



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:37 PM UTC

PDB ID : 6KC8 / pdb_00006kc8
Title : Crystal structure of WT Nme1Cas9 in complex with sgRNA and target DNA (ATATGATT PAM) in post-cleavage state
Authors : Sun, W.; Yang, J.; Cheng, Z.; Liu, C.; Wang, K.; Huang, X.; Wang, Y.
Deposited on : 2019-06-27
Resolution : 2.90 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

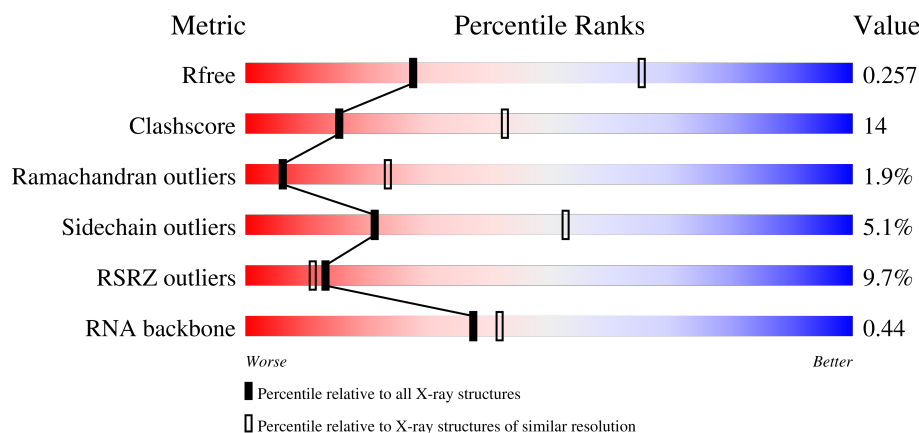
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



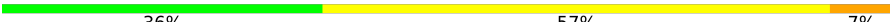
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	11% 65% 28% • •
2	B	135	3% 58% 31% 6% • •
3	C	21	62% 38%
4	D	11	55% 36% 9%

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Mol	Chain	Length	Quality of chain
5	P	14	 A horizontal bar chart showing the quality of chain 5. The bar is divided into three segments: green (36%), yellow (57%), and orange (7%).

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11793 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	1036	Total	C	N	O	S	0	0	0
			8094	5108	1493	1470	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP C9X1G5

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	P	0	0	0
			2746	1229	470	917	130			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*AP*GP*TP*TP*AP*AP*AP*TP*AP*GP*CP*AP*GP*AP*GP*TP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	P	0	0	0
			437	207	87	122	21			

- 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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	14	Total 285	C 139	N 53	O 80	P 13	0	0	0

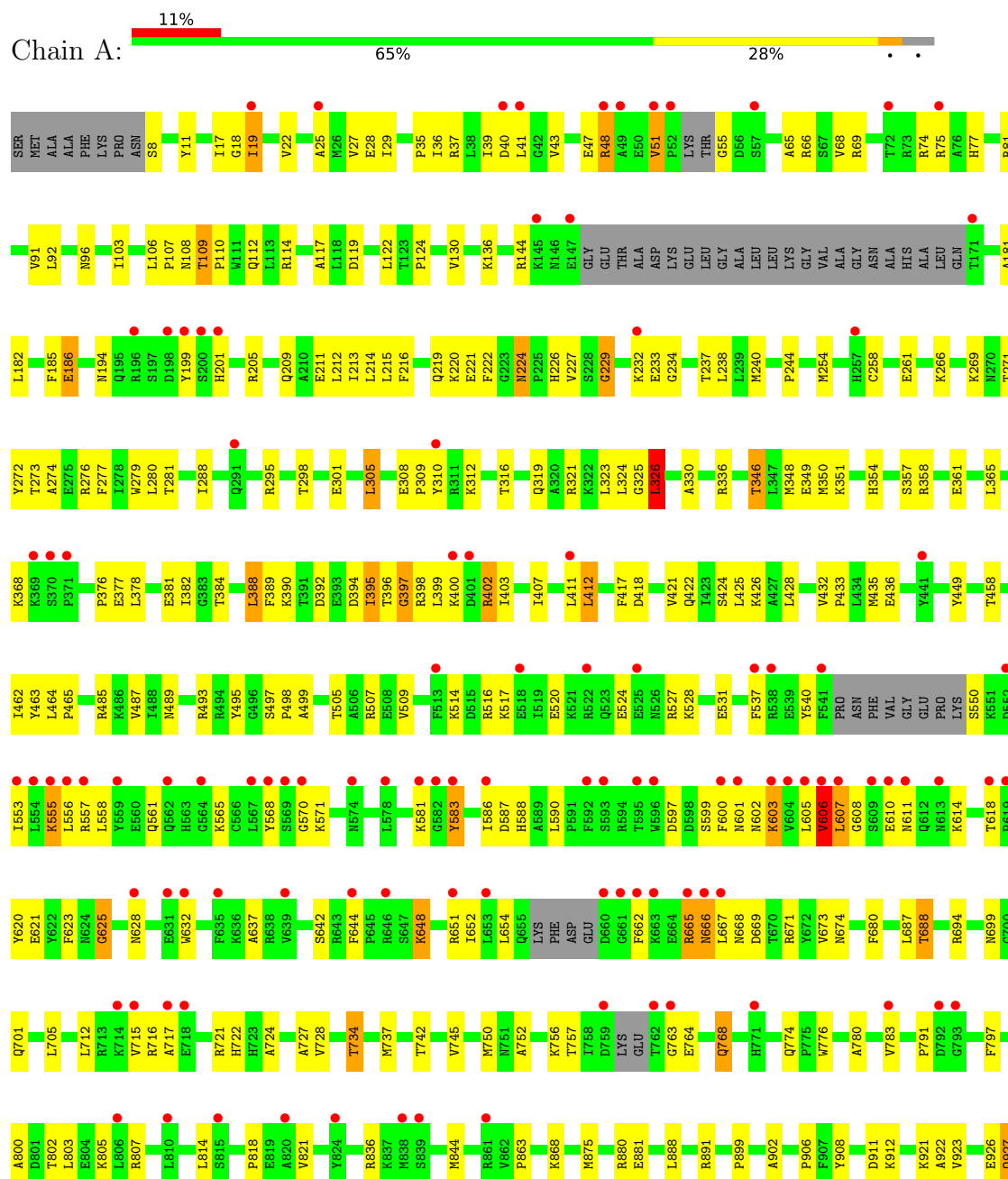
- Molecule 6 is water.

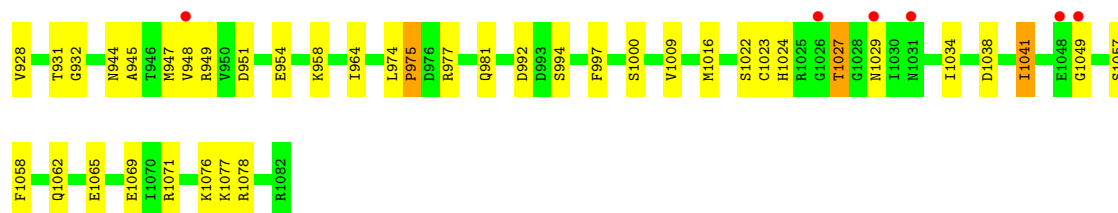
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total 6	O 6	0	0
6	B	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0

3 Residue-property plots

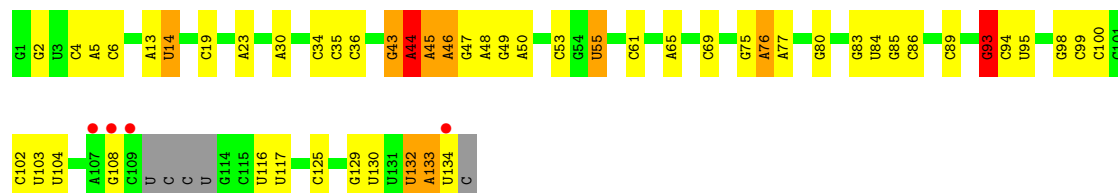
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

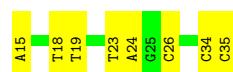




• Molecule 2: sgRNA



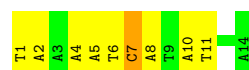
• Molecule 3: DNA (5'-D(P*AP*AP*GP*TP*TP*AP*AP*AP*TP*AP*GP*CP*AP*GP*AP*GP*TP*GP*AP*CP*C)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.60Å 159.52Å 117.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 2.90 49.35 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.7 (49.35-2.90) 83.3 (49.35-2.90)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.203 , 0.257 0.204 , 0.257	Depositor DCC
R_{free} test set	2422 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11793	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	1.03	2/8240 (0.0%)	1.43	17/11115 (0.2%)
2	B	0.55	0/3063	0.98	6/4763 (0.1%)
3	C	0.54	0/492	0.89	0/756
4	D	0.60	0/249	1.04	1/383 (0.3%)
5	P	0.54	0/320	1.03	1/492 (0.2%)
All	All	0.90	2/12364 (0.0%)	1.28	25/17509 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	LEU	C-O	5.50	1.31	1.24
1	A	18	GLY	N-CA	5.36	1.48	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	93	G	C2'-C3'-O3'	8.77	126.85	113.70
5	P	7	DC	C4'-C3'-O3'	7.75	121.63	110.00
2	B	23	A	C2'-C3'-O3'	-6.41	104.08	113.70
1	A	734	THR	CA-CB-OG1	-6.09	100.47	109.60
2	B	61	C	C3'-C2'-O2'	6.07	119.81	110.70
1	A	818	PRO	N-CA-C	5.97	121.68	113.98
1	A	394	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	818	PRO	CB-CA-C	-5.48	103.62	111.62
1	A	814	LEU	CA-C-N	5.47	127.92	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	814	LEU	C-N-CA	5.47	127.92	120.54
1	A	244	PRO	CA-C-N	5.46	128.15	120.28
1	A	244	PRO	C-N-CA	5.46	128.15	120.28
2	B	44	A	C2'-C3'-O3'	5.40	121.80	113.70
1	A	625	GLY	CA-C-N	5.40	127.78	120.38
1	A	625	GLY	C-N-CA	5.40	127.78	120.38
1	A	717	ALA	CA-C-N	5.29	127.37	120.28
1	A	717	ALA	C-N-CA	5.29	127.37	120.28
1	A	607	LEU	CA-C-N	5.19	126.67	120.13
1	A	607	LEU	C-N-CA	5.19	126.67	120.13
1	A	462	ILE	N-CA-C	-5.16	105.81	110.82
2	B	55	U	C3'-C2'-O2'	5.12	118.38	110.70
2	B	13	A	C3'-C2'-O2'	5.10	118.35	110.70
4	D	1	DA	C2'-C3'-O3'	-5.05	103.93	111.50
1	A	921	LYS	N-CA-C	-5.04	107.80	114.04
1	A	19	ILE	O-C-N	5.01	126.93	121.87

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ARG	Peptide
1	A	715	VAL	Peptide
1	A	975	PRO	Peptide

5.2 Too-close contacts [i](#)

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	8094	0	7936	263	0
2	B	2746	0	1394	29	0
3	C	437	0	236	8	0
4	D	223	0	129	5	0
5	P	285	0	161	6	0
6	A	6	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11793	0	9856	293	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 14.

All (293) 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:382:ILE:HD11	1:A:411:LEU:HD13	1.41	0.97
1:A:1069:GLU:OE2	1:A:1071:ARG:NH1	1.98	0.95
1:A:382:ILE:CD1	1:A:411:LEU:HD13	2.01	0.90
1:A:464:LEU:O	1:A:485:ARG:NH1	2.05	0.89
1:A:606:VAL:CG2	1:A:611:ASN:HD21	1.86	0.88
1:A:774:GLN:HG3	1:A:776:TRP:O	1.76	0.85
1:A:271:THR:HG21	1:A:425:LEU:HD21	1.59	0.84
1:A:558:LEU:HG	1:A:605:LEU:HD23	1.58	0.84
1:A:227:VAL:HB	1:A:232:LYS:HZ3	1.43	0.82
1:A:974:LEU:CD2	1:A:1078:ARG:HH21	1.94	0.80
1:A:611:ASN:HA	1:A:614:LYS:HE3	1.63	0.79
1:A:606:VAL:HG23	1:A:611:ASN:HD21	1.48	0.77
1:A:911:ASP:O	1:A:912:LYS:HB3	1.84	0.77
1:A:750:MET:HA	1:A:757:THR:HG22	1.67	0.77
2:B:44:A:O2'	2:B:45:A:OP1	2.00	0.75
1:A:181:ALA:HA	1:A:201:HIS:HE1	1.51	0.74
1:A:524:GLU:OE2	1:A:527:ARG:NH2	2.20	0.74
1:A:1034:ILE:HG21	1:A:1041:ILE:HD11	1.67	0.74
1:A:321:ARG:NH2	1:A:330:ALA:O	2.21	0.73
1:A:181:ALA:HA	1:A:201:HIS:CE1	2.25	0.72
1:A:403:ILE:CG1	1:A:407:ILE:HD11	2.20	0.71
1:A:600:PHE:HA	1:A:603:LYS:NZ	2.06	0.71
1:A:648:LYS:O	1:A:651:ARG:N	2.22	0.71
1:A:321:ARG:HG3	1:A:326:LEU:HD11	1.72	0.70
1:A:215:LEU:O	1:A:219:GLN:HB2	1.90	0.70
2:B:116:U:H2'	2:B:117:U:H6	1.56	0.70
1:A:728:VAL:HG21	1:A:783:VAL:HG21	1.73	0.69
1:A:258:CYS:HB2	1:A:424:SER:OG	1.93	0.69
1:A:109:THR:HG23	1:A:112:GLN:HE21	1.58	0.69
1:A:974:LEU:CD2	1:A:1078:ARG:NH2	2.55	0.69
1:A:880:ARG:NH1	2:B:36:C:O2	2.26	0.69
2:B:116:U:H2'	2:B:117:U:C6	2.28	0.68
1:A:605:LEU:HD12	1:A:605:LEU:C	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:THR:O	1:A:388:LEU:HD12	1.94	0.67
1:A:601:ASN:HA	1:A:648:LYS:HG2	1.77	0.67
1:A:301:GLU:HB3	1:A:324:LEU:CD2	2.24	0.66
1:A:312:LYS:O	1:A:354:HIS:NE2	2.29	0.66
1:A:803:LEU:HD21	1:A:807:ARG:CZ	2.26	0.65
1:A:389:PHE:HB2	1:A:395:ILE:HG22	1.78	0.65
1:A:517:LYS:NZ	1:A:520:GLU:OE2	2.24	0.64
5:P:7:DC:H2''	5:P:8:DA:O5'	1.97	0.64
3:C:23:DT:H2''	3:C:24:DA:H8	1.63	0.64
1:A:712:LEU:HD21	1:A:780:ALA:HA	1.80	0.62
1:A:305:LEU:HD21	1:A:324:LEU:HD11	1.80	0.62
1:A:557:ARG:O	1:A:561:GLN:OE1	2.17	0.62
1:A:687:LEU:O	1:A:694:ARG:NH1	2.32	0.62
1:A:875:MET:HE3	1:A:923:VAL:HG21	1.82	0.62
1:A:216:PHE:CD2	1:A:232:LYS:HD2	2.35	0.62
2:B:43:G:H5''	2:B:43:G:H8	1.64	0.62
1:A:992:ASP:OD1	1:A:994:SER:OG	2.18	0.61
1:A:28:GLU:OE1	1:A:37:ARG:NH2	2.32	0.61
1:A:227:VAL:HB	1:A:232:LYS:NZ	2.14	0.61
1:A:354:HIS:O	1:A:358:ARG:HG2	2.01	0.61
1:A:390:LYS:NZ	1:A:417:PHE:O	2.35	0.60
1:A:261:GLU:OE2	1:A:449:TYR:OH	2.14	0.60
2:B:46:A:C8	2:B:46:A:H5''	2.35	0.60
1:A:403:ILE:HD11	1:A:407:ILE:HD11	1.83	0.60
1:A:590:LEU:HD11	1:A:651:ARG:O	2.03	0.59
1:A:298:THR:N	1:A:301:GLU:OE1	2.32	0.59
1:A:51:VAL:O	1:A:55:GLY:HA2	2.02	0.59
1:A:279:TRP:HB2	1:A:348:MET:HE2	1.85	0.59
1:A:378:LEU:O	1:A:382:ILE:HG22	2.03	0.59
1:A:216:PHE:HD2	1:A:232:LYS:NZ	2.01	0.58
1:A:274:ALA:HB1	1:A:421:VAL:HG21	1.85	0.58
1:A:109:THR:N	1:A:110:PRO:HD3	2.18	0.58
1:A:276:ARG:NH1	1:A:436:GLU:OE2	2.36	0.58
1:A:516:ARG:HB2	3:C:26:DC:H5''	1.85	0.58
1:A:587:ASP:O	1:A:603:LYS:HA	2.04	0.58
1:A:1027:THR:HG22	1:A:1029:ASN:H	1.68	0.58
1:A:974:LEU:HD22	1:A:1078:ARG:HH21	1.69	0.58
1:A:899:PRO:HA	1:A:902:ALA:HB3	1.85	0.58
1:A:395:ILE:HD11	1:A:412:LEU:HG	1.84	0.57
1:A:728:VAL:HG21	1:A:783:VAL:CG2	2.34	0.57
1:A:974:LEU:HD23	1:A:1078:ARG:NH2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:ARG:HD2	2:B:125:C:O2'	2.04	0.57
1:A:11:TYR:CE2	1:A:498:PRO:HB3	2.40	0.57
1:A:106:LEU:HD12	1:A:107:PRO:HD2	1.87	0.57
1:A:555:LYS:CD	1:A:586:ILE:HD11	2.35	0.57
1:A:281:THR:HG22	1:A:435:MET:HE1	1.87	0.56
1:A:381:GLU:OE1	1:A:402:ARG:HD3	2.04	0.56
1:A:606:VAL:HG23	1:A:611:ASN:ND2	2.18	0.56
1:A:802:THR:HG23	1:A:805:LYS:HD3	1.87	0.56
2:B:76:A:P	2:B:76:A:H3'	2.45	0.56
1:A:605:LEU:O	1:A:606:VAL:HG13	2.06	0.56
1:A:880:ARG:NH2	2:B:53:C:O2	2.39	0.56
1:A:194:ASN:ND2	1:A:201:HIS:O	2.36	0.56
1:A:891:ARG:HD3	1:A:902:ALA:O	2.05	0.56
1:A:705:LEU:HD11	1:A:752:ALA:O	2.06	0.55
1:A:221:GLU:HG3	1:A:222:PHE:HD2	1.71	0.55
5:P:10:DA:H2''	5:P:11:DT:O5'	2.06	0.55
1:A:399:LEU:O	1:A:403:ILE:HG22	2.07	0.55
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.89	0.55
1:A:1076:LYS:HG3	1:A:1077:LYS:HG2	1.89	0.55
1:A:1071:ARG:HH12	2:B:102:C:H4'	1.73	0.54
1:A:321:ARG:HE	1:A:326:LEU:HD21	1.72	0.54
1:A:555:LYS:HD2	1:A:586:ILE:HD11	1.90	0.54
3:C:15:DA:H5''	3:C:15:DA:H8	1.73	0.54
1:A:277:PHE:O	1:A:281:THR:HG23	2.08	0.54
1:A:288:ILE:HD11	1:A:295:ARG:NH2	2.22	0.54
1:A:221:GLU:HG3	1:A:222:PHE:CD2	2.43	0.53
1:A:316:THR:HA	1:A:346:THR:HA	1.89	0.53
1:A:648:LYS:O	1:A:652:ILE:HD12	2.08	0.53
1:A:403:ILE:CD1	1:A:407:ILE:HD11	2.38	0.53
3:C:23:DT:H2''	3:C:24:DA:C8	2.42	0.53
1:A:527:ARG:HG2	1:A:531:GLU:OE1	2.08	0.53
1:A:665:ARG:NE	1:A:666:ASN:H	2.07	0.53
1:A:949:ARG:HD2	1:A:1000:SER:HB3	1.91	0.53
1:A:464:LEU:HD11	1:A:680:PHE:CD2	2.44	0.53
1:A:234:GLY:O	1:A:238:LEU:HD12	2.08	0.53
1:A:288:ILE:HD11	1:A:295:ARG:CZ	2.39	0.53
1:A:620:TYR:CE1	1:A:625:GLY:HA2	2.44	0.53
1:A:75:ARG:NH1	1:A:136:LYS:O	2.42	0.52
1:A:254:MET:HE1	3:C:19:DT:O2	2.09	0.52
1:A:975:PRO:O	1:A:1078:ARG:NH2	2.43	0.52
1:A:931:THR:OG1	1:A:932:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:THR:HG22	1:A:737:MET:SD	2.49	0.52
1:A:357:SER:O	1:A:361:GLU:HG3	2.10	0.51
1:A:25:ALA:HB1	1:A:728:VAL:HG12	1.92	0.51
1:A:185:PHE:CB	1:A:201:HIS:CE1	2.93	0.51
1:A:216:PHE:HD2	1:A:232:LYS:HZ2	1.57	0.51
1:A:463:TYR:OH	1:A:493:ARG:HG2	2.10	0.51
1:A:40:ASP:OD2	1:A:495:TYR:OH	2.22	0.51
1:A:108:ASN:C	1:A:110:PRO:HD3	2.36	0.51
1:A:601:ASN:HA	1:A:648:LYS:CG	2.40	0.51
1:A:881:GLU:OE2	2:B:35:C:O2'	2.28	0.51
1:A:233:GLU:O	1:A:237:THR:HG23	2.10	0.51
1:A:396:THR:O	1:A:399:LEU:N	2.43	0.51
1:A:421:VAL:HG12	1:A:422:GLN:H	1.76	0.50
2:B:76:A:H3'	2:B:76:A:OP2	2.12	0.50
1:A:418:ASP:OD1	1:A:418:ASP:N	2.44	0.50
1:A:668:ASN:HA	1:A:671:ARG:HD2	1.93	0.50
1:A:668:ASN:ND2	2:B:14:U:O2'	2.45	0.50
1:A:600:PHE:HA	1:A:603:LYS:CE	2.42	0.50
1:A:701:GLN:O	1:A:705:LEU:HD13	2.11	0.50
1:A:648:LYS:C	1:A:652:ILE:HD12	2.37	0.50
1:A:74:ARG:NH2	2:B:86:C:OP1	2.42	0.50
1:A:1024:HIS:CG	1:A:1027:THR:HB	2.47	0.50
1:A:280:LEU:CD1	1:A:432:VAL:HG13	2.42	0.50
5:P:1:DT:H2''	5:P:2:DA:C8	2.47	0.49
1:A:319:GLN:O	1:A:323:LEU:HG	2.12	0.49
1:A:628:ASN:HA	1:A:632:TRP:CD1	2.47	0.49
1:A:382:ILE:CD1	1:A:411:LEU:CD1	2.84	0.49
1:A:212:LEU:HD11	1:A:216:PHE:HE1	1.77	0.49
1:A:109:THR:HG22	1:A:109:THR:O	2.12	0.49
1:A:209:GLN:HB2	1:A:240:MET:HE3	1.95	0.49
1:A:605:LEU:HD12	1:A:606:VAL:N	2.27	0.49
1:A:28:GLU:O	1:A:36:ILE:HG12	2.13	0.49
1:A:28:GLU:HB2	1:A:39:ILE:HD11	1.94	0.49
1:A:43:VAL:HG21	1:A:721:ARG:HA	1.95	0.48
1:A:266:LYS:HD2	1:A:421:VAL:O	2.14	0.48
1:A:601:ASN:CB	1:A:648:LYS:HG3	2.43	0.48
1:A:606:VAL:HG21	1:A:611:ASN:HD21	1.73	0.48
2:B:5:A:H2'	2:B:6:C:C6	2.49	0.48
1:A:25:ALA:CB	1:A:728:VAL:HG12	2.44	0.48
1:A:951:ASP:OD2	1:A:1078:ARG:NH1	2.47	0.48
1:A:305:LEU:CD2	1:A:324:LEU:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ASP:O	1:A:673:VAL:HG23	2.13	0.48
2:B:4:C:H2'	2:B:5:A:C8	2.48	0.48
1:A:65:ALA:O	1:A:68:VAL:HG22	2.13	0.48
1:A:568:TYR:CD2	1:A:606:VAL:HG11	2.48	0.48
1:A:402:ARG:HB3	1:A:402:ARG:NH2	2.30	0.47
1:A:358:ARG:HH12	1:A:368:LYS:NZ	2.12	0.47
1:A:944:ASN:OD1	4:D:4:DT:OP1	2.32	0.47
1:A:875:MET:HE1	1:A:888:LEU:CD1	2.45	0.47
3:C:34:DC:H2''	3:C:35:DC:H5'	1.97	0.47
1:A:1065:GLU:H	1:A:1065:GLU:CD	2.22	0.47
1:A:288:ILE:HD11	1:A:295:ARG:NE	2.30	0.47
1:A:321:ARG:HA	1:A:326:LEU:HD21	1.97	0.47
1:A:527:ARG:O	1:A:531:GLU:OE2	2.33	0.47
5:P:4:DA:H2''	5:P:5:DA:H5''	1.97	0.47
1:A:220:LYS:HA	1:A:227:VAL:HG11	1.95	0.47
1:A:227:VAL:C	1:A:232:LYS:HD3	2.40	0.46
1:A:211:GLU:O	1:A:215:LEU:HG	2.15	0.46
1:A:875:MET:CE	1:A:923:VAL:HG21	2.45	0.46
2:B:103:U:H2'	2:B:104:U:H6	1.81	0.46
2:B:132:U:H4'	2:B:133:A:H5'	1.97	0.46
1:A:600:PHE:CA	1:A:603:LYS:NZ	2.77	0.46
1:A:791:PRO:HG2	1:A:797:PHE:CE1	2.51	0.46
1:A:600:PHE:C	1:A:603:LYS:HZ1	2.24	0.46
1:A:618:THR:HG23	1:A:621:GLU:H	1.80	0.46
1:A:964:ILE:HG12	1:A:975:PRO:HG2	1.97	0.46
1:A:421:VAL:HG12	1:A:422:GLN:N	2.31	0.46
1:A:17:ILE:HG23	1:A:22:VAL:HG12	1.98	0.46
1:A:261:GLU:OE1	1:A:426:LYS:HD3	2.15	0.46
1:A:396:THR:O	1:A:398:ARG:N	2.48	0.46
1:A:114:ARG:HG3	1:A:130:VAL:HG13	1.97	0.46
1:A:301:GLU:HB3	1:A:324:LEU:HD22	1.97	0.46
1:A:531:GLU:OE2	1:A:531:GLU:N	2.41	0.46
1:A:724:ALA:O	1:A:727:ALA:HB3	2.15	0.46
1:A:1009:VAL:HG22	1:A:1058:PHE:HD1	1.81	0.46
1:A:29:ILE:HG22	1:A:35:PRO:HA	1.98	0.45
1:A:667:LEU:O	1:A:671:ARG:HG3	2.16	0.45
1:A:553:ILE:HD12	1:A:553:ILE:H	1.82	0.45
1:A:1009:VAL:HG22	1:A:1058:PHE:CD1	2.52	0.45
4:D:1:DA:H2''	4:D:2:DT:H5'	1.99	0.45
1:A:402:ARG:HB3	1:A:402:ARG:HH21	1.82	0.45
1:A:485:ARG:NH1	1:A:489:ASN:ND2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:GLU:C	1:A:927:GLN:HG2	2.40	0.45
1:A:110:PRO:O	1:A:114:ARG:HB2	2.16	0.45
1:A:349:GLU:CD	1:A:351:LYS:HE3	2.42	0.45
1:A:537:PHE:HA	1:A:556:LEU:HD22	1.98	0.45
3:C:15:DA:H5''	3:C:15:DA:C8	2.52	0.45
1:A:403:ILE:HG13	1:A:407:ILE:HD11	1.96	0.45
1:A:499:ALA:HA	1:A:688:THR:HB	1.98	0.45
1:A:505:THR:O	1:A:699:ASN:HA	2.17	0.45
1:A:396:THR:O	1:A:397:GLY:C	2.61	0.44
1:A:583:TYR:O	1:A:608:GLY:N	2.49	0.44
1:A:600:PHE:HA	1:A:603:LYS:HZ2	1.78	0.44
2:B:34:C:H2'	2:B:35:C:O4'	2.18	0.44
1:A:1034:ILE:HD11	1:A:1038:ASP:H	1.83	0.44
1:A:17:ILE:HG12	1:A:22:VAL:HG12	1.98	0.44
1:A:875:MET:HE2	1:A:923:VAL:HB	1.99	0.44
1:A:11:TYR:HA	1:A:27:VAL:O	2.18	0.44
1:A:271:THR:HG22	1:A:274:ALA:H	1.81	0.44
1:A:757:THR:OG1	1:A:768:GLN:NE2	2.49	0.44
1:A:310:TYR:CE1	1:A:350:MET:HE2	2.52	0.44
1:A:377:GLU:O	1:A:381:GLU:HG3	2.16	0.44
1:A:66:ARG:NH1	2:B:19:C:OP2	2.50	0.44
1:A:119:ASP:C	1:A:222:PHE:HE1	2.25	0.44
1:A:109:THR:CG2	1:A:112:GLN:HE21	2.30	0.43
1:A:699:ASN:OD1	1:A:699:ASN:C	2.60	0.43
1:A:199:TYR:CD1	1:A:199:TYR:C	2.96	0.43
2:B:93:G:N2	2:B:129:G:C4	2.86	0.43
2:B:35:C:H2'	2:B:36:C:O4'	2.19	0.43
1:A:565:LYS:HG2	1:A:570:GLY:HA2	1.99	0.43
2:B:43:G:H5''	2:B:43:G:C8	2.49	0.43
1:A:17:ILE:HG12	1:A:22:VAL:CG1	2.49	0.43
1:A:868:LYS:HB2	1:A:868:LYS:NZ	2.33	0.43
1:A:17:ILE:HB	1:A:674:ASN:HD21	1.84	0.43
1:A:219:GLN:HG3	1:A:224:ASN:OD1	2.19	0.43
1:A:272:TYR:HE1	1:A:310:TYR:HE2	1.65	0.43
1:A:540:TYR:N	1:A:540:TYR:CD2	2.86	0.43
1:A:1071:ARG:NH1	2:B:102:C:H4'	2.33	0.43
1:A:205:ARG:HG2	1:A:240:MET:HE1	2.01	0.43
1:A:1016:MET:HE2	1:A:1016:MET:HB2	1.80	0.43
1:A:213:ILE:HD12	1:A:214:LEU:N	2.33	0.43
1:A:844:MET:CE	1:A:945:ALA:HA	2.49	0.43
1:A:1024:HIS:HE1	4:D:5:DG:N7	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:U:H2'	2:B:104:U:C6	2.54	0.42
1:A:308:GLU:HG3	1:A:323:LEU:CD1	2.49	0.42
1:A:600:PHE:HA	1:A:603:LYS:HE3	1.99	0.42
1:A:1024:HIS:CE1	4:D:5:DG:N7	2.88	0.42
1:A:392:ASP:CG	1:A:412:LEU:HD21	2.45	0.42
1:A:399:LEU:HB3	1:A:403:ILE:CG2	2.50	0.42
1:A:623:PHE:O	1:A:632:TRP:HB2	2.18	0.42
1:A:22:VAL:CG2	1:A:487:VAL:HG21	2.49	0.42
1:A:863:PRO:HA	1:A:922:ALA:HB2	2.01	0.42
1:A:325:GLY:O	1:A:326:LEU:HD12	2.19	0.42
1:A:588:HIS:HA	1:A:602:ASN:O	2.20	0.42
1:A:273:THR:HG22	1:A:428:LEU:HB3	2.00	0.42
1:A:947:MET:HE1	1:A:1023:CYS:HB3	2.02	0.42
1:A:28:GLU:C	1:A:36:ILE:HG12	2.45	0.42
1:A:651:ARG:HA	1:A:654:LEU:HD11	2.02	0.42
1:A:716:ARG:HE	1:A:722:HIS:HB2	1.84	0.42
1:A:309:PRO:HB2	1:A:350:MET:HG2	2.02	0.42
2:B:55:U:H6	2:B:55:U:O5'	2.02	0.42
1:A:229:GLY:CA	1:A:232:LYS:HG2	2.50	0.41
1:A:365:LEU:HD22	1:A:407:ILE:HG22	2.02	0.41
4:D:11:DA:C2	5:P:2:DA:C2	3.08	0.41
1:A:485:ARG:NH1	1:A:489:ASN:HD21	2.18	0.41
1:A:642:SER:C	1:A:644:PHE:H	2.28	0.41
1:A:906:PRO:HB2	1:A:908:TYR:CE1	2.55	0.41
1:A:117:ALA:HB2	1:A:122:LEU:HD11	2.02	0.41
1:A:880:ARG:HD2	2:B:36:C:O2'	2.19	0.41
1:A:974:LEU:HD23	1:A:1078:ARG:HH21	1.76	0.41
1:A:182:LEU:O	1:A:186:GLU:HB2	2.20	0.41
1:A:316:THR:HG22	1:A:319:GLN:HG3	2.01	0.41
1:A:601:ASN:HB2	1:A:651:ARG:HD3	2.03	0.41
1:A:768:GLN:OE1	1:A:768:GLN:N	2.54	0.41
1:A:1049:GLY:HA3	5:P:6:DT:H71	2.02	0.41
2:B:76:A:OP2	2:B:76:A:C8	2.74	0.41
1:A:11:TYR:CZ	1:A:498:PRO:HB3	2.55	0.41
1:A:509:VAL:HG12	1:A:745:VAL:HG21	2.02	0.41
1:A:583:TYR:O	1:A:607:LEU:HA	2.21	0.41
1:A:597:ASP:OD1	1:A:599:SER:OG	2.38	0.41
1:A:997:PHE:CE2	1:A:1078:ARG:HA	2.56	0.41
1:A:91:VAL:HG22	1:A:226:HIS:HB3	2.03	0.41
1:A:144:ARG:NH1	3:C:18:DT:OP1	2.53	0.41
1:A:528:LYS:HA	1:A:531:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:LEU:C	1:A:605:LEU:CD1	2.88	0.41
1:A:109:THR:HA	1:A:112:GLN:HE22	1.86	0.41
2:B:98:G:H2'	2:B:99:C:C6	2.56	0.41
1:A:65:ALA:O	1:A:69:ARG:HG3	2.20	0.40
1:A:77:HIS:NE2	1:A:81:ARG:HD2	2.36	0.40
1:A:396:THR:OG1	1:A:397:GLY:N	2.54	0.40
1:A:91:VAL:HA	1:A:226:HIS:CD2	2.56	0.40
1:A:216:PHE:CE2	1:A:232:LYS:HD2	2.56	0.40
1:A:992:ASP:OD1	1:A:992:ASP:N	2.53	0.40
1:A:392:ASP:O	1:A:396:THR:HG23	2.22	0.40
1:A:568:TYR:HB3	1:A:610:GLU:CD	2.46	0.40
1:A:951:ASP:OD2	1:A:964:ILE:HD11	2.21	0.40
1:A:954:GLU:HA	1:A:958:LYS:O	2.21	0.40
1:A:92:LEU:HD11	1:A:103:ILE:HD13	2.02	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	1024/1083 (95%)	908 (89%)	97 (10%)	19 (2%)	6	23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	GLY
1	A	662	PHE
1	A	666	ASN
1	A	764	GLU
1	A	800	ALA
1	A	981	GLN
1	A	48	ARG

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Mol	Chain	Res	Type
1	A	326	LEU
1	A	397	GLY
1	A	336	ARG
1	A	47	GLU
1	A	581	LYS
1	A	637	ALA
1	A	400	LYS
1	A	583	TYR
1	A	606	VAL
1	A	376	PRO
1	A	109	THR
1	A	763	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	809/933 (87%)	768 (95%)	41 (5%)	21 53

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	19	ILE
1	A	41	LEU
1	A	51	VAL
1	A	96	ASN
1	A	124	PRO
1	A	186	GLU
1	A	224	ASN
1	A	269	LYS
1	A	305	LEU
1	A	326	LEU
1	A	346	THR
1	A	395	ILE
1	A	402	ARG

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Mol	Chain	Res	Type
1	A	412	LEU
1	A	433	PRO
1	A	458	THR
1	A	497	SER
1	A	507	ARG
1	A	514	LYS
1	A	550	SER
1	A	555	LYS
1	A	571	LYS
1	A	603	LYS
1	A	606	VAL
1	A	648	LYS
1	A	665	ARG
1	A	688	THR
1	A	742	THR
1	A	756	LYS
1	A	768	GLN
1	A	821	VAL
1	A	927	GLN
1	A	928	VAL
1	A	948	VAL
1	A	977	ARG
1	A	1022	SER
1	A	1027	THR
1	A	1041	ILE
1	A	1057	SER
1	A	1062	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	195	GLN
1	A	201	HIS
1	A	526	ASN
1	A	617	GLN
1	A	624	ASN
1	A	668	ASN
1	A	674	ASN
1	A	722	HIS
1	A	1002	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	128/135 (94%)	30 (23%)	4 (3%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	14	U
2	B	30	A
2	B	43	G
2	B	44	A
2	B	45	A
2	B	46	A
2	B	47	G
2	B	48	A
2	B	49	G
2	B	50	A
2	B	65	A
2	B	69	C
2	B	75	G
2	B	76	A
2	B	77	A
2	B	80	G
2	B	83	G
2	B	84	U
2	B	85	G
2	B	89	C
2	B	93	G
2	B	94	C
2	B	95	U
2	B	100	C
2	B	108	G
2	B	130	U
2	B	132	U
2	B	133	A
2	B	134	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	44	A
2	B	46	A

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Mol	Chain	Res	Type
2	B	93	G
2	B	133	A

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	1036/1083 (95%)	0.65	114 (11%) 10 9	28, 66, 157, 227	0
2	B	130/135 (96%)	-0.10	4 (3%) 51 42	29, 52, 175, 221	0
3	C	21/21 (100%)	-0.85	0 100 100	31, 39, 54, 64	0
4	D	11/11 (100%)	-0.55	0 100 100	38, 49, 58, 58	0
5	P	14/14 (100%)	-0.82	0 100 100	33, 49, 54, 57	0
All	All	1212/1264 (95%)	0.52	118 (9%) 13 11	28, 64, 158, 227	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1048	GLU	6.9
1	A	198	ASP	5.8
1	A	793	GLY	5.8
1	A	556	LEU	5.7
1	A	541	PHE	5.4
1	A	52	PRO	5.1
1	A	762	THR	4.9
1	A	522	ARG	4.7
1	A	715	VAL	4.6
1	A	171	THR	4.5
1	A	401	ASP	4.1
1	A	605	LEU	4.1
1	A	370	SER	4.0
1	A	607	LEU	3.9
1	A	792	ASP	3.9
1	A	596	TRP	3.8
1	A	552	ASP	3.8
1	A	75	ARG	3.8
1	A	581	LYS	3.7
1	A	1026	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	639	VAL	3.7
1	A	717	ALA	3.7
1	A	49	ALA	3.7
1	A	51	VAL	3.5
1	A	604	VAL	3.5
1	A	783	VAL	3.5
1	A	513	PHE	3.4
1	A	718	GLU	3.4
1	A	578	LEU	3.4
1	A	25	ALA	3.4
1	A	759	ASP	3.4
1	A	635	PHE	3.3
1	A	145	LYS	3.2
1	A	553	ILE	3.2
1	A	200	SER	3.1
1	A	667	LEU	3.1
1	A	562	GLN	3.1
1	A	601	ASN	3.0
1	A	665	ARG	3.0
1	A	611	ASN	3.0
1	A	861	ARG	2.9
1	A	57	SER	2.9
1	A	839	SER	2.9
1	A	592	PHE	2.9
1	A	525	GLU	2.9
1	A	569	SER	2.9
1	A	582	GLY	2.8
1	A	232	LYS	2.8
1	A	400	LYS	2.8
1	A	666	ASN	2.8
1	A	838	MET	2.8
1	A	554	LEU	2.8
1	A	820	ALA	2.7
1	A	441	TYR	2.7
1	A	595	THR	2.7
1	A	518	GLU	2.7
1	A	600	PHE	2.7
1	A	644	PHE	2.7
1	A	618	THR	2.7
1	A	1029	ASN	2.7
1	A	40	ASP	2.6
1	A	810	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	196	ARG	2.6
1	A	537	PHE	2.6
2	B	134	U	2.5
1	A	763	GLY	2.5
1	A	199	TYR	2.5
1	A	557	ARG	2.5
1	A	603	LYS	2.5
1	A	646	ARG	2.5
1	A	806	LEU	2.4
1	A	619	PRO	2.4
1	A	593	SER	2.4
1	A	948	VAL	2.4
1	A	555	LYS	2.4
2	B	109	C	2.4
1	A	564	GLY	2.4
1	A	411	LEU	2.4
1	A	567	LEU	2.4
1	A	19	ILE	2.4
1	A	570	GLY	2.4
1	A	660	ASP	2.4
1	A	610	GLU	2.4
1	A	631	GLU	2.4
1	A	583	TYR	2.4
1	A	369	LYS	2.3
2	B	107	A	2.3
1	A	48	ARG	2.3
1	A	586	ILE	2.3
1	A	310	TYR	2.3
1	A	771	HIS	2.2
2	B	108	G	2.2
1	A	661	GLY	2.2
1	A	628	ASN	2.2
1	A	291	GLN	2.2
1	A	815	SER	2.2
1	A	662	PHE	2.2
1	A	613	ASN	2.2
1	A	632	TRP	2.2
1	A	609	SER	2.2
1	A	824	TYR	2.2
1	A	1031	ASN	2.2
1	A	559	TYR	2.2
1	A	653	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	72	THR	2.1
1	A	651	ARG	2.1
1	A	663	LYS	2.1
1	A	41	LEU	2.1
1	A	538	ARG	2.1
1	A	574	ASN	2.1
1	A	201	HIS	2.1
1	A	257	HIS	2.1
1	A	606	VAL	2.1
1	A	371	PRO	2.1
1	A	568	TYR	2.1
1	A	714	LYS	2.0
1	A	1049	GLY	2.0
1	A	147	GLU	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.