



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:21 pm BST

PDB ID : 5T98
Title : Crystal structure of BuGH2Awt
Authors : Pluinage, B.; Boraston, A.B.
Deposited on : 2016-09-09
Resolution : 2.60 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 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 : 2.11
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) : 2.11

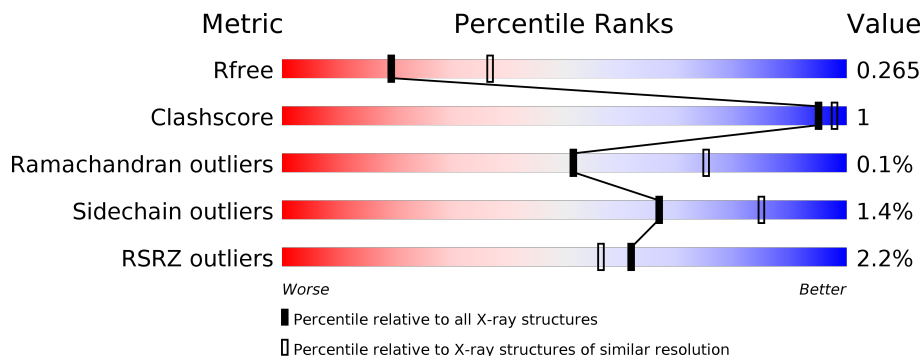
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	822	<p>2% 89% 8%</p>
1	B	822	<p>2% 88% 8%</p>

2 Entry composition [i](#)

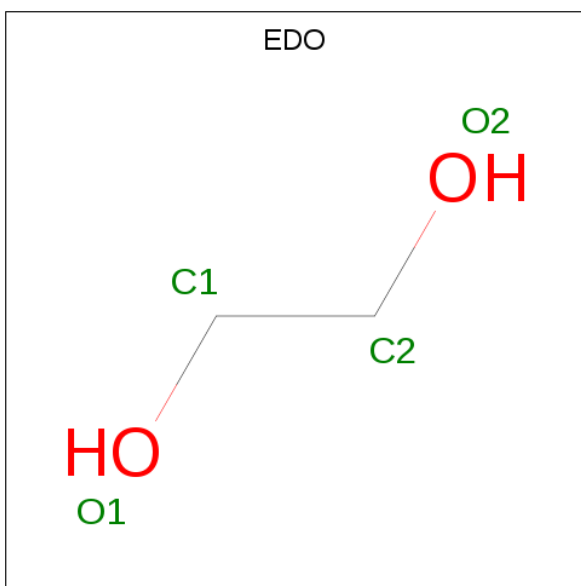
There are 4 unique types of molecules in this entry. The entry contains 12411 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycoside Hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	756	Total 5960	C 3801	N 1009	O 1121	S 29	0	1	0
1	B	755	Total 5972	C 3813	N 1013	O 1118	S 28	0	1	0

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



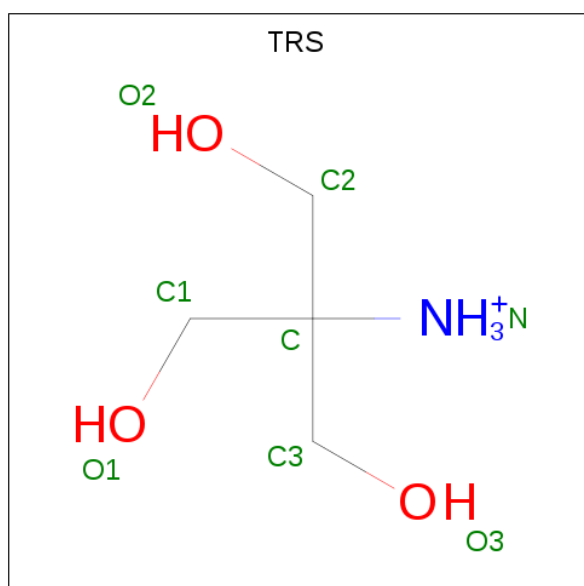
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

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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	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
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
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 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	205	Total	O	0	0
			205	205		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.83Å 120.31Å 143.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.29 – 2.60 29.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (92.29-2.60) 97.8 (29.85-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.209 , 0.263 0.212 , 0.265	Depositor DCC
R_{free} test set	3126 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.003 for k,h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12411	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: TRS, 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	0.44	0/6113	0.67	0/8299
1	B	0.43	0/6126	0.67	2/8312 (0.0%)
All	All	0.44	0/12239	0.67	2/16611 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	245	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5960	0	5675	10	0
1	B	5972	0	5716	18	0
2	A	32	0	48	0	0
2	B	32	0	48	0	0
3	A	8	0	12	1	0
3	B	8	0	12	0	0
4	A	194	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	205	0	0	1	0
All	All	12411	0	11511	28	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 (28) 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:56:ASN:HD21	1:A:196:ASN:HD22	1.28	0.78
1:B:758:ILE:HD11	1:B:843:ILE:HD11	1.70	0.73
1:B:545:VAL:HG13	1:B:551:ILE:HD11	1.82	0.59
1:B:833:SER:HB3	1:B:836:LEU:HD12	1.86	0.57
1:B:817:VAL:HB	1:B:827:MET:HE2	1.88	0.55
1:B:213:TYR:CD1	1:B:429:ARG:HG3	2.43	0.54
1:B:750:ALA:HB2	1:B:845:VAL:HG12	1.92	0.52
1:B:429:ARG:HD3	4:B:1121:HOH:O	2.10	0.51
1:A:443:ILE:HD12	1:A:446:GLN:HG3	1.92	0.50
1:A:750:ALA:HB2	1:A:845:VAL:HG12	1.94	0.49
1:A:498:TYR:CE1	1:A:522:SER:HB2	2.49	0.48
1:A:827:MET:HE3	1:A:829:ILE:HD11	1.95	0.47
1:A:141:VAL:HG11	1:A:160:ILE:HD13	1.97	0.47
1:A:399:GLU:HA	1:A:443:ILE:HG22	2.00	0.44
1:B:498:TYR:CE1	1:B:522:SER:HB2	2.53	0.44
1:B:641:LEU:HB2	1:B:642:PRO:HA	2.01	0.43
1:B:56:ASN:HB3	1:B:84:LEU:O	2.19	0.43
1:A:186:ARG:HH22	3:A:909:TRS:H12	1.84	0.42
1:B:532:LEU:HD21	1:B:653:PRO:HD2	2.02	0.42
1:B:833:SER:CB	1:B:836:LEU:HD12	2.48	0.42
1:B:677:LYS:HA	1:B:702:LEU:HD21	2.02	0.42
1:B:758:ILE:HD11	1:B:843:ILE:CD1	2.45	0.42
1:B:563:PHE:CE2	1:B:631:GLN:HG3	2.55	0.41
1:B:128:VAL:HG21	1:B:166:LEU:CD2	2.51	0.41
1:B:760:VAL:O	1:B:812:MET:HA	2.21	0.41
1:B:128:VAL:HG21	1:B:166:LEU:HD22	2.04	0.40
1:A:827:MET:CE	1:A:829:ILE:HD11	2.51	0.40
1:A:739:ILE:HD11	1:A:833:SER:CB	2.52	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	747/822 (91%)	718 (96%)	27 (4%)	2 (0%)	41	64
1	B	746/822 (91%)	722 (97%)	24 (3%)	0	100	100
All	All	1493/1644 (91%)	1440 (96%)	51 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	SER
1	A	152	PRO

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	624/705 (88%)	614 (98%)	10 (2%)	62	82
1	B	626/705 (89%)	619 (99%)	7 (1%)	73	88
All	All	1250/1410 (89%)	1233 (99%)	17 (1%)	67	85

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	82	LEU
1	A	88	TRP
1	A	316	ARG

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Mol	Chain	Res	Type
1	A	414	ASP
1	A	419	LYS
1	A	522	SER
1	A	609	SER
1	A	641	LEU
1	A	847	LEU
1	B	88	TRP
1	B	289	ASN
1	B	316	ARG
1	B	522	SER
1	B	560	ASP
1	B	609	SER
1	B	641	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	196	ASN
1	A	828	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	EDO	A	901	-	3,3,3	0.44	0	2,2,2	0.26	0
2	EDO	B	901	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	B	903	-	3,3,3	0.66	0	2,2,2	0.15	0
2	EDO	A	905	-	3,3,3	0.38	0	2,2,2	0.43	0
2	EDO	B	905	-	3,3,3	0.47	0	2,2,2	0.08	0
2	EDO	A	904	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	B	902	-	3,3,3	0.54	0	2,2,2	0.14	0
2	EDO	A	908	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	B	906	-	3,3,3	0.37	0	2,2,2	0.36	0
3	TRS	B	909	-	7,7,7	0.48	0	9,9,9	1.48	3 (33%)
2	EDO	A	903	-	3,3,3	0.47	0	2,2,2	0.28	0
2	EDO	B	907	-	3,3,3	0.52	0	2,2,2	0.47	0
2	EDO	A	907	-	3,3,3	0.41	0	2,2,2	0.40	0
3	TRS	A	909	-	7,7,7	0.58	0	9,9,9	2.08	3 (33%)
2	EDO	B	908	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	A	902	-	3,3,3	0.58	0	2,2,2	0.11	0
2	EDO	B	904	-	3,3,3	0.48	0	2,2,2	0.39	0
2	EDO	A	906	-	3,3,3	0.54	0	2,2,2	0.15	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	A	901	-	-	0/1/1/1	-
2	EDO	B	901	-	-	0/1/1/1	-
2	EDO	B	903	-	-	1/1/1/1	-
2	EDO	A	905	-	-	1/1/1/1	-
2	EDO	B	905	-	-	0/1/1/1	-
2	EDO	A	904	-	-	1/1/1/1	-
2	EDO	B	902	-	-	1/1/1/1	-
2	EDO	A	908	-	-	1/1/1/1	-
2	EDO	B	906	-	-	0/1/1/1	-
3	TRS	B	909	-	-	3/9/9/9	-
2	EDO	A	903	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	907	-	-	1/1/1/1	-
2	EDO	A	907	-	-	0/1/1/1	-
3	TRS	A	909	-	-	4/9/9/9	-
2	EDO	B	908	-	-	1/1/1/1	-
2	EDO	A	902	-	-	1/1/1/1	-
2	EDO	B	904	-	-	0/1/1/1	-
2	EDO	A	906	-	-	0/1/1/1	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	909	TRS	C1-C-N	3.72	119.09	107.98
3	A	909	TRS	C3-C-C2	3.31	121.08	110.81
3	A	909	TRS	C2-C-N	-2.83	99.54	107.98
3	B	909	TRS	C3-C-N	2.65	115.88	107.98
3	B	909	TRS	O3-C3-C	2.13	117.73	111.00
3	B	909	TRS	C3-C-C2	-2.10	104.31	110.81

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	909	TRS	C1-C-C3-O3
3	A	909	TRS	C2-C-C3-O3
2	A	904	EDO	O1-C1-C2-O2
2	B	902	EDO	O1-C1-C2-O2
2	B	908	EDO	O1-C1-C2-O2
2	B	903	EDO	O1-C1-C2-O2
2	A	902	EDO	O1-C1-C2-O2
3	A	909	TRS	N-C-C1-O1
2	A	908	EDO	O1-C1-C2-O2
3	B	909	TRS	C2-C-C1-O1
3	B	909	TRS	C3-C-C1-O1
2	A	903	EDO	O1-C1-C2-O2
2	A	905	EDO	O1-C1-C2-O2
2	B	907	EDO	O1-C1-C2-O2
3	B	909	TRS	N-C-C1-O1
3	A	909	TRS	N-C-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	909	TRS	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

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	756/822 (91%)	-0.17	17 (2%) 62 56	29, 45, 69, 103	0
1	B	755/822 (91%)	-0.23	16 (2%) 63 58	30, 45, 67, 107	0
All	All	1511/1644 (91%)	-0.20	33 (2%) 62 56	29, 45, 68, 107	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	THR	4.5
1	B	607	SER	4.0
1	A	50	THR	4.0
1	A	106	PRO	3.6
1	B	48	SER	3.5
1	B	105	LEU	3.4
1	A	607	SER	3.4
1	A	46	MET	2.9
1	A	847	LEU	2.9
1	B	93	PRO	2.9
1	B	108	HIS	2.8
1	A	552	GLY	2.8
1	B	50	THR	2.8
1	B	104	GLY	2.8
1	B	47	ALA	2.7
1	A	105	LEU	2.7
1	B	182	ASP	2.7
1	A	108	HIS	2.7
1	A	543	ASN	2.7
1	B	239	ASN	2.7
1	A	694	ASN	2.6
1	B	183	LEU	2.6
1	B	107	PHE	2.6
1	B	721	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	835	GLY	2.5
1	B	106	PRO	2.4
1	B	49	VAL	2.4
1	B	406	ASP	2.3
1	A	406	ASP	2.2
1	A	739	ILE	2.2
1	A	47	ALA	2.2
1	A	686	VAL	2.1
1	A	766	ASP	2.1

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 carbohydrates 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
3	TRS	B	909	8/8	0.73	0.25	58,61,63,65	0
3	TRS	A	909	8/8	0.76	0.33	63,70,76,77	0
2	EDO	B	907	4/4	0.77	0.31	60,65,65,66	0
2	EDO	B	903	4/4	0.85	0.30	50,52,55,57	0
2	EDO	B	904	4/4	0.86	0.17	63,66,66,68	0
2	EDO	B	906	4/4	0.88	0.23	55,55,56,58	0
2	EDO	B	908	4/4	0.89	0.23	58,58,58,59	0
2	EDO	A	908	4/4	0.91	0.15	56,56,57,58	0
2	EDO	B	902	4/4	0.92	0.20	43,46,46,47	0
2	EDO	A	905	4/4	0.92	0.30	39,41,41,44	0
2	EDO	B	901	4/4	0.93	0.31	42,43,43,44	0
2	EDO	B	905	4/4	0.93	0.15	41,42,43,43	0
2	EDO	A	906	4/4	0.93	0.14	47,48,48,50	0
2	EDO	A	904	4/4	0.94	0.21	35,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	903	4/4	0.95	0.19	49,50,50,51	0
2	EDO	A	902	4/4	0.95	0.15	42,43,44,45	0
2	EDO	A	907	4/4	0.97	0.22	40,40,41,41	0
2	EDO	A	901	4/4	0.97	0.13	34,36,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.