Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 06:53 PM JST

PDB ID	:	6M0V
Title	:	Crsytal structure of streptococcus thermophilus Cas9 in complex with the GGAA PAM
Authors	:	Zhang, Y.; Zhang, H.; Xu, X.; Wang, Y.; Chen, W.; Wang, Y.; Wu, Z.; Tang, N.; Wang, Y.; Zhao, S.; Gan, J.; Ji, Q.
Deposited on	:	2020-02-22
Resolution	:	3.00 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:

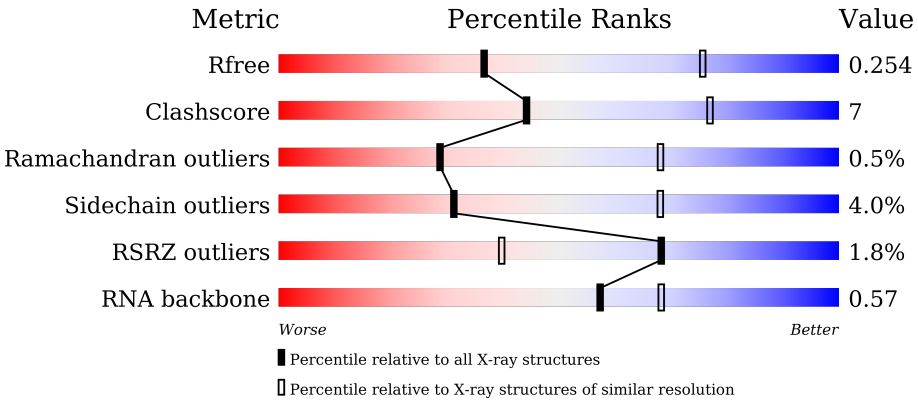
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=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	71	.% 70% 25% •
2	C	28	61% 39%
3	D	8	88% 12%
4	A	1122	2% 74% 16% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BA	C	101	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10482 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 (71-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	71	1500	670	271	488	71	0	0	0

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	28	561	272	91	171	27	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	8	166	79	38	42	7	0	0	0

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas9 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1030	8235	5215	1433	1570	17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q03LF7
A	1	GLY	-	expression tag	UNP Q03LF7
A	599	ALA	HIS	engineered mutation	UNP Q03LF7

- Molecule 5 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total Ba 4 4	0	0
5	C	1	Total Ba 1 1	0	0
5	A	5	Total Ba 5 5	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	6	Total O 6 6	0	0
7	C	1	Total O 1 1	0	0
7	A	2	Total O 2 2	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 (71-MER)

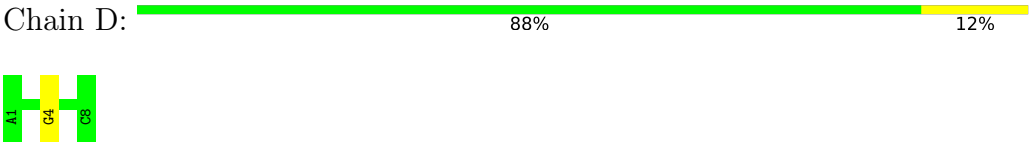
Chain B:

• Molecule 2: DNA (28-MER)

Chain C:

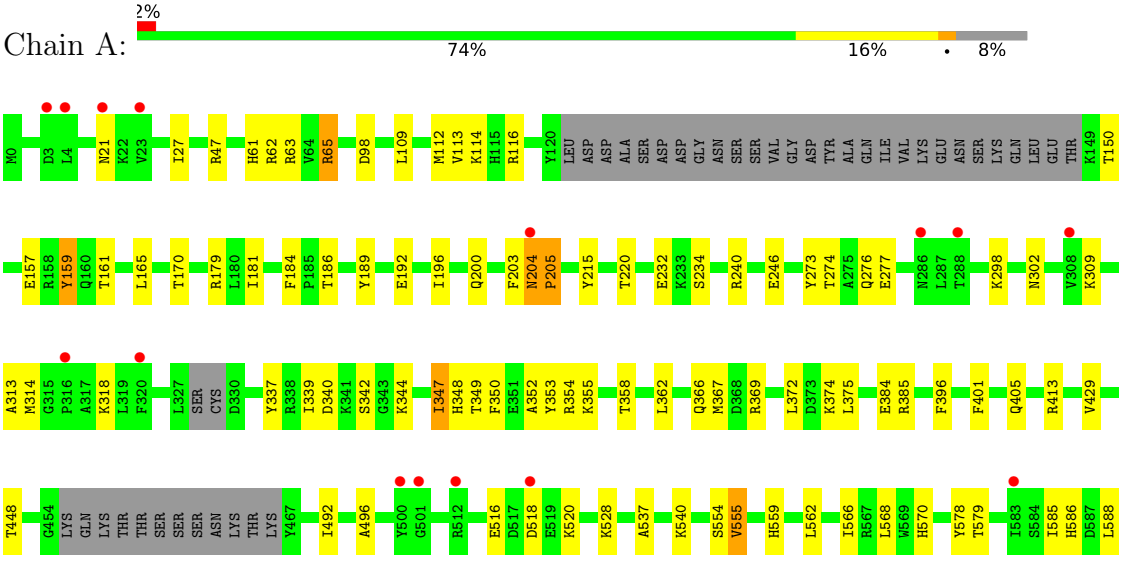
• Molecule 3: DNA (5'-D(*AP*AP*GP*GP*AP*AP*GP*C)-3')

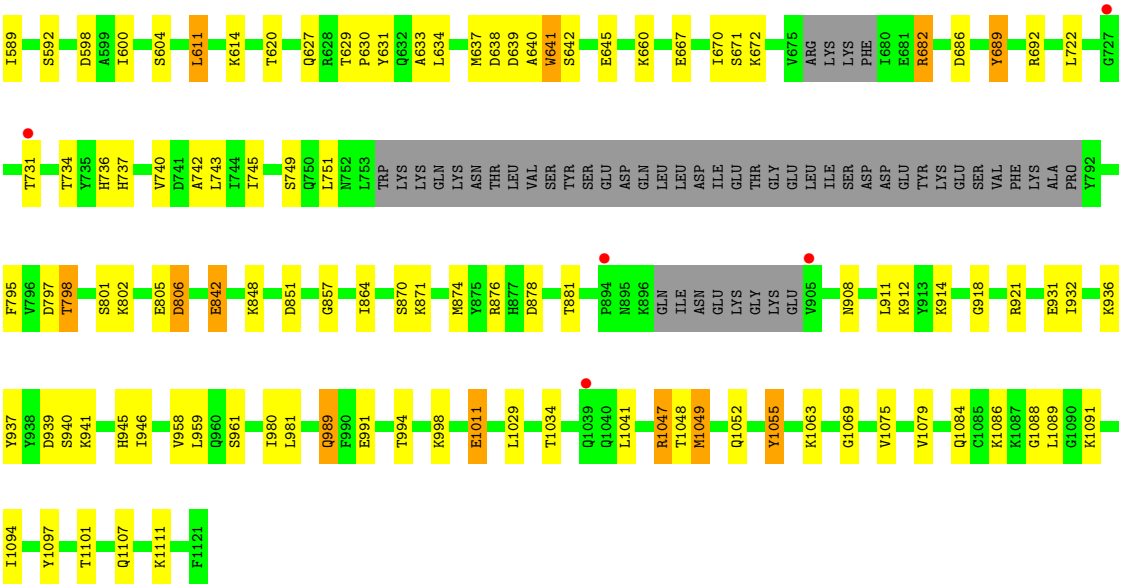
Chain D:



• Molecule 4: CRISPR-associated endonuclease Cas9 1

Chain A:




I589 S592 D598 A599 I600 S604 L611 K614 T620 Q627 R628 T629 P630 Y631 Q632 A633 L634 M637 D638 D639 A640 W641 S642 E645 K660 E667 I670 S671 K672 V675 ARG LYS LYS PHE I680 E681 R682 D686 Y689 R692 L722 G727
T731 T734 Y735 H736 H737 V740 D741 A742 L743 I744 I745 S749 Q750 L751 N752 L753 TRP LYS LYS GLN LYS ASN THR LEU VAL SER TYR SER GLU ASP GLN LEU LEU ASP ILE GLU THR GLY GLU LEU ILE SER ASP ASP GLU TYR LYS GLU SER VAL PHE LYS ALA PRO Y792
F795 V796 D797 T798 S801 K802 E805 D806 E842 K848 D851 G857 I864 S870 K871 M874 Y875 R876 H877 D878 T881 P894 N895 K896 GLN ILE ASN GLU LYS GLY LYS GLU V905 N908 L911 K912 Y913 K914 G918 R921 E931 I932 K936
Y937 Y938 D939 S940 K941 H945 I946 V958 L959 Q960 S961 I980 L981 Q989 F990 E991 T994 K998 E1011 L1029 T1034 Q1039 Q1040 L1041 R1047 T1048 M1049 Q1052 Y1055 K1063 G1069 V1075 V1079 Q1084 C1085 K1086 K1087 G1088 L1089 G1090 K1091
I1094 Y1097 T1101 Q1107 K1111 F1121

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	321.84Å 75.08Å 70.11Å 90.00° 93.21° 90.00°	Depositor
Resolution (Å)	48.82 – 3.00 48.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.82-3.00) 93.2 (48.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.213 , 0.257 0.214 , 0.254	Depositor DCC
R_{free} test set	1592 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10482	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BA, MG

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	0.36	1/1679 (0.1%)	0.82	0/2615
2	C	0.64	0/625	1.07	0/961
3	D	1.05	0/188	0.95	0/289
4	A	0.44	0/8378	0.51	0/11282
All	All	0.46	1/10870 (0.0%)	0.63	0/15147

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	U	O3'-P	-5.14	1.54	1.61

There are no bond angle outliers.

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	B	1500	0	751	11	0
2	C	561	0	321	10	0
3	D	166	0	90	1	0
4	A	8235	0	8116	118	0
5	A	5	0	0	0	0
5	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	A	1	0	0	0	0
7	A	2	0	0	0	0
7	B	6	0	0	0	0
7	C	1	0	0	0	0
All	All	10482	0	9278	129	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 7.

All (129) 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:A:314:MET:HG3	4:A:349:THR:HG23	1.58	0.85
4:A:937:TYR:HE1	4:A:939:ASP:HB2	1.39	0.85
4:A:937:TYR:CE1	4:A:939:ASP:HB2	2.13	0.84
4:A:159:TYR:HB2	4:A:165:LEU:HD21	1.63	0.80
4:A:27:ILE:HD13	4:A:743:LEU:HD13	1.60	0.80
4:A:722:LEU:HD23	4:A:722:LEU:O	1.84	0.77
4:A:347:ILE:HG13	4:A:348:HIS:H	1.52	0.73
4:A:981:LEU:HA	4:A:1011:GLU:HG2	1.72	0.72
4:A:347:ILE:HG13	4:A:348:HIS:N	2.05	0.71
4:A:314:MET:CG	4:A:349:THR:HG23	2.22	0.69
4:A:870:SER:O	4:A:876:ARG:NH2	2.25	0.69
4:A:734:THR:HG23	4:A:1063:LYS:HB3	1.78	0.66
2:C:24:DA:N6	2:C:25:DG:O6	2.30	0.65
2:C:28:DC:H5'	4:A:448:THR:HG22	1.79	0.64
4:A:1075:VAL:HG11	4:A:1094:ILE:HD13	1.81	0.62
4:A:309:LYS:HG2	4:A:353:TYR:CE2	2.34	0.61
2:C:10:DT:H2'	2:C:11:DC:C6	2.37	0.60
4:A:298:LYS:O	4:A:302:ASN:ND2	2.35	0.60
4:A:1047:ARG:NH1	4:A:1052:GLN:O	2.34	0.59
4:A:1075:VAL:HG11	4:A:1094:ILE:CD1	2.32	0.59
1:B:13:A:OP2	4:A:47:ARG:NH2	2.35	0.59
4:A:349:THR:O	4:A:349:THR:HG22	2.02	0.59
4:A:1055:TYR:HA	4:A:1088:GLY:HA2	1.84	0.59
4:A:232:GLU:OE2	4:A:232:GLU:HA	2.03	0.58
4:A:731:THR:HG21	4:A:736:HIS:HD2	1.69	0.56
4:A:639:ASP:O	4:A:640:ALA:HB2	2.05	0.56
1:B:45:A:H2'	1:B:46:A:C8	2.42	0.55
4:A:585:ILE:HA	4:A:588:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:374:LYS:HB3	4:A:396:PHE:CZ	2.42	0.55
2:C:27:DA:H2'	2:C:28:DC:C6	2.43	0.54
4:A:806:ASP:OD1	4:A:806:ASP:N	2.40	0.54
4:A:313:ALA:O	4:A:318:LYS:NZ	2.35	0.54
4:A:1029:LEU:O	4:A:1041:LEU:HD12	2.08	0.54
4:A:864:ILE:HG23	4:A:871:LYS:HD3	1.90	0.53
4:A:980:ILE:HD11	4:A:1089:LEU:HB2	1.90	0.53
4:A:642:SER:OG	4:A:645:GLU:HG3	2.07	0.53
4:A:62:ARG:HB3	4:A:113:VAL:HG13	1.91	0.53
4:A:842:GLU:HG2	4:A:941:LYS:HD3	1.91	0.52
4:A:340:ASP:N	4:A:344:LYS:O	2.34	0.52
4:A:851:ASP:O	4:A:857:GLY:HA3	2.10	0.52
1:B:36:A:C5	1:B:37:G:H1'	2.45	0.51
4:A:349:THR:HG22	4:A:354:ARG:NH1	2.26	0.50
1:B:48:G:OP2	4:A:114:LYS:NZ	2.45	0.50
4:A:204:ASN:N	4:A:205:PRO:HD3	2.27	0.50
4:A:737:HIS:HA	4:A:740:VAL:HG22	1.92	0.50
4:A:181:ILE:HD11	4:A:620:THR:HA	1.94	0.50
4:A:367:MET:HE1	4:A:375:LEU:HD12	1.92	0.50
4:A:921:ARG:NH2	4:A:931:GLU:OE1	2.45	0.49
4:A:562:LEU:HD11	4:A:589:ILE:HG12	1.94	0.49
4:A:731:THR:HG21	4:A:736:HIS:CD2	2.46	0.49
4:A:749:SER:C	4:A:751:LEU:H	2.16	0.49
4:A:342:SER:HA	4:A:528:LYS:HD2	1.94	0.49
1:B:60:U:O4	4:A:240:ARG:NH2	2.45	0.49
4:A:682:ARG:NE	4:A:686:ASP:OD2	2.31	0.49
4:A:274:THR:HG21	4:A:429:VAL:HG13	1.95	0.48
4:A:568:LEU:HD21	4:A:611:LEU:HD22	1.95	0.48
4:A:914:LYS:HA	4:A:918:GLY:O	2.12	0.48
4:A:355:LYS:O	4:A:358:THR:OG1	2.31	0.48
4:A:633:ALA:O	4:A:637:MET:HG3	2.13	0.48
1:B:49:A:OP2	4:A:63:ARG:NH2	2.43	0.47
2:C:19:DA:H4'	4:A:689:TYR:CZ	2.49	0.47
4:A:604:SER:HB2	4:A:627:GLN:HE21	1.79	0.47
4:A:537:ALA:HB1	4:A:566:ILE:HG22	1.97	0.47
4:A:742:ALA:HA	4:A:745:ILE:HD12	1.97	0.47
3:D:4:DG:O6	4:A:1086:LYS:NZ	2.45	0.47
4:A:384:GLU:HG2	4:A:385:ARG:H	1.80	0.47
4:A:795:PHE:O	4:A:798:THR:HB	2.15	0.47
4:A:555:VAL:HG22	4:A:589:ILE:CG2	2.45	0.46
1:B:3:G:H2'	1:B:4:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:61:HIS:CD2	4:A:65:ARG:HD3	2.50	0.46
2:C:20:DT:H2'	2:C:21:DC:C6	2.50	0.46
4:A:277:GLU:OE1	4:A:369:ARG:NH1	2.49	0.46
4:A:614:LYS:O	4:A:660:LYS:NZ	2.35	0.46
2:C:1:DG:HO5'	2:C:1:DG:H8	1.64	0.45
4:A:630:PRO:O	4:A:634:LEU:HB2	2.16	0.45
1:B:53:G:O2'	4:A:989:GLN:HG3	2.16	0.45
4:A:629:THR:CG2	4:A:670:ILE:HD11	2.46	0.45
4:A:492:ILE:O	4:A:496:ALA:N	2.48	0.45
4:A:170:THR:HG21	4:A:638:ASP:OD2	2.17	0.45
4:A:375:LEU:HD23	4:A:375:LEU:HA	1.75	0.45
4:A:578:TYR:O	4:A:641:TRP:HB2	2.17	0.45
4:A:874:MET:O	4:A:878:ASP:N	2.49	0.45
4:A:337:TYR:O	4:A:337:TYR:CD1	2.70	0.45
4:A:540:LYS:HD3	4:A:570:HIS:ND1	2.32	0.45
4:A:946:ILE:HB	4:A:959:LEU:HB2	1.99	0.44
2:C:19:DA:H2'	2:C:20:DT:C6	2.52	0.44
4:A:722:LEU:HD23	4:A:722:LEU:C	2.34	0.44
4:A:559:HIS:HE1	4:A:592:SER:CB	2.31	0.44
4:A:1069:GLY:H	4:A:1079:VAL:CG2	2.31	0.44
4:A:631:TYR:CD2	4:A:667:GLU:HA	2.53	0.44
4:A:908:ASN:HB3	4:A:911:LEU:HB3	1.99	0.44
4:A:109:LEU:HB3	4:A:215:TYR:CE1	2.53	0.44
4:A:170:THR:OG1	4:A:179:ARG:NE	2.51	0.44
4:A:181:ILE:HG13	4:A:620:THR:HG22	2.00	0.44
1:B:4:C:H2'	1:B:5:U:O4'	2.18	0.43
4:A:579:THR:HA	4:A:640:ALA:HA	1.99	0.43
4:A:945:HIS:HB2	4:A:958:VAL:HB	2.01	0.43
4:A:349:THR:O	4:A:350:PHE:HB2	2.18	0.43
4:A:555:VAL:HG22	4:A:589:ILE:HG23	2.00	0.43
4:A:203:PHE:C	4:A:205:PRO:HD3	2.38	0.43
4:A:276:GLN:OE1	4:A:352:ALA:HB3	2.18	0.43
1:B:41:C:O2'	4:A:874:MET:HA	2.20	0.42
1:B:35:A:OP2	1:B:35:A:H8	2.02	0.42
2:C:5:DC:N4	4:A:1084:GLN:OE1	2.52	0.42
4:A:736:HIS:CD2	4:A:805:GLU:OE1	2.72	0.42
4:A:362:LEU:HD21	4:A:405:GLN:HB3	2.01	0.42
4:A:1097:TYR:CE1	4:A:1111:LYS:HD2	2.55	0.42
4:A:1047:ARG:NH1	4:A:1049:MET:O	2.53	0.42
4:A:196:ILE:O	4:A:200:GLN:HG2	2.20	0.42
4:A:562:LEU:HD22	4:A:566:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:LYS:HE3	4:A:802:LYS:HB3	1.90	0.42
4:A:1069:GLY:H	4:A:1079:VAL:HG23	1.85	0.42
4:A:273:TYR:HB2	4:A:372:LEU:HD23	2.02	0.41
4:A:585:ILE:HD12	4:A:586:HIS:N	2.35	0.41
4:A:157:GLU:O	4:A:161:THR:HG23	2.20	0.41
4:A:516:GLU:O	4:A:520:LYS:N	2.30	0.41
4:A:150:THR:HB	4:A:192:GLU:HB2	2.01	0.41
4:A:276:GLN:CD	4:A:352:ALA:HB3	2.40	0.41
4:A:881:THR:HG21	4:A:932:ILE:HD11	2.02	0.41
4:A:848:LYS:HA	4:A:936:LYS:HA	2.02	0.41
4:A:1011:GLU:CD	4:A:1047:ARG:NH2	2.74	0.41
2:C:24:DA:H2"	4:A:339:ILE:HG22	2.03	0.41
4:A:184:PHE:HB2	4:A:189:TYR:CE2	2.56	0.41
4:A:912:LYS:HD3	4:A:912:LYS:HA	1.86	0.41
4:A:186:THR:HG22	4:A:220:THR:HG22	2.03	0.41
4:A:396:PHE:CG	4:A:401:PHE:HE2	2.39	0.41
4:A:991:GLU:OE2	4:A:994:THR:OG1	2.30	0.41
4:A:518:ASP:OD1	4:A:518:ASP:N	2.54	0.40
4:A:1101:THR:HG22	4:A:1107:GLN:HA	2.04	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
4	A	1016/1122 (91%)	948 (93%)	63 (6%)	5 (0%)	29 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	204	ASN
4	A	600	ILE

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Mol	Chain	Res	Type
4	A	205	PRO
4	A	1049	MET
4	A	961	SER

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	A	874/1000 (87%)	839 (96%)	35 (4%)	31 68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	ASN
4	A	65	ARG
4	A	98	ASP
4	A	112	MET
4	A	116	ARG
4	A	159	TYR
4	A	234	SER
4	A	246	GLU
4	A	347	ILE
4	A	366	GLN
4	A	413	ARG
4	A	554	SER
4	A	555	VAL
4	A	598	ASP
4	A	611	LEU
4	A	641	TRP
4	A	671	SER
4	A	672	LYS
4	A	682	ARG
4	A	689	TYR
4	A	692	ARG
4	A	797	ASP
4	A	798	THR

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Mol	Chain	Res	Type
4	A	801	SER
4	A	806	ASP
4	A	842	GLU
4	A	940	SER
4	A	989	GLN
4	A	998	LYS
4	A	1011	GLU
4	A	1034	THR
4	A	1047	ARG
4	A	1048	THR
4	A	1055	TYR
4	A	1091	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	627	GLN
4	A	736	HIS
4	A	880	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	69/71 (97%)	9 (13%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	34	A
1	B	35	A
1	B	37	G
1	B	51	A
1	B	53	G
1	B	54	G
1	B	57	U
1	B	59	A
1	B	61	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	71/71 (100%)	-0.25	1 (1%) 75 49	22, 35, 61, 107	0
2	C	28/28 (100%)	-0.34	0 100 100	27, 36, 75, 78	0
3	D	8/8 (100%)	-0.65	0 100 100	27, 32, 36, 43	0
4	A	1030/1122 (91%)	-0.11	20 (1%) 66 37	17, 57, 90, 112	0
All	All	1137/1229 (92%)	-0.13	21 (1%) 68 40	17, 55, 90, 112	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	204	ASN	3.4
1	B	0	G	3.2
4	A	23	VAL	3.1
4	A	727	GLY	3.1
4	A	316	PRO	3.0
4	A	21	ASN	2.9
4	A	894	PRO	2.9
4	A	308	VAL	2.7
4	A	3	ASP	2.6
4	A	288	THR	2.5
4	A	501	GLY	2.4
4	A	320	PHE	2.4
4	A	583	ILE	2.3
4	A	4	LEU	2.3
4	A	286	ASN	2.1
4	A	518	ASP	2.1
4	A	1039	GLN	2.1
4	A	512	ARG	2.0
4	A	500	TYR	2.0
4	A	905	VAL	2.0
4	A	731	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BA	C	101	1/1	0.59	0.42	245,245,245,245	0
6	MG	A	1206	1/1	0.77	0.17	41,41,41,41	0
5	BA	B	103	1/1	0.92	0.06	125,125,125,125	0
5	BA	A	1204	1/1	0.93	0.04	121,121,121,121	0
5	BA	A	1201	1/1	0.95	0.06	90,90,90,90	0
5	BA	B	104	1/1	0.96	0.07	114,114,114,114	0
5	BA	A	1203	1/1	0.98	0.04	122,122,122,122	0
5	BA	B	102	1/1	0.98	0.05	85,85,85,85	0
5	BA	A	1202	1/1	0.98	0.10	106,106,106,106	0
5	BA	A	1205	1/1	0.99	0.12	67,67,67,67	0
5	BA	B	101	1/1	0.99	0.14	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.