Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 09:53 PM JST

PDB ID	:	6AEG
Title	:	Crystal structure of xCas9 in complex with sgRNA and target DNA (GAT PAM)
Authors	:	Guo, M.; Ren, K.; Zhu, Y.; Huang, Z.
Deposited on	:	2018-08-04
Resolution	:	2.70 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:

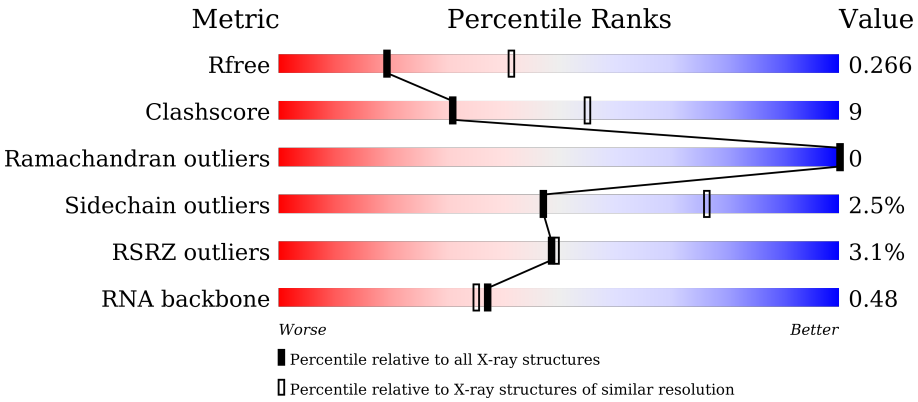
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

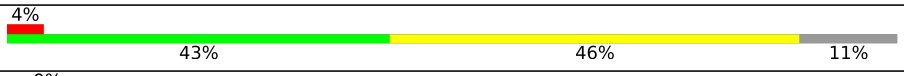
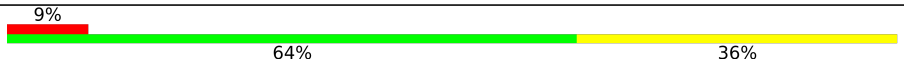
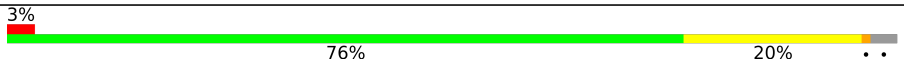
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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	100	
2	C	28	
3	D	11	
4	B	1368	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13362 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 RNA chain called RNA (95-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	95	2032	911	372	654	95	0	0	0

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	25	507	247	86	150	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	11	226	110	43	63	10	0	0	0

- Molecule 4 is a protein called DNA nuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	1322	10475	6690	1817	1947	21	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	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	694	ILE	MET	engineered mutation	UNP Q99ZW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1219	VAL	GLU	engineered mutation	UNP Q99ZW2

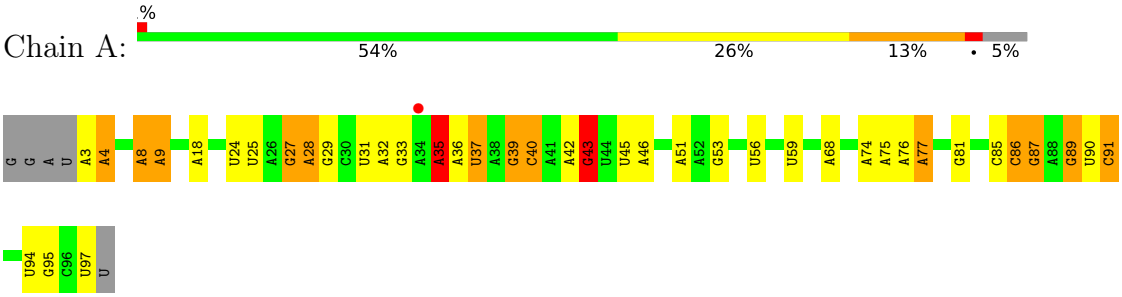
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0
5	C	10	Total O 10 10	0	0
5	D	6	Total O 6 6	0	0
5	B	80	Total O 80 80	0	0

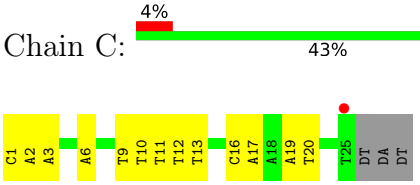
3 Residue-property plots (i)

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.

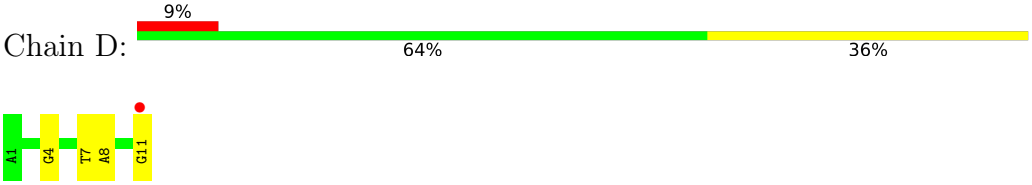
• Molecule 1: RNA (95-MER)



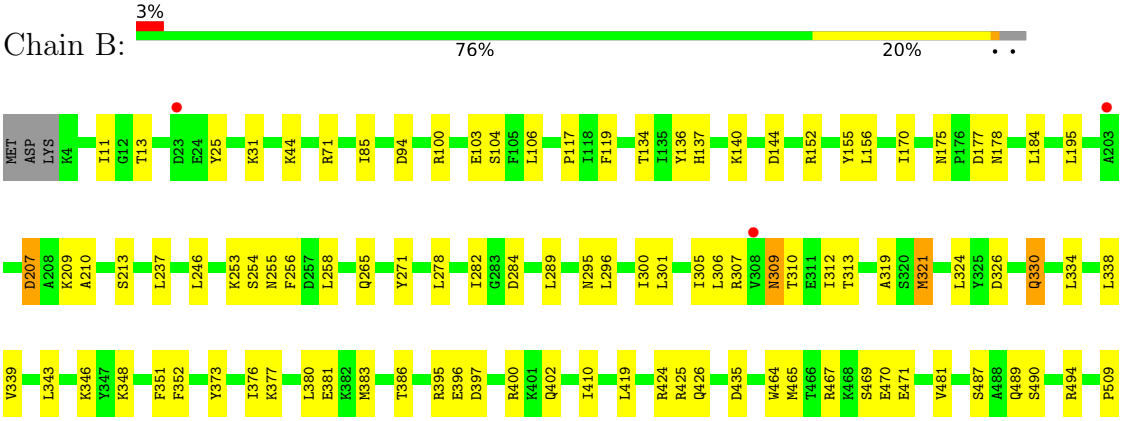
• Molecule 2: DNA (25-MER)

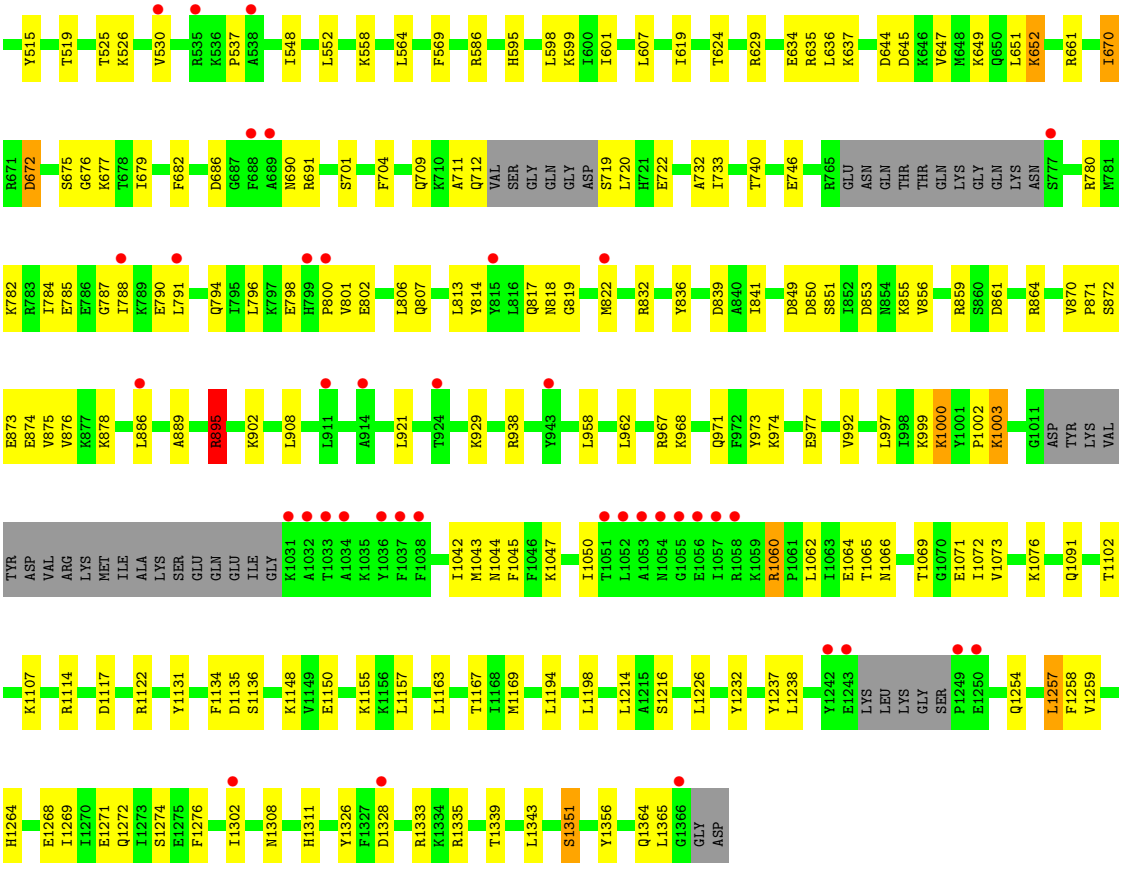


• Molecule 3: DNA (5'-D(*AP*AP*AP*GP*AP*TP*TP*AP*TP*TP*G)-3')



• Molecule 4: DNA nuclease




Y515 T519 T525 K526 V530 R535 K536 P537 A538 I548 L552 K558 L564 F569 R586 H595 L598 K599 I600 I601 L607 I619 T624 R629 E634 R635 L636 K637 D644 D645 K646 V647 M648 K649 Q650 L651 K652 R661 I670
R671 D672 S675 G676 K677 T678 I679 F682 D686 G687 F688 A689 N690 R691 S701 F704 Q709 K710 A711 Q712 VAL SER GLY GLN GLY ASP S719 L720 H721 E722 A732 I733 T740 E746 R765 GLU ASN GLN THR THR GLN LYS GLY GLN LYS ASN S777 R780 M781
K782 R783 I784 E785 E786 G787 I788 K789 E790 L791 Q794 I795 L796 K797 E798 H799 P800 V801 E802 L806 Q807 L813 Y814 Y815 L816 Q817 N818 G819 M822 R832 Y836 D839 A840 I841 D849 D850 S851 I852 D853 N854 K855 V856 R859 S860 D861 R864 V870 P871 S872
E873 E874 V875 V876 K877 K878 L886 A889 R895 K902 L908 L911 A914 L921 T924 K929 R938 Y943 L958 L962 R967 K968 Q971 F972 Y973 K974 E977 V992 L997 I998 K999 K1000 Y1001 P1002 K1003 G1011 ASP TYR LYS VAL
TYR ASP VAL ARG LYS MET ILE ALA LYS SER GLU GLN GLU ILE GLY K1031 A1032 T1033 A1034 K1035 Y1036 F1037 F1038 I1042 M1043 N1044 F1045 F1046 K1047 I1050 T1051 L1052 A1053 N1054 G1055 E1056 I1057 R1058 K1059 R1060 P1061 L1062 I1063 E1064 T1065 N1066 T1069 G1070 E1071 I1072 V1073 K1076 Q1091 T1102
K1107 R1114 D1117 R1122 Y1131 F1134 D1135 S1136 K1148 V1149 E1150 K1155 K1156 L1157 L1163 T1167 I1168 M1169 L1194 L1198 L1214 A1215 S1216 L1226 Y1232 Y1237 L1238 Y1242 E1243 LYS LEU LYS GLY SER P1249 E1250 Q1254 L1257 F1258 V1259
H1264 E1268 I1269 I1270 E1271 Q1272 I1273 S1274 E1275 F1276 I1302 N1308 H1311 Y1326 F1327 D1328 R1333 K1334 R1335 T1339 L1343 S1351 Y1356 Q1364 L1365 G1366 GLY ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.48Å 70.46Å 183.53Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	44.97 – 2.70 47.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	74.8 (44.97-2.70) 83.5 (47.11-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.215 , 0.263 0.217 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13362	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.40	0/2277	0.87	2/3546 (0.1%)
2	C	0.85	1/567 (0.2%)	1.13	2/873 (0.2%)
3	D	0.76	0/254	0.97	0/391
4	B	0.40	1/10664 (0.0%)	0.53	4/14393 (0.0%)
All	All	0.44	2/13762 (0.0%)	0.66	8/19203 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	DA	O3'-P	-6.33	1.53	1.61
4	B	672	ASP	CB-CG	-5.35	1.40	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	672	ASP	N-CA-C	-7.17	91.63	111.00
4	B	1257	LEU	CA-CB-CG	6.66	130.63	115.30
2	C	12	DT	O4'-C4'-C3'	-6.51	101.90	104.50
1	A	35	A	C8-N9-C4	-6.06	103.38	105.80
1	A	43	G	C4-C5-C6	5.83	122.30	118.80
2	C	13	DT	O4'-C4'-C3'	-5.78	102.19	104.50
4	B	312	ILE	N-CA-C	5.18	124.98	111.00
4	B	895	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2032	0	1021	26	1
2	C	507	0	288	9	0
3	D	226	0	127	4	0
4	B	10475	0	10378	200	1
5	A	26	0	0	3	0
5	B	80	0	0	5	0
5	C	10	0	0	1	0
5	D	6	0	0	1	0
All	All	13362	0	11814	227	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 9.

All (227) 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)
4:B:1308:ASN:OD1	4:B:1326:TYR:O	1.54	1.19
4:B:530:VAL:HG22	4:B:537:PRO:HA	1.32	1.10
4:B:870:VAL:HG22	4:B:871:PRO:HD2	1.41	0.99
4:B:1069:THR:HG22	4:B:1071:GLU:H	1.40	0.86
4:B:958:LEU:HD22	4:B:962:LEU:HD13	1.55	0.86
4:B:870:VAL:CG2	4:B:871:PRO:HD2	2.04	0.86
4:B:134:THR:HG22	4:B:137:HIS:ND1	1.98	0.79
4:B:256:PHE:HB2	4:B:258:LEU:HD11	1.67	0.75
4:B:746:GLU:OE1	4:B:1351:SER:OG	2.04	0.75
4:B:1050:ILE:HD11	4:B:1060:ARG:HD2	1.69	0.74
3:D:8:DA:OP1	4:B:1114:ARG:NH1	2.20	0.74
4:B:1254:GLN:HA	4:B:1257:LEU:HD23	1.69	0.74
4:B:395:ARG:NH1	4:B:397:ASP:OD2	2.21	0.73
4:B:817:GLN:OE1	4:B:822:MET:HG2	1.87	0.73
4:B:469:SER:HB3	4:B:481:VAL:HG13	1.71	0.73
1:A:46:A:N7	5:A:103:HOH:O	2.22	0.72
4:B:140:LYS:NZ	4:B:144:ASP:OD2	2.24	0.71
4:B:813:LEU:O	4:B:817:GLN:HG2	1.92	0.70
4:B:530:VAL:HG22	4:B:537:PRO:CA	2.17	0.69
4:B:1107:LYS:HG3	4:B:1136:SER:HB2	1.72	0.69
4:B:870:VAL:HG22	4:B:871:PRO:CD	2.21	0.69
4:B:849:ASP:OD2	4:B:895:ARG:NH2	2.26	0.68
4:B:321:MET:CE	4:B:402:GLN:HA	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:548:ILE:HG23	4:B:552:LEU:HD12	1.76	0.68
4:B:1272:GLN:O	5:B:1401:HOH:O	2.12	0.67
4:B:1042:ILE:HG23	4:B:1043:MET:HG2	1.77	0.67
4:B:921:LEU:HD11	4:B:1042:ILE:HG21	1.76	0.66
4:B:1308:ASN:CG	4:B:1326:TYR:O	2.32	0.66
4:B:796:LEU:HD12	4:B:800:PRO:HA	1.78	0.66
4:B:209:LYS:O	4:B:213:SER:OG	2.10	0.65
4:B:682:PHE:HE1	4:B:691:ARG:HH21	1.44	0.65
4:B:140:LYS:HD3	4:B:319:ALA:HB2	1.77	0.65
4:B:672:ASP:O	4:B:676:GLY:N	2.29	0.65
4:B:1102:THR:O	5:B:1402:HOH:O	2.15	0.64
1:A:27:G:H5'	1:A:28:A:H5"	1.79	0.64
3:D:4:DG:H5"	5:D:102:HOH:O	1.98	0.64
4:B:870:VAL:CG2	4:B:871:PRO:CD	2.76	0.64
4:B:1237:TYR:HD1	4:B:1238:LEU:HD23	1.63	0.63
4:B:134:THR:HG23	4:B:136:TYR:H	1.65	0.62
4:B:464:TRP:HB3	4:B:494:ARG:HD3	1.81	0.62
4:B:780:ARG:NH1	4:B:806:LEU:O	2.31	0.62
1:A:89:G:O6	4:B:1272:GLN:NE2	2.31	0.62
4:B:999:LYS:HB3	4:B:1073:VAL:HG22	1.81	0.62
1:A:27:G:H5'	1:A:28:A:C5'	2.30	0.61
1:A:77:A:N7	5:A:106:HOH:O	2.31	0.61
4:B:509:PRO:HB3	4:B:624:THR:HG21	1.80	0.61
1:A:53:G:OP2	5:A:102:HOH:O	2.16	0.61
4:B:237:LEU:HA	4:B:255:ASN:OD1	2.00	0.61
4:B:1066:ASN:HB3	4:B:1069:THR:HB	1.82	0.60
4:B:465:MET:HA	4:B:487:SER:HB3	1.82	0.60
4:B:1000:LYS:NZ	4:B:1064:GLU:OE1	2.33	0.60
4:B:307:ARG:NH1	4:B:397:ASP:OD1	2.33	0.60
4:B:170:ILE:HD13	4:B:301:LEU:HD11	1.84	0.60
4:B:119:PHE:HA	4:B:152:ARG:HH11	1.65	0.60
4:B:1150:GLU:OE1	4:B:1155:LYS:HE3	2.01	0.60
1:A:33:G:N2	1:A:36:A:OP2	2.31	0.60
4:B:85:ILE:O	5:B:1403:HOH:O	2.16	0.59
4:B:670:ILE:HD12	4:B:704:PHE:CE1	2.36	0.59
4:B:1150:GLU:CD	4:B:1155:LYS:HE3	2.23	0.59
4:B:380:LEU:O	4:B:386:THR:HG21	2.03	0.58
4:B:672:ASP:O	4:B:676:GLY:HA2	2.03	0.58
4:B:874:GLU:O	4:B:878:LYS:HG3	2.03	0.58
4:B:1163:LEU:HD13	4:B:1343:LEU:HD21	1.85	0.57
4:B:644:ASP:OD1	4:B:645:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:253:LYS:HG3	4:B:254:SER:N	2.20	0.57
4:B:343:LEU:HD13	4:B:346:LYS:HD2	1.86	0.57
4:B:207:ASP:HB3	4:B:210:ALA:HB3	1.87	0.57
1:A:94:U:H2'	1:A:95:G:C8	2.40	0.56
4:B:321:MET:HE2	4:B:402:GLN:HA	1.86	0.56
4:B:1167:THR:HG22	4:B:1169:MET:H	1.70	0.56
4:B:701:SER:OG	5:B:1404:HOH:O	2.18	0.55
4:B:958:LEU:HD22	4:B:962:LEU:CD1	2.31	0.55
4:B:1047:LYS:O	4:B:1076:LYS:NZ	2.40	0.55
1:A:3:A:H2'	1:A:4:A:H8	1.71	0.55
1:A:45:U:H4'	4:B:134:THR:OG1	2.07	0.55
4:B:321:MET:HE2	4:B:402:GLN:HG3	1.89	0.54
4:B:103:GLU:HG2	4:B:103:GLU:O	2.06	0.54
4:B:672:ASP:O	4:B:676:GLY:CA	2.56	0.54
4:B:1257:LEU:HD12	4:B:1258:PHE:CA	2.38	0.54
4:B:818:ASN:O	4:B:818:ASN:ND2	2.41	0.54
1:A:86:C:H5'	1:A:87:G:OP2	2.07	0.54
4:B:686:ASP:OD2	4:B:691:ARG:HG3	2.08	0.53
4:B:796:LEU:CD1	4:B:800:PRO:HA	2.37	0.53
4:B:780:ARG:NH1	4:B:807:GLN:HA	2.24	0.53
4:B:784:ILE:O	4:B:788:ILE:HG12	2.09	0.53
1:A:91:C:H5"	4:B:1091:GLN:HG3	1.90	0.52
4:B:134:THR:HG23	4:B:136:TYR:N	2.24	0.52
4:B:426:GLN:NE2	5:B:1416:HOH:O	2.42	0.52
4:B:1271:GLU:HA	4:B:1274:SER:HB3	1.90	0.52
1:A:94:U:H2'	1:A:95:G:H8	1.73	0.52
1:A:94:U:O4	4:B:31:LYS:NZ	2.43	0.52
4:B:321:MET:HE3	4:B:324:LEU:HD12	1.90	0.52
4:B:1117:ASP:OD1	4:B:1117:ASP:N	2.43	0.52
4:B:1122:ARG:HG2	4:B:1134:PHE:CE2	2.45	0.51
4:B:348:LYS:O	4:B:352:PHE:HB2	2.10	0.51
4:B:106:LEU:HA	4:B:1131:TYR:HE1	1.76	0.51
4:B:1044:ASN:HA	4:B:1047:LYS:HD2	1.92	0.51
2:C:9:DT:OP1	5:C:101:HOH:O	2.19	0.51
4:B:872:SER:OG	4:B:875:VAL:HG23	2.11	0.51
4:B:1148:LYS:HB3	4:B:1157:LEU:HB3	1.92	0.51
4:B:1065:THR:HG23	4:B:1072:ILE:HA	1.92	0.51
4:B:321:MET:HE1	4:B:402:GLN:HA	1.93	0.51
4:B:326:ASP:O	4:B:330:GLN:HG3	2.11	0.51
4:B:1232:TYR:HB3	4:B:1269:ILE:HD11	1.93	0.51
2:C:16:DC:H2'	2:C:17:DA:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:11:ILE:HD11	4:B:740:THR:HG21	1.93	0.50
4:B:619:ILE:HD13	4:B:651:LEU:HD21	1.92	0.50
1:A:33:G:O2'	1:A:35:A:N6	2.30	0.50
1:A:75:A:H2'	1:A:76:A:C8	2.45	0.50
4:B:309:ASN:ND2	4:B:309:ASN:H	2.10	0.50
4:B:1237:TYR:CD1	4:B:1238:LEU:HD23	2.45	0.50
4:B:321:MET:CE	4:B:324:LEU:HD12	2.42	0.50
4:B:558:LYS:HE2	4:B:586:ARG:NH2	2.27	0.50
4:B:902:LYS:NZ	4:B:908:LEU:HD23	2.27	0.50
4:B:1163:LEU:HD11	4:B:1198:LEU:HD12	1.94	0.50
4:B:790:GLU:CD	4:B:889:ALA:HA	2.32	0.49
4:B:1045:PHE:HA	4:B:1060:ARG:HD3	1.94	0.49
4:B:719:SER:OG	4:B:720:LEU:N	2.45	0.49
4:B:822:MET:HG3	4:B:856:VAL:CG1	2.42	0.49
2:C:1:DC:N3	3:D:11:DG:N2	2.48	0.49
2:C:16:DC:H2'	2:C:17:DA:C8	2.47	0.49
4:B:515:TYR:O	4:B:519:THR:HG23	2.13	0.49
4:B:850:ASP:O	4:B:855:LYS:NZ	2.44	0.49
4:B:1003:LYS:H	4:B:1003:LYS:HD2	1.78	0.49
4:B:902:LYS:HZ3	4:B:908:LEU:HD23	1.78	0.48
4:B:677:LYS:HG3	4:B:682:PHE:CE2	2.48	0.48
4:B:175:ASN:HB3	4:B:178:ASN:ND2	2.28	0.48
4:B:195:LEU:HD12	4:B:289:LEU:HD22	1.95	0.48
3:D:7:DT:H5"	4:B:1135:ASP:OD1	2.14	0.48
4:B:155:TYR:HD2	4:B:156:LEU:HD23	1.79	0.48
4:B:839:ASP:OD2	4:B:864:ARG:NE	2.40	0.48
4:B:1259:VAL:HG12	4:B:1302:ILE:HD13	1.96	0.48
1:A:4:A:OP1	4:B:661:ARG:NH2	2.47	0.48
4:B:601:ILE:HD11	4:B:607:LEU:HD11	1.96	0.48
4:B:782:LYS:HA	4:B:785:GLU:HB2	1.95	0.48
4:B:246:LEU:HD23	4:B:300:ILE:HG21	1.96	0.48
4:B:968:LYS:HA	4:B:973:TYR:CE1	2.49	0.48
4:B:489:GLN:OE1	4:B:635:ARG:NH2	2.47	0.47
4:B:558:LYS:HE2	4:B:586:ARG:HH21	1.79	0.47
4:B:634:GLU:HA	4:B:637:LYS:HD2	1.95	0.47
4:B:921:LEU:CD1	4:B:1042:ILE:HG21	2.42	0.47
4:B:469:SER:OG	4:B:470:GLU:N	2.47	0.47
1:A:43:G:O6	4:B:351:PHE:HB3	2.14	0.47
4:B:1050:ILE:CD1	4:B:1060:ARG:HD2	2.43	0.47
1:A:25:U:H1'	4:B:104:SER:O	2.14	0.46
4:B:305:ILE:HG22	4:B:306:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:305:ILE:HG23	4:B:410:ILE:HD13	1.98	0.46
4:B:709:GLN:C	4:B:711:ALA:H	2.19	0.46
1:A:18:A:H62	4:B:71:ARG:NH2	2.13	0.46
4:B:530:VAL:CG2	4:B:537:PRO:HA	2.24	0.46
4:B:558:LYS:HE2	4:B:586:ARG:HD2	1.98	0.46
4:B:801:VAL:HG22	4:B:802:GLU:H	1.79	0.46
1:A:39:G:H5'	1:A:40:C:OP2	2.16	0.46
4:B:967:ARG:NH2	4:B:974:LYS:HB2	2.30	0.46
4:B:373:TYR:HA	4:B:376:ILE:HG22	1.98	0.46
2:C:10:DT:H2'	2:C:11:DT:H71	1.96	0.45
2:C:19:DA:H2"	2:C:20:DT:O4'	2.15	0.45
4:B:564:LEU:O	4:B:569:PHE:HD2	1.99	0.45
4:B:711:ALA:HA	4:B:712:GLN:HA	1.67	0.45
4:B:471:GLU:H	4:B:471:GLU:HG2	1.63	0.45
4:B:784:ILE:HG23	4:B:788:ILE:HD11	1.98	0.45
4:B:644:ASP:HB3	4:B:647:VAL:HG23	1.99	0.45
4:B:1214:LEU:HD22	4:B:1216:SER:O	2.17	0.45
2:C:19:DA:H2"	2:C:20:DT:C5'	2.47	0.45
4:B:278:LEU:O	4:B:282:ILE:HG12	2.17	0.45
4:B:1163:LEU:HD22	4:B:1339:THR:HG21	1.99	0.45
4:B:1232:TYR:OH	4:B:1268:GLU:OE1	2.29	0.45
1:A:8:A:H2'	1:A:9:A:C8	2.51	0.45
1:A:81:G:N1	4:B:1356:TYR:HB3	2.32	0.45
4:B:31:LYS:HE3	4:B:44:LYS:NZ	2.33	0.44
4:B:490:SER:O	4:B:494:ARG:HG3	2.17	0.44
4:B:25:TYR:CD1	4:B:992:VAL:HG13	2.53	0.44
4:B:119:PHE:HA	4:B:152:ARG:NH1	2.33	0.44
4:B:1257:LEU:HD12	4:B:1258:PHE:HA	2.00	0.44
4:B:733:ILE:HD12	4:B:733:ILE:HA	1.85	0.44
4:B:1339:THR:HG22	4:B:1339:THR:O	2.18	0.44
4:B:636:LEU:HD13	4:B:651:LEU:HD23	1.99	0.44
4:B:525:THR:O	4:B:690:ASN:ND2	2.35	0.44
4:B:1194:LEU:HD22	4:B:1365:LEU:HD13	1.99	0.43
1:A:36:A:C5	1:A:37:U:H1'	2.53	0.43
4:B:1254:GLN:HA	4:B:1257:LEU:CD2	2.45	0.43
1:A:90:U:H4'	1:A:91:C:O4'	2.17	0.43
4:B:184:LEU:HD22	4:B:295:ASN:HB3	2.00	0.43
4:B:144:ASP:O	4:B:425:ARG:NH2	2.51	0.43
4:B:13:THR:HG23	4:B:732:ALA:HB1	1.99	0.43
4:B:1257:LEU:HD12	4:B:1258:PHE:N	2.33	0.43
4:B:377:LYS:NZ	4:B:381:GLU:OE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:A:O2'	1:A:4:A:H5'	2.18	0.43
2:C:2:DA:H2"	2:C:3:DA:O5'	2.17	0.43
4:B:558:LYS:CE	4:B:586:ARG:HD2	2.49	0.43
4:B:321:MET:SD	4:B:402:GLN:HB3	2.58	0.42
4:B:841:ILE:O	4:B:864:ARG:NH2	2.52	0.42
4:B:246:LEU:HD23	4:B:300:ILE:HD13	2.01	0.42
4:B:794:GLN:O	4:B:798:GLU:HG3	2.18	0.42
4:B:296:LEU:HA	4:B:296:LEU:HD12	1.84	0.42
4:B:675:SER:OG	4:B:677:LYS:HG2	2.20	0.42
4:B:679:ILE:HG13	4:B:704:PHE:CZ	2.55	0.42
4:B:814:TYR:O	4:B:819:GLY:N	2.45	0.42
4:B:977:GLU:OE2	4:B:977:GLU:N	2.38	0.42
4:B:334:LEU:O	4:B:338:LEU:HB2	2.19	0.42
4:B:1264:HIS:H	4:B:1264:HIS:CD2	2.37	0.42
4:B:100:ARG:NH1	4:B:117:PRO:O	2.50	0.42
4:B:787:GLY:O	4:B:791:LEU:HD12	2.20	0.42
4:B:971:GLN:HA	4:B:973:TYR:CE2	2.54	0.42
4:B:719:SER:HB3	4:B:722:GLU:HB2	2.01	0.42
4:B:265:GLN:O	4:B:271:TYR:HB2	2.20	0.41
4:B:396:GLU:O	4:B:400:ARG:HD3	2.20	0.41
4:B:836:TYR:CD1	4:B:859:ARG:HA	2.55	0.41
4:B:564:LEU:O	4:B:569:PHE:CD2	2.73	0.41
2:C:19:DA:H2"	2:C:20:DT:H5'	2.02	0.41
4:B:94:ASP:CG	4:B:100:ARG:HH22	2.23	0.41
4:B:886:LEU:HD23	4:B:886:LEU:HA	1.83	0.41
4:B:1364:GLN:C	4:B:1365:LEU:HD23	2.41	0.41
4:B:817:GLN:HG2	4:B:817:GLN:H	1.72	0.41
4:B:465:MET:SD	4:B:467:ARG:HG2	2.61	0.41
4:B:526:LYS:HA	4:B:526:LYS:HD2	1.90	0.41
4:B:598:LEU:HB2	4:B:607:LEU:HD22	2.02	0.41
4:B:997:LEU:HA	4:B:997:LEU:HD12	1.85	0.41
4:B:1002:PRO:HD2	4:B:1003:LYS:HZ2	1.86	0.41
4:B:1062:LEU:O	4:B:1076:LYS:HG3	2.21	0.41
4:B:649:LYS:O	4:B:652:LYS:HG2	2.21	0.40
4:B:851:SER:O	4:B:855:LYS:HE2	2.20	0.40
4:B:595:HIS:O	4:B:599:LYS:HG3	2.21	0.40
4:B:872:SER:O	4:B:876:VAL:HG23	2.21	0.40
4:B:1226:LEU:HD13	4:B:1276:PHE:CG	2.56	0.40
4:B:339:VAL:HA	4:B:383:MET:HE1	2.03	0.40
4:B:400:ARG:HE	4:B:400:ARG:HB3	1.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:U:OP1	4:B:424:ARG:NH1[3_445]	2.12	0.08

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	
4	B	1312/1368 (96%)	1226 (93%)	86 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	B	1103/1226 (90%)	1075 (98%)	28 (2%)	47	76

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	177	ASP
4	B	207	ASP
4	B	284	ASP
4	B	309	ASN
4	B	310	THR
4	B	313	THR

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Mol	Chain	Res	Type
4	B	321	MET
4	B	330	GLN
4	B	419	LEU
4	B	435	ASP
4	B	629	ARG
4	B	652	LYS
4	B	670	ILE
4	B	832	ARG
4	B	853	ASP
4	B	861	ASP
4	B	873	GLU
4	B	895	ARG
4	B	929	LYS
4	B	938	ARG
4	B	1000	LYS
4	B	1003	LYS
4	B	1060	ARG
4	B	1311	HIS
4	B	1328	ASP
4	B	1333	ARG
4	B	1335	ARG
4	B	1351	SER

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

Mol	Chain	Res	Type
4	B	309	ASN
4	B	330	GLN
4	B	650	GLN
4	B	668	ASN
4	B	1297	HIS
4	B	1308	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	94/100 (94%)	25 (26%)	4 (4%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	A
1	A	9	A
1	A	24	U
1	A	28	A
1	A	29	G
1	A	31	U
1	A	32	A
1	A	35	A
1	A	37	U
1	A	39	G
1	A	40	C
1	A	42	A
1	A	43	G
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	74	A
1	A	77	A
1	A	85	C
1	A	86	C
1	A	87	G
1	A	89	G
1	A	91	C
1	A	97	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	28	A
1	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	95/100 (95%)	-0.23	1 (1%) 80 82	12, 33, 82, 111	0
2	C	25/28 (89%)	0.17	1 (4%) 38 37	15, 26, 71, 91	0
3	D	11/11 (100%)	0.55	1 (9%) 9 7	22, 36, 78, 83	0
4	B	1322/1368 (96%)	0.14	42 (3%) 47 48	8, 35, 69, 108	0
All	All	1453/1507 (96%)	0.12	45 (3%) 49 49	8, 35, 71, 111	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	1054	ASN	8.2
4	B	1058	ARG	6.4
4	B	1052	LEU	6.1
4	B	1057	ILE	6.0
4	B	1032	ALA	5.5
4	B	1366	GLY	5.3
4	B	535	ARG	5.2
4	B	1053	ALA	4.7
2	C	25	DT	4.6
4	B	1031	LYS	4.5
4	B	23	ASP	4.1
4	B	1033	THR	3.8
4	B	1242	TYR	3.7
4	B	791	LEU	3.5
4	B	1243	GLU	3.5
3	D	11	DG	3.3
4	B	1249	PRO	3.3
4	B	1036	TYR	3.3
4	B	1056	GLU	3.2
4	B	799	HIS	3.2
4	B	914	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
4	B	1034	ALA	3.0
4	B	203	ALA	2.9
4	B	1037	PHE	2.7
4	B	800	PRO	2.7
4	B	777	SER	2.7
4	B	924	THR	2.5
4	B	1038	PHE	2.5
4	B	886	LEU	2.4
4	B	1055	GLY	2.4
4	B	1250	GLU	2.4
4	B	815	TYR	2.3
4	B	1302	ILE	2.3
4	B	689	ALA	2.3
4	B	822	MET	2.2
4	B	943	TYR	2.2
4	B	538	ALA	2.2
4	B	911	LEU	2.1
4	B	1051	THR	2.1
4	B	1328	ASP	2.1
4	B	788	ILE	2.1
1	A	34	A	2.1
4	B	530	VAL	2.1
4	B	688	PHE	2.0
4	B	308	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 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.