



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 10:25 AM JST

PDB ID : 5X7S  
Title : Crystal structure of Paenibacillus sp. 598K alpha-1,6-glucosyltransferase, terbium derivative  
Authors : Fujimoto, Z.; Kishine, N.; Suzuki, N.; Momma, M.; Ichinose, H.; Kimura, A.; Funane, K.  
Deposited on : 2017-02-27  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

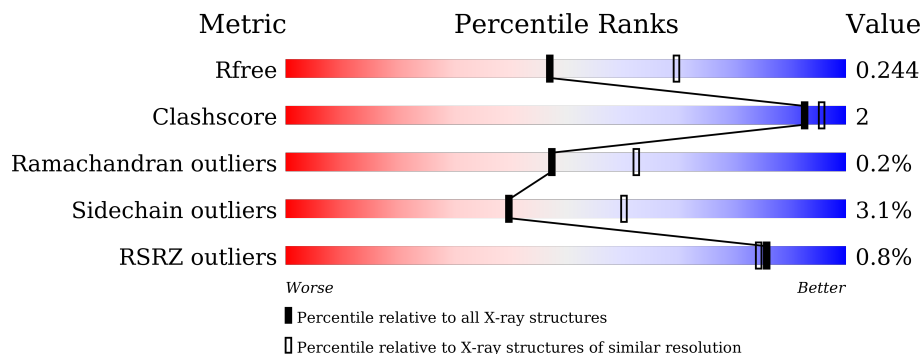
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1263	 92% 7%
1	B	1263	 92% 6%

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 20511 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
			Total	C	N	O	S			
1	A	1247	9607	6027	1634	1924	22	0	1	0
1	B	1247	9601	6023	1633	1923	22	0	0	0

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

*Continued on next page...*

Continued from previous page...

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

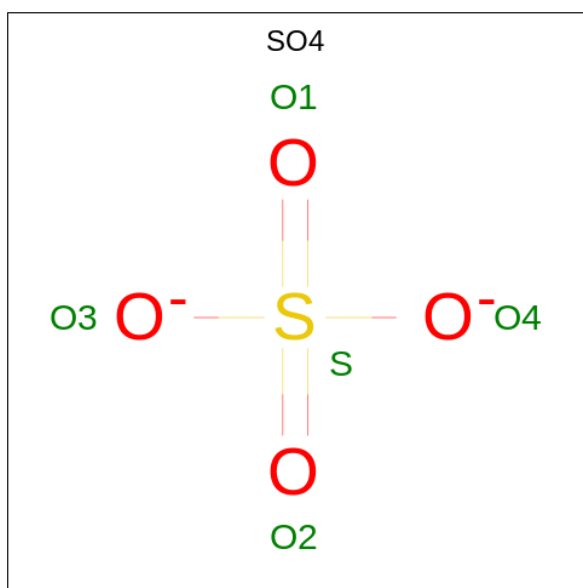
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Mg 4 4	0	0
4	B	3	Total Mg 3 3	0	0

- Molecule 5 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



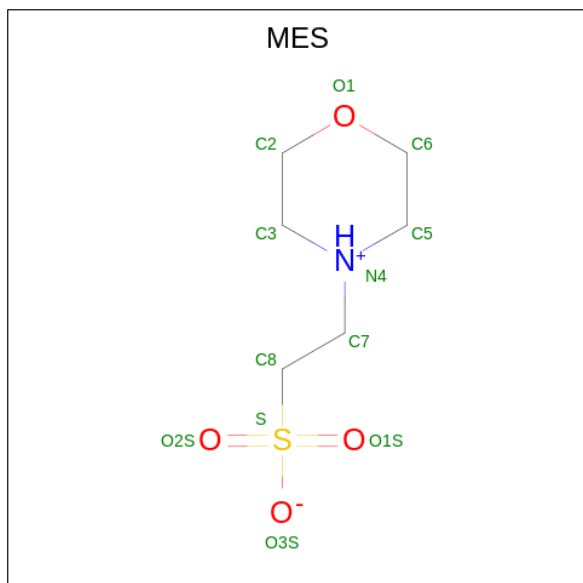
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total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

*Continued on next page...*

Continued from previous page...

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 8 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
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

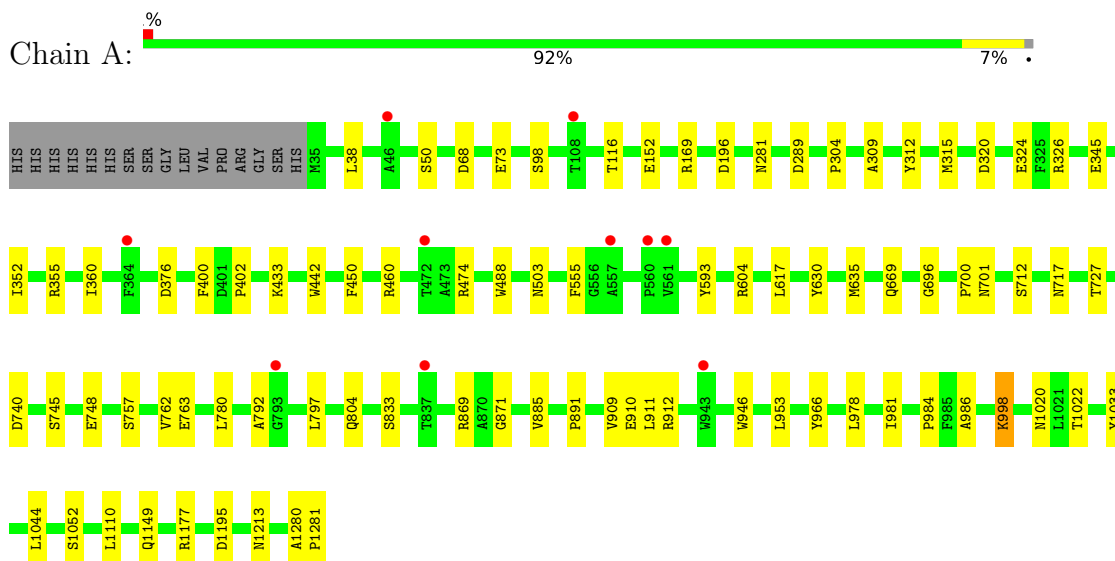
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	553	Total O 553 553	0	0
9	B	577	Total O 577 577	0	0

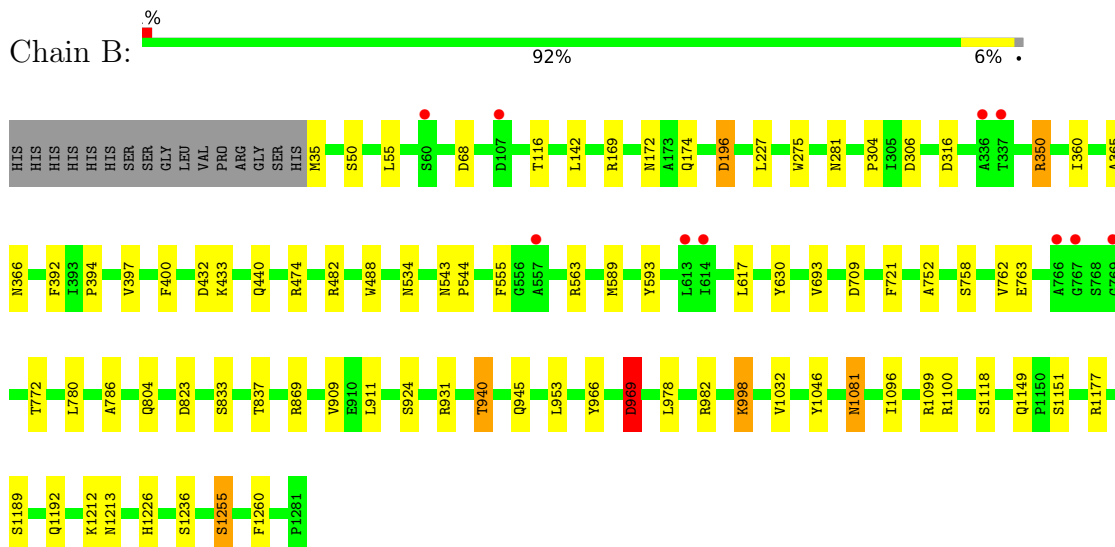
### 3 Residue-property plots [i](#)

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



- Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.81Å 270.92Å 133.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.54 – 2.40 48.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.4 (151.54-2.40) 92.4 (48.41-2.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.98 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.185 , 0.239 0.194 , 0.244	Depositor DCC
$R_{free}$ test set	5912 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtrriage
Anisotropy	0.684	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, MG, NI, CA, TB, MES

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	0.77	0/9872	0.86	11/13485 (0.1%)
1	B	0.75	0/9863	0.84	11/13473 (0.1%)
All	All	0.76	0/19735	0.85	22/26958 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	869	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	A	460	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	869	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	376	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	1195	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	320	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	474	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	196	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	316	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	869	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	289	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	1195	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	1099	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	196	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	1100	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	432	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	482	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	982	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	355	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	196	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	474	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	1100	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	9607	0	8962	28	0
1	B	9601	0	8954	31	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	4	0	0	0	0
4	B	3	0	0	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
6	A	30	0	0	0	0
6	B	45	0	0	0	0
7	A	24	0	26	0	0
7	B	24	0	26	0	0
8	A	16	0	24	0	0
8	B	12	0	18	0	0
9	A	553	0	0	2	0
9	B	577	0	0	2	0
All	All	20511	0	18010	56	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 (56) 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:360:ILE:HD13	1:B:397:VAL:HG12	1.48	0.94
1:B:911:LEU:HD11	1:B:978:LEU:HD22	1.66	0.76
1:A:617:LEU:HD12	1:A:630:TYR:HD2	1.59	0.66
1:A:617:LEU:HD12	1:A:630:TYR:CD2	2.32	0.65
1:A:909:VAL:HG21	1:A:953:LEU:HD12	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:THR:CG2	1:B:945:GLN:O	2.48	0.61
1:B:909:VAL:HG21	1:B:953:LEU:HD12	1.86	0.58
1:A:792:ALA:HB3	1:A:797:LEU:HD11	1.86	0.56
1:B:940:THR:HG21	1:B:945:GLN:O	2.06	0.56
1:A:593:TYR:CE1	1:B:304:PRO:HB2	2.42	0.55
1:A:998:LYS:NZ	9:A:2011:HOH:O	2.40	0.53
1:A:700:PRO:HA	1:A:717:ASN:O	2.09	0.52
1:A:38:LEU:O	9:A:2001:HOH:O	2.18	0.51
1:A:911:LEU:HD11	1:A:978:LEU:HD22	1.93	0.51
1:B:940:THR:HG23	1:B:945:GLN:O	2.10	0.50
1:B:433:LYS:NZ	1:B:440:GLN:HE21	2.09	0.49
1:A:304:PRO:HB2	1:B:593:TYR:CE1	2.49	0.48
1:B:786:ALA:HB2	1:B:823:ASP:HB3	1.96	0.47
1:A:740:ASP:HB3	1:A:745:SER:HB3	1.96	0.46
1:B:392:PHE:O	1:B:394:PRO:HD3	2.15	0.46
1:B:617:LEU:HD12	1:B:630:TYR:HD2	1.81	0.46
1:A:1044:LEU:HD21	1:A:1110:LEU:HD22	1.98	0.46
1:B:969:ASP:OD1	1:B:969:ASP:N	2.49	0.46
1:B:752:ALA:HB3	1:B:763:GLU:HB2	1.97	0.46
1:B:172:ASN:HB3	1:B:196:ASP:HB2	1.98	0.45
1:A:1280:ALA:O	1:A:1281:PRO:C	2.53	0.45
1:B:275:TRP:CE2	1:B:350:ARG:HG3	2.51	0.45
1:B:142:LEU:HD23	1:B:142:LEU:N	2.32	0.45
1:B:1046:TYR:CE1	1:B:1081:ASN:HB2	2.52	0.45
1:B:693:VAL:HG11	1:B:721:PHE:CD1	2.52	0.44
1:A:669:GLN:HG2	1:A:1033:TYR:CE2	2.53	0.44
1:A:871:GLY:O	1:A:885:VAL:HA	2.18	0.44
1:B:543:ASN:HB3	1:B:544:PRO:HD2	2.00	0.43
1:B:360:ILE:HD12	1:B:360:ILE:N	2.34	0.43
1:A:912:ARG:NH2	1:A:946:TRP:HB2	2.34	0.43
1:B:1032:VAL:HG21	1:B:1096:ILE:HD12	2.01	0.42
1:A:309:ALA:HA	1:A:352:ILE:HB	2.00	0.42
1:A:315:MET:HA	1:A:326:ARG:O	2.19	0.42
1:A:696:GLY:HA3	1:A:727:THR:HG21	2.00	0.42
1:B:762:VAL:HG11	1:B:780:LEU:HD13	2.01	0.42
1:A:402:PRO:HB2	1:A:450:PHE:HB3	2.01	0.42
1:A:910:GLU:O	1:A:981:ILE:HA	2.20	0.41
1:B:365:ALA:O	1:B:366:ASN:CB	2.68	0.41
1:B:924:SER:OG	1:B:931:ARG:NH2	2.50	0.41
1:B:1226:HIS:HA	1:B:1255:SER:O	2.20	0.41
1:B:709:ASP:OD1	1:B:709:ASP:N	2.52	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LYS:HD2	1:A:442:TRP:CE2	2.56	0.41
1:A:617:LEU:HD23	1:A:635:MET:HG2	2.02	0.41
1:B:804:GLN:HG3	9:B:2032:HOH:O	2.21	0.41
1:A:909:VAL:CG2	1:A:953:LEU:HD12	2.49	0.41
1:A:604:ARG:NH2	1:A:748:GLU:OE1	2.50	0.40
1:A:762:VAL:HG11	1:A:780:LEU:HD13	2.02	0.40
1:A:984:PRO:HB2	1:A:986:ALA:O	2.20	0.40
1:B:174:GLN:NE2	9:B:2030:HOH:O	2.45	0.40
1:B:998:LYS:HA	1:B:998:LYS:HD3	1.89	0.40
1:B:1189:SER:HA	1:B:1260:PHE:O	2.21	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	1246/1263 (99%)	1203 (96%)	41 (3%)	2 (0%)	47 62
1	B	1245/1263 (99%)	1205 (97%)	38 (3%)	2 (0%)	47 62
All	All	2491/2526 (99%)	2408 (97%)	79 (3%)	4 (0%)	47 62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	969	ASP
1	B	1213	ASN
1	A	312	TYR
1	A	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	998/1011 (99%)	970 (97%)	28 (3%)	43 63
1	B	997/1011 (99%)	964 (97%)	33 (3%)	38 57
All	All	1995/2022 (99%)	1934 (97%)	61 (3%)	40 60

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	68	ASP
1	A	73	GLU
1	A	98	SER
1	A	116	THR
1	A	152	GLU
1	A	169	ARG
1	A	281	ASN
1	A	324	GLU
1	A	345	GLU
1	A	400	PHE
1	A	488	TRP
1	A	503	ASN
1	A	555	PHE
1	A	701	ASN
1	A	712	SER
1	A	757	SER
1	A	763	GLU
1	A	804	GLN
1	A	833	SER
1	A	891	PRO
1	A	966	TYR
1	A	998	LYS
1	A	1020	ASN
1	A	1022	THR
1	A	1052	SER
1	A	1149	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1177	ARG
1	B	35	MET
1	B	50	SER
1	B	55	LEU
1	B	68	ASP
1	B	116	THR
1	B	169	ARG
1	B	227	LEU
1	B	281	ASN
1	B	306	ASP
1	B	350	ARG
1	B	400	PHE
1	B	488	TRP
1	B	534	ASN
1	B	555	PHE
1	B	563	ARG
1	B	589	MET
1	B	758	SER
1	B	772	THR
1	B	833	SER
1	B	837	THR
1	B	940	THR
1	B	966	TYR
1	B	969	ASP
1	B	998	LYS
1	B	1081	ASN
1	B	1118	SER
1	B	1149	GLN
1	B	1151	SER
1	B	1177	ARG
1	B	1192	GLN
1	B	1212	LYS
1	B	1236	SER
1	B	1255	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	405	GLN
1	A	1107	ASN
1	A	1149	GLN
1	A	1176	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	440	GLN
1	B	945	GLN
1	B	1248	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 48 ligands modelled in this entry, 22 are monoatomic - leaving 26 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
6	SO4	A	1703	-	4,4,4	0.44	0	6,6,6	0.81	0
6	SO4	B	1702	-	4,4,4	0.44	0	6,6,6	0.43	0
6	SO4	B	1711	-	4,4,4	0.40	0	6,6,6	0.17	0
6	SO4	B	1705	-	4,4,4	0.45	0	6,6,6	0.40	0
6	SO4	A	1701	-	4,4,4	0.54	0	6,6,6	0.46	0
6	SO4	B	1701	-	4,4,4	0.58	0	6,6,6	0.51	0
7	MES	B	1709	-	12,12,12	2.46	1 (8%)	14,16,16	1.30	2 (14%)
8	EDO	B	1803	-	3,3,3	0.72	0	2,2,2	0.09	0
6	SO4	A	1705	-	4,4,4	0.50	0	6,6,6	0.59	0
8	EDO	A	1803	-	3,3,3	0.57	0	2,2,2	0.60	0
6	SO4	B	1704	-	4,4,4	0.44	0	6,6,6	0.39	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	1710	-	4,4,4	0.49	0	6,6,6	0.28	0
8	EDO	A	1802	-	3,3,3	0.36	0	2,2,2	0.71	0
7	MES	B	1703	-	12,12,12	1.96	1 (8%)	14,16,16	1.71	2 (14%)
6	SO4	B	1708	-	4,4,4	0.60	0	6,6,6	0.76	0
6	SO4	A	1704	-	4,4,4	0.36	0	6,6,6	0.32	0
8	EDO	B	1801	-	3,3,3	0.76	0	2,2,2	0.66	0
6	SO4	A	1708	-	4,4,4	0.72	0	6,6,6	0.57	0
8	EDO	A	1804	-	3,3,3	0.75	0	2,2,2	0.32	0
6	SO4	B	1707	-	4,4,4	0.37	0	6,6,6	0.95	0
7	MES	A	1706	-	12,12,12	2.18	2 (16%)	14,16,16	1.73	3 (21%)
8	EDO	A	1801	-	3,3,3	0.62	0	2,2,2	0.35	0
6	SO4	B	1706	-	4,4,4	0.41	0	6,6,6	0.56	0
7	MES	A	1707	-	12,12,12	2.32	1 (8%)	14,16,16	1.79	3 (21%)
6	SO4	A	1702	-	4,4,4	0.50	0	6,6,6	0.45	0
8	EDO	B	1802	-	3,3,3	0.53	0	2,2,2	0.22	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	1804	-	-	0/1/1/1	-
7	MES	A	1707	-	-	3/6/14/14	0/1/1/1
7	MES	A	1706	-	-	0/6/14/14	0/1/1/1
8	EDO	A	1802	-	-	1/1/1/1	-
7	MES	B	1703	-	-	3/6/14/14	0/1/1/1
8	EDO	B	1802	-	-	0/1/1/1	-
8	EDO	B	1801	-	-	0/1/1/1	-
7	MES	B	1709	-	-	0/6/14/14	0/1/1/1
8	EDO	A	1801	-	-	0/1/1/1	-
8	EDO	B	1803	-	-	1/1/1/1	-
8	EDO	A	1803	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1709	MES	C8-S	-7.86	1.66	1.77
7	A	1707	MES	C8-S	-7.57	1.66	1.77
7	A	1706	MES	C8-S	-6.91	1.67	1.77
7	B	1703	MES	C8-S	-6.33	1.68	1.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1706	MES	O1S-S	2.00	1.50	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1706	MES	O3S-S-C8	4.68	113.33	105.77
7	A	1707	MES	O2S-S-C8	3.87	111.57	106.92
7	B	1703	MES	O2S-S-C8	3.75	111.43	106.92
7	B	1709	MES	O3S-S-C8	3.07	110.74	105.77
7	B	1703	MES	O3S-S-C8	3.02	110.66	105.77
7	A	1707	MES	O1-C6-C5	-2.79	105.65	111.80
7	A	1706	MES	O3S-S-O2S	-2.63	104.86	111.27
7	B	1709	MES	O2S-S-C8	-2.59	103.79	106.92
7	A	1706	MES	C6-C5-N4	-2.41	106.46	110.10
7	A	1707	MES	C7-N4-C5	-2.35	105.23	111.23

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1707	MES	N4-C7-C8-S
7	A	1707	MES	C7-C8-S-O1S
7	B	1703	MES	N4-C7-C8-S
8	B	1803	EDO	O1-C1-C2-O2
7	A	1707	MES	C7-C8-S-O3S
7	B	1703	MES	C8-C7-N4-C3
8	A	1802	EDO	O1-C1-C2-O2
8	A	1803	EDO	O1-C1-C2-O2
7	B	1703	MES	C8-C7-N4-C5

There are no ring outliers.

No monomer is involved in short contacts.

## 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	1247/1263 (98%)	-0.18	10 (0%) 86 84	33, 47, 64, 97	0
1	B	1247/1263 (98%)	-0.20	10 (0%) 86 84	29, 44, 62, 90	0
All	All	2494/2526 (98%)	-0.19	20 (0%) 86 84	29, 46, 63, 97	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	ALA	3.4
1	A	837	THR	3.2
1	A	943	TRP	2.7
1	B	337	THR	2.6
1	A	364	PHE	2.5
1	B	614	ILE	2.4
1	B	613	LEU	2.4
1	B	769	GLY	2.3
1	A	108	THR	2.3
1	A	46	ALA	2.3
1	B	767	GLY	2.3
1	A	560	PRO	2.2
1	A	557	ALA	2.2
1	A	793	GLY	2.2
1	A	472	THR	2.1
1	B	557	ALA	2.1
1	A	561	VAL	2.1
1	B	60	SER	2.1
1	B	766	ALA	2.0
1	B	107	ASP	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
6	SO4	A	1708	5/5	0.81	0.20	73,77,95,98	0
6	SO4	B	1705	5/5	0.82	0.21	99,99,108,109	0
4	MG	A	1603	1/1	0.86	0.14	95,95,95,95	0
7	MES	B	1703	12/12	0.86	0.28	87,94,111,116	0
6	SO4	B	1710	5/5	0.87	0.21	84,91,96,104	0
8	EDO	A	1804	4/4	0.88	0.20	45,54,55,62	0
6	SO4	B	1706	5/5	0.89	0.31	79,84,93,95	0
8	EDO	A	1803	4/4	0.89	0.18	52,59,61,64	0
7	MES	A	1707	12/12	0.89	0.26	75,80,101,103	0
8	EDO	B	1803	4/4	0.89	0.17	46,48,49,51	0
4	MG	B	1601	1/1	0.91	0.05	57,57,57,57	0
6	SO4	B	1708	5/5	0.91	0.27	58,75,84,92	0
8	EDO	A	1802	4/4	0.92	0.18	44,47,47,52	0
6	SO4	A	1703	5/5	0.93	0.17	66,68,83,89	0
6	SO4	A	1704	5/5	0.94	0.30	86,88,97,97	0
6	SO4	B	1711	5/5	0.94	0.17	97,98,99,102	0
6	SO4	B	1702	5/5	0.95	0.22	61,67,76,77	0
2	CA	A	1301	1/1	0.95	0.05	50,50,50,50	0
2	CA	B	1302	1/1	0.95	0.06	61,61,61,61	0
8	EDO	B	1801	4/4	0.95	0.12	42,43,45,48	0
5	TB	A	1606	1/1	0.95	0.06	42,42,42,42	1
2	CA	A	1302	1/1	0.96	0.07	59,59,59,59	0
4	MG	A	1604	1/1	0.96	0.04	56,56,56,56	0
3	NI	B	1501	1/1	0.96	0.04	76,76,76,76	0
8	EDO	A	1801	4/4	0.96	0.16	45,50,50,52	0
4	MG	B	1602	1/1	0.96	0.06	58,58,58,58	0
4	MG	B	1603	1/1	0.96	0.04	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	1601	1/1	0.96	0.04	50,50,50,50	0
5	TB	B	1604	1/1	0.96	0.10	44,44,44,44	1
8	EDO	B	1802	4/4	0.96	0.19	42,46,50,54	0
6	SO4	A	1701	5/5	0.96	0.12	48,55,67,67	0
6	SO4	B	1704	5/5	0.97	0.11	69,70,74,82	0
2	CA	B	1303	1/1	0.97	0.07	52,52,52,52	0
5	TB	A	1608	1/1	0.97	0.03	37,37,37,37	1
4	MG	A	1602	1/1	0.98	0.03	63,63,63,63	0
6	SO4	B	1701	5/5	0.98	0.19	52,54,66,66	0
7	MES	B	1709	12/12	0.98	0.15	48,51,57,59	0
6	SO4	A	1702	5/5	0.98	0.23	62,64,67,75	0
7	MES	A	1706	12/12	0.98	0.10	49,56,59,59	0
5	TB	B	1605	1/1	0.99	0.06	46,46,46,46	1
3	NI	A	1501	1/1	0.99	0.05	70,70,70,70	0
5	TB	A	1607	1/1	0.99	0.08	50,50,50,50	1
2	CA	A	1303	1/1	0.99	0.07	56,56,56,56	0
2	CA	B	1301	1/1	0.99	0.06	43,43,43,43	0
6	SO4	A	1705	5/5	0.99	0.10	51,51,55,57	0
6	SO4	B	1707	5/5	0.99	0.08	45,47,49,52	0
5	TB	A	1605	1/1	1.00	0.04	39,39,39,39	0
5	TB	B	1606	1/1	1.00	0.04	39,39,39,39	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.