



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:42 AM BST

PDB ID : 6DK2  
Title : Bacteroidetes AC2a SusD-like  
Authors : Koropatkin, N.M.  
Deposited on : 2018-05-28  
Resolution : 2.02 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.

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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 : 2.13.1  
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) : 2.13.1

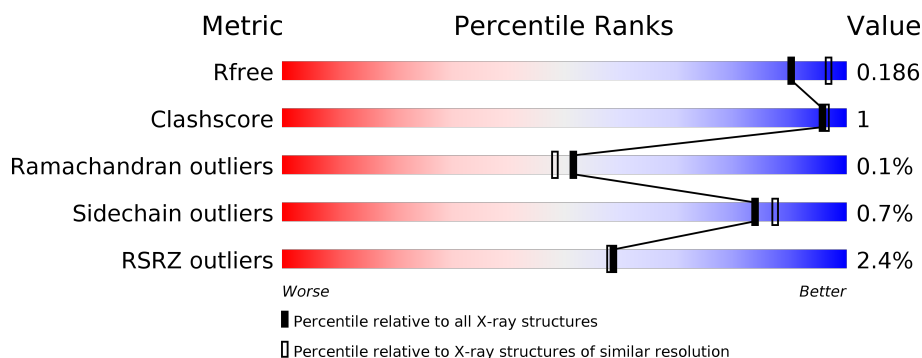
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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  $\geq 3$ , 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	529	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div></div> </div>
1	B	529	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9415 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 SusD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	4	0
			4139	2633	695	790	21			
1	B	515	Total	C	N	O	S	0	0	0
			4108	2615	686	786	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	-	expression tag	UNP A0A076ML24
B	32	SER	-	expression tag	UNP A0A076ML24

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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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		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	575	Total O 575 575	0	0

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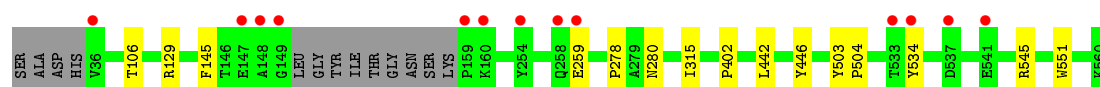
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	409	Total 409	O 409	0	0

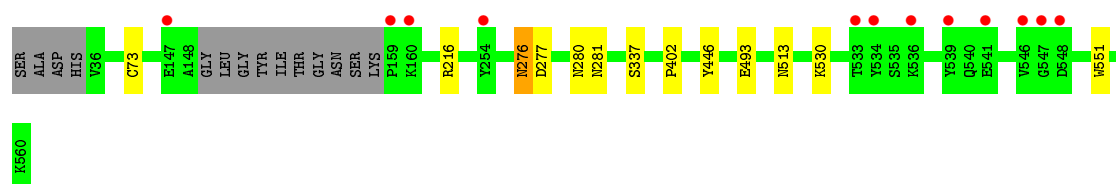
### 3 Residue-property plots [i](#)

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: SusD



- Molecule 1: SusD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.70Å 140.27Å 186.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.93 – 2.02 56.87 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.7 (56.93-2.02) 98.7 (56.87-2.02)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.152 , 0.176 0.163 , 0.186	Depositor DCC
$R_{free}$ test set	8391 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: CL, EDO, SO4

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	0.33	0/4261	0.49	0/5803
1	B	0.32	0/4221	0.49	0/5751
All	All	0.33	0/8482	0.49	0/11554

There are no bond length outliers.

There are no bond angle outliers.

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	4139	0	3919	9	0
1	B	4108	0	3880	8	0
2	A	40	0	0	1	0
2	B	30	0	0	0	0
3	A	76	0	114	3	0
3	B	36	0	54	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	575	0	0	2	0
5	B	409	0	0	0	0
All	All	9415	0	7967	18	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 (18) 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:73:CYS:SG	1:B:281:ASN:ND2	2.57	0.77
1:A:106:THR:HB	1:A:129[A]:ARG:NH1	2.10	0.66
1:A:106:THR:HB	1:A:129[A]:ARG:HH12	1.66	0.59
1:B:216:ARG:NH2	1:B:493:GLU:OE2	2.34	0.57
1:B:276:ASN:ND2	1:B:276:ASN:H	2.03	0.56
1:A:278:PRO:HG2	1:A:315:ILE:HD13	1.87	0.55
1:B:337:SER:HB2	3:B:607:EDO:H22	1.92	0.51
1:A:280[B]:ASN:ND2	1:B:513:ASN:OD1	2.46	0.48
1:A:402:PRO:HB3	3:A:617:EDO:H12	1.97	0.47
1:A:402:PRO:HG3	1:A:446:TYR:HB3	1.97	0.46
1:A:503:TYR:HA	1:A:504:PRO:C	2.36	0.46
1:A:129[A]:ARG:NH2	1:A:145:PHE:O	2.49	0.46
1:B:402:PRO:HG3	1:B:446:TYR:HB3	1.97	0.46
3:A:619:EDO:H11	5:A:874:HOH:O	2.17	0.44
1:A:545:ARG:NH1	2:A:601:SO4:O2	2.51	0.44
1:B:277:ASP:OD2	1:B:280:ASN:HB2	2.17	0.44
3:A:619:EDO:C1	5:A:874:HOH:O	2.66	0.43
1:B:337:SER:CB	3:B:607:EDO:H22	2.49	0.43

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	516/529 (98%)	501 (97%)	14 (3%)	1 (0%)	47	43
1	B	511/529 (97%)	496 (97%)	15 (3%)	0	100	100
All	All	1027/1058 (97%)	997 (97%)	29 (3%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	534	TYR

### 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	429/435 (99%)	426 (99%)	3 (1%)	84	87
1	B	425/435 (98%)	422 (99%)	3 (1%)	84	87
All	All	854/870 (98%)	848 (99%)	6 (1%)	84	87

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

Mol	Chain	Res	Type
1	A	259	GLU
1	A	442	LEU
1	A	551	TRP
1	B	276	ASN
1	B	530	LYS
1	B	551	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	276	ASN
1	B	281	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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	$\# Z  > 2$
3	EDO	A	614	-	3,3,3	0.45	0	2,2,2	0.23	0
3	EDO	B	609	-	3,3,3	0.44	0	2,2,2	0.31	0
3	EDO	A	622	-	3,3,3	0.52	0	2,2,2	0.17	0
3	EDO	B	613	-	3,3,3	0.57	0	2,2,2	0.15	0
2	SO4	A	603	-	4,4,4	0.41	0	6,6,6	0.11	0
3	EDO	A	612	-	3,3,3	0.44	0	2,2,2	0.28	0
2	SO4	A	607	-	4,4,4	0.36	0	6,6,6	0.06	0
3	EDO	A	627	-	3,3,3	0.58	0	2,2,2	0.13	0
3	EDO	A	623	-	3,3,3	0.46	0	2,2,2	0.25	0
3	EDO	B	612	-	3,3,3	0.41	0	2,2,2	0.39	0
3	EDO	B	607	-	3,3,3	0.60	0	2,2,2	0.16	0
3	EDO	B	614	-	3,3,3	0.47	0	2,2,2	0.30	0
2	SO4	A	605	-	4,4,4	0.40	0	6,6,6	0.06	0
2	SO4	B	602	-	4,4,4	0.37	0	6,6,6	0.08	0
3	EDO	A	625	-	3,3,3	0.45	0	2,2,2	0.29	0
3	EDO	A	624	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	621	-	3,3,3	0.52	0	2,2,2	0.39	0
3	EDO	A	609	-	3,3,3	0.54	0	2,2,2	0.18	0
3	EDO	A	620	-	3,3,3	0.59	0	2,2,2	0.21	0
3	EDO	A	610	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	B	610	-	3,3,3	0.49	0	2,2,2	0.26	0
3	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	604	-	4,4,4	0.36	0	6,6,6	0.07	0
2	SO4	B	603	-	4,4,4	0.37	0	6,6,6	0.04	0
3	EDO	A	615	-	3,3,3	0.68	0	2,2,2	0.30	0
3	EDO	B	615	-	3,3,3	0.58	0	2,2,2	0.19	0
3	EDO	A	617	-	3,3,3	0.46	0	2,2,2	0.43	0
3	EDO	B	611	-	3,3,3	0.42	0	2,2,2	0.47	0
3	EDO	A	613	-	3,3,3	0.42	0	2,2,2	0.31	0
2	SO4	B	605	-	4,4,4	0.34	0	6,6,6	0.08	0
3	EDO	A	626	-	3,3,3	0.58	0	2,2,2	0.01	0
2	SO4	A	602	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	A	608	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	B	606	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	B	601	-	4,4,4	0.35	0	6,6,6	0.09	0
3	EDO	A	618	-	3,3,3	0.67	0	2,2,2	0.32	0
3	EDO	A	616	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	619	-	3,3,3	0.37	0	2,2,2	0.38	0
3	EDO	B	608	-	3,3,3	0.51	0	2,2,2	0.23	0
2	SO4	A	606	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	B	604	-	4,4,4	0.39	0	6,6,6	0.06	0
2	SO4	A	601	-	4,4,4	0.36	0	6,6,6	0.10	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
3	EDO	A	614	-	-	0/1/1/1	-
3	EDO	B	609	-	-	0/1/1/1	-
3	EDO	A	622	-	-	1/1/1/1	-
3	EDO	B	613	-	-	1/1/1/1	-
3	EDO	A	612	-	-	1/1/1/1	-
3	EDO	A	627	-	-	1/1/1/1	-
3	EDO	A	623	-	-	1/1/1/1	-
3	EDO	B	612	-	-	1/1/1/1	-
3	EDO	B	607	-	-	1/1/1/1	-
3	EDO	B	614	-	-	1/1/1/1	-
3	EDO	A	625	-	-	1/1/1/1	-
3	EDO	A	624	-	-	1/1/1/1	-
3	EDO	A	621	-	-	0/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	A	620	-	-	1/1/1/1	-
3	EDO	A	610	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	610	-	-	1/1/1/1	-
3	EDO	A	611	-	-	1/1/1/1	-
3	EDO	B	615	-	-	0/1/1/1	-
3	EDO	A	617	-	-	1/1/1/1	-
3	EDO	B	611	-	-	0/1/1/1	-
3	EDO	A	613	-	-	1/1/1/1	-
3	EDO	A	626	-	-	1/1/1/1	-
3	EDO	A	615	-	-	1/1/1/1	-
3	EDO	A	618	-	-	1/1/1/1	-
3	EDO	A	616	-	-	0/1/1/1	-
3	EDO	A	619	-	-	1/1/1/1	-
3	EDO	B	608	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	612	EDO	O1-C1-C2-O2
3	B	612	EDO	O1-C1-C2-O2
3	B	614	EDO	O1-C1-C2-O2
3	A	625	EDO	O1-C1-C2-O2
3	A	609	EDO	O1-C1-C2-O2
3	A	611	EDO	O1-C1-C2-O2
3	A	617	EDO	O1-C1-C2-O2
3	A	613	EDO	O1-C1-C2-O2
3	A	618	EDO	O1-C1-C2-O2
3	B	613	EDO	O1-C1-C2-O2
3	A	624	EDO	O1-C1-C2-O2
3	A	610	EDO	O1-C1-C2-O2
3	A	622	EDO	O1-C1-C2-O2
3	A	627	EDO	O1-C1-C2-O2
3	B	607	EDO	O1-C1-C2-O2
3	B	610	EDO	O1-C1-C2-O2
3	A	626	EDO	O1-C1-C2-O2
3	B	608	EDO	O1-C1-C2-O2
3	A	620	EDO	O1-C1-C2-O2
3	A	615	EDO	O1-C1-C2-O2
3	A	619	EDO	O1-C1-C2-O2
3	A	623	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	607	EDO	2	0
3	A	617	EDO	1	0
3	A	619	EDO	2	0
2	A	601	SO4	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, 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	516/529 (97%)	-0.17	13 (2%) 57 57	27, 36, 61, 86	0
1	B	515/529 (97%)	-0.15	12 (2%) 60 59	35, 47, 70, 96	0
All	All	1031/1058 (97%)	-0.16	25 (2%) 59 58	27, 42, 65, 96	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	534	TYR	6.1
1	A	36	VAL	4.5
1	A	534	TYR	4.5
1	A	533	THR	4.2
1	A	149	GLY	4.1
1	B	547	GLY	3.0
1	B	147	GLU	2.9
1	B	533	THR	2.9
1	B	159	PRO	2.8
1	B	541	GLU	2.7
1	B	536	LYS	2.7
1	A	160	LYS	2.5
1	A	147	GLU	2.5
1	B	254	TYR	2.4
1	B	539	TYR	2.3
1	A	258	GLN	2.3
1	B	160	LYS	2.3
1	A	254	TYR	2.2
1	B	548	ASP	2.2
1	B	546	VAL	2.2
1	A	259	GLU	2.1
1	A	148	ALA	2.1
1	A	541	GLU	2.1
1	A	537	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	159	PRO	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 [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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	602	5/5	0.63	0.36	97,107,110,111	0
3	EDO	A	620	4/4	0.66	0.31	47,50,57,71	0
3	EDO	B	610	4/4	0.69	0.20	59,67,70,74	0
3	EDO	B	611	4/4	0.77	0.30	78,79,80,82	0
3	EDO	A	609	4/4	0.77	0.25	66,70,71,74	0
3	EDO	B	607	4/4	0.80	0.29	55,58,63,67	0
2	SO4	B	604	5/5	0.81	0.30	88,101,103,106	0
3	EDO	A	618	4/4	0.82	0.19	43,52,55,60	0
3	EDO	A	621	4/4	0.83	0.27	40,45,46,47	0
2	SO4	B	605	5/5	0.83	0.50	105,114,123,130	0
3	EDO	B	608	4/4	0.83	0.29	61,69,74,78	0
3	EDO	A	626	4/4	0.83	0.17	49,49,53,54	0
3	EDO	A	611	4/4	0.84	0.23	48,57,58,65	0
3	EDO	B	613	4/4	0.85	0.34	51,56,59,66	0
3	EDO	B	614	4/4	0.85	0.27	73,74,75,77	0
2	SO4	A	606	5/5	0.85	0.49	113,114,121,125	0
2	SO4	A	605	5/5	0.85	0.41	89,101,111,112	0
2	SO4	A	603	5/5	0.86	0.45	89,94,99,109	0
3	EDO	A	627	4/4	0.86	0.19	49,55,59,61	0
3	EDO	A	622	4/4	0.86	0.17	47,60,66,71	0
3	EDO	A	617	4/4	0.87	0.13	55,55,56,57	0
3	EDO	A	612	4/4	0.88	0.21	51,56,58,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	606	5/5	0.88	0.44	112,113,115,123	0
3	EDO	B	615	4/4	0.88	0.25	54,56,57,60	0
2	SO4	B	603	5/5	0.89	0.38	105,109,111,112	0
3	EDO	A	610	4/4	0.90	0.16	65,65,70,72	0
3	EDO	A	613	4/4	0.90	0.26	56,59,61,65	0
2	SO4	A	608	5/5	0.91	0.36	99,102,106,108	0
3	EDO	A	623	4/4	0.91	0.11	62,64,65,67	0
3	EDO	B	612	4/4	0.91	0.28	66,67,72,73	0
3	EDO	A	615	4/4	0.91	0.15	32,39,42,45	0
4	CL	B	616	1/1	0.91	0.26	75,75,75,75	0
3	EDO	A	614	4/4	0.91	0.22	46,48,49,51	0
2	SO4	A	604	5/5	0.92	0.29	80,81,90,93	0
3	EDO	A	616	4/4	0.92	0.24	54,56,61,61	0
2	SO4	B	602	5/5	0.92	0.17	86,88,92,93	0
3	EDO	A	625	4/4	0.92	0.20	52,58,61,71	0
2	SO4	B	601	5/5	0.92	0.31	99,105,112,112	0
2	SO4	A	601	5/5	0.92	0.46	115,115,119,119	0
3	EDO	A	624	4/4	0.93	0.12	64,65,69,73	0
3	EDO	B	609	4/4	0.93	0.11	65,65,65,74	0
4	CL	A	628	1/1	0.94	0.27	67,67,67,67	0
3	EDO	A	619	4/4	0.94	0.24	52,58,64,75	0
2	SO4	A	607	5/5	0.94	0.33	84,85,90,101	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.