



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 01:19 pm BST

PDB ID : 9S8A / pdb\_00009s8a  
Title : Amuc0451\_S1\_20  
Authors : Dey, D.; Cartmell, A.  
Deposited on : 2025-08-05  
Resolution : 1.60 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](mailto: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>.

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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 : 1.8.4, CSD as541be (2020)  
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

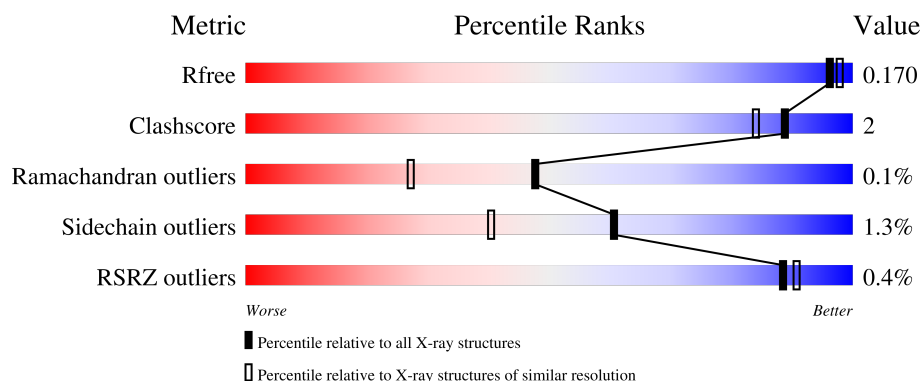
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	682	
1	B	682	

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
2	EDO	B	807	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11917 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 Sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	15	0
			5421	3419	976	1011	15			
1	B	682	Total	C	N	O	S	0	15	0
			5428	3429	978	1005	16			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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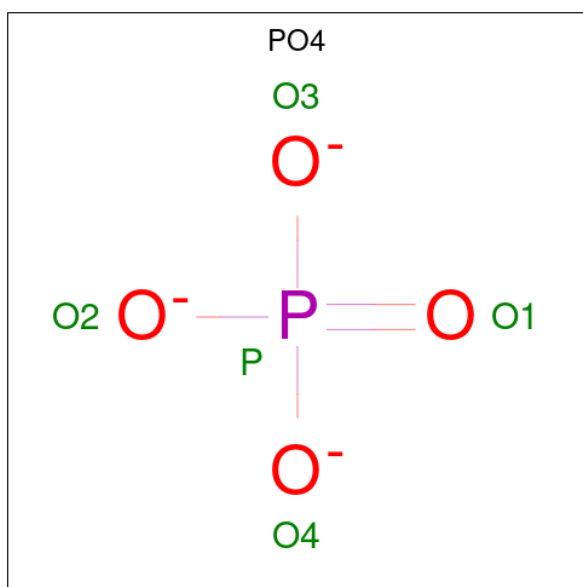
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Ca		0	0
			1	1			
3	B	1	Total	Ca		0	0
			1	1			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	441	Total	O		0	0
			441	441			

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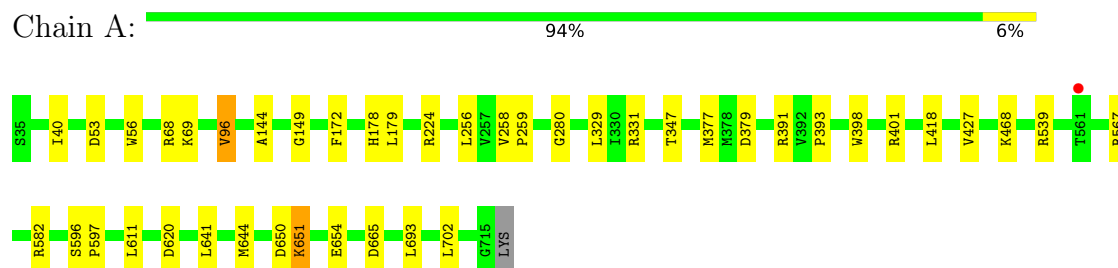
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	507	Total 507	O 507	0	0

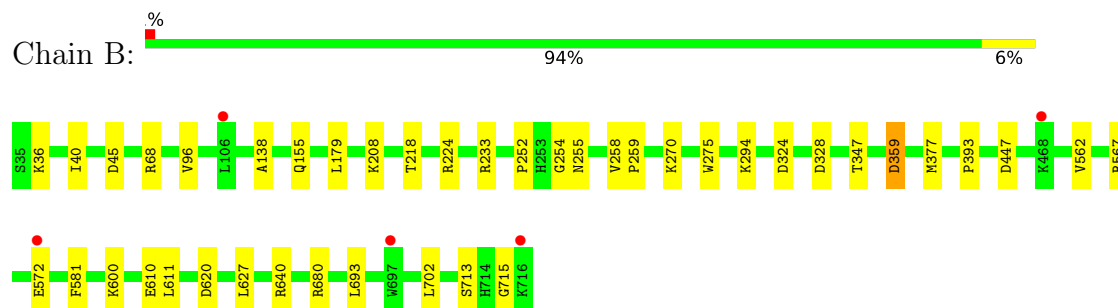
### 3 Residue-property plots [i](#)

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: Sulfatase



- Molecule 1: Sulfatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.66Å 59.90Å 123.72Å 90.00° 115.75° 90.00°	Depositor
Resolution (Å)	51.75 – 1.60 51.75 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.75-1.60) 100.0 (51.75-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.156 , 0.192 0.168 , 0.170	Depositor DCC
$R_{free}$ test set	10050 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, PO4

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	0.63	0/5567	1.03	6/7546 (0.1%)
1	B	0.71	1/5574 (0.0%)	1.09	7/7552 (0.1%)
All	All	0.67	1/11141 (0.0%)	1.06	13/15098 (0.1%)

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	3
1	B	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	ILE	C-O	7.94	1.32	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	620	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	620	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	427	VAL	N-CA-CB	6.25	116.14	111.83
1	B	359	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	324	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	379	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	665	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	218	THR	CA-CB-OG1	-5.54	101.29	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	572	GLU	CB-CG-CD	5.46	121.89	112.60
1	B	640	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	328	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	654	GLU	CB-CA-C	-5.23	104.07	110.08
1	A	650	ASP	CA-CB-CG	5.22	117.82	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	ARG	Sidechain
1	A	391	ARG	Sidechain
1	A	582	ARG	Sidechain
1	B	233	ARG	Sidechain
1	B	680[A]	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	5421	0	5273	20	0
1	B	5428	0	5304	22	0
2	A	52	0	78	2	0
2	B	56	0	84	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	441	0	0	4	0
5	B	507	0	0	0	0
All	All	11917	0	10739	42	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 2.

All (42) 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:280:GLY:N	5:A:901:HOH:O	2.20	0.73
1:B:581:PHE:HD2	2:B:807:EDO:H11	1.56	0.70
2:A:813:EDO:H11	1:B:179:LEU:HD21	1.78	0.64
1:A:651:LYS:NZ	5:A:902:HOH:O	2.30	0.63
1:B:627:LEU:HD11	1:B:693[A]:LEU:HD21	1.80	0.62
1:B:581:PHE:CD2	2:B:807:EDO:H11	2.36	0.61
1:B:567:ARG:NH1	1:B:715:GLY:O	2.33	0.58
1:A:539:ARG:HA	5:A:964:HOH:O	2.06	0.55
1:B:610:GLU:HG3	2:B:807:EDO:H12	1.90	0.54
1:B:693[B]:LEU:C	1:B:693[B]:LEU:HD23	2.34	0.53
1:A:149:GLY:O	1:A:178[B]:HIS:CE1	2.62	0.53
2:A:807:EDO:H12	1:B:155:GLN:OE1	2.09	0.53
1:B:258:VAL:HB	1:B:259:PRO:CD	2.39	0.52
1:A:40:ILE:HD13	1:A:329[B]:LEU:HD21	1.91	0.51
1:A:56:TRP:CD2	1:A:68[B]:ARG:HD3	2.44	0.51
1:A:641:LEU:O	1:A:644:MET:HG2	2.09	0.51
1:A:258:VAL:HB	1:A:259:PRO:CD	2.42	0.50
1:A:53:ASP:OD1	1:A:68[A]:ARG:NH1	2.28	0.49
1:B:45:ASP:O	1:B:252:PRO:HD2	2.14	0.47
1:B:627:LEU:C	1:B:627:LEU:HD23	2.40	0.46
1:B:627:LEU:CD1	1:B:693[A]:LEU:HD21	2.45	0.45
1:B:224:ARG:HD3	1:B:275:TRP:CH2	2.51	0.45
1:B:68[B]:ARG:HE	1:B:68[B]:ARG:HB3	1.27	0.45
1:B:36:LYS:NZ	1:B:138:ALA:O	2.50	0.45
1:A:258:VAL:HB	1:A:259:PRO:HD2	1.98	0.44
1:B:270:LYS:HA	1:B:270:LYS:HE2	1.99	0.43
1:B:258:VAL:HB	1:B:259:PRO:HD2	2.00	0.43
1:A:567:ARG:O	1:A:611:LEU:HA	2.18	0.43
1:B:567:ARG:O	1:B:611:LEU:HA	2.18	0.43
1:A:418:LEU:C	1:A:418:LEU:HD23	2.44	0.43
1:B:562[B]:VAL:HG12	1:B:713:SER:HB2	2.01	0.43
1:A:398:TRP:CZ2	1:A:401:ARG:HG3	2.53	0.43
1:A:693:LEU:C	1:A:693:LEU:HD23	2.44	0.43
1:B:347:THR:HA	1:B:393:PRO:O	2.19	0.42
1:A:596[A]:SER:HB2	1:A:597:PRO:CD	2.49	0.42
1:B:581:PHE:H	2:B:807:EDO:H11	1.83	0.42
1:A:56:TRP:CE3	1:A:68[B]:ARG:HD3	2.55	0.42
1:A:96[A]:VAL:HG22	5:A:1077:HOH:O	2.19	0.41
1:A:224:ARG:HA	1:A:224:ARG:HD2	1.93	0.41
1:A:347:THR:HA	1:A:393:PRO:O	2.20	0.41
1:B:254:GLY:HA2	1:B:255:ASN:C	2.46	0.41
1:A:144:ALA:O	1:A:172:PHE:HA	2.22	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	695/682 (102%)	676 (97%)	19 (3%)	0	100	100
1	B	695/682 (102%)	674 (97%)	20 (3%)	1 (0%)	48	27
All	All	1390/1364 (102%)	1350 (97%)	39 (3%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	359	ASP

### 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	572/557 (103%)	563 (98%)	9 (2%)	55	33
1	B	572/557 (103%)	564 (99%)	8 (1%)	59	38
All	All	1144/1114 (103%)	1127 (98%)	17 (2%)	61	35

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

Mol	Chain	Res	Type
1	A	69	LYS
1	A	96[A]	VAL

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Mol	Chain	Res	Type
1	A	96[B]	VAL
1	A	179	LEU
1	A	256	LEU
1	A	377	MET
1	A	468	LYS
1	A	651	LYS
1	A	702	LEU
1	B	96[A]	VAL
1	B	96[B]	VAL
1	B	208	LYS
1	B	294	LYS
1	B	377	MET
1	B	447	ASP
1	B	600	LYS
1	B	702	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	478	GLN
1	B	445	HIS
1	B	448	GLN
1	B	478	GLN

### 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 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	A	810	-	3,3,3	0.20	0	2,2,2	0.62	0
2	EDO	A	808	-	3,3,3	0.27	0	2,2,2	0.31	0
2	EDO	A	804	-	3,3,3	0.37	0	2,2,2	0.26	0
2	EDO	B	802	-	3,3,3	0.32	0	2,2,2	0.69	0
2	EDO	B	805	-	3,3,3	0.29	0	2,2,2	0.11	0
2	EDO	B	807	-	3,3,3	0.47	0	2,2,2	0.23	0
4	PO4	B	816	-	4,4,4	0.56	0	6,6,6	0.49	0
2	EDO	A	801	-	3,3,3	0.12	0	2,2,2	0.31	0
2	EDO	A	803	-	3,3,3	0.03	0	2,2,2	0.52	0
2	EDO	B	812	-	3,3,3	0.10	0	2,2,2	0.42	0
2	EDO	B	811	-	3,3,3	0.18	0	2,2,2	0.05	0
2	EDO	B	806	-	3,3,3	0.23	0	2,2,2	0.32	0
2	EDO	B	803	-	3,3,3	0.28	0	2,2,2	0.53	0
2	EDO	A	805	-	3,3,3	0.14	0	2,2,2	0.30	0
2	EDO	B	809	-	3,3,3	0.31	0	2,2,2	0.34	0
2	EDO	A	806	-	3,3,3	0.25	0	2,2,2	0.01	0
4	PO4	A	815	-	4,4,4	1.60	1 (25%)	6,6,6	0.77	0
2	EDO	B	814	-	3,3,3	0.11	0	2,2,2	0.21	0
2	EDO	A	812	-	3,3,3	0.30	0	2,2,2	0.17	0
2	EDO	B	813	-	3,3,3	0.13	0	2,2,2	0.42	0
2	EDO	B	810	-	3,3,3	0.20	0	2,2,2	0.19	0
2	EDO	A	809	-	3,3,3	0.16	0	2,2,2	0.16	0
2	EDO	A	807	-	3,3,3	0.12	0	2,2,2	0.25	0
2	EDO	A	802	-	3,3,3	0.13	0	2,2,2	0.15	0
2	EDO	B	801	-	3,3,3	0.20	0	2,2,2	0.26	0
2	EDO	B	808	-	3,3,3	0.35	0	2,2,2	0.29	0
2	EDO	A	813	-	3,3,3	0.14	0	2,2,2	0.39	0
2	EDO	B	804	-	3,3,3	0.17	0	2,2,2	0.17	0
2	EDO	A	811	-	3,3,3	0.19	0	2,2,2	0.31	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	810	-	-	0/1/1/1	-
2	EDO	A	808	-	-	0/1/1/1	-
2	EDO	A	804	-	-	0/1/1/1	-
2	EDO	B	802	-	-	1/1/1/1	-
2	EDO	B	805	-	-	1/1/1/1	-
2	EDO	B	807	-	-	0/1/1/1	-
2	EDO	A	801	-	-	0/1/1/1	-
2	EDO	A	803	-	-	0/1/1/1	-
2	EDO	B	812	-	-	0/1/1/1	-
2	EDO	B	811	-	-	1/1/1/1	-
2	EDO	B	806	-	-	0/1/1/1	-
2	EDO	B	803	-	-	0/1/1/1	-
2	EDO	A	805	-	-	1/1/1/1	-
2	EDO	B	809	-	-	0/1/1/1	-
2	EDO	A	806	-	-	1/1/1/1	-
2	EDO	B	814	-	-	1/1/1/1	-
2	EDO	A	812	-	-	0/1/1/1	-
2	EDO	B	813	-	-	1/1/1/1	-
2	EDO	B	810	-	-	1/1/1/1	-
2	EDO	A	809	-	-	0/1/1/1	-
2	EDO	A	807	-	-	1/1/1/1	-
2	EDO	A	802	-	-	0/1/1/1	-
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	B	808	-	-	1/1/1/1	-
2	EDO	A	813	-	-	1/1/1/1	-
2	EDO	B	804	-	-	0/1/1/1	-
2	EDO	A	811	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	815	PO4	P-O1	3.04	1.58	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	805	EDO	O1-C1-C2-O2
2	A	806	EDO	O1-C1-C2-O2
2	B	810	EDO	O1-C1-C2-O2
2	B	813	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	814	EDO	O1-C1-C2-O2
2	B	805	EDO	O1-C1-C2-O2
2	A	813	EDO	O1-C1-C2-O2
2	B	808	EDO	O1-C1-C2-O2
2	B	811	EDO	O1-C1-C2-O2
2	A	807	EDO	O1-C1-C2-O2
2	A	811	EDO	O1-C1-C2-O2
2	B	802	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	807	EDO	4	0
2	A	807	EDO	1	0
2	A	813	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	681/682 (99%)	-0.45	1 (0%)	92 92	9, 21, 36, 59	15 (2%)
1	B	682/682 (100%)	-0.46	5 (0%)	84 87	9, 21, 35, 56	15 (2%)
All	All	1363/1364 (99%)	-0.45	6 (0%)	88 91	9, 21, 36, 59	30 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	TRP	3.3
1	B	716	LYS	3.3
1	B	106	LEU	2.3
1	A	561	THR	2.1
1	B	572	GLU	2.0
1	B	468	LYS	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, 95<sup>th</sup> 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	B	810	4/4	0.82	0.15	47,47,47,52	0
2	EDO	A	806	4/4	0.86	0.14	41,44,45,47	0
2	EDO	A	809	4/4	0.87	0.16	39,41,43,50	0
2	EDO	B	813	4/4	0.87	0.16	49,49,54,59	0
2	EDO	B	801	4/4	0.88	0.14	42,43,44,46	0
2	EDO	B	808	4/4	0.88	0.19	50,54,57,57	0
2	EDO	B	811	4/4	0.91	0.12	31,35,37,44	0
2	EDO	A	813	4/4	0.92	0.15	47,48,49,49	0
2	EDO	B	812	4/4	0.92	0.10	39,40,40,42	0
2	EDO	A	810	4/4	0.92	0.15	31,34,34,37	0
2	EDO	A	807	4/4	0.93	0.11	56,56,60,61	0
2	EDO	A	805	4/4	0.93	0.11	39,39,42,43	0
2	EDO	B	803	4/4	0.93	0.08	28,29,29,33	0
2	EDO	A	804	4/4	0.93	0.10	35,41,41,44	0
2	EDO	B	805	4/4	0.94	0.11	42,45,45,48	0
2	EDO	B	814	4/4	0.94	0.13	37,37,39,39	0
2	EDO	A	808	4/4	0.95	0.08	24,24,27,28	0
2	EDO	A	811	4/4	0.95	0.10	27,31,32,36	0
2	EDO	A	812	4/4	0.95	0.07	29,31,31,31	0
2	EDO	A	802	4/4	0.95	0.09	30,30,31,31	0
2	EDO	B	809	4/4	0.95	0.10	49,50,50,50	0
2	EDO	B	807	4/4	0.96	0.19	23,24,25,27	0
2	EDO	A	803	4/4	0.96	0.08	27,27,28,31	0
2	EDO	A	801	4/4	0.97	0.09	23,24,25,25	0
2	EDO	B	804	4/4	0.98	0.04	20,20,21,22	0
2	EDO	B	806	4/4	0.98	0.05	24,25,26,26	0
3	CA	A	814	1/1	0.98	0.15	24,24,24,24	0
4	PO4	A	815	5/5	0.98	0.14	25,26,29,35	0
4	PO4	B	816	5/5	0.98	0.08	25,27,28,29	0
2	EDO	B	802	4/4	0.99	0.03	23,24,25,25	0
3	CA	B	815	1/1	0.99	0.09	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.