



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:10 am BST

PDB ID : 6K4S  
Title : Crystal structure of xCas9 in complex with sgRNA and DNA (TGC PAM)  
Authors : Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.  
Deposited on : 2019-05-26  
Resolution : 3.01 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](mailto: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.

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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 : 2.11  
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) : 2.11

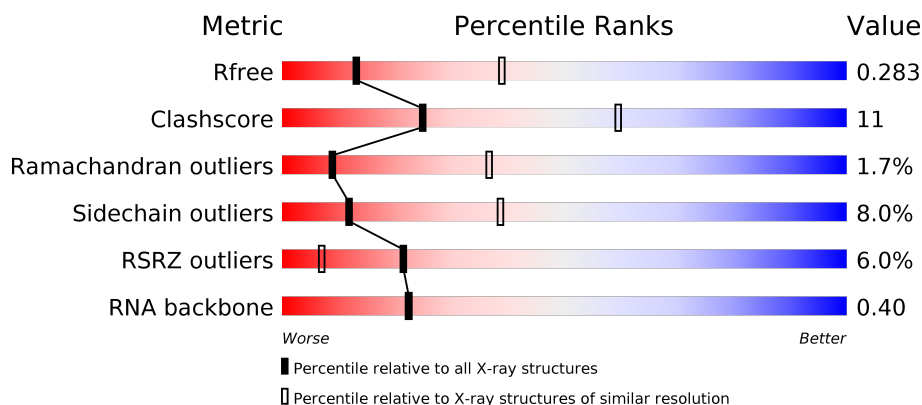
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)
RNA backbone	3102	1066 (3.30-2.74)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	B	1368	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• •</div> </div> </div>
2	A	83	<div> <div>•</div> <div> <div>42%</div> <div>33%</div> <div>18%</div> <div>• •</div> </div> </div>
3	C	28	<div> <div>4%</div> <div> <div>57%</div> <div>36%</div> <div>• •</div> </div> </div>
4	D	12	<div> <div>17%</div> <div> <div>42%</div> <div>42%</div> <div>8%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12412 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/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1308	Total	C	N	O	S	0	0	0
			9924	6324	1730	1854	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	80	LEU	CYS	engineered mutation	UNP Q99ZW2
B	262	THR	ALA	engineered mutation	UNP Q99ZW2
B	324	LEU	ARG	engineered mutation	UNP Q99ZW2
B	409	ILE	SER	engineered mutation	UNP Q99ZW2
B	480	LYS	GLU	engineered mutation	UNP Q99ZW2
B	543	ASP	GLU	engineered mutation	UNP Q99ZW2
B	574	GLU	CYS	engineered mutation	UNP Q99ZW2
B	694	ILE	MET	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1219	VAL	GLU	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	80	Total	C	N	O	P	0	0	0
			1710	768	313	549	80			

- Molecule 3 is a DNA chain called targeted DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	27	Total	C	N	O	P	0	0	0
			554	268	95	164	27			

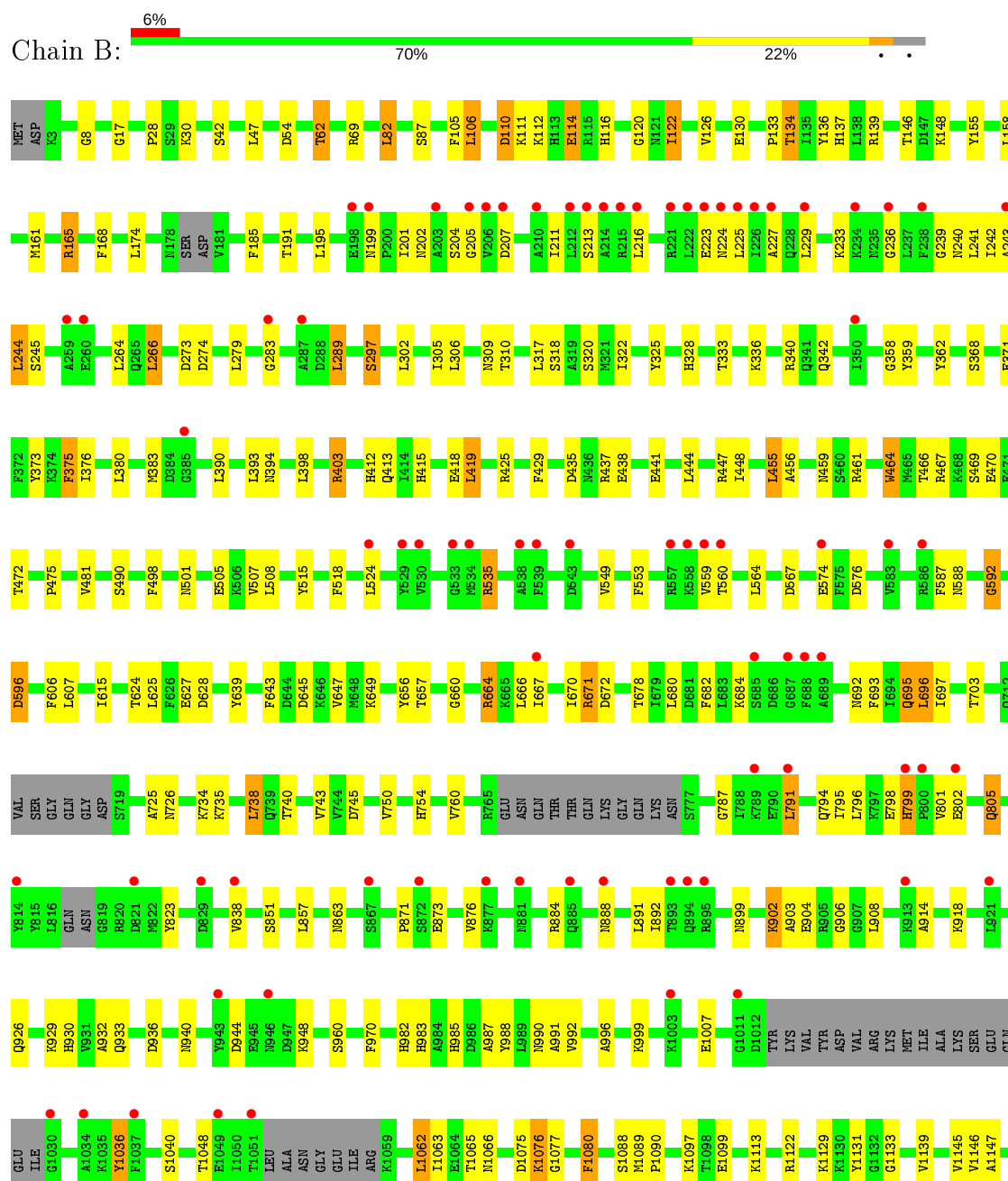
- Molecule 4 is a DNA chain called non-targeted DNA.

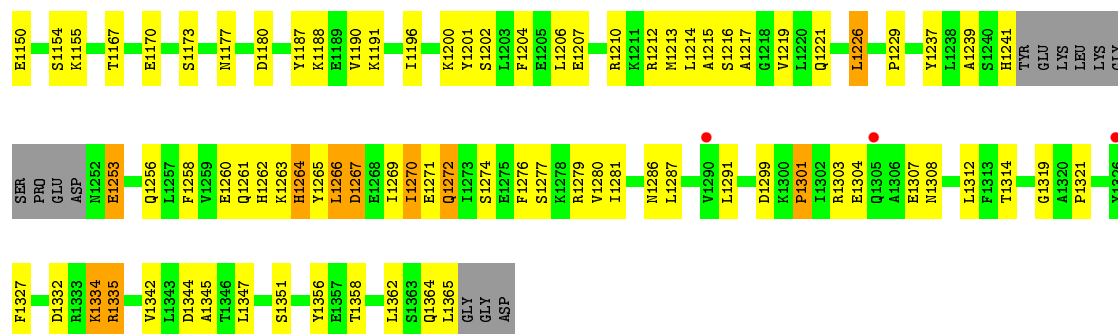
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total 224	C 109	N 41	O 64	P 10	0	0	0

### 3 Residue-property plots

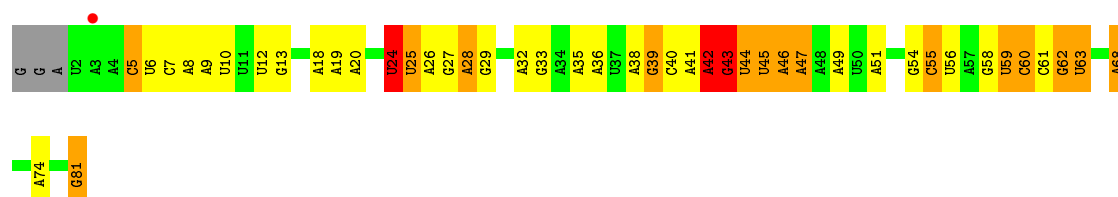
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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/Csn1

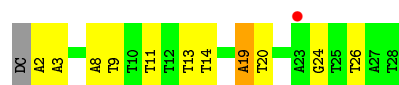




• Molecule 2: sgRNA



• Molecule 3: targeted DNA



• Molecule 4: non-targeted DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.46Å 70.36Å 188.90Å 90.00° 110.42° 90.00°	Depositor
Resolution (Å)	49.25 – 3.01 49.20 – 3.01	Depositor EDS
% Data completeness (in resolution range)	87.0 (49.25-3.01) 87.0 (49.20-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.237 , 0.285 0.237 , 0.283	Depositor DCC
$R_{free}$ test set	1913 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	B	0.78	0/10093	0.90	0/13650
2	A	1.09	18/1917 (0.9%)	0.92	0/2984
3	C	0.96	4/620 (0.6%)	0.85	0/955
4	D	0.90	3/251 (1.2%)	0.87	0/386
All	All	0.85	25/12881 (0.2%)	0.90	0/17975

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	12	U	O3'-P	-9.51	1.49	1.61
3	C	8	DA	O3'-P	-9.09	1.50	1.61
2	A	46	A	O3'-P	-8.65	1.50	1.61
2	A	45	U	O3'-P	-8.53	1.50	1.61
2	A	49	A	O3'-P	-8.53	1.50	1.61
2	A	61	C	O3'-P	-8.51	1.50	1.61
2	A	25	U	O3'-P	-8.43	1.51	1.61
2	A	42	A	O3'-P	-7.72	1.51	1.61
3	C	9	DT	O3'-P	-7.42	1.52	1.61
2	A	47	A	O3'-P	-7.41	1.52	1.61
2	A	24	U	O3'-P	-7.40	1.52	1.61
4	D	5	DT	O3'-P	-7.35	1.52	1.61
2	A	62	G	O3'-P	-7.16	1.52	1.61
3	C	11	DT	O3'-P	-6.61	1.53	1.61
3	C	19	DA	O3'-P	-6.19	1.53	1.61
2	A	60	C	O3'-P	-5.96	1.53	1.61
4	D	6	DG	O3'-P	-5.71	1.54	1.61
4	D	4	DA	O3'-P	-5.66	1.54	1.61
2	A	28	A	O3'-P	-5.64	1.54	1.61
2	A	5	C	O3'-P	-5.60	1.54	1.61
2	A	68	A	O3'-P	-5.17	1.54	1.61
2	A	43	G	O3'-P	-5.16	1.54	1.61
2	A	13	G	O3'-P	-5.15	1.54	1.61
2	A	27	G	O3'-P	-5.11	1.55	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	55	C	O3'-P	-5.06	1.55	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	B	9924	0	9432	220	0
2	A	1710	0	858	37	0
3	C	554	0	310	13	0
4	D	224	0	127	2	0
All	All	12412	0	10727	248	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 11.

All (248) 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)
3:C:19:DA:H2''	3:C:20:DT:C5'	1.64	1.27
3:C:19:DA:H2''	3:C:20:DT:H5''	1.13	1.10
3:C:19:DA:C2'	3:C:20:DT:H5''	1.88	1.03
1:B:241:LEU:HD11	1:B:289:LEU:HD13	1.44	0.99
3:C:19:DA:H2''	3:C:20:DT:H5'	1.51	0.92
1:B:1263:LYS:O	1:B:1264:HIS:HB2	1.74	0.87
1:B:241:LEU:CD1	1:B:289:LEU:HD13	2.08	0.83
2:A:42:A:H5''	2:A:42:A:H8	1.46	0.81
1:B:1265:TYR:O	1:B:1269:ILE:HG13	1.82	0.80
1:B:105:PHE:CD1	2:A:24:U:O2	2.36	0.79
1:B:191:THR:HG22	1:B:289:LEU:HD23	1.67	0.77
3:C:19:DA:C2'	3:C:20:DT:C5'	2.55	0.76
1:B:241:LEU:HD11	1:B:289:LEU:CD1	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:GLY:HA3	1:B:987:ALA:O	1.86	0.75
1:B:823:TYR:CB	1:B:863:ASN:HD22	2.01	0.74
1:B:725:ALA:O	1:B:734:LYS:NZ	2.20	0.74
1:B:1266:LEU:HD23	1:B:1266:LEU:N	2.01	0.73
1:B:876:VAL:HG21	1:B:903:ALA:HB3	1.68	0.73
1:B:518:PHE:CD1	1:B:667:ILE:HD12	2.23	0.73
1:B:340:ARG:NH2	2:A:41:A:OP2	2.22	0.71
2:A:46:A:H2'	2:A:47:A:C8	2.25	0.71
1:B:692:ASN:HD21	3:C:26:DT:H2''	1.58	0.68
1:B:936:ASP:OD1	1:B:940:ASN:ND2	2.27	0.67
1:B:926:GLN:O	1:B:930:HIS:ND1	2.26	0.66
1:B:1113:LYS:HB2	1:B:1129:LYS:O	1.96	0.66
1:B:191:THR:CG2	1:B:289:LEU:HD23	2.26	0.65
1:B:368:SER:OG	1:B:371:GLU:HG3	1.96	0.65
1:B:106:LEU:O	1:B:111:LYS:NZ	2.22	0.65
1:B:871:PRO:O	1:B:903:ALA:HB2	1.96	0.65
1:B:549:VAL:HA	1:B:553:PHE:HB2	1.79	0.65
1:B:838:VAL:HA	1:B:857:LEU:HA	1.77	0.65
1:B:1263:LYS:O	1:B:1264:HIS:CB	2.46	0.64
1:B:69:ARG:HD2	2:A:62:G:N7	2.12	0.63
1:B:795:ILE:O	1:B:799:HIS:HB2	1.98	0.63
2:A:42:A:H8	2:A:42:A:C5'	2.11	0.62
1:B:1196:ILE:HD11	1:B:1364:GLN:HE22	1.65	0.62
1:B:1266:LEU:O	1:B:1269:ILE:N	2.33	0.61
1:B:244:LEU:HD22	1:B:266:LEU:HD12	1.83	0.61
1:B:553:PHE:CG	1:B:559:VAL:HG21	2.35	0.61
1:B:191:THR:HG22	1:B:289:LEU:CD2	2.31	0.60
1:B:884:ARG:O	1:B:888:ASN:ND2	2.34	0.60
2:A:42:A:H5''	2:A:42:A:C8	2.33	0.59
2:A:42:A:C8	2:A:42:A:C5'	2.85	0.59
1:B:1287:LEU:O	1:B:1291:LEU:HG	2.02	0.59
1:B:1226:LEU:HD12	1:B:1226:LEU:C	2.22	0.59
1:B:1335:ARG:HH11	1:B:1335:ARG:CG	2.14	0.59
2:A:33:G:N2	2:A:36:A:OP2	2.35	0.59
1:B:1260:GLU:O	1:B:1263:LYS:HB2	2.04	0.58
1:B:518:PHE:CD1	1:B:667:ILE:CD1	2.86	0.58
1:B:114:GLU:OE2	1:B:116:HIS:HB2	2.03	0.58
1:B:114:GLU:HG3	1:B:120:GLY:O	2.04	0.58
1:B:1258:PHE:O	1:B:1261:GLN:O	2.22	0.58
1:B:419:LEU:HD13	1:B:444:LEU:HD12	1.85	0.58
1:B:899:ASN:O	1:B:902:LYS:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:HD1	2:A:24:U:O2	1.86	0.57
1:B:412:HIS:CE1	1:B:413:GLN:HE22	2.22	0.57
1:B:185:PHE:HE1	1:B:242:ILE:HD11	1.69	0.57
1:B:306:LEU:O	1:B:306:LEU:HD12	2.04	0.57
1:B:592:GLY:O	1:B:596:ASP:HB2	2.04	0.57
1:B:1215:ALA:HB3	1:B:1219:VAL:HG23	1.87	0.56
1:B:1139:VAL:HA	1:B:1167:THR:HA	1.88	0.56
1:B:1204:PHE:CD1	1:B:1342:VAL:HG13	2.42	0.55
2:A:46:A:H2'	2:A:47:A:H8	1.69	0.55
2:A:58:G:C2	2:A:60:C:O2	2.59	0.55
1:B:309:ASN:O	1:B:310:THR:HG22	2.07	0.55
1:B:740:THR:O	1:B:743:VAL:HB	2.07	0.55
1:B:110:ASP:OD2	1:B:1131:TYR:OH	2.21	0.55
1:B:1206:LEU:HD13	1:B:1210:ARG:NH2	2.22	0.55
1:B:390:LEU:O	1:B:394:ASN:ND2	2.40	0.54
1:B:535:ARG:HG3	1:B:535:ARG:HH11	1.72	0.54
1:B:264:LEU:HD22	1:B:274:ASP:HB3	1.89	0.54
1:B:672:ASP:OD2	1:B:703:THR:N	2.38	0.54
1:B:302:LEU:HA	1:B:305:ILE:HG12	1.90	0.54
1:B:54:ASP:O	1:B:735:LYS:NZ	2.38	0.54
1:B:615:ILE:HG23	1:B:639:TYR:CE1	2.43	0.53
1:B:524:LEU:HD12	1:B:587:PHE:HE2	1.73	0.53
1:B:760:VAL:HG11	1:B:990:ASN:O	2.09	0.53
4:D:6:DG:C4	4:D:7:DC:C5	2.96	0.53
1:B:518:PHE:CG	1:B:667:ILE:HD12	2.43	0.53
2:A:54:G:C6	2:A:55:C:N4	2.77	0.53
1:B:1308:ASN:OD1	1:B:1327:PHE:N	2.39	0.53
1:B:680:LEU:O	1:B:684:LYS:HG3	2.09	0.53
1:B:1150:GLU:HB2	1:B:1155:LYS:HA	1.90	0.53
1:B:279:LEU:O	1:B:283:GLY:N	2.40	0.53
1:B:1271:GLU:HA	1:B:1271:GLU:OE1	2.09	0.53
1:B:1145:VAL:HG21	1:B:1187:TYR:CZ	2.44	0.52
1:B:588:ASN:OD1	3:C:24:DG:N2	2.43	0.52
1:B:970:PHE:CD1	1:B:1080:PHE:HZ	2.27	0.52
1:B:1146:VAL:HG13	1:B:1191:LYS:HB2	1.91	0.52
1:B:158:LEU:HA	1:B:161:MET:HE3	1.90	0.52
1:B:695:GLN:O	1:B:697:ILE:N	2.43	0.52
1:B:475:PRO:HG3	2:A:59:U:O4	2.09	0.52
1:B:1145:VAL:HG21	1:B:1187:TYR:CE1	2.45	0.52
1:B:1321:PRO:HG2	1:B:1335:ARG:HA	1.92	0.52
1:B:1206:LEU:HD23	1:B:1345:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1253:GLU:O	1:B:1256:GLN:HB3	2.10	0.51
1:B:645:ASP:O	1:B:649:LYS:N	2.43	0.51
1:B:342:GLN:HE22	1:B:383:MET:HA	1.76	0.51
1:B:823:TYR:CB	1:B:863:ASN:ND2	2.73	0.51
1:B:1266:LEU:CD2	1:B:1266:LEU:N	2.72	0.50
1:B:1200:LYS:O	1:B:1201:TYR:HB2	2.11	0.50
1:B:105:PHE:CD1	2:A:24:U:C2	2.99	0.50
1:B:191:THR:O	1:B:195:LEU:HG	2.12	0.50
1:B:472:THR:HG23	2:A:59:U:OP2	2.11	0.49
1:B:615:ILE:HG23	1:B:639:TYR:CZ	2.47	0.49
1:B:1210:ARG:HE	1:B:1212:ARG:HH12	1.60	0.49
1:B:376:ILE:HG22	1:B:380:LEU:HG	1.95	0.49
1:B:507:VAL:CB	1:B:660:GLY:O	2.61	0.49
1:B:553:PHE:HZ	1:B:587:PHE:CD2	2.30	0.49
1:B:403:ARG:NH1	2:A:20:A:OP1	2.46	0.49
1:B:750:VAL:HG22	1:B:1356:TYR:OH	2.13	0.48
1:B:201:ILE:HG23	1:B:229:LEU:HD12	1.94	0.48
1:B:643:PHE:HB3	1:B:647:VAL:HB	1.94	0.48
1:B:501:ASN:HD22	1:B:666:LEU:CD1	2.25	0.48
1:B:318:SER:OG	1:B:418:GLU:OE1	2.23	0.48
1:B:1269:ILE:O	1:B:1270:ILE:C	2.51	0.48
1:B:515:TYR:OH	2:A:5:C:OP1	2.30	0.48
1:B:1207:GLU:OE2	1:B:1210:ARG:NH1	2.47	0.48
1:B:1237:TYR:CE1	1:B:1241:HIS:CE1	3.01	0.48
1:B:678:THR:O	1:B:682:PHE:HB2	2.13	0.48
1:B:795:ILE:HG22	1:B:796:LEU:HD23	1.96	0.48
1:B:1256:GLN:OE1	1:B:1256:GLN:HA	2.14	0.48
1:B:139:ARG:HH12	1:B:415:HIS:HD2	1.61	0.48
2:A:40:C:H2'	2:A:41:A:C8	2.49	0.48
1:B:122:ILE:O	1:B:126:VAL:HG23	2.13	0.47
1:B:403:ARG:HD2	2:A:20:A:OP1	2.14	0.47
1:B:692:ASN:O	1:B:696:LEU:HD13	2.14	0.47
1:B:1196:ILE:HD11	1:B:1364:GLN:NE2	2.28	0.47
1:B:982:HIS:HE2	1:B:983:HIS:CE1	2.33	0.47
1:B:1239:ALA:O	1:B:1303:ARG:HA	2.15	0.46
1:B:165:ARG:NH1	2:A:18:A:OP1	2.47	0.46
1:B:105:PHE:CE1	2:A:24:U:H1'	2.51	0.46
1:B:1075:ASP:O	1:B:1077:GLY:N	2.48	0.46
1:B:553:PHE:HA	1:B:559:VAL:CG2	2.46	0.46
1:B:1210:ARG:HE	1:B:1212:ARG:NH1	2.14	0.46
1:B:1301:PRO:HD2	1:B:1304:GLU:CD	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:THR:HG23	1:B:137:HIS:CE1	2.51	0.46
1:B:738:LEU:O	1:B:738:LEU:HD22	2.16	0.46
1:B:1356:TYR:HB3	2:A:81:G:N1	2.30	0.46
1:B:1308:ASN:N	1:B:1308:ASN:HD22	2.13	0.46
4:D:8:DT:H2''	4:D:9:DA:C5'	2.46	0.46
1:B:988:TYR:O	1:B:991:ALA:N	2.47	0.46
1:B:146:THR:O	1:B:146:THR:OG1	2.33	0.45
1:B:223:GLU:O	1:B:227:ALA:HB3	2.16	0.45
2:A:38:A:N6	2:A:39:G:C6	2.84	0.45
1:B:1221:GLN:HB2	1:B:1319:GLY:O	2.15	0.45
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.49	0.45
1:B:317:LEU:O	1:B:320:SER:N	2.50	0.45
1:B:393:LEU:HD23	1:B:393:LEU:O	2.17	0.45
1:B:1122:ARG:HD3	1:B:1133:GLY:HA2	1.98	0.45
1:B:802:GLU:HB2	1:B:805:GLN:HB2	1.99	0.45
1:B:805:GLN:HE21	1:B:805:GLN:HB3	1.60	0.45
1:B:467:ARG:NH2	2:A:59:U:OP1	2.50	0.45
1:B:787:GLY:O	1:B:791:LEU:HB2	2.16	0.45
1:B:467:ARG:HD3	1:B:470:GLU:HA	1.98	0.44
1:B:560:THR:O	1:B:564:LEU:CB	2.65	0.44
1:B:1048:THR:HG22	1:B:1076:LYS:HD3	1.98	0.44
1:B:1226:LEU:HB3	1:B:1276:PHE:CZ	2.52	0.44
1:B:982:HIS:NE2	1:B:983:HIS:NE2	2.65	0.44
1:B:1062:LEU:HD23	1:B:1063:ILE:HG13	1.98	0.44
1:B:1202:SER:O	1:B:1213:MET:HA	2.16	0.44
1:B:1269:ILE:O	1:B:1271:GLU:N	2.51	0.44
1:B:560:THR:O	1:B:564:LEU:N	2.51	0.44
1:B:876:VAL:CG2	1:B:903:ALA:HB3	2.42	0.44
1:B:373:TYR:CE1	1:B:398:LEU:HB3	2.52	0.44
1:B:325:TYR:O	1:B:328:HIS:HB3	2.18	0.44
1:B:456:ALA:HA	2:A:58:G:O2'	2.18	0.43
1:B:1089:MET:HA	1:B:1090:PRO:HD3	1.87	0.43
1:B:1344:ASP:HA	1:B:1362:LEU:O	2.18	0.43
1:B:133:PRO:HG2	1:B:137:HIS:CE1	2.53	0.43
1:B:148:LYS:HA	1:B:429:PHE:CD2	2.53	0.43
1:B:240:ASN:HA	1:B:243:ALA:HB3	1.99	0.43
1:B:322:ILE:O	1:B:325:TYR:HB3	2.18	0.43
1:B:333:THR:O	1:B:336:LYS:HB2	2.19	0.43
1:B:447:ARG:O	1:B:448:ILE:C	2.56	0.43
1:B:787:GLY:O	1:B:791:LEU:HD22	2.19	0.43
3:C:19:DA:C8	3:C:20:DT:H71	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1262:HIS:O	1:B:1265:TYR:CD2	2.72	0.43
1:B:1097:LYS:HE3	1:B:1099:GLU:CD	2.38	0.43
1:B:1204:PHE:CE1	1:B:1342:VAL:HG13	2.53	0.43
1:B:1216:SER:OG	1:B:1217:ALA:N	2.51	0.43
1:B:211:ILE:HD12	1:B:225:LEU:HA	2.00	0.43
1:B:671:ARG:NH2	1:B:678:THR:HG23	2.33	0.43
2:A:38:A:C6	2:A:39:G:C6	3.06	0.43
1:B:342:GLN:NE2	1:B:383:MET:HA	2.33	0.43
1:B:871:PRO:O	1:B:903:ALA:CB	2.66	0.43
1:B:929:LYS:O	1:B:932:ALA:HB3	2.19	0.43
1:B:1286:ASN:ND2	1:B:1332:ASP:O	2.52	0.43
1:B:1279:ARG:HG2	1:B:1280:VAL:HG13	2.00	0.43
1:B:168:PHE:CD2	1:B:412:HIS:CE1	3.06	0.43
3:C:2:DA:H2"	3:C:3:DA:C8	2.54	0.43
1:B:1266:LEU:HD23	1:B:1266:LEU:H	1.78	0.43
1:B:914:ALA:HB2	1:B:1036:TYR:HB2	2.01	0.42
1:B:666:LEU:C	1:B:666:LEU:HD23	2.39	0.42
2:A:38:A:C6	2:A:39:G:C5	3.07	0.42
1:B:1351:SER:HB3	1:B:1356:TYR:HB2	2.02	0.42
1:B:239:GLY:O	1:B:243:ALA:N	2.49	0.42
1:B:469:SER:CB	1:B:481:VAL:HG23	2.49	0.42
2:A:6:U:H2'	2:A:7:C:C6	2.55	0.42
1:B:918:LYS:NZ	1:B:1007:GLU:OE2	2.52	0.42
1:B:136:TYR:HE1	1:B:139:ARG:NH2	2.17	0.42
2:A:42:A:C6	2:A:43:G:C6	3.08	0.42
1:B:1065:THR:OG1	1:B:1066:ASN:N	2.52	0.42
1:B:358:GLY:HA2	1:B:375:PHE:CE1	2.55	0.42
1:B:359:TYR:O	1:B:362:TYR:HB3	2.20	0.42
1:B:116:HIS:CE1	1:B:122:ILE:HD13	2.55	0.42
1:B:236:GLY:O	1:B:240:ASN:ND2	2.53	0.42
1:B:1097:LYS:HE3	1:B:1099:GLU:OE2	2.19	0.42
1:B:245:SER:HA	1:B:297:SER:CB	2.50	0.42
1:B:625:LEU:HA	1:B:625:LEU:HD12	1.91	0.42
1:B:944:ASP:OD2	1:B:948:LYS:HB2	2.20	0.42
2:A:42:A:N6	2:A:43:G:C6	2.88	0.42
1:B:82:LEU:HD13	1:B:155:TYR:CE1	2.55	0.42
1:B:1036:TYR:O	1:B:1036:TYR:HD1	2.03	0.41
3:C:19:DA:H5"	3:C:19:DA:H8	1.85	0.41
1:B:1229:PRO:HD3	1:B:1272:GLN:NE2	2.35	0.41
1:B:985:HIS:O	1:B:988:TYR:HB3	2.19	0.41
1:B:1334:LYS:NZ	3:C:3:DA:OP2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1147:ALA:HB2	1:B:1190:VAL:HA	2.02	0.41
1:B:1277:SER:HA	1:B:1281:ILE:HB	2.02	0.41
1:B:1335:ARG:NH1	1:B:1335:ARG:CG	2.81	0.41
1:B:666:LEU:HD21	1:B:693:PHE:HE1	1.83	0.41
1:B:28:PRO:HG2	1:B:47:LEU:HD12	2.02	0.41
1:B:1147:ALA:HB1	1:B:1188:LYS:O	2.20	0.41
3:C:13:DT:H2'	3:C:14:DT:H6	1.85	0.41
2:A:19:A:H2'	2:A:20:A:O4'	2.20	0.41
1:B:1266:LEU:HB2	1:B:1267:ASP:H	1.75	0.41
1:B:873:GLU:HG3	1:B:904:GLU:HA	2.02	0.41
1:B:1177:ASN:ND2	1:B:1180:ASP:OD2	2.53	0.41
1:B:624:THR:HA	1:B:656:TYR:O	2.20	0.41
1:B:1170:GLU:O	1:B:1173:SER:HB3	2.21	0.41
1:B:62:THR:HG22	2:A:63:U:O2'	2.21	0.41
1:B:464:TRP:CD1	1:B:464:TRP:C	2.94	0.41
1:B:553:PHE:CD2	1:B:559:VAL:HG21	2.56	0.41
1:B:325:TYR:CD1	2:A:44:U:C2	3.08	0.41
1:B:437:ARG:O	1:B:441:GLU:HG3	2.20	0.41
1:B:501:ASN:HD22	1:B:666:LEU:HD11	1.85	0.41
1:B:498:PHE:HB3	1:B:505:GLU:O	2.21	0.41
1:B:508:LEU:HD21	1:B:664:ARG:HB2	2.02	0.41
1:B:996:ALA:O	1:B:999:LYS:N	2.53	0.41
1:B:111:LYS:NZ	2:A:25:U:O2'	2.27	0.40
1:B:1210:ARG:HG3	1:B:1280:VAL:HA	2.03	0.40
1:B:403:ARG:HH11	2:A:20:A:P	2.45	0.40
1:B:419:LEU:HD13	1:B:444:LEU:CD1	2.51	0.40
1:B:692:ASN:ND2	3:C:26:DT:H2''	2.32	0.40
1:B:459:ASN:ND2	2:A:56:U:H1'	2.37	0.40
1:B:1303:ARG:HD2	1:B:1307:GLU:OE2	2.21	0.40
1:B:17:GLY:HA3	1:B:983:HIS:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1292/1368 (94%)	1144 (88%)	126 (10%)	22 (2%)	9	37

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	LEU
1	B	607	LEU
1	B	114	GLU
1	B	696	LEU
1	B	906	GLY
1	B	908	LEU
1	B	992	VAL
1	B	30	LYS
1	B	204	SER
1	B	205	GLY
1	B	576	ASP
1	B	695	GLN
1	B	1076	LYS
1	B	1266	LEU
1	B	87	SER
1	B	464	TRP
1	B	574	GLU
1	B	1267	ASP
1	B	1301	PRO
1	B	1270	ILE
1	B	592	GLY
1	B	670	ILE

### 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	B	969/1226 (79%)	891 (92%)	78 (8%)	12	39



All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	SER
1	B	62	THR
1	B	82	LEU
1	B	106	LEU
1	B	110	ASP
1	B	112	LYS
1	B	122	ILE
1	B	130	GLU
1	B	134	THR
1	B	165	ARG
1	B	174	LEU
1	B	199	ASN
1	B	202	ASN
1	B	207	ASP
1	B	213	SER
1	B	216	LEU
1	B	224	ASN
1	B	233	LYS
1	B	244	LEU
1	B	266	LEU
1	B	273	ASP
1	B	289	LEU
1	B	297	SER
1	B	375	PHE
1	B	403	ARG
1	B	419	LEU
1	B	425	ARG
1	B	435	ASP
1	B	438	GLU
1	B	455	LEU
1	B	461	ARG
1	B	466	THR
1	B	490	SER
1	B	535	ARG
1	B	567	ASP
1	B	596	ASP
1	B	606	PHE
1	B	627	GLU
1	B	628	ASP
1	B	657	THR
1	B	664	ARG
1	B	671	ARG

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Mol	Chain	Res	Type
1	B	726	ASN
1	B	738	LEU
1	B	745	ASP
1	B	754	HIS
1	B	791	LEU
1	B	794	GLN
1	B	798	GLU
1	B	799	HIS
1	B	801	VAL
1	B	805	GLN
1	B	851	SER
1	B	891	LEU
1	B	892	ILE
1	B	902	LYS
1	B	933	GLN
1	B	960	SER
1	B	1036	TYR
1	B	1040	SER
1	B	1062	LEU
1	B	1080	PHE
1	B	1088	SER
1	B	1154	SER
1	B	1214	LEU
1	B	1226	LEU
1	B	1253	GLU
1	B	1264	HIS
1	B	1272	GLN
1	B	1274	SER
1	B	1299	ASP
1	B	1312	LEU
1	B	1314	THR
1	B	1334	LYS
1	B	1335	ARG
1	B	1347	LEU
1	B	1358	THR
1	B	1365	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	178	ASN

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Mol	Chain	Res	Type
1	B	342	GLN
1	B	413	GLN
1	B	415	HIS
1	B	459	ASN
1	B	501	ASN
1	B	504	ASN
1	B	511	HIS
1	B	692	ASN
1	B	805	GLN
1	B	863	ASN
1	B	888	ASN
1	B	1041	ASN
1	B	1364	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	79/83 (95%)	19 (24%)	4 (5%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	A
2	A	10	U
2	A	24	U
2	A	26	A
2	A	28	A
2	A	29	G
2	A	32	A
2	A	35	A
2	A	39	G
2	A	42	A
2	A	43	G
2	A	44	U
2	A	45	U
2	A	51	A
2	A	59	U
2	A	63	U
2	A	68	A
2	A	74	A
2	A	81	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	8	A
2	A	9	A
2	A	28	A
2	A	42	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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	1308/1368 (95%)	0.13	82 (6%) 20 6	25, 82, 155, 229	0
2	A	80/83 (96%)	-0.07	1 (1%) 77 51	26, 43, 122, 147	0
3	C	27/28 (96%)	0.08	1 (3%) 41 17	40, 71, 145, 186	0
4	D	11/12 (91%)	0.94	2 (18%) 1 0	63, 85, 159, 164	0
All	All	1426/1491 (95%)	0.12	86 (6%) 21 7	25, 78, 155, 229	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	ARG	13.7
1	B	214	ALA	10.8
1	B	225	LEU	10.6
1	B	216	LEU	10.0
1	B	224	ASN	8.4
1	B	226	ILE	7.6
1	B	229	LEU	6.2
1	B	213	SER	5.5
1	B	385	GLY	5.4
1	B	688	PHE	5.4
1	B	946	ASN	4.5
1	B	687	GLY	4.2
1	B	1030	GLY	4.2
1	B	867	SER	4.2
1	B	238	PHE	4.2
1	B	800	PRO	4.2
1	B	534	MET	4.1
1	B	586	ARG	4.0
1	B	893	THR	3.9
1	B	212	LEU	3.9
1	B	530	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	881	ASN	3.7
1	B	206	VAL	3.6
1	B	198	GLU	3.6
4	D	3	DA	3.5
1	B	685	SER	3.5
1	B	559	VAL	3.5
1	B	1003	LYS	3.4
4	D	2	DA	3.4
1	B	560	THR	3.4
1	B	872	SER	3.2
1	B	236	GLY	3.2
1	B	223	GLU	3.2
1	B	205	GLY	3.1
1	B	799	HIS	3.1
1	B	260	GLU	3.0
1	B	1305	GLN	3.0
1	B	529	TYR	3.0
1	B	667	ILE	2.9
1	B	1034	ALA	2.9
1	B	1051	THR	2.9
1	B	227	ALA	2.9
1	B	287	ALA	2.8
1	B	524	LEU	2.8
1	B	689	ALA	2.8
1	B	821	ASP	2.8
1	B	539	PHE	2.8
1	B	1049	GLU	2.8
1	B	894	GLN	2.7
1	B	558	LYS	2.7
1	B	1037	PHE	2.6
1	B	222	LEU	2.6
1	B	543	ASP	2.6
1	B	203	ALA	2.5
1	B	583	VAL	2.5
1	B	895	ARG	2.5
1	B	221	ARG	2.5
1	B	814	TYR	2.4
1	B	234	LYS	2.4
1	B	921	LEU	2.4
1	B	838	VAL	2.4
1	B	1326	TYR	2.3
1	B	538	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	885	GLN	2.3
1	B	1011	GLY	2.3
1	B	207	ASP	2.3
1	B	350	ILE	2.3
3	C	23	DA	2.3
1	B	210	ALA	2.2
1	B	913	LYS	2.2
1	B	1290	VAL	2.2
1	B	802	GLU	2.2
1	B	877	LYS	2.2
2	A	3	A	2.2
1	B	791	LEU	2.1
1	B	259	ALA	2.1
1	B	199	ASN	2.1
1	B	888	ASN	2.1
1	B	789	LYS	2.1
1	B	557	ARG	2.1
1	B	829	ASP	2.1
1	B	533	GLY	2.1
1	B	574	GLU	2.0
1	B	943	TYR	2.0
1	B	243	ALA	2.0
1	B	283	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.