



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:51 PM UTC

PDB ID : 1NH7 / pdb_00001nh7
Title : ATP PHOSPHORIBOSYLTRANSFERASE (ATP-PRTASE) FROM MYCOBACTERIUM TUBERCULOSIS
Authors : Cho, Y.; Sharma, V.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2002-12-18
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

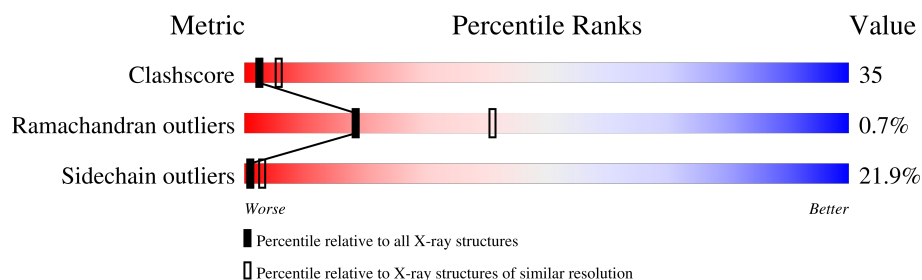
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	23% 37% 24% 6% 10%

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	A	1001	-	-	X	-
2	SO4	A	1004	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2272 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 ATP Phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2073	1306	368	391	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	HIS	-	expression tag	UNP P60759
A	-18	SER	-	expression tag	UNP P60759
A	-17	GLY	-	expression tag	UNP P60759
A	-16	ARG	-	expression tag	UNP P60759
A	-15	PRO	-	expression tag	UNP P60759
A	-14	VAL	-	expression tag	UNP P60759
A	-13	LEU	-	expression tag	UNP P60759
A	-12	GLY	-	expression tag	UNP P60759
A	-11	SER	-	expression tag	UNP P60759
A	-10	SER	-	expression tag	UNP P60759
A	-9	HIS	-	expression tag	UNP P60759
A	-8	HIS	-	expression tag	UNP P60759
A	-7	HIS	-	expression tag	UNP P60759
A	-6	HIS	-	expression tag	UNP P60759
A	-5	HIS	-	expression tag	UNP P60759
A	-4	HIS	-	expression tag	UNP P60759
A	-3	SER	-	expression tag	UNP P60759
A	-2	SER	-	expression tag	UNP P60759
A	-1	GLY	-	expression tag	UNP P60759
A	0	MET	-	expression tag	UNP P60759

- Molecule 2 is SULFATE ION (CCD ID: 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		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

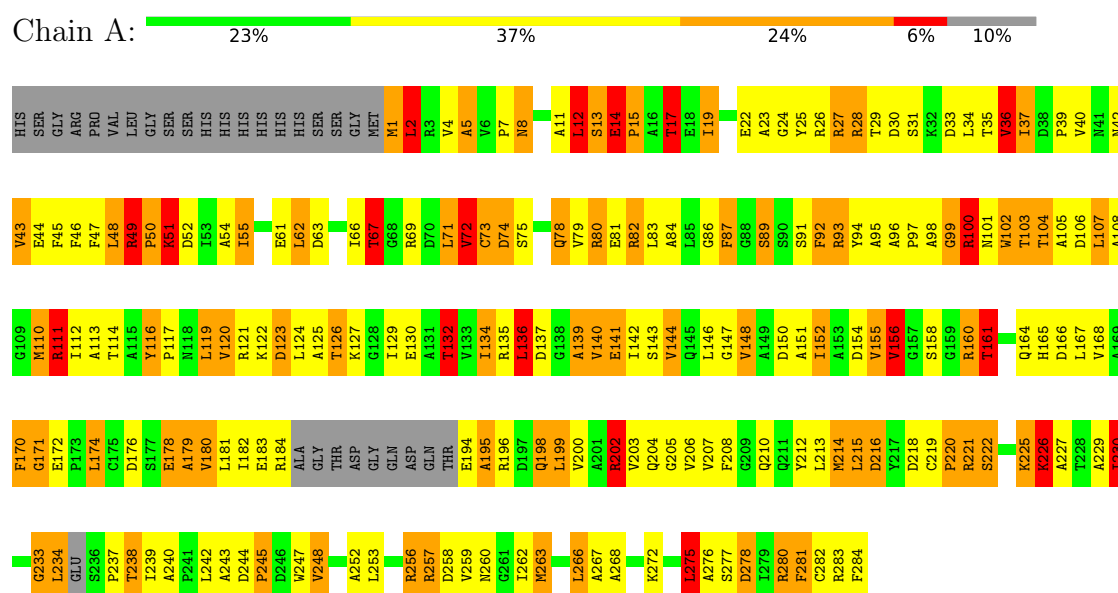
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: ATP Phosphoribosyltransferase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	132.54Å 132.54Å 110.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.74 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (27.74-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.192 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2272	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	2.75	151/2104 (7.2%)	2.28	109/2852 (3.8%)

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ALA	CA-CB	-12.18	1.36	1.53
1	A	81	GLU	C-O	-11.68	1.09	1.23
1	A	263	MET	SD-CE	-10.63	1.52	1.79
1	A	147	GLY	C-O	-10.41	1.09	1.23
1	A	239	ILE	C-O	-10.18	1.13	1.24
1	A	179	ALA	CA-CB	-10.08	1.36	1.53
1	A	11	ALA	CA-CB	-10.01	1.35	1.53
1	A	277	SER	C-O	-9.82	1.12	1.23
1	A	111	ARG	NE-CZ	9.79	1.43	1.33
1	A	113	ALA	CA-CB	-9.78	1.36	1.53
1	A	229	ALA	CA-C	9.46	1.66	1.52
1	A	71	LEU	C-O	-9.17	1.13	1.24
1	A	229	ALA	CA-CB	-9.07	1.37	1.53
1	A	11	ALA	C-O	-8.76	1.12	1.24
1	A	240	ALA	CA-CB	-8.70	1.42	1.53
1	A	4	VAL	CA-CB	8.64	1.65	1.54
1	A	257	ARG	CZ-NH1	8.61	1.44	1.32
1	A	282	CYS	CA-C	-8.41	1.42	1.52
1	A	14	GLU	C-O	-8.41	1.16	1.24
1	A	19	ILE	N-CA	-8.17	1.37	1.46
1	A	51	LYS	CE-NZ	-8.16	1.24	1.49
1	A	195	ALA	CA-CB	-8.09	1.39	1.53
1	A	66	ILE	CA-CB	8.09	1.64	1.54
1	A	207	VAL	CA-C	7.89	1.62	1.52
1	A	144	VAL	CA-CB	7.78	1.63	1.54
1	A	283	ARG	C-O	7.73	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ASP	N-CA	-7.73	1.37	1.46
1	A	203	VAL	C-O	-7.72	1.14	1.24
1	A	72	VAL	CA-CB	-7.68	1.43	1.54
1	A	72	VAL	C-O	-7.68	1.14	1.24
1	A	82	ARG	NE-CZ	7.66	1.41	1.33
1	A	89	SER	N-CA	-7.59	1.36	1.46
1	A	226	LYS	CE-NZ	7.56	1.72	1.49
1	A	110	MET	CG-SD	7.53	1.99	1.80
1	A	230	ILE	C-O	-7.51	1.14	1.23
1	A	61	GLU	CD-OE1	7.47	1.39	1.25
1	A	230	ILE	CA-CB	7.43	1.65	1.54
1	A	135	ARG	C-O	-7.43	1.14	1.23
1	A	124	LEU	CA-C	7.42	1.62	1.52
1	A	55	ILE	N-CA	-7.42	1.38	1.46
1	A	238	THR	C-O	-7.41	1.14	1.23
1	A	170	PHE	N-CA	-7.25	1.37	1.46
1	A	114	THR	N-CA	-7.21	1.37	1.46
1	A	134	ILE	C-O	-7.21	1.16	1.24
1	A	112	ILE	CA-CB	7.20	1.63	1.54
1	A	257	ARG	CZ-NH2	7.17	1.42	1.33
1	A	28	ARG	C-O	-7.09	1.14	1.23
1	A	164	GLN	N-CA	-7.02	1.36	1.46
1	A	144	VAL	N-CA	-6.99	1.38	1.46
1	A	31	SER	CA-C	-6.97	1.43	1.52
1	A	140	VAL	C-O	-6.92	1.15	1.24
1	A	33	ASP	C-O	-6.92	1.15	1.23
1	A	113	ALA	CA-C	-6.85	1.44	1.52
1	A	233	GLY	C-O	-6.84	1.14	1.23
1	A	148	VAL	CA-CB	6.83	1.63	1.54
1	A	282	CYS	C-O	-6.80	1.15	1.23
1	A	80	ARG	NE-CZ	6.78	1.40	1.33
1	A	204	GLN	C-O	-6.78	1.16	1.24
1	A	226	LYS	CA-C	-6.76	1.44	1.52
1	A	243	ALA	CA-CB	-6.63	1.42	1.53
1	A	218	ASP	CA-C	6.56	1.60	1.52
1	A	114	THR	CA-C	-6.52	1.44	1.52
1	A	239	ILE	CA-C	-6.50	1.44	1.52
1	A	280	ARG	CB-CG	-6.49	1.32	1.52
1	A	156	VAL	C-O	6.49	1.31	1.23
1	A	284	PHE	CA-C	-6.41	1.39	1.52
1	A	49	ARG	C-O	-6.41	1.15	1.24
1	A	111	ARG	C-O	-6.41	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	PHE	C-O	6.38	1.32	1.23
1	A	284	PHE	CA-CB	-6.37	1.40	1.53
1	A	42	ASN	CA-C	-6.36	1.44	1.53
1	A	196	ARG	CA-C	6.33	1.61	1.52
1	A	214	MET	SD-CE	6.33	1.95	1.79
1	A	1	MET	SD-CE	6.32	1.95	1.79
1	A	43	VAL	CB-CG1	-6.30	1.31	1.52
1	A	11	ALA	N-CA	-6.24	1.38	1.46
1	A	52	ASP	CA-C	6.23	1.61	1.52
1	A	12	LEU	CA-C	-6.23	1.44	1.52
1	A	4	VAL	CA-C	6.21	1.60	1.52
1	A	238	THR	N-CA	-6.19	1.37	1.46
1	A	137	ASP	C-O	-6.18	1.15	1.24
1	A	108	ALA	C-O	6.16	1.31	1.24
1	A	67	THR	CA-C	-6.11	1.44	1.53
1	A	93	ARG	CA-C	-6.09	1.45	1.52
1	A	5	ALA	N-CA	6.09	1.53	1.46
1	A	202	ARG	CB-CG	-6.08	1.34	1.52
1	A	202	ARG	NE-CZ	-6.06	1.26	1.33
1	A	79	VAL	C-O	-6.06	1.17	1.23
1	A	83	LEU	C-O	-6.05	1.16	1.24
1	A	156	VAL	CA-C	-6.02	1.46	1.52
1	A	121	ARG	C-O	-6.01	1.17	1.24
1	A	281	PHE	C-O	-6.01	1.16	1.23
1	A	27	ARG	CZ-NH2	-6.00	1.25	1.33
1	A	161	THR	CA-CB	5.99	1.62	1.53
1	A	182	ILE	C-O	-5.95	1.16	1.24
1	A	267	ALA	CA-CB	-5.94	1.43	1.53
1	A	257	ARG	C-O	-5.93	1.16	1.24
1	A	199	LEU	C-O	-5.89	1.17	1.24
1	A	111	ARG	N-CA	-5.87	1.38	1.46
1	A	132	THR	N-CA	-5.87	1.39	1.46
1	A	151	ALA	CA-C	-5.86	1.45	1.52
1	A	28	ARG	CA-C	-5.83	1.45	1.52
1	A	72	VAL	CA-C	-5.83	1.44	1.52
1	A	120	VAL	N-CA	5.72	1.53	1.46
1	A	13	SER	CA-C	5.65	1.60	1.52
1	A	125	ALA	N-CA	-5.64	1.39	1.46
1	A	120	VAL	CA-CB	5.62	1.60	1.54
1	A	23	ALA	CA-CB	-5.61	1.44	1.53
1	A	200	VAL	N-CA	-5.58	1.39	1.46
1	A	116	TYR	CB-CG	-5.55	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	MET	CA-C	5.54	1.60	1.53
1	A	25	TYR	CA-C	5.51	1.60	1.52
1	A	257	ARG	NE-CZ	5.47	1.39	1.33
1	A	125	ALA	CA-CB	-5.47	1.44	1.53
1	A	116	TYR	CA-CB	-5.44	1.46	1.53
1	A	14	GLU	CD-OE2	5.43	1.35	1.25
1	A	152	ILE	CA-CB	5.42	1.62	1.54
1	A	198	GLN	CA-CB	-5.42	1.44	1.53
1	A	135	ARG	CZ-NH2	-5.38	1.26	1.33
1	A	216	ASP	CB-CG	-5.38	1.38	1.52
1	A	206	VAL	C-O	-5.37	1.18	1.24
1	A	17	THR	CB-CG2	-5.37	1.34	1.52
1	A	202	ARG	CZ-NH2	-5.34	1.26	1.33
1	A	30	ASP	CA-CB	-5.33	1.45	1.53
1	A	86	GLY	C-O	-5.29	1.16	1.24
1	A	213	LEU	C-O	-5.29	1.17	1.23
1	A	156	VAL	CA-CB	5.27	1.59	1.53
1	A	63	ASP	C-O	-5.27	1.17	1.24
1	A	54	ALA	C-O	-5.25	1.18	1.24
1	A	39	PRO	C-N	-5.24	1.27	1.33
1	A	14	GLU	CG-CD	5.24	1.65	1.52
1	A	5	ALA	CA-CB	-5.22	1.45	1.53
1	A	216	ASP	CA-CB	-5.22	1.45	1.53
1	A	164	GLN	C-O	-5.21	1.17	1.24
1	A	220	PRO	N-CA	-5.19	1.41	1.47
1	A	194	GLU	CD-OE1	5.18	1.35	1.25
1	A	215	LEU	N-CA	-5.17	1.39	1.46
1	A	55	ILE	CG1-CD1	5.16	1.71	1.51
1	A	123	ASP	C-O	5.16	1.30	1.24
1	A	237	PRO	C-O	-5.16	1.17	1.23
1	A	139	ALA	C-O	5.15	1.31	1.23
1	A	262	ILE	C-O	-5.14	1.18	1.24
1	A	100	ARG	NE-CZ	5.11	1.38	1.33
1	A	260	ASN	CG-ND2	-5.11	1.22	1.33
1	A	8	ASN	C-O	-5.11	1.17	1.24
1	A	15	PRO	N-CA	-5.09	1.41	1.47
1	A	227	ALA	C-O	5.07	1.30	1.24
1	A	283	ARG	CZ-NH1	5.05	1.39	1.32
1	A	48	LEU	N-CA	-5.02	1.39	1.45
1	A	99	GLY	CA-C	5.02	1.58	1.51
1	A	1	MET	CG-SD	5.01	1.93	1.80

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	N-CA-C	12.83	124.61	108.45
1	A	207	VAL	N-CA-C	11.06	121.97	110.36
1	A	202	ARG	N-CA-C	-9.28	101.14	111.07
1	A	257	ARG	CA-C-N	-9.00	107.14	123.34
1	A	257	ARG	C-N-CA	-9.00	107.14	123.34
1	A	144	VAL	CB-CA-C	8.38	122.99	112.02
1	A	72	VAL	CB-CA-C	-8.18	101.28	112.24
1	A	73	CYS	N-CA-C	-8.13	103.11	112.87
1	A	156	VAL	CB-CA-C	-7.80	101.34	111.25
1	A	40	VAL	N-CA-C	7.77	117.88	110.42
1	A	42	ASN	N-CA-C	7.66	121.97	111.39
1	A	72	VAL	CA-CB-CG2	-7.65	97.40	110.40
1	A	230	ILE	N-CA-C	-7.48	103.66	111.58
1	A	195	ALA	N-CA-C	-7.45	104.17	113.18
1	A	284	PHE	N-CA-C	7.43	131.79	111.00
1	A	100	ARG	N-CA-C	7.39	121.54	109.94
1	A	26	ARG	CB-CA-C	-6.99	98.44	109.70
1	A	28	ARG	CA-C-O	-6.90	114.03	121.56
1	A	278	ASP	N-CA-C	6.90	119.22	110.24
1	A	280	ARG	CA-C-N	-6.87	111.37	122.36
1	A	280	ARG	C-N-CA	-6.87	111.37	122.36
1	A	181	LEU	CA-C-N	-6.79	112.67	122.45
1	A	181	LEU	C-N-CA	-6.79	112.67	122.45
1	A	103	THR	CA-C-N	-6.77	110.53	120.28
1	A	103	THR	C-N-CA	-6.77	110.53	120.28
1	A	36	VAL	CB-CA-C	-6.69	98.92	111.30
1	A	237	PRO	CB-CA-C	-6.62	102.91	111.39
1	A	75	SER	CA-C-N	-6.60	110.94	122.09
1	A	75	SER	C-N-CA	-6.60	110.94	122.09
1	A	148	VAL	N-CA-C	-6.57	107.09	113.53
1	A	152	ILE	CB-CA-C	-6.53	102.25	111.19
1	A	283	ARG	CA-C-N	-6.44	110.10	121.70
1	A	283	ARG	C-N-CA	-6.44	110.10	121.70
1	A	176	ASP	N-CA-C	-6.33	97.97	108.34
1	A	208	PHE	N-CA-C	-6.32	104.47	111.36
1	A	72	VAL	N-CA-C	-6.27	104.17	111.00
1	A	50	PRO	CA-C-N	-6.21	109.48	121.58
1	A	50	PRO	C-N-CA	-6.21	109.48	121.58
1	A	144	VAL	N-CA-CB	6.19	118.49	110.57
1	A	135	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	A	135	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	82	ARG	N-CA-C	-6.14	105.74	113.72
1	A	92	PHE	CA-C-N	-6.04	111.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	PHE	C-N-CA	-6.04	111.81	122.20
1	A	36	VAL	CA-C-N	-6.02	115.34	123.10
1	A	36	VAL	C-N-CA	-6.02	115.34	123.10
1	A	170	PHE	N-CA-C	-5.97	99.44	108.46
1	A	178	GLU	N-CA-C	5.94	118.97	110.24
1	A	51	LYS	CD-CE-NZ	-5.93	92.94	111.90
1	A	152	ILE	N-CA-C	5.92	117.36	108.96
1	A	51	LYS	CA-CB-CG	-5.91	102.28	114.10
1	A	14	GLU	CB-CG-CD	5.90	122.62	112.60
1	A	102	TRP	N-CA-C	5.86	118.11	110.43
1	A	17	THR	N-CA-CB	-5.84	101.30	110.30
1	A	110	MET	CA-C-N	-5.78	114.04	122.65
1	A	110	MET	C-N-CA	-5.78	114.04	122.65
1	A	148	VAL	CB-CA-C	5.78	116.31	110.65
1	A	282	CYS	CB-CA-C	-5.78	97.91	109.35
1	A	245	PRO	N-CD-CG	-5.76	94.56	103.20
1	A	155	VAL	CB-CA-C	5.75	118.63	111.15
1	A	179	ALA	N-CA-C	-5.75	102.53	110.35
1	A	73	CYS	CA-CB-SG	5.72	127.55	114.40
1	A	14	GLU	CA-CB-CG	5.71	125.51	114.10
1	A	120	VAL	N-CA-C	5.69	116.33	110.36
1	A	257	ARG	O-C-N	-5.66	114.65	122.46
1	A	222	SER	N-CA-C	-5.63	106.41	113.28
1	A	171	GLY	CA-C-O	-5.62	118.08	122.52
1	A	35	THR	N-CA-C	5.62	117.65	108.55
1	A	164	GLN	CA-CB-CG	-5.59	102.91	114.10
1	A	33	ASP	CA-C-O	-5.59	114.66	121.36
1	A	121	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	136	LEU	N-CA-C	-5.57	100.85	109.14
1	A	248	VAL	N-CA-C	-5.57	100.64	108.27
1	A	275	LEU	N-CA-CB	-5.50	102.14	110.77
1	A	74	ASP	CB-CG-OD2	5.48	131.01	118.40
1	A	45	PHE	N-CA-C	5.46	118.82	110.20
1	A	161	THR	CB-CA-C	5.45	119.94	110.68
1	A	136	LEU	CA-C-N	-5.42	114.08	122.49
1	A	136	LEU	C-N-CA	-5.42	114.08	122.49
1	A	86	GLY	O-C-N	-5.38	115.51	122.34
1	A	143	SER	N-CA-C	-5.37	106.23	112.89
1	A	268	ALA	CA-C-N	-5.34	114.11	122.56
1	A	268	ALA	C-N-CA	-5.34	114.11	122.56
1	A	24	GLY	N-CA-C	-5.32	107.92	115.43
1	A	256	ARG	CA-C-N	-5.30	110.68	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ARG	C-N-CA	-5.30	110.68	121.18
1	A	121	ARG	N-CA-C	5.30	116.74	111.07
1	A	146	LEU	CB-CG-CD2	-5.29	94.84	110.70
1	A	234	LEU	CA-CB-CG	5.28	134.77	116.30
1	A	100	ARG	CA-CB-CG	5.27	124.64	114.10
1	A	252	ALA	N-CA-C	5.23	117.97	109.24
1	A	137	ASP	CA-C-N	5.23	128.99	121.56
1	A	137	ASP	C-N-CA	5.23	128.99	121.56
1	A	180	VAL	N-CA-CB	-5.22	101.70	111.62
1	A	62	LEU	CA-CB-CG	5.22	134.56	116.30
1	A	67	THR	N-CA-CB	5.18	120.20	110.87
1	A	111	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	A	13	SER	N-CA-C	5.07	121.61	110.80
1	A	120	VAL	CB-CA-C	-5.06	105.41	111.88
1	A	26	ARG	N-CA-C	5.05	117.36	110.24
1	A	2	LEU	CA-C-N	-5.05	116.05	122.77
1	A	2	LEU	C-N-CA	-5.05	116.05	122.77
1	A	150	ASP	N-CA-C	-5.04	107.81	114.31
1	A	43	VAL	N-CA-C	5.03	117.05	108.86
1	A	258	ASP	CA-C-N	5.01	127.53	120.42
1	A	258	ASP	C-N-CA	5.01	127.53	120.42
1	A	205	GLY	CA-C-N	5.01	126.83	120.72
1	A	205	GLY	C-N-CA	5.01	126.83	120.72
1	A	245	PRO	N-CA-C	-5.00	107.33	113.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2073	0	2102	146	3
2	A	25	0	0	3	6
3	A	1	0	0	0	0
4	A	173	0	0	7	10
All	All	2272	0	2102	146	18

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 35.

All (146) 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:51:LYS:H	1:A:51:LYS:CD	1.24	1.48
1:A:226:LYS:CE	1:A:226:LYS:NZ	1.72	1.48
1:A:119:LEU:HD23	1:A:119:LEU:C	1.74	1.12
1:A:51:LYS:HD2	1:A:51:LYS:N	1.14	1.11
1:A:214:MET:HE1	4:A:3171:HOH:O	1.51	1.06
1:A:160:ARG:HH11	1:A:160:ARG:HG3	0.95	1.06
1:A:72:VAL:HG23	1:A:73:CYS:H	1.19	1.06
1:A:72:VAL:HG23	1:A:73:CYS:N	1.66	1.02
1:A:69:ARG:O	1:A:72:VAL:HG23	1.62	0.98
1:A:17:THR:HG21	2:A:1001:SO4:O3	1.63	0.98
1:A:100:ARG:HD3	1:A:101:ASN:C	1.89	0.96
1:A:225:LYS:HG2	1:A:226:LYS:HE2	1.47	0.96
1:A:160:ARG:HG3	1:A:160:ARG:NH1	1.72	0.95
1:A:275:LEU:HD12	1:A:275:LEU:C	1.84	0.94
1:A:110:MET:O	1:A:132:THR:HG23	1.70	0.92
1:A:225:LYS:HD2	1:A:225:LYS:H	1.33	0.89
1:A:107:LEU:HD12	1:A:110:MET:CE	2.04	0.87
1:A:55:ILE:H	1:A:55:ILE:HD12	1.38	0.87
1:A:160:ARG:HH11	1:A:160:ARG:CG	1.85	0.86
1:A:22:GLU:OE1	1:A:280:ARG:NH2	2.08	0.85
1:A:69:ARG:O	1:A:72:VAL:CG2	2.23	0.85
1:A:156:VAL:HG22	1:A:156:VAL:O	1.76	0.85
1:A:221:ARG:HH11	1:A:221:ARG:HG3	1.42	0.84
1:A:275:LEU:HD12	1:A:276:ALA:N	1.92	0.84
1:A:107:LEU:HD12	1:A:110:MET:HE3	1.65	0.79
1:A:103:THR:HG22	1:A:105:ALA:H	1.49	0.78
1:A:51:LYS:CD	1:A:51:LYS:N	1.99	0.77
1:A:51:LYS:O	1:A:55:ILE:HD13	1.85	0.77
1:A:119:LEU:C	1:A:119:LEU:CD2	2.57	0.77
1:A:89:SER:HB2	1:A:178:GLU:HG3	1.69	0.75
1:A:55:ILE:H	1:A:55:ILE:CD1	2.00	0.75
1:A:212:TYR:CE1	1:A:234:LEU:CD2	2.70	0.75
1:A:225:LYS:H	1:A:225:LYS:CD	2.00	0.74
1:A:37:ILE:O	1:A:37:ILE:HG13	1.88	0.73
1:A:156:VAL:O	1:A:156:VAL:HG13	1.90	0.72
1:A:167:LEU:N	1:A:167:LEU:HD23	1.86	0.71
1:A:225:LYS:CG	1:A:226:LYS:HE2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:HB1	1:A:97:PRO:CD	2.23	0.68
1:A:225:LYS:HG2	1:A:226:LYS:CE	2.22	0.68
1:A:100:ARG:O	4:A:3071:HOH:O	2.12	0.67
1:A:212:TYR:CE1	1:A:234:LEU:HD21	2.31	0.66
1:A:212:TYR:CZ	1:A:234:LEU:HD21	2.30	0.66
1:A:202:ARG:NH1	2:A:1002:SO4:O4	2.27	0.65
1:A:221:ARG:HG3	1:A:221:ARG:NH1	2.06	0.65
1:A:166:ASP:C	1:A:167:LEU:HD23	2.22	0.65
1:A:2:LEU:N	1:A:2:LEU:HD13	2.11	0.64
1:A:37:ILE:HG22	1:A:44:GLU:HG3	1.80	0.64
1:A:50:PRO:HD2	1:A:51:LYS:HZ3	1.62	0.63
1:A:55:ILE:HD12	1:A:55:ILE:N	2.13	0.63
1:A:69:ARG:HA	1:A:72:VAL:HG21	1.82	0.62
1:A:7:PRO:HA	1:A:48:LEU:O	2.00	0.62
1:A:256:ARG:NH1	4:A:3147:HOH:O	2.30	0.61
1:A:50:PRO:HD2	1:A:51:LYS:NZ	2.16	0.61
1:A:156:VAL:O	1:A:156:VAL:CG2	2.44	0.61
1:A:93:ARG:NH2	1:A:171:GLY:O	2.34	0.60
1:A:72:VAL:CG2	1:A:73:CYS:N	2.48	0.60
1:A:96:ALA:HB1	1:A:97:PRO:HD2	1.83	0.60
1:A:100:ARG:HD3	1:A:102:TRP:N	2.18	0.59
1:A:69:ARG:HA	1:A:72:VAL:CG2	2.34	0.57
1:A:92:PHE:HD2	1:A:155:VAL:CG1	2.15	0.57
1:A:72:VAL:C	1:A:74:ASP:N	2.60	0.57
1:A:100:ARG:HD3	1:A:101:ASN:O	2.04	0.57
1:A:8:ASN:ND2	1:A:49:ARG:HG2	2.20	0.57
1:A:8:ASN:HD21	1:A:49:ARG:HG2	1.70	0.56
1:A:119:LEU:HD23	1:A:120:VAL:N	2.19	0.56
1:A:272:LYS:HE2	4:A:3132:HOH:O	2.06	0.55
1:A:50:PRO:CD	1:A:51:LYS:HZ3	2.19	0.55
1:A:116:TYR:CD1	1:A:116:TYR:N	2.75	0.55
1:A:71:LEU:H	1:A:71:LEU:HD22	1.73	0.54
1:A:160:ARG:NH1	1:A:160:ARG:CG	2.54	0.54
1:A:242:LEU:HD12	1:A:247:TRP:HB3	1.89	0.54
1:A:222:SER:O	1:A:225:LYS:HD3	2.07	0.54
1:A:28:ARG:HA	1:A:36:VAL:HG22	1.90	0.53
1:A:72:VAL:O	1:A:73:CYS:C	2.49	0.53
1:A:107:LEU:HD11	1:A:170:PHE:HZ	1.72	0.53
1:A:230:ILE:HG21	1:A:266:LEU:HD13	1.91	0.53
1:A:69:ARG:C	1:A:72:VAL:CG2	2.82	0.52
1:A:158:SER:CB	1:A:160:ARG:NH1	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:THR:HG22	1:A:104:THR:N	2.24	0.52
1:A:50:PRO:HB3	1:A:67:THR:HG22	1.91	0.52
1:A:19:ILE:HD12	1:A:87:PHE:HE1	1.75	0.51
1:A:92:PHE:HD2	1:A:155:VAL:HG12	1.76	0.51
1:A:107:LEU:HA	1:A:110:MET:HE2	1.92	0.51
1:A:119:LEU:HD23	1:A:119:LEU:O	2.07	0.50
1:A:12:LEU:CD1	1:A:12:LEU:N	2.74	0.50
1:A:100:ARG:NH1	1:A:106:ASP:OD1	2.44	0.50
1:A:141:GLU:H	1:A:141:GLU:CD	2.19	0.50
1:A:233:GLY:HA2	1:A:253:LEU:O	2.12	0.49
1:A:225:LYS:HD2	1:A:225:LYS:N	2.15	0.49
1:A:72:VAL:C	1:A:74:ASP:H	2.21	0.49
1:A:94:TYR:OH	1:A:123:ASP:OD2	2.20	0.49
1:A:91:SER:O	1:A:156:VAL:HG12	2.13	0.48
1:A:139:ALA:O	1:A:142:ILE:HG22	2.13	0.48
1:A:259:VAL:O	1:A:263:MET:HG3	2.13	0.48
1:A:130:GLU:HB2	4:A:3103:HOH:O	2.13	0.48
1:A:28:ARG:HA	1:A:36:VAL:CG2	2.43	0.48
1:A:96:ALA:HB3	1:A:102:TRP:CE2	2.49	0.48
1:A:82:ARG:O	1:A:82:ARG:HG3	2.13	0.48
1:A:172:GLU:OE2	1:A:172:GLU:HA	2.13	0.47
1:A:87:PHE:CE2	1:A:179:ALA:HB2	2.49	0.47
1:A:225:LYS:CG	1:A:226:LYS:CE	2.89	0.47
1:A:198:GLN:O	1:A:202:ARG:HB2	2.15	0.47
1:A:78:GLN:NE2	1:A:184:ARG:HH21	2.13	0.47
1:A:17:THR:HG21	2:A:1001:SO4:S	2.55	0.46
1:A:91:SER:O	1:A:156:VAL:CG1	2.63	0.46
1:A:103:THR:O	1:A:104:THR:C	2.55	0.46
1:A:161:THR:O	1:A:165:HIS:ND1	2.40	0.46
1:A:80:ARG:N	1:A:183:GLU:O	2.40	0.46
1:A:74:ASP:HB2	1:A:119:LEU:HB2	1.98	0.46
1:A:5:ALA:HA	1:A:46:PHE:O	2.16	0.46
1:A:92:PHE:CD2	1:A:155:VAL:HG12	2.50	0.45
1:A:92:PHE:CD2	1:A:155:VAL:CG1	2.99	0.45
1:A:107:LEU:HD12	1:A:110:MET:HE2	1.95	0.45
1:A:219:CYS:HA	1:A:220:PRO:HD3	1.87	0.45
1:A:2:LEU:HD12	1:A:2:LEU:HA	1.34	0.45
1:A:34:LEU:HA	1:A:47:PHE:HB2	1.99	0.45
1:A:87:PHE:CE2	1:A:179:ALA:CB	3.00	0.45
1:A:27:ARG:NH1	4:A:3040:HOH:O	2.50	0.45
1:A:2:LEU:HD21	1:A:195:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.81	0.44
1:A:13:SER:O	1:A:17:THR:HB	2.18	0.44
1:A:106:ASP:O	1:A:110:MET:HE2	2.17	0.44
1:A:22:GLU:OE1	1:A:280:ARG:CZ	2.65	0.43
1:A:106:ASP:C	1:A:110:MET:HE2	2.43	0.43
1:A:244:ASP:HA	1:A:245:PRO:HD3	1.87	0.43
1:A:280:ARG:HA	1:A:280:ARG:HD2	1.83	0.43
1:A:174:LEU:N	1:A:174:LEU:HD23	2.33	0.43
1:A:92:PHE:O	1:A:93:ARG:HB3	2.19	0.42
1:A:95:ALA:HA	1:A:168:VAL:O	2.19	0.42
1:A:28:ARG:HB3	1:A:36:VAL:HG22	2.01	0.42
1:A:102:TRP:H	1:A:102:TRP:CD1	2.37	0.42
1:A:93:ARG:HB2	1:A:94:TYR:H	1.67	0.42
1:A:104:THR:CG2	1:A:107:LEU:HD22	2.49	0.42
1:A:51:LYS:H	1:A:51:LYS:HD2	0.35	0.42
1:A:140:VAL:HG21	1:A:154:ASP:HB2	2.01	0.42
1:A:199:LEU:C	1:A:199:LEU:HD23	2.45	0.42
1:A:167:LEU:HD23	1:A:167:LEU:HA	1.27	0.41
1:A:119:LEU:CD2	1:A:120:VAL:N	2.81	0.41
1:A:51:LYS:HG3	4:A:3005:HOH:O	2.20	0.41
1:A:116:TYR:HA	1:A:117:PRO:HD2	1.90	0.41
1:A:51:LYS:O	1:A:55:ILE:CD1	2.62	0.41
1:A:107:LEU:HA	1:A:110:MET:CE	2.50	0.41
1:A:111:ARG:HB3	1:A:134:ILE:CD1	2.51	0.41
1:A:215:LEU:HD23	1:A:276:ALA:HA	2.03	0.41
1:A:14:GLU:N	1:A:15:PRO:CD	2.84	0.40
1:A:123:ASP:O	1:A:126:THR:HB	2.21	0.40

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3067:HOH:O	4:A:3067:HOH:O[16_544]	0.55	1.65
4:A:3079:HOH:O	4:A:3079:HOH:O[16_544]	1.09	1.11
2:A:1004:SO4:O1	2:A:1004:SO4:O3[3_665]	1.23	0.97
4:A:3090:HOH:O	4:A:3090:HOH:O[16_544]	1.30	0.90
4:A:3167:HOH:O	4:A:3167:HOH:O[2_655]	1.35	0.85
2:A:1004:SO4:S	2:A:1004:SO4:O1[2_655]	1.39	0.81
2:A:1004:SO4:O1	2:A:1004:SO4:O4[3_665]	1.53	0.67
4:A:3119:HOH:O	4:A:3119:HOH:O[2_655]	1.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3043:HOH:O	4:A:3043:HOH:O[18_654]	1.57	0.63
4:A:3068:HOH:O	4:A:3068:HOH:O[6_765]	1.58	0.62
4:A:3124:HOH:O	4:A:3124:HOH:O[2_655]	1.82	0.38
4:A:3123:HOH:O	4:A:3165:HOH:O[3_665]	1.84	0.36
1:A:122:LYS:NZ	1:A:122:LYS:NZ[6_765]	1.85	0.35
1:A:278:ASP:O	2:A:1004:SO4:O2[3_665]	1.92	0.28
2:A:1004:SO4:S	2:A:1004:SO4:O3[3_665]	1.94	0.26
4:A:3118:HOH:O	4:A:3160:HOH:O[2_655]	2.06	0.14
1:A:104:THR:OG1	1:A:172:GLU:OE1[6_765]	2.07	0.13
2:A:1004:SO4:O3	2:A:1004:SO4:O3[2_655]	2.19	0.01

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	268/304 (88%)	255 (95%)	11 (4%)	2 (1%)	18 41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ALA
1	A	99	GLY

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	215/239 (90%)	168 (78%)	47 (22%)	1 3

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	12	LEU
1	A	14	GLU
1	A	17	THR
1	A	29	THR
1	A	36	VAL
1	A	37	ILE
1	A	43	VAL
1	A	49	ARG
1	A	51	LYS
1	A	62	LEU
1	A	67	THR
1	A	72	VAL
1	A	78	GLN
1	A	100	ARG
1	A	104	THR
1	A	107	LEU
1	A	111	ARG
1	A	119	LEU
1	A	126	THR
1	A	127	LYS
1	A	129	ILE
1	A	132	THR
1	A	136	LEU
1	A	141	GLU
1	A	144	VAL
1	A	148	VAL
1	A	152	ILE
1	A	156	VAL
1	A	160	ARG
1	A	161	THR
1	A	174	LEU
1	A	180	VAL
1	A	202	ARG
1	A	210	GLN
1	A	216	ASP
1	A	221	ARG

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Mol	Chain	Res	Type
1	A	225	LYS
1	A	226	LYS
1	A	230	ILE
1	A	238	THR
1	A	248	VAL
1	A	257	ARG
1	A	266	LEU
1	A	275	LEU
1	A	281	PHE

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	8	ASN
1	A	41	ASN
1	A	78	GLN
1	A	145	GLN
1	A	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
2	SO4	A	1002	-	4,4,4	0.69	0	6,6,6	2.03	1 (16%)
2	SO4	A	1001	-	4,4,4	0.54	0	6,6,6	1.05	0
2	SO4	A	1004	-	4,4,4	0.25	0	6,6,6	0.40	0
2	SO4	A	1003	-	4,4,4	1.14	0	6,6,6	1.30	1 (16%)
2	SO4	A	1005	-	4,4,4	0.61	0	6,6,6	0.65	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	SO4	O4-S-O3	-3.84	87.34	108.54
2	A	1003	SO4	O3-S-O2	-2.25	97.78	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	SO4	1	0
2	A	1001	SO4	2	0
2	A	1004	SO4	0	6

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.