



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2019 – 11:18 AM EDT

PDB ID : 6HQ6
Title : Bacterial beta-1,3-oligosaccharide phosphorylase from GH149
Authors : Kuhaudomlarp, S.; Stevenson, C.E.M.; Lawson, D.M.; Field, R.A.
Deposited on : 2018-09-24
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

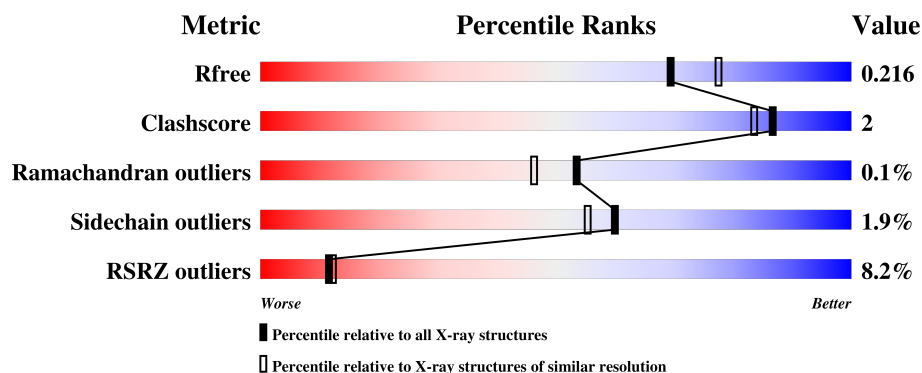
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.05 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}	111664	1449 (2.04-2.04)
Clashscore	122126	1524 (2.04-2.04)
Ramachandran outliers	120053	1512 (2.04-2.04)
Sidechain outliers	120020	1512 (2.04-2.04)
RSRZ outliers	108989	1429 (2.04-2.04)

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. 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	1175	 16% 91% 6% •
1	B	1175	 16% 90% 6% •

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
4	EDO	A	1207	-	-	X	-
5	CL	A	1218[B]	-	-	X	-

2 Entry composition [i](#)

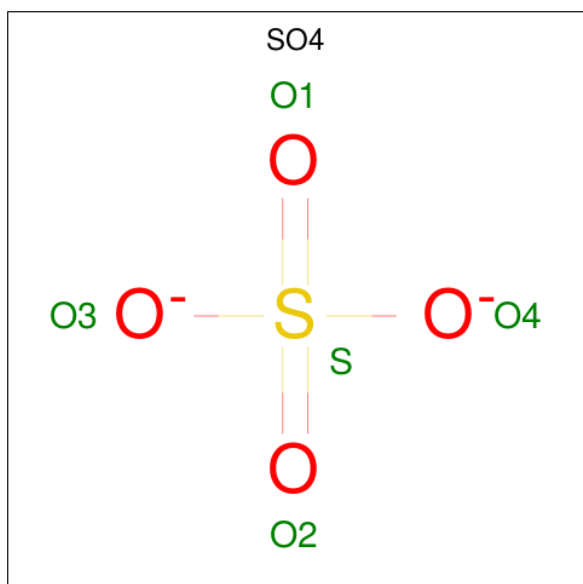
There are 6 unique types of molecules in this entry. The entry contains 18854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bacterial beta-1,3-oligosaccharide phosphorylase.

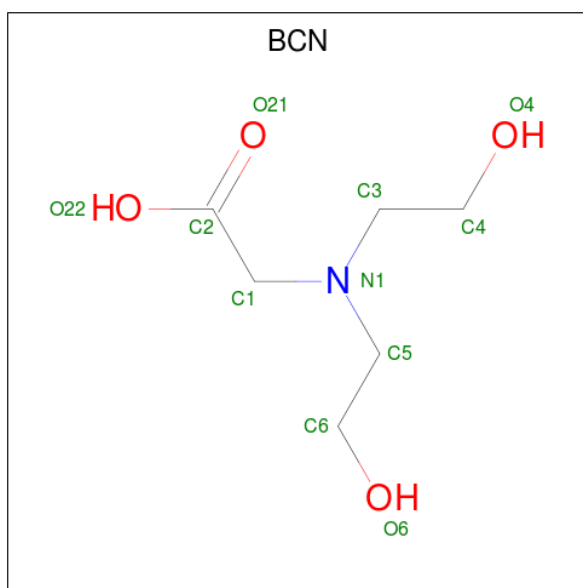
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1135	Total	C	N	O	S	0	3	0
			9084	5805	1507	1743	29			
1	B	1133	Total	C	N	O	S	0	0	0
			8754	5578	1453	1694	29			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



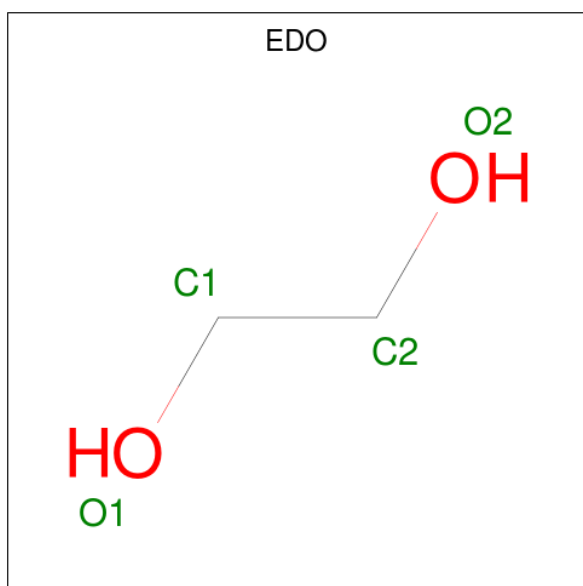
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	3	Total Cl 4 4	0	1

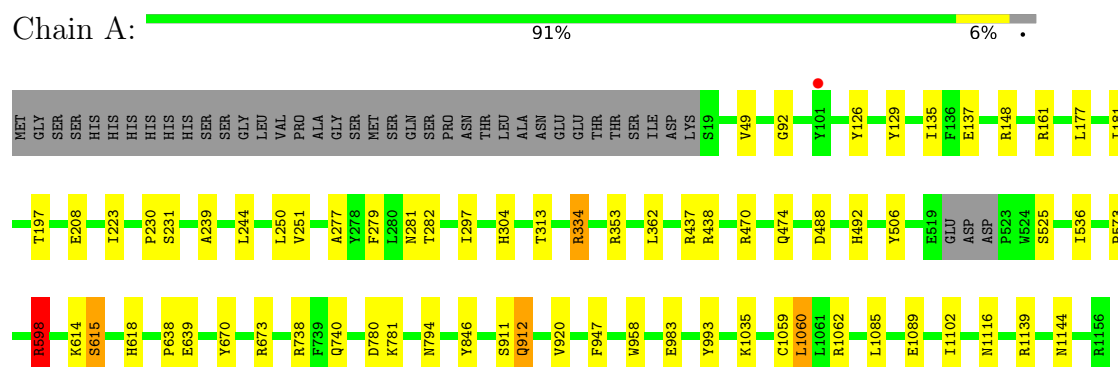
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	676	Total 708	O 708	0	32
6	B	189	Total 193	O 193	0	4

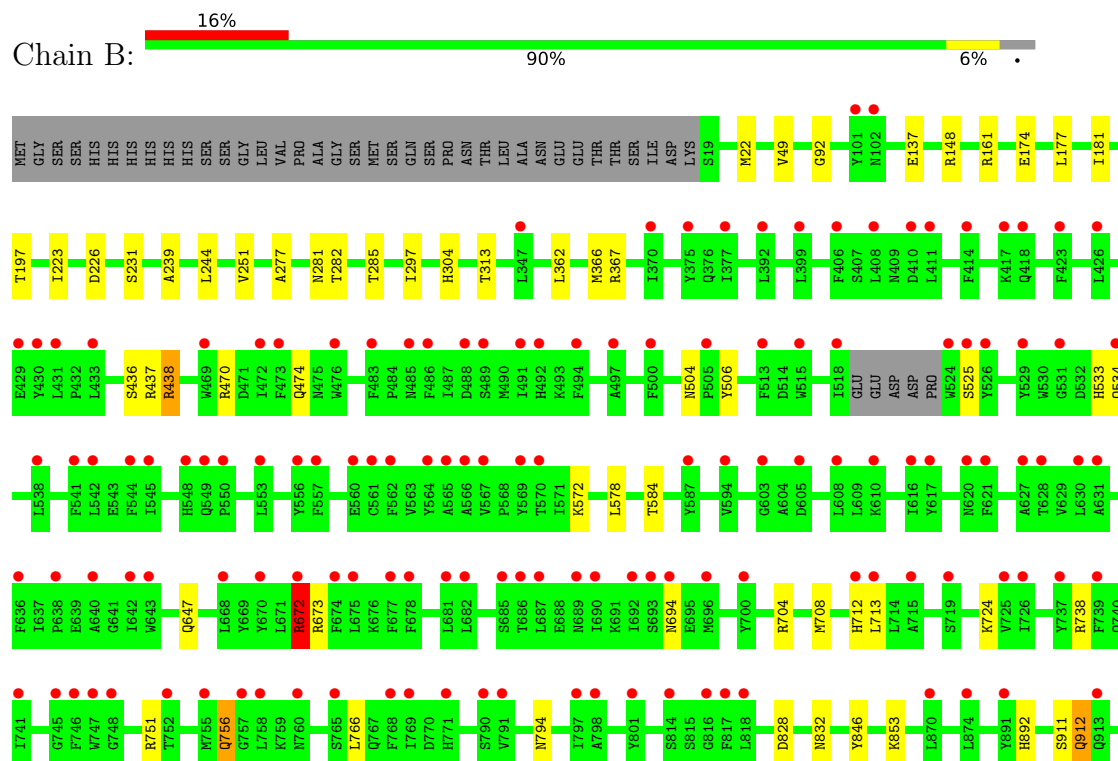
3 Residue-property plots

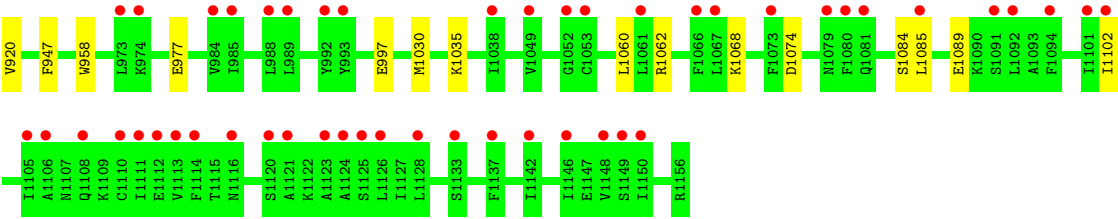
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Bacterial beta-1,3-oligosaccharide phosphorylase



- Molecule 1: Bacterial beta-1,3-oligosaccharide phosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.24Å 158.99Å 181.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.49 – 2.05 79.49 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.49-2.05) 100.0 (79.49-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.182 , 0.211 0.188 , 0.216	Depositor DCC
R_{free} test set	9118 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18854	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: BCN, 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	0.58	0/9284	0.68	3/12557 (0.0%)
1	B	0.46	0/8948	0.60	0/12154
All	All	0.53	0/18232	0.64	3/24711 (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	6
1	B	0	4
All	All	0	10

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1139	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	A	598	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	334	ARG	NE-CZ-NH2	5.16	122.88	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	353	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	438	ARG	Sidechain
1	A	598	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	9084	0	8782	38	0
1	B	8754	0	8107	43	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	11	0	12	0	0
3	B	11	0	12	0	0
4	A	48	0	72	7	0
4	B	20	0	30	1	0
5	A	4	0	0	2	0
5	B	1	0	0	0	0
6	A	708	0	0	2	0
6	B	193	0	0	0	0
All	All	18854	0	17015	79	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.

The worst 5 of 79 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:756:GLN:HA	1:B:756:GLN:HE21	1.29	0.96
1:B:438:ARG:HH11	1:B:438:ARG:HG2	1.30	0.93
1:A:912:GLN:HA	1:A:912:GLN:HE21	1.52	0.74
1:B:438:ARG:CG	1:B:438:ARG:HH11	2.01	0.74
1:B:504:ASN:HD22	1:B:534:GLN:HE21	1.37	0.72

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	1134/1175 (96%)	1102 (97%)	31 (3%)	1 (0%)	53	46
1	B	1129/1175 (96%)	1095 (97%)	33 (3%)	1 (0%)	53	46
All	All	2263/2350 (96%)	2197 (97%)	64 (3%)	2 (0%)	53	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	794	ASN
1	B	794	ASN

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	979/1041 (94%)	962 (98%)	17 (2%)	63	60
1	B	892/1041 (86%)	873 (98%)	19 (2%)	56	51
All	All	1871/2082 (90%)	1835 (98%)	36 (2%)	60	55

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1089	GLU
1	B	313	THR
1	B	1060	LEU
1	B	197	THR

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Mol	Chain	Res	Type
1	B	437	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	GLN
1	B	156	GLN
1	B	694	ASN
1	A	1144	ASN
1	B	712	HIS

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](#)

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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	SO4	A	1201	-	4,4,4	0.65	0	6,6,6	0.70	0
2	SO4	A	1202	-	4,4,4	0.24	0	6,6,6	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BCN	A	1203	-	7,10,10	0.44	0	8,11,11	1.30	1 (12%)
4	EDO	A	1204	-	3,3,3	0.50	0	2,2,2	0.34	0
4	EDO	A	1205	-	3,3,3	0.28	0	2,2,2	0.69	0
4	EDO	A	1206	-	3,3,3	0.37	0	2,2,2	0.30	0
4	EDO	A	1207	-	3,3,3	0.57	0	2,2,2	0.18	0
4	EDO	A	1208	-	3,3,3	0.53	0	2,2,2	0.10	0
4	EDO	A	1209	-	3,3,3	0.42	0	2,2,2	0.49	0
4	EDO	A	1210	-	3,3,3	0.42	0	2,2,2	0.77	0
4	EDO	A	1211	-	3,3,3	0.49	0	2,2,2	0.51	0
4	EDO	A	1212	-	3,3,3	0.54	0	2,2,2	0.34	0
4	EDO	A	1213	-	3,3,3	0.57	0	2,2,2	0.31	0
4	EDO	A	1214	-	3,3,3	0.40	0	2,2,2	0.22	0
4	EDO	A	1215	-	3,3,3	0.43	0	2,2,2	0.43	0
2	SO4	B	1201	-	4,4,4	0.45	0	6,6,6	0.30	0
2	SO4	B	1202	-	4,4,4	0.41	0	6,6,6	0.22	0
3	BCN	B	1203	-	7,10,10	0.54	0	8,11,11	1.26	1 (12%)
4	EDO	B	1204	-	3,3,3	0.57	0	2,2,2	0.19	0
4	EDO	B	1205	-	3,3,3	0.57	0	2,2,2	0.16	0
4	EDO	B	1206	-	3,3,3	0.64	0	2,2,2	0.10	0
4	EDO	B	1207	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	B	1208	-	3,3,3	0.31	0	2,2,2	0.55	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	BCN	A	1203	-	-	0/8/10/10	-
4	EDO	A	1204	-	-	0/1/1/1	-
4	EDO	A	1205	-	-	0/1/1/1	-
4	EDO	A	1206	-	-	0/1/1/1	-
4	EDO	A	1207	-	-	0/1/1/1	-
4	EDO	A	1208	-	-	0/1/1/1	-
4	EDO	A	1209	-	-	0/1/1/1	-
4	EDO	A	1210	-	-	1/1/1/1	-
4	EDO	A	1211	-	-	0/1/1/1	-
4	EDO	A	1212	-	-	1/1/1/1	-
4	EDO	A	1213	-	-	0/1/1/1	-
4	EDO	A	1214	-	-	1/1/1/1	-
4	EDO	A	1215	-	-	0/1/1/1	-
3	BCN	B	1203	-	-	1/8/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1204	-	-	0/1/1/1	-
4	EDO	B	1205	-	-	0/1/1/1	-
4	EDO	B	1206	-	-	1/1/1/1	-
4	EDO	B	1207	-	-	0/1/1/1	-
4	EDO	B	1208	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1203	BCN	C2-C1-N1	-3.03	109.17	113.48
3	B	1203	BCN	C2-C1-N1	-2.79	109.50	113.48

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1214	EDO	O1-C1-C2-O2
4	B	1206	EDO	O1-C1-C2-O2
4	A	1210	EDO	O1-C1-C2-O2
3	B	1203	BCN	N1-C3-C4-O4
4	B	1208	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1205	EDO	2	0
4	A	1207	EDO	4	0
4	A	1214	EDO	1	0
4	B	1206	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	1135/1175 (96%)	-0.10	1 (0%) 95 95	29, 44, 75, 108	0
1	B	1133/1175 (96%)	0.74	186 (16%) 1 1	36, 82, 124, 145	0
All	All	2268/2350 (96%)	0.32	187 (8%) 11 12	29, 58, 116, 145	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	PHE	8.5
1	B	1128	LEU	6.4
1	B	486	PHE	6.0
1	B	524	TRP	5.8
1	B	681	LEU	5.8

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(\AA^2)	Q<0.9
2	SO4	B	1202	5/5	0.72	0.13	116,122,130,137	0
3	BCN	B	1203	11/11	0.79	0.16	66,71,80,80	0
4	EDO	A	1211	4/4	0.84	0.14	47,57,59,65	0
5	CL	A	1217	1/1	0.86	0.14	103,103,103,103	0
4	EDO	B	1207	4/4	0.87	0.19	67,73,74,76	0
5	CL	B	1209	1/1	0.88	0.16	92,92,92,92	0
4	EDO	A	1215	4/4	0.89	0.23	65,68,71,74	0
5	CL	A	1218[A]	1/1	0.89	0.26	48,48,48,48	1
5	CL	A	1218[B]	1/1	0.89	0.26	67,67,67,67	1
4	EDO	B	1205	4/4	0.90	0.12	71,75,78,78	0
4	EDO	B	1206	4/4	0.90	0.23	64,66,71,72	0
4	EDO	A	1213	4/4	0.91	0.11	57,57,60,61	0
5	CL	A	1216	1/1	0.92	0.17	78,78,78,78	0
4	EDO	B	1204	4/4	0.92	0.11	55,60,60,63	0
4	EDO	A	1208	4/4	0.92	0.10	44,44,46,48	0
4	EDO	A	1209	4/4	0.93	0.14	42,47,52,58	0
4	EDO	A	1207	4/4	0.93	0.12	37,42,44,44	0
3	BCN	A	1203	11/11	0.94	0.12	34,39,45,46	0
4	EDO	A	1212	4/4	0.94	0.16	57,60,65,66	0
4	EDO	A	1206	4/4	0.94	0.13	52,52,57,57	0
2	SO4	B	1201	5/5	0.95	0.14	77,80,83,95	0
4	EDO	A	1210	4/4	0.96	0.15	33,35,36,42	0
4	EDO	A	1214	4/4	0.97	0.17	51,56,62,64	0
4	EDO	A	1204	4/4	0.97	0.13	35,36,36,37	0
4	EDO	B	1208	4/4	0.97	0.13	59,60,61,66	0
4	EDO	A	1205	4/4	0.97	0.24	45,45,46,47	0
2	SO4	A	1201	5/5	0.98	0.09	48,50,54,56	0
2	SO4	A	1202	5/5	0.99	0.14	48,50,51,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.