



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:05 PM UTC

PDB ID : 6JDQ / pdb_00006jdq
Title : Crystal structure of Nme1Cas9 in complex with sgRNA
Authors : Sun, W.; Yang, J.; Cheng, Z.; Liu, C.; Wang, K.; Huang, X.; Wang, Y.
Deposited on : 2019-02-02
Resolution : 2.95 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

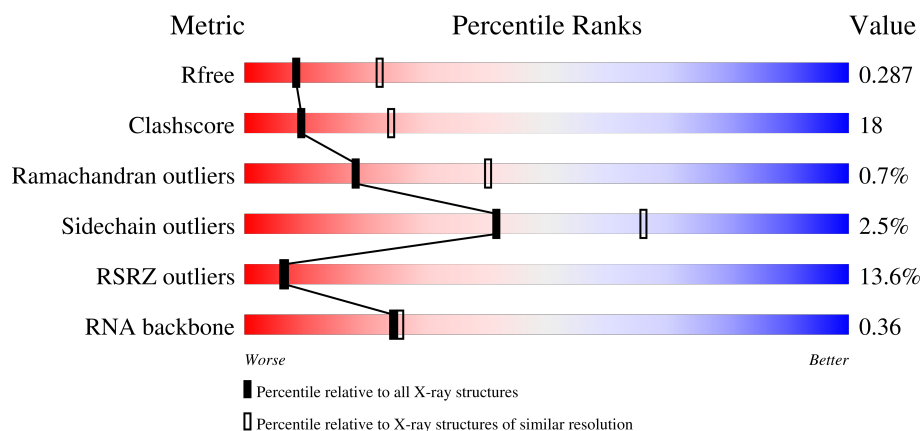
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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	1092	12% 65% 28% 5% ..
2	B	135	19% 21% 45% 16% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10857 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	1069	Total	C	N	O	S	0	3	0
			8365	5292	1514	1535	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1083	SER	-	expression tag	UNP C9X1G5
A	1084	GLU	-	expression tag	UNP C9X1G5
A	1085	HIS	-	expression tag	UNP C9X1G5
A	1086	HIS	-	expression tag	UNP C9X1G5
A	1087	HIS	-	expression tag	UNP C9X1G5
A	1088	HIS	-	expression tag	UNP C9X1G5
A	1089	HIS	-	expression tag	UNP C9X1G5
A	1090	HIS	-	expression tag	UNP C9X1G5
A	1091	HIS	-	expression tag	UNP C9X1G5
A	1092	HIS	-	expression tag	UNP C9X1G5

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	P	0	0	0
			2473	1107	426	823	117			

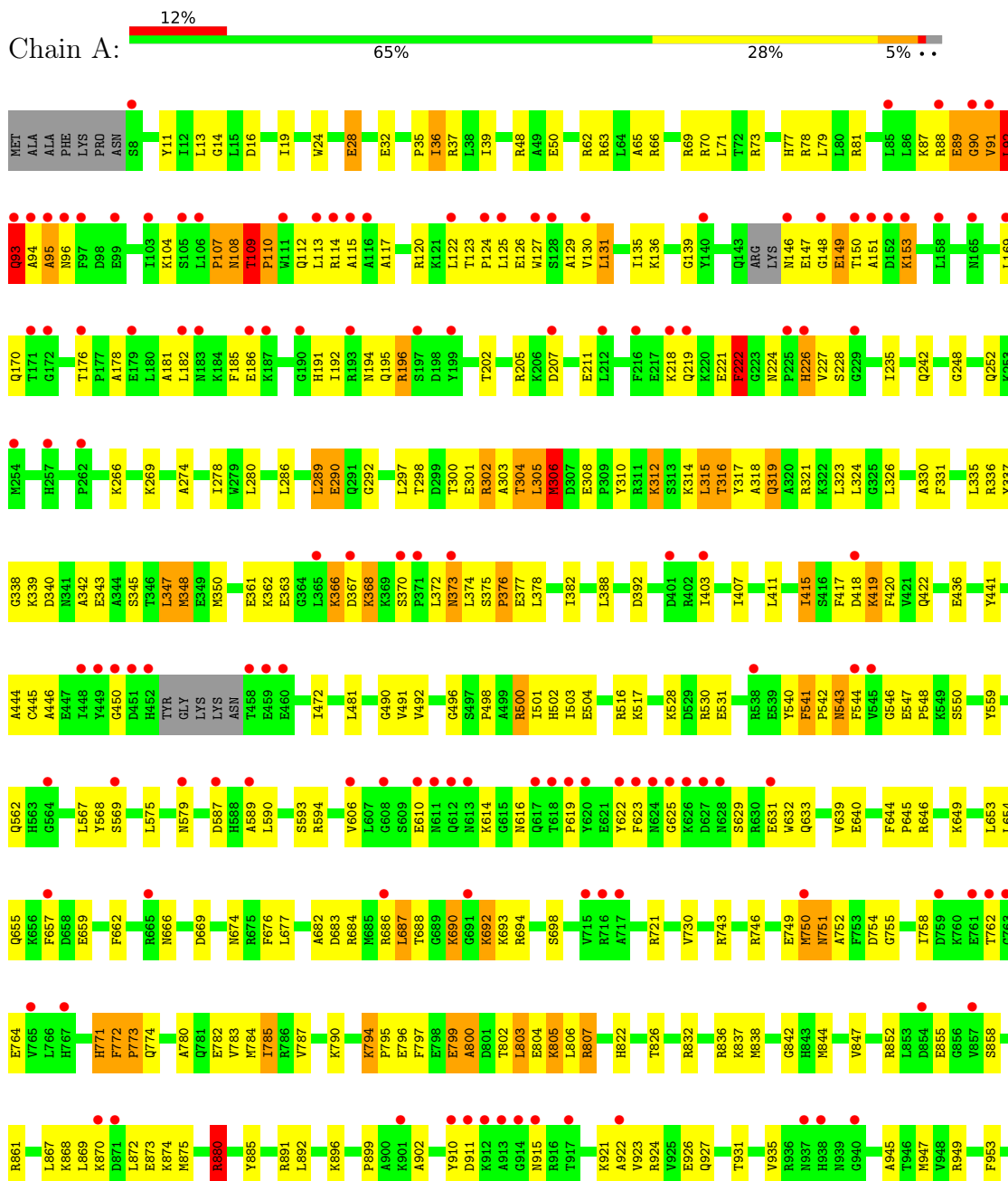
- Molecule 3 is water.

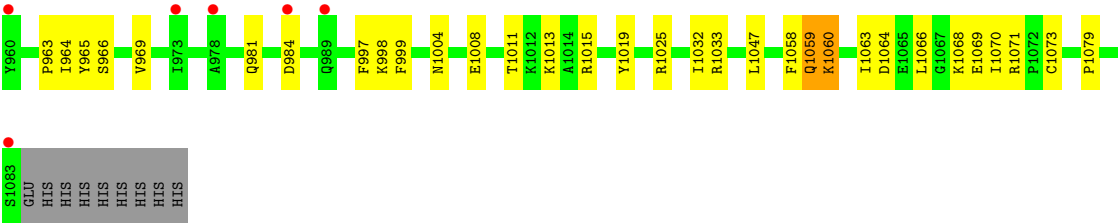
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	3	Total	O	0	0
			3	3		

3 Residue-property plots

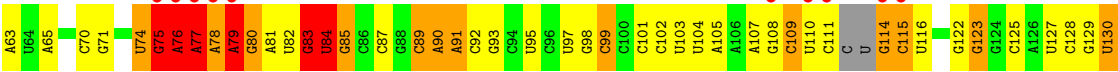
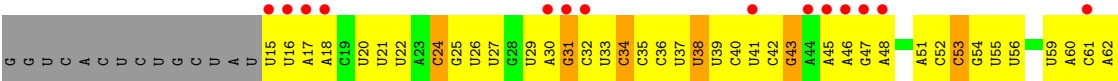
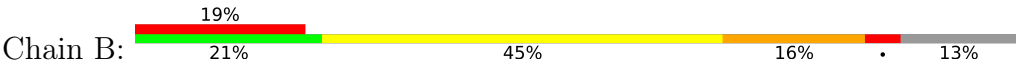
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.08Å 122.45Å 238.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.95 48.91 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.91-2.95) 98.6 (48.91-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.255 , 0.290 0.256 , 0.287	Depositor DCC
R_{free} test set	2258 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10857	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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	1.07	74/8529 (0.9%)	0.96	65/11518 (0.6%)
2	B	0.98	28/2759 (1.0%)	1.00	21/4290 (0.5%)
All	All	1.05	102/11288 (0.9%)	0.97	86/15808 (0.5%)

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
2	B	0	1

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	984	ASP	C-N	17.59	1.57	1.34
2	B	91	A	O3'-P	-10.63	1.45	1.61
2	B	130	U	O3'-P	-10.13	1.46	1.61
2	B	85	G	O3'-P	-9.51	1.46	1.61
1	A	348	MET	C-O	-8.88	1.13	1.23
2	B	92	C	O3'-P	-8.20	1.48	1.61
1	A	92	LEU	CA-C	-8.18	1.48	1.52
1	A	415	ILE	C-O	-7.81	1.15	1.24
1	A	39	ILE	C-O	-7.72	1.15	1.24
2	B	36	C	O3'-P	-7.52	1.49	1.61
1	A	543	ASN	CA-C	-7.51	1.44	1.53
2	B	122	G	O3'-P	-7.41	1.50	1.61
2	B	81	A	O3'-P	-7.40	1.50	1.61
1	A	500	ARG	C-O	-7.28	1.14	1.23
1	A	63	ARG	C-O	-7.22	1.15	1.24
2	B	89	C	O3'-P	-7.17	1.50	1.61
1	A	787	VAL	C-O	-7.15	1.15	1.24
1	A	803	LEU	CA-C	-7.14	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123	G	O3'-P	-7.06	1.50	1.61
2	B	35	C	O3'-P	-7.00	1.50	1.61
2	B	90	A	O3'-P	-6.98	1.50	1.61
1	A	782	GLU	C-O	-6.92	1.16	1.24
1	A	108	ASN	CA-C	-6.90	1.45	1.53
1	A	686	ARG	CA-C	-6.80	1.44	1.52
1	A	347	LEU	C-O	-6.76	1.14	1.23
1	A	645	PRO	C-O	-6.66	1.16	1.23
1	A	35	PRO	C-O	-6.64	1.16	1.23
1	A	417	PHE	C-O	-6.62	1.16	1.23
2	B	92	C	P-OP1	-6.58	1.35	1.49
1	A	784	MET	C-O	-6.44	1.16	1.24
1	A	335	LEU	C-O	-6.41	1.15	1.23
2	B	90	A	P-OP2	-6.40	1.36	1.49
2	B	53	C	O3'-P	-6.36	1.51	1.61
1	A	315	LEU	C-O	-6.33	1.16	1.24
1	A	419	LYS	C-O	-6.27	1.16	1.23
1	A	783	VAL	C-O	-6.24	1.16	1.24
2	B	91	A	P-OP1	-6.22	1.36	1.49
1	A	316	THR	C-O	-6.21	1.16	1.23
1	A	445	CYS	C-O	-6.19	1.16	1.24
1	A	89	GLU	CA-C	-6.19	1.47	1.53
1	A	780	ALA	C-O	-6.16	1.17	1.24
1	A	302	ARG	C-O	-6.16	1.17	1.24
1	A	372	LEU	CA-C	-6.14	1.45	1.52
2	B	93	G	O3'-P	-6.12	1.51	1.61
1	A	345	SER	C-O	-6.11	1.15	1.23
2	B	92	C	P-OP2	-6.10	1.36	1.49
1	A	807	ARG	C-O	-6.09	1.16	1.24
1	A	289	LEU	C-O	-6.08	1.17	1.24
1	A	799	GLU	C-O	-6.05	1.16	1.23
1	A	750	MET	C-O	-6.02	1.16	1.24
2	B	37	U	O3'-P	-6.00	1.52	1.61
2	B	84	U	O3'-P	-5.99	1.52	1.61
1	A	441	TYR	C-O	-5.98	1.17	1.24
1	A	785	ILE	C-O	-5.96	1.17	1.24
1	A	91	VAL	CA-C	-5.92	1.45	1.52
2	B	91	A	P-OP2	-5.92	1.37	1.49
1	A	444	ALA	C-O	-5.90	1.17	1.24
1	A	362	LYS	CA-C	-5.89	1.45	1.52
1	A	1060	LYS	C-O	-5.81	1.16	1.23
2	B	90	A	P-OP1	-5.80	1.37	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	LYS	C-O	-5.80	1.17	1.23
1	A	28	GLU	CA-C	-5.78	1.45	1.52
1	A	750	MET	CA-C	-5.77	1.45	1.52
1	A	342	ALA	C-O	-5.76	1.16	1.23
1	A	806	LEU	C-O	-5.76	1.17	1.24
2	B	83	G	O3'-P	-5.75	1.52	1.61
1	A	1058	PHE	C-O	-5.71	1.17	1.23
1	A	303	ALA	C-O	-5.71	1.17	1.24
1	A	774	GLN	C-O	-5.69	1.18	1.24
1	A	420	PHE	C-O	-5.68	1.16	1.23
1	A	319	GLN	C-O	-5.66	1.17	1.24
1	A	800	ALA	N-CA	-5.64	1.39	1.46
2	B	80	G	O3'-P	-5.60	1.52	1.61
1	A	90	GLY	CA-C	-5.46	1.44	1.51
1	A	686	ARG	C-O	-5.44	1.17	1.24
1	A	693	LYS	CA-C	-5.44	1.46	1.53
2	B	99	C	O3'-P	-5.42	1.53	1.61
1	A	224	ASN	CA-C	-5.42	1.46	1.52
2	B	89	C	P-OP1	-5.41	1.38	1.49
1	A	794	LYS	N-CA	-5.39	1.41	1.46
1	A	336	ARG	CA-C	-5.35	1.46	1.52
1	A	805	LYS	C-O	-5.33	1.17	1.24
2	B	89	C	P-OP2	-5.33	1.38	1.49
1	A	803	LEU	C-O	-5.32	1.17	1.24
2	B	131	U	O3'-P	-5.30	1.53	1.61
1	A	304	THR	C-O	-5.28	1.18	1.24
1	A	376	PRO	C-O	-5.26	1.17	1.24
1	A	880	ARG	C-O	-5.26	1.17	1.24
1	A	305	LEU	C-O	-5.25	1.17	1.24
1	A	339	LYS	C-O	-5.25	1.17	1.24
1	A	35	PRO	CA-C	-5.24	1.45	1.52
1	A	95	ALA	N-CA	-5.22	1.39	1.46
1	A	687	LEU	N-CA	-5.22	1.39	1.46
1	A	36	ILE	C-O	-5.21	1.17	1.24
1	A	547	GLU	CA-C	5.19	1.59	1.52
1	A	773	PRO	C-O	-5.17	1.16	1.23
1	A	90	GLY	C-O	-5.12	1.17	1.23
2	B	34	C	O3'-P	-5.09	1.53	1.61
1	A	93	GLN	CA-C	-5.08	1.46	1.52
1	A	800	ALA	CA-CB	-5.07	1.46	1.52
1	A	804	GLU	N-CA	-5.03	1.40	1.46
1	A	981	GLN	C-O	-5.03	1.18	1.23

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	984	ASP	O-C-N	-19.75	98.56	122.65
1	A	794	LYS	CA-C-N	17.02	138.01	119.28
1	A	794	LYS	C-N-CA	17.02	138.01	119.28
2	B	78	A	C4'-C3'-O3'	13.73	133.59	113.00
1	A	984	ASP	CA-C-N	13.72	140.03	120.28
1	A	984	ASP	C-N-CA	13.72	140.03	120.28
1	A	541	PHE	CA-C-N	12.84	132.84	118.85
1	A	541	PHE	C-N-CA	12.84	132.84	118.85
1	A	39	ILE	N-CA-C	12.35	122.14	110.53
1	A	149	GLU	N-CA-C	12.19	123.81	108.45
2	B	77	A	N9-C1'-C2'	12.08	132.12	114.00
1	A	92	LEU	N-CA-C	-11.71	90.03	108.30
2	B	78	A	C2'-C3'-O3'	-10.90	97.35	113.70
2	B	77	A	C4'-C3'-O3'	10.87	125.70	109.40
1	A	338	GLY	N-CA-C	10.77	125.66	112.73
1	A	306	MET	N-CA-C	10.68	122.92	111.28
1	A	546	GLY	O-C-N	10.21	135.98	122.70
1	A	543	ASN	N-CA-C	-10.09	96.66	110.68
1	A	339	LYS	N-CA-C	9.90	124.93	107.80
2	B	75	G	C2'-C3'-O3'	9.55	128.03	113.70
1	A	415	ILE	N-CA-C	9.52	121.20	109.30
2	B	101	C	C1'-C2'-O2'	-9.32	94.42	108.40
1	A	543	ASN	CA-C-N	-8.95	110.64	123.00
1	A	543	ASN	C-N-CA	-8.95	110.64	123.00
1	A	787	VAL	N-CA-C	8.94	119.75	110.72
1	A	546	GLY	CA-C-N	8.78	143.22	121.80
1	A	546	GLY	C-N-CA	8.78	143.22	121.80
1	A	109	THR	CA-C-N	8.55	130.53	119.84
1	A	109	THR	C-N-CA	8.55	130.53	119.84
1	A	108	ASN	N-CA-C	8.38	121.21	110.65
2	B	37	U	C4'-C3'-O3'	-8.32	100.52	113.00
1	A	92	LEU	O-C-N	8.03	126.77	120.83
2	B	93	G	C1'-C2'-O2'	-7.96	96.47	108.40
2	B	91	A	C1'-C2'-O2'	-7.89	96.57	108.40
2	B	90	A	N9-C1'-C2'	7.51	123.26	112.00
1	A	750	MET	N-CA-C	-7.29	96.64	108.52
1	A	93	GLN	N-CA-C	-7.21	95.44	110.80
2	B	79	A	C2'-C3'-O3'	-7.13	103.01	113.70
1	A	363	GLU	N-CA-C	7.10	122.04	112.88
1	A	772	PHE	CA-C-N	7.04	127.46	119.93
1	A	772	PHE	C-N-CA	7.04	127.46	119.93
1	A	107	PRO	N-CA-C	7.04	126.97	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	LEU	N-CA-C	-6.96	104.42	113.12
2	B	76	A	N9-C1'-C2'	6.95	122.43	112.00
2	B	80	G	C4'-C3'-O3'	-6.94	102.59	113.00
1	A	228	SER	N-CA-C	6.65	118.90	110.33
1	A	690	LYS	N-CA-C	6.49	118.89	111.11
1	A	644	PHE	CA-C-N	6.48	126.39	119.85
1	A	644	PHE	C-N-CA	6.48	126.39	119.85
1	A	1059	GLN	N-CA-C	6.39	118.66	109.14
1	A	771	HIS	N-CA-C	6.37	119.02	110.35
1	A	684	ARG	N-CA-C	6.19	120.97	113.17
1	A	153	LYS	N-CA-C	6.13	123.86	110.80
1	A	340	ASP	N-CA-C	6.10	123.79	110.80
1	A	150	THR	N-CA-C	6.08	118.65	109.23
2	B	77	A	O4'-C4'-C3'	-5.97	100.13	106.10
1	A	89	GLU	N-CA-C	5.88	117.20	107.20
1	A	683	ASP	N-CA-C	5.86	117.75	111.36
1	A	368	LYS	N-CA-CB	5.86	120.40	110.49
1	A	418	ASP	N-CA-C	5.83	123.22	110.80
2	B	93	G	N9-C1'-C2'	5.82	120.73	112.00
2	B	74	U	C1'-C2'-O2'	5.82	117.13	108.40
1	A	367	ASP	CA-C-N	5.77	132.56	121.54
1	A	367	ASP	C-N-CA	5.77	132.56	121.54
1	A	342	ALA	N-CA-C	-5.75	105.03	112.68
2	B	76	A	C1'-C2'-O2'	5.75	117.02	108.40
1	A	370	SER	CA-C-N	5.73	125.68	119.78
1	A	370	SER	C-N-CA	5.73	125.68	119.78
1	A	93	GLN	CA-C-N	5.72	130.97	122.74
1	A	93	GLN	C-N-CA	5.72	130.97	122.74
1	A	367	ASP	N-CA-C	5.71	117.18	111.07
2	B	78	A	N9-C1'-C2'	-5.67	103.49	112.00
1	A	548	PRO	CA-C-O	-5.65	115.07	122.19
1	A	224	ASN	N-CA-C	-5.64	98.32	109.10
1	A	89	GLU	CB-CA-C	-5.46	104.66	111.43
2	B	36	C	C2'-C3'-O3'	-5.35	105.68	113.70
1	A	222	PHE	N-CA-C	5.29	119.70	112.88
2	B	99	C	C1'-C2'-O2'	-5.21	100.58	108.40
1	A	803	LEU	CB-CA-C	-5.18	102.19	110.79
2	B	77	A	C5'-C4'-C3'	5.15	122.92	115.20
1	A	751	ASN	N-CA-C	5.12	121.71	110.80
1	A	92	LEU	CA-C-N	5.10	131.28	121.54
1	A	92	LEU	C-N-CA	5.10	131.28	121.54
1	A	39	ILE	N-CA-CB	-5.07	104.08	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	752	ALA	N-CA-C	5.04	118.39	111.54
1	A	373	ASN	N-CA-C	5.00	119.07	112.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	77	A	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	8365	0	8161	285	1
2	B	2473	0	1256	90	0
3	A	16	0	0	2	0
3	B	3	0	0	0	0
All	All	10857	0	9417	364	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 18.

All (364) 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:109:THR:H	1:A:110:PRO:HD3	1.11	1.15
1:A:218:LYS:O	1:A:222:PHE:CE2	2.05	1.10
2:B:74:U:H5''	2:B:74:U:H6	1.14	1.07
1:A:148:GLY:O	1:A:149:GLU:HG2	1.53	1.07
1:A:218:LYS:O	1:A:222:PHE:CD2	2.13	1.01
1:A:266:LYS:NZ	1:A:422:GLN:OE1	1.94	1.00
1:A:109:THR:N	1:A:110:PRO:HD3	1.73	0.99
2:B:38:U:H5''	2:B:38:U:H6	1.27	0.95
1:A:298:THR:OG1	1:A:301:GLU:OE1	1.84	0.95
1:A:91:VAL:CG2	1:A:124:PRO:HB3	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG23	1:A:124:PRO:HB3	1.49	0.94
2:B:79:A:H8	2:B:79:A:H5''	1.31	0.93
1:A:146:ASN:N	1:A:149:GLU:OE2	2.03	0.91
1:A:593:SER:OG	1:A:749:GLU:OE1	1.89	0.90
2:B:74:U:H5''	2:B:74:U:C6	2.07	0.89
1:A:319:GLN:HE21	1:A:323:LEU:CD1	1.87	0.87
1:A:109:THR:N	1:A:110:PRO:CD	2.38	0.86
1:A:131:LEU:O	1:A:135:ILE:HD12	1.76	0.85
1:A:319:GLN:NE2	1:A:323:LEU:CD1	2.40	0.85
1:A:131:LEU:HG	1:A:235:ILE:HD13	1.59	0.84
1:A:373:ASN:O	1:A:373:ASN:ND2	2.10	0.84
1:A:880:ARG:HH11	1:A:880:ARG:HG2	1.43	0.84
1:A:205:ARG:NH1	1:A:242:GLN:OE1	2.11	0.83
2:B:38:U:H5''	2:B:38:U:C6	2.13	0.83
1:A:500:ARG:NH2	1:A:690:LYS:HB2	1.95	0.81
1:A:308:GLU:OE1	1:A:312:LYS:HD3	1.81	0.79
1:A:131:LEU:HG	1:A:235:ILE:CD1	2.13	0.79
1:A:148:GLY:O	1:A:149:GLU:CG	2.31	0.79
1:A:298:THR:CB	1:A:301:GLU:OE1	2.30	0.79
1:A:562:GLN:HE22	1:A:567:LEU:HB2	1.48	0.78
2:B:15:U:H2'	2:B:16:U:H6	1.47	0.78
1:A:298:THR:N	1:A:301:GLU:OE1	2.18	0.77
2:B:74:U:H6	2:B:74:U:C5'	1.95	0.76
2:B:79:A:H5''	2:B:79:A:C8	2.18	0.76
1:A:109:THR:H	1:A:110:PRO:CD	1.95	0.76
1:A:688:THR:HG23	1:A:688:THR:O	1.85	0.75
1:A:266:LYS:HZ3	1:A:422:GLN:CD	1.95	0.75
1:A:692:LYS:HD3	1:A:692:LYS:H	1.52	0.75
1:A:880:ARG:HH11	1:A:880:ARG:CG	2.00	0.75
1:A:803:LEU:H	1:A:803:LEU:HD12	1.52	0.74
1:A:319:GLN:HE21	1:A:323:LEU:HD13	1.52	0.74
2:B:79:A:H8	2:B:79:A:C5'	2.00	0.73
1:A:218:LYS:C	1:A:222:PHE:HE2	1.97	0.73
1:A:743:ARG:NH2	3:A:1101:HOH:O	2.19	0.73
1:A:562:GLN:NE2	1:A:567:LEU:HB2	2.03	0.72
1:A:306:MET:O	1:A:306:MET:HG3	1.88	0.72
1:A:196:ARG:O	2:B:24:C:O2'	2.08	0.72
1:A:148:GLY:C	1:A:149:GLU:CG	2.62	0.72
1:A:218:LYS:C	1:A:222:PHE:CE2	2.68	0.72
1:A:368:LYS:O	1:A:368:LYS:HG2	1.89	0.72
1:A:298:THR:HG23	1:A:301:GLU:OE1	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:TYR:OH	1:A:614:LYS:NZ	2.22	0.71
1:A:181:ALA:O	1:A:185:PHE:HB2	1.91	0.71
1:A:375:SER:OG	1:A:376:PRO:HD2	1.90	0.71
1:A:289:LEU:HD12	1:A:331:PHE:CE1	2.26	0.71
2:B:17:A:H2'	2:B:18:A:H8	1.56	0.70
2:B:60:A:H2'	2:B:61:C:C6	2.27	0.70
2:B:76:A:C2	2:B:77:A:N6	2.59	0.70
2:B:133:A:OP2	2:B:133:A:O3'	2.05	0.70
1:A:308:GLU:OE1	1:A:312:LYS:CD	2.39	0.70
1:A:298:THR:HG1	1:A:301:GLU:CD	1.98	0.70
1:A:147:GLU:CB	1:A:392:ASP:OD2	2.41	0.69
1:A:594:ARG:NH2	1:A:659:GLU:OE2	2.22	0.69
2:B:15:U:H2'	2:B:16:U:C6	2.28	0.69
1:A:91:VAL:H	1:A:226:HIS:CD2	2.10	0.69
1:A:559:TYR:CZ	1:A:575:LEU:HG	2.28	0.69
1:A:91:VAL:HG21	1:A:124:PRO:HB3	1.74	0.68
1:A:319:GLN:NE2	1:A:323:LEU:HD11	2.09	0.67
1:A:96:ASN:O	1:A:104:LYS:N	2.20	0.66
1:A:148:GLY:C	1:A:149:GLU:HG2	2.19	0.66
1:A:682:ALA:O	1:A:694:ARG:NH2	2.28	0.66
1:A:807:ARG:NH2	1:A:822:HIS:O	2.24	0.66
1:A:298:THR:CG2	1:A:301:GLU:OE1	2.43	0.66
1:A:692:LYS:HD3	1:A:692:LYS:N	2.10	0.66
1:A:266:LYS:NZ	1:A:422:GLN:CD	2.51	0.65
2:B:42:C:H2'	2:B:43:G:H5'	1.78	0.65
1:A:191:HIS:CE1	1:A:195:GLN:HG3	2.31	0.65
1:A:147:GLU:CB	1:A:392:ASP:CG	2.70	0.65
1:A:227:VAL:HG12	1:A:227:VAL:O	1.96	0.65
2:B:16:U:H3'	2:B:17:A:H8	1.63	0.64
2:B:59:U:H2'	2:B:60:A:H8	1.62	0.64
1:A:178:ALA:O	1:A:182:LEU:HD12	1.97	0.64
2:B:76:A:C2	2:B:77:A:C6	2.86	0.64
1:A:503:ILE:HD13	1:A:677:LEU:HD23	1.80	0.64
1:A:331:PHE:HB2	1:A:337:TYR:CE2	2.34	0.63
1:A:587:ASP:OD2	1:A:614:LYS:NZ	2.21	0.63
1:A:869:LEU:HD11	1:A:892:LEU:HB3	1.80	0.62
2:B:54:G:H2'	2:B:55:U:O4'	1.99	0.62
1:A:502:HIS:HB3	1:A:730:VAL:HG22	1.81	0.62
2:B:17:A:H2'	2:B:18:A:C8	2.35	0.62
1:A:361:GLU:OE2	1:A:366:LYS:NZ	2.32	0.62
1:A:375:SER:OG	1:A:377:GLU:OE1	2.17	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:A:H2'	2:B:61:C:H6	1.64	0.62
1:A:290:GLU:OE1	1:A:330:ALA:HB2	2.00	0.61
2:B:41:U:H2'	2:B:42:C:C6	2.34	0.61
2:B:132:U:H4'	2:B:133:A:O5'	2.01	0.61
1:A:867:LEU:HD21	1:A:872:LEU:HB2	1.82	0.61
2:B:76:A:H2'	2:B:77:A:C8	2.35	0.60
1:A:880:ARG:NH2	2:B:53:C:O2	2.34	0.60
1:A:762:THR:HB	1:A:764:GLU:OE1	2.02	0.60
1:A:91:VAL:N	1:A:226:HIS:CD2	2.70	0.60
1:A:861:ARG:HH21	1:A:922:ALA:HB3	1.67	0.60
1:A:66:ARG:HD2	1:A:70:ARG:HH21	1.67	0.59
1:A:324:LEU:HB2	1:A:326:LEU:HG	1.84	0.59
1:A:321:ARG:NH2	1:A:343:GLU:OE2	2.33	0.59
1:A:290:GLU:OE1	1:A:330:ALA:N	2.35	0.59
2:B:76:A:H8	2:B:76:A:P	2.26	0.59
2:B:76:A:P	2:B:76:A:C8	2.96	0.59
1:A:79:LEU:HD11	1:A:136:LYS:HG3	1.85	0.58
1:A:758:ILE:CB	1:A:762:THR:OG1	2.52	0.58
1:A:297:LEU:HD22	1:A:301:GLU:HB3	1.84	0.58
1:A:500:ARG:HH22	1:A:690:LYS:HB2	1.67	0.58
1:A:569:SER:HB3	1:A:610[A]:GLU:HG2	1.86	0.58
1:A:870:LYS:H	1:A:870:LYS:HD2	1.68	0.58
1:A:113:LEU:HD13	1:A:126:GLU:HB3	1.86	0.57
1:A:319:GLN:HE21	1:A:323:LEU:HD11	1.64	0.57
1:A:222:PHE:CD2	1:A:222:PHE:N	2.72	0.57
1:A:947:MET:HE3	1:A:963:PRO:HB3	1.86	0.57
1:A:73:ARG:NH2	2:B:87:C:OP2	2.31	0.57
1:A:899:PRO:HA	1:A:902:ALA:HB3	1.87	0.57
1:A:698:SER:HB2	1:A:730:VAL:HG23	1.85	0.56
2:B:59:U:H2'	2:B:60:A:C8	2.40	0.56
2:B:75:G:C8	2:B:75:G:H3'	2.41	0.56
1:A:794:LYS:N	1:A:795:PRO:CD	2.64	0.56
1:A:1063:ILE:HG13	1:A:1070:ILE:HG12	1.87	0.56
2:B:38:U:C6	2:B:38:U:C5'	2.87	0.56
2:B:130:U:H2'	2:B:131:U:C6	2.40	0.56
1:A:112:GLN:HG3	1:A:182:LEU:HD21	1.88	0.56
1:A:88:ARG:C	1:A:89:GLU:HG2	2.31	0.56
1:A:290:GLU:OE1	1:A:330:ALA:CA	2.53	0.56
1:A:873:GLU:OE2	1:A:885:TYR:OH	2.24	0.56
1:A:541:PHE:O	1:A:544:PHE:HB2	2.06	0.56
1:A:640:GLU:HA	1:A:649:LYS:HE3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:THR:OG1	1:A:805:LYS:HG3	2.07	0.55
2:B:51:A:H2'	2:B:52:C:C6	2.42	0.55
1:A:91:VAL:HG13	1:A:91:VAL:O	2.06	0.55
1:A:302:ARG:HG3	1:A:302:ARG:HH11	1.72	0.55
2:B:82:U:O2'	2:B:83:G:H5'	2.07	0.55
1:A:375:SER:OG	1:A:376:PRO:CD	2.56	0.54
2:B:90:A:H2'	2:B:91:A:C8	2.41	0.54
1:A:373:ASN:HD22	1:A:373:ASN:C	2.04	0.54
1:A:248:GLY:HA2	1:A:388:LEU:HD22	1.90	0.54
1:A:868:LYS:HG2	1:A:899:PRO:HG3	1.90	0.54
1:A:568:TYR:CD2	1:A:606:VAL:HG11	2.43	0.53
1:A:117:ALA:HB2	1:A:122:LEU:HD11	1.90	0.53
1:A:374:LEU:N	1:A:374:LEU:HD23	2.22	0.53
1:A:88:ARG:O	1:A:89:GLU:HG2	2.09	0.53
1:A:266:LYS:HZ1	1:A:422:GLN:HE22	1.57	0.53
1:A:880:ARG:HG2	1:A:880:ARG:NH1	2.18	0.53
1:A:147:GLU:CB	1:A:392:ASP:OD1	2.56	0.53
1:A:292:GLY:HA3	1:A:653:LEU:O	2.09	0.53
1:A:317:TYR:CE1	1:A:347:LEU:HD13	2.43	0.53
1:A:181:ALA:HA	1:A:185:PHE:CD2	2.44	0.52
1:A:754:ASP:OD1	1:A:755:GLY:N	2.27	0.52
2:B:97:U:H2'	2:B:98:G:H8	1.74	0.52
2:B:79:A:C8	2:B:79:A:C5'	2.85	0.52
1:A:169:LEU:HD12	1:A:170:GLN:N	2.24	0.52
1:A:90:GLY:CA	1:A:226:HIS:HD2	2.23	0.52
1:A:500:ARG:HH11	1:A:694:ARG:HA	1.75	0.52
1:A:931:THR:HG21	1:A:1025:ARG:NH1	2.24	0.52
2:B:75:G:O5'	2:B:76:A:OP2	2.27	0.52
1:A:1011:THR:HG23	1:A:1013:LYS:H	1.75	0.52
2:B:70:C:H3'	2:B:71:G:H8	1.75	0.52
1:A:81:ARG:HH12	2:B:84:U:H4'	1.76	0.51
1:A:289:LEU:HD12	1:A:331:PHE:CZ	2.44	0.51
1:A:378:LEU:O	1:A:382:ILE:HG13	2.10	0.51
1:A:616:ASN:CB	1:A:749:GLU:OE2	2.58	0.51
2:B:38:U:H6	2:B:38:U:C5'	2.09	0.51
2:B:41:U:H2'	2:B:42:C:H6	1.73	0.51
1:A:115:ALA:HB2	1:A:182:LEU:HD13	1.92	0.51
1:A:304:THR:HG22	1:A:323:LEU:HD23	1.92	0.51
1:A:501:ILE:HG13	1:A:687:LEU:HD21	1.93	0.51
1:A:629:SER:OG	1:A:631:GLU:HG3	2.10	0.51
2:B:29:U:H2'	2:B:30:A:H8	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:C:H2'	2:B:116:U:H6	1.74	0.51
1:A:127:TRP:CZ3	1:A:219:GLN:HG3	2.44	0.51
2:B:76:A:N1	2:B:77:A:N6	2.58	0.51
1:A:407:ILE:O	1:A:411:LEU:HG	2.10	0.51
1:A:500:ARG:NH1	1:A:694:ARG:HA	2.25	0.51
2:B:16:U:H3'	2:B:17:A:C8	2.43	0.51
1:A:280:LEU:HD11	1:A:436:GLU:HG3	1.93	0.51
2:B:74:U:C6	2:B:74:U:C5'	2.83	0.51
1:A:500:ARG:NH2	1:A:690:LYS:CB	2.73	0.50
2:B:42:C:C2'	2:B:43:G:H5'	2.39	0.50
1:A:785:ILE:HD13	1:A:790:LYS:C	2.35	0.50
1:A:803:LEU:HG	1:A:826:THR:HG22	1.93	0.50
2:B:76:A:H8	2:B:76:A:O5'	1.93	0.50
1:A:28:GLU:OE1	1:A:37:ARG:NE	2.35	0.50
1:A:248:GLY:O	1:A:252:GLN:HG3	2.11	0.50
1:A:1060:LYS:HG2	1:A:1073:CYS:SG	2.51	0.50
2:B:76:A:C8	2:B:76:A:O5'	2.65	0.50
2:B:98:G:H2'	2:B:99:C:H6	1.76	0.50
2:B:62:A:H2'	2:B:63:A:C8	2.47	0.50
1:A:195:GLN:OE1	1:A:921:LYS:NZ	2.38	0.50
1:A:803:LEU:HD12	1:A:803:LEU:N	2.20	0.50
2:B:30:A:H2'	2:B:31:G:C8	2.47	0.50
1:A:136:LYS:NZ	2:B:62:A:OP2	2.37	0.50
1:A:500:ARG:HH11	1:A:500:ARG:HG2	1.77	0.50
1:A:266:LYS:HZ1	1:A:422:GLN:NE2	2.09	0.49
1:A:542:PRO:C	1:A:544:PHE:N	2.69	0.49
1:A:998:LYS:HE2	1:A:998:LYS:HA	1.94	0.49
1:A:629:SER:O	1:A:633:GLN:HG2	2.12	0.49
1:A:869:LEU:HD12	1:A:892:LEU:HD13	1.92	0.49
1:A:800:ALA:HB1	1:A:805:LYS:HB2	1.95	0.49
1:A:999:PHE:CE1	1:A:1059:GLN:HA	2.46	0.49
1:A:176:THR:HB	1:A:211:GLU:HG3	1.94	0.49
1:A:589:ALA:O	1:A:619:PRO:HD3	2.12	0.49
2:B:26:U:H2'	2:B:27:U:C6	2.47	0.49
2:B:104:U:H2'	2:B:105:A:H8	1.77	0.49
2:B:115:C:H2'	2:B:116:U:C6	2.48	0.49
1:A:528:LYS:O	1:A:531:GLU:HG2	2.12	0.48
2:B:76:A:H8	2:B:76:A:C5'	2.24	0.48
1:A:92:LEU:HD12	1:A:93:GLN:H	1.77	0.48
1:A:120:ARG:HD2	1:A:122:LEU:HD23	1.95	0.48
2:B:102:C:H2'	2:B:103:U:H6	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLU:OE2	1:A:516:ARG:NH2	2.46	0.48
1:A:120:ARG:NH2	1:A:126:GLU:OE2	2.46	0.48
1:A:838:MET:HG3	2:B:127:U:C5	2.49	0.48
1:A:542:PRO:HD2	1:A:543:ASN:H	1.79	0.48
1:A:92:LEU:HD13	1:A:94:ALA:HB2	1.95	0.47
1:A:139:GLY:O	2:B:22:U:H4'	2.13	0.47
1:A:541:PHE:CE1	1:A:579:ASN:ND2	2.82	0.47
1:A:794:LYS:HA	1:A:795:PRO:HD2	1.40	0.47
1:A:218:LYS:O	1:A:221:GLU:HB2	2.15	0.47
1:A:692:LYS:N	1:A:692:LYS:CD	2.73	0.47
1:A:870:LYS:H	1:A:870:LYS:CD	2.24	0.47
1:A:836:ARG:HH21	2:B:125:C:H4'	1.79	0.47
1:A:107:PRO:HD2	1:A:129:ALA:HB2	1.97	0.47
1:A:490:GLY:C	1:A:1066:LEU:HD11	2.40	0.47
1:A:653:LEU:O	1:A:655:GLN:HG3	2.14	0.47
1:A:924:ARG:HG3	2:B:56:U:OP1	2.14	0.47
1:A:87:LYS:HA	1:A:92:LEU:HB3	1.95	0.47
1:A:302:ARG:HG3	1:A:302:ARG:NH1	2.30	0.47
1:A:114:ARG:HG3	1:A:130:VAL:HB	1.97	0.47
1:A:361:GLU:HG3	1:A:366:LYS:HD3	1.95	0.47
1:A:949:ARG:CZ	1:A:1079:PRO:HG2	2.44	0.47
1:A:91:VAL:HG21	1:A:124:PRO:CB	2.45	0.47
1:A:852:ARG:NH2	1:A:926:GLU:OE2	2.45	0.47
1:A:1032:ILE:HD11	1:A:1047:LEU:HD12	1.97	0.47
2:B:109:C:H6	2:B:109:C:O5'	1.98	0.46
1:A:148:GLY:C	1:A:149:GLU:HG3	2.40	0.46
1:A:186:GLU:OE1	1:A:192:ILE:HD11	2.14	0.46
1:A:50:GLU:CD	1:A:516:ARG:HH22	2.24	0.46
1:A:91:VAL:HB	1:A:226:HIS:CE1	2.51	0.46
2:B:74:U:C6	2:B:74:U:C4'	2.98	0.46
1:A:298:THR:CA	1:A:301:GLU:OE1	2.64	0.46
1:A:337:TYR:OH	1:A:343:GLU:OE2	2.26	0.46
1:A:721:ARG:HH22	1:A:799:GLU:CD	2.24	0.46
1:A:965:TYR:O	1:A:969:VAL:HG23	2.16	0.46
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.81	0.46
1:A:207:ASP:N	1:A:207:ASP:OD1	2.49	0.46
1:A:832:ARG:HD2	1:A:1019:TYR:CD1	2.51	0.46
1:A:90:GLY:CA	1:A:226:HIS:CD2	2.99	0.45
1:A:331:PHE:HB2	1:A:337:TYR:CZ	2.50	0.45
1:A:274:ALA:O	1:A:278:ILE:HG13	2.17	0.45
1:A:88:ARG:C	1:A:89:GLU:CG	2.88	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:G:O2'	2:B:45:A:N7	2.43	0.45
2:B:76:A:C8	2:B:76:A:OP1	2.70	0.45
1:A:269:LYS:HE2	1:A:419:LYS:CB	2.47	0.45
1:A:286:LEU:HD23	1:A:297:LEU:HD11	1.97	0.45
2:B:104:U:H2'	2:B:105:A:C8	2.51	0.45
1:A:290:GLU:OE1	1:A:330:ALA:CB	2.63	0.45
1:A:319:GLN:NE2	1:A:323:LEU:HD13	2.20	0.45
2:B:31:G:H2'	2:B:32:C:H6	1.82	0.45
2:B:114:G:HO2'	2:B:115:C:P	2.40	0.45
1:A:348:MET:HE2	1:A:350:MET:SD	2.57	0.45
1:A:541:PHE:HE1	1:A:579:ASN:HD21	1.64	0.45
1:A:868:LYS:HG2	1:A:899:PRO:CG	2.46	0.45
1:A:874:LYS:O	1:A:926:GLU:HG2	2.17	0.45
1:A:910:TYR:HA	1:A:915:ASN:O	2.17	0.45
1:A:310:TYR:CZ	1:A:350:MET:HE2	2.52	0.44
1:A:378:LEU:HD13	1:A:403:ILE:HG22	1.98	0.44
1:A:517:LYS:HA	1:A:517:LYS:HD3	1.84	0.44
1:A:77:HIS:CE1	1:A:81:ARG:HD2	2.52	0.44
2:B:114:G:O2'	2:B:115:C:OP1	2.31	0.44
1:A:472:ILE:HD11	1:A:676:PHE:CD2	2.52	0.44
2:B:75:G:C8	2:B:75:G:C3'	3.00	0.44
1:A:122:LEU:HB3	1:A:126:GLU:HB2	1.99	0.44
1:A:844:MET:HE3	1:A:945:ALA:HA	2.00	0.44
1:A:90:GLY:HA3	1:A:226:HIS:CD2	2.52	0.44
1:A:194:ASN:ND2	1:A:202:THR:OG1	2.50	0.44
1:A:847:VAL:O	2:B:26:U:O2'	2.35	0.44
2:B:90:A:H2'	2:B:91:A:H8	1.82	0.44
1:A:16:ASP:HA	1:A:504:GLU:O	2.18	0.44
1:A:616:ASN:HB2	1:A:749:GLU:OE2	2.17	0.44
2:B:133:A:P	2:B:133:A:H3'	2.58	0.44
1:A:301:GLU:HG2	1:A:324:LEU:HD22	1.99	0.44
1:A:542:PRO:C	1:A:544:PHE:H	2.25	0.44
1:A:896:LYS:HB3	1:A:896:LYS:HE2	1.73	0.44
1:A:616:ASN:HB3	1:A:749:GLU:OE2	2.19	0.43
1:A:842:GLY:HA2	1:A:966:SER:OG	2.18	0.43
1:A:911:ASP:OD1	1:A:915:ASN:HB2	2.18	0.43
1:A:1064:ASP:HB2	1:A:1068:LYS:O	2.19	0.43
1:A:772:PHE:HA	1:A:773:PRO:HD3	1.74	0.43
1:A:891:ARG:HD3	1:A:902:ALA:O	2.19	0.43
1:A:953:PHE:CE2	1:A:997:PHE:HB2	2.54	0.43
1:A:562:GLN:NE2	1:A:567:LEU:HD13	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLY:HA2	1:A:632:TRP:CG	2.54	0.43
1:A:743:ARG:HG2	1:A:746:ARG:HH22	1.83	0.43
2:B:114:G:O4'	2:B:114:G:P	2.76	0.43
1:A:147:GLU:HA	1:A:392:ASP:OD1	2.19	0.43
2:B:62:A:H2'	2:B:63:A:H8	1.84	0.43
1:A:269:LYS:HE2	1:A:269:LYS:HB3	1.83	0.43
2:B:98:G:H2'	2:B:99:C:C6	2.52	0.43
1:A:855:GLU:H	1:A:855:GLU:HG3	1.69	0.43
1:A:191:HIS:CE1	1:A:195:GLN:CG	3.00	0.42
1:A:446:ALA:O	1:A:450:GLY:HA2	2.19	0.42
1:A:500:ARG:NH1	1:A:500:ARG:HG2	2.32	0.42
1:A:858:SER:O	1:A:927:GLN:N	2.41	0.42
1:A:13:LEU:HD13	1:A:491:VAL:HG11	2.01	0.42
1:A:837:LYS:HB2	1:A:837:LYS:HE3	1.74	0.42
1:A:949:ARG:HB3	1:A:964:ILE:HB	2.01	0.42
1:A:541:PHE:HA	1:A:542:PRO:HD3	1.69	0.42
2:B:45:A:OP2	2:B:45:A:H8	2.03	0.42
2:B:70:C:H2'	2:B:71:G:C8	2.55	0.42
2:B:102:C:H2'	2:B:103:U:C6	2.54	0.42
2:B:51:A:H2'	2:B:52:C:H6	1.85	0.42
1:A:14:GLY:O	1:A:24:TRP:HA	2.20	0.42
1:A:78:ARG:NE	3:A:1103:HOH:O	2.47	0.42
1:A:266:LYS:NZ	1:A:422:GLN:NE2	2.67	0.42
2:B:133:A:OP2	2:B:133:A:C3'	2.67	0.42
1:A:306:MET:HE2	1:A:306:MET:HB2	1.76	0.42
1:A:530:ARG:NH1	1:A:550:SER:OG	2.53	0.42
1:A:62:ARG:HD2	2:B:90:A:O4'	2.20	0.42
1:A:492:VAL:HA	1:A:496:GLY:O	2.20	0.41
2:B:31:G:H2'	2:B:32:C:C6	2.54	0.41
1:A:227:VAL:O	1:A:227:VAL:CG1	2.66	0.41
1:A:746:ARG:HG2	1:A:750:MET:HE2	2.02	0.41
2:B:25:G:H2'	2:B:26:U:H6	1.84	0.41
1:A:218:LYS:HB3	1:A:222:PHE:HE2	1.86	0.41
1:A:590:LEU:HD11	1:A:654:LEU:HD12	2.01	0.41
1:A:19:ILE:O	1:A:48:ARG:HB3	2.20	0.41
1:A:153:LYS:H	1:A:153:LYS:HG3	1.44	0.41
1:A:316:THR:HG22	1:A:318:ALA:H	1.86	0.41
1:A:623:PHE:O	1:A:632:TRP:HB2	2.20	0.41
1:A:847:VAL:HG22	1:A:935:VAL:HG21	2.02	0.41
1:A:109:THR:O	1:A:112:GLN:N	2.54	0.41
1:A:123:THR:HG22	1:A:125:LEU:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:PHE:O	1:A:666:ASN:ND2	2.53	0.41
1:A:869:LEU:HD11	1:A:892:LEU:CB	2.49	0.41
1:A:91:VAL:O	1:A:91:VAL:CG1	2.69	0.41
1:A:875:MET:HE3	1:A:923:VAL:HG21	2.02	0.41
1:A:135:ILE:HD11	1:A:235:ILE:HG23	2.03	0.41
2:B:133:A:P	2:B:133:A:C3'	3.09	0.41
1:A:87:LYS:O	1:A:92:LEU:HD23	2.21	0.41
1:A:669:ASP:OD1	1:A:674:ASN:ND2	2.53	0.41
2:B:97:U:H2'	2:B:98:G:C8	2.54	0.41
1:A:639:VAL:HG21	1:A:653:LEU:HD11	2.03	0.41
1:A:785:ILE:HD12	1:A:785:ILE:HG23	1.61	0.41
1:A:481:LEU:HD22	1:A:677:LEU:HD11	2.02	0.41
1:A:542:PRO:CD	1:A:543:ASN:H	2.34	0.41
1:A:610[B]:GLU:OE2	1:A:622:TYR:OH	2.15	0.41
1:A:377:GLU:CD	1:A:377:GLU:H	2.29	0.40
1:A:1004:ASN:OD1	1:A:1033:ARG:NH1	2.54	0.40
1:A:1008:GLU:OE2	1:A:1015:ARG:NH2	2.44	0.40
1:A:11:TYR:CE2	1:A:498:PRO:HB3	2.56	0.40
1:A:633:GLN:HG2	1:A:633:GLN:H	1.74	0.40
1:A:65:ALA:O	1:A:69:ARG:HG3	2.21	0.40
1:A:305:LEU:HA	1:A:305:LEU:HD23	1.83	0.40
1:A:315:LEU:HD23	1:A:347:LEU:HD23	2.02	0.40
1:A:654:LEU:HB3	1:A:657:PHE:HD2	1.86	0.40
1:A:1069:GLU:OE2	1:A:1071:ARG:NH2	2.41	0.40
1:A:910:TYR:CD1	1:A:915:ASN:C	2.99	0.40
2:B:128:C:H2'	2:B:129:G:H8	1.86	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)
1:A:319:GLN:OE1	1:A:915:ASN:ND2[3_455]	1.99	0.21

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	1066/1092 (98%)	1003 (94%)	56 (5%)	7 (1%)	18	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	109	THR
1	A	196	ARG
1	A	95	ALA
1	A	151	ALA
1	A	751	ASN
1	A	110	PRO

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	840/942 (89%)	819 (98%)	21 (2%)	42	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	36	ILE
1	A	92	LEU
1	A	108	ASN
1	A	109	THR
1	A	131	LEU
1	A	222	PHE
1	A	226	HIS
1	A	290	GLU
1	A	300	THR
1	A	306	MET
1	A	312	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	366	LYS
1	A	415	ILE
1	A	540	TYR
1	A	646	ARG
1	A	692	LYS
1	A	771	HIS
1	A	796	GLU
1	A	797	PHE
1	A	880	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	191	HIS
1	A	226	HIS
1	A	257	HIS
1	A	319	GLN
1	A	354	HIS
1	A	373	ASN
1	A	588	HIS
1	A	624	ASN
1	A	668	ASN
1	A	739	GLN
1	A	822	HIS
1	A	927	GLN
1	A	939	ASN
1	A	981	GLN
1	A	1059	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	116/135 (85%)	34 (29%)	7 (6%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	U
2	B	21	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	24	C
2	B	31	G
2	B	33	U
2	B	34	C
2	B	38	U
2	B	39	U
2	B	40	C
2	B	43	G
2	B	46	A
2	B	47	G
2	B	48	A
2	B	65	A
2	B	75	G
2	B	76	A
2	B	77	A
2	B	78	A
2	B	79	A
2	B	80	G
2	B	83	G
2	B	84	U
2	B	85	G
2	B	89	C
2	B	95	U
2	B	107	A
2	B	108	G
2	B	109	C
2	B	110	U
2	B	111	C
2	B	115	C
2	B	123	G
2	B	132	U
2	B	133	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	75	G
2	B	76	A
2	B	77	A
2	B	79	A
2	B	83	G
2	B	114	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	132	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 [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	1069/1092 (97%)	0.85	136 (12%) 8 7	11, 47, 76, 95	3 (0%)
2	B	117/135 (86%)	1.16	25 (21%) 2 2	17, 57, 126, 156	0
All	All	1186/1227 (96%)	0.88	161 (13%) 7 6	11, 48, 80, 156	3 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	914	GLY	6.6
1	A	225	PRO	4.8
1	A	913	ALA	4.8
1	A	97	PHE	4.8
1	A	103	ILE	4.8
2	B	17	A	4.4
1	A	105	SER	4.3
2	B	15	U	4.2
1	A	257	HIS	4.1
2	B	47	G	4.0
2	B	78	A	3.9
1	A	226	HIS	3.9
1	A	911	ASP	3.9
2	B	16	U	3.8
2	B	77	A	3.8
2	B	108	G	3.7
1	A	183	ASN	3.7
1	A	113	LEU	3.6
1	A	125	LEU	3.6
1	A	367	ASP	3.6
1	A	130	VAL	3.6
2	B	111	C	3.6
1	A	761	GLU	3.6
1	A	150	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	133	A	3.5
1	A	657	PHE	3.5
1	A	212	LEU	3.5
1	A	617	GLN	3.5
1	A	765	VAL	3.5
1	A	622	TYR	3.4
2	B	75	G	3.4
1	A	452	HIS	3.4
1	A	111	TRP	3.4
1	A	910	TYR	3.4
1	A	610[A]	GLU	3.3
1	A	631	GLU	3.3
1	A	140	TYR	3.3
1	A	759	ASP	3.3
1	A	199	TYR	3.2
2	B	76	A	3.2
1	A	619	PRO	3.2
1	A	176	THR	3.2
1	A	418	ASP	3.2
1	A	917	THR	3.2
1	A	115	ALA	3.1
1	A	124	PRO	3.1
1	A	153	LYS	3.1
1	A	116	ALA	3.0
1	A	451	ASP	3.0
1	A	564	GLY	3.0
1	A	691	GLY	3.0
1	A	1083	SER	3.0
1	A	458	THR	3.0
1	A	95	ALA	3.0
1	A	623	PHE	3.0
1	A	373	ASN	3.0
1	A	716	ARG	2.9
1	A	460	GLU	2.9
2	B	44	A	2.9
2	B	46	A	2.9
1	A	151	ALA	2.9
1	A	717	ALA	2.9
1	A	450	GLY	2.9
1	A	612	GLN	2.9
1	A	99	GLU	2.9
1	A	193	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	606	VAL	2.8
1	A	938	HIS	2.8
1	A	219	GLN	2.8
1	A	448	ILE	2.8
1	A	912	LYS	2.8
1	A	158	LEU	2.7
1	A	182	LEU	2.7
1	A	146	ASN	2.7
1	A	608	GLY	2.7
1	A	625	GLY	2.7
1	A	611	ASN	2.7
1	A	763	GLY	2.7
1	A	545	VAL	2.7
1	A	767	HIS	2.6
2	B	114	G	2.5
2	B	32	C	2.5
2	B	45	A	2.5
1	A	114	ARG	2.5
1	A	870	LYS	2.5
2	B	110	U	2.5
1	A	973	ILE	2.5
1	A	216	PHE	2.5
1	A	401	ASP	2.5
1	A	544	PHE	2.5
1	A	960	TYR	2.5
1	A	93	GLN	2.5
1	A	538[A]	ARG	2.5
2	B	31	G	2.5
1	A	628	ASN	2.5
1	A	262	PRO	2.4
1	A	626	LYS	2.4
1	A	624	ASN	2.4
2	B	30	A	2.4
1	A	91	VAL	2.4
1	A	106	LEU	2.4
1	A	750	MET	2.4
2	B	18	A	2.4
1	A	165	ASN	2.4
1	A	371	PRO	2.4
1	A	587	ASP	2.4
1	A	96	ASN	2.3
1	A	94	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	GLU	2.3
1	A	122	LEU	2.3
1	A	172	GLY	2.3
2	B	79	A	2.3
1	A	90	GLY	2.3
1	A	148	GLY	2.3
1	A	190	GLY	2.3
1	A	940	GLY	2.3
1	A	937	ASN	2.3
1	A	871	ASP	2.3
1	A	370	SER	2.3
1	A	569	SER	2.3
1	A	449	TYR	2.3
1	A	857	VAL	2.3
1	A	186	GLU	2.3
1	A	618	THR	2.3
1	A	620	TYR	2.3
1	A	187	LYS	2.2
1	A	85	LEU	2.2
1	A	901	LYS	2.2
1	A	8	SER	2.2
2	B	48	A	2.2
1	A	627	ASP	2.2
1	A	984	ASP	2.2
1	A	254	MET	2.2
1	A	978	ALA	2.2
1	A	88	ARG	2.2
1	A	989	GLN	2.2
1	A	171	THR	2.2
1	A	229	GLY	2.2
1	A	922	ALA	2.2
1	A	207	ASP	2.1
1	A	127	TRP	2.1
1	A	686	ARG	2.1
1	A	613	ASN	2.1
1	A	762	THR	2.1
1	A	459	GLU	2.1
1	A	915	ASN	2.1
1	A	365	LEU	2.1
1	A	197	SER	2.1
2	B	41	U	2.1
1	A	854	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	169	LEU	2.0
1	A	579	ASN	2.0
1	A	152	ASP	2.0
1	A	403	ILE	2.0
1	A	589	ALA	2.0
1	A	218	LYS	2.0
1	A	128	SER	2.0
1	A	665	ARG	2.0
2	B	61	C	2.0
2	B	115	C	2.0
1	A	715	VAL	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.