



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:25 AM UTC

PDB ID : 1WSF / pdb_00001wsf
Title : Co-crystal structure of E.coli RNase HI active site mutant (D134A*) with Mn²⁺
Authors : Tsunaka, Y.; Takano, K.; Matsumura, H.; Yamagata, Y.; Kanaya, S.
Deposited on : 2004-11-05
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

<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

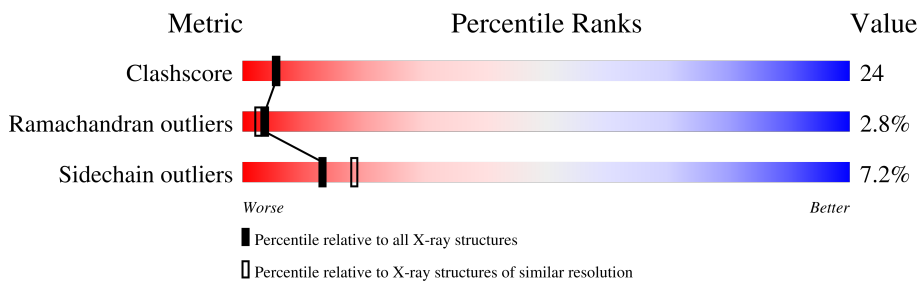
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	155	61% 34% 5% •
1	B	155	54% 40% 6% •
1	C	155	62% 30% 8%
1	D	155	59% 35% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5098 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 Ribonuclease HI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1230	772	226	225	7			
1	B	155	Total	C	N	O	S	0	0	0
			1230	772	226	225	7			
1	C	155	Total	C	N	O	S	0	0	0
			1230	772	226	225	7			
1	D	155	Total	C	N	O	S	0	0	0
			1231	772	226	226	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	LYS	engineered mutation	UNP P0A7Y4
A	134	ALA	ASP	engineered mutation	UNP P0A7Y4
B	87	ALA	LYS	engineered mutation	UNP P0A7Y4
B	134	ALA	ASP	engineered mutation	UNP P0A7Y4
C	87	ALA	LYS	engineered mutation	UNP P0A7Y4
C	134	ALA	ASP	engineered mutation	UNP P0A7Y4
D	87	ALA	LYS	engineered mutation	UNP P0A7Y4
D	134	ALA	ASP	engineered mutation	UNP P0A7Y4

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total 43	O 43	0	0
3	B	45	Total 45	O 45	0	0
3	C	46	Total 46	O 46	0	0
3	D	40	Total 40	O 40	0	0

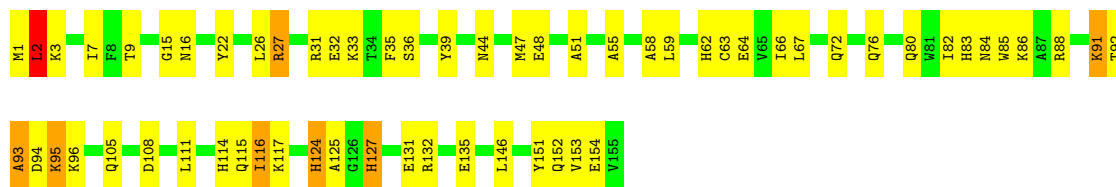
3 Residue-property plots

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.

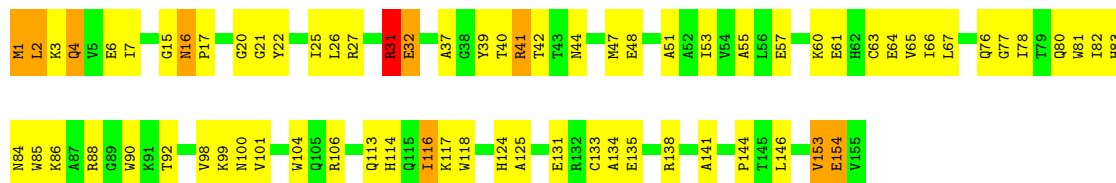
• Molecule 1: Ribonuclease HI

Chain A: 



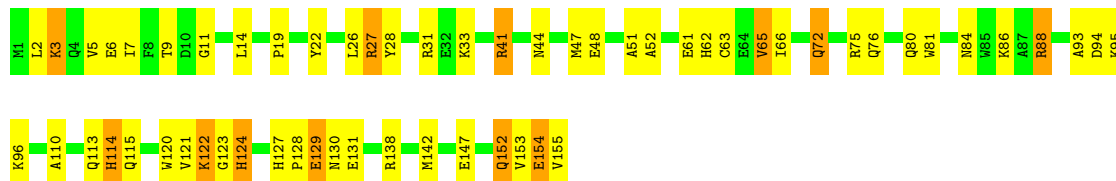
• Molecule 1: Ribonuclease HI

Chain B: 



• Molecule 1: Ribonuclease HI

Chain C: 



• Molecule 1: Ribonuclease HI

Chain D: 



A110	L111	G112	Q113	H114	Q115	I116	K117	W118	K122	G123	H124	A125	G126	M130	E131	R132	R138	A139	A140	A141	M142	R143	P144	V155
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.99Å 80.09Å 63.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5098	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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: MN

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	0.48	1/1258 (0.1%)	0.91	4/1702 (0.2%)
1	B	0.47	0/1258	0.88	4/1702 (0.2%)
1	C	0.48	0/1258	0.90	4/1702 (0.2%)
1	D	0.42	0/1259	0.90	4/1702 (0.2%)
All	All	0.46	1/5033 (0.0%)	0.90	16/6808 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	MET	SD-CE	5.11	1.92	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	VAL	N-CA-C	7.10	119.10	108.23
1	A	132	ARG	N-CA-C	-6.54	104.23	111.36
1	C	81	TRP	N-CA-C	6.46	122.65	114.31
1	B	64	GLU	N-CA-C	-6.26	98.52	108.73
1	B	40	THR	N-CA-C	5.86	118.42	111.33
1	D	27	ARG	N-CA-C	5.86	123.27	110.80
1	C	65	VAL	N-CA-C	5.85	116.36	108.17
1	A	115	GLN	N-CA-C	-5.76	99.34	108.73
1	C	95	LYS	N-CA-C	5.75	119.50	111.74
1	D	92	THR	N-CA-C	5.60	115.67	108.34
1	D	116	ILE	N-CA-C	5.59	116.15	107.99
1	A	64	GLU	N-CA-C	-5.50	99.55	108.41
1	D	28	TYR	N-CA-C	5.50	122.52	110.80
1	A	116	ILE	N-CA-C	5.33	116.27	108.53
1	B	116	ILE	N-CA-C	5.26	116.37	109.21
1	C	114	HIS	N-CA-C	5.00	116.59	109.14

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	1230	0	1210	51	0
1	B	1230	0	1210	66	0
1	C	1230	0	1210	58	0
1	D	1231	0	1210	63	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	43	0	0	4	0
3	B	45	0	0	5	0
3	C	46	0	0	5	0
3	D	40	0	0	11	0
All	All	5098	0	4840	232	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 24.

All (232) 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:B:42:THR:HG21	1:B:47:MET:HE2	1.24	1.09
1:B:31:ARG:O	1:B:32:GLU:HB3	1.65	0.94
1:B:20:GLY:C	1:B:47:MET:HE3	1.94	0.92
1:D:31:ARG:HG3	1:D:32:GLU:H	1.34	0.90
1:B:134:ALA:HB1	1:B:138:ARG:HH21	1.42	0.84
1:A:91:LYS:HG3	1:A:96:LYS:H	1.42	0.84
1:B:39:TYR:CD1	1:B:47:MET:HE1	2.13	0.83
1:B:2:LEU:HD12	1:B:2:LEU:H	1.43	0.83
1:B:39:TYR:HD1	1:B:47:MET:HE1	1.42	0.82
1:D:122:LYS:HB2	1:D:125:ALA:HB3	1.62	0.81
1:C:22:TYR:HB2	1:C:51:ALA:HB2	1.64	0.79
1:C:11:GLY:HA3	1:C:48:GLU:HG2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ARG:HG3	1:D:32:GLU:N	1.98	0.79
1:D:31:ARG:CG	1:D:32:GLU:H	1.97	0.78
1:D:49:LEU:HD23	1:D:74:VAL:HG22	1.67	0.76
1:A:91:LYS:HG3	1:A:96:LYS:N	2.01	0.75
1:B:1:MET:HE1	3:B:1033:HOH:O	1.86	0.75
1:B:65:VAL:HB	1:B:116:ILE:HD13	1.69	0.73
1:D:126:GLY:HA2	3:D:1030:HOH:O	1.86	0.73
1:A:26:LEU:HD23	1:A:33:LYS:HD2	1.70	0.73
1:C:147:GLU:HB3	3:C:166:HOH:O	1.88	0.72
1:A:2:LEU:HD23	1:A:2:LEU:H	1.55	0.71
1:A:15:GLY:HA3	3:A:1044:HOH:O	1.90	0.71
1:A:26:LEU:HD11	1:A:59:LEU:HD21	1.74	0.70
1:A:85:TRP:HE1	1:C:155:VAL:CG1	2.04	0.70
1:C:75:ARG:HG3	1:C:120:TRP:CD2	2.26	0.70
1:B:41:ARG:HG2	1:B:41:ARG:HH11	1.58	0.68
1:D:99:LYS:HE3	1:D:99:LYS:HA	1.75	0.68
1:B:31:ARG:O	1:B:32:GLU:CB	2.42	0.67
1:D:1:MET:HE2	1:D:3:LYS:H	1.61	0.66
1:C:76:GLN:NE2	3:C:190:HOH:O	2.29	0.66
1:A:151:TYR:OH	1:A:154:GLU:HG3	1.96	0.65
1:D:29:ARG:NE	1:D:29:ARG:HA	2.11	0.65
1:D:67:LEU:HD22	1:D:118:TRP:CZ3	2.31	0.65
1:D:28:TYR:HA	3:D:1041:HOH:O	1.97	0.64
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.62	0.64
1:A:26:LEU:HB3	1:A:33:LYS:HB2	1.81	0.63
1:B:82:ILE:HG23	1:B:83:HIS:N	2.12	0.63
1:D:2:LEU:O	1:D:3:LYS:HB3	1.98	0.63
1:B:26:LEU:O	1:B:32:GLU:HA	1.99	0.62
1:A:95:LYS:HA	1:A:95:LYS:HE2	1.81	0.62
1:C:88:ARG:NH1	1:C:93:ALA:HA	2.16	0.61
1:C:3:LYS:HE3	1:C:28:TYR:CZ	2.35	0.61
1:C:5:VAL:HG11	1:C:26:LEU:HD11	1.83	0.60
1:D:60:LYS:HB3	3:D:1019:HOH:O	2.00	0.60
1:B:41:ARG:HG2	1:B:41:ARG:NH1	2.16	0.60
1:A:125:ALA:HB3	3:A:1027:HOH:O	2.01	0.60
1:C:62:HIS:HD2	1:C:113:GLN:O	1.85	0.60
1:A:92:THR:O	1:A:95:LYS:N	2.35	0.59
1:C:138:ARG:O	1:C:142:MET:HG2	2.03	0.59
1:B:26:LEU:HD11	1:B:55:ALA:HB1	1.85	0.58
1:D:155:VAL:HG12	1:D:155:VAL:O	2.02	0.58
1:B:42:THR:HG21	1:B:47:MET:CE	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLU:OE2	1:D:28:TYR:HB2	2.04	0.58
1:B:66:ILE:HD12	1:B:117:LYS:O	2.04	0.57
1:B:2:LEU:HD12	1:B:2:LEU:N	2.16	0.57
1:A:2:LEU:H	1:A:2:LEU:CD2	2.18	0.57
1:A:44:ASN:O	1:A:48:GLU:HG3	2.05	0.56
1:A:88:ARG:HG2	1:A:95:LYS:NZ	2.20	0.56
1:B:3:LYS:HD3	1:B:61:GLU:CD	2.30	0.56
1:D:31:ARG:CG	1:D:32:GLU:N	2.63	0.56
1:D:28:TYR:O	1:D:29:ARG:HB2	2.03	0.56
3:A:1009:HOH:O	1:C:152:GLN:HG3	2.05	0.56
1:C:128:PRO:HB2	1:C:129:GLU:OE1	2.05	0.56
1:A:85:TRP:HE1	1:C:155:VAL:HG11	1.71	0.56
1:C:41:ARG:NH2	1:C:153:VAL:HG21	2.21	0.56
1:D:27:ARG:HD2	1:D:28:TYR:CD2	2.41	0.56
1:D:110:ALA:HA	3:D:1020:HOH:O	2.06	0.56
1:D:92:THR:HG23	1:D:98:VAL:HG12	1.87	0.55
1:B:2:LEU:H	1:B:2:LEU:CD1	2.17	0.55
1:A:66:ILE:HA	1:A:117:LYS:HG3	1.88	0.55
1:A:1:MET:HG3	1:A:62:HIS:HB2	1.87	0.55
1:D:78:ILE:CD1	1:D:111:LEU:HD11	2.36	0.55
1:B:63:CYS:O	1:B:114:HIS:HB3	2.08	0.54
1:D:78:ILE:HD12	1:D:111:LEU:HD11	1.87	0.54
1:A:131:GLU:O	1:A:135:GLU:HG3	2.05	0.54
1:C:41:ARG:CB	1:C:41:ARG:HH11	2.21	0.54
1:D:66:ILE:HG23	1:D:66:ILE:O	2.07	0.54
1:B:53:ILE:O	1:B:57:GLU:HG3	2.07	0.54
1:C:26:LEU:HB3	1:C:33:LYS:HB2	1.89	0.54
1:D:65:VAL:HB	1:D:116:ILE:CD1	2.37	0.54
1:D:8:PHE:HB3	1:D:130:ASN:HD22	1.73	0.54
1:B:82:ILE:HG23	1:B:83:HIS:H	1.72	0.53
1:D:5:VAL:HG13	3:D:1043:HOH:O	2.09	0.53
1:C:41:ARG:HD2	3:C:159:HOH:O	2.09	0.53
1:C:94:ASP:OD2	1:C:96:LYS:HG3	2.09	0.53
1:A:27:ARG:HG3	1:A:32:GLU:HG2	1.91	0.52
1:A:92:THR:O	1:A:93:ALA:C	2.52	0.52
1:C:121:VAL:HG12	1:C:122:LYS:N	2.24	0.52
1:D:41:ARG:HG2	1:D:41:ARG:NH1	2.23	0.52
1:C:2:LEU:O	1:C:3:LYS:C	2.53	0.52
1:D:3:LYS:HD2	1:D:29:ARG:NE	2.25	0.52
1:C:7:ILE:HD12	1:C:65:VAL:HG11	1.92	0.52
1:B:76:GLN:O	1:B:80:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLY:O	1:D:82:ILE:HG22	2.10	0.51
1:A:88:ARG:HG2	1:A:95:LYS:HZ1	1.74	0.51
1:A:84:ASN:O	1:A:88:ARG:HB2	2.11	0.50
1:C:14:LEU:HD12	1:C:19:PRO:HB2	1.93	0.50
1:A:92:THR:O	1:A:94:ASP:N	2.44	0.50
1:A:86:LYS:HE2	1:A:108:ASP:OD1	2.12	0.50
1:C:75:ARG:NH2	3:C:163:HOH:O	2.44	0.50
1:C:127:HIS:HB3	1:C:130:ASN:OD1	2.11	0.50
1:A:95:LYS:HE2	1:A:95:LYS:CA	2.42	0.50
1:B:85:TRP:O	1:B:90:TRP:N	2.39	0.50
1:D:1:MET:CE	1:D:3:LYS:H	2.25	0.50
1:B:134:ALA:HB1	1:B:138:ARG:NH2	2.20	0.50
1:D:44:ASN:ND2	3:D:1026:HOH:O	2.44	0.49
1:C:5:VAL:HG11	1:C:26:LEU:CD1	2.42	0.49
1:B:7:ILE:HD13	1:B:55:ALA:HB1	1.93	0.49
1:B:44:ASN:HB3	3:B:1032:HOH:O	2.11	0.49
1:C:76:GLN:O	1:C:80:GLN:HB2	2.13	0.49
1:C:72:GLN:H	1:C:72:GLN:NE2	2.09	0.49
1:A:35:PHE:O	1:A:36:SER:HB3	2.12	0.49
1:D:1:MET:HE2	1:D:3:LYS:N	2.27	0.49
1:B:57:GLU:CD	1:B:106:ARG:HH21	2.20	0.49
1:C:9:THR:HG21	1:C:52:ALA:HA	1.94	0.49
1:D:131:GLU:OE1	1:D:131:GLU:HA	2.13	0.48
1:A:16:ASN:C	1:A:16:ASN:HD22	2.20	0.48
1:B:76:GLN:HG2	1:B:80:GLN:NE2	2.28	0.48
1:C:44:ASN:O	1:C:48:GLU:HG3	2.13	0.48
1:D:65:VAL:HB	1:D:116:ILE:HD13	1.94	0.48
1:A:33:LYS:NZ	3:A:1002:HOH:O	2.47	0.48
1:D:3:LYS:HD2	1:D:29:ARG:HE	1.79	0.48
1:D:99:LYS:HA	1:D:99:LYS:CE	2.42	0.48
1:B:39:TYR:HA	1:B:146:LEU:O	2.13	0.48
1:B:98:VAL:HG22	1:B:101:VAL:HB	1.96	0.48
1:B:77:GLY:HA3	1:B:104:TRP:CH2	2.49	0.48
1:D:89:GLY:O	1:D:90:TRP:C	2.56	0.48
1:B:21:GLY:N	1:B:47:MET:HE3	2.29	0.48
1:C:122:LYS:N	1:C:122:LYS:HD2	2.29	0.47
1:B:6:GLU:HA	1:B:66:ILE:HG23	1.96	0.47
1:C:6:GLU:OE2	1:C:27:ARG:NH2	2.47	0.47
1:C:5:VAL:HG12	1:C:6:GLU:N	2.28	0.47
1:B:86:LYS:C	1:B:88:ARG:H	2.22	0.47
1:D:4:GLN:HA	1:D:64:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:PHE:O	1:D:36:SER:HB3	2.14	0.47
1:B:22:TYR:HB2	1:B:51:ALA:HB2	1.96	0.47
1:B:67:LEU:HD22	1:B:118:TRP:CZ3	2.49	0.47
1:D:111:LEU:HD21	1:D:118:TRP:HZ2	1.79	0.47
1:A:94:ASP:OD2	1:A:94:ASP:C	2.58	0.47
1:D:44:ASN:O	1:D:48:GLU:HG3	2.15	0.47
1:B:22:TYR:CE2	1:B:37:ALA:HB3	2.50	0.46
1:C:63:CYS:O	1:C:114:HIS:HB3	2.15	0.46
1:D:42:THR:OG1	1:D:47:MET:HE3	2.15	0.46
1:A:127:HIS:ND1	1:A:127:HIS:N	2.62	0.46
1:B:84:ASN:O	1:B:85:TRP:C	2.58	0.46
1:B:153:VAL:O	1:B:154:GLU:HB2	2.15	0.46
1:A:39:TYR:HA	1:A:146:LEU:O	2.15	0.46
1:A:96:LYS:HZ1	1:C:152:GLN:HG3	1.81	0.46
1:A:55:ALA:O	1:A:58:ALA:HB3	2.16	0.46
1:C:2:LEU:O	1:C:3:LYS:O	2.33	0.46
1:D:110:ALA:O	1:D:113:GLN:HB2	2.16	0.45
1:B:82:ILE:CG2	1:B:83:HIS:N	2.78	0.45
1:C:129:GLU:OE1	1:C:129:GLU:N	2.49	0.45
1:A:117:LYS:HG3	1:A:117:LYS:O	2.16	0.45
1:C:41:ARG:HH11	1:C:41:ARG:HB3	1.82	0.45
1:D:141:ALA:O	1:D:144:PRO:HD3	2.16	0.45
1:D:22:TYR:CZ	1:D:54:VAL:HG21	2.51	0.45
1:B:141:ALA:O	1:B:144:PRO:HD3	2.16	0.45
1:D:47:MET:HE2	1:D:47:MET:HA	1.98	0.45
1:A:63:CYS:O	1:A:114:HIS:HB3	2.16	0.45
1:A:85:TRP:NE1	1:C:155:VAL:CG1	2.75	0.45
1:D:63:CYS:O	1:D:114:HIS:HB3	2.16	0.45
1:B:44:ASN:O	1:B:48:GLU:HG3	2.16	0.45
1:C:47:MET:HA	1:C:47:MET:HE2	1.98	0.45
1:C:115:GLN:OE1	1:C:115:GLN:HA	2.17	0.45
1:D:92:THR:CG2	1:D:98:VAL:HG12	2.47	0.45
1:C:88:ARG:HH12	1:C:93:ALA:HA	1.80	0.44
1:D:2:LEU:O	1:D:3:LYS:CB	2.65	0.44
1:D:16:ASN:O	1:D:16:ASN:CG	2.61	0.44
1:D:8:PHE:HB3	1:D:130:ASN:ND2	2.32	0.44
1:A:66:ILE:HA	1:A:117:LYS:CG	2.48	0.44
1:A:82:ILE:HG23	1:A:83:HIS:N	2.32	0.44
1:B:15:GLY:O	1:B:16:ASN:HB2	2.17	0.44
1:C:5:VAL:CG1	1:C:6:GLU:N	2.80	0.44
1:C:3:LYS:HE3	1:C:28:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLN:H	1:C:72:GLN:HE21	1.64	0.44
1:C:121:VAL:HG12	1:C:122:LYS:H	1.83	0.44
1:D:27:ARG:HD2	1:D:28:TYR:H	1.83	0.44
1:A:7:ILE:HB	1:A:67:LEU:HD23	2.00	0.43
1:D:28:TYR:HD1	3:D:1041:HOH:O	2.01	0.43
1:D:45:ASN:HB3	1:D:73:TYR:CE2	2.52	0.43
1:D:115:GLN:HA	3:D:1021:HOH:O	2.17	0.43
1:A:66:ILE:O	1:A:66:ILE:HG23	2.18	0.43
1:B:4:GLN:HE21	1:B:4:GLN:HB3	1.58	0.43
1:B:17:PRO:HD3	3:B:1047:HOH:O	2.19	0.43
1:A:111:LEU:HD22	1:A:116:ILE:HG13	2.00	0.43
1:B:99:LYS:O	1:B:100:ASN:HB2	2.19	0.43
1:C:110:ALA:O	1:C:113:GLN:HB2	2.19	0.43
1:C:124:HIS:HA	3:C:200:HOH:O	2.18	0.43
1:B:124:HIS:CE1	3:B:1003:HOH:O	2.71	0.43
1:C:84:ASN:O	1:C:88:ARG:CG	2.67	0.43
1:D:138:ARG:O	1:D:142:MET:HG2	2.19	0.43
1:B:77:GLY:HA2	1:B:81:TRP:CE3	2.53	0.42
1:B:78:ILE:HG13	1:B:118:TRP:CZ2	2.54	0.42
1:C:31:ARG:H	1:C:31:ARG:HG2	1.54	0.42
1:B:86:LYS:NZ	1:B:86:LYS:HB3	2.34	0.42
1:A:1:MET:HG3	1:A:62:HIS:CB	2.49	0.42
1:B:7:ILE:HG12	1:B:26:LEU:HD12	2.01	0.42
1:B:131:GLU:O	1:B:135:GLU:HG3	2.19	0.42
1:D:99:LYS:HE3	1:D:99:LYS:CA	2.44	0.42
1:D:27:ARG:C	3:D:1043:HOH:O	2.62	0.42
1:A:124:HIS:CD2	1:A:124:HIS:H	2.36	0.42
1:C:3:LYS:HE3	1:C:28:TYR:CE1	2.55	0.42
1:A:9:THR:HB	1:A:51:ALA:HB1	2.00	0.42
1:C:75:ARG:HG3	1:C:120:TRP:CE3	2.55	0.42
1:A:76:GLN:O	1:A:80:GLN:HB2	2.20	0.42
1:B:82:ILE:CG2	1:B:83:HIS:H	2.33	0.42
1:A:92:THR:HG22	1:C:155:VAL:HG23	2.02	0.41
1:B:57:GLU:OE1	1:B:106:ARG:NH2	2.54	0.41
1:B:66:ILE:HG23	1:B:66:ILE:O	2.20	0.41
1:D:140:ALA:HA	3:D:1024:HOH:O	2.19	0.41
1:A:2:LEU:HD23	1:A:2:LEU:N	2.30	0.41
1:B:98:VAL:CG2	1:B:101:VAL:HB	2.50	0.41
1:C:152:GLN:O	1:C:154:GLU:HG3	2.20	0.41
1:B:3:LYS:HD3	1:B:61:GLU:OE2	2.21	0.41
1:B:20:GLY:O	1:B:47:MET:HE3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TRP:NE1	1:C:155:VAL:HG11	2.34	0.41
1:D:29:ARG:HB2	3:D:1039:HOH:O	2.19	0.41
1:D:67:LEU:HD13	1:D:118:TRP:CH2	2.55	0.41
1:B:1:MET:SD	1:B:1:MET:C	3.03	0.41
1:A:22:TYR:HB2	1:A:51:ALA:HB2	2.02	0.41
1:B:41:ARG:HH11	1:B:41:ARG:CG	2.31	0.41
1:C:121:VAL:HG13	1:C:127:HIS:CE1	2.56	0.41
1:B:25:ILE:HG13	1:B:133:CYS:SG	2.61	0.40
1:C:152:GLN:C	1:C:152:GLN:CD	2.90	0.40
1:B:125:ALA:HB3	3:B:1024:HOH:O	2.21	0.40
1:B:44:ASN:ND2	1:B:48:GLU:CD	2.79	0.40
1:A:151:TYR:CE1	1:A:153:VAL:HA	2.56	0.40
1:B:84:ASN:O	1:B:88:ARG:HG2	2.22	0.40
1:C:88:ARG:NH1	1:C:93:ALA:CA	2.82	0.40
1:D:114:HIS:HB2	1:D:116:ILE:HD11	2.02	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	153/155 (99%)	138 (90%)	11 (7%)	4 (3%)	4	3
1	B	153/155 (99%)	139 (91%)	9 (6%)	5 (3%)	3	2
1	C	153/155 (99%)	141 (92%)	9 (6%)	3 (2%)	6	5
1	D	153/155 (99%)	127 (83%)	21 (14%)	5 (3%)	3	2
All	All	612/620 (99%)	545 (89%)	50 (8%)	17 (3%)	4	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ALA
1	B	31	ARG
1	B	32	GLU
1	C	3	LYS
1	D	28	TYR
1	D	29	ARG
1	D	88	ARG
1	A	95	LYS
1	B	154	GLU
1	C	123	GLY
1	C	124	HIS
1	A	2	LEU
1	A	3	LYS
1	B	92	THR
1	D	90	TRP
1	B	16	ASN
1	D	36	SER

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	125/125 (100%)	116 (93%)	9 (7%)	13	18
1	B	125/125 (100%)	117 (94%)	8 (6%)	16	23
1	C	125/125 (100%)	113 (90%)	12 (10%)	8	10
1	D	125/125 (100%)	118 (94%)	7 (6%)	19	28
All	All	500/500 (100%)	464 (93%)	36 (7%)	13	18

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	27	ARG
1	A	31	ARG
1	A	72	GLN
1	A	91	LYS

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Mol	Chain	Res	Type
1	A	105	GLN
1	A	124	HIS
1	A	127	HIS
1	A	152	GLN
1	B	1	MET
1	B	2	LEU
1	B	4	GLN
1	B	27	ARG
1	B	31	ARG
1	B	41	ARG
1	B	60	LYS
1	B	113	GLN
1	C	27	ARG
1	C	41	ARG
1	C	61	GLU
1	C	66	ILE
1	C	72	GLN
1	C	86	LYS
1	C	88	ARG
1	C	122	LYS
1	C	129	GLU
1	C	131	GLU
1	C	152	GLN
1	C	154	GLU
1	D	27	ARG
1	D	72	GLN
1	D	99	LYS
1	D	117	LYS
1	D	124	HIS
1	D	131	GLU
1	D	132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	45	ASN
1	A	100	ASN
1	A	105	GLN
1	A	124	HIS
1	B	44	ASN
1	B	62	HIS

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Mol	Chain	Res	Type
1	B	72	GLN
1	B	80	GLN
1	B	105	GLN
1	B	113	GLN
1	B	115	GLN
1	B	124	HIS
1	B	143	ASN
1	C	45	ASN
1	C	62	HIS
1	C	72	GLN
1	C	76	GLN
1	C	105	GLN
1	C	113	GLN
1	C	143	ASN
1	D	45	ASN
1	D	72	GLN
1	D	84	ASN
1	D	124	HIS
1	D	130	ASN
1	D	143	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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

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 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.