-2.03	106.98	111.85

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	607	7D8	CAG-CAH-CAL-OAM
4	A	618	EDO	O1-C1-C2-O2
4	A	614	EDO	O1-C1-C2-O2
3	A	607	7D8	CAA-CAH-CAL-OAM
4	A	616	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	611	EDO	O1-C1-C2-O2
4	A	613	EDO	O1-C1-C2-O2
4	A	615	EDO	O1-C1-C2-O2
4	A	617	EDO	O1-C1-C2-O2
3	A	607	7D8	CAI-CAH-CAL-OAM

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	619	EDO	1	0
4	A	614	EDO	1	0

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	539/575 (93%)	-0.07	6 (1%) 78 84	8, 20, 38, 52	16 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-13	HIS	4.8
1	A	74	PHE	3.0
1	A	166[A]	LYS	2.8
1	A	341	ASN	2.5
1	A	76	PHE	2.2
1	A	484	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	615	4/4	0.78	0.20	32,40,44,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	606	5/5	0.80	0.10	42,63,72,74	0
4	EDO	A	618	4/4	0.82	0.20	46,50,51,57	0
4	EDO	A	614	4/4	0.83	0.18	36,39,40,47	0
4	EDO	A	613	4/4	0.85	0.16	33,38,41,45	0
4	EDO	A	616	4/4	0.87	0.15	37,41,44,45	0
4	EDO	A	612	4/4	0.88	0.16	21,33,41,44	0
4	EDO	A	611	4/4	0.88	0.16	36,37,45,46	0
2	SO4	A	603	5/5	0.92	0.10	35,40,41,46	0
4	EDO	A	617	4/4	0.92	0.11	40,43,45,47	0
2	SO4	A	604	5/5	0.92	0.08	35,39,52,52	0
4	EDO	A	619	4/4	0.92	0.13	33,41,46,51	0
2	SO4	A	605	5/5	0.93	0.09	33,33,36,41	5
4	EDO	A	608	4/4	0.95	0.09	18,20,20,22	0
2	SO4	A	602	5/5	0.97	0.06	27,28,31,42	0
2	SO4	A	601	5/5	0.98	0.06	23,24,25,30	0
4	EDO	A	609	4/4	0.98	0.05	19,21,23,23	0
4	EDO	A	610	4/4	0.98	0.06	19,19,22,22	0
3	7D8	A	607	12/12	0.98	0.04	15,16,16,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.