



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 PM GMT

PDB ID : 4X7P
Title : Crystal structure of apo S. aureus TarM
Authors : Worrall, L.J.; Sobhanifar, S.; Gruninger, R.J.; Strynadka, N.C.
Deposited on : 2014-12-09
Resolution : 3.40 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

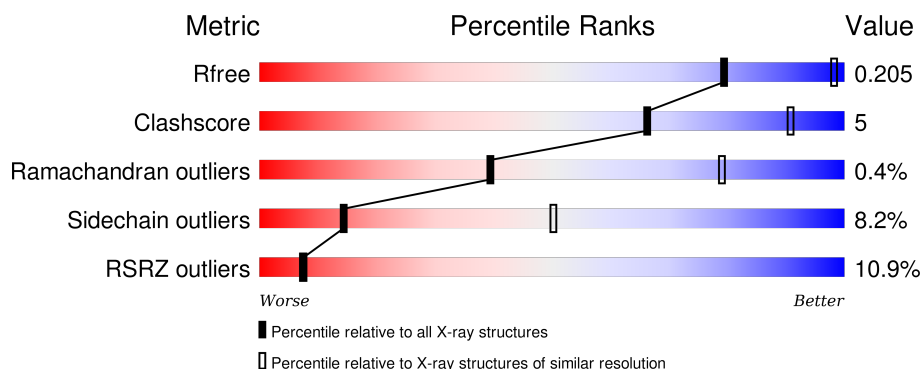
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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. 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	493	<div> <div>21%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
1	B	493	<div> <div>%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8146 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 TarM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			4033	2581	681	752	19			
1	B	493	Total	C	N	O	S	0	0	0
			4033	2581	681	752	19			

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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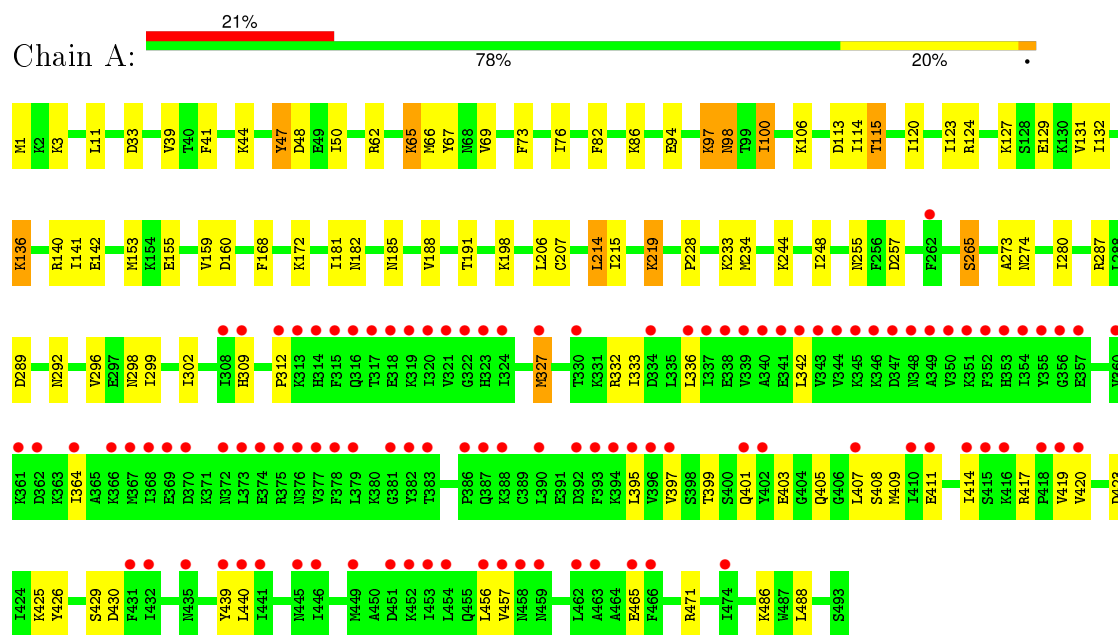
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: TarM



• Molecule 1: TarM



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	208.60Å 208.60Å 120.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.33 – 3.40 78.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.33-3.40) 99.8 (78.93-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.01Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.173 , 0.187 0.184 , 0.205	Depositor DCC
R_{free} test set	2101 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.4	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 59812 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8146	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.47	0/4110	0.67	0/5516
1	B	0.44	0/4110	0.67	0/5516
All	All	0.45	0/8220	0.67	0/11032

There are no bond length outliers.

There are no bond angle outliers.

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	4033	0	4057	46	0
1	B	4033	0	4057	38	0
2	A	40	0	0	1	0
2	B	40	0	0	1	0
All	All	8146	0	8114	79	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 5.

All (79) 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:114:ILE:CG1	1:B:114:ILE:CD1	1.74	1.57
1:A:114:ILE:CG1	1:A:114:ILE:CD1	1.83	1.50
1:B:287:ARG:HG3	1:B:299:ILE:HG22	1.79	0.65
1:A:287:ARG:HG3	1:A:299:ILE:HG22	1.79	0.64
1:B:39:VAL:HG22	1:B:67:TYR:HB2	1.81	0.63
1:B:280:ILE:HG12	1:B:302:ILE:HD12	1.83	0.60
1:B:312:PRO:HG2	1:B:417:ARG:HH21	1.68	0.58
1:A:312:PRO:HG2	1:A:417:ARG:HH21	1.70	0.57
1:A:191:THR:HG21	1:A:206:LEU:HD22	1.88	0.56
1:A:207:CYS:HB2	1:A:233:LYS:HG2	1.88	0.55
1:A:65:LYS:HE3	1:B:446:ILE:HD11	1.90	0.53
1:B:73:PHE:HA	1:B:76:ILE:HD12	1.92	0.51
1:A:280:ILE:HG12	1:A:302:ILE:HD12	1.93	0.51
1:A:214:LEU:HD23	1:A:215:ILE:HG13	1.94	0.50
1:B:409:MET:HG2	1:B:419:VAL:HG11	1.94	0.49
1:A:153:MET:HG3	1:A:168:PHE:CD1	2.48	0.49
1:A:228:PRO:HB2	1:A:265:SER:HB2	1.95	0.49
1:A:395:LEU:HD22	1:A:456:LEU:HB3	1.95	0.49
1:A:411:GLU:HA	1:A:414:ILE:HD12	1.95	0.48
1:B:332:ARG:HG3	1:B:401:GLN:HG2	1.95	0.48
1:B:274:ASN:HA	1:B:298:ASN:HD22	1.79	0.48
1:A:98:ASN:HD21	1:A:115:THR:HG22	1.78	0.48
1:B:411:GLU:HA	1:B:414:ILE:HD12	1.96	0.48
1:A:113:ASP:HB2	1:A:120:ILE:HD11	1.94	0.48
1:B:228:PRO:HB2	1:B:265:SER:HB2	1.95	0.48
1:A:332:ARG:HG3	1:A:401:GLN:HG2	1.96	0.48
1:A:409:MET:HG2	1:A:419:VAL:HG11	1.94	0.48
1:A:274:ASN:HA	1:A:298:ASN:HD22	1.78	0.48
1:B:395:LEU:HD22	1:B:456:LEU:HB3	1.95	0.47
1:A:94:GLU:O	1:A:97:LYS:HB2	2.14	0.47
1:B:124:ARG:NH2	2:B:504:SO4:O2	2.47	0.47
1:B:113:ASP:HB2	1:B:120:ILE:HD11	1.95	0.47
1:A:41:PHE:HA	1:A:69:VAL:HG12	1.97	0.47
1:A:82:PHE:HE1	1:B:329:PRO:HG2	1.81	0.46
1:A:336:LEU:HD11	1:A:397:VAL:HG13	1.98	0.46
1:B:94:GLU:O	1:B:97:LYS:HB2	2.16	0.46
1:A:44:LYS:HB2	1:A:47:TYR:CD2	2.50	0.46
1:B:327:MET:HG3	1:B:333:ILE:HD13	1.98	0.46
1:A:136:LYS:HB2	1:A:141:ILE:HG12	1.98	0.45
1:A:327:MET:HG3	1:A:333:ILE:HD13	1.98	0.45
1:B:273:ALA:HB3	1:B:296:VAL:HG21	1.98	0.45
1:A:153:MET:HG3	1:A:168:PHE:HD1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HB3	1:A:296:VAL:HG21	1.98	0.45
1:A:39:VAL:HG22	1:A:67:TYR:HB2	1.98	0.45
1:A:76:ILE:HG23	1:B:256:PHE:HB3	1.98	0.45
1:B:136:LYS:HB2	1:B:141:ILE:HG12	1.99	0.45
1:A:234:MET:HG2	1:A:244:LYS:HD3	1.99	0.44
1:B:182:ASN:HB3	1:B:185:ASN:OD1	2.18	0.44
1:B:181:ILE:HD12	1:B:188:VAL:HG22	1.98	0.44
1:B:336:LEU:HD11	1:B:397:VAL:HG13	1.98	0.44
1:A:73:PHE:HA	1:A:76:ILE:HD12	1.99	0.44
1:B:219:LYS:H	1:B:219:LYS:CD	2.30	0.44
1:B:423:ASP:HB2	1:B:440:LEU:HG	2.00	0.44
1:A:198:LYS:HE3	1:B:259:THR:HG22	1.99	0.44
1:A:123:ILE:HG12	1:A:132:ILE:HG12	1.99	0.44
1:A:11:LEU:HD12	1:A:66:MET:HE3	2.00	0.44
1:A:181:ILE:HD12	1:A:188:VAL:HG22	2.00	0.43
1:B:113:ASP:CG	1:B:116:THR:HG22	2.38	0.43
1:A:219:LYS:H	1:A:219:LYS:CD	2.31	0.43
1:B:98:ASN:HD21	1:B:115:THR:HG22	1.84	0.43
1:B:123:ILE:HG12	1:B:132:ILE:HG12	2.00	0.43
1:B:69:VAL:O	1:B:72:TYR:HB3	2.18	0.43
1:B:234:MET:HG2	1:B:244:LYS:HD3	2.01	0.43
1:A:182:ASN:HB3	1:A:185:ASN:OD1	2.19	0.42
1:A:124:ARG:NH2	2:A:504:SO4:O2	2.52	0.42
1:A:62:ARG:HD2	1:B:345:LYS:NZ	2.34	0.42
1:B:309:HIS:O	1:B:471:ARG:NH2	2.53	0.42
1:A:47:TYR:CE1	1:A:66:MET:HE1	2.54	0.42
1:A:44:LYS:HD3	1:A:50:ILE:HD13	2.01	0.42
1:B:420:VAL:HG22	1:B:439:TYR:HB2	2.00	0.42
1:A:309:HIS:O	1:A:471:ARG:NH2	2.53	0.41
1:A:423:ASP:HB2	1:A:440:LEU:HG	2.01	0.41
1:B:11:LEU:HD12	1:B:66:MET:HE3	2.02	0.41
1:B:47:TYR:CE1	1:B:66:MET:HE1	2.55	0.41
1:A:100:ILE:CG2	1:A:114:ILE:HB	2.50	0.41
1:A:425:LYS:HA	1:A:426:TYR:HA	1.88	0.41
1:B:191:THR:HG21	1:B:206:LEU:HD22	2.03	0.41
1:A:142:GLU:HA	1:A:155:GLU:O	2.20	0.40
1:A:420:VAL:HG22	1:A:439:TYR:HB2	2.02	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	491/493 (100%)	458 (93%)	31 (6%)	2 (0%)	39	79
1	B	491/493 (100%)	459 (94%)	30 (6%)	2 (0%)	39	79
All	All	982/986 (100%)	917 (93%)	61 (6%)	4 (0%)	39	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	B	97	LYS
1	A	405	GLN
1	B	405	GLN

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	449/449 (100%)	409 (91%)	40 (9%)	12	45
1	B	449/449 (100%)	415 (92%)	34 (8%)	16	54
All	All	898/898 (100%)	824 (92%)	74 (8%)	14	50

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	33	ASP
1	A	47	TYR
1	A	48	ASP
1	A	65	LYS
1	A	86	LYS
1	A	98	ASN
1	A	100	ILE
1	A	106	LYS
1	A	115	THR
1	A	127	LYS
1	A	129	GLU
1	A	131	VAL
1	A	136	LYS
1	A	140	ARG
1	A	159	VAL
1	A	160	ASP
1	A	172	LYS
1	A	214	LEU
1	A	219	LYS
1	A	248	ILE
1	A	255	ASN
1	A	257	ASP
1	A	265	SER
1	A	289	ASP
1	A	292	ASN
1	A	327	MET
1	A	342	LEU
1	A	364	ILE
1	A	399	THR
1	A	403	GLU
1	A	407	LEU
1	A	408	SER
1	A	429	SER
1	A	430	ASP
1	A	457	VAL
1	A	465	GLU
1	A	486	LYS
1	A	488	LEU
1	B	1	MET
1	B	33	ASP
1	B	47	TYR
1	B	48	ASP

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Mol	Chain	Res	Type
1	B	65	LYS
1	B	98	ASN
1	B	100	ILE
1	B	106	LYS
1	B	115	THR
1	B	127	LYS
1	B	129	GLU
1	B	131	VAL
1	B	140	ARG
1	B	159	VAL
1	B	160	ASP
1	B	172	LYS
1	B	219	LYS
1	B	248	ILE
1	B	255	ASN
1	B	257	ASP
1	B	265	SER
1	B	289	ASP
1	B	292	ASN
1	B	327	MET
1	B	342	LEU
1	B	364	ILE
1	B	399	THR
1	B	403	GLU
1	B	407	LEU
1	B	408	SER
1	B	429	SER
1	B	430	ASP
1	B	457	VAL
1	B	465	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	149	ASN
1	A	184	ASN
1	A	196	ASN
1	A	298	ASN
1	A	309	HIS
1	A	314	HIS
1	A	387	GLN

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Mol	Chain	Res	Type
1	A	435	ASN
1	B	149	ASN
1	B	196	ASN
1	B	298	ASN
1	B	309	HIS
1	B	314	HIS
1	B	435	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 ⓘ

16 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	501	-	4,4,4	0.35	0	6,6,6	0.21	0
2	SO4	A	502	-	4,4,4	0.55	0	6,6,6	0.24	0
2	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.17	0
2	SO4	A	504	-	4,4,4	0.19	0	6,6,6	0.17	0
2	SO4	A	505	-	4,4,4	0.48	0	6,6,6	0.10	0
2	SO4	A	506	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	A	507	-	4,4,4	0.23	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	508	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	B	501	-	4,4,4	0.37	0	6,6,6	0.14	0
2	SO4	B	502	-	4,4,4	0.48	0	6,6,6	0.15	0
2	SO4	B	503	-	4,4,4	0.30	0	6,6,6	0.16	0
2	SO4	B	504	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	B	505	-	4,4,4	0.10	0	6,6,6	0.16	0
2	SO4	B	506	-	4,4,4	0.24	0	6,6,6	0.19	0
2	SO4	B	507	-	4,4,4	0.21	0	6,6,6	0.32	0
2	SO4	B	508	-	4,4,4	0.19	0	6,6,6	0.10	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
2	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	SO4	A	507	-	-	0/0/0/0	0/0/0/0
2	SO4	A	508	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
2	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	SO4	B	507	-	-	0/0/0/0	0/0/0/0
2	SO4	B	508	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	SO4	1	0
2	B	504	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 ⓘ

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	493/493 (100%)	1.09	104 (21%) 1 1	35, 80, 259, 264	0
1	B	493/493 (100%)	0.26	3 (0%) 90 86	54, 83, 123, 147	0
All	All	986/986 (100%)	0.68	107 (10%) 7 7	35, 83, 253, 264	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	VAL	9.2
1	A	321	VAL	8.6
1	A	395	LEU	8.1
1	A	322	GLY	7.9
1	A	320	ILE	7.1
1	A	356	GLY	7.0
1	A	453	ILE	7.0
1	A	454	LEU	6.9
1	A	338	GLU	6.9
1	A	346	LYS	6.6
1	A	352	PHE	6.5
1	A	396	VAL	6.2
1	A	340	ALA	6.1
1	A	377	VAL	6.0
1	A	456	LEU	6.0
1	A	375	ARG	6.0
1	A	342	LEU	5.9
1	A	353	HIS	5.7
1	A	327	MET	5.2
1	A	394	LYS	5.0
1	A	419	VAL	5.0
1	A	420	VAL	4.9
1	A	376	ASN	4.8
1	A	357	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	315	PHE	4.8
1	A	369	GLU	4.6
1	A	466	PHE	4.6
1	A	397	VAL	4.5
1	A	418	PRO	4.5
1	A	373	LEU	4.5
1	A	344	VAL	4.4
1	A	341	GLU	4.3
1	A	368	ILE	4.3
1	A	337	ILE	4.2
1	A	439	TYR	4.1
1	A	449	MET	4.1
1	A	432	ILE	4.1
1	A	317	THR	4.1
1	A	458	ASN	4.1
1	A	378	PHE	3.9
1	A	374	GLU	3.9
1	A	336	LEU	3.9
1	A	451	ASP	3.8
1	A	318	GLU	3.8
1	A	324	ILE	3.7
1	A	393	PHE	3.7
1	A	351	LYS	3.6
1	A	435	ASN	3.6
1	A	474	ILE	3.5
1	A	463	ALA	3.5
1	A	386	PRO	3.5
1	A	392	ASP	3.5
1	A	452	LYS	3.5
1	A	316	GLN	3.5
1	A	401	GLN	3.4
1	A	440	LEU	3.3
1	A	348	ASN	3.3
1	A	379	LEU	3.3
1	A	387	GLN	3.3
1	A	415	SER	3.3
1	A	314	HIS	3.2
1	A	350	VAL	3.2
1	A	411	GLU	3.2
1	A	319	LYS	3.2
1	A	355	TYR	3.2
1	A	462	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	390	LEU	3.0
1	A	366	LYS	3.0
1	A	313	LYS	2.9
1	A	312	PRO	2.9
1	A	339	VAL	2.9
1	A	367	MET	2.9
1	A	410	ILE	2.9
1	A	360	VAL	2.9
1	A	354	ILE	2.9
1	A	330	THR	2.8
1	A	372	ASN	2.8
1	A	262	PHE	2.8
1	B	395	LEU	2.7
1	A	388	LYS	2.7
1	A	364	ILE	2.7
1	A	370	ASP	2.7
1	A	416	LYS	2.6
1	A	309	HIS	2.6
1	A	334	ASP	2.6
1	A	441	ILE	2.5
1	A	465	GLU	2.5
1	A	323	HIS	2.5
1	A	446	ILE	2.4
1	A	362	ASP	2.4
1	A	349	ALA	2.4
1	A	345	LYS	2.4
1	A	459	ASN	2.4
1	A	308	ILE	2.3
1	A	431	PHE	2.3
1	A	347	ASP	2.3
1	A	383	THR	2.3
1	A	457	VAL	2.3
1	A	382	TYR	2.2
1	A	361	LYS	2.2
1	A	414	ILE	2.2
1	A	445	ASN	2.2
1	A	381	GLY	2.1
1	A	407	LEU	2.1
1	B	373	LEU	2.1
1	B	345	LYS	2.1
1	A	402	TYR	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	506	5/5	0.91	0.32	1.66	147,148,148,151	0
2	SO4	A	502	5/5	0.95	0.30	1.50	92,93,94,95	0
2	SO4	A	503	5/5	0.97	0.29	0.47	83,84,90,90	0
2	SO4	A	501	5/5	0.98	0.24	-0.11	70,73,75,79	0
2	SO4	B	502	5/5	0.96	0.23	-0.25	91,92,92,93	0
2	SO4	A	506	5/5	0.94	0.21	-0.98	117,117,118,119	0
2	SO4	B	503	5/5	0.93	0.23	-1.01	109,109,109,110	0
2	SO4	B	504	5/5	0.93	0.15	-	134,134,136,137	0
2	SO4	A	504	5/5	0.95	0.18	-	121,122,124,124	0
2	SO4	B	501	5/5	0.89	0.21	-	128,129,130,131	0
2	SO4	A	505	5/5	0.97	0.24	-	97,98,99,100	0
2	SO4	A	508	5/5	0.78	0.23	-	163,164,166,166	0
2	SO4	B	508	5/5	0.86	0.25	-	172,172,173,173	0
2	SO4	B	505	5/5	0.86	0.26	-	139,140,141,143	0
2	SO4	B	507	5/5	0.74	0.19	-	129,130,131,132	0
2	SO4	A	507	5/5	0.85	0.14	-	126,127,128,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.