



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:15 PM UTC

PDB ID : 4E6H / pdb_00004e6h
Title : CRYSTAL STRUCTURE OF THE HAT domain of k. lactis RNA14
Authors : Paulson, A.R.; Tong, L.
Deposited on : 2012-03-15
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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

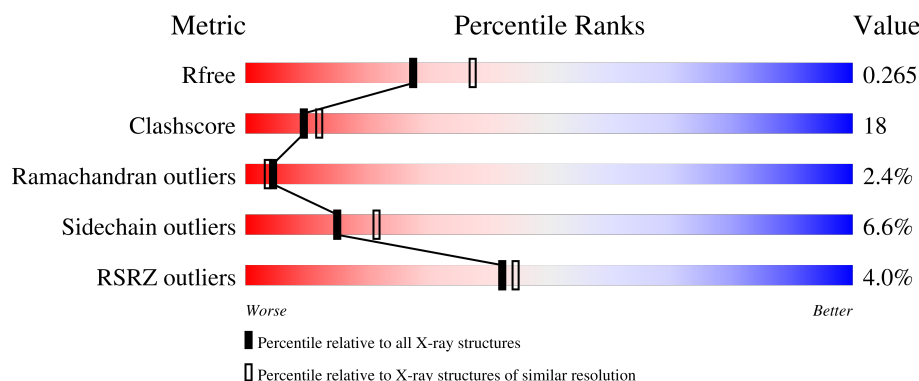
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	679	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4838 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 mRNA 3'-end-processing protein RNA14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4608	2967	764	852	25	0	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP Q6CII8
A	-16	GLY	-	expression tag	UNP Q6CII8
A	-15	SER	-	expression tag	UNP Q6CII8
A	-14	SER	-	expression tag	UNP Q6CII8
A	-13	HIS	-	expression tag	UNP Q6CII8
A	-12	HIS	-	expression tag	UNP Q6CII8
A	-11	HIS	-	expression tag	UNP Q6CII8
A	-10	HIS	-	expression tag	UNP Q6CII8
A	-9	HIS	-	expression tag	UNP Q6CII8
A	-8	HIS	-	expression tag	UNP Q6CII8
A	-7	SER	-	expression tag	UNP Q6CII8
A	-6	SER	-	expression tag	UNP Q6CII8
A	-5	GLY	-	expression tag	UNP Q6CII8
A	-4	LEU	-	expression tag	UNP Q6CII8
A	-3	VAL	-	expression tag	UNP Q6CII8
A	-2	PRO	-	expression tag	UNP Q6CII8
A	-1	ARG	-	expression tag	UNP Q6CII8
A	0	GLY	-	expression tag	UNP Q6CII8
A	1	SER	-	expression tag	UNP Q6CII8
A	2	HIS	-	expression tag	UNP Q6CII8
A	3	MET	-	expression tag	UNP Q6CII8
A	4	ALA	-	expression tag	UNP Q6CII8
A	5	SER	-	expression tag	UNP Q6CII8
A	6	MET	-	expression tag	UNP Q6CII8
A	7	THR	-	expression tag	UNP Q6CII8
A	8	GLY	-	expression tag	UNP Q6CII8
A	9	GLY	-	expression tag	UNP Q6CII8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLN	-	expression tag	UNP Q6CII8
A	11	GLN	-	expression tag	UNP Q6CII8
A	12	MET	-	expression tag	UNP Q6CII8
A	13	GLY	-	expression tag	UNP Q6CII8
A	14	ARG	-	expression tag	UNP Q6CII8
A	15	GLY	-	expression tag	UNP Q6CII8
A	16	SER	-	expression tag	UNP Q6CII8
A	17	MET	-	expression tag	UNP Q6CII8

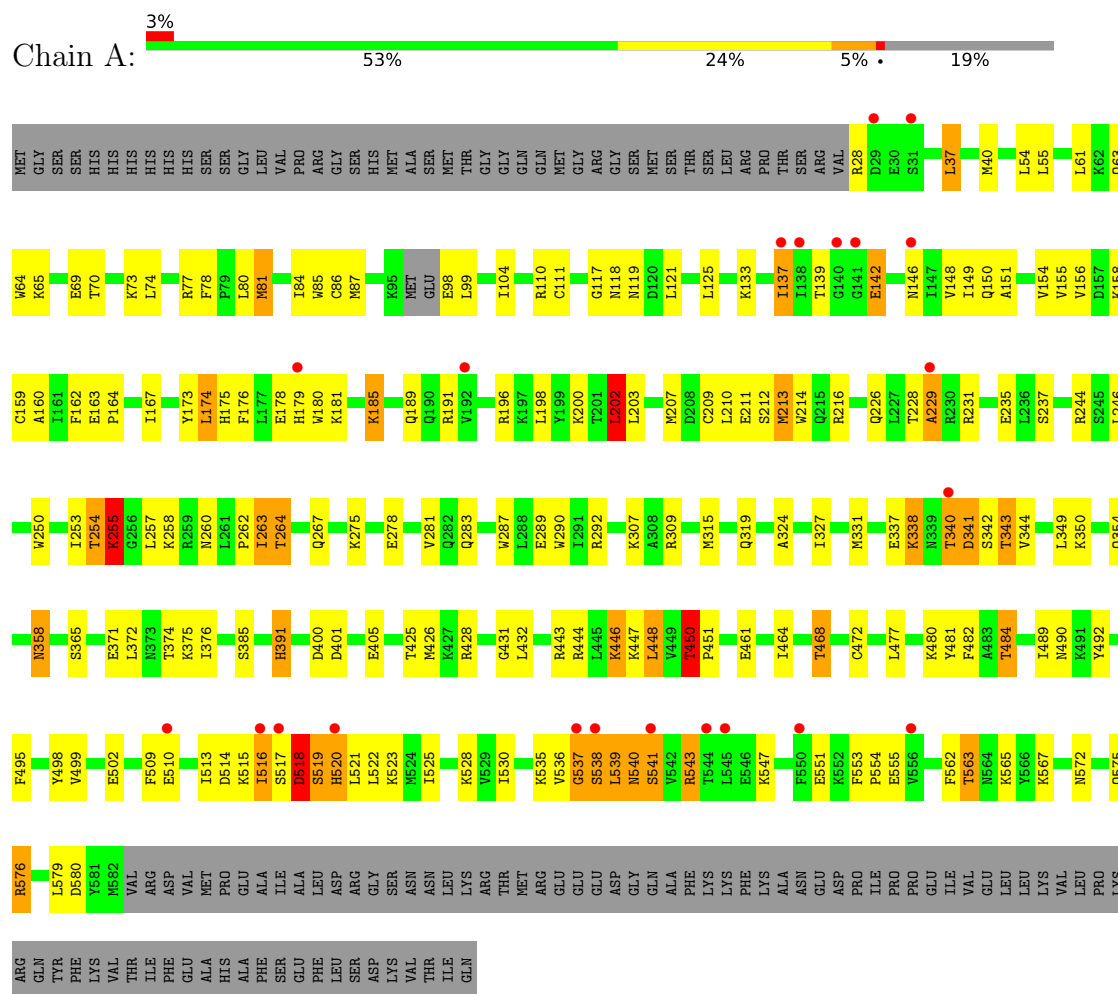
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	230	Total O 230 230	0	0

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 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: mRNA 3'-end-processing protein RNA14



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.35Å 59.79Å 123.48Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	29.32 – 2.30 29.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.32-2.30) 89.2 (29.32-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.270 0.204 , 0.265	Depositor DCC
R_{free} test set	1782 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4838	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.85	1/4708 (0.0%)	1.13	35/6363 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	MET	SD-CE	-9.59	1.55	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	GLY	N-CA-C	8.58	122.71	112.33
1	A	104	ILE	N-CA-C	8.49	119.29	110.72
1	A	516	ILE	N-CA-C	7.81	119.06	109.30
1	A	344	VAL	N-CA-C	7.42	117.55	110.42
1	A	163	GLU	CA-C-N	-7.14	112.44	119.87
1	A	163	GLU	C-N-CA	-7.14	112.44	119.87
1	A	492	TYR	N-CA-C	-7.09	103.48	111.07
1	A	401	ASP	CA-C-N	6.87	126.57	119.56
1	A	401	ASP	C-N-CA	6.87	126.57	119.56
1	A	562	PHE	CA-C-N	6.53	129.03	120.28
1	A	562	PHE	C-N-CA	6.53	129.03	120.28
1	A	160	ALA	N-CA-C	6.49	120.06	111.75
1	A	401	ASP	N-CA-CB	6.37	118.99	111.09
1	A	156	VAL	CB-CA-C	-6.31	103.90	111.97
1	A	446	LYS	CB-CA-C	-6.10	109.53	116.54
1	A	513	ILE	N-CA-C	6.07	117.54	110.62
1	A	482	PHE	N-CA-C	5.86	120.03	112.41
1	A	535	LYS	N-CA-C	-5.82	104.89	112.23
1	A	121	LEU	N-CA-C	5.82	118.37	111.33
1	A	576	ARG	N-CA-C	5.59	117.37	111.28
1	A	375	LYS	N-CA-C	-5.53	101.25	109.11
1	A	400	ASP	N-CA-C	5.50	117.35	111.36
1	A	64	TRP	N-CA-C	5.45	118.72	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	ASN	N-CA-C	-5.43	105.44	111.36
1	A	448	LEU	N-CA-C	-5.38	105.45	112.23
1	A	450	THR	CA-C-N	5.37	125.69	119.47
1	A	450	THR	C-N-CA	5.37	125.69	119.47
1	A	77	ARG	CG-CD-NE	-5.34	100.24	112.00
1	A	278	GLU	N-CA-C	5.34	118.93	109.96
1	A	202	LEU	N-CA-C	5.32	116.76	111.07
1	A	541	SER	N-CA-C	-5.29	105.20	110.97
1	A	432	LEU	N-CA-C	5.20	117.62	111.33
1	A	155	VAL	N-CA-C	-5.19	105.48	110.72
1	A	523	LYS	N-CA-C	-5.09	105.42	110.97
1	A	210	LEU	N-CA-C	5.07	119.68	111.37

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	4608	0	4608	164	0
2	A	230	0	0	17	0
All	All	4838	0	4608	164	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 18.

All (164) 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:258:LYS:HG3	1:A:260:ASN:HD21	1.28	0.98
1:A:202:LEU:HD21	1:A:213:MET:HG2	1.47	0.97
1:A:563:THR:CG2	1:A:572:ASN:HD21	1.80	0.93
1:A:580:ASP:HB2	2:A:736:HOH:O	1.70	0.91
1:A:450:THR:HG23	1:A:451:PRO:HD2	1.58	0.83
1:A:185:LYS:HD2	1:A:185:LYS:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ARG:HH11	1:A:543:ARG:HG2	1.47	0.80
1:A:258:LYS:HG3	1:A:260:ASN:ND2	1.96	0.80
1:A:180:TRP:CE3	1:A:191:ARG:HG3	2.16	0.79
1:A:547:LYS:O	1:A:551:GLU:HG3	1.82	0.79
1:A:81:MET:HE1	1:A:319:GLN:HA	1.65	0.78
1:A:563:THR:HG23	1:A:572:ASN:HD21	1.47	0.78
1:A:28:ARG:N	2:A:730:HOH:O	2.15	0.78
1:A:258:LYS:H	1:A:283:GLN:HE22	1.33	0.77
1:A:519:SER:O	1:A:521:LEU:N	2.19	0.75
1:A:264:THR:HB	1:A:267:GLN:OE1	1.86	0.74
1:A:350:LYS:NZ	1:A:354:GLN:HE21	1.85	0.74
1:A:509:PHE:CE1	1:A:525:ILE:HG22	2.23	0.74
1:A:444:ARG:HH11	1:A:444:ARG:HG2	1.53	0.74
1:A:537:GLY:O	1:A:538:SER:HB3	1.87	0.73
1:A:167:ILE:HG13	1:A:209:CYS:HB3	1.68	0.72
1:A:250:TRP:O	1:A:254:THR:HB	1.89	0.72
1:A:231:ARG:O	1:A:235:GLU:HG3	1.90	0.72
1:A:81:MET:CE	1:A:319:GLN:HA	2.20	0.71
1:A:181:LYS:HD2	1:A:181:LYS:O	1.90	0.71
1:A:65:LYS:O	1:A:69:GLU:HG3	1.92	0.70
1:A:563:THR:HG22	1:A:572:ASN:HD21	1.57	0.69
1:A:538:SER:OG	1:A:539:LEU:N	2.22	0.69
1:A:490:ASN:ND2	1:A:528:LYS:HE3	2.07	0.69
1:A:307:LYS:HD3	1:A:338:LYS:HG3	1.73	0.69
1:A:174:LEU:HD13	1:A:216:ARG:NH2	2.10	0.67
1:A:563:THR:HG21	1:A:575:GLN:HG3	1.74	0.67
1:A:258:LYS:H	1:A:283:GLN:NE2	1.93	0.67
1:A:563:THR:HG23	1:A:572:ASN:ND2	2.10	0.67
1:A:258:LYS:CG	1:A:260:ASN:HD21	2.07	0.66
1:A:536:VAL:HG12	1:A:536:VAL:O	1.93	0.66
1:A:158:LYS:HD2	2:A:900:HOH:O	1.96	0.66
1:A:207:MET:HE2	1:A:209:CYS:SG	2.36	0.65
1:A:99:LEU:HD11	1:A:133:LYS:HD2	1.78	0.64
1:A:391:HIS:HD2	2:A:727:HOH:O	1.81	0.63
1:A:315:MET:HG3	1:A:331:MET:HE1	1.80	0.62
1:A:61:LEU:HD12	1:A:63:GLN:NE2	2.14	0.62
1:A:110:ARG:HD2	2:A:706:HOH:O	2.00	0.62
1:A:350:LYS:HZ3	1:A:354:GLN:HE21	1.47	0.62
1:A:444:ARG:HG2	1:A:444:ARG:NH1	2.13	0.61
1:A:450:THR:HG23	1:A:451:PRO:CD	2.28	0.61
1:A:99:LEU:CD1	1:A:133:LYS:HD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:PHE:CZ	1:A:499:VAL:HG21	2.35	0.60
1:A:146:ASN:O	1:A:150:GLN:HG2	1.99	0.60
1:A:371:GLU:OE1	1:A:428:ARG:NH2	2.34	0.60
1:A:537:GLY:O	1:A:538:SER:CB	2.49	0.60
1:A:263:ILE:HG22	2:A:757:HOH:O	2.02	0.59
1:A:538:SER:C	1:A:540:ASN:H	2.12	0.58
1:A:538:SER:OG	1:A:541:SER:HB2	2.03	0.58
1:A:543:ARG:HG2	1:A:543:ARG:NH1	2.17	0.58
1:A:207:MET:CE	1:A:209:CYS:SG	2.92	0.57
1:A:477:LEU:HD12	1:A:480:LYS:HD2	1.85	0.57
1:A:81:MET:HE2	1:A:319:GLN:HG3	1.86	0.57
1:A:37:LEU:HD12	1:A:40:MET:CE	2.34	0.57
1:A:374:THR:HG22	1:A:374:THR:O	2.04	0.57
1:A:174:LEU:HD13	1:A:216:ARG:CZ	2.35	0.56
1:A:37:LEU:HD12	1:A:40:MET:HE3	1.86	0.56
1:A:78:PHE:HB3	1:A:81:MET:HG3	1.87	0.56
1:A:307:LYS:CD	1:A:338:LYS:HG3	2.35	0.56
1:A:484:THR:HB	2:A:819:HOH:O	2.05	0.56
1:A:263:ILE:HG12	1:A:263:ILE:O	2.06	0.55
1:A:509:PHE:HE1	1:A:525:ILE:HG22	1.70	0.55
1:A:151:ALA:O	1:A:154:VAL:HG12	2.07	0.55
1:A:181:LYS:O	1:A:181:LYS:CD	2.54	0.55
1:A:538:SER:O	1:A:540:ASN:N	2.33	0.54
1:A:196:ARG:HG2	1:A:200:LYS:HE2	1.88	0.54
1:A:86:CYS:HB3	1:A:263:ILE:HG13	1.89	0.54
1:A:81:MET:HE3	2:A:707:HOH:O	2.08	0.53
1:A:253:ILE:HG23	1:A:289:GLU:HG2	1.90	0.53
1:A:87:MET:CE	1:A:262:PRO:HG2	2.38	0.53
1:A:555:GLU:HB2	2:A:810:HOH:O	2.08	0.53
1:A:119:ASN:OD1	1:A:159:CYS:HB2	2.08	0.52
1:A:538:SER:C	1:A:540:ASN:N	2.67	0.52
1:A:358:ASN:C	1:A:358:ASN:HD22	2.16	0.51
1:A:518:ASP:HB3	1:A:520:HIS:CE1	2.45	0.51
1:A:551:GLU:O	1:A:554:PRO:HD3	2.10	0.51
1:A:519:SER:O	1:A:522:LEU:N	2.37	0.51
1:A:139:THR:HG22	1:A:139:THR:O	2.10	0.51
1:A:489:ILE:HG21	1:A:516:ILE:HD11	1.93	0.51
1:A:78:PHE:HB3	1:A:81:MET:CG	2.41	0.51
1:A:257:LEU:HD11	1:A:287:TRP:CE2	2.46	0.51
1:A:340:THR:O	1:A:341:ASP:HB3	2.11	0.51
1:A:202:LEU:C	1:A:202:LEU:HD12	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD13	1:A:214:TRP:HE3	1.76	0.50
1:A:55:LEU:HG	1:A:70:THR:HG21	1.93	0.50
1:A:538:SER:CB	1:A:541:SER:HB2	2.41	0.50
1:A:517:SER:O	1:A:518:ASP:O	2.30	0.50
1:A:563:THR:HG23	1:A:572:ASN:OD1	2.11	0.50
1:A:162:PHE:HA	1:A:309:ARG:NH1	2.27	0.49
1:A:149:ILE:HG13	1:A:176:PHE:HE2	1.77	0.49
1:A:167:ILE:CG1	1:A:209:CYS:HB3	2.39	0.49
1:A:371:GLU:CD	1:A:428:ARG:HH21	2.20	0.49
1:A:253:ILE:CG2	1:A:289:GLU:HG2	2.43	0.49
1:A:520:HIS:CG	1:A:521:LEU:H	2.30	0.49
1:A:518:ASP:N	2:A:783:HOH:O	2.43	0.48
1:A:576:ARG:HD3	2:A:838:HOH:O	2.11	0.48
1:A:468:THR:HG23	1:A:472:CYS:SG	2.53	0.48
1:A:536:VAL:O	1:A:537:GLY:O	2.31	0.48
1:A:175:HIS:O	1:A:179:HIS:HB2	2.13	0.48
1:A:250:TRP:CH2	1:A:254:THR:HG21	2.49	0.48
1:A:142:GLU:HB3	2:A:867:HOH:O	2.14	0.47
1:A:484:THR:HG22	2:A:855:HOH:O	2.13	0.47
1:A:350:LYS:HZ2	1:A:354:GLN:HE21	1.60	0.47
1:A:518:ASP:O	1:A:519:SER:O	2.32	0.47
1:A:499:VAL:O	1:A:499:VAL:HG12	2.14	0.47
1:A:563:THR:HG23	1:A:572:ASN:CG	2.40	0.47
1:A:73:LYS:NZ	2:A:824:HOH:O	2.47	0.47
1:A:341:ASP:C	1:A:343:THR:H	2.23	0.47
1:A:281:VAL:HG23	2:A:763:HOH:O	2.15	0.46
1:A:37:LEU:HD23	1:A:54:LEU:HA	1.96	0.46
1:A:142:GLU:OE1	1:A:142:GLU:HA	2.15	0.46
1:A:81:MET:HE2	1:A:81:MET:HA	1.97	0.46
1:A:498:TYR:CD2	1:A:498:TYR:C	2.94	0.46
1:A:461:GLU:O	1:A:464:ILE:HD12	2.16	0.46
1:A:563:THR:CG2	1:A:575:GLN:HG3	2.43	0.46
1:A:137:ILE:HD12	1:A:137:ILE:H	1.81	0.45
1:A:174:LEU:HD22	1:A:178:GLU:HG3	1.98	0.45
1:A:81:MET:HE1	1:A:319:GLN:CA	2.42	0.45
1:A:337:GLU:O	1:A:338:LYS:C	2.60	0.45
1:A:446:LYS:HG2	1:A:481:TYR:OH	2.17	0.45
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.75	0.44
1:A:563:THR:CG2	1:A:572:ASN:ND2	2.62	0.44
1:A:137:ILE:H	1:A:137:ILE:CD1	2.28	0.44
1:A:211:GLU:HG3	1:A:244:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:O	1:A:229:ALA:C	2.60	0.44
1:A:290:TRP:C	1:A:290:TRP:CD1	2.96	0.44
1:A:495:PHE:O	1:A:499:VAL:HG23	2.18	0.44
1:A:520:HIS:CG	1:A:521:LEU:N	2.86	0.43
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.88	0.43
1:A:349:LEU:HD13	1:A:365:SER:HB3	2.00	0.43
1:A:530:ILE:HG22	1:A:565:LYS:HG3	2.00	0.43
1:A:137:ILE:HD12	1:A:137:ILE:N	2.34	0.43
1:A:85:TRP:CD2	1:A:111:CYS:HB3	2.54	0.43
1:A:244:ARG:HE	1:A:244:ARG:HB3	1.50	0.43
1:A:425:THR:HG22	1:A:426:MET:HE2	1.99	0.43
1:A:167:ILE:HG13	1:A:209:CYS:CB	2.45	0.42
1:A:254:THR:O	1:A:255:LYS:C	2.62	0.42
1:A:264:THR:HG22	1:A:267:GLN:H	1.84	0.42
1:A:74:LEU:HD13	1:A:84:ILE:HD13	2.01	0.42
1:A:567:LYS:HG2	1:A:572:ASN:HA	2.01	0.42
1:A:162:PHE:O	1:A:164:PRO:HD3	2.19	0.42
1:A:148:VAL:O	1:A:151:ALA:HB3	2.19	0.42
1:A:258:LYS:CG	1:A:260:ASN:ND2	2.73	0.42
1:A:117:GLY:O	1:A:315:MET:HE1	2.20	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.91	0.42
1:A:553:PHE:O	1:A:554:PRO:C	2.60	0.42
1:A:340:THR:O	1:A:341:ASP:CB	2.68	0.42
1:A:173:TYR:CE2	1:A:198:LEU:HD13	2.55	0.41
1:A:254:THR:O	1:A:254:THR:CG2	2.68	0.41
1:A:554:PRO:O	1:A:555:GLU:HB2	2.20	0.41
1:A:324:ALA:O	1:A:327:ILE:HG22	2.20	0.41
1:A:575:GLN:HA	1:A:579:LEU:HB2	2.03	0.41
1:A:254:THR:O	1:A:254:THR:HG23	2.21	0.41
1:A:80:LEU:HA	1:A:118:ASN:HD21	1.86	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.87	0.41
1:A:447:LYS:HD2	2:A:773:HOH:O	2.21	0.41
1:A:289:GLU:CB	1:A:292:ARG:NH2	2.85	0.40
1:A:553:PHE:C	1:A:554:PRO:O	2.63	0.40
1:A:447:LYS:CD	2:A:773:HOH:O	2.69	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	549/679 (81%)	503 (92%)	33 (6%)	13 (2%)	4 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	255	LYS
1	A	518	ASP
1	A	519	SER
1	A	520	HIS
1	A	537	GLY
1	A	538	SER
1	A	338	LYS
1	A	229	ALA
1	A	340	THR
1	A	341	ASP
1	A	342	SER
1	A	142	GLU

5.3.2 Protein sidechains [i](#)

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	514/624 (82%)	480 (93%)	34 (7%)	15 21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	98	GLU
1	A	137	ILE
1	A	174	LEU
1	A	185	LYS
1	A	189	GLN
1	A	202	LEU
1	A	212	SER
1	A	213	MET
1	A	226	GLN
1	A	254	THR
1	A	255	LYS
1	A	263	ILE
1	A	264	THR
1	A	275	LYS
1	A	343	THR
1	A	358	ASN
1	A	372	LEU
1	A	376	ILE
1	A	385	SER
1	A	391	HIS
1	A	405	GLU
1	A	443	ARG
1	A	450	THR
1	A	468	THR
1	A	484	THR
1	A	502	GLU
1	A	510	GLU
1	A	514	ASP
1	A	515	LYS
1	A	518	ASP
1	A	539	LEU
1	A	543	ARG
1	A	563	THR

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	63	GLN
1	A	66	GLN
1	A	83	ASN
1	A	118	ASN

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	193	GLN
1	A	260	ASN
1	A	277	ASN
1	A	282	GLN
1	A	283	GLN
1	A	319	GLN
1	A	330	ASN
1	A	333	ASN
1	A	335	GLN
1	A	353	GLN
1	A	354	GLN
1	A	358	ASN
1	A	391	HIS
1	A	457	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 ⓘ

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	553/679 (81%)	0.12	22 (3%) 42 44	29, 53, 90, 121	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	SER	3.5
1	A	29	ASP	3.4
1	A	537	GLY	3.2
1	A	340	THR	3.0
1	A	137	ILE	2.9
1	A	538	SER	2.9
1	A	141	GLY	2.8
1	A	140	GLY	2.8
1	A	138	ILE	2.8
1	A	510	GLU	2.7
1	A	545	LEU	2.7
1	A	556	VAL	2.7
1	A	541	SER	2.7
1	A	550	PHE	2.6
1	A	520	HIS	2.5
1	A	544	THR	2.4
1	A	31	SER	2.3
1	A	179	HIS	2.3
1	A	146	ASN	2.2
1	A	229	ALA	2.2
1	A	516	ILE	2.1
1	A	192	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.