



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:03 am BST

PDB ID : 1JXI  
Title : 4-Amino-5-hydroxymethyl-2-methylpyrimidine Phosphate Kinase from  
Salmonella typhimurium complexed with 4-Amino-5-hydroxymethyl-2-methylpyrimidine  
Authors : Cheng, G.; Bennett, E.M.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2001-09-07  
Resolution : 2.64 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](mailto: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.

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

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

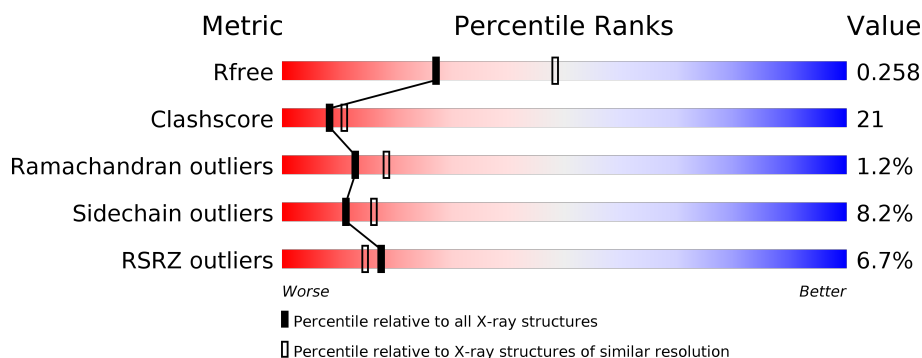
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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  $\geq 3$ , 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	A	288	
1	B	288	

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
3	HMH	A	2001	-	X	-	-
3	HMH	B	2002	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3918 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 PHOSPHOMETHYLPYRIMIDINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1902	1194	342	356	10			
1	B	254	Total	C	N	O	S	0	0	0
			1902	1194	342	356	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P55882
A	-20	GLY	-	EXPRESSION TAG	UNP P55882
A	-19	HIS	-	EXPRESSION TAG	UNP P55882
A	-18	HIS	-	EXPRESSION TAG	UNP P55882
A	-17	HIS	-	EXPRESSION TAG	UNP P55882
A	-16	HIS	-	EXPRESSION TAG	UNP P55882
A	-15	HIS	-	EXPRESSION TAG	UNP P55882
A	-14	HIS	-	EXPRESSION TAG	UNP P55882
A	-13	HIS	-	EXPRESSION TAG	UNP P55882
A	-12	HIS	-	EXPRESSION TAG	UNP P55882
A	-11	HIS	-	EXPRESSION TAG	UNP P55882
A	-10	HIS	-	EXPRESSION TAG	UNP P55882
A	-9	SER	-	EXPRESSION TAG	UNP P55882
A	-8	SER	-	EXPRESSION TAG	UNP P55882
A	-7	GLY	-	EXPRESSION TAG	UNP P55882
A	-6	TYR	-	EXPRESSION TAG	UNP P55882
A	-5	HIS	-	EXPRESSION TAG	UNP P55882
A	-4	ILE	-	EXPRESSION TAG	UNP P55882
A	-3	GLN	-	EXPRESSION TAG	UNP P55882
A	-2	GLY	-	EXPRESSION TAG	UNP P55882
A	-1	ARG	-	EXPRESSION TAG	UNP P55882
A	0	HIS	-	EXPRESSION TAG	UNP P55882
B	-21	MET	-	EXPRESSION TAG	UNP P55882
B	-20	GLY	-	EXPRESSION TAG	UNP P55882
B	-19	HIS	-	EXPRESSION TAG	UNP P55882

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	EXPRESSION TAG	UNP P55882
B	-17	HIS	-	EXPRESSION TAG	UNP P55882
B	-16	HIS	-	EXPRESSION TAG	UNP P55882
B	-15	HIS	-	EXPRESSION TAG	UNP P55882
B	-14	HIS	-	EXPRESSION TAG	UNP P55882
B	-13	HIS	-	EXPRESSION TAG	UNP P55882
B	-12	HIS	-	EXPRESSION TAG	UNP P55882
B	-11	HIS	-	EXPRESSION TAG	UNP P55882
B	-10	HIS	-	EXPRESSION TAG	UNP P55882
B	-9	SER	-	EXPRESSION TAG	UNP P55882
B	-8	SER	-	EXPRESSION TAG	UNP P55882
B	-7	GLY	-	EXPRESSION TAG	UNP P55882
B	-6	TYR	-	EXPRESSION TAG	UNP P55882
B	-5	HIS	-	EXPRESSION TAG	UNP P55882
B	-4	ILE	-	EXPRESSION TAG	UNP P55882
B	-3	GLN	-	EXPRESSION TAG	UNP P55882
B	-2	GLY	-	EXPRESSION TAG	UNP P55882
B	-1	ARG	-	EXPRESSION TAG	UNP P55882
B	0	HIS	-	EXPRESSION TAG	UNP P55882

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



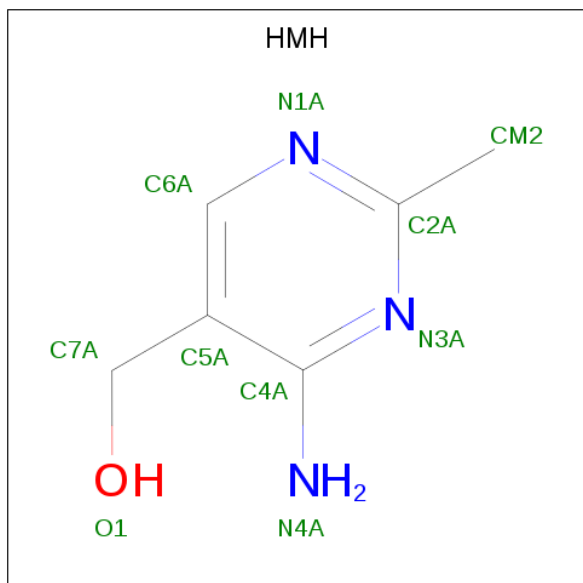
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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

- Molecule 3 is 4-AMINO-5-HYDROXYMETHYL-2-METHYLPYRIMIDINE (three-letter code: HMH) (formula: C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	3	1		
3	B	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	35	Total	O	0	0
			35	35		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.75Å 77.75Å 183.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.64 24.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-2.64) 99.5 (24.94-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.91 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.270 0.222 , 0.258	Depositor DCC
$R_{free}$ test set	1986 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7208e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/1935	0.61	0/2631
1	B	0.36	0/1935	0.61	0/2631
All	All	0.36	0/3870	0.61	0/5262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1902	0	1893	86	0
1	B	1902	0	1893	85	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	10	0	9	2	0
3	B	10	0	9	2	0
4	A	39	0	0	3	0
4	B	35	0	0	3	0
All	All	3918	0	3804	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (160) 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)
3:B:2002:HMH:O1	3:B:2002:HMH:C7A	1.63	1.45
3:A:2001:HMH:C7A	3:A:2001:HMH:O1	1.63	1.44
1:B:154:THR:HG22	1:B:157:GLU:HG3	1.41	1.02
1:A:154:THR:HG22	1:A:157:GLU:HG3	1.42	1.02
1:A:207:ASN:HD22	1:A:257:GLY:H	1.20	0.89
1:B:207:ASN:HD22	1:B:257:GLY:H	1.23	0.86
1:A:60:VAL:HG21	1:A:86:ILE:HD12	1.56	0.86
1:B:60:VAL:HG21	1:B:86:ILE:HD12	1.58	0.85
1:A:29:ALA:HA	1:A:265:TRP:CH2	2.16	0.80
1:B:29:ALA:HA	1:B:265:TRP:CH2	2.17	0.80
1:A:75:THR:HG21	1:A:220:ALA:O	1.82	0.79
1:A:46:THR:CG2	1:A:255:GLY:H	1.96	0.79
1:A:207:ASN:ND2	1:A:257:GLY:H	1.82	0.78
1:B:46:THR:CG2	1:B:255:GLY:H	1.97	0.78
1:A:126:ARG:HA	1:A:130:LEU:HD22	1.67	0.76
1:B:207:ASN:ND2	1:B:257:GLY:H	1.83	0.75
1:A:117:LEU:HB2	1:A:122:ILE:HD11	1.68	0.75
1:B:75:THR:HG21	1:B:220:ALA:O	1.86	0.75
1:B:117:LEU:HB2	1:B:122:ILE:HD11	1.69	0.75
1:A:228:SER:O	1:A:232:THR:HG22	1.87	0.74
1:B:126:ARG:HA	1:B:130:LEU:HD22	1.69	0.73
1:B:228:SER:O	1:B:232:THR:HG22	1.88	0.73
1:A:154:THR:CG2	1:A:157:GLU:HG3	2.19	0.72
1:B:191:THR:HG22	1:B:193:GLU:H	1.54	0.71
1:A:191:THR:HG22	1:A:193:GLU:H	1.56	0.70
1:A:45:ASN:HD21	1:B:70:ASP:HB2	1.56	0.70
1:A:70:ASP:HB2	1:B:45:ASN:HD21	1.55	0.70
1:A:191:THR:CG2	1:A:193:GLU:HG2	2.23	0.69
1:B:154:THR:CG2	1:B:157:GLU:HG3	2.18	0.69
1:A:126:ARG:HD3	4:A:2006:HOH:O	1.91	0.69
1:B:191:THR:CG2	1:B:193:GLU:HG2	2.23	0.68
1:B:42:VAL:HG22	1:B:44:GLU:HB2	1.77	0.66
1:A:42:VAL:HG22	1:A:44:GLU:HB2	1.78	0.66
1:B:126:ARG:HD2	4:B:2013:HOH:O	1.95	0.66
1:B:158:MET:HG2	1:B:175:MET:HE3	1.79	0.64
1:A:223:ARG:HB3	1:A:224:PRO:HD3	1.83	0.61
3:B:2002:HMH:HO1	3:B:2002:HMH:C7A	2.07	0.60
1:A:46:THR:HG23	1:A:255:GLY:H	1.66	0.59
1:B:29:ALA:HA	1:B:265:TRP:CZ3	2.37	0.59
1:B:95:GLN:HB2	1:B:132:GLN:HE22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:MET:HG2	1:A:175:MET:HE3	1.83	0.59
1:A:37:VAL:HG21	1:A:64:LEU:HD13	1.85	0.59
1:A:191:THR:HG21	1:A:193:GLU:HG2	1.84	0.58
1:A:95:GLN:HB2	1:A:132:GLN:HE22	1.68	0.58
1:B:191:THR:HG21	1:B:193:GLU:HG2	1.84	0.58
1:B:191:THR:HG22	1:B:192:ARG:N	2.16	0.58
1:B:117:LEU:CB	1:B:122:ILE:HD11	2.34	0.58
1:A:191:THR:HG22	1:A:192:ARG:N	2.18	0.58
1:A:191:THR:HG22	1:A:193:GLU:HG2	1.86	0.58
3:A:2001:HMH:HO1	3:A:2001:HMH:C7A	2.07	0.58
1:A:117:LEU:CB	1:A:122:ILE:HD11	2.34	0.57
1:B:93:ARG:HH11	1:B:93:ARG:HG2	1.68	0.57
1:A:29:ALA:HA	1:A:265:TRP:CZ3	2.38	0.57
1:A:229:TRP:HA	1:A:232:THR:CG2	2.35	0.57
1:B:12:THR:O	1:B:42:VAL:HG13	2.05	0.57
1:B:191:THR:HG22	1:B:193:GLU:HG2	1.86	0.56
1:B:223:ARG:HB3	1:B:224:PRO:HD3	1.87	0.56
1:B:45:ASN:HB2	1:B:50:GLN:HE22	1.69	0.56
1:B:37:VAL:HG21	1:B:64:LEU:HD13	1.86	0.56
1:B:61:ALA:HB1	1:B:93:ARG:NH2	2.20	0.56
1:B:46:THR:HG23	1:B:255:GLY:H	1.68	0.56
1:A:45:ASN:HB2	1:A:50:GLN:HE22	1.70	0.56
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.70	0.56
1:B:118:SER:HB3	1:B:121:ALA:CB	2.36	0.56
1:A:118:SER:HB3	1:A:121:ALA:CB	2.36	0.56
1:A:61:ALA:HB1	1:A:93:ARG:NH2	2.20	0.55
1:B:77:LYS:HD3	1:B:77:LYS:C	2.27	0.55
1:B:38:ILE:H	1:B:63:GLN:HE22	1.54	0.55
1:A:38:ILE:H	1:A:63:GLN:NE2	2.05	0.54
1:B:139:ASN:OD1	1:B:141:PRO:HD2	2.06	0.54
1:A:88:GLU:OE1	1:A:128:ARG:HD3	2.08	0.54
1:B:38:ILE:H	1:B:63:GLN:NE2	2.05	0.54
1:A:266:TRP:CE2	1:B:31:GLY:HA2	2.43	0.54
1:A:125:LEU:HD23	1:A:130:LEU:HD13	1.88	0.54
1:A:139:ASN:OD1	1:A:141:PRO:HD2	2.08	0.54
1:B:229:TRP:HA	1:B:232:THR:CG2	2.38	0.54
1:A:12:THR:O	1:A:42:VAL:HG13	2.07	0.53
1:A:38:ILE:H	1:A:63:GLN:HE22	1.55	0.53
1:B:10:ALA:HB1	4:B:2014:HOH:O	2.07	0.53
1:B:88:GLU:OE1	1:B:128:ARG:HD3	2.08	0.53
1:B:125:LEU:HD23	1:B:130:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ALA:HB1	4:A:2023:HOH:O	2.08	0.52
1:A:260:HIS:HE1	1:A:266:TRP:OXT	1.92	0.52
1:A:88:GLU:OE2	1:A:128:ARG:NH1	2.42	0.52
1:B:122:ILE:O	1:B:126:ARG:HG2	2.09	0.52
1:B:191:THR:CG2	1:B:192:ARG:N	2.73	0.52
1:A:77:LYS:C	1:A:77:LYS:HD3	2.31	0.51
1:A:31:GLY:HA2	1:B:266:TRP:CE2	2.46	0.51
1:A:223:ARG:HD3	1:A:229:TRP:CZ3	2.45	0.51
1:A:60:VAL:O	1:A:64:LEU:HD22	2.10	0.51
1:B:214:THR:OG1	1:B:261:HIS:HE1	1.93	0.51
1:A:109:LEU:HG	1:A:110:ALA:H	1.77	0.50
1:B:109:LEU:HG	1:B:110:ALA:H	1.76	0.50
1:B:260:HIS:HE1	1:B:266:TRP:OXT	1.94	0.50
1:B:60:VAL:O	1:B:64:LEU:HD22	2.11	0.50
1:A:122:ILE:O	1:A:126:ARG:HG2	2.12	0.50
1:A:191:THR:CG2	1:A:192:ARG:N	2.75	0.50
1:A:265:TRP:CE3	1:B:265:TRP:CZ3	3.00	0.50
1:B:118:SER:HB3	1:B:121:ALA:HB2	1.93	0.50
1:A:118:SER:HB3	1:A:121:ALA:HB2	1.93	0.50
1:B:223:ARG:HD3	1:B:229:TRP:CZ3	2.47	0.50
1:A:265:TRP:CZ3	1:B:265:TRP:CE3	3.00	0.50
1:B:136:ILE:HG12	1:B:138:PRO:HD3	1.94	0.50
1:A:136:ILE:HG12	1:A:138:PRO:HD3	1.93	0.49
1:A:70:ASP:CB	1:B:45:ASN:HD21	2.26	0.48
1:A:154:THR:HG23	1:A:157:GLU:H	1.79	0.48
1:A:214:THR:OG1	1:A:261:HIS:HE1	1.97	0.48
1:A:45:ASN:HD21	1:B:70:ASP:CB	2.26	0.48
1:A:123:GLU:O	1:A:127:VAL:HG23	2.13	0.47
1:B:45:ASN:OD1	1:B:46:THR:N	2.47	0.47
1:A:46:THR:HG23	1:A:255:GLY:N	2.28	0.47
1:B:154:THR:HG23	1:B:157:GLU:H	1.79	0.47
1:B:225:ARG:HD2	4:B:2008:HOH:O	2.15	0.47
1:A:45:ASN:OD1	1:A:46:THR:N	2.47	0.47
1:B:88:GLU:OE2	1:B:128:ARG:NH1	2.48	0.46
1:A:266:TRP:CD1	1:B:31:GLY:HA2	2.51	0.46
1:B:123:GLU:O	1:B:127:VAL:HG23	2.16	0.46
1:A:93:ARG:NH1	1:A:93:ARG:HG2	2.31	0.45
1:A:70:ASP:OD2	1:B:46:THR:HB	2.17	0.45
1:A:109:LEU:HA	1:A:115:PRO:HA	1.99	0.45
1:A:207:ASN:HD22	1:A:257:GLY:N	2.02	0.45
1:B:93:ARG:NH1	1:B:93:ARG:HG2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HA	1:B:115:PRO:HA	1.99	0.45
1:B:207:ASN:HD22	1:B:257:GLY:N	2.03	0.45
1:A:125:LEU:C	1:A:125:LEU:HD23	2.38	0.44
1:A:57:PRO:HA	1:A:86:ILE:CD1	2.47	0.44
1:B:46:THR:HG23	1:B:255:GLY:N	2.30	0.44
1:A:265:TRP:CE3	1:B:265:TRP:CE3	3.06	0.44
1:A:125:LEU:CD2	1:A:130:LEU:HD13	2.47	0.44
1:A:20:ILE:O	1:A:24:LEU:HB2	2.18	0.44
1:A:31:GLY:HA2	1:B:266:TRP:CD1	2.53	0.43
1:B:20:ILE:O	1:B:24:LEU:HB2	2.18	0.43
1:A:266:TRP:NE1	1:B:31:GLY:HA2	2.34	0.43
1:B:125:LEU:HD23	1:B:125:LEU:C	2.39	0.43
1:B:125:LEU:CD2	1:B:130:LEU:HD13	2.49	0.42
1:B:115:PRO:C	1:B:117:LEU:H	2.22	0.42
1:B:193:GLU:OE1	1:B:193:GLU:N	2.53	0.42
1:A:115:PRO:C	1:A:117:LEU:H	2.22	0.42
1:A:253:GLY:HA2	1:B:70:ASP:O	2.19	0.42
1:B:57:PRO:HA	1:B:86:ILE:CD1	2.49	0.42
1:A:118:SER:HB3	1:A:121:ALA:HB3	2.02	0.41
1:A:223:ARG:HD3	1:A:229:TRP:CH2	2.55	0.41
1:B:20:ILE:HG13	1:B:21:GLN:N	2.35	0.41
1:B:118:SER:HB3	1:B:121:ALA:HB3	2.02	0.41
1:B:262:PHE:HD1	1:B:265:TRP:CE3	2.38	0.41
1:A:46:THR:HG21	1:A:253:GLY:HA3	2.03	0.41
1:A:46:THR:HG23	1:A:255:GLY:CA	2.50	0.41
1:A:46:THR:HB	1:B:70:ASP:OD2	2.20	0.41
1:A:229:TRP:HA	1:A:232:THR:HG23	2.02	0.41
1:A:262:PHE:HD1	1:A:265:TRP:CE3	2.38	0.41
1:B:46:THR:HG21	1:B:253:GLY:HA3	2.03	0.41
1:B:2:GLN:O	1:B:225:ARG:NH2	2.46	0.41
1:B:45:ASN:HB2	1:B:50:GLN:NE2	2.35	0.41
1:A:193:GLU:OE1	1:A:193:GLU:N	2.53	0.41
1:A:223:ARG:HD2	1:A:232:THR:HG21	2.03	0.41
1:A:71:VAL:HA	4:A:2029:HOH:O	2.20	0.40
1:A:44:GLU:HG3	1:A:49:VAL:HG22	2.03	0.40
1:A:45:ASN:HB2	1:A:50:GLN:NE2	2.36	0.40
1:B:46:THR:HG23	1:B:255:GLY:CA	2.52	0.40
1:B:44:GLU:HG3	1:B:49:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/288 (86%)	236 (95%)	9 (4%)	3 (1%)	13	18
1	B	248/288 (86%)	234 (94%)	11 (4%)	3 (1%)	13	18
All	All	496/576 (86%)	470 (95%)	20 (4%)	6 (1%)	13	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	B	114	ASP
1	A	109	LEU
1	B	109	LEU
1	B	116	LEU
1	A	116	LEU

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/228 (85%)	178 (92%)	16 (8%)	11	16
1	B	194/228 (85%)	178 (92%)	16 (8%)	11	16
All	All	388/456 (85%)	356 (92%)	32 (8%)	11	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	24	LEU
1	A	42	VAL
1	A	46	THR
1	A	75	THR
1	A	77	LYS
1	A	94	LEU
1	A	100	ARG
1	A	117	LEU
1	A	130	LEU
1	A	193	GLU
1	A	222	LEU
1	A	225	ARG
1	A	232	THR
1	A	241	SER
1	A	252	VAL
1	B	2	GLN
1	B	24	LEU
1	B	42	VAL
1	B	46	THR
1	B	75	THR
1	B	77	LYS
1	B	94	LEU
1	B	100	ARG
1	B	117	LEU
1	B	130	LEU
1	B	193	GLU
1	B	222	LEU
1	B	225	ARG
1	B	232	THR
1	B	241	SER
1	B	252	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	63	GLN
1	A	161	GLN
1	A	207	ASN
1	A	246	GLN
1	A	260	HIS
1	A	261	HIS

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Mol	Chain	Res	Type
1	B	2	GLN
1	B	50	GLN
1	B	63	GLN
1	B	161	GLN
1	B	207	ASN
1	B	260	HIS
1	B	261	HIS

### 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](#)

6 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	B	2006	-	4,4,4	0.31	0	6,6,6	0.10	0
3	HMH	B	2002	-	10,10,10	3.93	6 (60%)	12,13,13	2.11	5 (41%)
2	SO4	A	2005	-	4,4,4	0.28	0	6,6,6	0.13	0
3	HMH	A	2001	-	10,10,10	3.88	6 (60%)	12,13,13	2.16	5 (41%)
2	SO4	B	2004	-	4,4,4	0.35	0	6,6,6	0.13	0
2	SO4	A	2003	-	4,4,4	0.38	0	6,6,6	0.08	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
3	HMH	B	2002	-	-	2/2/2/2	0/1/1/1
3	HMH	A	2001	-	-	0/2/2/2	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	HMH	C4A-N3A	6.77	1.44	1.35
3	B	2002	HMH	C5A-C4A	6.43	1.53	1.42
3	B	2002	HMH	C4A-N3A	6.13	1.43	1.35
3	A	2001	HMH	C5A-C4A	5.75	1.52	1.42
3	B	2002	HMH	O1-C7A	5.28	1.63	1.41
3	A	2001	HMH	O1-C7A	5.23	1.63	1.41
3	B	2002	HMH	C2A-N1A	5.22	1.42	1.34
3	A	2001	HMH	C2A-N1A	4.85	1.42	1.34
3	B	2002	HMH	C6A-N1A	3.77	1.42	1.34
3	A	2001	HMH	C6A-N1A	3.68	1.42	1.34
3	A	2001	HMH	C6A-C5A	2.52	1.43	1.37
3	B	2002	HMH	C6A-C5A	2.36	1.42	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	HMH	C7A-C5A-C6A	5.15	127.74	119.37
3	B	2002	HMH	C7A-C5A-C6A	5.01	127.52	119.37
3	A	2001	HMH	CM2-C2A-N3A	2.87	121.63	117.15
3	B	2002	HMH	CM2-C2A-N3A	2.69	121.35	117.15
3	B	2002	HMH	O1-C7A-C5A	2.38	118.59	111.87
3	A	2001	HMH	O1-C7A-C5A	2.30	118.35	111.87
3	B	2002	HMH	C2A-N3A-C4A	2.14	121.42	118.08
3	A	2001	HMH	C2A-N3A-C4A	2.07	121.31	118.08
3	A	2001	HMH	C6A-N1A-C2A	2.06	119.47	115.96
3	B	2002	HMH	C6A-N1A-C2A	2.01	119.39	115.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	HMH	C6A-C5A-C7A-O1

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Mol	Chain	Res	Type	Atoms
3	B	2002	HMH	C4A-C5A-C7A-O1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2002	HMH	2	0
3	A	2001	HMH	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/288 (88%)	0.15	17 (6%) 17 15	23, 38, 78, 130	0
1	B	254/288 (88%)	0.18	17 (6%) 17 15	23, 38, 76, 129	0
All	All	508/576 (88%)	0.16	34 (6%) 17 15	23, 38, 76, 130	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	ASP	9.4
1	A	114	ASP	7.7
1	A	110	ALA	6.7
1	A	116	LEU	6.6
1	B	115	PRO	5.6
1	B	117	LEU	5.0
1	B	113	GLY	4.6
1	A	112	SER	4.4
1	A	109	LEU	4.2
1	A	227	ARG	4.0
1	A	111	LYS	4.0
1	A	117	LEU	3.9
1	B	153	ARG	3.9
1	A	113	GLY	3.8
1	B	112	SER	3.6
1	B	116	LEU	3.6
1	B	110	ALA	3.2
1	B	111	LYS	3.1
1	A	115	PRO	3.1
1	B	20	ILE	3.0
1	B	227	ARG	3.0
1	B	206	LYS	2.9
1	A	203	VAL	2.8
1	A	192	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	2.6
1	B	109	LEU	2.6
1	B	151	HIS	2.5
1	A	153	ARG	2.4
1	B	100	ARG	2.4
1	B	192	ARG	2.4
1	A	204	ASN	2.3
1	B	154	THR	2.2
1	A	206	LYS	2.1
1	A	54	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	2006	5/5	0.85	0.24	74,75,76,76	5
2	SO4	A	2005	5/5	0.87	0.24	86,87,88,88	0
2	SO4	A	2003	5/5	0.87	0.18	63,63,63,65	0
3	HMH	A	2001	10/10	0.92	0.17	44,47,50,56	0
2	SO4	B	2004	5/5	0.92	0.14	63,63,65,65	0
3	HMH	B	2002	10/10	0.92	0.20	53,54,56,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.