



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:51 AM UTC

PDB ID : 6HQ6 / pdb_00006hq6
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 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

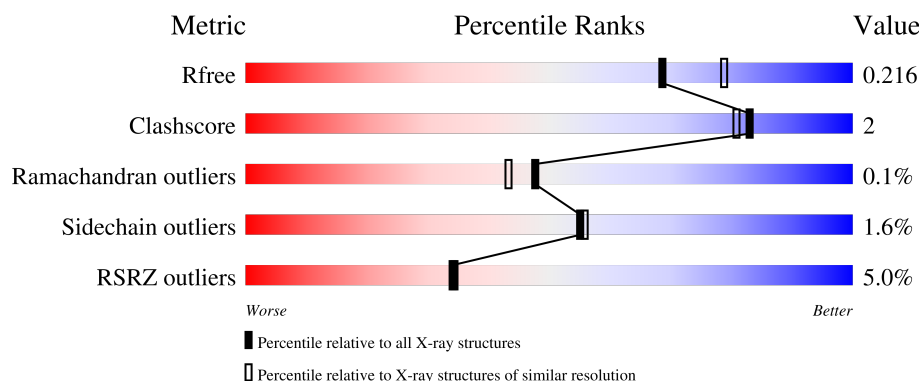
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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	1175	
1	B	1175	

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](#)

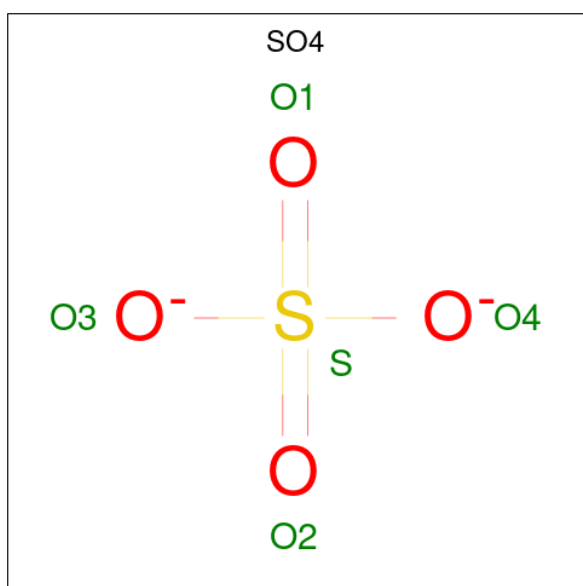
There are 6 unique types of molecules in this entry. The entry contains 18854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

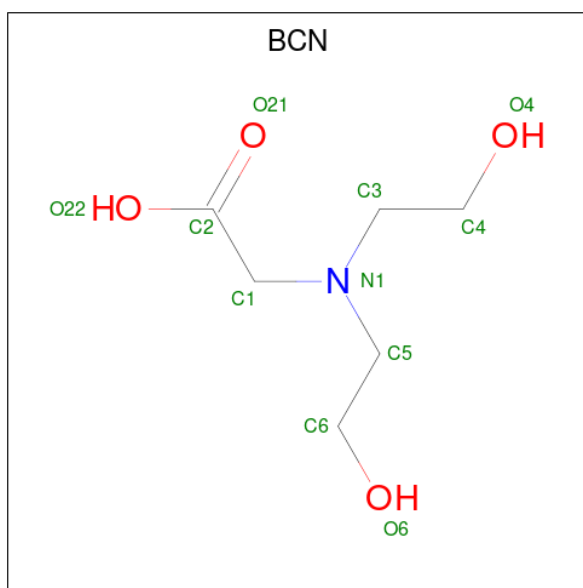
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1135	Total	C	N	O	S	0	3	0
			9084	5805	1507	1743	29			
1	B	1133	Total	C	N	O	S	0	0	0
			8754	5578	1453	1694	29			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



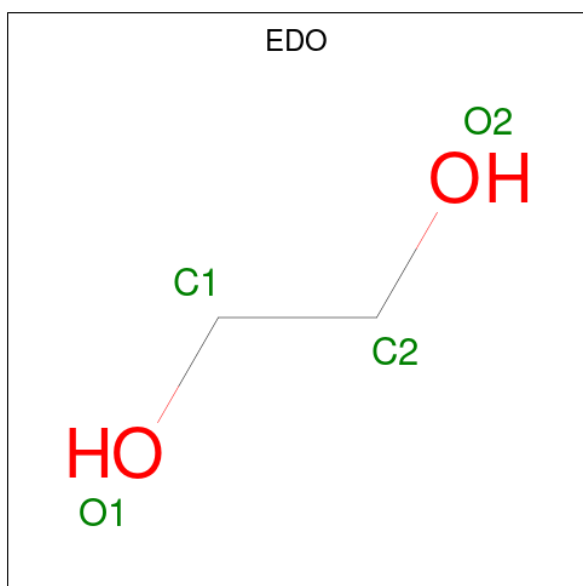
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

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

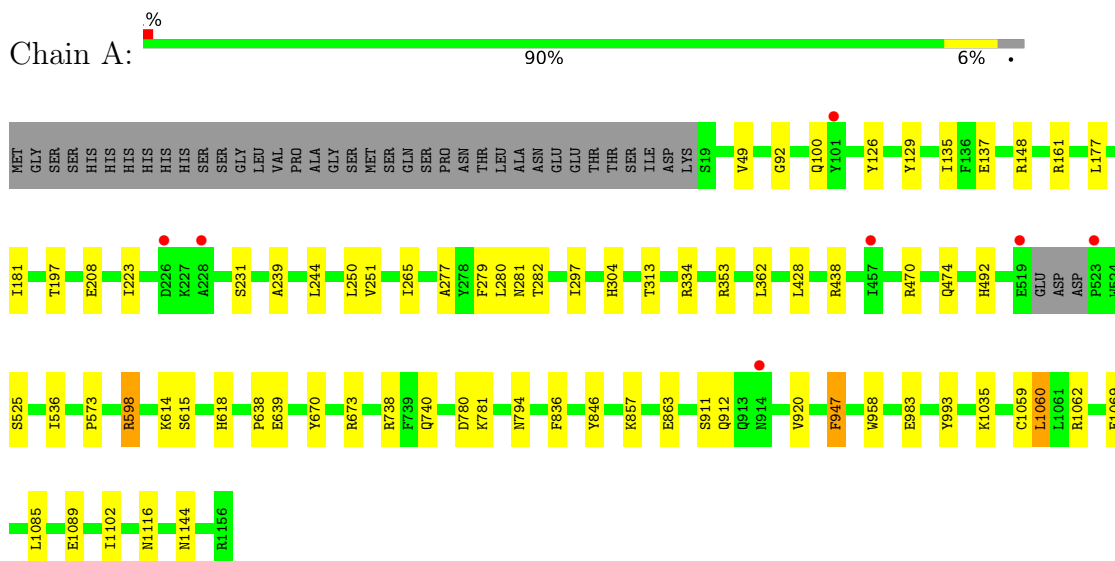
- Molecule 6 is water.

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

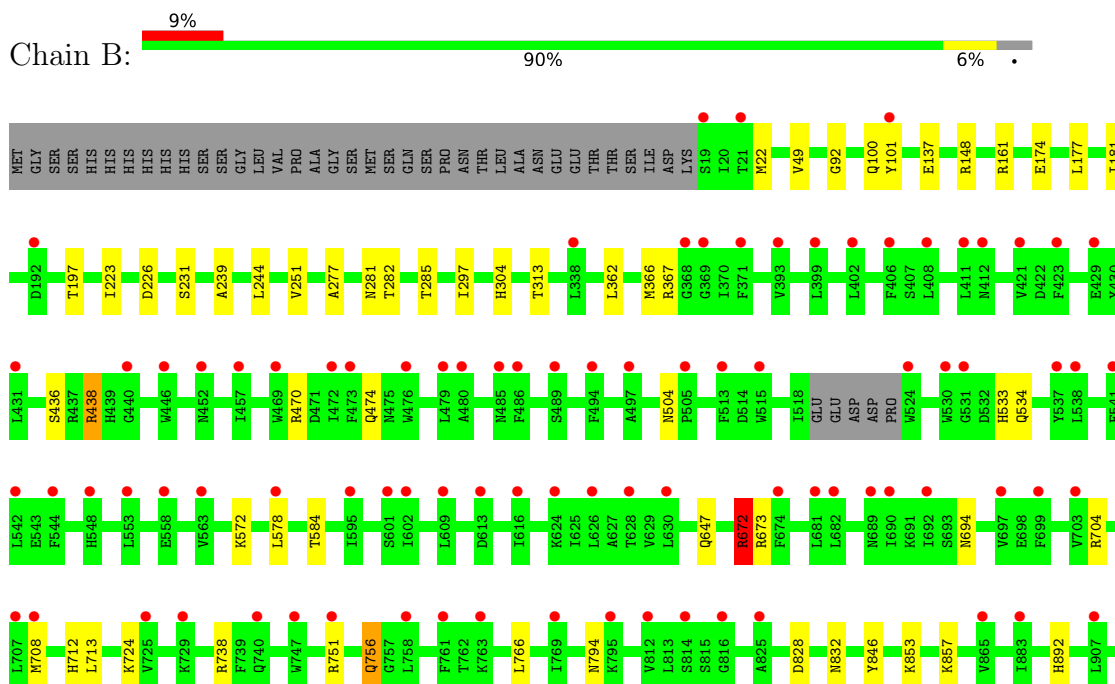
3 Residue-property plots [i](#)

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: 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 (4.87%)	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)	0.34 , 58.9	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, EDO, SO4, CL

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	0.87	1/9284 (0.0%)	0.95	2/12557 (0.0%)
1	B	0.74	0/8948	0.91	2/12154 (0.0%)
All	All	0.81	1/18232 (0.0%)	0.93	4/24711 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	836	PHE	C-O	-5.05	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1069	GLU	CB-CG-CD	5.54	122.02	112.60
1	B	947	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	947	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	101	TYR	CB-CA-C	5.03	117.88	110.14

There are no chirality outliers.

All (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
1	A	438	ARG	Sidechain
1	A	598	ARG	Sidechain
1	A	673	ARG	Sidechain
1	B	1062	ARG	Sidechain
1	B	161	ARG	Sidechain
1	B	672	ARG	Sidechain
1	B	673	ARG	Sidechain

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	9084	0	8782	40	0
1	B	8754	0	8107	45	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	3	0
6	B	193	0	0	1	0
All	All	18854	0	17015	83	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 (83) 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:HE21	1:B:756:GLN:HA	1.29	0.96
1:B:438:ARG:HH11	1:B:438:ARG:HG2	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:GLN:HE21	1:A:912:GLN:HA	1.52	0.74
1:B:438:ARG:HH11	1:B:438:ARG:CG	2.01	0.74
1:B:504:ASN:HD22	1:B:534:GLN:HE21	1.37	0.72
1:A:857:LYS:NZ	6:A:1301:HOH:O	2.22	0.71
1:B:367:ARG:CA	1:B:1030:MET:HE3	2.21	0.70
1:A:958:TRP:CG	4:A:1207:EDO:H21	2.28	0.69
1:B:504:ASN:HD21	1:B:533:HIS:HB3	1.59	0.66
1:B:912:GLN:HE21	1:B:912:GLN:HA	1.61	0.65
1:A:1116:ASN:HA	1:A:1144:ASN:HD21	1.63	0.64
1:B:438:ARG:CG	1:B:438:ARG:NH1	2.62	0.61
1:B:49:VAL:HG11	1:B:362:LEU:HD21	1.82	0.60
6:A:1909[B]:HOH:O	1:B:304:HIS:HD2	1.85	0.60
1:B:367:ARG:CB	1:B:1030:MET:HE3	2.34	0.57
1:B:367:ARG:HA	1:B:1030:MET:HE3	1.88	0.55
1:A:492:HIS:HD2	6:A:1634:HOH:O	1.89	0.55
1:A:993[B]:TYR:CE1	1:A:1062:ARG:NH2	2.74	0.54
1:B:438:ARG:HG2	1:B:438:ARG:NH1	2.10	0.54
1:B:756:GLN:HA	1:B:756:GLN:NE2	2.11	0.53
1:A:470:ARG:HG2	1:A:474:GLN:NE2	2.25	0.52
1:B:470:ARG:HG2	1:B:474:GLN:NE2	2.24	0.52
1:A:738:ARG:HG3	4:A:1205:EDO:H12	1.92	0.52
1:B:584:THR:H	1:B:647:GLN:NE2	2.08	0.51
1:A:598:ARG:NH2	1:A:615:SER:O	2.42	0.50
1:B:672:ARG:HH21	1:B:766:LEU:HD22	1.76	0.49
1:B:244:LEU:HD22	1:B:282:THR:HG21	1.95	0.49
1:A:49:VAL:HG21	1:A:362:LEU:HD21	1.95	0.49
1:A:304:HIS:CE1	1:B:892:HIS:CE1	3.01	0.49
1:B:367:ARG:HB2	1:B:1030:MET:HE3	1.95	0.48
1:B:712:HIS:CE1	1:B:713:LEU:HD12	2.47	0.48
1:B:756:GLN:HE21	1:B:756:GLN:CA	2.10	0.48
1:A:573:PRO:HG3	4:A:1205:EDO:H22	1.96	0.47
1:B:578:LEU:HD21	1:B:724:LYS:NZ	2.29	0.47
1:B:704:ARG:HG2	1:B:708:MET:SD	2.54	0.47
1:B:912:GLN:HE21	1:B:912:GLN:CA	2.25	0.47
1:B:174:GLU:OE1	1:B:285:THR:OG1	2.26	0.47
1:B:958:TRP:CD1	4:B:1206:EDO:H21	2.50	0.47
1:B:1074:ASP:OD1	1:B:1084:SER:OG	2.32	0.47
1:A:912:GLN:HA	1:A:912:GLN:NE2	2.25	0.46
1:B:223:ILE:HB	1:B:231:SER:OG	2.16	0.46
1:B:367:ARG:HA	1:B:1030:MET:CE	2.45	0.46
1:A:1085:LEU:HD13	1:A:1102:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ASN:HD22	1:B:751:ARG:CG	2.28	0.46
1:A:137:GLU:OE2	1:A:148:ARG:HD3	2.16	0.45
1:B:572:LYS:O	1:B:738:ARG:NH2	2.49	0.45
1:B:137:GLU:OE2	1:B:148:ARG:HD3	2.16	0.45
1:A:958:TRP:CD1	4:A:1207:EDO:H21	2.52	0.45
1:A:177:LEU:C	1:A:177:LEU:HD12	2.42	0.45
1:B:177:LEU:C	1:B:177:LEU:HD12	2.42	0.45
1:B:828:ASP:O	1:B:832:ASN:ND2	2.50	0.45
1:B:1085:LEU:HD13	1:B:1102:ILE:HD11	1.99	0.45
1:A:911:SER:HB3	1:A:920:VAL:HG11	2.00	0.44
1:A:1116:ASN:HA	1:A:1144:ASN:ND2	2.32	0.44
1:A:49:VAL:HG21	1:A:362:LEU:CD2	2.48	0.44
1:A:223:ILE:HB	1:A:231:SER:OG	2.18	0.44
1:A:958:TRP:CD1	4:A:1207:EDO:C2	3.01	0.44
1:B:177:LEU:O	1:B:281:ASN:HA	2.17	0.44
1:A:244:LEU:HD22	1:A:282:THR:HG21	2.00	0.44
1:B:911:SER:HB3	1:B:920:VAL:HG11	1.99	0.44
1:A:251:VAL:HA	1:A:277:ALA:O	2.18	0.43
1:B:367:ARG:N	1:B:1030:MET:HE3	2.34	0.43
1:A:92:GLY:O	1:A:181:ILE:HA	2.18	0.43
1:A:618:HIS:ND1	5:A:1218[B]:CL:CL	2.77	0.43
1:B:92:GLY:O	1:B:181:ILE:HA	2.19	0.42
1:A:177:LEU:O	1:A:281:ASN:HA	2.18	0.42
1:A:129:TYR:HB3	4:A:1214:EDO:C2	2.50	0.42
1:A:780:ASP:O	1:A:781:LYS:HB2	2.20	0.41
1:A:993[B]:TYR:CE1	1:A:1062:ARG:CZ	3.03	0.41
1:B:366:MET:O	1:B:436:SER:HA	2.20	0.41
1:A:1059:CYS:SG	1:A:1060:LEU:HD13	2.61	0.41
1:B:857:LYS:NZ	6:B:1304:HOH:O	2.44	0.41
1:A:250:LEU:HB2	1:A:279:PHE:HB2	2.02	0.41
1:A:536:ILE:HD13	1:A:670:TYR:CD1	2.55	0.41
1:A:614:LYS:HG3	5:A:1218[B]:CL:CL	2.58	0.41
1:B:239:ALA:HA	1:B:297:ILE:O	2.20	0.41
1:B:251:VAL:HA	1:B:277:ALA:O	2.20	0.41
1:A:958:TRP:CG	4:A:1207:EDO:C2	3.03	0.40
1:A:208:GLU:OE1	1:B:853:LYS:HB3	2.22	0.40
1:A:638:PRO:O	1:A:639:GLU:HB2	2.22	0.40
1:A:239:ALA:HA	1:A:297:ILE:O	2.21	0.40
1:A:265:ILE:HD12	1:A:265:ILE:C	2.47	0.40
1:A:126:TYR:HB2	1:A:135:ILE:HB	2.04	0.40

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%)	48	43
1	B	1129/1175 (96%)	1095 (97%)	33 (3%)	1 (0%)	48	43
All	All	2263/2350 (96%)	2197 (97%)	64 (3%)	2 (0%)	48	43

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%)	965 (99%)	14 (1%)	59	60
1	B	892/1041 (86%)	876 (98%)	16 (2%)	51	51
All	All	1871/2082 (90%)	1841 (98%)	30 (2%)	55	56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	197	THR
1	A	280	LEU
1	A	313	THR

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Mol	Chain	Res	Type
1	A	428	LEU
1	A	525	SER
1	A	740	GLN
1	A	846	TYR
1	A	863	GLU
1	A	947	PHE
1	A	983	GLU
1	A	1035	LYS
1	A	1060	LEU
1	A	1089	GLU
1	B	22	MET
1	B	100	GLN
1	B	197	THR
1	B	226	ASP
1	B	313	THR
1	B	438	ARG
1	B	672	ARG
1	B	756	GLN
1	B	846	TYR
1	B	912	GLN
1	B	947	PHE
1	B	977	GLU
1	B	997	GLU
1	B	1035	LYS
1	B	1060	LEU
1	B	1089	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	100	GLN
1	A	150	GLN
1	A	156	GLN
1	A	351	ASN
1	A	492	HIS
1	A	534	GLN
1	A	680	GLN
1	A	684	ASN
1	A	710	ASN
1	A	712	HIS
1	A	912	GLN

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Mol	Chain	Res	Type
1	A	1116	ASN
1	A	1144	ASN
1	B	38	ASN
1	B	100	GLN
1	B	156	GLN
1	B	194	GLN
1	B	351	ASN
1	B	504	ASN
1	B	647	GLN
1	B	680	GLN
1	B	684	ASN
1	B	694	ASN
1	B	712	HIS
1	B	756	GLN
1	B	898	ASN
1	B	912	GLN
1	B	914	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 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
3	BCN	B	1203	-	10,10,10	0.78	0	11,11,11	0.96	0
3	BCN	A	1203	-	10,10,10	0.71	0	11,11,11	0.97	0
4	EDO	A	1210	-	3,3,3	0.36	0	2,2,2	0.80	0
4	EDO	A	1205	-	3,3,3	0.24	0	2,2,2	0.69	0
4	EDO	B	1206	-	3,3,3	0.59	0	2,2,2	0.06	0
4	EDO	A	1209	-	3,3,3	0.39	0	2,2,2	0.52	0
2	SO4	B	1202	-	4,4,4	0.43	0	6,6,6	0.22	0
4	EDO	B	1208	-	3,3,3	0.27	0	2,2,2	0.58	0
4	EDO	A	1213	-	3,3,3	0.53	0	2,2,2	0.35	0
4	EDO	B	1205	-	3,3,3	0.52	0	2,2,2	0.19	0
4	EDO	B	1207	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	B	1204	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	A	1207	-	3,3,3	0.49	0	2,2,2	0.13	0
4	EDO	A	1206	-	3,3,3	0.33	0	2,2,2	0.34	0
4	EDO	A	1208	-	3,3,3	0.49	0	2,2,2	0.15	0
4	EDO	A	1214	-	3,3,3	0.36	0	2,2,2	0.24	0
4	EDO	A	1215	-	3,3,3	0.40	0	2,2,2	0.47	0
2	SO4	A	1202	-	4,4,4	0.19	0	6,6,6	0.70	0
2	SO4	A	1201	-	4,4,4	0.65	0	6,6,6	0.68	0
4	EDO	A	1204	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	A	1211	-	3,3,3	0.46	0	2,2,2	0.53	0
2	SO4	B	1201	-	4,4,4	0.47	0	6,6,6	0.26	0
4	EDO	A	1212	-	3,3,3	0.50	0	2,2,2	0.38	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	B	1203	-	-	3/10/10/10	-
3	BCN	A	1203	-	-	0/10/10/10	-
4	EDO	A	1210	-	-	1/1/1/1	-
4	EDO	A	1205	-	-	0/1/1/1	-
4	EDO	B	1206	-	-	1/1/1/1	-
4	EDO	A	1209	-	-	0/1/1/1	-
4	EDO	B	1208	-	-	1/1/1/1	-
4	EDO	A	1213	-	-	0/1/1/1	-
4	EDO	B	1205	-	-	0/1/1/1	-
4	EDO	B	1207	-	-	0/1/1/1	-
4	EDO	B	1204	-	-	0/1/1/1	-
4	EDO	A	1207	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1206	-	-	0/1/1/1	-
4	EDO	A	1208	-	-	0/1/1/1	-
4	EDO	A	1214	-	-	1/1/1/1	-
4	EDO	A	1215	-	-	0/1/1/1	-
4	EDO	A	1204	-	-	0/1/1/1	-
4	EDO	A	1211	-	-	0/1/1/1	-
4	EDO	A	1212	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1214	EDO	O1-C1-C2-O2
3	B	1203	BCN	N1-C1-C2-O22
3	B	1203	BCN	N1-C1-C2-O21
4	B	1206	EDO	O1-C1-C2-O2
4	A	1210	EDO	O1-C1-C2-O2
4	A	1212	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	B	1206	EDO	1	0
4	A	1207	EDO	4	0
4	A	1214	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

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	1135/1175 (96%)	-0.18	7 (0%) 85 87	18, 44, 75, 108	3 (0%)
1	B	1133/1175 (96%)	0.75	106 (9%) 14 14	36, 82, 124, 145	0
All	All	2268/2350 (96%)	0.28	113 (4%) 34 34	18, 58, 116, 145	3 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	PHE	4.6
1	B	541	PHE	4.0
1	B	747	TRP	3.9
1	B	697	VAL	3.9
1	A	101	TYR	3.8
1	B	421	VAL	3.8
1	A	228	ALA	3.7
1	B	537	TYR	3.7
1	B	524	TRP	3.6
1	A	523	PRO	3.6
1	B	399	LEU	3.6
1	B	563	VAL	3.4
1	B	423	PHE	3.3
1	B	469	TRP	3.3
1	B	602	ILE	3.3
1	A	914	ASN	3.2
1	B	476	TRP	3.1
1	B	480	ALA	3.1
1	B	626	LEU	3.1
1	B	707	LEU	3.1
1	B	497	ALA	3.1
1	B	816	GLY	3.0
1	B	457	ILE	3.0
1	B	489	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	486	PHE	2.9
1	B	494	PHE	2.9
1	B	814	SER	2.9
1	B	1105	ILE	2.9
1	B	1113	VAL	2.8
1	B	1155	LEU	2.8
1	B	431	LEU	2.8
1	B	558	GLU	2.8
1	B	479	LEU	2.8
1	B	452	ASN	2.7
1	B	613	ASP	2.7
1	B	624	LYS	2.7
1	B	472	ILE	2.7
1	B	429	GLU	2.6
1	B	674	PHE	2.6
1	B	630	LEU	2.6
1	B	1151	LEU	2.6
1	B	1106	ALA	2.6
1	B	699	PHE	2.6
1	B	758	LEU	2.6
1	B	907	LEU	2.6
1	B	408	LEU	2.5
1	A	519	GLU	2.5
1	B	440	GLY	2.5
1	B	1038	ILE	2.5
1	B	101	TYR	2.5
1	B	919	LEU	2.5
1	B	371	PHE	2.5
1	B	595	ILE	2.5
1	B	993	TYR	2.4
1	B	411	LEU	2.4
1	B	542	LEU	2.4
1	B	708	MET	2.4
1	B	538	LEU	2.4
1	B	192	ASP	2.4
1	B	725	VAL	2.4
1	B	930	ILE	2.4
1	B	988	LEU	2.4
1	B	368	GLY	2.4
1	B	769	ILE	2.4
1	B	968	VAL	2.4
1	B	1136	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	689	ASN	2.3
1	B	812	VAL	2.3
1	B	609	LEU	2.3
1	B	761	PHE	2.3
1	A	457	ILE	2.3
1	B	505	PRO	2.3
1	B	369	GLY	2.3
1	B	751	ARG	2.3
1	B	21	THR	2.3
1	B	578	LEU	2.3
1	B	682	LEU	2.3
1	B	531	GLY	2.2
1	B	530	TRP	2.2
1	B	883	ILE	2.2
1	B	1131	GLN	2.2
1	B	338	LEU	2.2
1	B	964	LEU	2.2
1	B	729	LYS	2.2
1	B	412	ASN	2.2
1	B	513	PHE	2.1
1	B	692	ILE	2.1
1	B	393	VAL	2.1
1	B	703	VAL	2.1
1	A	226	ASP	2.1
1	B	628	THR	2.1
1	B	446	TRP	2.1
1	B	825	ALA	2.1
1	B	19	SER	2.1
1	B	548	HIS	2.1
1	B	1101	ILE	2.1
1	B	406	PHE	2.1
1	B	763	LYS	2.1
1	B	402	LEU	2.1
1	B	681	LEU	2.1
1	B	544	PHE	2.1
1	B	984	VAL	2.1
1	B	601	SER	2.1
1	B	1123	ALA	2.1
1	B	485	ASN	2.0
1	B	740	GLN	2.0
1	B	616	ILE	2.0
1	B	690	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	865	VAL	2.0
1	B	515	TRP	2.0
1	B	553	LEU	2.0
1	B	1061	LEU	2.0
1	B	795	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, 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
2	SO4	B	1202	5/5	0.74	0.10	116,122,130,137	0
4	EDO	A	1211	4/4	0.84	0.18	47,57,59,65	0
5	CL	A	1217	1/1	0.84	0.23	103,103,103,103	0
4	EDO	B	1206	4/4	0.86	0.15	64,66,71,72	0
3	BCN	B	1203	11/11	0.86	0.13	66,71,80,80	0
4	EDO	B	1205	4/4	0.89	0.16	71,75,78,78	0
4	EDO	B	1207	4/4	0.90	0.14	67,73,74,76	0
4	EDO	A	1208	4/4	0.91	0.14	44,44,46,48	0
5	CL	A	1218[A]	1/1	0.92	0.20	48,48,48,48	1
5	CL	A	1218[B]	1/1	0.92	0.20	67,67,67,67	1
5	CL	B	1209	1/1	0.92	0.10	92,92,92,92	0
2	SO4	B	1201	5/5	0.93	0.08	77,80,83,95	0
5	CL	A	1216	1/1	0.94	0.09	78,78,78,78	0
4	EDO	A	1215	4/4	0.94	0.13	65,68,71,74	0
4	EDO	A	1205	4/4	0.94	0.20	45,45,46,47	0
4	EDO	A	1213	4/4	0.94	0.08	57,57,60,61	0
4	EDO	A	1214	4/4	0.94	0.12	51,56,62,64	0
4	EDO	B	1204	4/4	0.95	0.11	55,60,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	1209	4/4	0.95	0.10	42,47,52,58	0
4	EDO	A	1206	4/4	0.95	0.09	52,52,57,57	0
4	EDO	A	1212	4/4	0.95	0.11	57,60,65,66	0
4	EDO	B	1208	4/4	0.95	0.09	59,60,61,66	0
4	EDO	A	1207	4/4	0.96	0.10	37,42,44,44	0
3	BCN	A	1203	11/11	0.96	0.07	34,39,45,46	0
2	SO4	A	1202	5/5	0.96	0.07	48,50,51,62	0
4	EDO	A	1210	4/4	0.97	0.06	33,35,36,42	0
2	SO4	A	1201	5/5	0.97	0.10	48,50,54,56	0
4	EDO	A	1204	4/4	0.98	0.05	35,36,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.