



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 1V8D / pdb_00001v8d
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

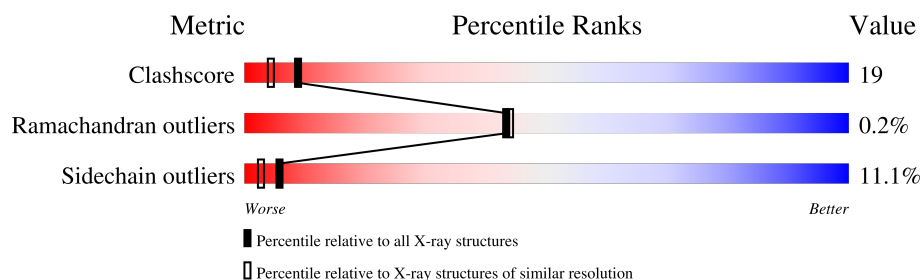
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

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 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 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

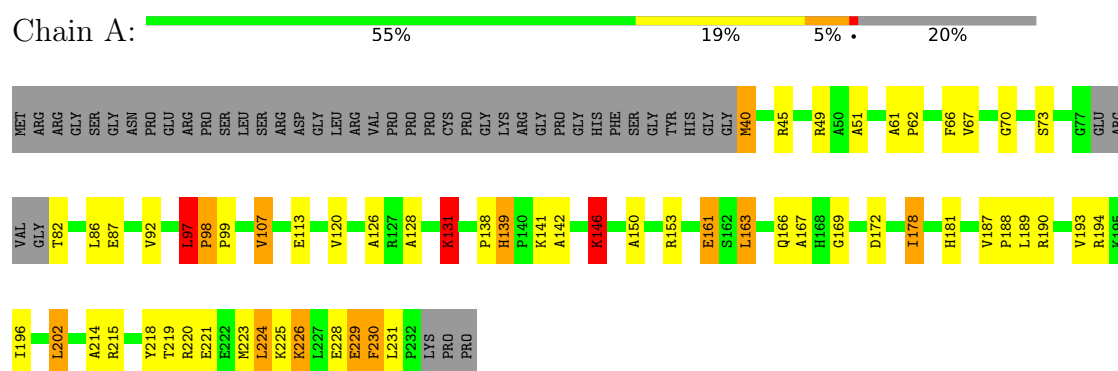
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	128	Total	O	0	0
			128	128		
3	C	102	Total	O	0	0
			102	102		

3 Residue-property plots [i](#)

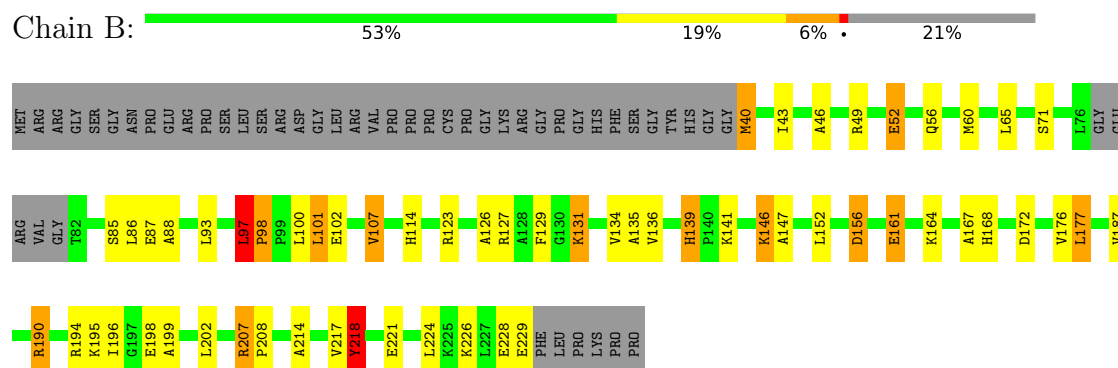
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

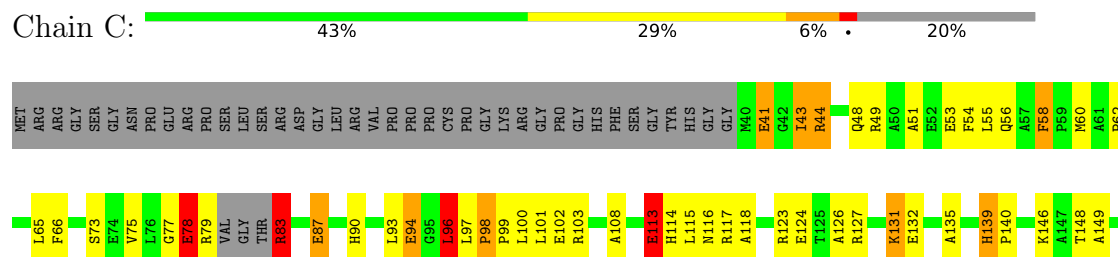
- Molecule 1: hypothetical protein (TT1679)

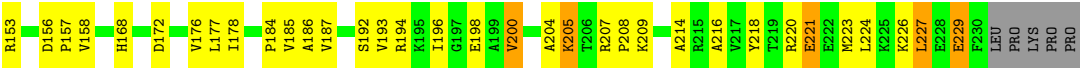


- Molecule 1: hypothetical protein (TT1679)



- Molecule 1: hypothetical protein (TT1679)





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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	1.65	13/1449 (0.9%)	1.51	18/1954 (0.9%)
1	B	1.63	14/1417 (1.0%)	1.50	15/1910 (0.8%)
1	C	1.40	7/1446 (0.5%)	1.45	17/1947 (0.9%)
All	All	1.56	34/4312 (0.8%)	1.49	50/5811 (0.9%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	MET	SD-CE	-8.92	1.57	1.79
1	A	67	VAL	CA-CB	8.74	1.64	1.54
1	B	135	ALA	CA-CB	7.72	1.64	1.53
1	A	107	VAL	CA-CB	7.24	1.62	1.54
1	B	136	VAL	CA-CB	6.74	1.60	1.55
1	B	199	ALA	CA-CB	6.62	1.63	1.53
1	C	218	TYR	CA-C	-6.22	1.44	1.52
1	A	128	ALA	CA-CB	6.10	1.63	1.53
1	A	61	ALA	CA-CB	6.03	1.62	1.53
1	A	62	PRO	CA-C	5.98	1.59	1.52
1	A	51	ALA	N-CA	-5.95	1.39	1.46
1	B	187	VAL	CA-C	5.94	1.59	1.52
1	A	167	ALA	CA-CB	5.87	1.63	1.53
1	B	107	VAL	CA-CB	5.82	1.62	1.54
1	C	139	HIS	CA-C	5.80	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	ALA	CA-CB	5.80	1.62	1.53
1	B	177	LEU	C-O	5.77	1.31	1.24
1	A	150	ALA	CA-CB	-5.75	1.44	1.53
1	C	204	ALA	CA-CB	5.65	1.65	1.54
1	C	135	ALA	CA-CB	5.62	1.60	1.53
1	B	114	HIS	CA-C	5.46	1.60	1.52
1	C	216	ALA	CA-CB	5.46	1.62	1.53
1	B	134	VAL	CA-CB	5.43	1.62	1.54
1	B	176	VAL	CA-CB	5.43	1.61	1.54
1	A	169	GLY	C-O	-5.35	1.18	1.23
1	A	193	VAL	CA-CB	-5.35	1.47	1.53
1	B	52	GLU	CA-C	5.29	1.59	1.52
1	A	166	GLN	CA-C	5.26	1.60	1.52
1	C	186	ALA	CA-CB	5.24	1.61	1.53
1	C	108	ALA	CA-C	5.22	1.58	1.52
1	A	120	VAL	CA-CB	5.20	1.60	1.54
1	B	85	SER	CA-C	5.18	1.58	1.52
1	A	178	ILE	CA-CB	5.15	1.61	1.54
1	B	101	LEU	CG-CD2	-5.07	1.35	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	ILE	N-CA-C	-9.29	92.51	107.28
1	A	139	HIS	N-CA-C	-9.27	97.50	108.25
1	C	43	ILE	N-CA-C	-9.04	102.05	110.82
1	C	113	GLU	N-CA-C	7.83	122.26	112.87
1	B	98	PRO	N-CA-C	7.56	119.93	110.70
1	A	214	ALA	N-CA-C	7.51	120.35	111.71
1	B	218	TYR	N-CA-C	7.38	122.00	112.41
1	B	147	ALA	N-CA-C	-7.34	103.35	111.36
1	B	97	LEU	N-CA-C	7.26	122.62	112.75
1	C	205	LYS	N-CA-C	-7.18	99.61	109.95
1	A	218	TYR	N-CA-C	6.99	122.79	112.94
1	C	118	ALA	N-CA-C	-6.69	101.67	110.43
1	A	97	LEU	CA-C-N	-6.59	113.59	120.38
1	A	97	LEU	C-N-CA	-6.59	113.59	120.38
1	C	73	SER	N-CA-C	-6.52	104.25	111.36
1	C	97	LEU	N-CA-C	6.52	124.22	109.81
1	B	214	ALA	N-CA-C	6.25	119.75	111.75
1	A	97	LEU	N-CA-C	6.21	123.54	109.81
1	A	163	LEU	N-CA-C	-6.07	105.05	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	GLU	N-CA-C	6.02	117.92	111.36
1	A	146	LYS	CG-CD-CE	-6.01	97.47	111.30
1	C	139	HIS	CB-CA-C	5.95	118.90	109.55
1	A	98	PRO	N-CA-C	5.88	117.87	110.70
1	A	70	GLY	N-CA-C	5.86	119.05	110.38
1	B	196	ILE	N-CA-C	-5.77	98.10	107.28
1	C	58	PHE	CA-C-N	5.64	126.89	119.84
1	C	58	PHE	C-N-CA	5.64	126.89	119.84
1	A	189	LEU	CA-C-N	-5.61	114.96	122.42
1	A	189	LEU	C-N-CA	-5.61	114.96	122.42
1	B	56	GLN	N-CA-C	-5.57	105.28	111.36
1	B	46	ALA	N-CA-C	-5.55	105.13	111.07
1	A	230	PHE	N-CA-C	-5.49	105.70	112.72
1	A	131	LYS	CG-CD-CE	-5.48	98.70	111.30
1	C	83	ARG	CA-C-N	5.43	125.42	120.21
1	C	83	ARG	C-N-CA	5.43	125.42	120.21
1	A	153	ARG	N-CA-C	5.41	119.99	112.90
1	B	114	HIS	N-CA-C	-5.39	105.96	112.54
1	C	56	GLN	N-CA-C	-5.28	105.42	111.07
1	C	214	ALA	N-CA-C	5.15	117.63	111.71
1	A	228	GLU	N-CA-C	-5.14	105.37	110.97
1	A	120	VAL	CB-CA-C	-5.12	104.50	111.15
1	B	139	HIS	CB-CA-C	5.10	117.88	109.97
1	B	87	GLU	CB-CA-C	-5.09	102.89	110.88
1	C	96	LEU	N-CA-C	5.07	117.93	111.69
1	C	208	PRO	N-CA-C	5.07	119.26	111.21
1	B	156	ASP	CA-C-N	5.06	125.50	120.14
1	B	156	ASP	C-N-CA	5.06	125.50	120.14
1	C	78	GLU	N-CA-C	5.04	119.27	113.18
1	B	97	LEU	CA-C-N	-5.03	115.20	120.38
1	B	97	LEU	C-N-CA	-5.03	115.20	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	218	TYR	Sidechain

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	1424	0	1488	51	0
1	B	1394	0	1458	46	0
1	C	1422	0	1482	71	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	161	1

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 19.

All (161) 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:231:LEU:HD23	3:A:1540:HOH:O	1.40	1.19
1:C:131:LYS:HZ2	1:C:131:LYS:HA	1.05	1.16
1:B:228:GLU:O	1:B:229:GLU:HG3	1.48	1.11
1:B:40:MET:HE3	1:B:43:ILE:HD12	1.36	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:C:131:LYS:HZ2	1:C:131:LYS:CA	1.77	0.97
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:54:PHE:HE1	1:C:60:MET:HE2	1.36	0.88
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:A:231:LEU:HA	3:A:1540:HOH:O	1.79	0.83
1:A:190:ARG:NH2	1:A:194:ARG:HH22	1.77	0.83
1:C:83:ARG:HD3	3:C:335:HOH:O	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:O	1:C:94:GLU:HB2	1.80	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:C:60:MET:HE1	1:C:66:PHE:HD2	1.49	0.77
1:A:172:ASP:HB3	1:A:202:LEU:HG	1.67	0.77
1:C:221:GLU:N	1:C:221:GLU:OE1	2.18	0.76
1:C:54:PHE:CE1	1:C:60:MET:HE2	2.22	0.72
1:C:124:GLU:OE2	1:C:127:ARG:NH1	2.23	0.71
1:C:131:LYS:NZ	1:C:131:LYS:CA	2.46	0.70
1:C:60:MET:HE1	1:C:66:PHE:CD2	2.26	0.70
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:N	1:C:41:GLU:OE2	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:A:229:GLU:O	3:A:1533:HOH:O	2.12	0.66
1:B:146:LYS:HB2	1:B:146:LYS:HZ3	1.59	0.66
1:C:149:ALA:O	1:C:153:ARG:HG3	1.95	0.66
1:A:139:HIS:CE1	1:A:142:ALA:HB3	2.31	0.66
1:B:40:MET:HE3	1:B:43:ILE:CD1	2.22	0.65
1:C:200:VAL:HG12	3:C:248:HOH:O	1.94	0.65
1:C:221:GLU:CD	1:C:221:GLU:H	2.04	0.65
1:C:55:LEU:HD13	1:C:103:ARG:CD	2.27	0.65
1:C:49:ARG:HH11	1:C:193:VAL:HG23	1.62	0.63
1:B:65:LEU:H	1:B:168:HIS:HD2	1.47	0.62
1:B:146:LYS:HZ3	1:B:146:LYS:CB	2.13	0.62
1:C:49:ARG:NH1	1:C:192:SER:OG	2.31	0.62
1:C:126:ALA:HA	1:C:131:LYS:HG3	1.81	0.62
1:B:127:ARG:HH11	1:B:127:ARG:HG2	1.65	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:C:113:GLU:H	1:C:113:GLU:CD	2.08	0.61
1:A:86:LEU:HD11	1:C:227:LEU:HD11	1.83	0.61
1:B:194:ARG:NH2	1:B:195:LYS:NZ	2.50	0.60
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:A:49:ARG:HD3	3:A:1464:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:NZ	3:A:1513:HOH:O	2.35	0.59
1:A:141:LYS:HG2	3:A:1432:HOH:O	2.00	0.59
1:B:194:ARG:CZ	1:B:195:LYS:HZ3	2.14	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: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:OE2	1:B:52:GLU:HA	2.04	0.57
1:A:226:LYS:HG2	1:B:139:HIS:CD2	2.40	0.57
1:A:40:MET:HE3	1:A:87:GLU:HB2	1.87	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:B:139:HIS:HD2	3:B:362:HOH:O	1.90	0.53
1:B:146:LYS:CB	1:B:146:LYS:NZ	2.58	0.53
1:C:65:LEU:H	1:C:168:HIS:CD2	2.12	0.53
1:C:87:GLU:CD	1:C:87:GLU:H	2.16	0.53
1:A:146:LYS:CB	1:A:146:LYS:NZ	2.66	0.53
1:B:131:LYS:NZ	1:B:131:LYS:HA	2.24	0.53
1:C:78:GLU:O	1:C:79:ARG:C	2.52	0.52
1:A:97:LEU:HD11	1:A:107:VAL:HG11	1.91	0.52
1:A:225:LYS:O	1:A:229:GLU:HG3	2.09	0.52
1:C:87:GLU:CD	1:C:87:GLU:N	2.69	0.51
1:C:44:ARG:HH12	1:C:48:GLN:NE2	2.09	0.51
1:A:223:MET:HE3	1:A:224:LEU:HD13	1.93	0.50
1:B:194:ARG:NH2	1:B:195:LYS:HZ1	2.09	0.50
1:C:54:PHE:HE1	1:C:60:MET:CE	2.15	0.50
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:C:146:LYS:HZ2	1:C:146:LYS:HB3	1.77	0.49
1:C:131:LYS:HZ2	1:C:131:LYS:CB	2.23	0.49
1:A:219:THR:HB	1:A:221:GLU:OE2	2.13	0.48
1:C:94:GLU:HA	1:C:94:GLU:OE1	2.13	0.48
1:C:123:ARG:HD2	1:C:156:ASP:OD2	2.14	0.48
1:A:146:LYS:CB	1:A:146:LYS:HZ3	2.27	0.48
1:C:123:ARG:HH11	1:C:156:ASP:CG	2.22	0.47
1:A:131:LYS:HE3	1:A:131:LYS:HB3	1.62	0.47
1:B:93:LEU:HB3	1:B:97:LEU:HD22	1.96	0.47
1:A:190:ARG:HA	1:A:194:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:H	1:A:221:GLU:CD	2.23	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: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: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:114:HIS:C	1:C:115:LEU:HD23	2.41	0.45
1:C:55:LEU:HD13	1:C:103:ARG:HD2	1.97	0.45
1:C:83:ARG:NH1	3:C:335:HOH:O	2.20	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
3:A:1421:HOH:O	1:C:209:LYS:HG3	2.16	0.44
1:C:49:ARG:HH11	1:C:193:VAL:CG2	2.26	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:161:GLU:OE1	3:B:297:HOH:O	2.21	0.44
1:B:221:GLU:H	1:B:221:GLU:CD	2.26	0.44
1:B:131:LYS:HA	1:B:131:LYS:HZ3	1.81	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:A:40:MET:HE3	1:A:87:GLU:CB	2.48	0.43
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:A:49:ARG:HG2	3:A:1479:HOH:O	2.18	0.43
1:C:93:LEU:HD12	1:C:153:ARG:HD3	2.00	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:A:146:LYS:HZ2	1:A:146:LYS:HG3	0.94	0.43
1:B:131:LYS:HZ2	1:B:131:LYS:HG3	1.05	0.43
1:B:40:MET:HE2	1:B:88:ALA:HA	2.00	0.42
1:C:83:ARG:HE	1:C:83:ARG:HB2	1.71	0.42
1:A:215:ARG:HD2	1:B:141:LYS:O	2.20	0.42
1:B:100:LEU:HA	1:B:100:LEU:HD23	1.81	0.42
1:C:98:PRO:CB	1:C:99:PRO:HD3	2.39	0.42
1:A:49:ARG:NH2	3:A:1464:HOH:O	2.26	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	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MET:HE3	1:B:168:HIS:HB2	2.02	0.42
1:A:187:VAL:HA	1:A:188:PRO:HD3	1.86	0.41
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.92	0.41
1:A:146:LYS:HZ3	1:A:146:LYS:HA	1.86	0.41
1:C:54:PHE:O	1:C:58:PHE:N	2.46	0.41
1:B:190:ARG:NH1	3:B:363:HOH:O	2.02	0.41
1:C:220:ARG:HG3	1:C:223:MET:CE	2.51	0.41
1:A:113:GLU:H	1:A:113:GLU:HG3	1.49	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:163:LEU:HD12	1:A:181:HIS:HB3	2.01	0.41
1:C:184:PRO:HA	1:C:185:VAL:HA	1.86	0.41
1:A:194:ARG:NH1	3:A:1529:HOH:O	2.54	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:138:PRO:O	1:C:223:MET:HG3	2.21	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

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	Interatomic distance (Å)	Clash overlap (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%)	24	20
1	B	181/235 (77%)	174 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	184/235 (78%)	178 (97%)	6 (3%)	0	100	100
All	All	550/705 (78%)	532 (97%)	17 (3%)	1 (0%)	43	44

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%)	132 (92%)	11 (8%)	12	7
1	B	140/179 (78%)	126 (90%)	14 (10%)	7	3
1	C	142/179 (79%)	120 (84%)	22 (16%)	2	1
All	All	425/537 (79%)	378 (89%)	47 (11%)	6	3

All (47) 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	196	ILE
1	A	202	LEU
1	A	224	LEU
1	A	226	LYS
1	B	49	ARG
1	B	71	SER
1	B	97	LEU

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Mol	Chain	Res	Type
1	B	101	LEU
1	B	131	LYS
1	B	146	LYS
1	B	152	LEU
1	B	161	GLU
1	B	177	LEU
1	B	190	ARG
1	B	198	GLU
1	B	207	ARG
1	B	217	VAL
1	B	224	LEU
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	98	PRO
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	194	ARG
1	C	200	VAL
1	C	221	GLU
1	C	224	LEU
1	C	226	LYS
1	C	227	LEU
1	C	229	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	B	48	GLN
1	B	139	HIS
1	B	166	GLN
1	B	168	HIS

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Mol	Chain	Res	Type
1	C	48	GLN
1	C	90	HIS
1	C	166	GLN
1	C	168	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.