



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 PM UTC

PDB ID : 6KC7 / pdb_00006kc7
Title : Crystal structure of Nme1Cas9 in complex with sgRNA and target DNA (ATATGATT PAM) in seed-base paring state
Authors : Sun, W.; Yang, J.; Cheng, Z.; Liu, C.; Wang, K.; Huang, X.; Wang, Y.
Deposited on : 2019-06-27
Resolution : 3.30 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

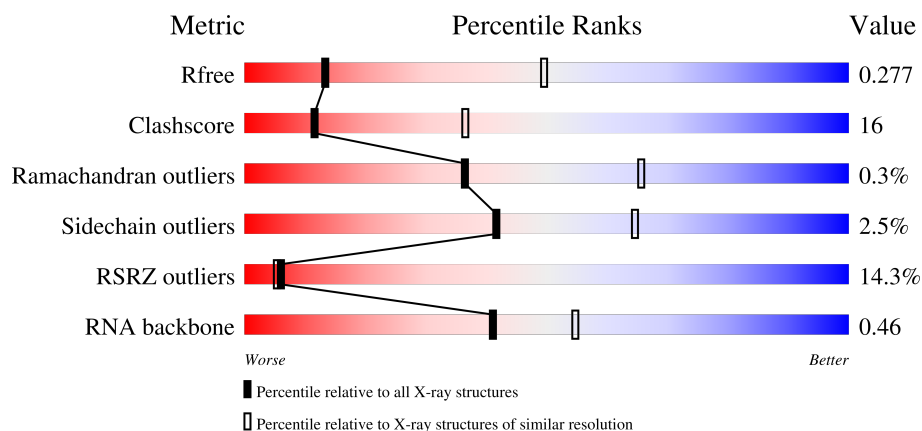
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 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	1083	
2	B	135	
3	C	19	
4	D	11	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10502 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 CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	0
			7540	4775	1393	1352	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP C9X1G5
A	588	ALA	HIS	engineered mutation	UNP C9X1G5

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	111	Total	C	N	O	P	0	0	0
			2350	1052	409	778	111			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*AP*AP*AP*TP*CP*AP*TP*AP*TP*GP*TP*AP*AP*AP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	19	Total	C	N	O	P	0	0	0
			389	189	72	110	18			

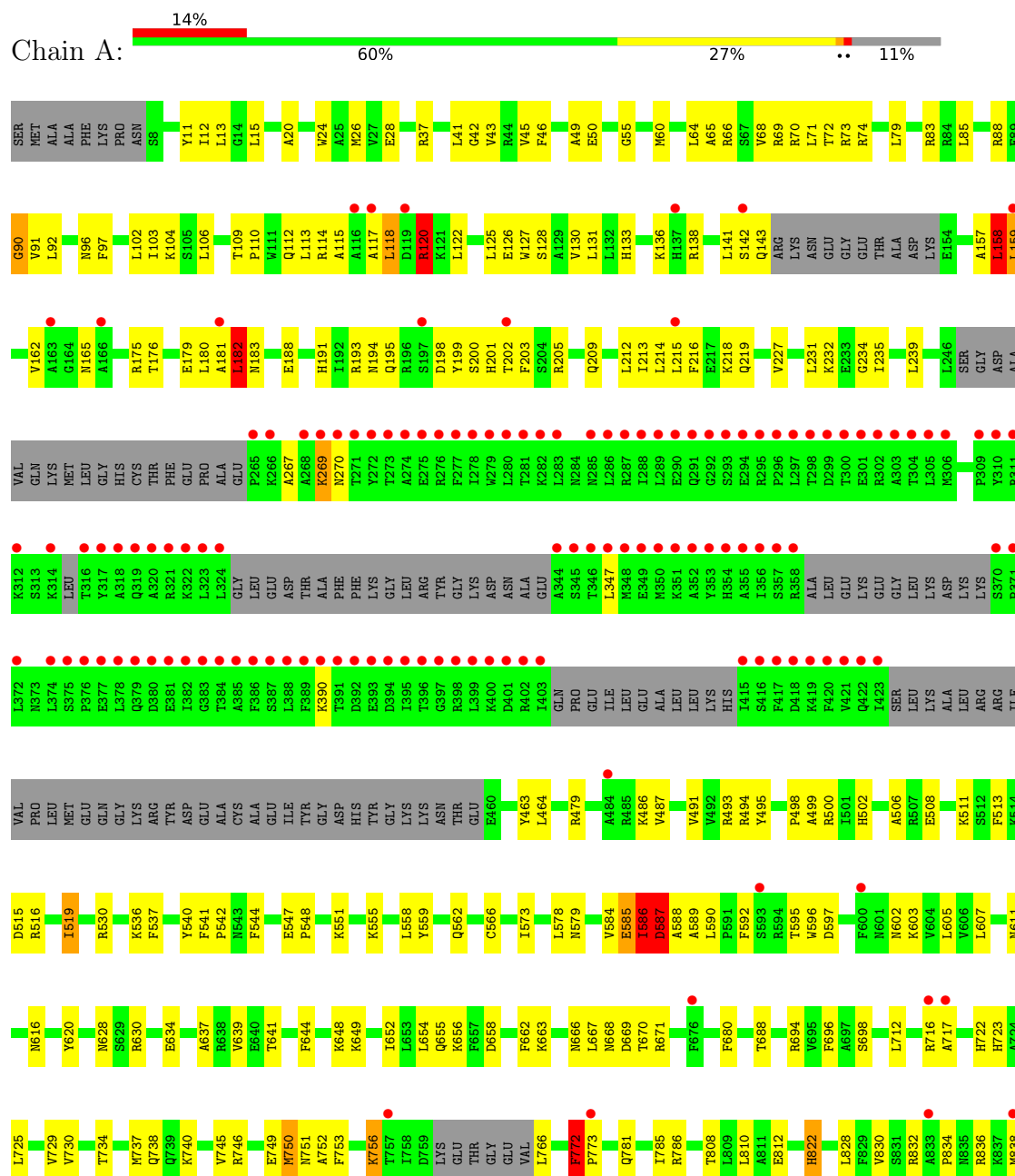
- Molecule 4 is a DNA chain called DNA (5'-D(*AP*TP*AP*TP*GP*AP*TP*TP*TP*TP*A)-3').

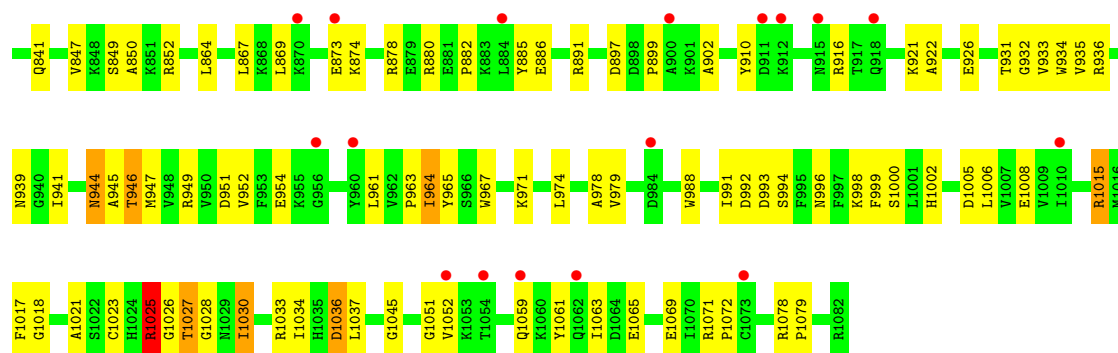
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			223	110	37	66	10			

3 Residue-property plots

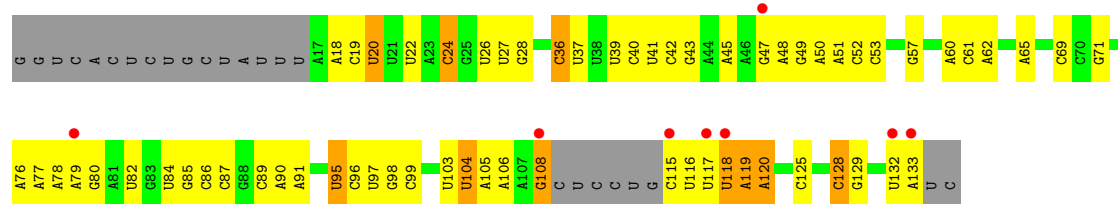
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endonuclease Cas9





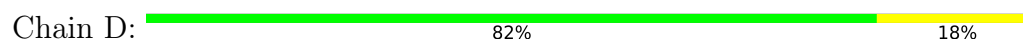
• Molecule 2: sgRNA



• Molecule 3: DNA (5'-D(*TP*AP*AP*AP*AP*TP*CP*AP*TP*AP*TP*GP*TP*AP*AP*AP*GP*TP*T)-3')



• Molecule 4: DNA (5'-D(*AP*TP*AP*TP*GP*AP*TP*TP*TP*TP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.58Å 72.51Å 115.15Å 90.00° 104.67° 90.00°	Depositor
Resolution (Å)	46.20 – 3.30 46.20 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.0 (46.20-3.30) 86.1 (46.20-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.253 , 0.275 0.253 , 0.277	Depositor DCC
R_{free} test set	1251 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10502	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.75	28/7684 (0.4%)	0.74	18/10368 (0.2%)
2	B	0.15	0/2623	0.40	0/4079
3	C	0.26	0/437	0.53	0/673
4	D	0.26	0/249	0.52	0/383
All	All	0.64	28/10993 (0.3%)	0.65	18/15503 (0.1%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	ILE	C-O	-9.44	1.14	1.24
1	A	933	VAL	C-O	-8.88	1.13	1.24
1	A	751	ASN	CA-C	-8.36	1.44	1.52
1	A	181	ALA	CA-C	-7.75	1.43	1.52
1	A	519	ILE	CA-CB	-7.59	1.43	1.54
1	A	181	ALA	C-O	-7.30	1.15	1.24
1	A	588	ALA	N-CA	-7.25	1.37	1.46
1	A	1037	LEU	C-O	-7.03	1.15	1.24
1	A	585	GLU	C-O	-6.96	1.15	1.23
1	A	935	VAL	C-O	-6.26	1.16	1.24
1	A	935	VAL	CA-CB	-6.21	1.46	1.54
1	A	1026	GLY	C-O	-6.07	1.15	1.23
1	A	1027	THR	C-O	-5.97	1.16	1.24
1	A	834	PRO	C-O	-5.90	1.28	1.24
1	A	933	VAL	CA-CB	-5.76	1.46	1.54
1	A	934	TRP	C-O	-5.74	1.16	1.23
1	A	834	PRO	CA-C	-5.70	1.47	1.52
1	A	772	PHE	C-O	-5.52	1.17	1.24
1	A	586	ILE	C-O	-5.35	1.18	1.24
1	A	751	ASN	C-O	-5.33	1.19	1.24
1	A	158	LEU	CA-C	-5.31	1.46	1.52
1	A	519	ILE	C-O	-5.29	1.17	1.24
1	A	180	LEU	CA-C	-5.25	1.46	1.52
1	A	1025	ARG	CA-C	-5.21	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	ALA	C-O	-5.16	1.17	1.24
1	A	1025	ARG	C-O	-5.05	1.18	1.24
1	A	515	ASP	CA-C	-5.03	1.46	1.52
1	A	515	ASP	C-O	-5.00	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	ARG	N-CA-C	10.24	125.37	111.24
1	A	587	ASP	N-CA-C	8.66	123.72	109.95
1	A	120	ARG	N-CA-C	8.59	122.54	109.23
1	A	590	LEU	N-CA-C	-7.75	100.32	109.93
1	A	267	ALA	N-CA-C	7.45	120.64	109.25
1	A	1036	ASP	N-CA-C	-6.84	98.06	109.07
1	A	269	LYS	N-CA-C	6.16	117.69	110.97
1	A	158	LEU	N-CA-C	-6.09	104.58	112.68
1	A	90	GLY	N-CA-C	5.90	123.74	115.43
1	A	750	MET	CB-CG-SD	-5.42	96.46	112.70
1	A	182	LEU	CA-C-N	-5.39	112.63	120.29
1	A	182	LEU	C-N-CA	-5.39	112.63	120.29
1	A	933	VAL	N-CA-C	-5.30	98.31	109.34
1	A	588	ALA	N-CA-C	-5.27	99.16	108.23
1	A	590	LEU	CA-C-N	5.09	125.07	120.03
1	A	590	LEU	C-N-CA	5.09	125.07	120.03
1	A	935	VAL	CB-CA-C	-5.07	102.97	111.29
1	A	717	ALA	N-CA-C	5.00	121.46	110.80

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	7540	0	7382	278	0
2	B	2350	0	1193	52	0
3	C	389	0	218	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	223	0	129	2	0
All	All	10502	0	8922	310	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 16.

All (310) 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:175:ARG:HB2	1:A:179:GLU:OE2	1.58	1.02
1:A:808:THR:O	1:A:812:GLU:HB2	1.70	0.92
1:A:974:LEU:HD21	1:A:1078:ARG:HH12	1.44	0.83
1:A:1008:GLU:HB2	1:A:1017:PHE:CD1	2.13	0.83
1:A:974:LEU:HD21	1:A:1078:ARG:NH1	1.97	0.79
1:A:113:LEU:HD13	1:A:126:GLU:HB3	1.67	0.77
1:A:756:LYS:O	1:A:766:LEU:HB2	1.85	0.75
3:C:13:DT:H2''	3:C:14:DA:H5''	1.66	0.75
1:A:194:ASN:HD21	1:A:199:TYR:HA	1.51	0.75
1:A:880:ARG:HD2	2:B:36:C:O2'	1.87	0.74
1:A:118:LEU:N	1:A:118:LEU:HD12	2.03	0.74
1:A:212:LEU:HD21	1:A:235:ILE:HG22	1.70	0.73
1:A:1008:GLU:HB2	1:A:1017:PHE:HD1	1.49	0.72
1:A:194:ASN:ND2	1:A:199:TYR:HA	2.04	0.72
1:A:931:THR:HB	1:A:1025:ARG:HH11	1.55	0.72
1:A:118:LEU:HD12	1:A:118:LEU:H	1.54	0.71
2:B:119:A:H2'	2:B:120:A:C8	2.25	0.71
1:A:74:ARG:NH2	2:B:86:C:OP1	2.23	0.70
1:A:120:ARG:NH1	1:A:122:LEU:HD23	2.06	0.70
1:A:120:ARG:NH1	1:A:122:LEU:CD2	2.55	0.70
1:A:961:LEU:HD11	1:A:1052:VAL:HG21	1.74	0.70
1:A:573:ILE:HG12	1:A:607:LEU:HD21	1.73	0.69
1:A:671:ARG:HG3	1:A:671:ARG:HH11	1.56	0.69
1:A:45:VAL:HG23	1:A:832:ARG:HG2	1.75	0.66
1:A:500:ARG:HH12	1:A:694:ARG:HA	1.59	0.66
1:A:92:LEU:CD1	1:A:103:ILE:HG12	2.25	0.66
1:A:28:GLU:OE1	1:A:37:ARG:NE	2.29	0.66
2:B:117:U:H2'	2:B:118:U:C6	2.32	0.65
1:A:944:ASN:ND2	1:A:944:ASN:H	1.95	0.64
1:A:671:ARG:HG3	1:A:671:ARG:NH1	2.12	0.64
1:A:644:PHE:HB3	1:A:648:LYS:HB3	1.79	0.64
1:A:41:LEU:O	1:A:828:LEU:HD21	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:NE2	2:B:20:U:O2	2.30	0.64
2:B:119:A:H2'	2:B:120:A:H8	1.63	0.64
1:A:159:LEU:HD23	1:A:159:LEU:O	1.98	0.63
1:A:70:ARG:NH1	2:B:20:U:OP2	2.31	0.63
1:A:1008:GLU:HB3	1:A:1061:TYR:HE2	1.63	0.63
2:B:116:U:H2'	2:B:117:U:H6	1.63	0.63
1:A:13:LEU:HD13	1:A:491:VAL:HG11	1.81	0.62
1:A:92:LEU:HD12	1:A:97:PHE:CE2	2.35	0.62
1:A:944:ASN:H	1:A:944:ASN:HD22	1.46	0.62
1:A:91:VAL:HG12	1:A:92:LEU:CD2	2.29	0.62
1:A:1078:ARG:HG2	1:A:1079:PRO:HD2	1.81	0.61
1:A:891:ARG:NH1	1:A:902:ALA:O	2.29	0.61
1:A:138:ARG:O	1:A:205:ARG:HG3	2.00	0.61
1:A:120:ARG:HH12	1:A:122:LEU:HD23	1.63	0.61
1:A:60:MET:O	1:A:64:LEU:HD23	2.00	0.61
1:A:1015:ARG:CG	1:A:1015:ARG:HH21	2.14	0.61
1:A:194:ASN:OD1	1:A:201:HIS:HB2	2.00	0.61
1:A:949:ARG:NH1	1:A:1000:SER:OG	2.33	0.60
2:B:105:A:H2'	2:B:106:A:C8	2.36	0.60
1:A:122:LEU:HD22	1:A:126:GLU:HB2	1.83	0.60
1:A:96:ASN:O	1:A:104:LYS:N	2.34	0.60
1:A:931:THR:CB	1:A:1025:ARG:HH11	2.15	0.59
1:A:952:VAL:HG22	1:A:961:LEU:HD23	1.84	0.59
1:A:193:ARG:NH1	2:B:24:C:OP2	2.35	0.59
1:A:43:VAL:HB	1:A:830:VAL:HG13	1.84	0.59
1:A:68:VAL:O	1:A:72:THR:HG23	2.02	0.59
1:A:584:VAL:HB	1:A:605:LEU:HD11	1.85	0.59
1:A:511:LYS:O	1:A:516:ARG:NH1	2.36	0.59
1:A:722:HIS:O	1:A:725:LEU:HB2	2.02	0.59
2:B:117:U:H2'	2:B:118:U:H6	1.67	0.59
1:A:92:LEU:CD1	1:A:97:PHE:HE2	2.15	0.58
1:A:620:TYR:CE1	1:A:655:GLN:HG2	2.38	0.58
1:A:947:MET:HE3	1:A:1023:CYS:HB3	1.85	0.58
1:A:587:ASP:O	1:A:603:LYS:HA	2.03	0.58
1:A:194:ASN:ND2	1:A:198:ASP:O	2.35	0.58
1:A:500:ARG:NH1	1:A:694:ARG:HA	2.18	0.58
1:A:836:ARG:NH1	1:A:1005:ASP:OD1	2.36	0.58
1:A:1036:ASP:OD1	1:A:1036:ASP:N	2.28	0.58
1:A:595:THR:O	1:A:666:ASN:ND2	2.36	0.58
1:A:92:LEU:HD12	1:A:97:PHE:HE2	1.68	0.58
1:A:162:VAL:HG22	1:A:202:THR:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ALA:HB2	1:A:941:ILE:HB	1.86	0.58
2:B:104:U:H2'	2:B:105:A:C8	2.38	0.58
1:A:110:PRO:HG2	2:B:60:A:H4'	1.85	0.58
1:A:878:ARG:HB2	1:A:885:TYR:CE1	2.39	0.58
3:C:1:DT:H2'	3:C:2:DA:C8	2.39	0.58
1:A:867:LEU:HD23	1:A:867:LEU:O	2.04	0.57
1:A:616:ASN:HB3	1:A:749:GLU:OE2	2.04	0.57
1:A:639:VAL:HG22	1:A:649:LYS:HG3	1.86	0.57
1:A:988:TRP:HH2	1:A:1025:ARG:HD2	1.68	0.57
1:A:494:ARG:HB3	1:A:495:TYR:HD2	1.70	0.57
1:A:530:ARG:HG2	1:A:530:ARG:HH21	1.68	0.57
2:B:90:A:H2'	2:B:91:A:C8	2.40	0.57
2:B:116:U:H2'	2:B:117:U:C6	2.39	0.57
2:B:118:U:H2'	2:B:119:A:C8	2.39	0.57
1:A:26:MET:HE1	1:A:495:TYR:CD1	2.40	0.57
1:A:1061:TYR:CE1	1:A:1072:PRO:HG3	2.39	0.56
1:A:628:ASN:ND2	1:A:628:ASN:O	2.38	0.56
1:A:947:MET:CE	1:A:1023:CYS:HB3	2.34	0.56
1:A:136:LYS:HE3	2:B:62:A:OP2	2.06	0.56
1:A:945:ALA:O	4:D:3:DA:H5''	2.04	0.56
1:A:193:ARG:HH11	2:B:24:C:P	2.28	0.56
1:A:79:LEU:O	1:A:83:ARG:HG3	2.05	0.56
1:A:464:LEU:HG	1:A:680:PHE:HE2	1.71	0.56
1:A:644:PHE:CD2	1:A:648:LYS:HD3	2.40	0.56
1:A:198:ASP:OD1	1:A:199:TYR:N	2.38	0.56
1:A:65:ALA:O	1:A:69:ARG:HG3	2.06	0.56
1:A:648:LYS:O	1:A:652:ILE:HG13	2.06	0.56
1:A:781:GLN:O	1:A:785:ILE:HG12	2.06	0.56
1:A:1030:ILE:O	1:A:1030:ILE:HG13	2.00	0.56
1:A:42:GLY:HA2	1:A:828:LEU:HD21	1.88	0.56
1:A:1065:GLU:H	1:A:1065:GLU:CD	2.14	0.55
1:A:954:GLU:O	1:A:996:ASN:HB2	2.06	0.55
1:A:127:TRP:O	1:A:131:LEU:HD13	2.05	0.55
1:A:891:ARG:HH11	1:A:891:ARG:HB3	1.71	0.55
1:A:92:LEU:HD21	1:A:128:SER:OG	2.06	0.54
2:B:98:G:H2'	2:B:99:C:H6	1.73	0.54
1:A:66:ARG:HG3	1:A:69:ARG:HH21	1.73	0.54
1:A:88:ARG:C	1:A:90:GLY:H	2.15	0.54
1:A:630:ARG:O	1:A:634:GLU:HG3	2.08	0.54
1:A:670:THR:HG22	1:A:670:THR:O	2.08	0.54
1:A:109:THR:O	1:A:113:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:U:H2'	2:B:40:C:C6	2.43	0.54
1:A:540:TYR:O	1:A:542:PRO:HD3	2.08	0.54
1:A:202:THR:HG22	1:A:203:PHE:H	1.73	0.54
1:A:750:MET:O	1:A:750:MET:HG3	2.08	0.54
1:A:781:GLN:N	1:A:781:GLN:OE1	2.41	0.54
1:A:91:VAL:HG12	1:A:92:LEU:HD23	1.90	0.53
1:A:878:ARG:HB2	1:A:885:TYR:CD1	2.42	0.53
2:B:60:A:H2'	2:B:61:C:C6	2.43	0.53
1:A:734:THR:O	1:A:738:GLN:HG3	2.09	0.53
1:A:786:ARG:HD2	1:A:810:LEU:HD11	1.89	0.53
1:A:159:LEU:HD23	1:A:159:LEU:C	2.33	0.53
1:A:994:SER:O	1:A:994:SER:OG	2.25	0.53
1:A:822:HIS:N	1:A:822:HIS:CD2	2.75	0.53
1:A:88:ARG:NH1	2:B:82:U:OP1	2.37	0.53
1:A:566:CYS:HB2	1:A:607:LEU:HG	1.91	0.53
1:A:1006:LEU:HD12	1:A:1018:GLY:O	2.09	0.53
2:B:98:G:H2'	2:B:99:C:C6	2.44	0.53
1:A:114:ARG:O	1:A:118:LEU:HD11	2.09	0.52
1:A:115:ALA:O	1:A:118:LEU:CD1	2.57	0.52
1:A:66:ARG:NH2	2:B:18:A:H5'	2.25	0.52
1:A:979:VAL:HG22	1:A:988:TRP:CH2	2.44	0.52
1:A:694:ARG:HG3	1:A:694:ARG:HH11	1.73	0.52
1:A:723:HIS:H	1:A:723:HIS:CD2	2.26	0.52
1:A:841:GLN:O	1:A:946:THR:HG23	2.09	0.52
1:A:157:ALA:N	3:C:16:DA:OP1	2.37	0.52
1:A:11:TYR:CE2	1:A:498:PRO:HB3	2.45	0.51
1:A:37:ARG:HH11	1:A:37:ARG:HG2	1.74	0.51
1:A:70:ARG:HA	1:A:73:ARG:HG2	1.92	0.51
1:A:209:GLN:O	1:A:213:ILE:HG13	2.11	0.51
1:A:963:PRO:HB2	1:A:965:TYR:HE2	1.75	0.51
1:A:1015:ARG:CG	1:A:1015:ARG:NH2	2.72	0.51
2:B:104:U:H2'	2:B:105:A:H8	1.76	0.51
1:A:71:LEU:HD11	2:B:22:U:H5	1.76	0.51
1:A:899:PRO:HA	1:A:902:ALA:HB3	1.93	0.51
1:A:486:LYS:HE3	2:B:125:C:OP1	2.11	0.51
1:A:537:PHE:HZ	1:A:579:ASN:ND2	2.08	0.51
1:A:891:ARG:NH1	1:A:891:ARG:HB3	2.25	0.50
1:A:1008:GLU:HB3	1:A:1061:TYR:CE2	2.44	0.50
1:A:195:GLN:HE21	1:A:921:LYS:NZ	2.09	0.50
1:A:530:ARG:HG2	1:A:530:ARG:NH2	2.27	0.50
1:A:112:GLN:HG3	1:A:182:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HH22	2:B:18:A:H5'	1.77	0.49
1:A:120:ARG:HH11	1:A:122:LEU:HD21	1.77	0.49
3:C:7:DC:H4'	3:C:8:DA:OP1	2.10	0.49
1:A:494:ARG:HD3	1:A:495:TYR:HE2	1.78	0.49
1:A:159:LEU:C	1:A:159:LEU:CD2	2.86	0.49
1:A:115:ALA:O	1:A:118:LEU:HD12	2.12	0.49
1:A:195:GLN:HE21	1:A:921:LYS:HZ1	1.60	0.49
1:A:637:ALA:O	1:A:641:THR:HG23	2.13	0.49
1:A:541:PHE:HB3	1:A:544:PHE:HB2	1.93	0.49
1:A:551:LYS:O	1:A:555:LYS:HG3	2.13	0.49
1:A:944:ASN:ND2	1:A:944:ASN:N	2.58	0.49
1:A:979:VAL:HG11	1:A:1028:GLY:HA2	1.95	0.48
1:A:562:GLN:OE1	1:A:605:LEU:N	2.42	0.48
2:B:90:A:H2'	2:B:91:A:H8	1.79	0.48
1:A:102:LEU:HD21	2:B:62:A:H5'	1.94	0.48
1:A:1069:GLU:OE2	1:A:1071:ARG:NH2	2.32	0.48
1:A:998:LYS:HA	1:A:998:LYS:HD3	1.65	0.48
1:A:978:ALA:HB2	1:A:991:ILE:HD11	1.95	0.48
1:A:1015:ARG:NH2	1:A:1015:ARG:HG2	2.28	0.48
2:B:79:A:H2'	2:B:80:G:H8	1.79	0.48
1:A:597:ASP:HB3	1:A:602:ASN:ND2	2.29	0.47
1:A:55:GLY:HA3	1:A:513:PHE:CD2	2.49	0.47
1:A:88:ARG:C	1:A:90:GLY:N	2.72	0.47
1:A:165:ASN:ND2	1:A:200:SER:O	2.32	0.47
1:A:218:LYS:HD2	1:A:218:LYS:HA	1.61	0.47
1:A:463:TYR:CZ	1:A:493:ARG:HG2	2.49	0.47
1:A:910:TYR:CE1	1:A:916:ARG:HB3	2.50	0.47
1:A:390:LYS:HE3	3:C:19:DT:H5''	1.96	0.47
1:A:1034:ILE:HG12	1:A:1045:GLY:O	2.15	0.47
2:B:39:U:H2'	2:B:40:C:H6	1.78	0.47
1:A:85:LEU:HD21	1:A:234:GLY:HA3	1.97	0.47
1:A:120:ARG:NH1	1:A:122:LEU:HD21	2.30	0.47
1:A:596:TRP:CD1	1:A:663:LYS:HD2	2.50	0.46
1:A:847:VAL:O	2:B:26:U:O2'	2.31	0.46
1:A:964:ILE:O	1:A:964:ILE:HG22	2.16	0.46
1:A:112:GLN:CD	1:A:112:GLN:H	2.24	0.46
1:A:885:TYR:HD2	1:A:885:TYR:O	1.98	0.46
1:A:70:ARG:NH2	2:B:19:C:OP1	2.40	0.46
1:A:216:PHE:CE2	1:A:232:LYS:HB2	2.51	0.46
1:A:537:PHE:HD1	1:A:548:PRO:HG3	1.81	0.46
1:A:698:SER:HB2	1:A:730:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:LEU:HA	1:A:828:LEU:HD23	1.54	0.46
1:A:12:ILE:HG12	1:A:500:ARG:HB2	1.98	0.46
1:A:73:ARG:NH1	2:B:87:C:C5	2.84	0.46
1:A:694:ARG:HG3	1:A:694:ARG:NH1	2.29	0.46
1:A:537:PHE:HZ	1:A:579:ASN:HD21	1.63	0.45
1:A:49:ALA:HB2	1:A:479:ARG:HD2	1.98	0.45
1:A:199:TYR:OH	3:C:14:DA:N3	2.36	0.45
1:A:999:PHE:CE1	1:A:1059:GLN:HA	2.50	0.45
1:A:133:HIS:CD2	2:B:60:A:H5''	2.52	0.45
1:A:869:LEU:O	1:A:873:GLU:HG2	2.17	0.45
1:A:1008:GLU:OE2	1:A:1015:ARG:NE	2.49	0.45
1:A:745:VAL:O	1:A:749:GLU:HG3	2.17	0.45
1:A:537:PHE:CZ	1:A:579:ASN:ND2	2.85	0.45
1:A:967:TRP:O	1:A:971:LYS:HG3	2.17	0.45
1:A:73:ARG:NH1	2:B:87:C:H5	2.13	0.45
1:A:88:ARG:O	1:A:90:GLY:N	2.50	0.45
1:A:1027:THR:HG22	1:A:1027:THR:O	2.16	0.45
1:A:1051:GLY:N	3:C:5:DA:OP2	2.50	0.44
1:A:558:LEU:HD12	1:A:586:ILE:HG22	1.99	0.44
1:A:772:PHE:HA	1:A:773:PRO:HD3	1.83	0.44
1:A:658:ASP:O	1:A:662:PHE:HB2	2.18	0.44
1:A:852:ARG:NH2	1:A:926:GLU:OE1	2.50	0.44
1:A:932:GLY:HA3	1:A:941:ILE:HG12	1.98	0.44
1:A:547:GLU:HG3	1:A:548:PRO:CD	2.47	0.44
1:A:92:LEU:HD12	1:A:103:ILE:HG12	1.99	0.44
1:A:97:PHE:CE2	1:A:103:ILE:HG13	2.53	0.44
1:A:586:ILE:HG21	1:A:586:ILE:HD13	1.69	0.44
1:A:120:ARG:HB2	1:A:120:ARG:NH2	2.33	0.44
1:A:547:GLU:HG3	1:A:548:PRO:HD2	2.00	0.44
1:A:559:TYR:C	1:A:559:TYR:CD2	2.95	0.44
1:A:864:LEU:HA	1:A:867:LEU:HD22	1.99	0.44
1:A:874:LYS:HB3	1:A:874:LYS:HE3	1.81	0.44
1:A:949:ARG:NH1	1:A:951:ASP:OD1	2.51	0.44
1:A:158:LEU:HD11	1:A:202:THR:HG21	1.99	0.44
1:A:737:MET:HE3	1:A:740:LYS:HD2	2.00	0.44
1:A:841:GLN:O	1:A:946:THR:CG2	2.65	0.44
1:A:114:ARG:HG2	1:A:130:VAL:CG2	2.48	0.44
1:A:494:ARG:HB3	1:A:495:TYR:CD2	2.51	0.44
1:A:506:ALA:O	1:A:671:ARG:NH2	2.51	0.44
1:A:592:PHE:HD2	1:A:745:VAL:HG11	1.83	0.44
1:A:1006:LEU:HD22	1:A:1063:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LYS:HB2	1:A:536:LYS:HE2	1.67	0.43
1:A:656:LYS:HB3	1:A:656:LYS:HE2	1.51	0.43
1:A:103:ILE:HD12	1:A:103:ILE:H	1.83	0.43
1:A:114:ARG:CG	1:A:130:VAL:HG23	2.48	0.43
1:A:118:LEU:HG	1:A:215:LEU:CD2	2.48	0.43
1:A:191:HIS:CD2	1:A:195:GLN:NE2	2.87	0.43
1:A:24:TRP:CD1	1:A:487:VAL:HG11	2.53	0.43
2:B:20:U:H5''	2:B:20:U:H6	1.83	0.43
2:B:105:A:H2'	2:B:106:A:H8	1.83	0.43
1:A:113:LEU:O	1:A:117:ALA:N	2.50	0.43
1:A:922:ALA:N	2:B:57:G:OP1	2.51	0.43
1:A:1021:ALA:HB2	1:A:1033:ARG:HG3	2.00	0.43
1:A:114:ARG:HG2	1:A:130:VAL:HG23	2.00	0.43
1:A:508:GLU:H	1:A:508:GLU:HG2	1.65	0.43
1:A:585:GLU:OE1	1:A:611:ASN:ND2	2.52	0.43
1:A:849:SER:HB2	2:B:28:G:OP1	2.19	0.43
1:A:541:PHE:HZ	1:A:578:LEU:HB3	1.82	0.43
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.86	0.42
1:A:944:ASN:ND2	4:D:4:DT:OP1	2.52	0.42
2:B:118:U:C2	2:B:119:A:C8	3.07	0.42
3:C:1:DT:H3'	3:C:2:DA:C8	2.53	0.42
1:A:847:VAL:O	2:B:27:U:H5'	2.18	0.42
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.96	0.42
1:A:103:ILE:HB	1:A:106:LEU:HD11	2.00	0.42
1:A:216:PHE:CD2	1:A:232:LYS:HB2	2.55	0.42
2:B:95:U:H2'	2:B:96:C:H6	1.84	0.42
2:B:128:C:H2'	2:B:129:G:H8	1.84	0.42
1:A:141:LEU:HG	1:A:142:SER:H	1.84	0.42
1:A:110:PRO:CG	2:B:60:A:H4'	2.49	0.42
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.87	0.42
1:A:130:VAL:HG13	1:A:131:LEU:CD1	2.49	0.42
1:A:138:ARG:HB2	1:A:239:LEU:HD12	2.02	0.42
1:A:662:PHE:HD1	1:A:666:ASN:HD21	1.66	0.42
1:A:499:ALA:HA	1:A:688:THR:HG23	2.00	0.42
1:A:1027:THR:O	1:A:1027:THR:CG2	2.67	0.42
1:A:50:GLU:OE2	1:A:516:ARG:NH2	2.53	0.41
1:A:176:THR:HG22	1:A:179:GLU:HB3	2.02	0.41
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.86	0.41
1:A:838:MET:HE2	1:A:838:MET:HB3	1.99	0.41
1:A:188:GLU:OE1	1:A:188:GLU:HA	2.20	0.41
1:A:537:PHE:CD1	1:A:548:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:ARG:O	1:A:749:GLU:HB2	2.20	0.41
1:A:15:LEU:HD23	1:A:24:TRP:HB3	2.03	0.41
1:A:931:THR:OG1	1:A:1025:ARG:NH1	2.54	0.41
1:A:669:ASP:OD2	1:A:671:ARG:HG3	2.20	0.41
1:A:97:PHE:N	1:A:97:PHE:CD2	2.88	0.41
1:A:519:ILE:O	1:A:519:ILE:HG22	2.19	0.41
1:A:668:ASN:OD1	1:A:696:PHE:HE1	2.03	0.41
1:A:20:ALA:HA	1:A:46:PHE:CE2	2.56	0.41
1:A:42:GLY:HA2	1:A:828:LEU:CD2	2.50	0.41
1:A:141:LEU:HD13	1:A:205:ARG:HD2	2.02	0.41
2:B:115:C:H2'	2:B:116:U:C6	2.55	0.41
1:A:138:ARG:HD2	1:A:205:ARG:NH1	2.36	0.41
1:A:219:GLN:CB	1:A:227:VAL:HG21	2.51	0.41
1:A:712:LEU:HD12	1:A:729:VAL:CG2	2.51	0.41
1:A:882:PRO:O	1:A:886:GLU:HG2	2.21	0.41
1:A:936:ARG:O	1:A:939:ASN:HB2	2.21	0.41
2:B:97:U:H2'	2:B:98:G:H8	1.86	0.41
1:A:936:ARG:HD3	1:A:936:ARG:HA	1.80	0.41
2:B:51:A:H2'	2:B:52:C:C6	2.56	0.41
1:A:70:ARG:NH1	2:B:20:U:P	2.95	0.40
1:A:191:HIS:O	1:A:191:HIS:ND1	2.55	0.40
1:A:752:ALA:HA	1:A:756:LYS:HE3	2.03	0.40
2:B:108:G:H8	2:B:108:G:OP2	2.04	0.40
1:A:11:TYR:CZ	1:A:498:PRO:HB3	2.57	0.40
1:A:999:PHE:HE1	1:A:1059:GLN:HA	1.85	0.40
1:A:1008:GLU:HB2	1:A:1017:PHE:CE1	2.54	0.40
1:A:131:LEU:HG	1:A:235:ILE:HD13	2.02	0.40
1:A:502:HIS:HD2	1:A:696:PHE:HB3	1.87	0.40
1:A:663:LYS:HG2	1:A:667:LEU:HD11	2.04	0.40
1:A:836:ARG:HB3	1:A:1002:HIS:CG	2.57	0.40
2:B:79:A:H2'	2:B:80:G:C8	2.55	0.40
1:A:992:ASP:HB2	1:A:993:ASP:H	1.60	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	945/1083 (87%)	864 (91%)	78 (8%)	3 (0%)	36 65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	A	897	ASP
1	A	772	PHE

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	753/932 (81%)	734 (98%)	19 (2%)	42 64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	120	ARG
1	A	158	LEU
1	A	159	LEU
1	A	182	LEU
1	A	183	ASN
1	A	269	LYS
1	A	347	LEU
1	A	586	ILE
1	A	587	ASP
1	A	753	PHE
1	A	756	LYS
1	A	772	PHE
1	A	822	HIS

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Mol	Chain	Res	Type
1	A	944	ASN
1	A	946	THR
1	A	964	ILE
1	A	1015	ARG
1	A	1025	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	183	ASN
1	A	195	GLN
1	A	242	GLN
1	A	270	ASN
1	A	379	GLN
1	A	561	GLN
1	A	704	ASN
1	A	722	HIS
1	A	822	HIS
1	A	866	GLN
1	A	944	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	109/135 (80%)	31 (28%)	1 (0%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	U
2	B	24	C
2	B	36	C
2	B	37	U
2	B	42	C
2	B	43	G
2	B	45	A
2	B	47	G
2	B	48	A
2	B	49	G

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Mol	Chain	Res	Type
2	B	50	A
2	B	53	C
2	B	65	A
2	B	69	C
2	B	71	G
2	B	76	A
2	B	77	A
2	B	78	A
2	B	84	U
2	B	85	G
2	B	89	C
2	B	95	U
2	B	103	U
2	B	104	U
2	B	108	G
2	B	118	U
2	B	119	A
2	B	120	A
2	B	128	C
2	B	132	U
2	B	133	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	41	U

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](#)

There are no ligands in this entry.

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 ⓘ

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	963/1083 (88%)	0.98	150 (15%) 5 4	12, 36, 71, 110	117 (12%)
2	B	111/135 (82%)	0.77	8 (7%) 21 15	13, 49, 138, 158	0
3	C	19/19 (100%)	0.38	0 100 100	15, 36, 47, 50	0
4	D	11/11 (100%)	0.32	0 100 100	14, 22, 61, 69	0
All	All	1104/1248 (88%)	0.94	158 (14%) 6 5	12, 37, 74, 158	117 (10%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ALA	8.6
1	A	293	SER	8.1
1	A	292	GLY	7.8
1	A	344	ALA	7.7
1	A	389	PHE	6.6
1	A	291	GLN	6.4
1	A	387	SER	6.2
1	A	378	LEU	6.0
1	A	398	ARG	6.0
1	A	288	ILE	5.8
1	A	382	ILE	5.7
1	A	403	ILE	5.6
1	A	320	ALA	5.6
1	A	309	PRO	5.6
1	A	383	GLY	5.5
1	A	395	ILE	5.4
1	A	358	ARG	5.4
1	A	353	TYR	5.1
1	A	289	LEU	5.1
1	A	394	ASP	5.0
1	A	391	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	310	TYR	5.0
1	A	900	ALA	4.8
1	A	305	LEU	4.8
2	B	133	A	4.8
1	A	352	ALA	4.7
1	A	347	LEU	4.7
1	A	317	TYR	4.7
1	A	918	GLN	4.6
1	A	417	PHE	4.6
1	A	355	ALA	4.6
1	A	324	LEU	4.6
1	A	415	ILE	4.5
1	A	388	LEU	4.5
1	A	370	SER	4.5
1	A	379	GLN	4.5
1	A	294	GLU	4.5
1	A	280	LEU	4.5
1	A	311	ARG	4.5
1	A	386	PHE	4.4
1	A	420	PHE	4.4
1	A	318	ALA	4.4
1	A	380	ASP	4.4
1	A	376	PRO	4.3
1	A	316	THR	4.3
1	A	319	GLN	4.2
1	A	323	LEU	4.2
1	A	390	LYS	4.2
1	A	272	TYR	4.1
1	A	314	LYS	4.1
1	A	273	THR	4.1
1	A	270	ASN	4.1
1	A	286	LEU	4.1
1	A	287	ARG	4.0
1	A	271	THR	4.0
1	A	312	LYS	4.0
1	A	282	LYS	3.9
2	B	132	U	3.9
1	A	298	THR	3.9
1	A	1054	THR	3.9
1	A	306	MET	3.9
1	A	301	GLU	3.8
1	A	377	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	423	ILE	3.8
1	A	346	THR	3.8
1	A	393	GLU	3.7
1	A	354	HIS	3.7
1	A	422	GLN	3.6
1	A	357	SER	3.6
1	A	266	LYS	3.6
1	A	351	LYS	3.6
1	A	396	THR	3.6
1	A	276	ARG	3.5
1	A	295	ARG	3.5
1	A	418	ASP	3.5
1	A	265	PRO	3.5
1	A	402	ARG	3.5
1	A	884	LEU	3.4
1	A	321	ARG	3.4
1	A	375	SER	3.4
1	A	392	ASP	3.4
1	A	348	MET	3.4
1	A	116	ALA	3.3
1	A	419	LYS	3.3
2	B	117	U	3.3
1	A	281	THR	3.3
1	A	716	ARG	3.3
1	A	296	PRO	3.3
1	A	300	THR	3.3
1	A	279	TRP	3.2
1	A	303	ALA	3.2
1	A	1059	GLN	3.2
1	A	416	SER	3.2
1	A	277	PHE	3.1
1	A	371	PRO	3.1
1	A	278	ILE	3.1
1	A	350	MET	3.1
1	A	372	LEU	3.1
1	A	119	ASP	3.1
1	A	397	GLY	3.0
1	A	297	LEU	3.0
1	A	290	GLU	3.0
1	A	283	LEU	3.0
1	A	838	MET	3.0
1	A	274	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	384	THR	3.0
1	A	717	ALA	2.9
1	A	984	ASP	2.9
2	B	115	C	2.8
1	A	117	ALA	2.8
1	A	356	ILE	2.8
2	B	108	G	2.8
1	A	345	SER	2.7
1	A	401	ASP	2.7
1	A	421	VAL	2.7
1	A	1073	CYS	2.7
1	A	757	THR	2.7
1	A	159	LEU	2.7
1	A	285	ASN	2.7
1	A	381	GLU	2.6
1	A	268	ALA	2.6
2	B	118	U	2.6
1	A	304	THR	2.6
1	A	302	ARG	2.6
1	A	600	PHE	2.6
1	A	400	LYS	2.5
1	A	1010	ILE	2.5
1	A	1062	GLN	2.5
1	A	593	SER	2.4
1	A	322	LYS	2.4
1	A	163	ALA	2.4
1	A	202	THR	2.4
1	A	299	ASP	2.4
1	A	275	GLU	2.4
1	A	484	ALA	2.3
1	A	870	LYS	2.3
2	B	47	G	2.3
1	A	399	LEU	2.3
1	A	349	GLU	2.3
1	A	912	LYS	2.3
1	A	773	PRO	2.3
1	A	137	HIS	2.3
1	A	915	ASN	2.2
1	A	142	SER	2.2
1	A	374	LEU	2.2
1	A	215	LEU	2.2
1	A	166	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1052	VAL	2.2
1	A	181	ALA	2.2
1	A	911	ASP	2.2
1	A	873	GLU	2.1
1	A	676	PHE	2.1
1	A	269	LYS	2.1
1	A	833	ALA	2.1
2	B	79	A	2.0
1	A	197	SER	2.0
1	A	960	TYR	2.0
1	A	956	GLY	2.0

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.