Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 01:02 AM JST

PDB ID	:	6KC8
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:

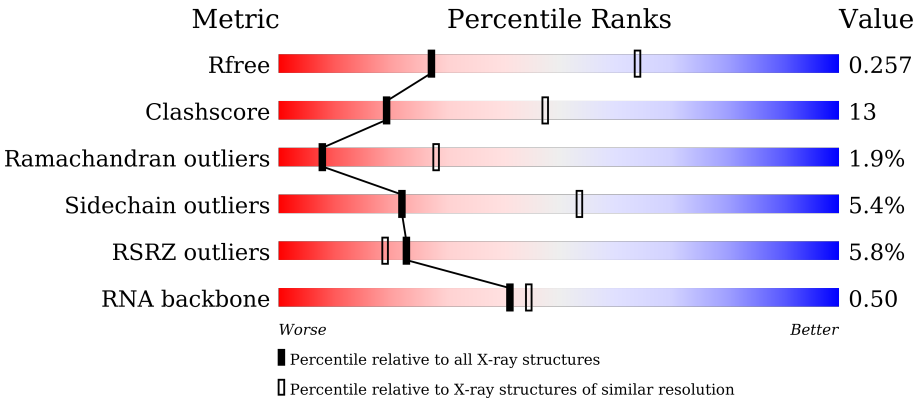
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 <=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	6% 67% 27%
2	B	135	6% 58% 30% 7%
3	C	21	57% 29% 14%
4	D	11	55% 36% 9%

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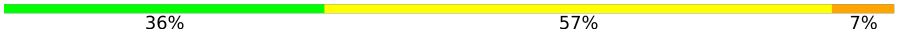
Mol	Chain	Length	Quality of chain
5	P	14	

2 Entry composition (i)

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	C	N	O	P	0	0	0
			285	139	53	80	13			

- Molecule 6 is water.

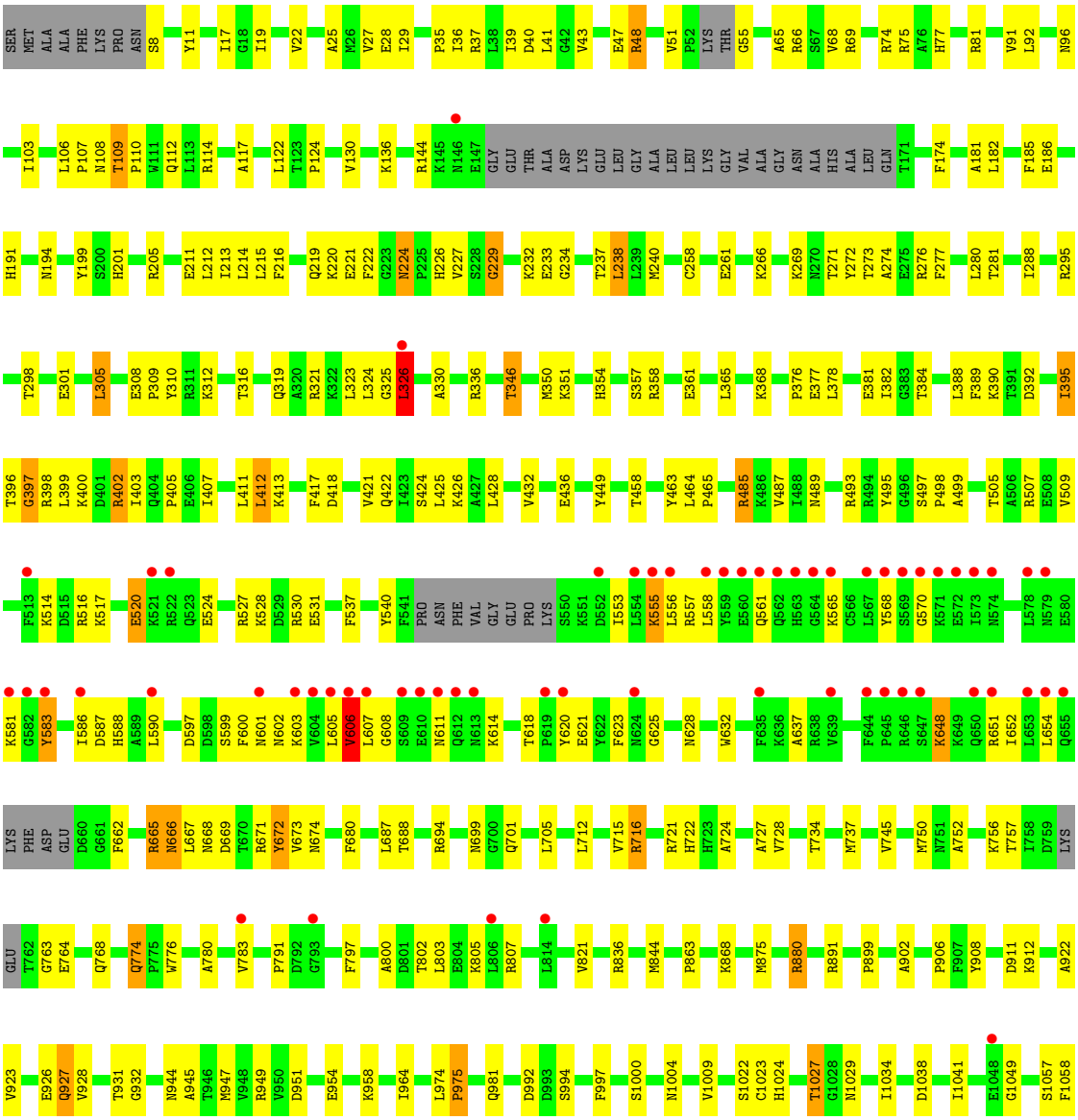
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

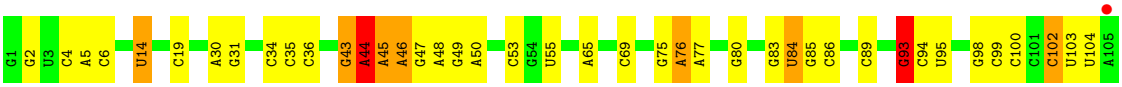
- Molecule 1: CRISPR-associated endonuclease Cas9

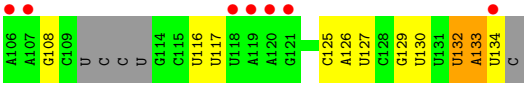
Chain A:



• Molecule 2: sgRNA

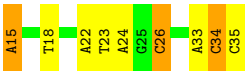
Chain B:





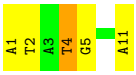
• Molecule 3: DNA (5'-D(P*AP*AP*GP*TP*TP*AP*AP*AP*TP*AP*GP*CP*AP*GP*AP*GP*TP*GP*AP*CP*C)-3')

Chain C:



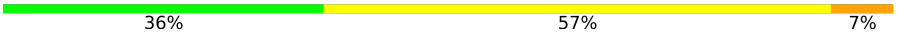
• Molecule 4: DNA (5'-D(*AP*TP*AP*TP*GP*AP*TP*TP*TP*TP*A)-3')

Chain D:



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

Chain P:



4 Data and refinement statistics (i)

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 49.30 – 2.89	Depositor EDS
% Data completeness (in resolution range)	82.7 (49.35-2.90) 82.7 (49.30-2.89)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.20%)	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)	0.28 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	1/8240 (0.0%)	0.86	1/11115 (0.0%)
2	B	0.60	0/3063	0.89	5/4763 (0.1%)
3	C	0.83	1/492 (0.2%)	1.08	5/756 (0.7%)
4	D	0.73	0/249	1.06	1/383 (0.3%)
5	P	0.68	0/320	1.01	1/492 (0.2%)
All	All	0.67	2/12364 (0.0%)	0.89	13/17509 (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)
3	C	15	DA	OP3-P	-9.02	1.50	1.61
1	A	520	GLU	CD-OE1	5.14	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	26	DC	O5'-P-OP2	-9.30	97.33	105.70
2	B	93	G	C2'-C3'-O3'	7.89	126.85	109.50
3	C	26	DC	O5'-P-OP1	7.49	119.69	110.70
3	C	22	DA	O5'-P-OP2	-7.12	99.30	105.70
5	P	5	DA	O5'-P-OP1	-6.15	100.17	105.70
2	B	102	C	O5'-P-OP2	-5.79	100.49	105.70
3	C	33	DA	O5'-P-OP2	-5.52	100.73	105.70
2	B	31	G	O5'-P-OP1	5.40	117.18	110.70
1	A	672	TYR	CB-CG-CD2	-5.36	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4	DT	O5'-P-OP2	-5.22	101.00	105.70
2	B	44	A	C2'-C3'-O3'	5.06	121.80	113.70
3	C	34	DC	C1'-O4'-C4'	-5.06	105.04	110.10
2	B	84	U	O5'-P-OP1	-5.02	101.18	105.70

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	247	0
2	B	2746	0	1394	29	0
3	C	437	0	236	7	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
All	All	11793	0	9856	278	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 13.

All (278) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:605:LEU:HD12	1:A:605:LEU:C	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:600:PHE:HA	1:A:603:LYS:HZ2	1.64	0.61
1:A:390:LYS:NZ	1:A:417:PHE:O	2.35	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: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:261:GLU:OE2	1:A:449:TYR:OH	2.14	0.57
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:844:MET:HE3	1:A:945:ALA:HA	1.89	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:227:VAL:HB	1:A:232:LYS:HZ1	1.72	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: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
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: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:601:ASN:HA	1:A:648:LYS:CG	2.40	0.51
1:A:600:PHE:CA	1:A:603:LYS:HZ2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:MET:HE2	1:A:923:VAL:HB	1.94	0.50
2:B:126:A:HO2'	2:B:127:U:H6	1.59	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: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: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
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:216:PHE:HD2	1:A:232:LYS:HZ2	1.62	0.47
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
3:C:34:DC:H2"	3:C:35:DC:H5'	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:MET:CE	1:A:923:VAL:HG21	2.45	0.47
1:A:211:GLU:O	1:A:215:LEU:HG	2.15	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:791:PRO:HG2	1:A:797:PHE:CE1	2.51	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:108:ASN:C	1:A:110:PRO:HD3	2.36	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
1:A:648:LYS:C	1:A:652:ILE:HD12	2.37	0.45
1:A:110:PRO:O	1:A:114:ARG:HB2	2.16	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:600:PHE:CA	1:A:603:LYS:NZ	2.77	0.45
1:A:583:TYR:O	1:A:608:GLY:N	2.49	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:CG2	1:A:112:GLN:HE21	2.30	0.43
1:A:599:SER:O	1:A:603:LYS:NZ	2.42	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:947:MET:HE1	1:A:1023:CYS:HB3	2.01	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: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
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:227:VAL:C	1:A:232:LYS:HD3	2.40	0.42
1:A:1024:HIS:CE1	4:D:5:DG:N7	2.88	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:1065:GLU:H	1:A:1065:GLU:CD	2.22	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:926:GLU:C	1:A:927:GLN:HG2	2.40	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:22:VAL:HG23	1:A:22:VAL:O	2.21	0.40
1:A:205:ARG:HG2	1:A:240:MET:HE2	2.03	0.40
1:A:392:ASP:O	1:A:396:THR:HG23	2.22	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%)	8 28

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
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 (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	809/933 (87%)	765 (95%)	44 (5%)	22 54

All (44) 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	96	ASN
1	A	124	PRO
1	A	174	PHE
1	A	191	HIS
1	A	199	TYR
1	A	224	ASN
1	A	238	LEU
1	A	269	LYS
1	A	305	LEU
1	A	326	LEU
1	A	346	THR
1	A	351	LYS
1	A	395	ILE
1	A	402	ARG
1	A	405	PRO
1	A	412	LEU
1	A	413	LYS
1	A	458	THR
1	A	485	ARG
1	A	497	SER
1	A	507	ARG
1	A	514	LYS
1	A	530	ARG
1	A	555	LYS
1	A	606	VAL
1	A	648	LYS
1	A	665	ARG
1	A	672	TYR
1	A	716	ARG
1	A	756	LYS
1	A	774	GLN
1	A	821	VAL
1	A	880	ARG
1	A	927	GLN
1	A	928	VAL
1	A	1004	ASN
1	A	1022	SER
1	A	1027	THR
1	A	1057	SER
1	A	1062	GLN

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Mol	Chain	Res	Type
1	A	1078	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	143	GLN
1	A	201	HIS
1	A	219	GLN
1	A	668	ASN
1	A	674	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	128/135 (94%)	29 (22%)	4 (3%)

All (29) 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

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Mol	Chain	Res	Type
2	B	89	C
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
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 monosaccharides 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, 95^{th} 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%)	0.13	62 (5%) 21 18	28, 66, 157, 227	0
2	B	130/135 (96%)	0.15	8 (6%) 20 16	29, 52, 175, 221	0
3	C	21/21 (100%)	-0.65	0 100 100	31, 39, 54, 64	0
4	D	11/11 (100%)	-0.49	0 100 100	38, 49, 58, 58	0
5	P	14/14 (100%)	-0.45	0 100 100	33, 49, 54, 57	0
All	All	1212/1264 (95%)	0.10	70 (5%) 23 19	28, 64, 158, 227	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	LEU	7.0
1	A	556	LEU	6.7
1	A	562	GLN	6.2
1	A	582	GLY	6.2
1	A	610	GLU	5.8
1	A	604	VAL	5.5
1	A	564	GLY	5.4
1	A	624	ASN	5.2
1	A	639	VAL	5.1
1	A	583	TYR	4.7
1	A	559	TYR	4.5
1	A	567	LEU	4.4
1	A	578	LEU	4.4
1	A	565	LYS	4.4
1	A	601	ASN	4.4
1	A	653	LEU	4.0
2	B	119	A	3.9
1	A	619	PRO	3.9
1	A	793	GLY	3.9
1	A	571	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	611	ASN	3.7
1	A	606	VAL	3.6
1	A	552	ASP	3.6
1	A	572	GLU	3.5
1	A	651	ARG	3.4
1	A	590	LEU	3.4
1	A	620	TYR	3.4
2	B	134	U	3.3
1	A	645	PRO	3.3
1	A	563	HIS	3.3
2	B	105	A	3.3
1	A	646	ARG	3.2
1	A	569	SER	3.2
1	A	607	LEU	3.2
1	A	573	ILE	3.2
1	A	146	ASN	3.2
1	A	574	ASN	3.1
1	A	1048	GLU	3.1
1	A	568	TYR	3.1
1	A	644	PHE	3.0
1	A	555	LYS	3.0
1	A	326	LEU	2.9
1	A	612	GLN	2.8
2	B	120	A	2.8
1	A	655	GLN	2.8
1	A	554	LEU	2.7
1	A	558	LEU	2.7
1	A	654	LEU	2.7
1	A	609	SER	2.6
1	A	561	GLN	2.5
1	A	581	LYS	2.5
1	A	513	PHE	2.5
1	A	806	LEU	2.5
1	A	647	SER	2.4
1	A	650	GLN	2.4
2	B	118	U	2.4
1	A	522	ARG	2.4
1	A	521	LYS	2.3
1	A	613	ASN	2.3
1	A	603	LYS	2.3
1	A	560	GLU	2.3
2	B	121	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	579	ASN	2.2
1	A	814	LEU	2.1
1	A	570	GLY	2.1
1	A	783	VAL	2.1
1	A	586	ILE	2.1
2	B	107	A	2.1
2	B	106	A	2.0
1	A	635	PHE	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 monosaccharides 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.