



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:21 PM GMT

PDB ID : 1JXH
Title : 4-Amino-5-hydroxymethyl-2-methylpyrimidine Phosphate Kinase from
Salmonella typhimurium
Authors : Cheng, G.; Bennett, E.M.; Begley, T.P.; Ealick, S.E.
Deposited on : 2001-09-07
Resolution : 2.30 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

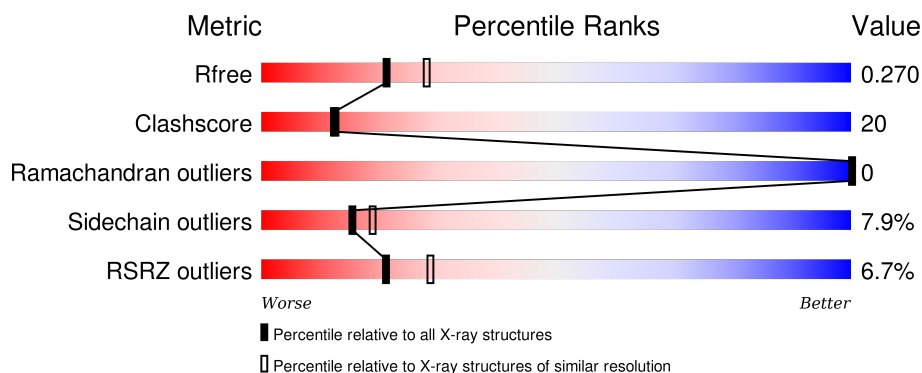
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>22%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	288	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>•</div> <div>14%</div> </div> </div>

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	2001	-	-	-	X
2	SO4	B	2004	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3923 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	248	Total	C	N	O	S	0	0	0
			1882	1181	340	351	10			
1	B	248	Total	C	N	O	S	0	0	0
			1882	1181	340	351	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: O₄S).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	68	Total	O	0	0
			68	68		

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.

Chain A:

Amino Acid	Percentage
MET	6%
GLY	61%
HIS	22%
LEU	6%
GLU	14%
ASP	
ALA	
GLN	
SER	
PRO	
THR	
ILE	
GLN	
ARG	
HIS	
MET	
T75	
T76	
K77	
T78	
E88	
R93	
I94	
Q95	
R100	
M101	
V102	
T106	
I107	
M108	
I109	
A110	
L116	
E123	
T124	
I125	
R126	
I127	
R128	
I129	
L130	
P131	
Q132	
V133	
I136	
T137	
P138	
M139	
L140	
A144	
A145	
L146	
A149	
P150	
H151	
A152	
R153	
T154	
E157	
C174	

Chain B:

MET	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	TYR	HIS	ILE	GLN	ARG	HIS	M1	I4	A10	G11	T12	I20	L24	S28	A29	L30	G31	V37	I38	V42	A43	E44	N45	T46	Q50	P57	V60	A61	A62	Q63	L64	D70					
T75	T76	K77	I86	V87	E88	R93	L94	Q95	R100	M101	V102	V103	I104	D105	T106	M108	V107	A109	L116	L123	T124	R125	R126	V127	R128	L129	L130	P131	Q132	V133	I136	T137	P138	N139	L140	A144	A145	L146	A149	P150	H151	A152	T153	L154	P155	Q156			
E157	G177	GLY	HIS	LEU	GLU	ASP	ALA	GLN	SER	PRO	D187	T191	R192	E193	F198	SER	ALA	PRO	R202	V203	M204	T205	K206	N207	A220	A221	L222	R223	P224	R225	E226	R227	S228	W229	T232	V233	E234	E235	V252	E253	E254	G255	L256	G257	H260	E261	F262	V265	W266

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.72Å 77.72Å 183.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 35.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.30) 99.8 (35.21-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.272 0.232 , 0.270	Depositor DCC
R_{free} test set	2603 reflections (10.11%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 33624 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3923	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 23.69 % 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 4.4379e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/1913	0.59	0/2597
1	B	0.33	0/1913	0.59	0/2597
All	All	0.33	0/3826	0.59	0/5194

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	1882	0	1893	80	0
1	B	1882	0	1893	77	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	71	0	0	6	0
3	B	68	0	0	2	0
All	All	3923	0	3786	149	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 20.

All (149) 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:213:CYS:HB3	3:A:2069:HOH:O	1.75	0.85
1:A:228:SER:O	1:A:232:THR:HG22	1.83	0.79
1:B:154:THR:HG22	1:B:157:GLU:HG3	1.64	0.78
1:A:46:THR:CG2	1:A:255:GLY:H	1.96	0.78
1:B:46:THR:CG2	1:B:255:GLY:H	1.97	0.77
1:A:154:THR:HG22	1:A:157:GLU:HG3	1.66	0.77
1:A:29:ALA:HA	1:A:265:TRP:CH2	2.20	0.77
1:B:228:SER:O	1:B:232:THR:HG22	1.84	0.77
1:B:29:ALA:HA	1:B:265:TRP:CH2	2.20	0.76
1:A:45:ASN:HD21	1:B:70:ASP:HB2	1.51	0.75
1:B:60:VAL:HG21	1:B:86:ILE:HD12	1.69	0.75
1:A:70:ASP:HB2	1:B:45:ASN:HD21	1.52	0.73
1:A:60:VAL:HG21	1:A:86:ILE:HD12	1.69	0.72
1:A:126:ARG:HA	1:A:130:LEU:HD22	1.72	0.71
1:B:126:ARG:HA	1:B:130:LEU:HD22	1.73	0.69
1:A:22:ALA:HB3	3:A:2069:HOH:O	1.94	0.68
1:B:45:ASN:HB2	1:B:50:GLN:HE22	1.60	0.67
1:A:95:GLN:HB2	1:A:132:GLN:HE22	1.61	0.66
1:B:95:GLN:HB2	1:B:132:GLN:HE22	1.60	0.66
1:B:100:ARG:HH11	1:B:100:ARG:HB3	1.60	0.66
1:B:29:ALA:HA	1:B:265:TRP:CZ3	2.31	0.65
1:A:29:ALA:HA	1:A:265:TRP:CZ3	2.30	0.65
1:B:10:ALA:HB1	3:B:2019:HOH:O	1.96	0.65
1:A:45:ASN:HB2	1:A:50:GLN:HE22	1.61	0.65
1:A:100:ARG:HH11	1:A:100:ARG:HB3	1.63	0.64
1:B:46:THR:HG21	1:B:253:GLY:HA3	1.81	0.63
1:A:46:THR:HG21	1:A:253:GLY:HA3	1.82	0.62
1:B:126:ARG:HB3	3:B:2064:HOH:O	2.02	0.59
1:A:4:ILE:HD12	1:A:224:PRO:HG2	1.83	0.59
1:A:10:ALA:HB1	3:A:2012:HOH:O	2.02	0.59
1:A:42:VAL:HG22	1:A:44:GLU:HB2	1.85	0.59
1:B:4:ILE:HD12	1:B:224:PRO:HG2	1.84	0.58
1:B:136:ILE:HG12	1:B:138:PRO:HD3	1.84	0.58
1:B:42:VAL:HG22	1:B:44:GLU:HB2	1.85	0.58
1:A:229:TRP:HA	1:A:232:THR:HG23	1.86	0.57
1:A:136:ILE:HG12	1:A:138:PRO:HD3	1.85	0.57
1:A:37:VAL:HG21	1:A:64:LEU:HD13	1.86	0.57
1:B:75:THR:HG22	1:B:101:ASN:HB3	1.87	0.56
1:B:191:THR:HG22	1:B:192:ARG:N	2.19	0.56
1:B:46:THR:HG23	1:B:255:GLY:H	1.69	0.56
1:B:60:VAL:O	1:B:64:LEU:HD22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:O	1:A:64:LEU:HD22	2.05	0.56
1:A:191:THR:HG22	1:A:192:ARG:N	2.20	0.56
1:B:229:TRP:HA	1:B:232:THR:HG23	1.88	0.55
1:A:46:THR:HG23	1:A:255:GLY:H	1.69	0.55
1:B:223:ARG:HB3	1:B:224:PRO:HD3	1.89	0.54
1:B:226:HIS:NE2	1:B:235:GLU:OE1	2.40	0.54
1:A:223:ARG:HB3	1:A:224:PRO:HD3	1.89	0.54
1:A:75:THR:HG22	1:A:101:ASN:HB3	1.91	0.53
1:A:225:ARG:HD2	3:A:2017:HOH:O	2.09	0.53
1:B:37:VAL:HG21	1:B:64:LEU:HD13	1.89	0.53
1:A:38:ILE:H	1:A:63:GLN:HE22	1.57	0.52
1:A:229:TRP:HA	1:A:232:THR:CG2	2.39	0.52
1:B:229:TRP:HA	1:B:232:THR:CG2	2.39	0.52
1:A:75:THR:HG21	1:A:220:ALA:O	2.10	0.51
1:B:38:ILE:H	1:B:63:GLN:HE22	1.57	0.51
1:B:100:ARG:HH11	1:B:100:ARG:CB	2.24	0.51
1:B:38:ILE:H	1:B:63:GLN:NE2	2.09	0.51
1:A:38:ILE:H	1:A:63:GLN:NE2	2.09	0.50
1:B:207:ASN:ND2	1:B:257:GLY:H	2.09	0.50
1:A:226:HIS:NE2	1:A:235:GLU:OE1	2.42	0.50
1:B:75:THR:HG21	1:B:220:ALA:O	2.12	0.50
1:A:207:ASN:ND2	1:A:257:GLY:H	2.09	0.50
1:B:61:ALA:HB1	1:B:93:ARG:NH2	2.27	0.50
1:A:109:LEU:O	1:A:109:LEU:HG	2.12	0.49
1:A:61:ALA:HB1	1:A:93:ARG:NH2	2.27	0.49
1:B:123:GLU:HA	1:B:126:ARG:HD3	1.95	0.49
1:A:106:THR:HG21	1:A:138:PRO:HB3	1.95	0.49
1:A:126:ARG:NH2	1:A:146:LEU:O	2.45	0.48
1:A:125:LEU:HD23	1:A:130:LEU:HD13	1.94	0.48
1:A:260:HIS:HD2	3:A:2066:HOH:O	1.96	0.48
1:B:45:ASN:HB2	1:B:50:GLN:NE2	2.27	0.48
1:B:12:THR:O	1:B:42:VAL:HG13	2.14	0.48
1:B:77:LYS:HD3	1:B:77:LYS:C	2.33	0.48
1:A:123:GLU:HA	1:A:126:ARG:HD3	1.96	0.48
1:B:125:LEU:HD23	1:B:130:LEU:HD13	1.95	0.48
1:B:109:LEU:O	1:B:109:LEU:HG	2.13	0.48
1:A:46:THR:HG21	1:A:255:GLY:H	1.75	0.48
1:A:45:ASN:HB2	1:A:50:GLN:NE2	2.28	0.48
1:B:126:ARG:NH2	1:B:146:LEU:O	2.47	0.47
1:B:106:THR:HG21	1:B:138:PRO:HB3	1.96	0.47
1:B:140:LEU:HD23	1:B:151:HIS:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ALA:HB1	1:B:149:ALA:O	2.14	0.47
1:A:77:LYS:HD3	1:A:77:LYS:C	2.34	0.47
1:A:75:THR:HG22	1:A:101:ASN:CB	2.44	0.47
1:B:75:THR:HG22	1:B:101:ASN:CB	2.45	0.47
1:B:140:LEU:HD23	1:B:151:HIS:CE1	2.50	0.46
1:A:144:ALA:HB1	1:A:149:ALA:O	2.15	0.46
1:A:70:ASP:CB	1:B:45:ASN:HD21	2.25	0.46
1:A:46:THR:HG23	1:A:255:GLY:N	2.30	0.46
1:A:100:ARG:HH11	1:A:100:ARG:CB	2.28	0.46
1:A:140:LEU:HD23	1:A:151:HIS:CE1	2.50	0.46
1:A:75:THR:HG21	1:A:224:PRO:HD3	1.98	0.45
1:A:46:THR:HG23	1:A:255:GLY:CA	2.47	0.45
1:B:46:THR:HG23	1:B:255:GLY:N	2.31	0.45
1:B:75:THR:HG21	1:B:224:PRO:HD3	1.99	0.45
1:A:28:SER:O	1:A:265:TRP:HH2	1.99	0.45
1:A:140:LEU:HD23	1:A:151:HIS:HE1	1.80	0.45
1:B:20:ILE:O	1:B:24:LEU:HB2	2.17	0.45
1:A:12:THR:O	1:A:42:VAL:HG13	2.15	0.45
1:A:191:THR:CG2	1:A:193:GLU:HG2	2.46	0.45
1:A:265:TRP:CE3	1:B:265:TRP:CZ3	3.05	0.45
1:A:262:PHE:HD1	1:A:265:TRP:CE3	2.35	0.45
1:A:265:TRP:CZ3	1:B:265:TRP:CE3	3.05	0.45
1:B:46:THR:HG23	1:B:255:GLY:CA	2.48	0.44
1:B:46:THR:HG21	1:B:255:GLY:H	1.76	0.44
1:A:20:ILE:O	1:A:24:LEU:HB2	2.18	0.44
1:B:28:SER:O	1:B:265:TRP:HH2	2.01	0.44
1:B:46:THR:HG21	1:B:253:GLY:CA	2.47	0.44
1:B:262:PHE:HD1	1:B:265:TRP:CE3	2.36	0.44
1:B:191:THR:CG2	1:B:193:GLU:HG2	2.47	0.44
1:B:93:ARG:HG2	1:B:93:ARG:HH11	1.83	0.44
1:B:191:THR:CG2	1:B:192:ARG:N	2.81	0.43
1:A:45:ASN:HD21	1:B:70:ASP:CB	2.24	0.43
1:B:88:GLU:OE1	1:B:128:ARG:HD3	2.18	0.43
1:A:260:HIS:HE1	1:A:266:TRP:OXT	2.00	0.43
1:B:123:GLU:O	1:B:126:ARG:HG2	2.18	0.43
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.84	0.43
1:B:260:HIS:HE1	1:B:266:TRP:OXT	2.01	0.43
1:A:57:PRO:HA	1:A:86:ILE:CD1	2.49	0.43
1:A:191:THR:CG2	1:A:192:ARG:N	2.82	0.42
1:A:88:GLU:OE1	1:A:128:ARG:HD3	2.19	0.42
1:B:229:TRP:O	1:B:233:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:HG21	1:A:253:GLY:CA	2.48	0.42
1:A:191:THR:HG22	1:A:193:GLU:HG2	2.01	0.42
1:A:191:THR:HG22	1:A:193:GLU:H	1.85	0.42
1:B:154:THR:CG2	1:B:157:GLU:HG3	2.43	0.42
1:A:154:THR:CG2	1:A:157:GLU:HG3	2.44	0.41
1:B:57:PRO:HA	1:B:86:ILE:CD1	2.49	0.41
1:B:191:THR:HG22	1:B:193:GLU:H	1.84	0.41
1:A:123:GLU:O	1:A:126:ARG:HG2	2.19	0.41
1:A:57:PRO:HA	1:A:86:ILE:HD13	2.03	0.41
1:A:45:ASN:OD1	1:A:46:THR:N	2.54	0.41
1:B:191:THR:HG22	1:B:193:GLU:HG2	2.03	0.41
1:A:223:ARG:HD2	1:A:232:THR:HG21	2.02	0.41
1:A:262:PHE:CZ	1:B:28:SER:HB3	2.56	0.41
1:B:45:ASN:OD1	1:B:46:THR:N	2.54	0.41
1:B:123:GLU:HA	1:B:126:ARG:CD	2.51	0.41
1:B:223:ARG:HD2	1:B:232:THR:HG21	2.02	0.41
1:B:57:PRO:HA	1:B:86:ILE:HD13	2.03	0.41
1:A:60:VAL:O	1:A:64:LEU:CD2	2.69	0.41
1:A:266:TRP:CE2	1:B:31:GLY:HA2	2.56	0.41
1:A:108:MET:O	1:A:109:LEU:C	2.59	0.40
1:A:125:LEU:C	1:A:125:LEU:HD23	2.42	0.40
1:B:75:THR:HG23	1:B:224:PRO:HG3	2.04	0.40
1:A:223:ARG:HD3	1:A:229:TRP:CZ3	2.57	0.40
1:B:108:MET:O	1:B:109:LEU:C	2.59	0.40
1:A:116:LEU:HD22	3:A:2072:HOH:O	2.21	0.40
1:B:125:LEU:HD23	1:B:125:LEU:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/288 (83%)	233 (97%)	7 (3%)	0	100	100
1	B	240/288 (83%)	233 (97%)	7 (3%)	0	100	100
All	All	480/576 (83%)	466 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	196/228 (86%)	181 (92%)	15 (8%)	16	20
1	B	196/228 (86%)	180 (92%)	16 (8%)	14	17
All	All	392/456 (86%)	361 (92%)	31 (8%)	15	19

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	24	LEU
1	A	42	VAL
1	A	46	THR
1	A	64	LEU
1	A	77	LYS
1	A	94	LEU
1	A	100	ARG
1	A	130	LEU
1	A	133	VAL
1	A	193	GLU
1	A	222	LEU
1	A	225	ARG
1	A	232	THR
1	A	252	VAL
1	B	4	ILE
1	B	24	LEU
1	B	42	VAL

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Mol	Chain	Res	Type
1	B	46	THR
1	B	64	LEU
1	B	75	THR
1	B	77	LYS
1	B	94	LEU
1	B	100	ARG
1	B	130	LEU
1	B	133	VAL
1	B	193	GLU
1	B	222	LEU
1	B	225	ARG
1	B	232	THR
1	B	252	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	63	GLN
1	A	132	GLN
1	A	156	GLN
1	A	161	GLN
1	A	196	GLN
1	A	207	ASN
1	A	246	GLN
1	A	260	HIS
1	A	261	HIS
1	B	50	GLN
1	B	63	GLN
1	B	132	GLN
1	B	156	GLN
1	B	161	GLN
1	B	196	GLN
1	B	207	ASN
1	B	246	GLN
1	B	260	HIS
1	B	261	HIS

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	2001	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	A	2003	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	B	2002	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	B	2004	-	4,4,4	0.26	0	6,6,6	0.06	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	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2004	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	248/288 (86%)	0.32	16 (6%) 22 30	25, 38, 64, 90	0
1	B	248/288 (86%)	0.42	17 (6%) 20 27	25, 38, 64, 90	0
All	All	496/576 (86%)	0.37	33 (6%) 21 29	25, 38, 65, 90	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	VAL	6.6
1	A	202	ARG	6.0
1	B	153	ARG	5.6
1	B	203	VAL	5.5
1	B	204	ASN	4.6
1	B	109	LEU	4.0
1	A	227	ARG	4.0
1	A	204	ASN	3.9
1	A	265	TRP	3.8
1	A	206	LYS	3.8
1	B	192	ARG	3.8
1	A	193	GLU	3.7
1	A	153	ARG	3.5
1	B	100	ARG	3.2
1	B	202	ARG	3.1
1	B	227	ARG	3.0
1	B	154	THR	3.0
1	B	193	GLU	2.9
1	A	192	ARG	2.9
1	B	206	LYS	2.9
1	A	123	GLU	2.8
1	B	156	GLN	2.7
1	B	104	LEU	2.6
1	B	116	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	109	LEU	2.5
1	B	20	ILE	2.5
1	A	20	ILE	2.4
1	B	103	VAL	2.4
1	B	265	TRP	2.3
1	A	100	ARG	2.3
1	A	126	ARG	2.2
1	A	102	VAL	2.2
1	A	197	ARG	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	2001	5/5	0.70	0.24	5.63	76,76,77,79	0
2	SO4	B	2004	5/5	0.83	0.20	2.02	67,67,67,69	5
2	SO4	B	2002	5/5	0.83	0.18	1.68	70,71,71,74	0
2	SO4	A	2003	5/5	0.86	0.20	1.67	60,62,63,63	5

6.5 Other polymers [i](#)

There are no such residues in this entry.