Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:38 pm BST

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
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:

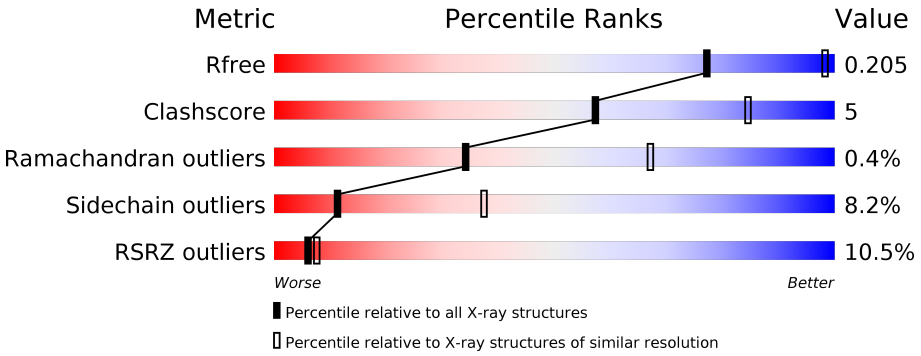
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (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 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 <=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	21% 78% 20%
1	B	493	81% 18%

2 Entry composition

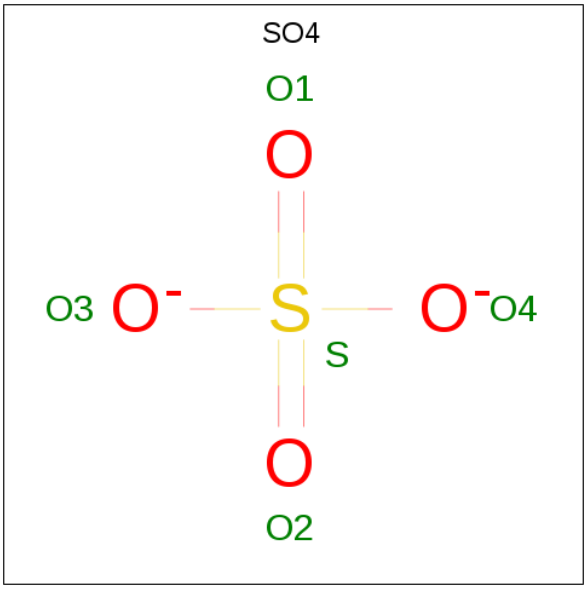
There are 2 unique types of molecules in this entry. The entry contains 8146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: O_4S).



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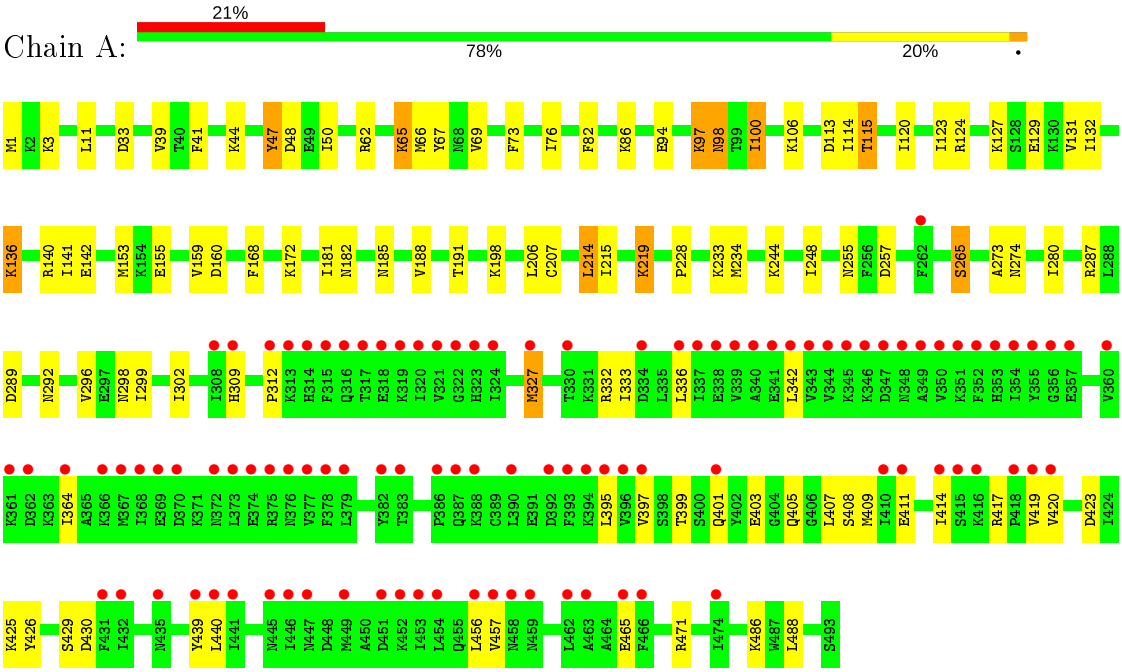
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0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

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.

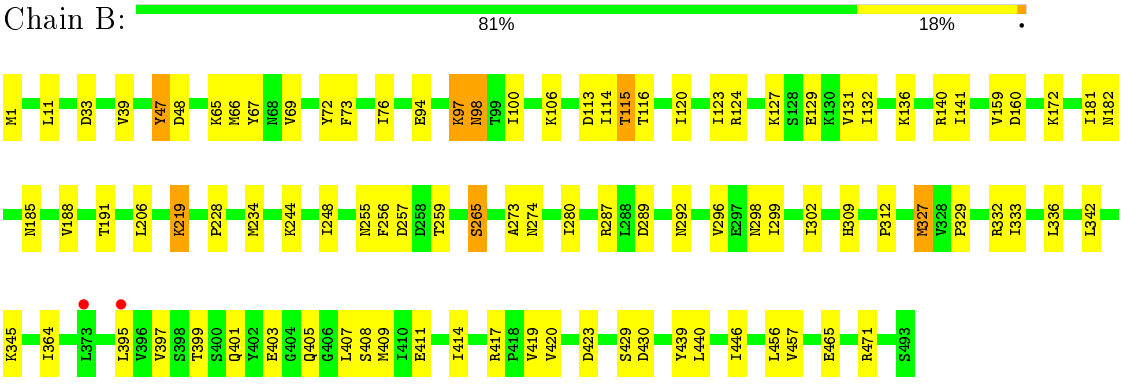
- Molecule 1: TarM

Chain A:



- Molecule 1: TarM

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.71 (at 3.01Å)	Xtriage
Refinement program	BUSTER, REFMAC	Depositor
R, R_{free}	0.173 , 0.187 0.184 , 0.205	Depositor DCC
R_{free} test set	3022 reflections (5.05%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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:A:98:ASN:HD21	1:A:115:THR:HG22	1.78	0.48
1:B:274:ASN:HA	1:B:298:ASN:HD22	1.79	0.48
1:B:332:ARG:HG3	1:B:401:GLN:HG2	1.95	0.48
1:A:113:ASP:HB2	1:A:120:ILE:HD11	1.94	0.48
1:B:411:GLU:HA	1:B:414:ILE:HD12	1.96	0.48
1:A:332:ARG:HG3	1:A:401:GLN:HG2	1.96	0.48
1:B:228:PRO:HB2	1:B:265:SER:HB2	1.95	0.48
1:A:274:ASN:HA	1:A:298:ASN:HD22	1.78	0.48
1:A:409:MET:HG2	1:A:419:VAL:HG11	1.94	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:336:LEU:HD11	1:A:397:VAL:HG13	1.98	0.46
1:A:82:PHE:HE1	1:B:329:PRO:HG2	1.81	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:A:123:ILE:HG12	1:A:132:ILE:HG12	1.99	0.44
1:A:198:LYS:HE3	1:B:259:THR:HG22	1.99	0.44
1:B:423:ASP:HB2	1:B:440:LEU:HG	2.00	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 (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	491/493 (100%)	458 (93%)	31 (6%)	2 (0%)	34 67
1	B	491/493 (100%)	459 (94%)	30 (6%)	2 (0%)	34 67
All	All	982/986 (100%)	917 (93%)	61 (6%)	4 (0%)	34 67

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 (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	449/449 (100%)	409 (91%)	40 (9%)	9 33
1	B	449/449 (100%)	415 (92%)	34 (8%)	13 41
All	All	898/898 (100%)	824 (92%)	74 (8%)	11 37

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	506	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.34	0
2	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	B	507	-	4,4,4	0.17	0	6,6,6	0.40	0
2	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	506	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	A	504	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	B	501	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	508	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	508	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	B	502	-	4,4,4	0.21	0	6,6,6	0.22	0
2	SO4	A	502	-	4,4,4	0.29	0	6,6,6	0.25	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	B	504	SO4	1	0
2	A	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, 95^{th} 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%)	1.03	102 (20%) 1 1	35, 80, 259, 264	0
1	B	493/493 (100%)	0.22	2 (0%) 92 92	54, 83, 123, 147	0
All	All	986/986 (100%)	0.63	104 (10%) 6 7	35, 83, 253, 264	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	VAL	9.1
1	A	321	VAL	8.3
1	A	395	LEU	8.0
1	A	322	GLY	7.2
1	A	320	ILE	7.0
1	A	453	ILE	6.8
1	A	454	LEU	6.5
1	A	338	GLU	6.5
1	A	346	LYS	6.3
1	A	356	GLY	6.3
1	A	352	PHE	6.2
1	A	396	VAL	6.1
1	A	342	LEU	6.0
1	A	340	ALA	6.0
1	A	456	LEU	5.9
1	A	375	ARG	5.9
1	A	377	VAL	5.8
1	A	353	HIS	5.4
1	A	419	VAL	4.9
1	A	420	VAL	4.8
1	A	315	PHE	4.7
1	A	327	MET	4.7
1	A	376	ASN	4.7
1	A	394	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	418	PRO	4.5
1	A	357	GLU	4.5
1	A	344	VAL	4.5
1	A	341	GLU	4.3
1	A	373	LEU	4.3
1	A	397	VAL	4.2
1	A	369	GLU	4.2
1	A	466	PHE	4.2
1	A	337	ILE	4.2
1	A	439	TYR	4.2
1	A	432	ILE	4.1
1	A	368	ILE	4.1
1	A	336	LEU	3.9
1	A	458	ASN	3.9
1	A	324	ILE	3.9
1	A	374	GLU	3.8
1	A	317	THR	3.8
1	A	449	MET	3.7
1	A	378	PHE	3.7
1	A	451	ASP	3.7
1	A	351	LYS	3.7
1	A	318	GLU	3.7
1	A	474	ILE	3.6
1	A	386	PRO	3.6
1	A	452	LYS	3.5
1	A	379	LEU	3.5
1	A	350	VAL	3.5
1	A	393	PHE	3.5
1	A	435	ASN	3.4
1	A	319	LYS	3.4
1	A	440	LEU	3.3
1	A	415	SER	3.3
1	A	392	ASP	3.3
1	A	463	ALA	3.3
1	A	401	GLN	3.1
1	A	314	HIS	3.1
1	A	390	LEU	3.1
1	A	316	GLN	3.0
1	A	462	LEU	3.0
1	A	387	GLN	2.9
1	A	312	PRO	2.9
1	A	366	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	348	ASN	2.8
1	A	370	ASP	2.8
1	A	355	TYR	2.8
1	B	395	LEU	2.8
1	A	313	LYS	2.7
1	A	339	VAL	2.7
1	A	411	GLU	2.7
1	A	364	ILE	2.7
1	A	330	THR	2.7
1	A	372	ASN	2.7
1	A	410	ILE	2.7
1	A	367	MET	2.6
1	A	354	ILE	2.6
1	A	388	LYS	2.6
1	A	416	LYS	2.6
1	A	360	VAL	2.5
1	A	345	LYS	2.5
1	A	262	PHE	2.5
1	A	441	ILE	2.5
1	A	323	HIS	2.5
1	A	309	HIS	2.4
1	A	308	ILE	2.4
1	A	334	ASP	2.4
1	A	446	ILE	2.4
1	A	362	ASP	2.3
1	A	431	PHE	2.3
1	A	349	ALA	2.3
1	A	457	VAL	2.3
1	A	465	GLU	2.3
1	A	459	ASN	2.2
1	A	383	THR	2.2
1	A	414	ILE	2.2
1	A	361	LYS	2.2
1	A	347	ASP	2.1
1	A	382	TYR	2.1
1	A	447	ASN	2.1
1	A	445	ASN	2.1
1	B	373	LEU	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, 95^{th} 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^2)	Q<0.9
2	SO4	B	507	5/5	0.72	0.21	129,130,131,132	0
2	SO4	A	508	5/5	0.79	0.22	163,164,166,166	0
2	SO4	A	507	5/5	0.85	0.14	126,127,128,129	0
2	SO4	B	505	5/5	0.85	0.26	139,140,141,143	0
2	SO4	B	508	5/5	0.86	0.25	172,172,173,173	0
2	SO4	B	501	5/5	0.89	0.21	128,129,130,131	0
2	SO4	B	506	5/5	0.91	0.30	147,148,148,151	0
2	SO4	B	503	5/5	0.93	0.23	109,109,109,110	0
2	SO4	B	504	5/5	0.93	0.15	134,134,136,137	0
2	SO4	A	506	5/5	0.94	0.21	117,117,118,119	0
2	SO4	A	504	5/5	0.95	0.18	121,122,124,124	0
2	SO4	A	502	5/5	0.95	0.30	92,93,94,95	0
2	SO4	B	502	5/5	0.96	0.23	91,92,92,93	0
2	SO4	A	505	5/5	0.97	0.23	97,98,99,100	0
2	SO4	A	503	5/5	0.97	0.28	83,84,90,90	0
2	SO4	A	501	5/5	0.98	0.23	70,73,75,79	0

6.5 Other polymers (i)

There are no such residues in this entry.