



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:13 AM GMT

PDB ID : 4M6R  
Title : Structural and biochemical basis for the inhibition of cell death by APIP, a methionine salvage enzyme  
Authors : Kang, W.; Hong, S.H.; Lee, H.M.; Kim, N.Y.; Lim, Y.C.; Le, L.T.M.; Lim, B.; Kim, H.C.; Kim, T.Y.; Ashida, H.; Yokota, A.; Hah, S.S.; Chun, K.H.; Jung, Y.K.; Yang, J.K.  
Deposited on : 2013-08-10  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

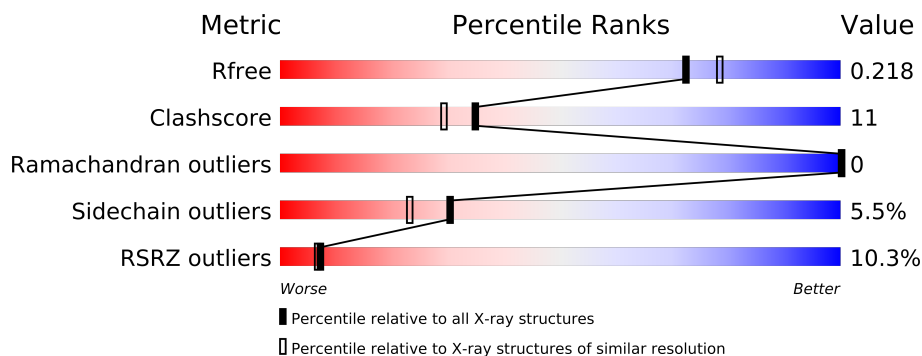
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
1	C	224	
1	D	224	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7620 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Methylthioribulose-1-phosphatedehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1767	1125	298	326	18			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1125	298	326	18			
1	C	224	Total	C	N	O	S	0	0	0
			1767	1125	298	326	18			
1	D	221	Total	C	N	O	S	0	0	0
			1748	1112	295	323	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP Q96GX9
B	19	MET	-	EXPRESSION TAG	UNP Q96GX9
C	19	MET	-	EXPRESSION TAG	UNP Q96GX9
D	19	MET	-	EXPRESSION TAG	UNP Q96GX9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

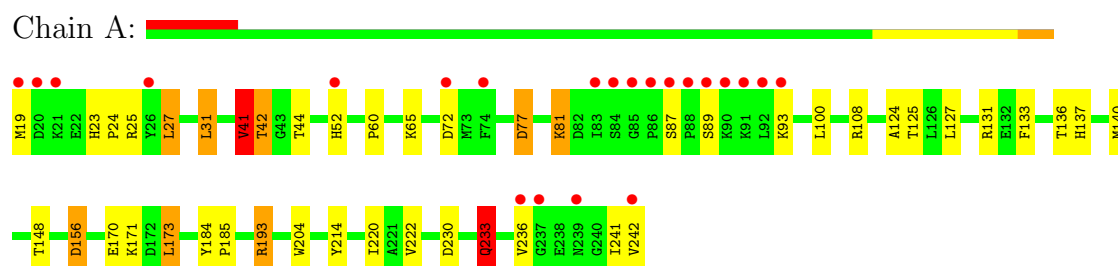
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	157	Total 157	O 157	0	0
3	C	127	Total 127	O 127	0	0
3	D	138	Total 138	O 138	0	0

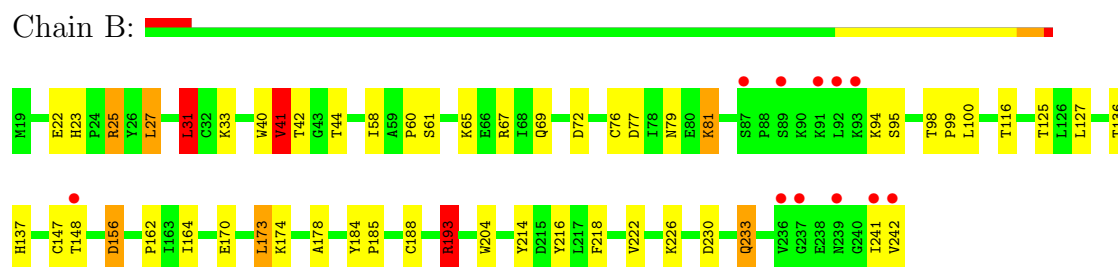
### 3 Residue-property plots

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.

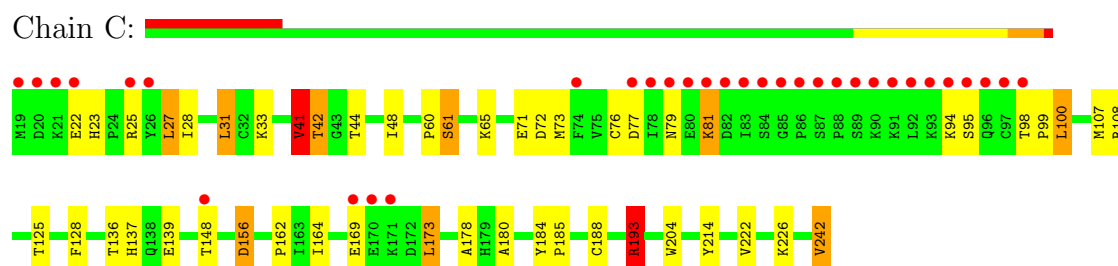
- Molecule 1: Methylthioribulose-1-phosphatedehydratase



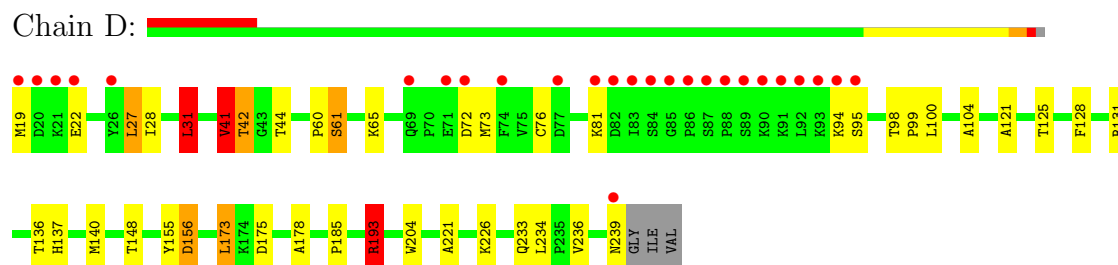
- Molecule 1: Methylthioribulose-1-phosphatedehydratase



- Molecule 1: Methylthioribulose-1-phosphatedehydratase



- Molecule 1: Methylthioribulose-1-phosphatedehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.03Å 107.73Å 192.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 40.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.00) 96.0 (40.59-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.181 , 0.220 0.182 , 0.218	Depositor DCC
$R_{free}$ test set	3616 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.2	EDS
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72021 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.22	7/1810 (0.4%)	1.16	10/2442 (0.4%)
1	B	1.21	7/1810 (0.4%)	1.18	10/2442 (0.4%)
1	C	1.21	7/1810 (0.4%)	1.27	9/2442 (0.4%)
1	D	1.23	8/1791 (0.4%)	1.26	10/2416 (0.4%)
All	All	1.22	29/7221 (0.4%)	1.22	39/9742 (0.4%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	156	ASP	CB-CG	-10.25	1.30	1.51
1	D	128	PHE	CE2-CZ	7.82	1.52	1.37
1	B	156	ASP	CB-CG	-7.33	1.36	1.51
1	C	156	ASP	CB-CG	-7.30	1.36	1.51
1	A	156	ASP	CB-CG	-7.15	1.36	1.51
1	A	193	ARG	CD-NE	-6.77	1.34	1.46
1	C	178	ALA	CA-CB	6.58	1.66	1.52
1	D	193	ARG	CD-NE	-6.34	1.35	1.46
1	A	133	PHE	CE1-CZ	6.32	1.49	1.37
1	B	214	TYR	CD2-CE2	6.09	1.48	1.39
1	C	214	TYR	CD2-CE2	5.80	1.48	1.39
1	C	193	ARG	CD-NE	-5.66	1.36	1.46
1	D	128	PHE	CG-CD1	5.64	1.47	1.38
1	B	193	ARG	CD-NE	-5.59	1.36	1.46
1	C	180	ALA	CA-CB	5.55	1.64	1.52
1	D	178	ALA	CA-CB	5.43	1.63	1.52
1	C	128	PHE	CE2-CZ	5.39	1.47	1.37
1	B	178	ALA	CA-CB	5.38	1.63	1.52
1	C	139	GLU	CG-CD	5.37	1.60	1.51
1	A	233	GLN	CB-CG	-5.34	1.38	1.52
1	B	216	TYR	CD1-CE1	5.32	1.47	1.39
1	A	214	TYR	CD2-CE2	5.31	1.47	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	121	ALA	CA-CB	5.25	1.63	1.52
1	D	221	ALA	CA-CB	5.20	1.63	1.52
1	A	124	ALA	CA-CB	5.15	1.63	1.52
1	B	214	TYR	CD1-CE1	5.13	1.47	1.39
1	B	218	PHE	CE2-CZ	5.04	1.47	1.37
1	D	104	ALA	CA-CB	5.04	1.63	1.52
1	A	184	TYR	CD1-CE1	-5.01	1.31	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	ARG	NE-CZ-NH2	-26.00	107.30	120.30
1	D	193	ARG	NE-CZ-NH2	-23.83	108.39	120.30
1	C	193	ARG	NE-CZ-NH1	22.69	131.65	120.30
1	D	193	ARG	NE-CZ-NH1	21.50	131.05	120.30
1	A	193	ARG	NE-CZ-NH2	-20.92	109.84	120.30
1	B	193	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	B	193	ARG	NE-CZ-NH1	18.70	129.65	120.30
1	A	193	ARG	NE-CZ-NH1	17.70	129.15	120.30
1	D	156	ASP	CB-CG-OD1	-16.39	103.55	118.30
1	B	156	ASP	CB-CG-OD1	-12.21	107.31	118.30
1	C	156	ASP	CB-CG-OD1	-11.64	107.82	118.30
1	A	156	ASP	CB-CG-OD1	-10.44	108.91	118.30
1	A	41	VAL	CG1-CB-CG2	10.00	126.91	110.90
1	C	41	VAL	CG1-CB-CG2	8.85	125.05	110.90
1	B	41	VAL	CG1-CB-CG2	8.77	124.93	110.90
1	D	41	VAL	CG1-CB-CG2	8.52	124.53	110.90
1	C	193	ARG	CD-NE-CZ	8.19	135.07	123.60
1	D	193	ARG	CD-NE-CZ	7.84	134.57	123.60
1	B	127	LEU	CA-CB-CG	-6.56	100.22	115.30
1	B	193	ARG	CD-NE-CZ	6.53	132.75	123.60
1	A	193	ARG	CD-NE-CZ	6.43	132.60	123.60
1	B	31	LEU	CB-CG-CD1	6.42	121.92	111.00
1	C	108	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	127	LEU	CA-CB-CG	-6.17	101.12	115.30
1	A	108	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	D	156	ASP	OD1-CG-OD2	6.12	134.92	123.30
1	D	156	ASP	N-CA-CB	-5.96	99.88	110.60
1	A	108	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	C	156	ASP	N-CA-CB	-5.67	100.40	110.60
1	B	25	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	156	ASP	CB-CG-OD2	5.49	123.24	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ASP	CB-CG-OD1	5.35	123.12	118.30
1	D	175	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	100	LEU	CA-CB-CG	-5.24	103.25	115.30
1	C	156	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	156	ASP	CB-CA-C	-5.13	100.13	110.40
1	A	156	ASP	N-CA-CB	-5.07	101.47	110.60
1	B	67	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	31	LEU	CB-CG-CD1	5.00	119.51	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1767	0	1756	34	0
1	B	1767	0	1756	44	0
1	C	1767	0	1756	41	0
1	D	1748	0	1733	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	145	0	0	16	0
3	B	157	0	0	19	0
3	C	127	0	0	19	0
3	D	138	0	0	16	0
All	All	7620	0	7001	151	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:226:LYS:HG3	3:D:476:HOH:O	1.24	1.29
1:B:58:ILE:HD13	3:B:531:HOH:O	1.30	1.29
1:B:58:ILE:CD1	3:B:531:HOH:O	1.83	1.23
1:A:93:LYS:HG2	3:A:441:HOH:O	1.38	1.23
1:B:174:LYS:HE3	3:B:543:HOH:O	1.45	1.17
1:D:236:VAL:HA	3:D:519:HOH:O	1.59	1.01
1:C:188:CYS:SG	3:C:506:HOH:O	2.18	1.00
1:A:87:SER:HB2	3:A:476:HOH:O	1.62	0.96
1:C:222:VAL:HG21	3:C:494:HOH:O	1.71	0.91
1:B:148:THR:HG23	1:B:185:PRO:O	1.74	0.86
1:C:169:GLU:HB3	3:C:493:HOH:O	1.77	0.85
1:C:48:ILE:O	3:C:467:HOH:O	1.95	0.83
1:B:42:THR:HB	3:B:411:HOH:O	1.76	0.83
1:D:131:ARG:HD3	3:D:528:HOH:O	1.79	0.82
1:D:42:THR:OG1	3:D:527:HOH:O	1.96	0.82
1:D:233:GLN:HE21	1:D:234:LEU:H	1.27	0.82
1:D:233:GLN:OE1	3:D:510:HOH:O	1.97	0.81
1:C:148:THR:HG23	1:C:185:PRO:O	1.79	0.81
1:A:89:SER:HB3	3:A:528:HOH:O	1.82	0.79
1:D:148:THR:HG23	1:D:185:PRO:O	1.82	0.78
1:A:148:THR:HG23	1:A:185:PRO:O	1.84	0.77
1:B:226:LYS:HD2	3:B:449:HOH:O	1.84	0.74
1:C:222:VAL:CG2	3:C:494:HOH:O	2.34	0.73
1:B:22:GLU:OE2	3:B:454:HOH:O	2.06	0.73
1:B:72:ASP:OD1	3:B:504:HOH:O	2.08	0.72
3:C:431:HOH:O	1:D:42:THR:HG21	1.91	0.71
3:A:429:HOH:O	1:B:42:THR:HG21	1.91	0.70
1:A:42:THR:HB	3:A:412:HOH:O	1.92	0.69
1:A:89:SER:CB	3:A:528:HOH:O	2.38	0.69
1:B:148:THR:HG22	3:B:498:HOH:O	1.93	0.69
1:C:148:THR:CG2	3:C:487:HOH:O	2.41	0.69
1:A:230:ASP:HB3	1:A:233:GLN:HG2	1.74	0.69
1:C:169:GLU:C	3:C:493:HOH:O	2.32	0.68
1:C:65:LYS:HE3	3:C:436:HOH:O	1.94	0.68
1:B:100:LEU:HD21	1:B:173:LEU:HD13	1.75	0.67
1:B:147:CYS:HA	3:B:471:HOH:O	1.95	0.65
1:D:233:GLN:HE21	1:D:234:LEU:N	1.95	0.64
1:C:148:THR:HG21	3:C:487:HOH:O	1.97	0.64
1:A:42:THR:HG21	3:D:411:HOH:O	1.97	0.64
1:A:170:GLU:O	3:A:452:HOH:O	2.15	0.63
1:C:100:LEU:HD21	1:C:173:LEU:HD13	1.79	0.63
1:C:33:LYS:HE2	3:C:449:HOH:O	1.98	0.63
3:A:429:HOH:O	1:B:42:THR:CG2	2.48	0.62

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:136:THR:OG1	1:A:137:HIS:HD2	1.84	0.61
1:D:226:LYS:HD3	3:D:525:HOH:O	1.99	0.61
1:A:100:LEU:HD21	1:A:173:LEU:HD13	1.82	0.61
1:D:131:ARG:CD	3:D:528:HOH:O	2.42	0.61
1:B:230:ASP:HB3	1:B:233:GLN:HG2	1.83	0.60
1:D:22:GLU:HB3	3:D:516:HOH:O	2.02	0.60
1:C:242:VAL:C	3:C:489:HOH:O	2.40	0.59
1:C:27:LEU:HD11	1:C:204:TRP:CE2	2.38	0.59
1:C:27:LEU:HD22	1:C:31:LEU:HD22	1.83	0.59
1:D:226:LYS:CG	3:D:476:HOH:O	2.05	0.59
1:C:42:THR:HB	3:C:404:HOH:O	2.03	0.58
1:B:98:THR:HG23	3:B:531:HOH:O	2.04	0.58
1:D:60:PRO:HG3	1:D:72:ASP:HB3	1.87	0.57
1:A:72:ASP:OD1	3:A:516:HOH:O	2.17	0.57
1:A:60:PRO:HG3	1:A:72:ASP:HB3	1.88	0.56
1:D:136:THR:OG1	1:D:137:HIS:HD2	1.89	0.56
1:B:125:THR:O	1:B:193:ARG:HD3	2.06	0.56
1:B:60:PRO:HG3	1:B:72:ASP:HB3	1.87	0.55
1:D:100:LEU:HD21	1:D:173:LEU:HD13	1.89	0.55
1:C:136:THR:OG1	1:C:137:HIS:HD2	1.90	0.54
1:C:25:ARG:HD2	3:C:471:HOH:O	2.07	0.54
1:D:125:THR:O	1:D:193:ARG:HD3	2.08	0.54
1:A:87:SER:CB	3:A:476:HOH:O	2.34	0.54
1:B:41:VAL:HG13	1:B:65:LYS:HB2	1.90	0.54
1:A:27:LEU:HD11	1:A:204:TRP:CE2	2.43	0.54
1:A:140:MET:CE	1:B:42:THR:HG22	2.38	0.53
1:A:100:LEU:CD2	1:A:173:LEU:HD13	2.38	0.53
1:C:100:LEU:CD2	1:C:173:LEU:HD13	2.39	0.52
3:B:409:HOH:O	1:C:42:THR:HG21	2.08	0.52
1:A:27:LEU:HD22	1:A:31:LEU:HD22	1.92	0.52
1:B:100:LEU:CD2	1:B:173:LEU:HD13	2.40	0.52
1:C:148:THR:HG22	3:C:487:HOH:O	2.06	0.52
1:C:41:VAL:HG13	1:C:65:LYS:HB2	1.92	0.51
1:B:241:ILE:HB	1:C:164:ILE:HG22	1.92	0.51
1:B:58:ILE:HD11	3:B:531:HOH:O	1.79	0.51
1:D:131:ARG:NH2	3:D:467:HOH:O	2.42	0.51
1:B:27:LEU:HD22	1:B:31:LEU:HD22	1.91	0.51
1:D:137:HIS:HE1	3:D:422:HOH:O	1.93	0.51
1:C:226:LYS:HE3	3:C:492:HOH:O	2.12	0.50
1:C:61:SER:HB2	1:C:95:SER:HA	1.93	0.50
1:C:162:PRO:HB3	1:C:184:TYR:CD2	2.47	0.50
1:C:98:THR:HB	1:C:99:PRO:HD3	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:27:LEU:HD22	1:D:31:LEU:HD22	1.93	0.50
1:C:77:ASP:OD1	1:C:81:LYS:HG2	2.12	0.49
1:A:44:THR:O	1:A:65:LYS:NZ	2.46	0.49
1:D:131:ARG:NE	3:D:467:HOH:O	2.14	0.49
1:C:28:ILE:HG21	1:C:73:MET:HE1	1.94	0.49
1:B:77:ASP:OD1	1:B:81:LYS:HG2	2.12	0.49
1:C:41:VAL:HG13	1:C:65:LYS:CB	2.43	0.49
1:A:42:THR:HG22	1:D:140:MET:CE	2.43	0.48
1:C:44:THR:O	1:C:65:LYS:NZ	2.46	0.48
1:C:107:MET:C	3:C:507:HOH:O	2.51	0.48
1:B:61:SER:HB2	1:B:95:SER:HA	1.94	0.48
1:D:76:CYS:HB3	1:D:94:LYS:NZ	2.29	0.48
1:A:241:ILE:HB	1:B:164:ILE:HG22	1.94	0.48
1:B:23:HIS:CE1	1:B:25:ARG:HG3	2.49	0.48
1:C:60:PRO:HG3	1:C:72:ASP:HB3	1.96	0.48
1:D:61:SER:HB2	1:D:95:SER:HA	1.96	0.47
1:D:100:LEU:CD2	1:D:173:LEU:HD13	2.44	0.47
1:B:136:THR:OG1	1:B:137:HIS:HD2	1.96	0.47
1:D:76:CYS:HB3	1:D:94:LYS:HZ3	1.79	0.47
1:D:27:LEU:HD11	1:D:204:TRP:CE2	2.49	0.47
1:B:98:THR:HB	1:B:99:PRO:HD3	1.96	0.47
1:B:76:CYS:HB3	1:B:94:LYS:NZ	2.29	0.47
1:C:100:LEU:N	1:C:100:LEU:HD12	2.31	0.46
1:A:41:VAL:HG13	1:A:65:LYS:HB2	1.97	0.46
1:D:233:GLN:NE2	1:D:234:LEU:H	2.06	0.45
1:B:170:GLU:O	3:B:527:HOH:O	2.20	0.45
1:A:140:MET:HE1	1:B:42:THR:HG22	1.98	0.45
1:C:23:HIS:CE1	1:C:25:ARG:HG3	2.52	0.45
1:A:131:ARG:HB3	3:A:513:HOH:O	2.16	0.45
1:D:28:ILE:HG21	1:D:73:MET:HE1	1.99	0.45
1:D:131:ARG:NE	3:D:528:HOH:O	2.50	0.44
1:C:22:GLU:HG3	3:C:476:HOH:O	2.17	0.44
1:D:98:THR:HB	1:D:99:PRO:HD3	1.99	0.44
1:A:19:MET:HG3	3:A:526:HOH:O	2.18	0.44
1:B:40:TRP:HB3	1:B:116:THR:HB	2.00	0.44
1:D:41:VAL:HG13	1:D:65:LYS:HB2	2.00	0.43
1:D:41:VAL:HG13	1:D:65:LYS:CB	2.48	0.43
1:A:23:HIS:CE1	1:A:25:ARG:HG3	2.53	0.43
1:B:188:CYS:SG	3:B:512:HOH:O	2.08	0.43
1:B:27:LEU:HD11	1:B:204:TRP:CE2	2.53	0.43
1:D:44:THR:O	1:D:65:LYS:NZ	2.47	0.43
1:C:41:VAL:HG13	1:C:41:VAL:O	2.18	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:137:HIS:HA	1:D:155:TYR:O	2.19	0.43
1:A:131:ARG:HD2	3:A:480:HOH:O	2.18	0.43
1:C:125:THR:O	1:C:193:ARG:HD3	2.19	0.42
1:A:24:PRO:HG2	1:A:52:HIS:HB2	2.00	0.42
1:A:65:LYS:HE3	3:A:511:HOH:O	2.18	0.42
1:B:148:THR:CG2	3:B:498:HOH:O	2.57	0.42
1:A:222:VAL:HG21	3:A:413:HOH:O	2.19	0.42
1:D:42:THR:HB	3:D:428:HOH:O	2.20	0.42
3:C:431:HOH:O	1:D:42:THR:CG2	2.60	0.41
1:C:79:ASN:HB2	1:C:81:LYS:HE2	2.01	0.41
1:C:71:GLU:H	1:C:71:GLU:CD	2.24	0.41
1:B:79:ASN:HB2	1:B:81:LYS:HE2	2.02	0.41
1:A:125:THR:O	1:A:193:ARG:HD3	2.21	0.41
1:B:33:LYS:HE2	3:B:520:HOH:O	2.20	0.41
1:A:77:ASP:OD1	1:A:81:LYS:HG2	2.21	0.41
1:B:44:THR:O	1:B:65:LYS:NZ	2.52	0.41
1:B:222:VAL:CG2	3:B:479:HOH:O	2.69	0.41
1:B:69:GLN:HB2	1:B:72:ASP:OD2	2.21	0.41
1:A:193:ARG:HD2	3:A:427:HOH:O	2.20	0.41
1:C:76:CYS:HB3	1:C:94:LYS:NZ	2.36	0.41
1:A:42:THR:CG2	3:D:411:HOH:O	2.64	0.40
1:B:77:ASP:HB2	3:B:459:HOH:O	2.20	0.40
1:B:222:VAL:HG21	3:B:479:HOH:O	2.20	0.40
1:B:162:PRO:HB3	1:B:184:TYR:CD2	2.57	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	222/224 (99%)	216 (97%)	6 (3%)	0	100	100
1	B	222/224 (99%)	214 (96%)	8 (4%)	0	100	100
1	C	222/224 (99%)	214 (96%)	8 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	219/224 (98%)	213 (97%)	6 (3%)	0	100	100
All	All	885/896 (99%)	857 (97%)	28 (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	193/193 (100%)	181 (94%)	12 (6%)	26	18
1	B	193/193 (100%)	184 (95%)	9 (5%)	36	29
1	C	193/193 (100%)	183 (95%)	10 (5%)	32	25
1	D	191/193 (99%)	180 (94%)	11 (6%)	28	21
All	All	770/772 (100%)	728 (94%)	42 (6%)	30	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	31	LEU
1	A	41	VAL
1	A	42	THR
1	A	81	LYS
1	A	156	ASP
1	A	171	LYS
1	A	173	LEU
1	A	220	ILE
1	A	233	GLN
1	A	236	VAL
1	A	242	VAL
1	B	27	LEU
1	B	31	LEU
1	B	41	VAL
1	B	81	LYS
1	B	156	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	173	LEU
1	B	193	ARG
1	B	233	GLN
1	B	242	VAL
1	C	27	LEU
1	C	31	LEU
1	C	41	VAL
1	C	42	THR
1	C	61	SER
1	C	81	LYS
1	C	156	ASP
1	C	173	LEU
1	C	193	ARG
1	C	242	VAL
1	D	19	MET
1	D	27	LEU
1	D	31	LEU
1	D	41	VAL
1	D	42	THR
1	D	61	SER
1	D	81	LYS
1	D	156	ASP
1	D	173	LEU
1	D	193	ARG
1	D	239	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	137	HIS
1	A	138	GLN
1	B	34	GLN
1	B	137	HIS
1	C	34	GLN
1	C	137	HIS
1	D	34	GLN
1	D	137	HIS
1	D	138	GLN
1	D	233	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

## 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, 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	224/224 (100%)	0.39	22 (9%) 8 7	12, 27, 59, 75	0
1	B	224/224 (100%)	0.21	11 (4%) 28 28	12, 26, 58, 65	0
1	C	224/224 (100%)	0.79	33 (14%) 3 3	13, 27, 59, 76	0
1	D	221/224 (98%)	0.51	26 (11%) 5 5	12, 26, 59, 70	0
All	All	893/896 (99%)	0.48	92 (10%) 7 7	12, 26, 59, 76	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	SER	10.3
1	C	85	GLY	9.4
1	C	88	PRO	8.9
1	C	86	PRO	8.9
1	C	87	SER	8.7
1	C	92	LEU	8.3
1	C	19	MET	7.9
1	C	79	ASN	7.8
1	C	83	ILE	7.6
1	C	97	CYS	7.1
1	C	78	ILE	7.0
1	C	82	ASP	7.0
1	D	88	PRO	7.0
1	D	91	LYS	6.7
1	D	89	SER	6.6
1	C	90	LYS	6.6
1	A	91	LYS	6.2
1	A	19	MET	6.2
1	A	87	SER	6.0
1	C	84	SER	5.9
1	A	89	SER	5.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	86	PRO	5.8
1	C	74	PHE	5.7
1	D	19	MET	5.6
1	D	86	PRO	5.6
1	C	96	GLN	5.6
1	A	84	SER	5.5
1	D	21	LYS	5.4
1	D	92	LEU	5.2
1	D	87	SER	5.2
1	C	93	LYS	5.1
1	C	91	LYS	5.1
1	D	93	LYS	5.1
1	C	21	LYS	4.8
1	B	242	VAL	4.6
1	D	20	ASP	4.5
1	D	81	LYS	4.5
1	C	95	SER	4.4
1	A	88	PRO	4.3
1	B	236	VAL	4.2
1	D	85	GLY	4.2
1	C	77	ASP	4.2
1	D	90	LYS	4.2
1	D	239	ASN	4.1
1	C	26	TYR	4.1
1	D	83	ILE	4.1
1	A	236	VAL	4.0
1	A	242	VAL	3.9
1	B	237	GLY	3.9
1	A	239	ASN	3.8
1	C	148	THR	3.7
1	C	94	LYS	3.6
1	D	82	ASP	3.5
1	A	26	TYR	3.4
1	A	93	LYS	3.4
1	D	84	SER	3.3
1	A	85	GLY	3.3
1	C	98	THR	3.3
1	C	20	ASP	3.2
1	C	80	GLU	3.2
1	B	241	ILE	3.2
1	B	91	LYS	3.1
1	D	71	GLU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	239	ASN	3.0
1	D	72	ASP	3.0
1	A	83	ILE	3.0
1	D	26	TYR	2.9
1	C	169	GLU	2.8
1	B	89	SER	2.8
1	A	90	LYS	2.8
1	C	81	LYS	2.6
1	D	22	GLU	2.6
1	A	237	GLY	2.5
1	A	20	ASP	2.5
1	D	95	SER	2.5
1	B	93	LYS	2.5
1	D	77	ASP	2.5
1	C	171	LYS	2.5
1	C	22	GLU	2.5
1	D	69	GLN	2.4
1	B	92	LEU	2.4
1	A	92	LEU	2.3
1	D	74	PHE	2.3
1	B	148	THR	2.3
1	A	74	PHE	2.3
1	A	21	LYS	2.2
1	D	94	LYS	2.2
1	C	170	GLU	2.2
1	C	25	ARG	2.2
1	A	72	ASP	2.1
1	A	52	HIS	2.1
1	B	87	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	301	1/1	0.08	-0.68	18,18,18,18	0
2	ZN	A	301	1/1	0.08	-1.67	20,20,20,20	0
2	ZN	B	301	1/1	0.06	-2.21	17,17,17,17	0
2	ZN	D	301	1/1	0.07	-2.83	19,19,19,19	0

## 6.5 Other polymers

There are no such residues in this entry.