



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 AM UTC

PDB ID : 2ULL / pdb_00002ull
Title : MULTIPLE CONFORMATION STRUCTURE OF ALPHA-LYTIC PROTEASE AT 120 K
Authors : Rader, S.D.; Agard, D.A.
Deposited on : 1996-11-26
Resolution : 1.50 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)
Xtrriage (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

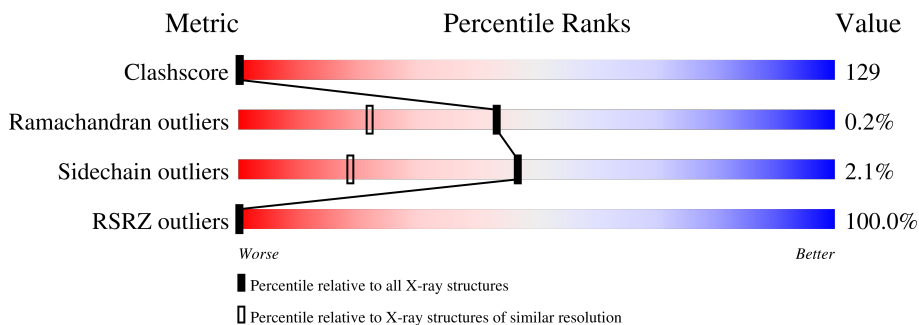
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	1-A	198	 100% 97%
1	10-A	198	 98%
1	11-A	198	 98%
1	12-A	198	 98%
1	13-A	198	 98%
1	14-A	198	 98%
1	15-A	198	 97%

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Mol	Chain	Length	Quality of chain
1	16-A	198	98%
1	2-A	198	98%
1	3-A	198	97%
1	4-A	198	97%
1	5-A	198	97%
1	6-A	198	98%
1	7-A	198	98%
1	8-A	198	98%
1	9-A	198	98%

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
2	SO4	1-A	4	-	X	-	-
2	SO4	10-A	4	-	X	-	-
2	SO4	11-A	4	-	X	-	-
2	SO4	12-A	4	-	X	-	-
2	SO4	13-A	4	-	X	-	-
2	SO4	14-A	4	-	X	-	-
2	SO4	15-A	4	-	X	-	-
2	SO4	16-A	4	-	X	-	-
2	SO4	2-A	4	-	X	-	-
2	SO4	3-A	4	-	X	-	-
2	SO4	4-A	4	-	X	-	-
2	SO4	5-A	4	-	X	-	-
2	SO4	6-A	4	-	X	-	-
2	SO4	7-A	4	-	X	-	-
2	SO4	8-A	4	-	X	-	-
2	SO4	9-A	4	-	X	-	-
3	TAM	1-A	1	-	X	-	-
3	TAM	10-A	1	-	X	-	-
3	TAM	11-A	1	-	X	-	-
3	TAM	12-A	1	-	X	-	-
3	TAM	13-A	1	-	X	-	-
3	TAM	14-A	1	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TAM	15-A	1	-	X	-	-
3	TAM	16-A	1	-	X	-	-
3	TAM	2-A	1	-	X	-	-
3	TAM	3-A	1	-	X	-	-
3	TAM	4-A	1	-	X	-	-
3	TAM	5-A	1	-	X	-	-
3	TAM	6-A	1	-	X	-	-
3	TAM	7-A	1	-	X	-	-
3	TAM	8-A	1	-	X	-	-
3	TAM	9-A	1	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27440 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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	198	1391	846	262	275	8	0	0	0
1	2-A	198	1391	846	262	275	8	0	0	0
1	3-A	198	1391	846	262	275	8	0	0	0
1	4-A	198	1391	846	262	275	8	0	0	0
1	5-A	198	1391	846	262	275	8	0	0	0
1	6-A	198	1391	846	262	275	8	0	0	0
1	7-A	198	1391	846	262	275	8	0	0	0
1	8-A	198	1391	846	262	275	8	0	0	0
1	9-A	198	1391	846	262	275	8	0	0	0
1	10-A	198	1391	846	262	275	8	0	0	0
1	11-A	198	1391	846	262	275	8	0	0	0
1	12-A	198	1391	846	262	275	8	0	0	0
1	13-A	198	1391	846	262	275	8	0	0	0
1	14-A	198	1391	846	262	275	8	0	0	0
1	15-A	198	1391	846	262	275	8	0	0	0
1	16-A	198	1391	846	262	275	8	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		

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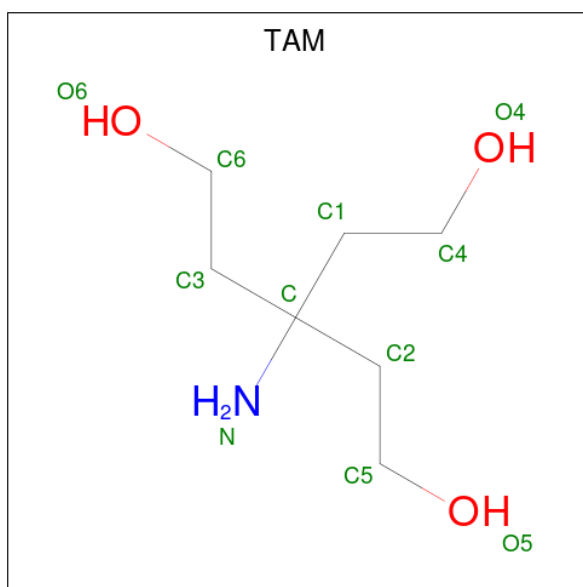
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	14-A	1	5	4	1	0	0
2	15-A	1	5	4	1	0	0
2	16-A	1	5	4	1	0	0
2	1-A	1	5	4	1	0	0
2	2-A	1	5	4	1	0	0
2	3-A	1	5	4	1	0	0
2	4-A	1	5	4	1	0	0
2	5-A	1	5	4	1	0	0
2	6-A	1	5	4	1	0	0
2	7-A	1	5	4	1	0	0
2	8-A	1	5	4	1	0	0
2	9-A	1	5	4	1	0	0
2	10-A	1	5	4	1	0	0
2	11-A	1	5	4	1	0	0
2	12-A	1	5	4	1	0	0
2	13-A	1	5	4	1	0	0
2	14-A	1	5	4	1	0	0
2	15-A	1	5	4	1	0	0
2	16-A	1	5	4	1	0	0
2	1-A	1	5	4	1	0	0
2	2-A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	3-A	1	Total 5	O 4	S 1	0	0
2	4-A	1	Total 5	O 4	S 1	0	0
2	5-A	1	Total 5	O 4	S 1	0	0
2	6-A	1	Total 5	O 4	S 1	0	0
2	7-A	1	Total 5	O 4	S 1	0	0
2	8-A	1	Total 5	O 4	S 1	0	0
2	9-A	1	Total 5	O 4	S 1	0	0
2	10-A	1	Total 5	O 4	S 1	0	0
2	11-A	1	Total 5	O 4	S 1	0	0
2	12-A	1	Total 5	O 4	S 1	0	0
2	13-A	1	Total 5	O 4	S 1	0	0
2	14-A	1	Total 5	O 4	S 1	0	0
2	15-A	1	Total 5	O 4	S 1	0	0
2	16-A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	1	Total C N 8 7 1	0	0
3	2-A	1	Total C N 8 7 1	0	0
3	3-A	1	Total C N 8 7 1	0	0
3	4-A	1	Total C N 8 7 1	0	0
3	5-A	1	Total C N 8 7 1	0	0
3	6-A	1	Total C N 8 7 1	0	0
3	7-A	1	Total C N 8 7 1	0	0
3	8-A	1	Total C N 8 7 1	0	0
3	9-A	1	Total C N 8 7 1	0	0
3	10-A	1	Total C N 8 7 1	0	0
3	11-A	1	Total C N 8 7 1	0	0
3	12-A	1	Total C N 8 7 1	0	0
3	13-A	1	Total C N 8 7 1	0	0
3	14-A	1	Total C N 8 7 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	15-A	1	Total	C	N	0	0
			8	7	1		
3	16-A	1	Total	C	N	0	0
			8	7	1		

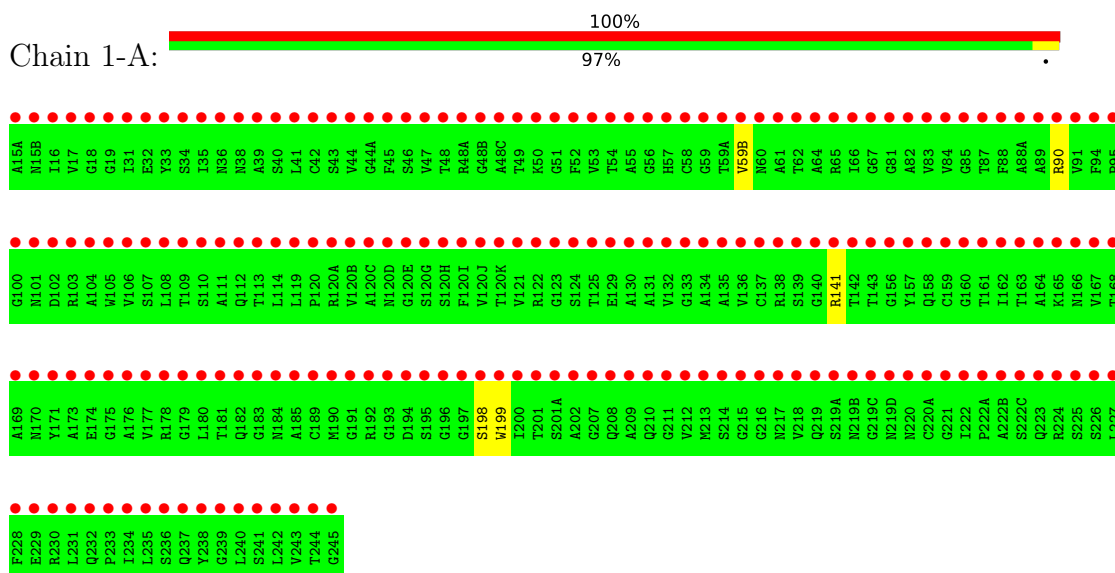
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	301	Total	O	2	0
			301	301		
4	2-A	301	Total	O	2	0
			301	301		
4	3-A	301	Total	O	2	0
			301	301		
4	4-A	301	Total	O	2	0
			301	301		
4	5-A	301	Total	O	2	0
			301	301		
4	6-A	301	Total	O	2	0
			301	301		
4	7-A	301	Total	O	2	0
			301	301		
4	8-A	301	Total	O	2	0
			301	301		
4	9-A	301	Total	O	2	0
			301	301		
4	10-A	301	Total	O	2	0
			301	301		
4	11-A	301	Total	O	2	0
			301	301		
4	12-A	301	Total	O	2	0
			301	301		
4	13-A	301	Total	O	2	0
			301	301		
4	14-A	301	Total	O	2	0
			301	301		
4	15-A	301	Total	O	2	0
			301	301		
4	16-A	301	Total	O	2	0
			301	301		

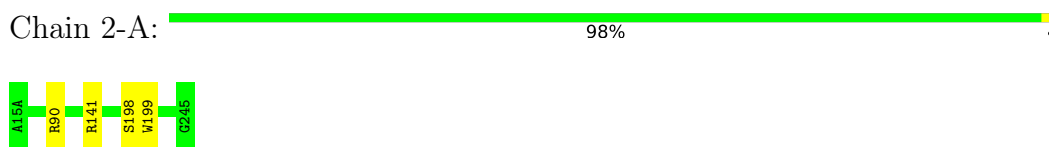
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

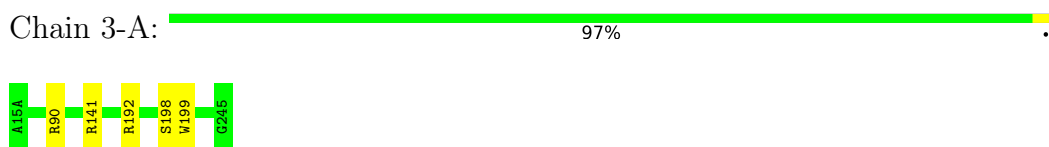
- Molecule 1: ALPHA-LYTIC PROTEASE



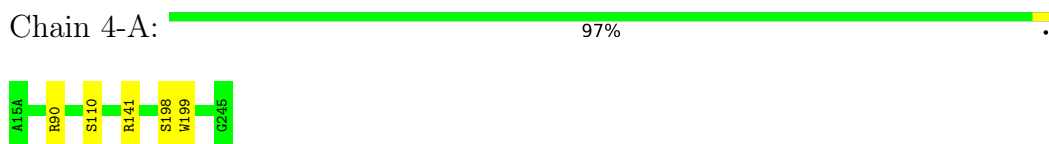
- Molecule 1: ALPHA-LYTIC PROTEASE



- Molecule 1: ALPHA-LYTIC PROTEASE



- Molecule 1: ALPHA-LYTIC PROTEASE



● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 5-A:  97%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 6-A:  98%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 7-A:  98%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 8-A:  98%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 9-A:  98%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 10-A:  98%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 11-A:  98%

● Molecule 1: ALPHA-LYTIC PROTEASE

Chain 12-A:  98% .



• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 13-A:  98% .



• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 14-A:  98% .



• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 15-A:  97% .



• Molecule 1: ALPHA-LYTIC PROTEASE

Chain 16-A:  98% .



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 65.80Å 79.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 1.50 6.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (6.00-1.50) 97.2 (6.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 1.48Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.165 , 0.192 0.500 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	5.5	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.05 , 2.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.48	EDS
Total number of atoms	27440	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: TAM, 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	1-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	2-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	3-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	4-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	5-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	6-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	7-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	8-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	9-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	10-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	11-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	12-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	13-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	14-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	15-A	0.25	0/1409	0.52	1/1909 (0.1%)
1	16-A	0.25	0/1409	0.52	1/1909 (0.1%)
All	All	0.25	0/22544	0.52	16/30544 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	2-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	3-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	4-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	5-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	6-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	7-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	8-A	199	TRP	N-CA-C	-5.38	99.64	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	10-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	11-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	12-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	13-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	14-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	15-A	199	TRP	N-CA-C	-5.38	99.64	108.41
1	16-A	199	TRP	N-CA-C	-5.38	99.64	108.41

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	1-A	1391	0	1363	0	0
1	2-A	1391	0	1361	0	0
1	3-A	1391	0	1363	0	0
1	4-A	1391	0	1361	0	0
1	5-A	1391	0	1363	0	0
1	6-A	1391	0	1363	0	0
1	7-A	1391	0	1365	0	0
1	8-A	1391	0	1361	0	0
1	9-A	1391	0	1363	0	0
1	10-A	1391	0	1363	0	0
1	11-A	1391	0	1361	0	0
1	12-A	1391	0	1361	0	0
1	13-A	1391	0	1363	0	0
1	14-A	1391	0	1361	0	0
1	15-A	1391	0	1361	0	0
1	16-A	1391	0	1363	0	0
2	1-A	15	0	0	0	0
2	2-A	15	0	0	0	0
2	3-A	15	0	0	0	0
2	4-A	15	0	0	0	0
2	5-A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-A	15	0	0	0	0
2	7-A	15	0	0	0	0
2	8-A	15	0	0	0	0
2	9-A	15	0	0	0	0
2	10-A	15	0	0	0	0
2	11-A	15	0	0	0	0
2	12-A	15	0	0	0	0
2	13-A	15	0	0	0	0
2	14-A	15	0	0	0	0
2	15-A	15	0	0	0	0
2	16-A	15	0	0	0	0
3	1-A	8	0	8	4	0
3	2-A	8	0	8	4	0
3	3-A	8	0	8	4	0
3	4-A	8	0	8	4	0
3	5-A	8	0	8	4	0
3	6-A	8	0	8	4	0
3	7-A	8	0	8	4	0
3	8-A	8	0	8	4	0
3	9-A	8	0	8	4	0
3	10-A	8	0	8	4	0
3	11-A	8	0	8	4	0
3	12-A	8	0	8	4	0
3	13-A	8	0	8	4	0
3	14-A	8	0	8	4	0
3	15-A	8	0	8	4	0
3	16-A	8	0	8	4	0
4	1-A	301	0	0	4	0
4	2-A	301	0	0	4	0
4	3-A	301	0	0	4	0
4	4-A	301	0	0	4	0
4	5-A	301	0	0	4	0
4	6-A	301	0	0	4	0
4	7-A	301	0	0	4	0
4	8-A	301	0	0	4	0
4	9-A	301	0	0	4	0
4	10-A	301	0	0	4	0
4	11-A	301	0	0	4	0
4	12-A	301	0	0	4	0
4	13-A	301	0	0	4	0
4	14-A	301	0	0	4	0
4	15-A	301	0	0	4	0

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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	1-A	196/198 (99%)	183 (93%)	12 (6%)	1 (0%)	24	8
1	2-A	196/198 (99%)	184 (94%)	12 (6%)	0	100	100
1	3-A	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	8
1	4-A	196/198 (99%)	182 (93%)	13 (7%)	1 (0%)	24	8
1	5-A	196/198 (99%)	185 (94%)	10 (5%)	1 (0%)	24	8
1	6-A	196/198 (99%)	185 (94%)	11 (6%)	0	100	100
1	7-A	196/198 (99%)	180 (92%)	16 (8%)	0	100	100
1	8-A	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
1	9-A	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
1	10-A	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
1	11-A	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
1	12-A	196/198 (99%)	184 (94%)	12 (6%)	0	100	100
1	13-A	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
1	14-A	196/198 (99%)	184 (94%)	12 (6%)	0	100	100
1	15-A	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	8
1	16-A	196/198 (99%)	183 (93%)	13 (7%)	0	100	100
All	All	3136/3168 (99%)	2952 (94%)	179 (6%)	5 (0%)	43	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	5-A	110	SER
1	15-A	67	GLY
1	4-A	110	SER
1	3-A	192	ARG
1	1-A	59(B)	VAL

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	1-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	2-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	3-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	4-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	5-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	6-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	7-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	8-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	9-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	10-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	11-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	12-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	13-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	14-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	15-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
1	16-A	142/142 (100%)	139 (98%)	3 (2%)	47	19
All	All	2272/2272 (100%)	2224 (98%)	48 (2%)	47	19

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	90	ARG
1	1-A	141	ARG
1	1-A	198	SER
1	2-A	90	ARG
1	2-A	141	ARG
1	2-A	198	SER
1	3-A	90	ARG
1	3-A	141	ARG
1	3-A	198	SER
1	4-A	90	ARG
1	4-A	141	ARG
1	4-A	198	SER
1	5-A	90	ARG
1	5-A	141	ARG

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Mol	Chain	Res	Type
1	5-A	198	SER
1	6-A	90	ARG
1	6-A	141	ARG
1	6-A	198	SER
1	7-A	90	ARG
1	7-A	141	ARG
1	7-A	198	SER
1	8-A	90	ARG
1	8-A	141	ARG
1	8-A	198	SER
1	9-A	90	ARG
1	9-A	141	ARG
1	9-A	198	SER
1	10-A	90	ARG
1	10-A	141	ARG
1	10-A	198	SER
1	11-A	90	ARG
1	11-A	141	ARG
1	11-A	198	SER
1	12-A	90	ARG
1	12-A	141	ARG
1	12-A	198	SER
1	13-A	90	ARG
1	13-A	141	ARG
1	13-A	198	SER
1	14-A	90	ARG
1	14-A	141	ARG
1	14-A	198	SER
1	15-A	90	ARG
1	15-A	141	ARG
1	15-A	198	SER
1	16-A	90	ARG
1	16-A	141	ARG
1	16-A	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	101	ASN
1	1-A	166	ASN
1	1-A	219(B)	ASN
1	2-A	60	ASN

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Mol	Chain	Res	Type
1	2-A	101	ASN
1	2-A	120(D)	ASN
1	2-A	166	ASN
1	2-A	170	ASN
1	3-A	101	ASN
1	3-A	112	GLN
1	3-A	166	ASN
1	3-A	170	ASN
1	4-A	60	ASN
1	4-A	101	ASN
1	4-A	112	GLN
1	4-A	166	ASN
1	5-A	60	ASN
1	5-A	101	ASN
1	5-A	112	GLN
1	5-A	166	ASN
1	5-A	208	GLN
1	6-A	38	ASN
1	6-A	60	ASN
1	6-A	101	ASN
1	6-A	112	GLN
1	6-A	166	ASN
1	6-A	170	ASN
1	7-A	38	ASN
1	7-A	60	ASN
1	7-A	101	ASN
1	7-A	112	GLN
1	7-A	120(D)	ASN
1	8-A	101	ASN
1	8-A	112	GLN
1	8-A	120(D)	ASN
1	8-A	219	GLN
1	9-A	60	ASN
1	9-A	101	ASN
1	9-A	166	ASN
1	9-A	182	GLN
1	10-A	60	ASN
1	10-A	101	ASN
1	10-A	112	GLN
1	10-A	166	ASN
1	11-A	101	ASN
1	11-A	112	GLN

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Mol	Chain	Res	Type
1	11-A	158	GLN
1	11-A	166	ASN
1	12-A	60	ASN
1	12-A	101	ASN
1	12-A	112	GLN
1	12-A	166	ASN
1	13-A	60	ASN
1	13-A	101	ASN
1	13-A	112	GLN
1	13-A	166	ASN
1	13-A	170	ASN
1	13-A	223	GLN
1	14-A	60	ASN
1	14-A	101	ASN
1	14-A	112	GLN
1	14-A	166	ASN
1	15-A	101	ASN
1	15-A	120(D)	ASN
1	15-A	166	ASN
1	15-A	182	GLN
1	16-A	60	ASN
1	16-A	120(D)	ASN
1	16-A	166	ASN
1	16-A	232	GLN

5.3.3 RNA [i](#)

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](#)

64 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	11-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	5-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	7-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	1-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	7-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
3	TAM	5-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	10-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	8-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	15-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	12-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	6-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	10-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	14-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	12-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	13-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	3-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
3	TAM	2-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	2-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	11-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	8-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	3-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	6-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
3	TAM	13-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
3	TAM	15-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
3	TAM	1-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	4-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	3-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	15-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	9-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAM	4-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	6-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	3-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	15-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	13-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	8-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	7-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	9-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	1-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	16-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	11-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	2-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	4-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	2-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	12-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	13-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
2	SO4	5-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
3	TAM	14-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	12-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	16-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	10-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	10-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	14-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	14-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	5-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
3	TAM	11-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	4-A	3	-	4,4,4	1.55	1 (25%)	6,6,6	0.95	0
2	SO4	16-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	7-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	1-A	4	-	4,4,4	1.51	1 (25%)	6,6,6	5.55	5 (83%)
3	TAM	9-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)
2	SO4	6-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	9-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
2	SO4	8-A	2	-	4,4,4	0.99	0	6,6,6	2.48	2 (33%)
3	TAM	16-A	1	-	7,7,10	2.12	4 (57%)	6,9,12	5.88	4 (66%)

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
3	TAM	6-A	1	-	-	3/9/9/12	-
3	TAM	15-A	1	-	-	3/9/9/12	-
3	TAM	1-A	1	-	-	3/9/9/12	-
3	TAM	12-A	1	-	-	3/9/9/12	-
3	TAM	3-A	1	-	-	3/9/9/12	-
3	TAM	5-A	1	-	-	3/9/9/12	-
3	TAM	11-A	1	-	-	3/9/9/12	-
3	TAM	4-A	1	-	-	3/9/9/12	-
3	TAM	14-A	1	-	-	3/9/9/12	-
3	TAM	7-A	1	-	-	3/9/9/12	-
3	TAM	9-A	1	-	-	3/9/9/12	-
3	TAM	10-A	1	-	-	3/9/9/12	-
3	TAM	2-A	1	-	-	3/9/9/12	-
3	TAM	13-A	1	-	-	3/9/9/12	-
3	TAM	16-A	1	-	-	3/9/9/12	-
3	TAM	8-A	1	-	-	3/9/9/12	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	2-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	3-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	4-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	5-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	6-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	7-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	8-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	9-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	10-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	11-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	12-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	13-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	14-A	1	TAM	C5-C2	-2.88	1.40	1.51
3	15-A	1	TAM	C5-C2	-2.88	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-A	1	TAM	C5-C2	-2.88	1.40	1.51
2	1-A	3	SO4	O1-S	2.67	1.60	1.44
2	2-A	3	SO4	O1-S	2.67	1.60	1.44
2	3-A	3	SO4	O1-S	2.67	1.60	1.44
2	4-A	3	SO4	O1-S	2.67	1.60	1.44
2	5-A	3	SO4	O1-S	2.67	1.60	1.44
2	6-A	3	SO4	O1-S	2.67	1.60	1.44
2	7-A	3	SO4	O1-S	2.67	1.60	1.44
2	8-A	3	SO4	O1-S	2.67	1.60	1.44
2	9-A	3	SO4	O1-S	2.67	1.60	1.44
2	10-A	3	SO4	O1-S	2.67	1.60	1.44
2	11-A	3	SO4	O1-S	2.67	1.60	1.44
2	12-A	3	SO4	O1-S	2.67	1.60	1.44
2	13-A	3	SO4	O1-S	2.67	1.60	1.44
2	14-A	3	SO4	O1-S	2.67	1.60	1.44
2	15-A	3	SO4	O1-S	2.67	1.60	1.44
2	16-A	3	SO4	O1-S	2.67	1.60	1.44
3	1-A	1	TAM	C-N	-2.58	1.41	1.49
3	2-A	1	TAM	C-N	-2.58	1.41	1.49
3	3-A	1	TAM	C-N	-2.58	1.41	1.49
3	4-A	1	TAM	C-N	-2.58	1.41	1.49
3	5-A	1	TAM	C-N	-2.58	1.41	1.49
3	6-A	1	TAM	C-N	-2.58	1.41	1.49
3	7-A	1	TAM	C-N	-2.58	1.41	1.49
3	8-A	1	TAM	C-N	-2.58	1.41	1.49
3	9-A	1	TAM	C-N	-2.58	1.41	1.49
3	10-A	1	TAM	C-N	-2.58	1.41	1.49
3	11-A	1	TAM	C-N	-2.58	1.41	1.49
3	12-A	1	TAM	C-N	-2.58	1.41	1.49
3	13-A	1	TAM	C-N	-2.58	1.41	1.49
3	14-A	1	TAM	C-N	-2.58	1.41	1.49
3	15-A	1	TAM	C-N	-2.58	1.41	1.49
3	16-A	1	TAM	C-N	-2.58	1.41	1.49
3	1-A	1	TAM	C2-C	-2.55	1.49	1.53
3	2-A	1	TAM	C2-C	-2.55	1.49	1.53
3	3-A	1	TAM	C2-C	-2.55	1.49	1.53
3	4-A	1	TAM	C2-C	-2.55	1.49	1.53
3	5-A	1	TAM	C2-C	-2.55	1.49	1.53
3	6-A	1	TAM	C2-C	-2.55	1.49	1.53
3	7-A	1	TAM	C2-C	-2.55	1.49	1.53
3	8-A	1	TAM	C2-C	-2.55	1.49	1.53
3	9-A	1	TAM	C2-C	-2.55	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-A	1	TAM	C2-C	-2.55	1.49	1.53
3	11-A	1	TAM	C2-C	-2.55	1.49	1.53
3	12-A	1	TAM	C2-C	-2.55	1.49	1.53
3	13-A	1	TAM	C2-C	-2.55	1.49	1.53
3	14-A	1	TAM	C2-C	-2.55	1.49	1.53
3	15-A	1	TAM	C2-C	-2.55	1.49	1.53
3	16-A	1	TAM	C2-C	-2.55	1.49	1.53
3	1-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	2-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	3-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	4-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	5-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	6-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	7-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	8-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	9-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	10-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	11-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	12-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	13-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	14-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	15-A	1	TAM	C6-C3	-2.46	1.41	1.51
3	16-A	1	TAM	C6-C3	-2.46	1.41	1.51
2	1-A	4	SO4	O2-S	-2.05	1.32	1.44
2	2-A	4	SO4	O2-S	-2.05	1.32	1.44
2	3-A	4	SO4	O2-S	-2.05	1.32	1.44
2	4-A	4	SO4	O2-S	-2.05	1.32	1.44
2	5-A	4	SO4	O2-S	-2.05	1.32	1.44
2	6-A	4	SO4	O2-S	-2.05	1.32	1.44
2	7-A	4	SO4	O2-S	-2.05	1.32	1.44
2	8-A	4	SO4	O2-S	-2.05	1.32	1.44
2	9-A	4	SO4	O2-S	-2.05	1.32	1.44
2	10-A	4	SO4	O2-S	-2.05	1.32	1.44
2	11-A	4	SO4	O2-S	-2.05	1.32	1.44
2	12-A	4	SO4	O2-S	-2.05	1.32	1.44
2	13-A	4	SO4	O2-S	-2.05	1.32	1.44
2	14-A	4	SO4	O2-S	-2.05	1.32	1.44
2	15-A	4	SO4	O2-S	-2.05	1.32	1.44
2	16-A	4	SO4	O2-S	-2.05	1.32	1.44

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	2-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	3-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	4-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	5-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	6-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	7-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	8-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	9-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	10-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	11-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	12-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	13-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	14-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	15-A	1	TAM	C3-C-C1	12.62	134.15	110.67
3	16-A	1	TAM	C3-C-C1	12.62	134.15	110.67
2	1-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	2-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	3-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	4-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	5-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	6-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	7-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	8-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	9-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	10-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	11-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	12-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	13-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	14-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	15-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	16-A	4	SO4	O3-S-O1	-10.30	55.72	109.56
2	1-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	2-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	3-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	4-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	5-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	6-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	7-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	8-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	9-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	10-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	11-A	4	SO4	O4-S-O1	7.65	149.53	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	13-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	14-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	15-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	16-A	4	SO4	O4-S-O1	7.65	149.53	109.56
2	1-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	2-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	3-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	4-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	5-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	6-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	7-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	8-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	9-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	10-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	11-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	12-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	13-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	14-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	15-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
2	16-A	2	SO4	O3-S-O1	-4.73	84.85	109.56
3	1-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	2-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	3-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	4-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	5-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	6-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	7-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	8-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	9-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	10-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	11-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	12-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	13-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	14-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	15-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	16-A	1	TAM	C3-C-C2	-4.56	102.20	110.67
3	1-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	2-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	3-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	4-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	5-A	1	TAM	C1-C-N	-4.38	97.09	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	7-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	8-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	9-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	10-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	11-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	12-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	13-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	14-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	15-A	1	TAM	C1-C-N	-4.38	97.09	108.22
3	16-A	1	TAM	C1-C-N	-4.38	97.09	108.22
2	1-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	2-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	3-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	4-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	5-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	6-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	7-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	8-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	9-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	10-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	11-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	12-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	13-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	14-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	15-A	2	SO4	O3-S-O2	3.19	126.26	109.56
2	16-A	2	SO4	O3-S-O2	3.19	126.26	109.56
3	1-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	2-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	3-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	4-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	5-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	6-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	7-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	8-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	9-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	10-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	11-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	12-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	13-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	14-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
3	15-A	1	TAM	C1-C-C2	-2.80	105.47	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	16-A	1	TAM	C1-C-C2	-2.80	105.47	110.67
2	1-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	2-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	3-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	4-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	5-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	6-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	7-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	8-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	9-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	10-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	11-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	12-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	13-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	14-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	15-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	16-A	4	SO4	O3-S-O2	2.78	124.11	109.56
2	1-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	2-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	3-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	4-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	5-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	6-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	7-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	8-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	9-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	10-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	11-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	12-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	13-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	14-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	15-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	16-A	4	SO4	O2-S-O1	-2.58	90.91	109.06
2	1-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	2-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	3-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	4-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	5-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	6-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	7-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	8-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	9-A	4	SO4	O4-S-O3	2.43	121.95	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	11-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	12-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	13-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	14-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	15-A	4	SO4	O4-S-O3	2.43	121.95	108.54
2	16-A	4	SO4	O4-S-O3	2.43	121.95	108.54

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1-A	1	TAM	C2-C-C1-C4
3	1-A	1	TAM	C3-C-C1-C4
3	1-A	1	TAM	N-C-C1-C4
3	2-A	1	TAM	C2-C-C1-C4
3	2-A	1	TAM	C3-C-C1-C4
3	2-A	1	TAM	N-C-C1-C4
3	3-A	1	TAM	C2-C-C1-C4
3	3-A	1	TAM	C3-C-C1-C4
3	3-A	1	TAM	N-C-C1-C4
3	4-A	1	TAM	C2-C-C1-C4
3	4-A	1	TAM	C3-C-C1-C4
3	4-A	1	TAM	N-C-C1-C4
3	5-A	1	TAM	C2-C-C1-C4
3	5-A	1	TAM	C3-C-C1-C4
3	5-A	1	TAM	N-C-C1-C4
3	6-A	1	TAM	C2-C-C1-C4
3	6-A	1	TAM	C3-C-C1-C4
3	6-A	1	TAM	N-C-C1-C4
3	7-A	1	TAM	C2-C-C1-C4
3	7-A	1	TAM	C3-C-C1-C4
3	7-A	1	TAM	N-C-C1-C4
3	8-A	1	TAM	C2-C-C1-C4
3	8-A	1	TAM	C3-C-C1-C4
3	8-A	1	TAM	N-C-C1-C4
3	9-A	1	TAM	C2-C-C1-C4
3	9-A	1	TAM	C3-C-C1-C4
3	9-A	1	TAM	N-C-C1-C4
3	10-A	1	TAM	C2-C-C1-C4
3	10-A	1	TAM	C3-C-C1-C4
3	10-A	1	TAM	N-C-C1-C4

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Mol	Chain	Res	Type	Atoms
3	11-A	1	TAM	C2-C-C1-C4
3	11-A	1	TAM	C3-C-C1-C4
3	11-A	1	TAM	N-C-C1-C4
3	12-A	1	TAM	C2-C-C1-C4
3	12-A	1	TAM	C3-C-C1-C4
3	12-A	1	TAM	N-C-C1-C4
3	13-A	1	TAM	C2-C-C1-C4
3	13-A	1	TAM	C3-C-C1-C4
3	13-A	1	TAM	N-C-C1-C4
3	14-A	1	TAM	C2-C-C1-C4
3	14-A	1	TAM	C3-C-C1-C4
3	14-A	1	TAM	N-C-C1-C4
3	15-A	1	TAM	C2-C-C1-C4
3	15-A	1	TAM	C3-C-C1-C4
3	15-A	1	TAM	N-C-C1-C4
3	16-A	1	TAM	C2-C-C1-C4
3	16-A	1	TAM	C3-C-C1-C4
3	16-A	1	TAM	N-C-C1-C4

There are no ring outliers.

16 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	5-A	1	TAM	4	0
3	10-A	1	TAM	4	0
3	12-A	1	TAM	4	0
3	2-A	1	TAM	4	0
3	8-A	1	TAM	4	0
3	6-A	1	TAM	4	0
3	13-A	1	TAM	4	0
3	15-A	1	TAM	4	0
3	1-A	1	TAM	4	0
3	3-A	1	TAM	4	0
3	4-A	1	TAM	4	0
3	14-A	1	TAM	4	0
3	11-A	1	TAM	4	0
3	7-A	1	TAM	4	0
3	9-A	1	TAM	4	0
3	16-A	1	TAM	4	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	1-A	198/198 (100%)	13.31	198 (100%) 0 0	0, 0, 0, 0	198 (100%)
1	2-A	0/198	-	-	-	-
1	3-A	0/198	-	-	-	-
1	4-A	0/198	-	-	-	-
1	5-A	0/198	-	-	-	-
1	6-A	0/198	-	-	-	-
1	7-A	0/198	-	-	-	-
1	8-A	0/198	-	-	-	-
1	9-A	0/198	-	-	-	-
1	10-A	0/198	-	-	-	-
1	11-A	0/198	-	-	-	-
1	12-A	0/198	-	-	-	-
1	13-A	0/198	-	-	-	-
1	14-A	0/198	-	-	-	-
1	15-A	0/198	-	-	-	-
1	16-A	0/198	-	-	-	-
All	All	198/3168 (6%)	13.31	198 (100%) 0 0	0, 0, 0, 0	198 (100%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	218	VAL	35.6
1	1-A	59(B)	VAL	34.1
1	1-A	60	ASN	29.4
1	1-A	111	ALA	26.5
1	1-A	178	ARG	25.2
1	1-A	162	ILE	22.4
1	1-A	120(H)	SER	22.3
1	1-A	168	THR	21.1
1	1-A	94	PHE	21.0
1	1-A	161	THR	20.5
1	1-A	106	VAL	20.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	41	LEU	20.1
1	1-A	104	ALA	20.0
1	1-A	222(A)	PRO	19.9
1	1-A	88	PHE	19.7
1	1-A	44	VAL	19.0
1	1-A	35	ILE	19.0
1	1-A	167	VAL	18.8
1	1-A	47	VAL	18.7
1	1-A	200	ILE	18.7
1	1-A	136	VAL	18.5
1	1-A	120(E)	GLY	18.1
1	1-A	45	PHE	18.1
1	1-A	109	THR	18.0
1	1-A	82	ALA	17.6
1	1-A	16	ILE	17.5
1	1-A	108	LEU	17.3
1	1-A	199	TRP	17.1
1	1-A	112	GLN	16.8
1	1-A	163	THR	16.6
1	1-A	219(B)	ASN	16.6
1	1-A	219	GLN	16.5
1	1-A	105	TRP	16.4
1	1-A	201(A)	SER	16.3
1	1-A	209	ALA	16.3
1	1-A	171	TYR	16.3
1	1-A	52	PHE	16.3
1	1-A	66	ILE	16.2
1	1-A	231	LEU	16.2
1	1-A	91	VAL	16.1
1	1-A	87	THR	16.1
1	1-A	119	LEU	16.1
1	1-A	189	CYS	16.0
1	1-A	19	GLY	16.0
1	1-A	120(B)	VAL	16.0
1	1-A	39	ALA	15.9
1	1-A	120(K)	THR	15.6
1	1-A	31	ILE	15.6
1	1-A	59	GLY	15.5
1	1-A	222(B)	ALA	15.4
1	1-A	53	VAL	15.2
1	1-A	54	THR	15.1
1	1-A	169	ALA	15.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	234	ILE	15.0
1	1-A	59(A)	THR	15.0
1	1-A	235	LEU	14.9
1	1-A	238	TYR	14.9
1	1-A	55	ALA	14.9
1	1-A	192	ARG	14.8
1	1-A	202	ALA	14.8
1	1-A	183	GLY	14.8
1	1-A	131	ALA	14.8
1	1-A	228	PHE	14.7
1	1-A	236	SER	14.7
1	1-A	237	GLN	14.7
1	1-A	226	SER	14.6
1	1-A	222	ILE	14.5
1	1-A	207	GLY	14.5
1	1-A	143	THR	14.4
1	1-A	15(A)	ALA	14.2
1	1-A	17	VAL	14.1
1	1-A	227	LEU	14.1
1	1-A	135	ALA	14.0
1	1-A	177	VAL	14.0
1	1-A	243	VAL	13.9
1	1-A	196	GLY	13.9
1	1-A	134	ALA	13.9
1	1-A	242	LEU	13.7
1	1-A	222(C)	SER	13.7
1	1-A	244	THR	13.6
1	1-A	120(C)	ALA	13.6
1	1-A	32	GLU	13.5
1	1-A	95	PRO	13.5
1	1-A	176	ALA	13.4
1	1-A	239	GLY	13.4
1	1-A	81	GLY	13.4
1	1-A	181	THR	13.4
1	1-A	61	ALA	13.4
1	1-A	83	VAL	13.3
1	1-A	225	SER	13.1
1	1-A	182	GLN	13.1
1	1-A	90	ARG	13.0
1	1-A	166	ASN	13.0
1	1-A	42	CYS	13.0
1	1-A	46	SER	13.0

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Mol	Chain	Res	Type	RSRZ
1	1-A	137	CYS	13.0
1	1-A	84	VAL	12.9
1	1-A	58	CYS	12.9
1	1-A	89	ALA	12.9
1	1-A	157	TYR	12.9
1	1-A	240	LEU	12.9
1	1-A	212	VAL	12.7
1	1-A	220(A)	CYS	12.7
1	1-A	197	GLY	12.6
1	1-A	180	LEU	12.6
1	1-A	120(I)	PHE	12.5
1	1-A	179	GLY	12.4
1	1-A	141	ARG	12.2
1	1-A	140	GLY	12.1
1	1-A	48	THR	12.0
1	1-A	48(C)	ALA	12.0
1	1-A	139	SER	12.0
1	1-A	195	SER	12.0
1	1-A	33	TYR	11.9
1	1-A	191	GLY	11.9
1	1-A	50	LYS	11.8
1	1-A	120(D)	ASN	11.7
1	1-A	120(J)	VAL	11.7
1	1-A	216	GLY	11.7
1	1-A	221	GLY	11.6
1	1-A	194	ASP	11.5
1	1-A	100	GLY	11.5
1	1-A	184	ASN	11.5
1	1-A	232	GLN	11.5
1	1-A	210	GLN	11.3
1	1-A	113	THR	11.3
1	1-A	233	PRO	11.3
1	1-A	18	GLY	11.2
1	1-A	120	PRO	11.2
1	1-A	201	THR	11.2
1	1-A	38	ASN	11.1
1	1-A	223	GLN	11.1
1	1-A	88(A)	ALA	11.0
1	1-A	64	ALA	10.9
1	1-A	198	SER	10.9
1	1-A	241	SER	10.8
1	1-A	34	SER	10.7

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Mol	Chain	Res	Type	RSRZ
1	1-A	132	VAL	10.7
1	1-A	120(A)	ARG	10.7
1	1-A	229	GLU	10.6
1	1-A	170	ASN	10.6
1	1-A	219(A)	SER	10.6
1	1-A	164	ALA	10.5
1	1-A	121	VAL	10.4
1	1-A	185	ALA	10.4
1	1-A	56	GLY	10.3
1	1-A	67	GLY	10.3
1	1-A	40	SER	10.3
1	1-A	175	GLY	10.3
1	1-A	125	THR	10.2
1	1-A	36	ASN	10.2
1	1-A	158	GLN	10.1
1	1-A	114	LEU	10.1
1	1-A	142	THR	10.0
1	1-A	193	GLY	9.9
1	1-A	219(D)	ASN	9.9
1	1-A	49	THR	9.8
1	1-A	62	THR	9.8
1	1-A	110	SER	9.7
1	1-A	130	ALA	9.7
1	1-A	48(B)	GLY	9.6
1	1-A	43	SER	9.6
1	1-A	211	GLY	9.6
1	1-A	120(G)	SER	9.6
1	1-A	138	ARG	9.6
1	1-A	173	ALA	9.3
1	1-A	85	GLY	9.3
1	1-A	102	ASP	9.3
1	1-A	159	CYS	9.3
1	1-A	217	ASN	9.3
1	1-A	224	ARG	9.1
1	1-A	57	HIS	9.1
1	1-A	213	MET	9.0
1	1-A	48(A)	ARG	8.9
1	1-A	129	GLU	8.9
1	1-A	230	ARG	8.8
1	1-A	44(A)	GLY	8.8
1	1-A	156	GLY	8.7
1	1-A	51	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	133	GLY	8.4
1	1-A	103	ARG	8.4
1	1-A	124	SER	8.4
1	1-A	214	SER	8.3
1	1-A	101	ASN	8.3
1	1-A	245	GLY	8.3
1	1-A	190	MET	8.2
1	1-A	123	GLY	8.2
1	1-A	122	ARG	8.1
1	1-A	15(B)	ASN	8.1
1	1-A	107	SER	8.1
1	1-A	220	ASN	8.0
1	1-A	208	GLN	7.7
1	1-A	219(C)	GLY	7.2
1	1-A	215	GLY	7.1
1	1-A	165	LYS	6.6
1	1-A	65	ARG	6.4
1	1-A	160	GLY	6.3
1	1-A	174	GLU	6.3

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 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(Å ²)	Q<0.9
3	TAM	1-A	1	8/11	0.75	0.16	7,8,10,11	8
2	SO4	2-A	2	5/5	-	-	9,9,10,10	5
2	SO4	3-A	2	5/5	-	-	9,9,10,10	5
2	SO4	4-A	2	5/5	-	-	9,9,10,10	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	5-A	2	5/5	-	-	9,9,10,10	5
2	SO4	6-A	2	5/5	-	-	9,9,10,10	5
2	SO4	7-A	2	5/5	-	-	9,9,10,10	5
2	SO4	8-A	2	5/5	-	-	9,9,10,10	5
2	SO4	9-A	2	5/5	-	-	9,9,10,10	5
2	SO4	10-A	2	5/5	-	-	9,9,10,10	5
2	SO4	11-A	2	5/5	-	-	9,9,10,10	5
2	SO4	12-A	2	5/5	-	-	9,9,10,10	5
2	SO4	13-A	2	5/5	-	-	9,9,10,10	5
2	SO4	14-A	2	5/5	-	-	9,9,10,10	5
2	SO4	15-A	2	5/5	-	-	9,9,10,10	5
2	SO4	16-A	2	5/5	-	-	9,9,10,10	5
2	SO4	1-A	4	5/5	0.83	0.23	18,18,19,19	5
2	SO4	2-A	3	5/5	-	-	6,6,6,7	5
2	SO4	3-A	3	5/5	-	-	6,6,6,7	5
2	SO4	4-A	3	5/5	-	-	6,6,6,7	5
2	SO4	5-A	3	5/5	-	-	6,6,6,7	5
2	SO4	6-A	3	5/5	-	-	6,6,6,7	5
2	SO4	7-A	3	5/5	-	-	6,6,6,7	5
2	SO4	8-A	3	5/5	-	-	6,6,6,7	5
2	SO4	9-A	3	5/5	-	-	6,6,6,7	5
2	SO4	10-A	3	5/5	-	-	6,6,6,7	5
2	SO4	11-A	3	5/5	-	-	6,6,6,7	5
2	SO4	12-A	3	5/5	-	-	6,6,6,7	5
2	SO4	13-A	3	5/5	-	-	6,6,6,7	5
2	SO4	14-A	3	5/5	-	-	6,6,6,7	5
2	SO4	15-A	3	5/5	-	-	6,6,6,7	5
2	SO4	16-A	3	5/5	-	-	6,6,6,7	5
2	SO4	1-A	2	5/5	0.91	0.10	9,9,10,10	5
2	SO4	2-A	4	5/5	-	-	18,18,19,19	5
2	SO4	3-A	4	5/5	-	-	18,18,19,19	5
2	SO4	4-A	4	5/5	-	-	18,18,19,19	5
2	SO4	5-A	4	5/5	-	-	18,18,19,19	5
2	SO4	6-A	4	5/5	-	-	18,18,19,19	5
2	SO4	7-A	4	5/5	-	-	18,18,19,19	5
2	SO4	8-A	4	5/5	-	-	18,18,19,19	5
2	SO4	9-A	4	5/5	-	-	18,18,19,19	5
2	SO4	10-A	4	5/5	-	-	18,18,19,19	5
2	SO4	11-A	4	5/5	-	-	18,18,19,19	5
2	SO4	12-A	4	5/5	-	-	18,18,19,19	5
2	SO4	13-A	4	5/5	-	-	18,18,19,19	5
2	SO4	14-A	4	5/5	-	-	18,18,19,19	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	15-A	4	5/5	-	-	18,18,19,19	5
2	SO4	16-A	4	5/5	-	-	18,18,19,19	5
2	SO4	1-A	3	5/5	0.99	0.11	6,6,6,7	5
3	TAM	2-A	1	8/11	-	-	7,8,10,11	8
3	TAM	3-A	1	8/11	-	-	7,8,10,11	8
3	TAM	4-A	1	8/11	-	-	7,8,10,11	8
3	TAM	5-A	1	8/11	-	-	7,8,10,11	8
3	TAM	6-A	1	8/11	-	-	7,8,10,11	8
3	TAM	7-A	1	8/11	-	-	7,8,10,11	8
3	TAM	8-A	1	8/11	-	-	7,8,10,11	8
3	TAM	9-A	1	8/11	-	-	7,8,10,11	8
3	TAM	10-A	1	8/11	-	-	7,8,10,11	8
3	TAM	11-A	1	8/11	-	-	7,8,10,11	8
3	TAM	12-A	1	8/11	-	-	7,8,10,11	8
3	TAM	13-A	1	8/11	-	-	7,8,10,11	8
3	TAM	14-A	1	8/11	-	-	7,8,10,11	8
3	TAM	15-A	1	8/11	-	-	7,8,10,11	8
3	TAM	16-A	1	8/11	-	-	7,8,10,11	8

6.5 Other polymers [i](#)

There are no such residues in this entry.