



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:23 PM UTC

PDB ID : 5OSS / pdb_00005oss
Title : Beta-glucosidase from *Thermotoga maritima* in complex with Gluco-1H-imidazole
Authors : Offen, W.A.; Schroeder, S.P.; Davies, G.J.; Overkleeft, H.S.
Deposited on : 2017-08-18
Resolution : 1.70 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

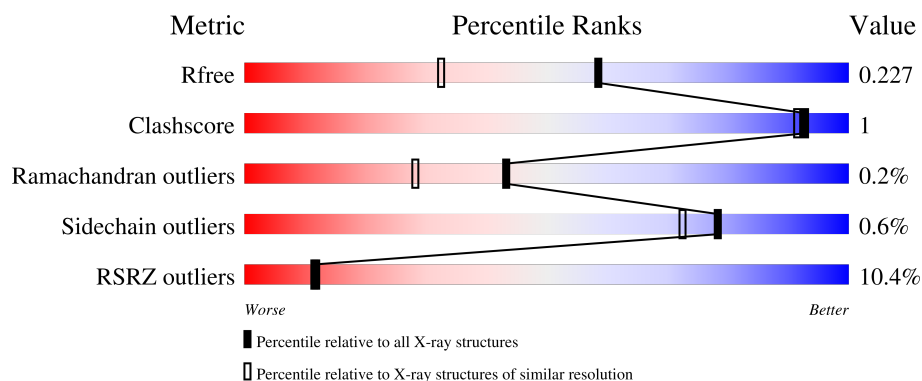
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	468	5% 90% 5% 5%
1	B	468	15% 90% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7660 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 Beta-glucosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	6	0
			3632	2365	612	649	6			
1	B	443	Total	C	N	O	S	0	6	0
			3599	2341	609	643	6			

There are 46 discrepancies between the modelled and reference sequences:

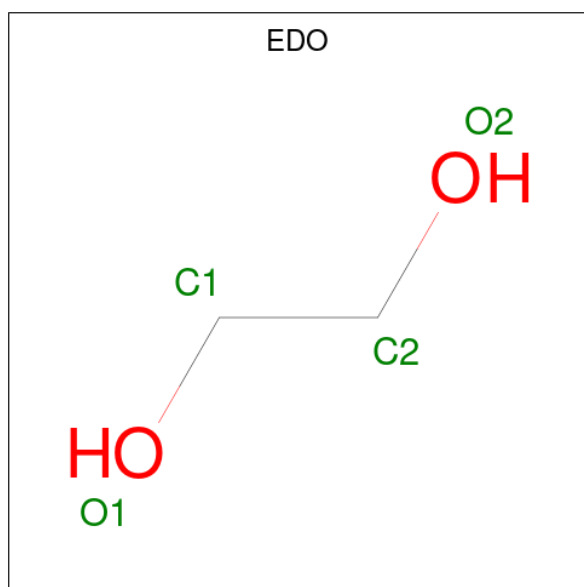
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q08638
A	-20	GLY	-	expression tag	UNP Q08638
A	-19	SER	-	expression tag	UNP Q08638
A	-18	SER	-	expression tag	UNP Q08638
A	-17	HIS	-	expression tag	UNP Q08638
A	-16	HIS	-	expression tag	UNP Q08638
A	-15	HIS	-	expression tag	UNP Q08638
A	-14	HIS	-	expression tag	UNP Q08638
A	-13	HIS	-	expression tag	UNP Q08638
A	-12	HIS	-	expression tag	UNP Q08638
A	-11	SER	-	expression tag	UNP Q08638
A	-10	SER	-	expression tag	UNP Q08638
A	-9	GLY	-	expression tag	UNP Q08638
A	-8	LEU	-	expression tag	UNP Q08638
A	-7	VAL	-	expression tag	UNP Q08638
A	-6	PRO	-	expression tag	UNP Q08638
A	-5	ARG	-	expression tag	UNP Q08638
A	-4	GLY	-	expression tag	UNP Q08638
A	-3	SER	-	expression tag	UNP Q08638
A	-2	HIS	-	expression tag	UNP Q08638
A	-1	MET	-	expression tag	UNP Q08638
A	0	ALA	-	expression tag	UNP Q08638
A	1	SER	-	expression tag	UNP Q08638
B	-21	MET	-	initiating methionine	UNP Q08638
B	-20	GLY	-	expression tag	UNP Q08638

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP Q08638
B	-18	SER	-	expression tag	UNP Q08638
B	-17	HIS	-	expression tag	UNP Q08638
B	-16	HIS	-	expression tag	UNP Q08638
B	-15	HIS	-	expression tag	UNP Q08638
B	-14	HIS	-	expression tag	UNP Q08638
B	-13	HIS	-	expression tag	UNP Q08638
B	-12	HIS	-	expression tag	UNP Q08638
B	-11	SER	-	expression tag	UNP Q08638
B	-10	SER	-	expression tag	UNP Q08638
B	-9	GLY	-	expression tag	UNP Q08638
B	-8	LEU	-	expression tag	UNP Q08638
B	-7	VAL	-	expression tag	UNP Q08638
B	-6	PRO	-	expression tag	UNP Q08638
B	-5	ARG	-	expression tag	UNP Q08638
B	-4	GLY	-	expression tag	UNP Q08638
B	-3	SER	-	expression tag	UNP Q08638
B	-2	HIS	-	expression tag	UNP Q08638
B	-1	MET	-	expression tag	UNP Q08638
B	0	ALA	-	expression tag	UNP Q08638
B	1	SER	-	expression tag	UNP Q08638

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



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

Continued on next page...

Continued from previous page...

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

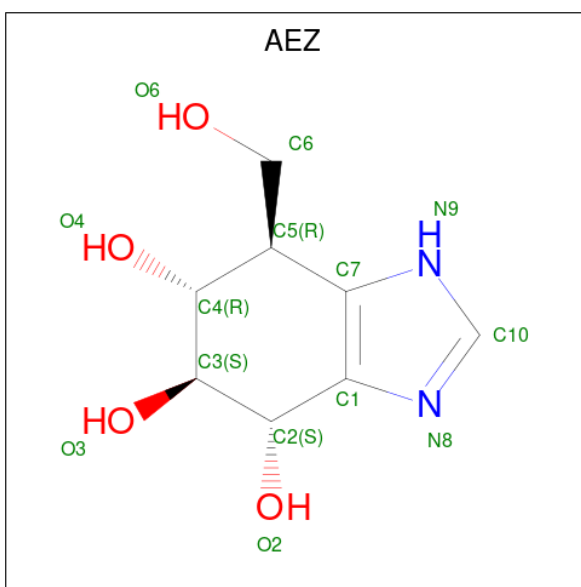
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0

- Molecule 5 is (4 {S},5 {S},6 {R},7 {R})-7-(hydroxymethyl)-4,5,6,7-tetrahydro-1 {H}-benzimidazole-4,5,6-triol (CCD ID: AEZ) (formula: C₈H₁₂N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	2	4		

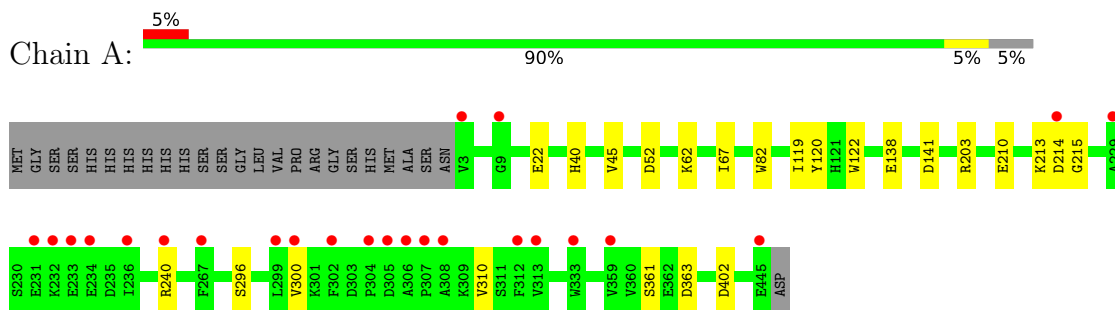
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total	O	0	0
			224	224		
6	B	143	Total	O	0	2
			145	145		

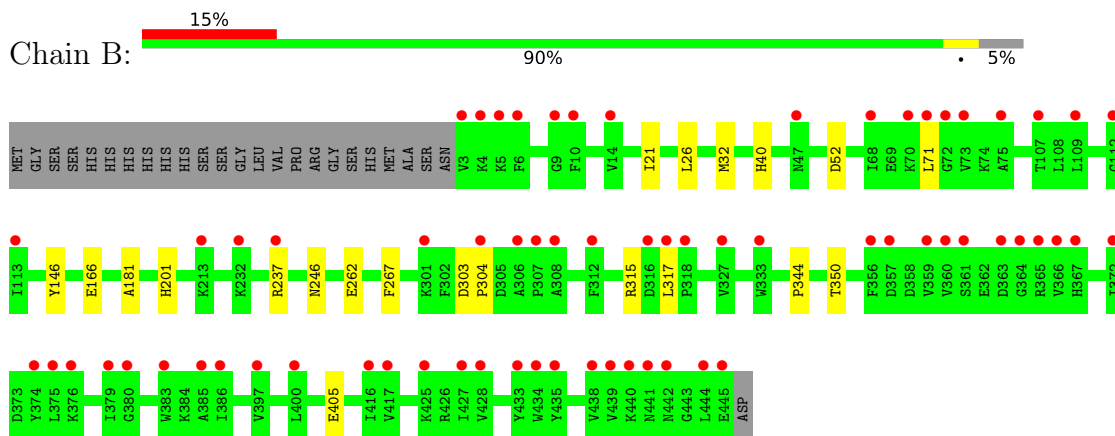
3 Residue-property plots [i](#)

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: Beta-glucosidase A



- Molecule 1: Beta-glucosidase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.32Å 94.62Å 113.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.77 – 1.70 72.66 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.77-1.70) 99.9 (72.66-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.186 , 0.222 0.197 , 0.227	Depositor DCC
R_{free} test set	5629 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: AEZ, CL, EDO, NA

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	1.26	5/3751 (0.1%)	1.10	6/5103 (0.1%)
1	B	1.18	7/3716 (0.2%)	1.06	1/5061 (0.0%)
All	All	1.22	12/7467 (0.2%)	1.08	7/10164 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	344	PRO	CA-C	12.09	1.58	1.51
1	A	215	GLY	N-CA	9.71	1.52	1.44
1	B	344	PRO	C-O	-7.12	1.19	1.25
1	B	201	HIS	C-O	6.74	1.31	1.24
1	B	262	GLU	CA-CB	6.25	1.63	1.53
1	A	62	LYS	N-CA	5.83	1.53	1.46
1	B	146	TYR	N-CA	-5.58	1.39	1.46
1	A	120	TYR	CA-C	-5.42	1.46	1.52
1	A	119	ILE	CA-C	5.26	1.59	1.52
1	B	267	PHE	N-CA	5.19	1.52	1.46
1	B	181	ALA	CA-C	5.18	1.58	1.53
1	A	45	VAL	N-CA	5.15	1.52	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ASP	N-CA-C	6.60	121.50	113.38
1	B	21	ILE	N-CA-C	6.56	119.96	113.53
1	A	296	SER	N-CA-C	6.50	119.05	109.24
1	A	67	ILE	N-CA-C	6.33	116.49	110.42
1	A	22	GLU	N-CA-C	6.22	118.14	111.36
1	A	402	ASP	N-CA-C	-5.27	102.59	110.23
1	A	82	TRP	CA-CB-CG	5.07	123.23	113.60

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	3632	0	3455	11	0
1	B	3599	0	3370	10	0
2	A	32	0	47	0	0
2	B	12	0	18	0	0
3	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	14	0	0	2	0
6	A	224	0	0	4	0
6	B	145	0	0	3	0
All	All	7660	0	6890	21	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 (21) 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:203[B]:ARG:HG3	1:A:203[B]:ARG:NH2	1.65	1.00
1:A:203[B]:ARG:HG3	1:A:203[B]:ARG:HH21	0.85	0.99
1:A:203[B]:ARG:HH21	1:A:203[B]:ARG:CG	1.78	0.94
1:A:52:ASP:OD2	6:A:604:HOH:O	1.90	0.88
1:A:40:HIS:NE2	6:A:604:HOH:O	2.07	0.70
1:A:138:GLU:OE2	6:A:605:HOH:O	2.09	0.70
1:B:52:ASP:OD2	6:B:604:HOH:O	2.09	0.69
1:B:40:HIS:NE2	6:B:604:HOH:O	2.16	0.65
1:B:304:PRO:O	6:B:605:HOH:O	2.15	0.63
1:B:237[A]:ARG:HH21	1:B:237[A]:ARG:HG3	1.65	0.60
1:A:210:GLU:OE2	6:A:606:HOH:O	2.16	0.58
1:B:315:ARG:HB3	1:B:317:LEU:HD13	1.90	0.54
1:A:300:VAL:HG13	1:A:310:VAL:HG13	1.93	0.51
1:A:40:HIS:HE1	1:A:52:ASP:OD1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:OE2	5:B:505:AEZ:N8	2.49	0.46
1:A:141:ASP:OD1	1:A:203[A]:ARG:NH1	2.44	0.45
1:B:237[A]:ARG:HG3	1:B:237[A]:ARG:NH2	2.28	0.45
1:B:26:LEU:HD21	1:B:32:MET:HG2	1.99	0.44
1:A:361:SER:HB2	1:A:363:ASP:OD1	2.18	0.43
1:B:405:GLU:OE2	5:B:505:AEZ:O6	2.38	0.41
1:B:303:ASP:OD1	1:B:303:ASP:C	2.64	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	447/468 (96%)	437 (98%)	8 (2%)	2 (0%)	30	16
1	B	447/468 (96%)	435 (97%)	12 (3%)	0	100	100
All	All	894/936 (96%)	872 (98%)	20 (2%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	A	122	TRP

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	367/399 (92%)	365 (100%)	2 (0%)	81	76
1	B	356/399 (89%)	353 (99%)	3 (1%)	73	65
All	All	723/798 (91%)	718 (99%)	5 (1%)	78	69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240[A]	ARG
1	A	240[B]	ARG
1	B	71	LEU
1	B	246	ASN
1	B	350	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	129	GLN
1	A	253	ASN
1	A	387	GLN
1	B	253	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	EDO	B	501	-	3,3,3	0.35	0	2,2,2	0.38	0
2	EDO	B	503	-	3,3,3	0.35	0	2,2,2	0.88	0
2	EDO	B	502	-	3,3,3	0.41	0	2,2,2	0.43	0
2	EDO	A	503	-	3,3,3	0.42	0	2,2,2	0.55	0
2	EDO	A	501	-	3,3,3	0.38	0	2,2,2	0.93	0
5	AEZ	B	505	-	12,15,15	3.30	3 (25%)	10,22,22	2.43	3 (30%)
2	EDO	A	506	-	3,3,3	0.25	0	2,2,2	0.89	0
2	EDO	A	505	-	3,3,3	0.50	0	2,2,2	0.11	0
2	EDO	A	504	-	3,3,3	0.41	0	2,2,2	0.56	0
2	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	A	507[A]	-	3,3,3	0.62	0	2,2,2	0.41	0
2	EDO	A	507[B]	-	3,3,3	0.57	0	2,2,2	0.28	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	EDO	B	501	-	-	0/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
5	AEZ	B	505	-	-	0/2/22/22	0/2/2/2
2	EDO	A	506	-	-	1/1/1/1	-
2	EDO	A	505	-	-	1/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	A	507[A]	-	-	1/1/1/1	-
2	EDO	A	507[B]	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	AEZ	C7-C1	10.14	1.48	1.36
5	B	505	AEZ	C1-N8	-3.53	1.33	1.39
5	B	505	AEZ	C6-C5	-2.76	1.49	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	AEZ	C10-N8-C1	5.08	110.91	104.83
5	B	505	AEZ	N9-C10-N8	-3.92	108.44	112.98
5	B	505	AEZ	C4-C3-C2	3.54	115.81	110.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	EDO	O1-C1-C2-O2
2	A	507[A]	EDO	O1-C1-C2-O2
2	B	503	EDO	O1-C1-C2-O2
2	A	506	EDO	O1-C1-C2-O2
2	A	507[B]	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	A	505	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	AEZ	2	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

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	443/468 (94%)	0.38	24 (5%) 31 34	16, 32, 48, 64	33 (7%)
1	B	443/468 (94%)	1.00	68 (15%) 5 4	15, 40, 58, 70	44 (9%)
All	All	886/936 (94%)	0.69	92 (10%) 11 12	15, 35, 55, 70	77 (8%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	VAL	10.3
1	B	307	PRO	9.3
1	A	306	ALA	9.1
1	A	3	VAL	8.8
1	B	359	VAL	6.5
1	A	305	ASP	5.6
1	B	3	VAL	5.5
1	B	434	TRP	5.1
1	A	236	ILE	5.0
1	B	367	HIS	4.9
1	B	317	LEU	4.8
1	B	71	LEU	4.7
1	B	365	ARG	4.5
1	A	312	PHE	4.5
1	A	233	GLU	4.4
1	B	68	ILE	4.3
1	A	307	PRO	4.2
1	A	304	PRO	4.1
1	B	439	VAL	4.1
1	B	375	LEU	4.1
1	B	376	LYS	3.9
1	B	316	ASP	3.9
1	B	364	GLY	3.8
1	B	357	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	372	ILE	3.8
1	B	213	LYS	3.5
1	B	363	ASP	3.5
1	B	441	ASN	3.4
1	B	445	GLU	3.3
1	B	232	LYS	3.2
1	B	237[A]	ARG	3.1
1	B	361	SER	3.1
1	B	333	TRP	3.0
1	B	428	VAL	3.0
1	B	70	LYS	3.0
1	A	300	VAL	2.9
1	A	234	GLU	2.9
1	B	113	ILE	2.9
1	B	442	ASN	2.9
1	A	231	GLU	2.9
1	B	4	LYS	2.9
1	B	5	LYS	2.8
1	A	333	TRP	2.8
1	A	229	ALA	2.8
1	B	366	VAL	2.8
1	B	306	ALA	2.8
1	A	308	ALA	2.7
1	B	73	VAL	2.7
1	A	302	PHE	2.7
1	B	400	LEU	2.7
1	B	304	PRO	2.7
1	B	444	LEU	2.7
1	A	214	ASP	2.7
1	B	308	ALA	2.7
1	B	9	GLY	2.6
1	A	313	VAL	2.6
1	B	417	VAL	2.6
1	B	433	TYR	2.6
1	B	438	VAL	2.6
1	B	374	TYR	2.6
1	B	6	PHE	2.5
1	B	301	LYS	2.4
1	A	445	GLU	2.4
1	B	312	PHE	2.4
1	B	383	TRP	2.4
1	B	435	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	397	VAL	2.4
1	B	416	ILE	2.3
1	A	267	PHE	2.3
1	B	356	PHE	2.3
1	B	425	LYS	2.3
1	B	75	ALA	2.3
1	B	440	LYS	2.3
1	A	359	VAL	2.3
1	B	14	VAL	2.3
1	A	240[A]	ARG	2.2
1	B	385	ALA	2.2
1	B	380	GLY	2.2
1	B	427	ILE	2.2
1	A	232	LYS	2.2
1	B	386	ILE	2.2
1	A	299	LEU	2.1
1	B	109	LEU	2.1
1	B	10	PHE	2.1
1	B	72	GLY	2.1
1	B	112	GLY	2.1
1	B	318	PRO	2.1
1	A	9	GLY	2.1
1	B	327	VAL	2.1
1	B	107	THR	2.1
1	B	47	ASN	2.0
1	B	379	ILE	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($\text{\AA}^2$)	Q<0.9
2	EDO	A	505	4/4	0.83	0.22	43,46,48,49	4
2	EDO	A	504	4/4	0.84	0.19	38,38,39,44	4
2	EDO	A	503	4/4	0.84	0.19	35,37,39,42	4
2	EDO	B	503	4/4	0.84	0.25	34,36,37,39	4
2	EDO	B	502	4/4	0.85	0.25	34,35,36,37	4
2	EDO	A	502	4/4	0.85	0.33	37,38,38,38	4
2	EDO	A	506	4/4	0.86	0.28	41,42,43,45	4
2	EDO	A	507[A]	4/4	0.89	0.13	32,33,34,39	4
2	EDO	A	507[B]	4/4	0.89	0.13	32,34,35,40	4
2	EDO	B	501	4/4	0.91	0.16	34,40,40,44	4
5	AEZ	B	505	14/14	0.92	0.10	29,39,44,48	14
2	EDO	A	501	4/4	0.93	0.12	36,46,48,49	0
3	CL	A	508	1/1	0.96	0.14	48,48,48,48	0
4	NA	B	504	1/1	0.98	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.