



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:10 pm BST

PDB ID : 3T69
Title : Crystal structure of a putative 2-dehydro-3-deoxygalactonokinase protein from *Sinorhizobium meliloti*
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Deposited on : 2011-07-28
Resolution : 2.55 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 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	:	2.11
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)	:	2.11

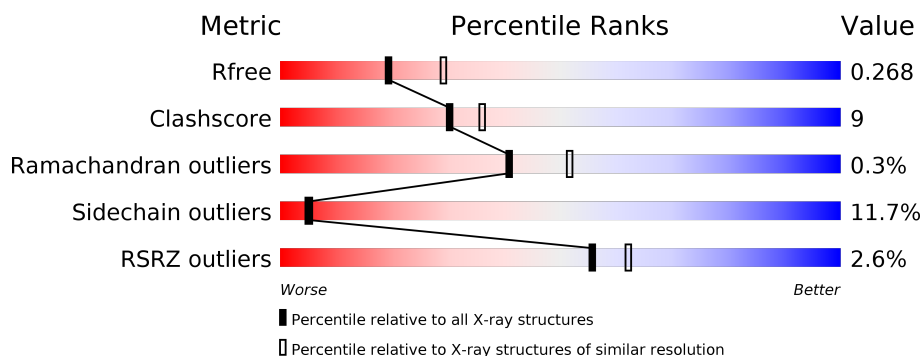
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	330	<div> <div> <div></div> <div>76%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	330	<div> <div>4%</div> <div>70%</div> <div>20%</div> <div>•</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4491 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 Putative 2-dehydro-3-deoxygalactonokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2198	1372	404	414	8			
1	B	304	Total	C	N	O	S	0	0	0
			2204	1381	396	419	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q92RN7
A	2	VAL	-	EXPRESSION TAG	UNP Q92RN7
A	309	ALA	-	EXPRESSION TAG	UNP Q92RN7
A	310	GLU	-	EXPRESSION TAG	UNP Q92RN7
A	311	ASN	-	EXPRESSION TAG	UNP Q92RN7
A	312	LEU	-	EXPRESSION TAG	UNP Q92RN7
A	313	TYR	-	EXPRESSION TAG	UNP Q92RN7
A	314	PHE	-	EXPRESSION TAG	UNP Q92RN7
A	315	GLN	-	EXPRESSION TAG	UNP Q92RN7
A	316	SER	-	EXPRESSION TAG	UNP Q92RN7
A	317	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	318	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	319	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	320	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	321	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	322	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	323	TRP	-	EXPRESSION TAG	UNP Q92RN7
A	324	SER	-	EXPRESSION TAG	UNP Q92RN7
A	325	HIS	-	EXPRESSION TAG	UNP Q92RN7
A	326	PRO	-	EXPRESSION TAG	UNP Q92RN7
A	327	GLN	-	EXPRESSION TAG	UNP Q92RN7
A	328	PHE	-	EXPRESSION TAG	UNP Q92RN7
A	329	GLU	-	EXPRESSION TAG	UNP Q92RN7
A	330	LYS	-	EXPRESSION TAG	UNP Q92RN7
B	1	MET	-	EXPRESSION TAG	UNP Q92RN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	VAL	-	EXPRESSION TAG	UNP Q92RN7
B	309	ALA	-	EXPRESSION TAG	UNP Q92RN7
B	310	GLU	-	EXPRESSION TAG	UNP Q92RN7
B	311	ASN	-	EXPRESSION TAG	UNP Q92RN7
B	312	LEU	-	EXPRESSION TAG	UNP Q92RN7
B	313	TYR	-	EXPRESSION TAG	UNP Q92RN7
B	314	PHE	-	EXPRESSION TAG	UNP Q92RN7
B	315	GLN	-	EXPRESSION TAG	UNP Q92RN7
B	316	SER	-	EXPRESSION TAG	UNP Q92RN7
B	317	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	318	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	319	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	320	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	321	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	322	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	323	TRP	-	EXPRESSION TAG	UNP Q92RN7
B	324	SER	-	EXPRESSION TAG	UNP Q92RN7
B	325	HIS	-	EXPRESSION TAG	UNP Q92RN7
B	326	PRO	-	EXPRESSION TAG	UNP Q92RN7
B	327	GLN	-	EXPRESSION TAG	UNP Q92RN7
B	328	PHE	-	EXPRESSION TAG	UNP Q92RN7
B	329	GLU	-	EXPRESSION TAG	UNP Q92RN7
B	330	LYS	-	EXPRESSION TAG	UNP Q92RN7

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	30	Total	O	0	0
			30	30		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.40Å 109.74Å 121.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.46 – 2.55 43.46 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.46-2.55) 97.2 (43.46-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.277 0.213 , 0.268	Depositor DCC
R_{free} test set	1360 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4491	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.97	1/2238 (0.0%)	0.92	2/3043 (0.1%)
1	B	0.86	1/2244 (0.0%)	0.92	0/3054
All	All	0.92	2/4482 (0.0%)	0.92	2/6097 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ARG	CG-CD	5.22	1.65	1.51
1	B	93	GLU	CG-CD	5.13	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	126	ARG	CG-CD-NE	-5.03	101.23	111.80

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	2198	0	2172	35	0
1	B	2204	0	2136	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	0	0
2	B	15	0	0	1	0
3	A	34	0	0	1	0
3	B	30	0	0	2	0
All	All	4491	0	4308	81	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 9.

All (81) 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:49:HIS:CD2	3:B:349:HOH:O	2.25	0.89
1:B:40:MET:CE	1:B:72:MET:HB3	2.05	0.85
1:A:260:ASP:CG	1:A:261:GLY:HA3	1.97	0.83
1:B:308:LEU:HD23	1:B:308:LEU:H	1.44	0.82
1:B:260:ASP:N	1:B:261:GLY:HA3	1.97	0.80
1:B:11:ALA:HB1	1:B:298:LEU:HD13	1.63	0.79
1:A:40:MET:HE3	1:A:72:MET:HB3	1.66	0.77
1:A:40:MET:CE	1:A:75:ALA:HB3	2.15	0.77
1:B:260:ASP:H	1:B:261:GLY:HA3	1.48	0.77
1:B:40:MET:HE3	1:B:72:MET:HB3	1.68	0.73
1:A:40:MET:HE2	1:A:75:ALA:HB3	1.71	0.72
1:B:40:MET:HE2	1:B:72:MET:HB3	1.70	0.71
1:B:131:GLN:HG2	1:B:294:VAL:HG13	1.73	0.70
1:B:76:ARG:HB2	1:B:77:GLN:HE21	1.58	0.68
1:A:223:ARG:NH1	1:A:226:GLN:OE1	2.26	0.68
1:A:8:TYR:HA	1:A:24:ILE:O	1.95	0.66
1:B:308:LEU:CD2	1:B:308:LEU:H	2.10	0.65
1:B:49:HIS:HD2	3:B:349:HOH:O	1.73	0.64
1:A:109:ARG:CZ	1:A:305:ILE:HD13	2.28	0.63
1:A:131:GLN:HG2	1:A:294:VAL:HG13	1.81	0.62
1:B:9:TYR:OH	1:B:299:SER:HB2	2.01	0.61
1:A:171:THR:HG21	1:A:248:GLU:HB2	1.84	0.60
1:B:171:THR:HG21	1:B:248:GLU:HB2	1.83	0.59
1:B:185:SER:O	1:B:189:ALA:HB2	2.02	0.59
1:B:8:TYR:OH	1:B:308:LEU:HD22	2.02	0.59
1:A:260:ASP:CG	1:A:261:GLY:CA	2.70	0.59
1:B:48:PHE:HB3	1:B:79:TRP:CD1	2.38	0.57
1:A:67:ILE:CD1	1:A:106:ARG:HD3	2.35	0.57
1:A:260:ASP:OD2	1:A:260:ASP:N	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD11	1:B:67:ILE:HD11	1.87	0.55
1:A:109:ARG:CZ	1:A:305:ILE:CD1	2.85	0.55
1:B:88:PRO:HA	1:B:163:VAL:O	2.07	0.55
1:A:253:LEU:HD22	1:A:259:VAL:HG11	1.89	0.54
1:B:35:ARG:HG2	1:B:35:ARG:HH11	1.72	0.53
1:B:48:PHE:O	1:B:48:PHE:CD2	2.62	0.53
1:A:260:ASP:OD1	1:A:261:GLY:CA	2.58	0.52
1:B:14:TRP:CH2	1:B:48:PHE:HE2	2.27	0.52
1:A:182:THR:HG22	1:B:177:THR:HG21	1.92	0.52
1:B:291:ASP:HA	1:B:294:VAL:CG2	2.41	0.51
1:B:68:ILE:HD11	1:B:111:LEU:HD21	1.93	0.50
1:A:109:ARG:NH1	1:A:305:ILE:HD13	2.27	0.50
1:A:40:MET:CE	1:A:72:MET:HB3	2.38	0.50
1:B:117:ARG:O	1:B:118:ASP:C	2.51	0.49
1:B:38:GLU:HA	1:B:42:THR:OG1	2.13	0.49
1:A:66:PRO:C	1:A:67:ILE:HG13	2.33	0.48
1:B:160:ASP:O	1:B:161:ASP:HB2	2.12	0.48
1:A:101:ILE:HD11	1:A:110:ILE:HD11	1.96	0.48
1:A:260:ASP:OD1	1:A:261:GLY:HA2	2.14	0.48
1:A:67:ILE:HD11	1:A:106:ARG:HD3	1.96	0.47
1:B:8:TYR:C	1:B:65:LEU:HD11	2.34	0.47
1:A:127:GLY:N	1:A:129:GLU:OE1	2.42	0.47
1:B:118:ASP:CG	1:B:120:ARG:O	2.53	0.47
1:B:12:VAL:HB	1:B:69:ILE:HG12	1.97	0.46
1:B:270:LEU:HD11	1:B:274:TYR:HE2	1.80	0.46
1:A:219:LEU:O	1:A:222:VAL:HG13	2.16	0.46
1:A:98:ALA:HB2	1:A:111:LEU:HD23	1.96	0.45
1:A:118:ASP:C	1:A:118:ASP:OD2	2.55	0.45
1:B:155:TRP:CE3	1:B:252:ALA:HB1	2.52	0.45
1:A:180:ARG:NH2	3:A:354:HOH:O	2.50	0.45
1:A:305:ILE:HD11	1:A:306:TRP:CE2	2.52	0.45
1:B:203:ASP:O	1:B:207:ARG:HG2	2.16	0.45
1:B:308:LEU:N	1:B:308:LEU:CD2	2.78	0.45
1:B:130:THR:O	1:B:297:GLY:HA3	2.17	0.45
1:B:154:LYS:HE3	1:B:168:THR:OG1	2.17	0.44
1:A:67:ILE:HD12	1:A:106:ARG:HD3	1.99	0.44
1:B:48:PHE:O	1:B:48:PHE:HD2	2.00	0.43
1:B:77:GLN:NE2	1:B:77:GLN:H	2.16	0.43
1:B:223:ARG:HG3	1:B:223:ARG:O	2.10	0.43
1:A:305:ILE:HG13	1:A:306:TRP:CD2	2.54	0.43
1:B:76:ARG:NH2	2:B:331:SO4:O2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASP:CB	1:A:261:GLY:CA	2.98	0.41
1:A:260:ASP:CB	1:A:261:GLY:HA3	2.50	0.41
1:A:67:ILE:HD12	1:A:106:ARG:CD	2.49	0.41
1:B:148:MET:HA	1:B:149:PRO:HD2	1.94	0.41
1:B:185:SER:O	1:B:189:ALA:CB	2.68	0.41
1:B:27:ASP:CG	1:B:29:ALA:H	2.23	0.41
1:B:8:TYR:HB3	1:B:24:ILE:O	2.21	0.41
1:B:27:ASP:OD1	1:B:29:ALA:CB	2.69	0.41
1:B:50:THR:HG22	1:B:51:ILE:N	2.36	0.40
1:A:117:ARG:O	1:A:118:ASP:C	2.60	0.40
1:A:40:MET:HE3	1:A:72:MET:O	2.21	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	299/330 (91%)	285 (95%)	12 (4%)	2 (1%)	22	30
1	B	298/330 (90%)	281 (94%)	17 (6%)	0	100	100
All	All	597/660 (90%)	566 (95%)	29 (5%)	2 (0%)	41	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLY
1	A	26	GLU

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	210/238 (88%)	184 (88%)	26 (12%)	4	4
1	B	208/238 (87%)	185 (89%)	23 (11%)	6	6
All	All	418/476 (88%)	369 (88%)	49 (12%)	5	5

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	TYR
1	A	14	TRP
1	A	16	THR
1	A	20	ARG
1	A	26	GLU
1	A	27	ASP
1	A	40	MET
1	A	97	ARG
1	A	117	ARG
1	A	119	ARG
1	A	124	VAL
1	A	125	MET
1	A	126	ARG
1	A	129	GLU
1	A	143	SER
1	A	157	ARG
1	A	158	LEU
1	A	171	THR
1	A	177	THR
1	A	208	THR
1	A	209	ARG
1	A	259	VAL
1	A	260	ASP
1	A	294	VAL
1	A	305	ILE
1	A	308	LEU
1	B	8	TYR

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Mol	Chain	Res	Type
1	B	31	LEU
1	B	38	GLU
1	B	46	THR
1	B	48	PHE
1	B	50	THR
1	B	77	GLN
1	B	91	LEU
1	B	97	ARG
1	B	106	ARG
1	B	124	VAL
1	B	154	LYS
1	B	157	ARG
1	B	193	THR
1	B	209	ARG
1	B	222	VAL
1	B	223	ARG
1	B	262	VAL
1	B	294	VAL
1	B	305	ILE
1	B	308	LEU
1	B	310	GLU
1	B	312	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	B	77	GLN

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 [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	332	-	4,4,4	0.22	0	6,6,6	0.93	0
2	SO4	B	332	-	4,4,4	0.27	0	6,6,6	0.69	0
2	SO4	B	333	-	4,4,4	0.21	0	6,6,6	0.38	0
2	SO4	B	331	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	A	331	-	4,4,4	0.10	0	6,6,6	0.42	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	331	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	301/330 (91%)	-0.18	3 (0%) 82 86	29, 40, 56, 75	0
1	B	304/330 (92%)	0.14	13 (4%) 35 42	35, 54, 76, 82	0
All	All	605/660 (91%)	-0.02	16 (2%) 56 62	29, 46, 73, 82	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	ALA	3.4
1	B	141	ALA	3.3
1	B	137	ALA	3.1
1	B	142	GLY	2.9
1	B	46	THR	2.9
1	A	256	SER	2.6
1	B	258	SER	2.6
1	B	160	ASP	2.6
1	B	285	VAL	2.2
1	B	190	GLU	2.2
1	A	257	GLY	2.2
1	B	138	HIS	2.1
1	B	56	LEU	2.1
1	A	195	ALA	2.0
1	B	143	SER	2.0
1	B	27	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	332	5/5	0.92	0.32	35,39,41,41	5
2	SO4	B	333	5/5	0.94	0.20	38,38,40,43	5
2	SO4	A	331	5/5	0.95	0.42	33,34,36,37	5
2	SO4	B	332	5/5	0.96	0.29	30,30,31,33	5
2	SO4	B	331	5/5	0.97	0.23	35,36,36,36	5

6.5 Other polymers [i](#)

There are no such residues in this entry.