



# Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 03:20 PM GMT

PDB ID : 1V8D  
Title : Crystal structure of the conserved hypothetical protein TT1679 from *Thermus thermophilus*  
Authors : Kishishita, S.; Terada, T.; Shirouzu, M.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-01-05  
Resolution : 2.16 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>

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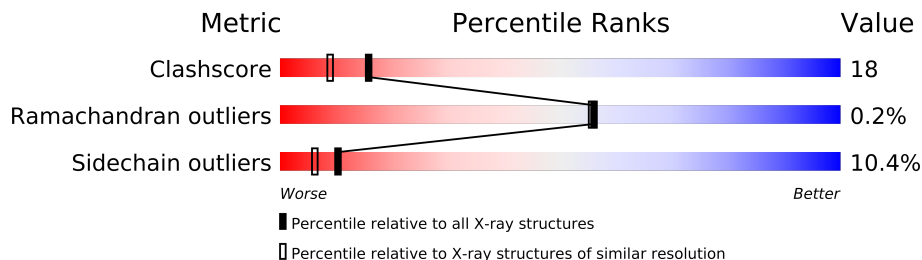
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.16 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	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	235	
1	B	235	
1	C	235	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4610 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 hypothetical protein (TT1679).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1424	907	263	247	7			
1	B	185	Total	C	N	O	S	0	0	0
			1394	885	259	243	7			
1	C	188	Total	C	N	O	S	0	0	0
			1422	903	265	247	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	128	Total	O	0	0
			128	128		
3	C	102	Total	O	0	0
			102	102		



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.80Å 115.22Å 75.27Å 90.00° 129.76° 90.00°	Depositor
Resolution (Å)	34.55 – 2.16	Depositor
% Data completeness (in resolution range)	89.6 (34.55-2.16)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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: 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	1.36	11/1449 (0.8%)	1.28	14/1954 (0.7%)
1	B	1.34	10/1417 (0.7%)	1.25	8/1910 (0.4%)
1	C	1.20	4/1446 (0.3%)	1.13	4/1947 (0.2%)
All	All	1.30	25/4312 (0.6%)	1.22	26/5811 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	GLU	CD-OE2	6.38	1.32	1.25
1	C	204	ALA	CA-CB	6.35	1.65	1.52
1	B	161	GLU	CB-CG	-6.21	1.40	1.52
1	C	185	VAL	CB-CG1	6.08	1.65	1.52
1	B	135	ALA	CA-CB	5.92	1.64	1.52
1	B	134	VAL	CB-CG2	5.91	1.65	1.52
1	B	124	GLU	CG-CD	5.90	1.60	1.51
1	B	58	PHE	CE2-CZ	5.87	1.48	1.37
1	C	133	GLU	CD-OE2	5.79	1.32	1.25
1	A	124	GLU	CG-CD	5.76	1.60	1.51
1	A	161	GLU	CD-OE1	5.68	1.31	1.25
1	C	218	TYR	CE1-CZ	5.64	1.45	1.38
1	A	124	GLU	CD-OE1	5.59	1.31	1.25
1	B	132	GLU	CG-CD	5.50	1.60	1.51
1	A	187	VAL	CB-CG1	5.50	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	ALA	CA-CB	5.37	1.63	1.52
1	A	205	LYS	CE-NZ	5.36	1.62	1.49
1	A	132	GLU	CD-OE2	5.36	1.31	1.25
1	A	132	GLU	CG-CD	5.28	1.59	1.51
1	B	136	VAL	CB-CG2	5.19	1.63	1.52
1	A	128	ALA	CA-CB	5.18	1.63	1.52
1	A	167	ALA	CA-CB	5.17	1.63	1.52
1	A	102	GLU	CD-OE2	5.10	1.31	1.25
1	B	117	ARG	CG-CD	5.09	1.64	1.51
1	B	133	GLU	CG-CD	5.07	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	A	183	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	C	183	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	C	183	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	183	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	215	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	183	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	183	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	A	103	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	103	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	C	194	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	C	196	ILE	N-CA-C	-6.85	92.51	111.00
1	A	202	LEU	CA-CB-CG	6.73	130.78	115.30
1	B	156	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	172	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	156	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	153	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	A	156	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	202	LEU	CB-CG-CD2	5.45	120.26	111.00
1	A	123	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	45	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	123	ARG	CG-CD-NE	-5.13	101.03	111.80
1	A	127	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	194	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	97	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	215	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	218	TYR	Sidechain

## 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	1424	0	1488	49	0
1	B	1394	0	1458	46	0
1	C	1422	0	1482	72	0
2	A	2	0	0	0	0
3	A	138	0	0	16	0
3	B	128	0	0	4	1
3	C	102	0	0	10	0
All	All	4610	0	4428	160	1

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 18.

All (160) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:LEU:HD23	3:A:1540:HOH:O	1.40	1.19
1:B:228:GLU:O	1:B:229:GLU:HG3	1.48	1.11
1:C:131:LYS:HA	1:C:131:LYS:HZ2	1.17	1.06
1:A:172:ASP:O	1:A:202:LEU:HD23	1.56	1.05
1:A:131:LYS:HE2	1:A:163:LEU:HA	1.38	1.02
1:C:131:LYS:HA	1:C:131:LYS:NZ	1.76	0.99
1:A:126:ALA:HA	1:A:131:LYS:HG3	1.51	0.93
1:C:90:HIS:CD2	1:C:153:ARG:HD2	2.06	0.89
1:C:65:LEU:H	1:C:168:HIS:HD2	1.20	0.89
1:B:40:MET:CE	1:B:43:ILE:HD12	2.02	0.89
1:C:90:HIS:HD2	1:C:153:ARG:HD2	1.40	0.87
1:C:229:GLU:HG2	3:C:300:HOH:O	1.74	0.86
1:C:131:LYS:CA	1:C:131:LYS:HZ2	1.91	0.83
1:A:231:LEU:HA	3:A:1540:HOH:O	1.79	0.83
1:C:83:ARG:HD3	3:C:335:HOH:O	1.79	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ARG:NH2	1:A:194:ARG:HH22	1.77	0.83
1:A:161:GLU:HG3	3:A:1503:HOH:O	1.80	0.82
1:C:98:PRO:HB2	1:C:99:PRO:HD3	1.61	0.82
1:C:90:HIS:O	1:C:94:GLU:HB2	1.80	0.80
1:B:40:MET:HE3	1:B:43:ILE:HD12	1.61	0.80
1:B:98:PRO:O	1:B:102:GLU:HG3	1.82	0.80
1:B:129:PHE:HB3	1:B:131:LYS:HE2	1.63	0.79
1:A:190:ARG:HH21	1:A:194:ARG:HH22	1.28	0.78
1:C:51:ALA:HB2	1:C:96:LEU:HD23	1.65	0.78
1:A:172:ASP:HB3	1:A:202:LEU:HG	1.67	0.77
1:C:131:LYS:CA	1:C:131:LYS:NZ	2.46	0.76
1:C:221:GLU:OE1	1:C:221:GLU:N	2.18	0.76
1:B:131:LYS:HA	1:B:131:LYS:HZ3	1.54	0.72
1:A:146:LYS:CB	1:A:146:LYS:HZ3	2.02	0.72
1:C:124:GLU:OE2	1:C:127:ARG:NH1	2.23	0.71
1:A:190:ARG:NH2	1:A:194:ARG:NH2	2.41	0.69
1:C:176:VAL:O	1:C:177:LEU:HB2	1.94	0.68
1:C:41:GLU:OE2	1:C:41:GLU:N	2.27	0.67
1:C:116:ASN:O	1:C:117:ARG:HB2	1.95	0.67
1:B:194:ARG:CZ	1:B:195:LYS:NZ	2.58	0.67
1:C:55:LEU:HD13	1:C:103:ARG:HD3	1.77	0.66
1:B:40:MET:HE2	1:B:43:ILE:HD12	1.77	0.66
1:A:229:GLU:O	3:A:1533:HOH:O	2.12	0.66
1:C:149:ALA:O	1:C:153:ARG:HG3	1.95	0.66
1:B:146:LYS:HB2	1:B:146:LYS:HZ3	1.59	0.66
1:A:139:HIS:CE1	1:A:142:ALA:HB3	2.31	0.66
1:C:200:VAL:HG12	3:C:248:HOH:O	1.94	0.65
1:C:55:LEU:HD13	1:C:103:ARG:CD	2.27	0.65
1:C:60:MET:HE1	1:C:66:PHE:HD2	1.62	0.64
1:B:131:LYS:CA	1:B:131:LYS:HZ3	2.11	0.63
1:C:49:ARG:HH11	1:C:193:VAL:HG23	1.62	0.63
1:C:54:PHE:HE1	1:C:60:MET:HE1	1.63	0.63
1:B:65:LEU:H	1:B:168:HIS:HD2	1.47	0.62
1:B:146:LYS:CB	1:B:146:LYS:HZ3	2.13	0.62
1:C:126:ALA:HA	1:C:131:LYS:HG3	1.81	0.62
1:C:49:ARG:NH1	1:C:192:SER:OG	2.31	0.62
1:B:228:GLU:O	1:B:229:GLU:CG	2.38	0.62
1:C:77:GLY:O	3:C:333:HOH:O	2.16	0.62
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.65	0.62
1:A:86:LEU:HD11	1:C:227:LEU:HD11	1.83	0.61
1:C:221:GLU:H	1:C:221:GLU:CD	2.04	0.60
1:B:194:ARG:NH2	1:B:195:LYS:NZ	2.50	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:PHE:CB	1:B:131:LYS:HE2	2.30	0.60
1:B:40:MET:CE	1:B:43:ILE:CD1	2.77	0.59
1:A:190:ARG:HD2	1:A:194:ARG:HH22	1.67	0.59
1:C:54:PHE:HE1	1:C:60:MET:CE	2.15	0.59
1:A:141:LYS:NZ	3:A:1513:HOH:O	2.35	0.59
1:A:49:ARG:HD3	3:A:1464:HOH:O	2.03	0.59
1:A:141:LYS:HG2	3:A:1432:HOH:O	2.00	0.59
1:B:123:ARG:HD2	1:B:156:ASP:OD2	2.03	0.58
1:A:190:ARG:HH21	1:A:194:ARG:NH2	2.00	0.58
1:C:53:GLU:OE1	1:C:192:SER:OG	2.22	0.58
1:B:194:ARG:CZ	1:B:195:LYS:HZ3	2.16	0.57
1:A:190:ARG:HD2	1:A:194:ARG:NH2	2.19	0.57
1:B:97:LEU:HD11	1:B:107:VAL:HG11	1.87	0.57
1:B:52:GLU:HA	1:B:52:GLU:OE2	2.04	0.57
1:A:226:LYS:HG2	1:B:139:HIS:CD2	2.40	0.57
1:C:113:GLU:CD	1:C:113:GLU:H	2.08	0.56
1:B:40:MET:HE3	1:B:43:ILE:CD1	2.33	0.56
1:A:139:HIS:HD2	3:A:1432:HOH:O	1.89	0.56
1:C:123:ARG:NH1	1:C:156:ASP:OD1	2.39	0.55
1:C:49:ARG:HD3	1:C:193:VAL:HG22	1.88	0.55
1:C:126:ALA:HA	1:C:131:LYS:CG	2.38	0.54
1:C:60:MET:HE1	1:C:66:PHE:CD2	2.41	0.54
1:B:146:LYS:NZ	1:B:146:LYS:CB	2.58	0.53
1:B:139:HIS:HD2	3:B:362:HOH:O	1.90	0.53
1:C:65:LEU:H	1:C:168:HIS:CD2	2.12	0.53
1:B:131:LYS:HA	1:B:131:LYS:NZ	2.24	0.53
1:A:225:LYS:O	1:A:229:GLU:HG3	2.09	0.52
1:A:97:LEU:HD11	1:A:107:VAL:HG11	1.91	0.52
1:A:146:LYS:CA	1:A:146:LYS:HZ3	2.23	0.51
1:C:44:ARG:HH12	1:C:48:GLN:NE2	2.09	0.51
1:B:172:ASP:HB3	1:B:202:LEU:HB2	1.93	0.50
1:A:98:PRO:N	1:A:99:PRO:HD2	2.27	0.50
1:A:146:LYS:HA	1:A:146:LYS:HZ3	1.77	0.49
1:A:223:MET:HE3	1:A:224:LEU:HD13	1.93	0.49
1:C:94:GLU:OE1	1:C:94:GLU:HA	2.13	0.48
1:A:219:THR:HB	1:A:221:GLU:OE2	2.13	0.48
1:C:87:GLU:H	1:C:87:GLU:CD	2.16	0.48
1:C:123:ARG:HD2	1:C:156:ASP:OD2	2.14	0.48
1:C:78:GLU:O	1:C:79:ARG:C	2.52	0.47
1:A:146:LYS:HZ2	1:A:146:LYS:HG3	1.26	0.47
1:A:131:LYS:HB3	1:A:131:LYS:HE3	1.62	0.47
1:B:93:LEU:HB3	1:B:97:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:190:ARG:HA	1:A:194:ARG:HH12	1.80	0.47
1:A:190:ARG:CD	1:A:194:ARG:HH22	2.28	0.47
1:C:62:PRO:HD2	3:C:308:HOH:O	2.15	0.47
1:C:54:PHE:CE1	1:C:60:MET:HE1	2.48	0.46
1:B:164:LYS:HE2	3:B:265:HOH:O	2.15	0.46
1:B:52:GLU:OE2	1:B:52:GLU:CA	2.60	0.46
1:C:87:GLU:N	1:C:87:GLU:CD	2.69	0.46
1:C:140:PRO:HD3	1:C:148:THR:HG21	1.97	0.46
3:A:1533:HOH:O	1:B:141:LYS:NZ	2.49	0.46
1:C:205:LYS:CE	3:C:244:HOH:O	2.63	0.46
1:A:45:ARG:HD2	3:A:1443:HOH:O	2.16	0.45
1:B:207:ARG:HB2	1:B:208:PRO:HD2	1.97	0.45
1:C:83:ARG:NH1	3:C:335:HOH:O	2.20	0.45
1:C:55:LEU:HD13	1:C:103:ARG:HD2	1.97	0.45
1:C:131:LYS:HA	1:C:131:LYS:HZ3	1.73	0.45
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.29	0.45
1:C:227:LEU:HD13	1:C:227:LEU:HA	1.81	0.45
1:C:146:LYS:HB3	1:C:146:LYS:HZ2	1.82	0.45
1:C:49:ARG:HH11	1:C:193:VAL:CG2	2.26	0.44
3:A:1421:HOH:O	1:C:209:LYS:HG3	2.16	0.44
1:C:98:PRO:O	1:C:102:GLU:HG3	2.18	0.44
1:C:198:GLU:HB3	3:C:316:HOH:O	2.18	0.44
1:B:194:ARG:NH2	1:B:195:LYS:HZ3	2.15	0.44
1:B:161:GLU:OE1	3:B:297:HOH:O	2.21	0.44
1:C:187:VAL:HG21	1:C:207:ARG:HD3	1.99	0.44
1:B:218:TYR:CD1	1:B:218:TYR:N	2.86	0.44
1:B:126:ALA:HA	1:B:131:LYS:HB2	2.00	0.43
1:C:172:ASP:HB2	1:C:178:ILE:HG12	2.00	0.43
1:C:93:LEU:HD12	1:C:153:ARG:HD3	2.00	0.43
1:A:49:ARG:HG2	3:A:1479:HOH:O	2.18	0.43
1:C:205:LYS:HE3	3:C:244:HOH:O	2.18	0.43
1:A:178:ILE:HG12	3:A:1489:HOH:O	2.17	0.43
1:C:123:ARG:HH11	1:C:156:ASP:CG	2.22	0.43
1:C:131:LYS:HZ2	1:C:131:LYS:CB	2.32	0.43
1:C:83:ARG:HE	1:C:83:ARG:HB2	1.71	0.42
1:C:98:PRO:CB	1:C:99:PRO:HD3	2.39	0.42
1:A:215:ARG:HD2	1:B:141:LYS:O	2.20	0.42
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.81	0.42
1:A:49:ARG:NH2	3:A:1464:HOH:O	2.26	0.42
1:A:221:GLU:CD	1:A:221:GLU:H	2.23	0.42
1:A:92:VAL:HG11	1:A:146:LYS:HE3	2.01	0.42
1:A:220:ARG:NH1	1:A:224:LEU:HD11	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:VAL:HA	1:A:188:PRO:HD3	1.86	0.41
1:B:86:LEU:HA	1:B:86:LEU:HD23	1.92	0.41
1:C:54:PHE:O	1:C:58:PHE:N	2.46	0.41
1:C:220:ARG:HG3	1:C:223:MET:CE	2.51	0.41
1:B:190:ARG:NH1	3:B:363:HOH:O	2.02	0.41
1:A:221:GLU:HG2	3:A:1523:HOH:O	2.20	0.41
1:B:226:LYS:HG2	1:C:139:HIS:CD2	2.56	0.41
1:A:113:GLU:H	1:A:113:GLU:HG3	1.49	0.41
1:A:163:LEU:HD12	1:A:181:HIS:HB3	2.01	0.41
1:B:194:ARG:NH2	1:B:195:LYS:HZ1	2.18	0.41
1:C:184:PRO:HA	1:C:185:VAL:HA	1.86	0.41
1:B:40:MET:HE1	1:B:88:ALA:HB2	2.02	0.40
1:A:194:ARG:NH1	3:A:1529:HOH:O	2.54	0.40
1:C:114:HIS:C	1:C:115:LEU:HD23	2.41	0.40
1:A:231:LEU:HD21	1:B:86:LEU:HD12	2.02	0.40
1:C:43:ILE:HD12	1:C:75:VAL:CG1	2.51	0.40
1:A:230:PHE:HD1	1:B:141:LYS:HE3	1.87	0.40
1:C:198:GLU:CG	3:C:316:HOH:O	2.69	0.40
1:A:138:PRO:O	1:C:223:MET:HG3	2.21	0.40

All (1) 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	Distance(Å)	Clash(Å)
3:B:357:HOH:O	3:B:357:HOH:O[2_555]	0.98	1.22

## 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	185/235 (79%)	180 (97%)	4 (2%)	1 (0%)	38	31
1	B	181/235 (77%)	174 (96%)	7 (4%)	0	100	100
1	C	184/235 (78%)	178 (97%)	6 (3%)	0	100	100
All	All	550/705 (78%)	532 (97%)	17 (3%)	1 (0%)	56	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLU

### 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	143/179 (80%)	133 (93%)	10 (7%)	21	16
1	B	140/179 (78%)	126 (90%)	14 (10%)	11	6
1	C	142/179 (79%)	122 (86%)	20 (14%)	5	2
All	All	425/537 (79%)	381 (90%)	44 (10%)	10	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	A	66	PHE
1	A	73	SER
1	A	82	THR
1	A	97	LEU
1	A	131	LYS
1	A	146	LYS
1	A	202	LEU
1	A	220	ARG
1	A	224	LEU
1	B	49	ARG
1	B	71	SER
1	B	97	LEU
1	B	101	LEU
1	B	131	LYS
1	B	146	LYS
1	B	152	LEU
1	B	161	GLU
1	B	190	ARG
1	B	198	GLU
1	B	207	ARG
1	B	217	VAL

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Mol	Chain	Res	Type
1	B	224	LEU
1	B	226	LYS
1	C	40	MET
1	C	41	GLU
1	C	44	ARG
1	C	78	GLU
1	C	83	ARG
1	C	87	GLU
1	C	94	GLU
1	C	96	LEU
1	C	100	LEU
1	C	101	LEU
1	C	113	GLU
1	C	131	LYS
1	C	132	GLU
1	C	157	PRO
1	C	158	VAL
1	C	180	MET
1	C	194	ARG
1	C	221	GLU
1	C	224	LEU
1	C	227	LEU

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	48	GLN
1	A	139	HIS
1	A	166	GLN
1	B	48	GLN
1	B	139	HIS
1	B	166	GLN
1	B	168	HIS
1	C	48	GLN
1	C	90	HIS
1	C	166	GLN
1	C	168	HIS

### 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 2 ligands modelled in this entry, 2 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 ⓘ

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.