



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 02:07 AM EST

PDB ID : 3WNP  
Title : D308A, F268V, D469Y, A513V, and Y515S quintuple mutant of *Bacillus circulans* T-3040 cycloisomaltooligosaccharide glucanotransferase complexed with isomaltoundecaose  
Authors : Suzuki, R.; Suzuki, N.; Fujimoto, Z.; Momma, M.; Kimura, K.; Kitamura, S.; Kimura, A.; Funane, K.  
Deposited on : unknown  
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

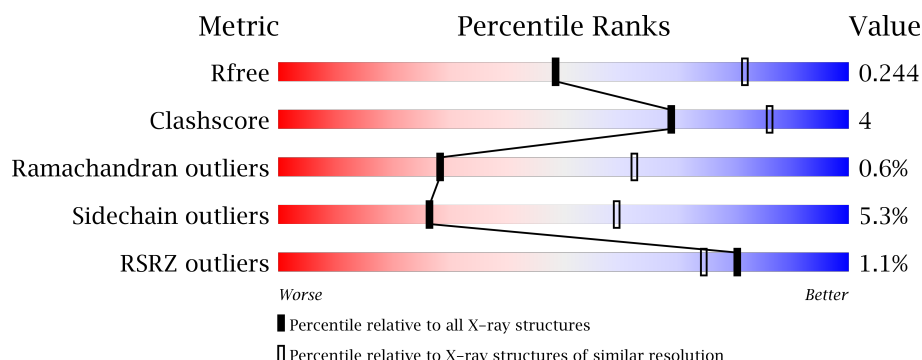
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	710	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">83% 14% ..</div> </div> </div>
1	B	710	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">83% 15% ..</div> </div> </div>

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
3	NA	A	802	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11337 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 Cycloisomaltooligosaccharide glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5497	3454	923	1105	15			
1	B	699	Total	C	N	O	S	0	0	0
			5497	3454	923	1105	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	EXPRESSION TAG	UNP P94286
A	38	GLY	-	EXPRESSION TAG	UNP P94286
A	268	VAL	PHE	ENGINEERED MUTATION	UNP P94286
A	278	PHE	SER	SEE REMARK 999	UNP P94286
A	308	ALA	ASP	ENGINEERED MUTATION	UNP P94286
A	469	TYR	ASP	ENGINEERED MUTATION	UNP P94286
A	513	VAL	ALA	ENGINEERED MUTATION	UNP P94286
A	515	SER	TYR	ENGINEERED MUTATION	UNP P94286
A	739	LEU	-	EXPRESSION TAG	UNP P94286
A	740	GLU	-	EXPRESSION TAG	UNP P94286
A	741	HIS	-	EXPRESSION TAG	UNP P94286
A	742	HIS	-	EXPRESSION TAG	UNP P94286
A	743	HIS	-	EXPRESSION TAG	UNP P94286
A	744	HIS	-	EXPRESSION TAG	UNP P94286
A	745	HIS	-	EXPRESSION TAG	UNP P94286
A	746	HIS	-	EXPRESSION TAG	UNP P94286
B	37	MET	-	EXPRESSION TAG	UNP P94286
B	38	GLY	-	EXPRESSION TAG	UNP P94286
B	268	VAL	PHE	ENGINEERED MUTATION	UNP P94286
B	278	PHE	SER	SEE REMARK 999	UNP P94286
B	308	ALA	ASP	ENGINEERED MUTATION	UNP P94286
B	469	TYR	ASP	ENGINEERED MUTATION	UNP P94286
B	513	VAL	ALA	ENGINEERED MUTATION	UNP P94286
B	515	SER	TYR	ENGINEERED MUTATION	UNP P94286
B	739	LEU	-	EXPRESSION TAG	UNP P94286

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Chain	Residue	Modelled	Actual	Comment	Reference
B	740	GLU	-	EXPRESSION TAG	UNP P94286
B	741	HIS	-	EXPRESSION TAG	UNP P94286
B	742	HIS	-	EXPRESSION TAG	UNP P94286
B	743	HIS	-	EXPRESSION TAG	UNP P94286
B	744	HIS	-	EXPRESSION TAG	UNP P94286
B	745	HIS	-	EXPRESSION TAG	UNP P94286
B	746	HIS	-	EXPRESSION TAG	UNP P94286

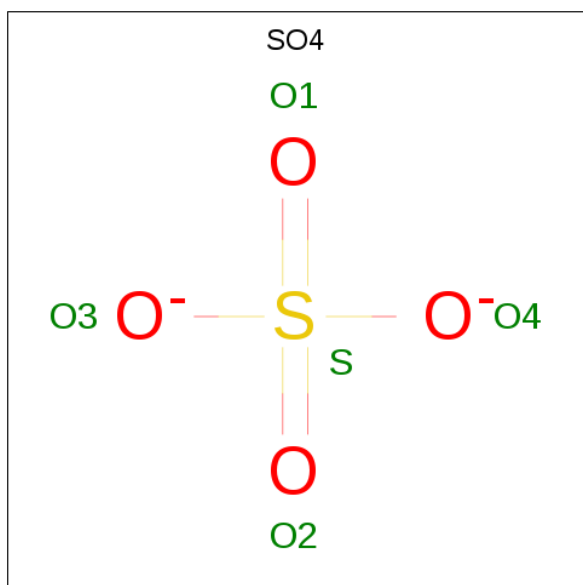
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

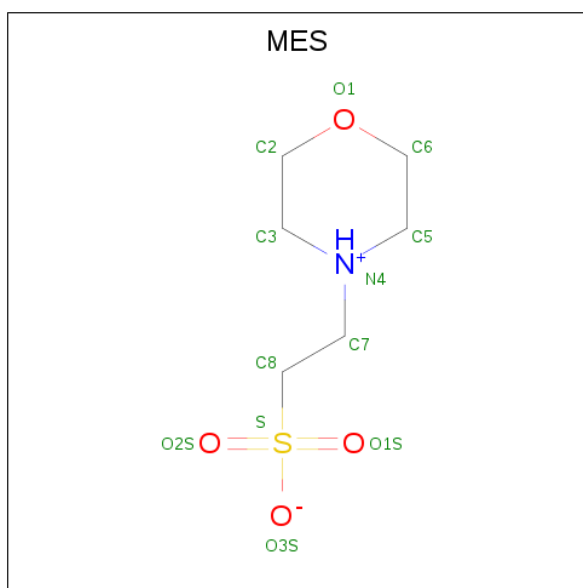
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0

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



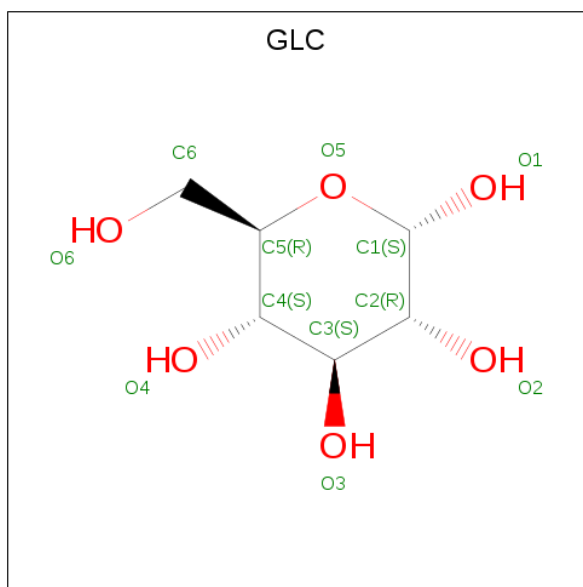
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



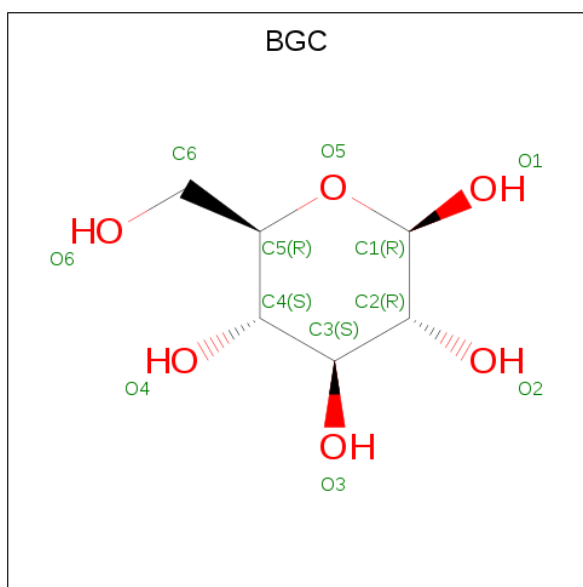
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 8 is water.

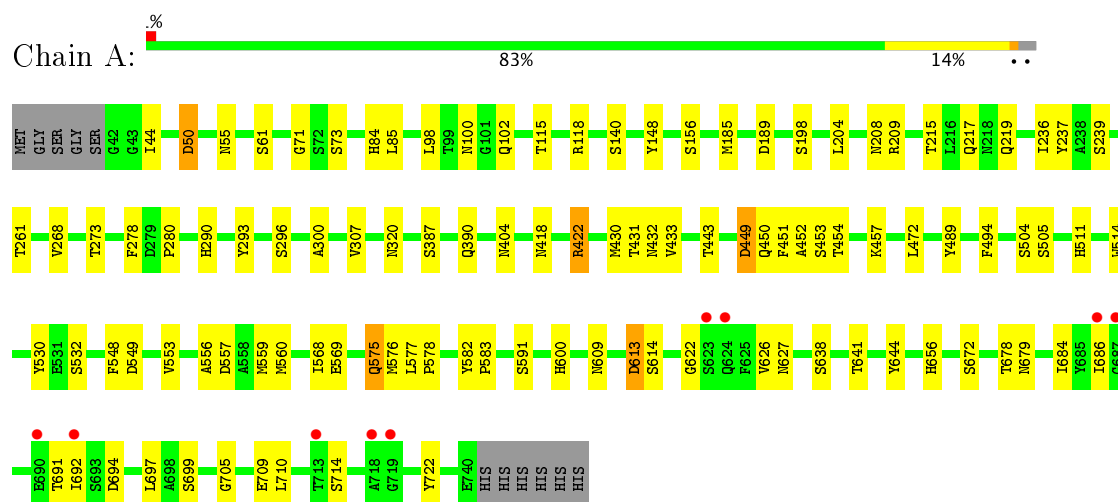
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	77	Total	O	0	0
			77	77		
8	B	88	Total	O	0	0
			88	88		



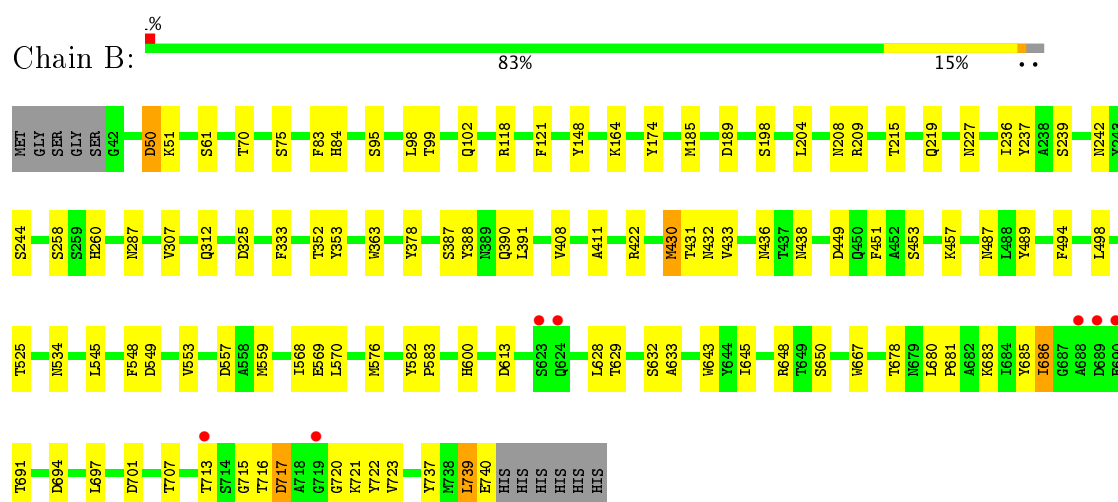
### 3 Residue-property plots [i](#)

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: Cycloisomaltooligosaccharide glucanotransferase



#### • Molecule 1: Cycloisomaltooligosaccharide glucanotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.99Å 172.81Å 172.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.85 – 2.80 41.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.85-2.80) 97.0 (41.81-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.187 , 0.243 0.191 , 0.244	Depositor DCC
$R_{free}$ test set	2243 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 25.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.408 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: BGC, NA, CA, GLC, SO4, 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	0.58	0/5636	0.74	0/7677
1	B	0.59	0/5636	0.75	1/7677 (0.0%)
All	All	0.58	0/11272	0.74	1/15354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ASP	CB-CG-OD1	5.71	123.44	118.30

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	5497	0	5111	47	0
1	B	5497	0	5111	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	13	0	0
5	B	12	0	13	0	0
6	A	33	0	28	0	0
6	B	33	0	28	0	0
7	A	12	0	11	0	0
7	B	12	0	11	0	0
8	A	77	0	0	0	0
8	B	88	0	0	0	0
All	All	11337	0	10326	92	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 4.

All (92) 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:452:ALA:O	1:A:530:TYR:CZ	2.45	0.70
1:B:84:HIS:CE1	1:B:118:ARG:HD2	2.33	0.64
1:A:556:ALA:O	1:A:560:MET:HG3	1.99	0.63
1:A:575:GLN:HE21	1:A:575:GLN:HA	1.66	0.61
1:B:436:ASN:HB2	1:B:449:ASP:OD2	1.99	0.61
1:A:118:ARG:HA	1:A:609:ASN:HD21	1.66	0.58
1:B:387:SER:OG	1:B:390:GLN:HG3	2.04	0.58
1:A:609:ASN:O	1:A:613:ASP:HB2	2.04	0.57
1:B:717:ASP:O	1:B:720:GLY:O	2.23	0.57
1:B:174:TYR:CE2	1:B:570:LEU:HD22	2.40	0.56
1:B:430:MET:HB3	1:B:433:VAL:HG23	1.87	0.56
1:B:84:HIS:HE1	1:B:118:ARG:HD2	1.69	0.55
1:A:50:ASP:OD1	1:A:61:SER:HB2	2.07	0.54
1:B:715:GLY:HA3	1:B:722:TYR:CZ	2.43	0.54
1:A:489:TYR:CE1	1:A:494:PHE:HB2	2.43	0.53
1:A:55:ASN:OD1	1:A:140:SER:HA	2.09	0.52
1:B:716:THR:O	1:B:717:ASP:HB3	2.08	0.52
1:A:472:LEU:O	1:A:514:TRP:HA	2.09	0.52
1:B:431:THR:HB	1:B:457:LYS:HB2	1.90	0.52
1:B:548:PHE:CE2	1:B:576:MET:HB3	2.44	0.51
1:A:582:TYR:N	1:A:583:PRO:CD	2.74	0.51
1:B:391:LEU:HD23	1:B:559:MET:HE2	1.92	0.50
1:A:575:GLN:HE21	1:A:575:GLN:CA	2.24	0.50
1:B:50:ASP:OD1	1:B:61:SER:HB2	2.12	0.50
1:A:557:ASP:HB3	1:A:600:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:VAL:HG22	1:A:684:ILE:HG12	1.93	0.49
1:B:215:THR:O	1:B:219:GLN:HG3	2.13	0.49
1:B:629:THR:HB	1:B:681:PRO:HG2	1.93	0.49
1:B:487:ASN:OD1	1:B:534:ASN:ND2	2.42	0.49
1:B:391:LEU:HD23	1:B:559:MET:CE	2.43	0.49
1:A:577:LEU:HD11	1:A:582:TYR:HA	1.95	0.48
1:A:714:SER:HB2	1:A:722:TYR:O	2.13	0.48
1:B:739:LEU:HD12	1:B:740:GLU:H	1.77	0.48
1:B:236:ILE:HG13	1:B:333:PHE:CE1	2.48	0.48
1:A:569:GLU:O	1:A:576:MET:HA	2.14	0.48
1:B:489:TYR:CE2	1:B:494:PHE:HB2	2.48	0.48
1:A:699:SER:O	1:A:705:GLY:HA2	2.15	0.47
1:A:548:PHE:CE2	1:A:576:MET:HB3	2.50	0.47
1:A:278:PHE:O	1:A:280:PRO:HD3	2.15	0.47
1:B:204:LEU:HA	1:B:209:ARG:O	2.15	0.47
1:B:431:THR:O	1:B:432:ASN:HB2	2.13	0.47
1:B:686:ILE:HD11	1:B:723:VAL:HG23	1.96	0.47
1:B:189:ASP:HB3	1:B:239:SER:HA	1.98	0.46
1:A:418:ASN:HB2	1:A:511:HIS:CE1	2.51	0.46
1:A:44:ILE:HG22	1:A:44:ILE:O	2.16	0.46
1:A:638:SER:O	1:A:641:THR:HG23	2.15	0.46
1:B:628:LEU:HD12	1:B:633:ALA:HB2	1.98	0.46
1:B:715:GLY:HA3	1:B:722:TYR:CE1	2.51	0.46
1:A:692:ILE:HG22	1:A:692:ILE:O	2.14	0.46
1:B:98:LEU:HB2	1:B:102:GLN:HB3	1.98	0.45
1:B:707:THR:HG21	1:B:737:TYR:OH	2.17	0.45
1:B:557:ASP:HB3	1:B:600:HIS:CE1	2.51	0.45
1:A:98:LEU:HD22	1:A:102:GLN:HG3	1.99	0.44
1:B:569:GLU:O	1:B:576:MET:HA	2.18	0.44
1:A:290:HIS:O	1:A:293:TYR:HB2	2.17	0.44
1:A:268:VAL:HG22	1:A:273:THR:O	2.17	0.44
1:B:51:LYS:HD3	1:B:227:ASN:ND2	2.33	0.44
1:A:387:SER:OG	1:A:390:GLN:HG3	2.18	0.44
1:A:236:ILE:HB	1:A:307:VAL:CG1	2.47	0.44
1:B:411:ALA:HB1	1:B:667:TRP:CH2	2.53	0.44
1:A:217:GLN:HA	1:A:217:GLN:NE2	2.33	0.43
1:A:422:ARG:NH1	1:A:443:THR:HB	2.33	0.43
1:A:505:SER:HB3	1:B:242:ASN:ND2	2.32	0.43
1:A:709:GLU:C	1:A:710:LEU:HD23	2.39	0.43
1:B:388:TYR:CE1	1:B:667:TRP:HA	2.53	0.43
1:A:215:THR:O	1:A:219:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TYR:HA	1:B:408:VAL:O	2.18	0.43
1:B:685:TYR:CD2	1:B:721:LYS:O	2.72	0.43
1:A:549:ASP:O	1:A:553:VAL:HG23	2.19	0.43
1:B:260:HIS:ND1	1:B:260:HIS:O	2.52	0.43
1:A:71:GLY:N	1:A:100:ASN:OD1	2.51	0.42
1:A:577:LEU:HA	1:A:578:PRO:HD3	1.87	0.42
1:B:83:PHE:HB2	1:B:121:PHE:HB3	2.00	0.42
1:B:582:TYR:N	1:B:583:PRO:CD	2.83	0.42
1:A:189:ASP:HB3	1:A:239:SER:HA	2.02	0.42
1:A:422:ARG:NH1	1:A:443:THR:CB	2.83	0.42
1:A:320:ASN:HA	1:A:320:ASN:HD22	1.72	0.42
1:A:431:THR:HB	1:A:457:LYS:HB2	2.02	0.42
1:B:549:ASP:O	1:B:553:VAL:HG23	2.19	0.42
1:B:236:ILE:HB	1:B:307:VAL:CG1	2.50	0.41
1:A:644:TYR:HA	1:A:656:HIS:O	2.20	0.41
1:B:643:TRP:CH2	1:B:645:ILE:HD11	2.55	0.41
1:A:449:ASP:O	1:A:450:GLN:C	2.58	0.41
1:A:568:ILE:O	1:A:568:ILE:HG23	2.21	0.41
1:B:312:GLN:HA	1:B:363:TRP:CZ3	2.55	0.41
1:A:432:ASN:C	1:A:433:VAL:HG13	2.41	0.41
1:B:683:LYS:HE2	1:B:722:TYR:CG	2.56	0.40
1:A:204:LEU:HA	1:A:209:ARG:O	2.21	0.40
1:A:84:HIS:CE1	1:A:118:ARG:HD2	2.57	0.40
1:B:568:ILE:HG23	1:B:568:ILE:O	2.20	0.40
1:A:296:SER:O	1:A:300:ALA:HB3	2.22	0.40
1:B:352:THR:OG1	1:B:353:TYR:N	2.55	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	697/710 (98%)	649 (93%)	42 (6%)	6 (1%)	20	52
1	B	697/710 (98%)	645 (92%)	50 (7%)	2 (0%)	44	77
All	All	1394/1420 (98%)	1294 (93%)	92 (7%)	8 (1%)	28	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	591	SER
1	A	679	ASN
1	B	686	ILE
1	A	622	GLY
1	B	717	ASP
1	A	85	LEU
1	A	504	SER

### 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	588/597 (98%)	560 (95%)	28 (5%)	30	63
1	B	588/597 (98%)	554 (94%)	34 (6%)	23	55
All	All	1176/1194 (98%)	1114 (95%)	62 (5%)	26	59

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	115	THR
1	A	148	TYR
1	A	156	SER
1	A	185	MET
1	A	198	SER
1	A	208	ASN
1	A	237	TYR

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Mol	Chain	Res	Type
1	A	261	THR
1	A	404	ASN
1	A	422	ARG
1	A	430	MET
1	A	449	ASP
1	A	451	PHE
1	A	453	SER
1	A	454	THR
1	A	532	SER
1	A	559	MET
1	A	575	GLN
1	A	613	ASP
1	A	614	SER
1	A	627	ASN
1	A	672	SER
1	A	678	THR
1	A	686	ILE
1	A	691	THR
1	A	694	ASP
1	A	697	LEU
1	B	50	ASP
1	B	70	THR
1	B	75	SER
1	B	95	SER
1	B	99	THR
1	B	148	TYR
1	B	164	LYS
1	B	185	MET
1	B	198	SER
1	B	208	ASN
1	B	237	TYR
1	B	244	SER
1	B	258	SER
1	B	287	ASN
1	B	422	ARG
1	B	430	MET
1	B	438	ASN
1	B	451	PHE
1	B	453	SER
1	B	498	LEU
1	B	525	THR
1	B	545	LEU

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Mol	Chain	Res	Type
1	B	613	ASP
1	B	632	SER
1	B	648	ARG
1	B	650	SER
1	B	678	THR
1	B	680	LEU
1	B	691	THR
1	B	694	ASP
1	B	697	LEU
1	B	701	ASP
1	B	713	THR
1	B	739	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	315	ASN
1	A	320	ASN
1	A	404	ASN
1	A	479	ASN
1	A	493	ASN
1	A	496	GLN
1	A	521	GLN
1	A	600	HIS
1	A	619	ASN
1	A	666	GLN
1	B	84	HIS
1	B	242	ASN
1	B	287	ASN
1	B	320	ASN
1	B	438	ASN
1	B	479	ASN
1	B	521	GLN
1	B	600	HIS
1	B	646	ASN
1	B	679	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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$
4	SO4	A	803	-	4,4,4	0.43	0	6,6,6	0.80	0
4	SO4	A	804	-	4,4,4	0.53	0	6,6,6	0.37	0
4	SO4	A	805	-	4,4,4	0.51	0	6,6,6	0.55	0
4	SO4	A	806	-	4,4,4	0.43	0	6,6,6	0.58	0
4	SO4	A	807	-	4,4,4	0.49	0	6,6,6	0.28	0
4	SO4	A	808	-	4,4,4	0.50	0	6,6,6	0.20	0
5	MES	A	809	-	12,12,12	2.11	1 (8%)	14,16,16	2.04	4 (28%)
6	GLC	A	818	6	11,11,12	0.81	0	13,15,17	1.34	2 (15%)
6	GLC	A	819	6	11,11,12	0.94	1 (9%)	13,15,17	1.05	1 (7%)
6	GLC	A	820	7,6	11,11,12	0.73	0	13,15,17	1.17	1 (7%)
7	BGC	A	821	6	12,12,12	0.42	0	17,17,17	0.98	0
4	SO4	B	803	-	4,4,4	0.52	0	6,6,6	0.79	0
4	SO4	B	804	-	4,4,4	0.50	0	6,6,6	0.35	0
4	SO4	B	805	-	4,4,4	0.41	0	6,6,6	0.46	0
4	SO4	B	806	-	4,4,4	0.51	0	6,6,6	0.21	0
4	SO4	B	807	-	4,4,4	0.47	0	6,6,6	0.11	0
4	SO4	B	808	-	4,4,4	0.49	0	6,6,6	0.21	0
5	MES	B	809	-	12,12,12	1.99	1 (8%)	14,16,16	1.89	3 (21%)
6	GLC	B	818	6	11,11,12	0.93	0	13,15,17	1.37	2 (15%)
6	GLC	B	819	6	11,11,12	0.81	0	13,15,17	1.84	3 (23%)
6	GLC	B	820	7,6	11,11,12	0.58	0	13,15,17	1.64	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BGC	B	821	6	12,12,12	0.51	0	17,17,17	1.13	1 (5%)

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
4	SO4	A	803	-	-	0/0/0/0	0/0/0/0
4	SO4	A	804	-	-	0/0/0/0	0/0/0/0
4	SO4	A	805	-	-	0/0/0/0	0/0/0/0
4	SO4	A	806	-	-	0/0/0/0	0/0/0/0
4	SO4	A	807	-	-	0/0/0/0	0/0/0/0
4	SO4	A	808	-	-	0/0/0/0	0/0/0/0
5	MES	A	809	-	-	0/6/14/14	0/1/1/1
6	GLC	A	818	6	-	0/2/19/22	0/1/1/1
6	GLC	A	819	6	-	0/2/19/22	0/1/1/1
6	GLC	A	820	7,6	-	0/2/19/22	0/1/1/1
7	BGC	A	821	6	-	0/2/22/22	0/1/1/1
4	SO4	B	803	-	-	0/0/0/0	0/0/0/0
4	SO4	B	804	-	-	0/0/0/0	0/0/0/0
4	SO4	B	805	-	-	0/0/0/0	0/0/0/0
4	SO4	B	806	-	-	0/0/0/0	0/0/0/0
4	SO4	B	807	-	-	0/0/0/0	0/0/0/0
4	SO4	B	808	-	-	0/0/0/0	0/0/0/0
5	MES	B	809	-	-	0/6/14/14	0/1/1/1
6	GLC	B	818	6	-	0/2/19/22	0/1/1/1
6	GLC	B	819	6	-	0/2/19/22	0/1/1/1
6	GLC	B	820	7,6	-	0/2/19/22	0/1/1/1
7	BGC	B	821	6	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	809	MES	C8-S	-6.92	1.67	1.77
5	B	809	MES	C8-S	-6.52	1.67	1.77
6	A	819	GLC	C2-C3	2.08	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	819	GLC	O5-C1-C2	-4.13	104.31	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	820	GLC	O3-C3-C2	-2.87	104.81	110.02
6	A	819	GLC	O5-C1-C2	-2.73	106.51	110.79
6	B	819	GLC	O4-C4-C3	-2.64	104.62	110.36
5	A	809	MES	O3S-S-O2S	-2.49	105.67	111.37
7	B	821	BGC	C3-C4-C5	-2.20	106.34	110.22
5	B	809	MES	O2S-S-O1S	-2.11	106.54	113.86
6	B	820	GLC	O3-C3-C4	-2.10	105.79	110.36
5	A	809	MES	O1-C6-C5	-2.04	107.27	111.83
6	A	820	GLC	O2-C2-C3	-2.03	106.18	110.17
6	B	820	GLC	C1-O5-C5	2.01	114.94	112.17
6	B	818	GLC	O3-C3-C4	2.03	114.77	110.36
6	B	820	GLC	C3-C4-C5	2.32	114.30	110.22
6	A	818	GLC	C3-C4-C5	2.46	114.56	110.22
6	A	818	GLC	C1-O5-C5	2.75	115.96	112.17
6	B	818	GLC	C3-C4-C5	2.86	115.26	110.22
6	B	819	GLC	C1-C2-C3	3.25	113.77	109.65
5	A	809	MES	O3S-S-C8	4.33	111.38	106.06
5	A	809	MES	O2S-S-C8	4.46	110.62	106.79
5	B	809	MES	O1S-S-C8	4.54	110.69	106.79
5	B	809	MES	O3S-S-C8	4.57	111.68	106.06

There are no chirality outliers.

There are no torsion outliers.

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 [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, 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	699/710 (98%)	-0.09	9 (1%) 77 71	39, 65, 104, 176	0
1	B	699/710 (98%)	-0.13	7 (1%) 82 77	39, 65, 106, 150	0
All	All	1398/1420 (98%)	-0.11	16 (1%) 80 74	39, 65, 106, 176	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	624	GLN	6.6
1	B	624	GLN	4.9
1	B	688	ALA	4.0
1	A	690	GLU	3.2
1	A	623	SER	3.1
1	B	713	THR	3.0
1	A	686	ILE	3.0
1	A	713	THR	2.7
1	B	623	SER	2.6
1	B	689	ASP	2.6
1	A	718	ALA	2.6
1	B	690	GLU	2.5
1	A	719	GLY	2.2
1	B	719	GLY	2.2
1	A	692	ILE	2.1
1	A	687	GLY	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	802	1/1	0.93	0.26	3.22	93,93,93,93	0
5	MES	B	809	12/12	0.96	0.21	0.82	57,69,82,84	0
6	GLC	A	818	11/12	0.88	0.19	0.80	58,68,74,77	0
5	MES	A	809	12/12	0.97	0.17	0.33	60,65,74,76	0
4	SO4	A	805	5/5	0.86	0.18	0.07	86,91,100,112	0
6	GLC	B	818	11/12	0.87	0.16	-0.33	56,74,80,80	0
7	BGC	B	821	12/12	0.98	0.17	-0.83	39,44,48,49	0
2	CA	B	801	1/1	0.99	0.11	-0.93	67,67,67,67	0
7	BGC	A	821	12/12	0.98	0.17	-1.52	44,48,51,55	0
6	GLC	A	820	11/12	0.98	0.14	-1.53	42,47,51,59	0
2	CA	A	801	1/1	0.99	0.07	-1.58	67,67,67,67	0
6	GLC	B	820	11/12	0.97	0.14	-1.74	44,48,51,63	0
3	NA	B	802	1/1	0.94	0.11	-1.81	81,81,81,81	0
6	GLC	B	819	11/12	0.96	0.13	-2.08	59,62,63,69	0
6	GLC	A	819	11/12	0.96	0.12	-3.10	51,57,60,61	0
4	SO4	B	807	5/5	0.94	0.17	-	93,104,106,109	0
4	SO4	B	808	5/5	0.85	0.24	-	110,115,127,135	0
4	SO4	B	803	5/5	0.98	0.10	-	69,70,73,74	0
4	SO4	A	807	5/5	0.92	0.19	-	92,113,116,117	0
4	SO4	A	806	5/5	0.80	0.19	-	108,114,123,129	0
4	SO4	A	808	5/5	0.92	0.15	-	89,94,106,107	0
4	SO4	A	804	5/5	0.79	0.25	-	107,109,115,125	0
4	SO4	B	806	5/5	0.89	0.18	-	88,97,109,121	0
4	SO4	B	804	5/5	0.91	0.13	-	87,88,102,106	0
4	SO4	B	805	5/5	0.83	0.20	-	99,106,112,124	0
4	SO4	A	803	5/5	0.97	0.14	-	66,68,72,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.