



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:52 PM UTC

PDB ID : 3WAJ / pdb_00003waj
Title : Crystal structure of the Archaeoglobus fulgidus oligosaccharyltransferase (O29867_ARCFU) complex with Zn and sulfate
Authors : Matsumoto, S.; Shimada, A.; Kohda, D.
Deposited on : 2013-05-03
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

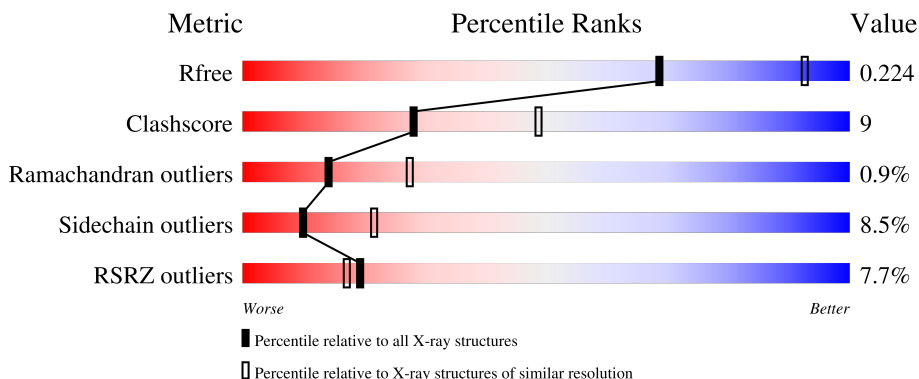
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	875	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6525 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 Transmembrane oligosaccharyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	793	Total	C	N	O	S	0	0	0
			6368	4233	1007	1112	16			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	869	GLU	-	expression tag	UNP O29867
A	870	LEU	-	expression tag	UNP O29867
A	871	ALA	-	expression tag	UNP O29867
A	872	LEU	-	expression tag	UNP O29867
A	873	VAL	-	expression tag	UNP O29867
A	874	PRO	-	expression tag	UNP O29867
A	875	ARG	-	expression tag	UNP O29867

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total	O	0	0
			151	151		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.19Å 108.96Å 56.07Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	38.81 – 2.50 38.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.81-2.50) 98.7 (38.81-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.182 , 0.216 0.192 , 0.224	Depositor DCC
R_{free} test set	2429 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6525	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	1/6573 (0.0%)	0.88	20/8970 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	PRO	N-CD	10.79	1.62	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ARG	N-CA-C	13.80	130.37	111.74
1	A	404	SER	N-CA-C	8.21	121.64	110.55
1	A	148	PRO	N-CA-CB	6.88	110.47	103.25
1	A	277	SER	CA-C-N	-6.63	113.09	120.45
1	A	277	SER	C-N-CA	-6.63	113.09	120.45
1	A	196	ARG	N-CA-C	-6.25	105.56	113.43
1	A	392	ILE	CB-CA-C	-6.06	103.95	111.70
1	A	832	TYR	CA-C-N	5.80	125.41	119.56
1	A	832	TYR	C-N-CA	5.80	125.41	119.56
1	A	148	PRO	CA-N-CD	-5.77	103.92	112.00
1	A	404	SER	N-CA-CB	-5.77	101.68	110.45
1	A	331	PHE	N-CA-C	-5.74	107.27	114.56
1	A	403	ARG	CB-CA-C	-5.69	103.65	111.73
1	A	473	PHE	N-CA-C	-5.46	106.46	113.23
1	A	734	TYR	N-CA-C	-5.26	106.89	113.15
1	A	568	ASN	CB-CA-C	-5.18	100.84	108.87
1	A	663	ILE	CB-CA-C	5.12	117.99	110.98
1	A	851	ILE	CB-CA-C	-5.12	103.77	110.98
1	A	483	TYR	CA-C-N	-5.11	114.56	119.87
1	A	483	TYR	C-N-CA	-5.11	114.56	119.87

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	6368	0	6273	113	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	151	0	0	14	0
All	All	6525	0	6273	113	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 (113) 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:183:ARG:HG3	1:A:197:GLN:HE22	1.08	1.14
1:A:398:ARG:HD3	1:A:402:ARG:HD3	1.32	1.05
1:A:398:ARG:CD	1:A:402:ARG:HD3	1.86	1.05
1:A:398:ARG:CG	1:A:402:ARG:HD3	1.92	0.98
1:A:543:GLU:OE2	4:A:1096:HOH:O	1.82	0.98
1:A:56:GLU:OE1	4:A:1138:HOH:O	1.86	0.94
1:A:398:ARG:HG2	1:A:402:ARG:HD3	1.48	0.91
1:A:183:ARG:CG	1:A:197:GLN:HE22	1.84	0.89
1:A:740:MET:SD	4:A:1046:HOH:O	2.31	0.87
1:A:398:ARG:HD3	1:A:402:ARG:CD	2.10	0.81
1:A:446:VAL:HG11	1:A:477:ILE:HD11	1.63	0.80
1:A:402:ARG:O	1:A:403:ARG:HG2	1.82	0.79
1:A:653:ASN:OD1	4:A:1112:HOH:O	2.01	0.77
1:A:183:ARG:HG3	1:A:197:GLN:NE2	1.94	0.77
1:A:398:ARG:HG2	1:A:402:ARG:CD	2.17	0.75
1:A:27:LEU:O	1:A:493:SER:OG	2.04	0.74
1:A:147:VAL:O	4:A:1021:HOH:O	2.08	0.72
1:A:755:TYR:OH	4:A:1126:HOH:O	2.06	0.71
1:A:830:SER:OG	4:A:1066:HOH:O	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:GLN:NE2	4:A:1089:HOH:O	2.08	0.69
1:A:383:ALA:H	1:A:485:THR:HG22	1.58	0.69
1:A:786:VAL:HB	1:A:790:VAL:HG21	1.74	0.68
1:A:695:MET:HE3	1:A:698:GLU:HB3	1.78	0.66
1:A:395:SER:O	4:A:1065:HOH:O	2.14	0.65
1:A:653:ASN:OD1	1:A:653:ASN:N	2.30	0.64
1:A:131:VAL:HG21	1:A:410:LEU:HD13	1.81	0.62
1:A:802:ASN:HB3	1:A:833:PRO:HB2	1.83	0.61
1:A:72:THR:OG1	1:A:568:ASN:OD1	2.19	0.60
1:A:150:GLN:NE2	1:A:425:ASN:O	2.25	0.59
1:A:788:ALA:HA	1:A:790:VAL:H	1.68	0.59
1:A:543:GLU:H	1:A:543:GLU:CD	2.11	0.58
1:A:20:ALA:N	4:A:1095:HOH:O	2.37	0.57
1:A:398:ARG:O	1:A:402:ARG:HG2	2.04	0.57
1:A:188:ASP:O	4:A:1058:HOH:O	2.18	0.56
1:A:271:PHE:HE1	1:A:278:PRO:HG2	1.71	0.56
1:A:121:ILE:HG13	1:A:141:ALA:HB1	1.89	0.55
1:A:188:ASP:N	1:A:188:ASP:OD1	2.40	0.55
1:A:619:TYR:OH	1:A:677:THR:HG21	2.08	0.54
1:A:398:ARG:HG2	1:A:402:ARG:CG	2.38	0.54
1:A:383:ALA:H	1:A:485:THR:CG2	2.20	0.54
1:A:186:GLY:O	1:A:187:HIS:HB2	2.08	0.53
1:A:388:GLY:O	1:A:392:ILE:HG12	2.09	0.52
1:A:655:GLN:HA	1:A:658:ILE:HD12	1.92	0.52
1:A:184:TRP:CE3	1:A:193:LEU:HD13	2.44	0.52
1:A:121:ILE:HG22	1:A:122:LEU:HD23	1.91	0.52
1:A:182:ASN:O	1:A:183:ARG:HB2	2.10	0.51
1:A:694:ARG:HD3	1:A:825:PRO:O	2.11	0.51
1:A:320:VAL:O	1:A:324:THR:HG23	2.10	0.50
1:A:286:GLY:O	1:A:290:ILE:HG12	2.11	0.50
1:A:470:ARG:C	1:A:472:ALA:H	2.20	0.50
1:A:446:VAL:HG11	1:A:477:ILE:CD1	2.40	0.50
1:A:297:ILE:HG22	1:A:316:MET:HG3	1.94	0.50
1:A:675:TYR:CE1	1:A:751:TYR:HB2	2.46	0.50
1:A:128:THR:HG22	1:A:437:VAL:HG22	1.94	0.50
1:A:695:MET:HG2	1:A:834:VAL:HG21	1.94	0.49
1:A:402:ARG:C	1:A:403:ARG:HG2	2.38	0.49
1:A:183:ARG:C	1:A:185:LYS:H	2.20	0.49
1:A:639:GLY:HA3	1:A:652:ALA:O	2.12	0.49
1:A:443:LEU:C	1:A:445:VAL:H	2.21	0.49
1:A:124:VAL:O	1:A:128:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NH1	1:A:155:SER:OG	2.46	0.48
1:A:55:ILE:HD13	1:A:90:GLY:HA3	1.94	0.48
1:A:842:ILE:HD12	1:A:849:LYS:HB2	1.95	0.48
1:A:571:GLN:O	4:A:1054:HOH:O	2.20	0.48
1:A:481:ALA:O	1:A:485:THR:HG23	2.14	0.47
1:A:801:THR:HA	1:A:834:VAL:HG22	1.96	0.47
1:A:398:ARG:O	1:A:402:ARG:CG	2.62	0.47
1:A:686:ASP:OD1	1:A:772:LYS:NZ	2.39	0.47
1:A:21:ALA:O	1:A:25:VAL:HG23	2.14	0.47
1:A:16:VAL:HG12	4:A:1088:HOH:O	2.14	0.47
1:A:183:ARG:C	1:A:185:LYS:N	2.71	0.47
1:A:261:TYR:CZ	1:A:280:GLN:HB2	2.50	0.47
1:A:551:TRP:HE3	1:A:569:PRO:HA	1.80	0.47
1:A:206:ILE:HA	1:A:260:ILE:CD1	2.45	0.46
1:A:555:HIS:CE1	1:A:569:PRO:HD2	2.50	0.46
1:A:199:ALA:O	1:A:203:ILE:HG12	2.16	0.46
1:A:374:LEU:O	1:A:377:ALA:N	2.37	0.46
1:A:399:PHE:N	4:A:1065:HOH:O	2.47	0.46
1:A:568:ASN:HB3	1:A:570:PHE:H	1.80	0.45
1:A:121:ILE:HD11	1:A:145:ALA:HB2	1.99	0.45
1:A:235:LEU:HD22	1:A:238:PHE:HE2	1.81	0.45
1:A:230:PHE:CD1	1:A:324:THR:HG21	2.52	0.44
1:A:53:ARG:HD3	1:A:53:ARG:C	2.42	0.44
1:A:120:ALA:O	1:A:123:PRO:HD2	2.17	0.44
1:A:637:TYR:HB3	1:A:668:ARG:HG2	1.99	0.44
1:A:523:TYR:CE2	1:A:541:PRO:HG2	2.52	0.44
1:A:551:TRP:CE3	1:A:569:PRO:HA	2.53	0.44
1:A:18:VAL:O	1:A:22:LEU:HG	2.18	0.44
1:A:143:LEU:HD22	1:A:384:LEU:HD21	2.01	0.43
1:A:151:PHE:O	1:A:155:SER:HB2	2.18	0.43
1:A:290:ILE:HD12	1:A:327:ILE:HD13	2.00	0.43
1:A:718:SER:O	1:A:722:GLN:HG2	2.19	0.43
1:A:306:PHE:HB3	1:A:315:GLY:HA3	2.00	0.43
1:A:381:PHE:HB2	1:A:385:PHE:HB2	2.00	0.43
1:A:35:SER:HB2	1:A:496:ALA:HB3	2.01	0.42
1:A:634:GLU:OE1	1:A:668:ARG:NH1	2.34	0.42
1:A:309:VAL:HG23	1:A:311:LEU:HG	2.01	0.42
1:A:694:ARG:HB2	1:A:826:TYR:CE1	2.54	0.42
1:A:316:MET:HB3	1:A:317:PRO:HD3	2.01	0.42
1:A:695:MET:CE	1:A:698:GLU:HB3	2.47	0.42
1:A:408:MET:HE2	1:A:408:MET:HB3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:CG	1:A:63:PRO:HA	2.54	0.42
1:A:613:GLU:HG2	1:A:740:MET:SD	2.59	0.42
1:A:19:ILE:O	1:A:23:ILE:HG13	2.20	0.41
1:A:130:GLU:CD	1:A:179:LEU:HD23	2.45	0.41
1:A:447:PHE:O	1:A:451:HIS:HB2	2.20	0.41
1:A:540:TYR:HA	1:A:541:PRO:HD3	1.82	0.41
1:A:183:ARG:CG	1:A:197:GLN:NE2	2.68	0.41
1:A:271:PHE:CE1	1:A:278:PRO:HG2	2.53	0.41
1:A:866:LEU:HD12	1:A:866:LEU:HA	1.96	0.41
1:A:128:THR:HB	1:A:437:VAL:HG13	2.02	0.40
1:A:317:PRO:O	1:A:321:ILE:HG12	2.21	0.40
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.83	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	785/875 (90%)	746 (95%)	32 (4%)	7 (1%)	14	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	PRO
1	A	187	HIS
1	A	183	ARG
1	A	471	VAL
1	A	444	SER
1	A	845	GLY
1	A	445	VAL

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	657/727 (90%)	601 (92%)	56 (8%)	10	22

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	27	LEU
1	A	30	LEU
1	A	38	THR
1	A	41	VAL
1	A	86	LEU
1	A	105	LEU
1	A	128	THR
1	A	129	ARG
1	A	130	GLU
1	A	138	VAL
1	A	146	ILE
1	A	156	ILE
1	A	157	LEU
1	A	184	TRP
1	A	188	ASP
1	A	196	ARG
1	A	238	PHE
1	A	282	LEU
1	A	323	LEU
1	A	328	MET
1	A	374	LEU
1	A	392	ILE
1	A	393	LEU
1	A	399	PHE
1	A	400	LEU
1	A	417	MET
1	A	418	PHE
1	A	426	ARG
1	A	441	LEU

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Mol	Chain	Res	Type
1	A	445	VAL
1	A	450	LEU
1	A	451	HIS
1	A	475	LEU
1	A	479	LEU
1	A	485	THR
1	A	488	LEU
1	A	543	GLU
1	A	566	ILE
1	A	605	VAL
1	A	653	ASN
1	A	663	ILE
1	A	673	LEU
1	A	730	MET
1	A	736	VAL
1	A	777	VAL
1	A	813	VAL
1	A	816	LYS
1	A	819	THR
1	A	835	LYS
1	A	842	ILE
1	A	846	ASN
1	A	847	VAL
1	A	851	ILE
1	A	852	THR
1	A	867	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	170	GLN
1	A	197	GLN
1	A	301	ASN
1	A	789	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	902	-	4,4,4	0.29	0	6,6,6	0.26	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.

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, 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	793/875 (90%)	0.24	61 (7%) 19 17	26, 50, 100, 151	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	TYR	9.0
1	A	187	HIS	5.2
1	A	333	VAL	5.0
1	A	181	TYR	4.8
1	A	787	SER	4.6
1	A	469	PHE	4.6
1	A	422	TRP	4.6
1	A	471	VAL	4.4
1	A	474	ALA	4.3
1	A	374	LEU	4.3
1	A	185	LYS	4.2
1	A	188	ASP	4.1
1	A	186	GLY	4.0
1	A	477	ILE	3.7
1	A	332	PHE	3.7
1	A	193	LEU	3.7
1	A	788	ALA	3.7
1	A	183	ARG	3.4
1	A	238	PHE	3.3
1	A	313	ARG	3.2
1	A	472	ALA	3.1
1	A	184	TRP	3.1
1	A	476	LEU	3.0
1	A	239	VAL	3.0
1	A	17	LEU	3.0
1	A	16	VAL	2.9
1	A	448	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	734	TYR	2.8
1	A	447	PHE	2.7
1	A	854	TYR	2.7
1	A	485	THR	2.7
1	A	451	HIS	2.7
1	A	19	ILE	2.6
1	A	475	LEU	2.6
1	A	473	PHE	2.6
1	A	868	LEU	2.5
1	A	15	SER	2.5
1	A	180	ALA	2.5
1	A	421	LEU	2.4
1	A	182	ASN	2.4
1	A	423	GLY	2.4
1	A	404	SER	2.4
1	A	449	LYS	2.4
1	A	450	LEU	2.3
1	A	484	PRO	2.3
1	A	179	LEU	2.3
1	A	326	LEU	2.3
1	A	397	TYR	2.3
1	A	445	VAL	2.2
1	A	133	ASP	2.2
1	A	786	VAL	2.2
1	A	480	ALA	2.1
1	A	444	SER	2.1
1	A	195	ALA	2.1
1	A	543	GLU	2.1
1	A	402	ARG	2.0
1	A	330	LEU	2.0
1	A	487	ILE	2.0
1	A	816	LYS	2.0
1	A	237	GLY	2.0
1	A	483	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	902	5/5	0.98	0.05	50,53,57,60	0
2	ZN	A	901	1/1	0.99	0.07	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.