Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 10:30 AM JST

PDB ID	:	5X7O
Title	:	Crystal structure of Paenibacillus sp. 598K alpha-1,6-glucosyltransferase
Authors	:	Fujimoto, Z.; Suzuki, N.; Kishine, N.; Momma, M.; Ichinose, H.; Kimura, A.; Funane, K.
Deposited on	:	2017-02-27
Resolution	:	2.00 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:

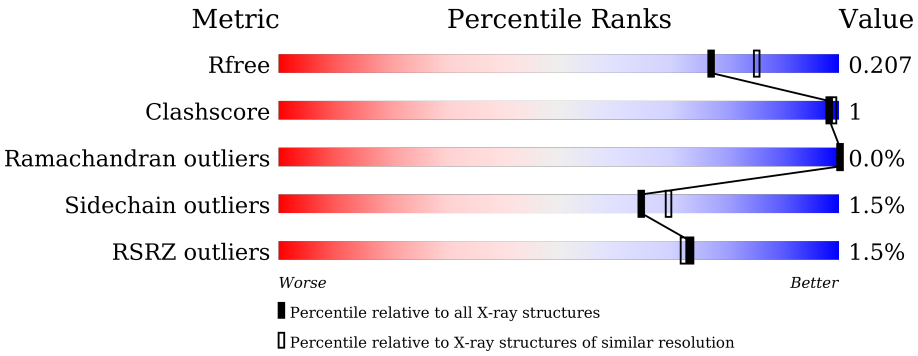
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 <=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	1263	2% 96%
1	B	1263	3% 97%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21429 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 family 31 alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1247	Total	C	N	O	S	0	12	0
			9655	6057	1641	1934	23			
1	B	1247	Total	C	N	O	S	0	5	0
			9622	6036	1638	1926	22			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP A0A193PKW5
A	20	HIS	-	expression tag	UNP A0A193PKW5
A	21	HIS	-	expression tag	UNP A0A193PKW5
A	22	HIS	-	expression tag	UNP A0A193PKW5
A	23	HIS	-	expression tag	UNP A0A193PKW5
A	24	HIS	-	expression tag	UNP A0A193PKW5
A	25	SER	-	expression tag	UNP A0A193PKW5
A	26	SER	-	expression tag	UNP A0A193PKW5
A	27	GLY	-	expression tag	UNP A0A193PKW5
A	28	LEU	-	expression tag	UNP A0A193PKW5
A	29	VAL	-	expression tag	UNP A0A193PKW5
A	30	PRO	-	expression tag	UNP A0A193PKW5
A	31	ARG	-	expression tag	UNP A0A193PKW5
A	32	GLY	-	expression tag	UNP A0A193PKW5
A	33	SER	-	expression tag	UNP A0A193PKW5
A	34	HIS	-	expression tag	UNP A0A193PKW5
A	35	MET	-	expression tag	UNP A0A193PKW5
B	19	HIS	-	expression tag	UNP A0A193PKW5
B	20	HIS	-	expression tag	UNP A0A193PKW5
B	21	HIS	-	expression tag	UNP A0A193PKW5
B	22	HIS	-	expression tag	UNP A0A193PKW5
B	23	HIS	-	expression tag	UNP A0A193PKW5
B	24	HIS	-	expression tag	UNP A0A193PKW5
B	25	SER	-	expression tag	UNP A0A193PKW5
B	26	SER	-	expression tag	UNP A0A193PKW5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLY	-	expression tag	UNP A0A193PKW5
B	28	LEU	-	expression tag	UNP A0A193PKW5
B	29	VAL	-	expression tag	UNP A0A193PKW5
B	30	PRO	-	expression tag	UNP A0A193PKW5
B	31	ARG	-	expression tag	UNP A0A193PKW5
B	32	GLY	-	expression tag	UNP A0A193PKW5
B	33	SER	-	expression tag	UNP A0A193PKW5
B	34	HIS	-	expression tag	UNP A0A193PKW5
B	35	MET	-	expression tag	UNP A0A193PKW5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

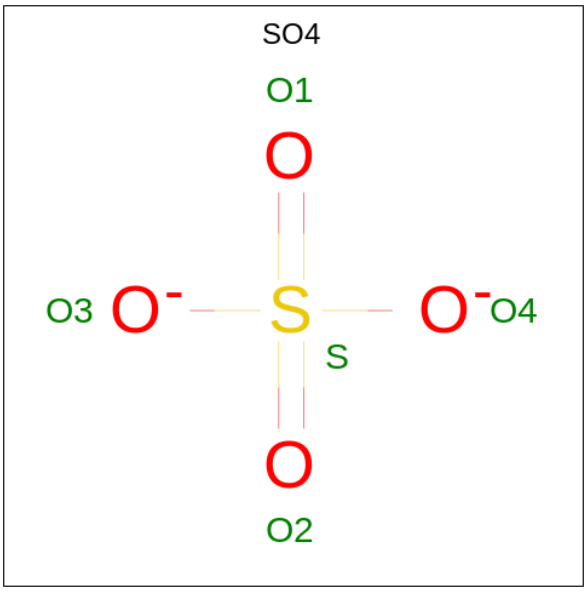
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total Mg 8 8	0	0
4	B	7	Total Mg 7 7	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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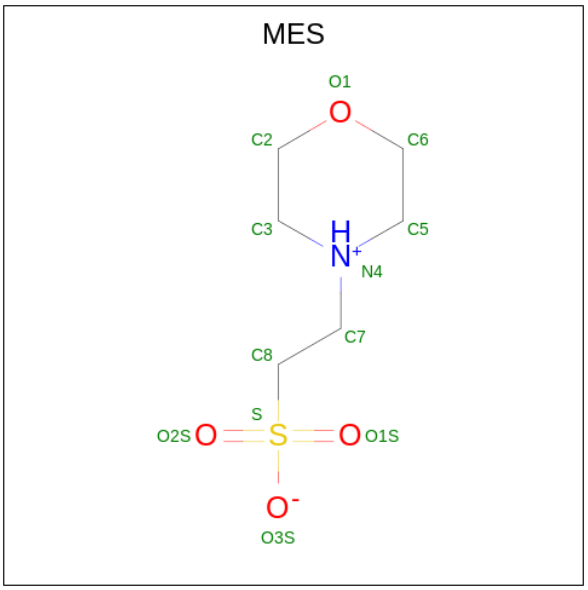
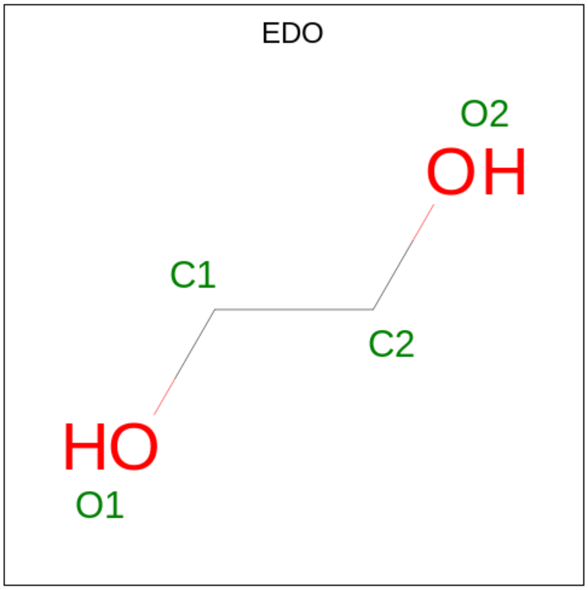
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 12 6 1 4 1	0	0
6	A	1	Total C N O S 12 6 1 4 1	0	0
6	B	1	Total C N O S 12 6 1 4 1	0	0
6	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is water.

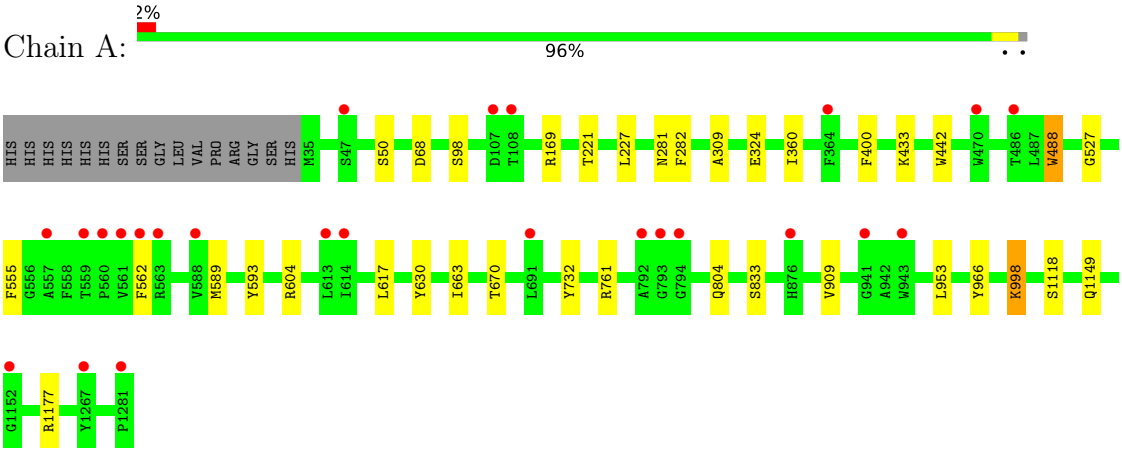
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	979	Total O 979 979	0	0
8	B	975	Total O 975 975	0	0

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.

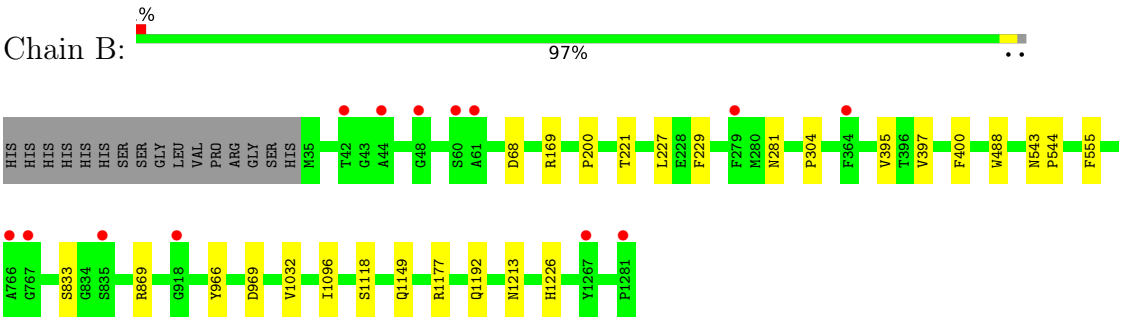
• Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase

Chain A:



• Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	184.16Å 271.93Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.48 – 2.00 47.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (152.48-2.00) 99.3 (47.52-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.166 , 0.199 0.176 , 0.207	Depositor DCC
R_{free} test set	11196 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21429	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, MG, MES, EDO, CA, NI

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	0.46	0/9966	0.68	0/13612
1	B	0.46	0/9903	0.68	1/13527 (0.0%)
All	All	0.46	0/19869	0.68	1/27139 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	869	ARG	NE-CZ-NH1	5.38	122.99	120.30

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	9655	0	8998	17	0
1	B	9622	0	8974	9	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	0	0	0
4	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	30	0	0	0	0
5	B	45	0	0	0	0
6	A	24	0	26	0	0
6	B	24	0	26	0	0
7	A	28	0	42	0	0
7	B	24	0	36	0	0
8	A	979	0	0	2	0
8	B	975	0	0	0	0
All	All	21429	0	18102	22	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 (22) 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:617:LEU:HD12	1:A:630[B]:TYR:CD2	2.25	0.71
1:A:360:ILE:HD13	1:B:397:VAL:HG12	1.77	0.66
1:A:663:ILE:HG12	1:A:670[A]:THR:HG22	1.89	0.55
1:A:617:LEU:HD12	1:A:630[B]:TYR:CE2	2.43	0.53
1:A:221:THR:HG22	1:A:227:LEU:HD12	1.92	0.50
1:B:543:ASN:HB3	1:B:544:PRO:HD2	1.94	0.50
1:A:360:ILE:HD12	1:B:395[A]:VAL:CG1	2.43	0.49
1:A:433:LYS:HD2	1:A:442:TRP:CE2	2.50	0.47
1:A:909:VAL:HG21	1:A:953:LEU:HD12	1.96	0.47
1:A:282:PHE:CG	1:A:309:ALA:HB3	2.52	0.45
1:A:360:ILE:HD12	1:B:395[A]:VAL:HG11	1.99	0.44
1:A:604:ARG:HD3	1:A:732:TYR:CD1	2.53	0.44
1:A:562:PHE:HE2	1:A:589[B]:MET:SD	2.41	0.43
1:B:200:PRO:HB3	1:B:229:PHE:CE1	2.55	0.42
1:B:1032:VAL:HG21	1:B:1096:ILE:HD12	2.01	0.42
1:A:488:TRP:HA	1:A:527:GLY:O	2.19	0.42
1:B:221:THR:HG22	1:B:227:LEU:HD12	2.02	0.41
1:A:761:ARG:NH1	8:A:2012:HOH:O	2.47	0.41
1:A:593:TYR:CE1	1:B:304:PRO:HB2	2.56	0.41
1:A:604:ARG:HD2	1:A:732:TYR:CE1	2.56	0.41
1:B:1226:HIS:CD2	1:B:1226:HIS:H	2.38	0.41
1:A:998:LYS:NZ	8:A:2038:HOH:O	2.53	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	1257/1263 (100%)	1233 (98%)	24 (2%)	0	100 100
1	B	1250/1263 (99%)	1221 (98%)	28 (2%)	1 (0%)	51 49
All	All	2507/2526 (99%)	2454 (98%)	52 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1213	ASN

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	1009/1011 (100%)	993 (98%)	16 (2%)	62 67
1	B	1001/1011 (99%)	988 (99%)	13 (1%)	69 74
All	All	2010/2022 (99%)	1981 (99%)	29 (1%)	65 72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	68	ASP
1	A	98	SER
1	A	169	ARG
1	A	281	ASN

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Mol	Chain	Res	Type
1	A	324	GLU
1	A	400	PHE
1	A	488	TRP
1	A	555	PHE
1	A	804	GLN
1	A	833	SER
1	A	966	TYR
1	A	998	LYS
1	A	1118	SER
1	A	1149	GLN
1	A	1177	ARG
1	B	68	ASP
1	B	169	ARG
1	B	281	ASN
1	B	400	PHE
1	B	488	TRP
1	B	555	PHE
1	B	833	SER
1	B	966	TYR
1	B	969	ASP
1	B	1118	SER
1	B	1149	GLN
1	B	1177	ARG
1	B	1192	GLN

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

Mol	Chain	Res	Type
1	B	440	GLN
1	B	1226	HIS
1	B	1250	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 23 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
5	SO4	B	1706	-	4,4,4	0.30	0	6,6,6	0.47	0
7	EDO	B	1806	-	3,3,3	0.58	0	2,2,2	0.07	0
5	SO4	B	1708	-	4,4,4	0.40	0	6,6,6	0.21	0
7	EDO	B	1801	-	3,3,3	0.48	0	2,2,2	0.01	0
5	SO4	B	1703	-	4,4,4	0.37	0	6,6,6	0.14	0
5	SO4	B	1709	-	4,4,4	0.36	0	6,6,6	0.10	0
7	EDO	B	1802	-	3,3,3	0.39	0	2,2,2	0.34	0
5	SO4	B	1707	-	4,4,4	0.40	0	6,6,6	0.33	0
5	SO4	A	1703	-	4,4,4	0.37	0	6,6,6	0.27	0
6	MES	B	1711	-	12,12,12	2.18	1 (8%)	14,16,16	1.00	0
5	SO4	A	1706	-	4,4,4	0.38	0	6,6,6	0.26	0
7	EDO	A	1802	-	3,3,3	0.36	0	2,2,2	0.47	0
5	SO4	B	1702	-	4,4,4	0.32	0	6,6,6	0.18	0
5	SO4	A	1705	-	4,4,4	0.28	0	6,6,6	0.52	0
5	SO4	B	1705	-	4,4,4	0.39	0	6,6,6	0.10	0
7	EDO	A	1801	-	3,3,3	0.38	0	2,2,2	0.39	0
5	SO4	A	1701	-	4,4,4	0.40	0	6,6,6	0.16	0
7	EDO	B	1804	-	3,3,3	0.43	0	2,2,2	0.51	0
7	EDO	B	1803	-	3,3,3	0.35	0	2,2,2	0.45	0
5	SO4	B	1701	-	4,4,4	0.39	0	6,6,6	0.19	0
5	SO4	B	1704	-	4,4,4	0.35	0	6,6,6	0.11	0
6	MES	B	1710	-	12,12,12	2.21	1 (8%)	14,16,16	1.33	2 (14%)
7	EDO	A	1807	-	3,3,3	0.62	0	2,2,2	0.19	0
5	SO4	A	1704	-	4,4,4	0.34	0	6,6,6	0.16	0
6	MES	A	1707	-	12,12,12	2.32	1 (8%)	14,16,16	1.35	1 (7%)
7	EDO	A	1803	-	3,3,3	0.36	0	2,2,2	0.46	0
5	SO4	A	1702	-	4,4,4	0.32	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	EDO	B	1805	-	3,3,3	0.50	0	2,2,2	0.28	0
7	EDO	A	1805	-	3,3,3	0.41	0	2,2,2	0.44	0
7	EDO	A	1804	-	3,3,3	0.47	0	2,2,2	0.63	0
7	EDO	A	1806	-	3,3,3	0.54	0	2,2,2	0.04	0
6	MES	A	1708	-	12,12,12	2.24	1 (8%)	14,16,16	1.69	1 (7%)

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
7	EDO	A	1803	-	-	1/1/1/1	-
7	EDO	A	1807	-	-	0/1/1/1	-
7	EDO	B	1806	-	-	1/1/1/1	-
7	EDO	A	1801	-	-	0/1/1/1	-
7	EDO	B	1801	-	-	0/1/1/1	-
7	EDO	B	1804	-	-	1/1/1/1	-
7	EDO	B	1803	-	-	1/1/1/1	-
7	EDO	A	1802	-	-	0/1/1/1	-
6	MES	B	1710	-	-	0/6/14/14	0/1/1/1
7	EDO	B	1802	-	-	0/1/1/1	-
7	EDO	B	1805	-	-	1/1/1/1	-
7	EDO	A	1805	-	-	0/1/1/1	-
6	MES	A	1707	-	-	0/6/14/14	0/1/1/1
7	EDO	A	1804	-	-	0/1/1/1	-
7	EDO	A	1806	-	-	0/1/1/1	-
6	MES	B	1711	-	-	0/6/14/14	0/1/1/1
6	MES	A	1708	-	-	3/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1707	MES	C8-S	-7.68	1.66	1.77
6	A	1708	MES	C8-S	-7.46	1.66	1.77
6	B	1710	MES	C8-S	-7.38	1.67	1.77
6	B	1711	MES	C8-S	-7.15	1.67	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1708	MES	O2S-S-C8	4.93	112.85	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1707	MES	O3S-S-C8	3.43	111.31	105.77
6	B	1710	MES	O1S-S-C8	2.92	110.44	106.92
6	B	1710	MES	O3S-S-C8	2.01	109.03	105.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1708	MES	C7-C8-S-O3S
7	B	1804	EDO	O1-C1-C2-O2
7	B	1803	EDO	O1-C1-C2-O2
7	B	1806	EDO	O1-C1-C2-O2
6	A	1708	MES	C7-C8-S-O1S
6	A	1708	MES	C7-C8-S-O2S
7	A	1803	EDO	O1-C1-C2-O2
7	B	1805	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	1247/1263 (98%)	-0.05	25 (2%)	65	63	22, 33, 48, 83	0
1	B	1247/1263 (98%)	-0.11	13 (1%)	82	81	23, 33, 47, 71	0
All	All	2494/2526 (98%)	-0.08	38 (1%)	73	72	22, 33, 48, 83	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	PHE	5.5
1	A	1281	PRO	3.5
1	A	1267	TYR	3.4
1	A	557	ALA	3.0
1	A	794	GLY	3.0
1	A	792	ALA	2.9
1	A	588	VAL	2.8
1	B	1267	TYR	2.7
1	B	767	GLY	2.7
1	B	61	ALA	2.6
1	B	48	GLY	2.5
1	A	562	PHE	2.5
1	B	1281	PRO	2.5
1	A	561	VAL	2.4
1	A	941	GLY	2.4
1	B	835	SER	2.3
1	B	364	PHE	2.3
1	A	470	TRP	2.3
1	A	560	PRO	2.2
1	A	614	ILE	2.2
1	B	60	SER	2.2
1	A	943	TRP	2.2
1	A	559	THR	2.2
1	B	42	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	44	ALA	2.1
1	B	279	PHE	2.1
1	A	108	THR	2.1
1	B	766	ALA	2.1
1	A	613	LEU	2.1
1	A	107	ASP	2.1
1	A	563[A]	ARG	2.1
1	A	1152	GLY	2.1
1	A	47	SER	2.1
1	A	876	HIS	2.0
1	A	793	GLY	2.0
1	A	486	THR	2.0
1	B	918	GLY	2.0
1	A	691	LEU	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^{th} 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
4	MG	B	1606	1/1	0.59	0.19	77,77,77,77	0
4	MG	B	1601	1/1	0.78	0.30	61,61,61,61	0
6	MES	A	1708	12/12	0.80	0.33	86,88,91,93	0
5	SO4	A	1706	5/5	0.81	0.25	71,77,85,92	0
7	EDO	B	1805	4/4	0.82	0.15	58,58,60,61	0
7	EDO	A	1807	4/4	0.83	0.27	48,49,50,51	0
6	MES	B	1710	12/12	0.83	0.38	86,91,97,101	0
4	MG	A	1605	1/1	0.84	0.13	65,65,65,65	0
7	EDO	A	1803	4/4	0.84	0.21	50,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	1707	5/5	0.85	0.22	54,62,72,73	0
5	SO4	B	1703	5/5	0.86	0.19	82,84,88,91	0
7	EDO	A	1805	4/4	0.86	0.13	59,59,59,60	0
5	SO4	A	1704	5/5	0.87	0.42	84,90,91,94	0
7	EDO	B	1803	4/4	0.88	0.27	53,59,59,63	0
5	SO4	B	1708	5/5	0.88	0.24	77,80,82,86	0
7	EDO	B	1806	4/4	0.88	0.19	47,47,49,52	0
5	SO4	B	1709	5/5	0.90	0.30	83,83,88,88	0
7	EDO	A	1806	4/4	0.90	0.17	49,51,52,53	0
5	SO4	B	1704	5/5	0.91	0.15	76,77,80,81	0
7	EDO	A	1804	4/4	0.91	0.16	35,44,44,50	0
7	EDO	B	1804	4/4	0.91	0.17	34,37,38,45	0
5	SO4	A	1703	5/5	0.91	0.19	81,81,84,85	0
4	MG	A	1607	1/1	0.91	0.17	74,74,74,74	0
5	SO4	B	1705	5/5	0.92	0.29	83,90,91,93	0
5	SO4	A	1701	5/5	0.92	0.21	60,62,66,69	0
4	MG	A	1604	1/1	0.92	0.28	84,84,84,84	0
5	SO4	B	1702	5/5	0.93	0.34	70,74,75,76	0
4	MG	B	1604	1/1	0.93	0.14	61,61,61,61	0
4	MG	A	1603	1/1	0.93	0.16	60,60,60,60	0
5	SO4	B	1701	5/5	0.94	0.21	61,63,67,71	0
7	EDO	B	1801	4/4	0.94	0.14	35,36,37,38	0
7	EDO	A	1802	4/4	0.94	0.13	39,39,40,42	0
4	MG	B	1603	1/1	0.95	0.13	62,62,62,62	0
7	EDO	A	1801	4/4	0.95	0.15	35,38,38,38	0
2	CA	A	1303	1/1	0.95	0.08	34,34,34,34	0
7	EDO	B	1802	4/4	0.95	0.15	36,39,41,43	0
4	MG	A	1602	1/1	0.96	0.03	39,39,39,39	0
5	SO4	A	1702	5/5	0.96	0.28	64,66,66,68	0
4	MG	B	1605	1/1	0.97	0.09	39,39,39,39	0
6	MES	B	1711	12/12	0.97	0.11	38,41,44,45	0
4	MG	A	1606	1/1	0.97	0.09	48,48,48,48	0
2	CA	A	1302	1/1	0.97	0.05	40,40,40,40	0
4	MG	A	1608	1/1	0.97	0.25	64,64,64,64	0
2	CA	B	1303	1/1	0.98	0.08	36,36,36,36	0
6	MES	A	1707	12/12	0.98	0.08	37,41,42,43	0
2	CA	A	1301	1/1	0.98	0.04	35,35,35,35	0
5	SO4	B	1706	5/5	0.98	0.08	44,45,47,47	0
4	MG	B	1607	1/1	0.98	0.12	27,27,27,27	0
5	SO4	A	1705	5/5	0.98	0.08	40,43,46,46	0
3	NI	B	1501	1/1	0.99	0.04	49,49,49,49	0
4	MG	A	1601	1/1	0.99	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	B	1302	1/1	0.99	0.05	40,40,40,40	0
4	MG	B	1602	1/1	0.99	0.07	42,42,42,42	0
3	NI	A	1501	1/1	0.99	0.03	51,51,51,51	0
2	CA	B	1301	1/1	1.00	0.06	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.