Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:05 PM GMT

PDB ID	:	1NH7
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

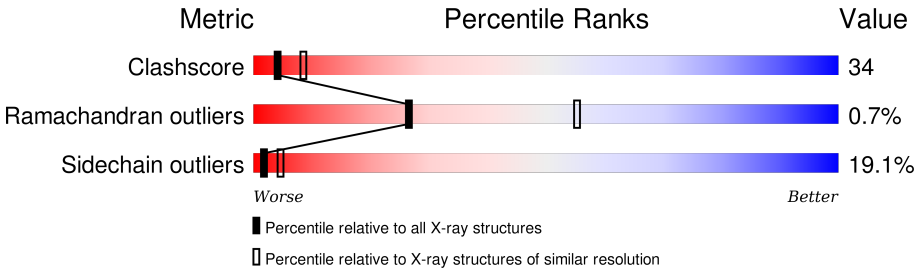
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	34% 34% 17% 5% 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	1003	-	X	-	-
2	SO4	A	1004	-	-	X	-

2 Entry composition (i)

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.

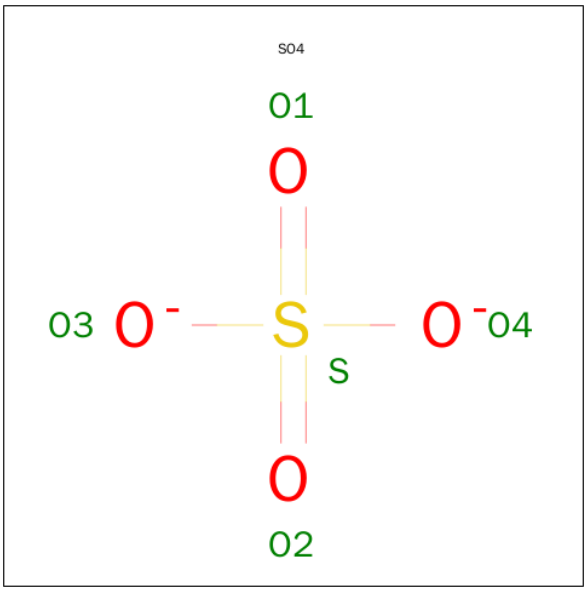
- Molecule 1 is a protein called ATP Phosphoribosyltransferase.

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 (three-letter code: SO4) (formula: O_4S).



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	A	1	Total O S 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

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

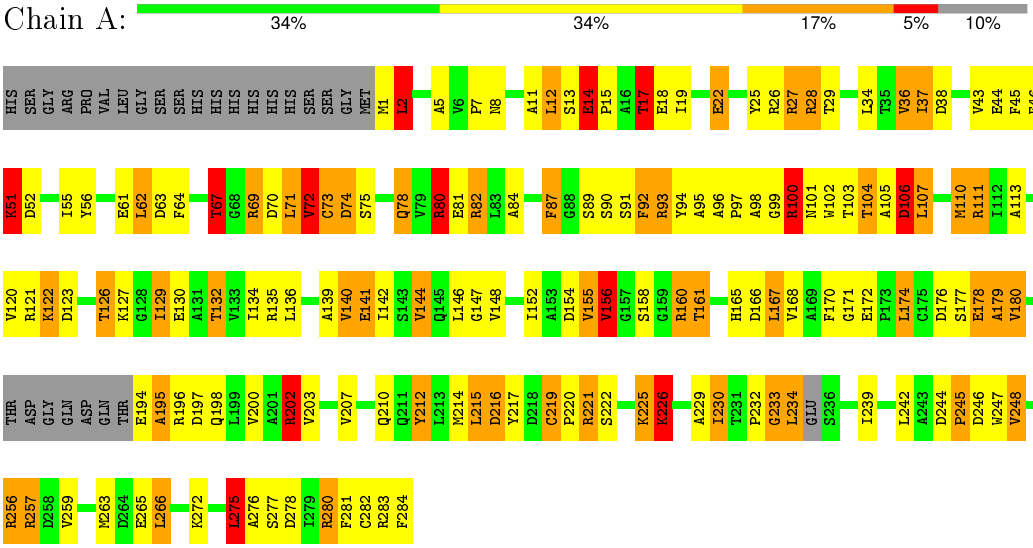
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

Note EDS was not executed.

- Molecule 1: ATP Phosphoribosyltransferase

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	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: MG, 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	2.21	69/2104 (3.3%)	2.00	76/2852 (2.7%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CD-OE1	12.63	1.39	1.25
1	A	43	VAL	CB-CG1	-10.04	1.31	1.52
1	A	51	LYS	CE-NZ	-9.67	1.24	1.49
1	A	226	LYS	CE-NZ	9.19	1.72	1.49
1	A	14	GLU	CD-OE2	9.11	1.35	1.25
1	A	257	ARG	CZ-NH1	9.04	1.44	1.33
1	A	14	GLU	CG-CD	8.79	1.65	1.51
1	A	194	GLU	CD-OE1	8.68	1.35	1.25
1	A	147	GLY	C-O	-8.61	1.09	1.23
1	A	111	ARG	NE-CZ	8.28	1.43	1.33
1	A	116	TYR	CB-CG	-8.14	1.39	1.51
1	A	11	ALA	CA-CB	-8.04	1.35	1.52
1	A	179	ALA	CA-CB	-7.72	1.36	1.52
1	A	84	ALA	CA-CB	-7.67	1.36	1.52
1	A	113	ALA	CA-CB	-7.55	1.36	1.52
1	A	257	ARG	CZ-NH2	7.48	1.42	1.33
1	A	155	VAL	CB-CG2	-7.45	1.37	1.52
1	A	203	VAL	CB-CG1	-7.39	1.37	1.52
1	A	280	ARG	CB-CG	-7.25	1.32	1.52
1	A	81	GLU	C-O	-7.09	1.09	1.23
1	A	229	ALA	CA-CB	-7.09	1.37	1.52
1	A	110	MET	CG-SD	7.08	1.99	1.81
1	A	25	TYR	CD1-CE1	-6.99	1.28	1.39
1	A	61	GLU	CG-CD	6.82	1.62	1.51
1	A	202	ARG	CB-CG	-6.79	1.34	1.52
1	A	90	SER	CB-OG	-6.62	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ARG	NE-CZ	6.48	1.41	1.33
1	A	282	CYS	CB-SG	-6.45	1.71	1.82
1	A	216	ASP	CB-CG	-6.26	1.38	1.51
1	A	195	ALA	CA-CB	-6.24	1.39	1.52
1	A	45	PHE	CE1-CZ	6.20	1.49	1.37
1	A	265	GLU	CD-OE1	6.17	1.32	1.25
1	A	87	PHE	CD1-CE1	6.04	1.51	1.39
1	A	284	PHE	CA-CB	-6.01	1.40	1.53
1	A	212	TYR	CB-CG	-6.01	1.42	1.51
1	A	277	SER	C-O	-5.83	1.12	1.23
1	A	80	ARG	NE-CZ	5.74	1.40	1.33
1	A	18	GLU	CD-OE1	5.72	1.31	1.25
1	A	61	GLU	CD-OE2	5.72	1.31	1.25
1	A	56	TYR	CE2-CZ	-5.70	1.31	1.38
1	A	64	PHE	CD2-CE2	5.69	1.50	1.39
1	A	27	ARG	CZ-NH2	-5.69	1.25	1.33
1	A	248	VAL	CB-CG1	-5.65	1.41	1.52
1	A	233	GLY	C-O	-5.60	1.14	1.23
1	A	122	LYS	CD-CE	5.58	1.65	1.51
1	A	11	ALA	C-O	-5.54	1.12	1.23
1	A	140	VAL	CB-CG1	-5.51	1.41	1.52
1	A	239	ILE	C-O	-5.42	1.13	1.23
1	A	178	GLU	CD-OE2	-5.39	1.19	1.25
1	A	203	VAL	CB-CG2	-5.36	1.41	1.52
1	A	177	SER	CB-OG	5.34	1.49	1.42
1	A	82	ARG	CG-CD	5.32	1.65	1.51
1	A	92	PHE	CD2-CE2	5.32	1.49	1.39
1	A	17	THR	CB-CG2	-5.31	1.34	1.52
1	A	71	LEU	C-O	-5.30	1.13	1.23
1	A	127	LYS	CE-NZ	5.23	1.62	1.49
1	A	283	ARG	CZ-NH1	5.21	1.39	1.33
1	A	69	ARG	CB-CG	5.19	1.66	1.52
1	A	72	VAL	CA-CB	-5.18	1.43	1.54
1	A	284	PHE	CA-C	-5.18	1.39	1.52
1	A	283	ARG	C-O	5.14	1.33	1.23
1	A	202	ARG	NE-CZ	-5.13	1.26	1.33
1	A	135	ARG	CZ-NH2	-5.08	1.26	1.33
1	A	232	PRO	CG-CD	-5.06	1.33	1.50
1	A	217	TYR	CB-CG	-5.05	1.44	1.51
1	A	141	GLU	CD-OE2	5.03	1.31	1.25
1	A	194	GLU	CD-OE2	5.03	1.31	1.25
1	A	202	ARG	CZ-NH2	-5.03	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	CYS	CB-SG	-5.02	1.73	1.81

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	ARG	NE-CZ-NH1	14.71	127.65	120.30
1	A	74	ASP	CB-CG-OD2	14.12	131.01	118.30
1	A	135	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	A	111	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	A	278	ASP	CB-CG-OD2	11.56	128.70	118.30
1	A	63	ASP	CB-CG-OD2	11.25	128.42	118.30
1	A	52	ASP	CB-CG-OD2	10.65	127.89	118.30
1	A	63	ASP	CB-CG-OD1	-9.85	109.43	118.30
1	A	80	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	257	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	146	LEU	CB-CG-CD2	-9.51	94.84	111.00
1	A	72	VAL	CA-CB-CG2	-9.00	97.40	110.90
1	A	121	ARG	NE-CZ-NH1	-8.77	115.91	120.30
1	A	38	ASP	CB-CG-OD1	8.58	126.02	118.30
1	A	234	LEU	CA-CB-CG	8.46	134.77	115.30
1	A	62	LEU	CA-CB-CG	8.37	134.56	115.30
1	A	62	LEU	CB-CG-CD1	8.33	125.17	111.00
1	A	51	LYS	CD-CE-NZ	-8.16	92.94	111.70
1	A	26	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	246	ASP	CB-CG-OD2	7.87	125.39	118.30
1	A	27	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	167	LEU	CB-CG-CD2	-7.74	97.84	111.00
1	A	196	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	284	PHE	N-CA-C	7.70	131.79	111.00
1	A	73	CYS	CA-CB-SG	7.53	127.55	114.00
1	A	26	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	197	ASP	CB-CG-OD2	7.27	124.85	118.30
1	A	119	LEU	CB-CG-CD2	-7.25	98.68	111.00
1	A	70	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	202	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	106	ASP	CB-CG-OD2	7.16	124.75	118.30
1	A	275	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	A	129	ILE	CG1-CB-CG2	-6.68	96.71	111.40
1	A	256	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	82	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	36	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	111	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	LEU	CB-CG-CD2	-6.40	100.11	111.00
1	A	176	ASP	CB-CG-OD1	6.37	124.04	118.30
1	A	226	LYS	CD-CE-NZ	6.30	126.20	111.70
1	A	246	ASP	OD1-CG-OD2	-6.29	111.35	123.30
1	A	28	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	282	CYS	CB-CA-C	-6.24	97.91	110.40
1	A	93	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	A	27	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	167	LEU	CA-CB-CG	-6.17	101.12	115.30
1	A	144	VAL	CB-CA-C	6.10	122.99	111.40
1	A	74	ASP	OD1-CG-OD2	-6.05	111.80	123.30
1	A	202	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	2	LEU	CB-CG-CD1	-6.02	100.76	111.00
1	A	26	ARG	CB-CA-C	-5.98	98.44	110.40
1	A	43	VAL	CA-CB-CG1	-5.90	102.05	110.90
1	A	93	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	257	ARG	C-N-CA	-5.82	107.14	121.70
1	A	207	VAL	CA-CB-CG2	-5.79	102.22	110.90
1	A	180	VAL	CG1-CB-CG2	5.78	120.15	110.90
1	A	245	PRO	N-CD-CG	-5.76	94.56	103.20
1	A	257	ARG	NH1-CZ-NH2	5.75	125.73	119.40
1	A	52	ASP	OD1-CG-OD2	-5.67	112.53	123.30
1	A	38	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	14	GLU	CA-CB-CG	5.51	125.51	113.40
1	A	246	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	251	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	75	SER	C-N-CA	-5.41	110.94	122.30
1	A	22	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	A	18	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	72	VAL	CB-CA-C	-5.32	101.28	111.40
1	A	156	VAL	CB-CA-C	-5.29	101.34	111.40
1	A	215	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	67	THR	N-CA-CB	5.21	120.20	110.30
1	A	100	ARG	CA-CB-CG	5.11	124.64	113.40
1	A	230	ILE	CG1-CB-CG2	-5.06	100.28	111.40
1	A	51	LYS	CA-CB-CG	-5.05	102.28	113.40
1	A	93	ARG	N-CA-C	5.04	124.61	111.00
1	A	257	ARG	O-C-N	-5.03	114.65	122.70
1	A	200	VAL	CG1-CB-CG2	-5.01	102.89	110.90

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	141	2
2	A	25	0	0	3	5
3	A	1	0	0	0	0
4	A	173	0	0	7	10
All	All	2272	0	2102	141	17

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 34.

All (141) 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:CD	1:A:51:LYS:H	1.24	1.48
1:A:226:LYS:CE	1:A:226:LYS:NZ	1.72	1.48
1:A:214:MET:HE1	4:A:3171:HOH:O	1.45	1.15
1:A:51:LYS:N	1:A:51:LYS:HD2	1.14	1.11
1:A:160:ARG:HG3	1:A:160:ARG:HH11	0.95	1.06
1:A:72:VAL:HG23	1:A:73:CYS:H	1.19	1.06
1:A:119:LEU:C	1:A:119:LEU:HD23	1.74	1.05
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: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:100:ARG:HD3	1:A:101:ASN:C	1.89	0.92
1:A:110:MET:O	1:A:132:THR:HG23	1.70	0.92
1:A:275:LEU:C	1:A:275:LEU:HD12	1.84	0.90
1:A:225:LYS:H	1:A:225:LYS:HD2	1.33	0.89
1:A:107:LEU:HD12	1:A:110:MET:CE	2.04	0.87
1:A:55:ILE:HD12	1:A:55:ILE:H	1.38	0.87
1:A:160:ARG:CG	1:A:160:ARG:HH11	1.85	0.86
1:A:69:ARG:O	1:A:72:VAL:CG2	2.23	0.85
1:A:22:GLU:OE1	1:A:280:ARG:NH2	2.08	0.85
1:A:156:VAL:HG22	1:A:156:VAL:O	1.76	0.85
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD12	1:A:276:ALA:N	1.92	0.84
1:A:107:LEU:HD12	1:A:110:MET:HE3	1.60	0.82
1:A:103:THR:HG22	1:A:105:ALA:H	1.49	0.78
1:A:51:LYS:N	1:A:51:LYS:CD	1.99	0.77
1:A:51:LYS:O	1:A:55:ILE:HD13	1.85	0.77
1:A:89:SER:HB2	1:A:178:GLU:HG3	1.69	0.75
1:A:55:ILE:CD1	1:A:55:ILE:H	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:107:LEU:HA	1:A:110:MET:HE3	1.69	0.74
1:A:37:ILE:O	1:A:37:ILE:HG13	1.88	0.73
1:A:156:VAL:HG13	1:A:156:VAL:O	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
1:A:119:LEU:C	1:A:119:LEU:CD2	2.57	0.69
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:221:ARG:HG3	1:A:221:ARG:NH1	2.06	0.65
1:A:202:ARG:NH1	2:A:1002:SO4:O4	2.27	0.65
1:A:2:LEU:HD13	1:A:2:LEU:N	2.11	0.64
1:A:37:ILE:HG22	1:A:44:GLU:HG3	1.80	0.64
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:CG2	1:A:156:VAL:O	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:166:ASP:C	1:A:167:LEU:HD23	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PRO:HD2	1:A:51:LYS:HZ1	1.71	0.56
1:A:272:LYS:HE2	4:A:3132:HOH:O	2.06	0.55
1:A:116:TYR:CD1	1:A:116:TYR:N	2.75	0.55
1:A:160:ARG:CG	1:A:160:ARG:NH1	2.54	0.54
1:A:71:LEU:HD22	1:A:71:LEU:H	1.73	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:72:VAL:C	1:A:74:ASP:N	2.60	0.53
1:A:28:ARG:HA	1:A:36:VAL:HG22	1.90	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:158:SER:CB	1:A:160:ARG:NH1	2.72	0.52
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:119:LEU:O	1:A:119:LEU:HD23	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:233:GLY:HA2	1:A:253:LEU:O	2.12	0.49
1:A:225:LYS:N	1:A:225:LYS:HD2	2.15	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:259:VAL:O	1:A:263:MET:HG3	2.13	0.48
1:A:139:ALA:O	1:A:142:ILE:HG22	2.13	0.48
1:A:72:VAL:O	1:A:73:CYS:C	2.49	0.48
1:A:130:GLU:HB2	4:A:3103:HOH:O	2.13	0.48
1:A:51:LYS:HZ3	1:A:51:LYS:H	1.62	0.48
1:A:96:ALA:HB3	1:A:102:TRP:CE2	2.49	0.48
1:A:28:ARG:HA	1:A:36:VAL:CG2	2.43	0.48
1:A:82:ARG:HG3	1:A:82:ARG:O	2.13	0.48
1:A:69:ARG:C	1:A:72:VAL:CG2	2.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:CYS:HA	1:A:220:PRO:HD3	1.87	0.45
1:A:141:GLU:H	1:A:141:GLU:CD	2.19	0.45
1:A:2:LEU:HA	1:A:2:LEU:HD12	1.34	0.45
1:A:87:PHE:CE2	1:A:179:ALA:CB	3.00	0.45
1:A:34:LEU:HA	1:A:47:PHE:HB2	1.99	0.45
1:A:27:ARG:NH1	4:A:3040:HOH:O	2.50	0.45
1:A:72:VAL:C	1:A:74:ASP:H	2.21	0.44
1:A:2:LEU:HD21	1:A:195:ALA:O	2.17	0.44
1:A:136:LEU:HA	1:A:136:LEU:HD12	1.81	0.44
1:A:13:SER:O	1:A:17:THR:HB	2.18	0.44
1:A:22:GLU:OE1	1:A:280:ARG:CZ	2.65	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:93:ARG:HB2	1:A:94:TYR:H	1.67	0.42
1:A:50:PRO:CD	1:A:51:LYS:NZ	2.83	0.42
1:A:104:THR:CG2	1:A:107:LEU:HD22	2.49	0.42
1:A:51:LYS:HD2	1:A:51:LYS:H	0.35	0.42
1:A:140:VAL:HG21	1:A:154:ASP:HB2	2.01	0.42
1:A:167:LEU:HA	1:A:167:LEU:HD23	1.27	0.41
1:A:103:THR:O	1:A:104:THR:C	2.55	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:215:LEU:HD23	1:A:276:ALA:HA	2.03	0.41
1:A:111:ARG:HB3	1:A:134:ILE:CD1	2.51	0.41
1:A:123:ASP:O	1:A:126:THR:HB	2.21	0.40
1:A:14:GLU:N	1:A:15:PRO:CD	2.84	0.40

All (17) 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
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
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%)	26 55

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%)	174 (81%)	41 (19%)	2 4

All (41) 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	37	ILE
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	80	ARG
1	A	100	ARG
1	A	104	THR
1	A	106	ASP
1	A	107	LEU
1	A	119	LEU
1	A	126	THR
1	A	129	ILE
1	A	132	THR
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

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Mol	Chain	Res	Type
1	A	202	ARG
1	A	210	GLN
1	A	216	ASP
1	A	221	ARG
1	A	225	LYS
1	A	226	LYS
1	A	248	VAL
1	A	257	ARG
1	A	266	LEU
1	A	275	LEU
1	A	281	PHE

Some 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 (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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1001	-	4,4,4	0.79	0	6,6,6	0.98	0
2	SO4	A	1002	-	4,4,4	1.61	1 (25%)	6,6,6	2.37	1 (16%)
2	SO4	A	1003	-	4,4,4	2.55	4 (100%)	6,6,6	1.04	0
2	SO4	A	1004	1	4,4,4	0.31	0	6,6,6	0.26	0
2	SO4	A	1005	-	4,4,4	1.14	0	6,6,6	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1004	1	-	0/0/0/0	0/0/0/0
2	SO4	A	1005	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	SO4	O4-S	-3.08	1.36	1.47
2	A	1003	SO4	O3-S	-2.60	1.38	1.47
2	A	1003	SO4	O1-S	-2.24	1.39	1.47
2	A	1002	SO4	O2-S	-2.24	1.39	1.47
2	A	1003	SO4	O2-S	-2.17	1.39	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1002	SO4	O4-S-O3	-5.32	87.34	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SO4	2	0
2	A	1002	SO4	1	0
2	A	1004	SO4	0	5

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.