Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 06:47 pm BST

PDB ID	:	4ZT0
Title	:	Crystal structure of catalytically-active Streptococcus pyogenes Cas9 in complex with single-guide RNA at 2.9 Angstrom resolution
Authors	:	Jiang, F.; Doudna, J.A.
Deposited on	:	2015-05-14
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

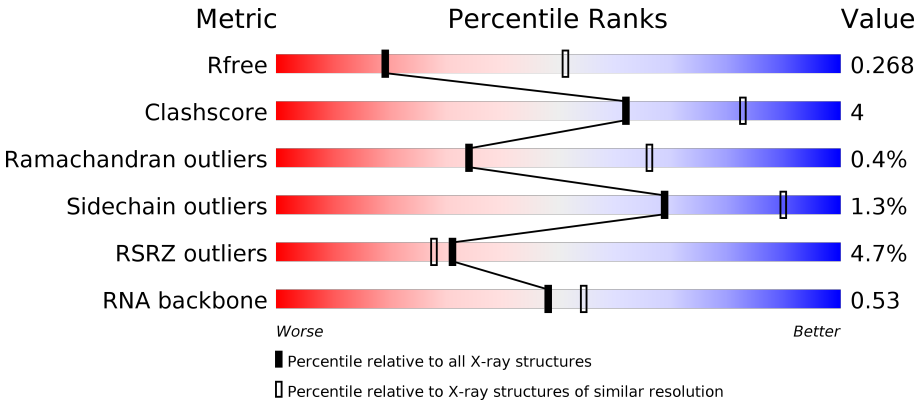
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (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 on 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	1369	4% 87% 12%
1	C	1369	6% 83% 11% 5%
2	B	85	% 49% 31% 5% 15%
2	D	85	44% 36% 5% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23790 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	1364	Total	C	N	O	S	Se	0	0	0
			10654	6778	1829	2025	2	20			
1	C	1296	Total	C	N	O	S	Se	0	0	0
			10046	6393	1728	1904	2	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0C6FZC2
A	1	MSE	-	expression tag	UNP A0A0C6FZC2
C	0	SER	-	expression tag	UNP A0A0C6FZC2
C	1	MSE	-	expression tag	UNP A0A0C6FZC2

- Molecule 2 is a RNA chain called single-guide RNA.

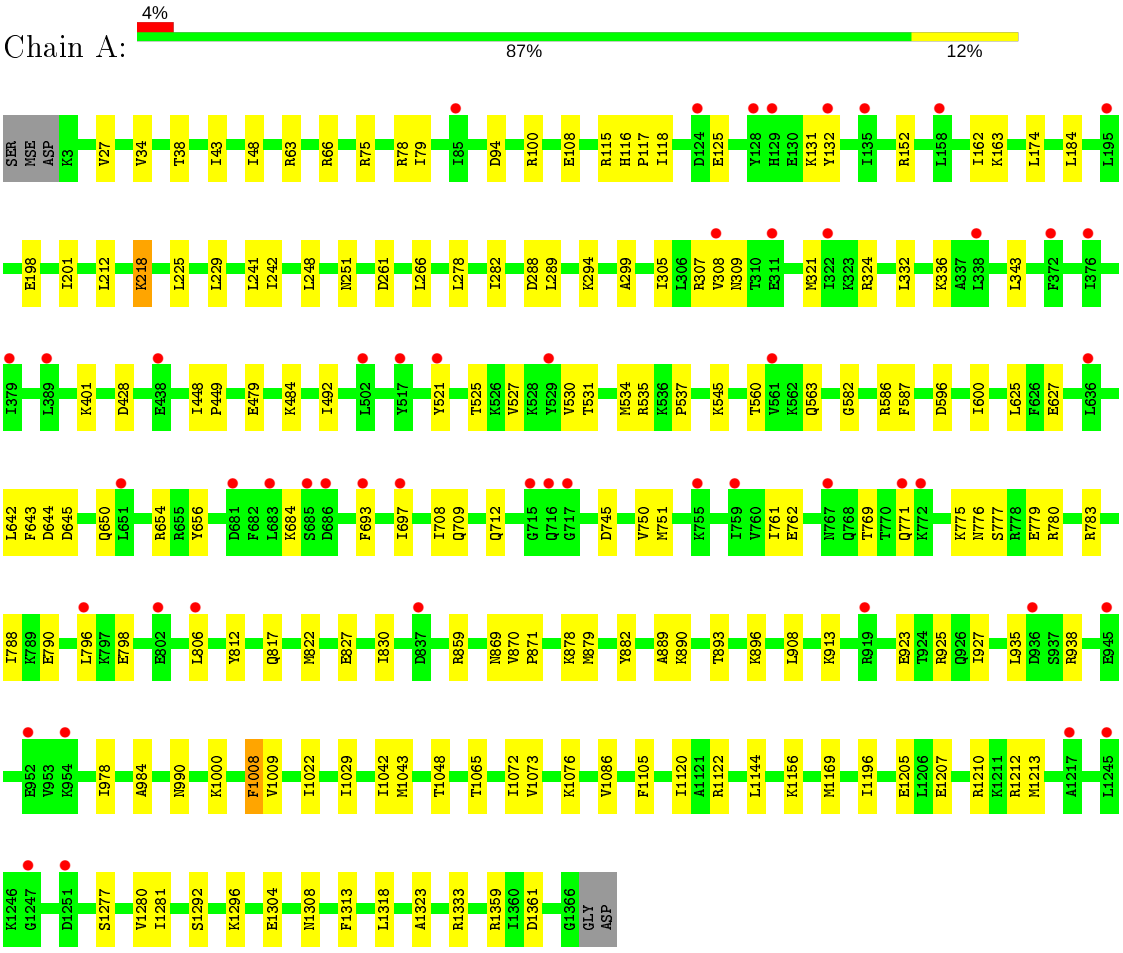
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	P	0	0	0
			1545	692	285	496	72			
2	D	72	Total	C	N	O	P	0	0	0
			1545	692	285	496	72			

3 Residue-property plots (i)

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.

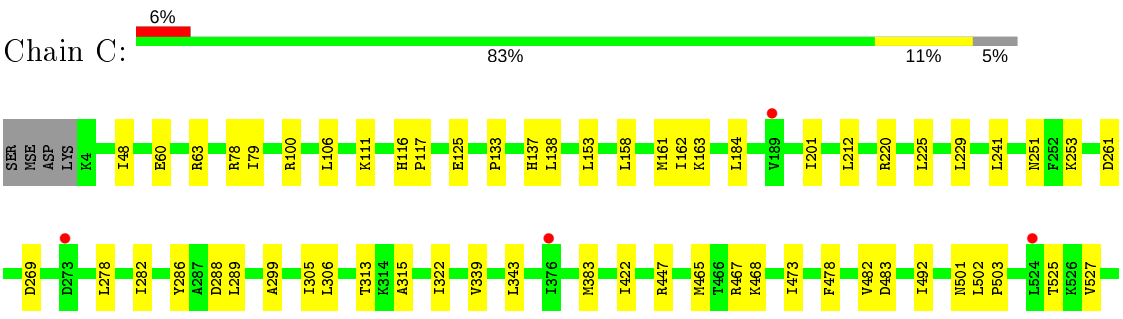
- Molecule 1: CRISPR-associated endonuclease Cas9

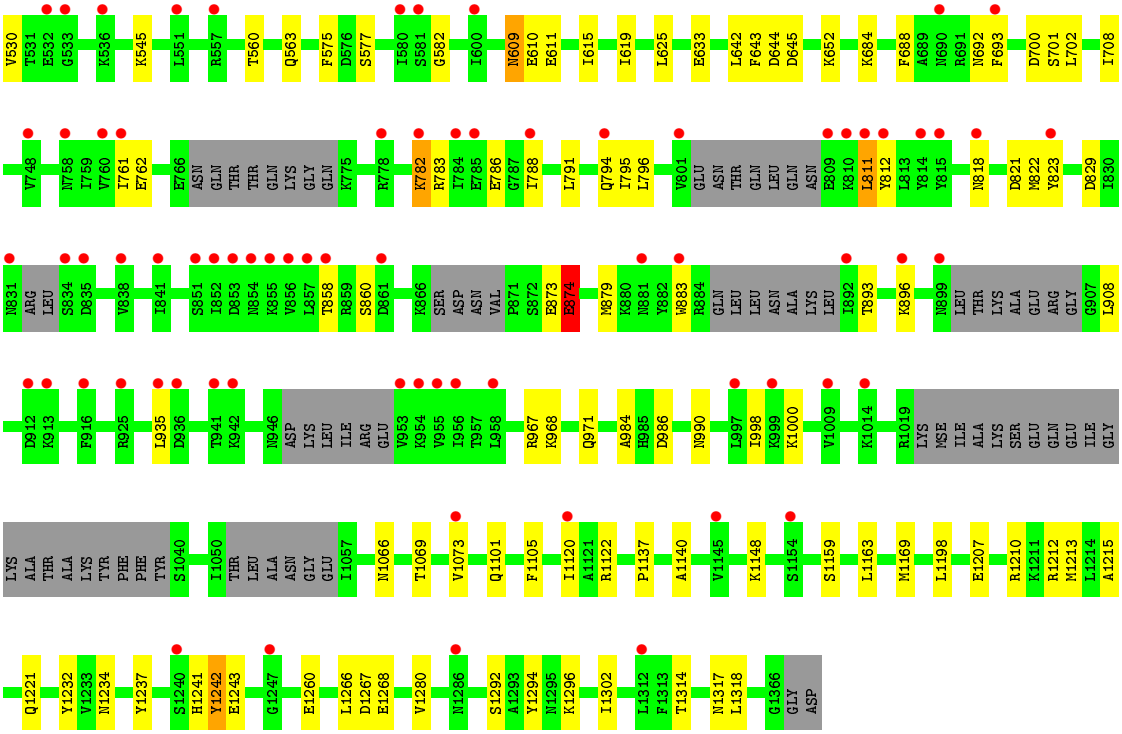
Chain A:



- Molecule 1: CRISPR-associated endonuclease Cas9

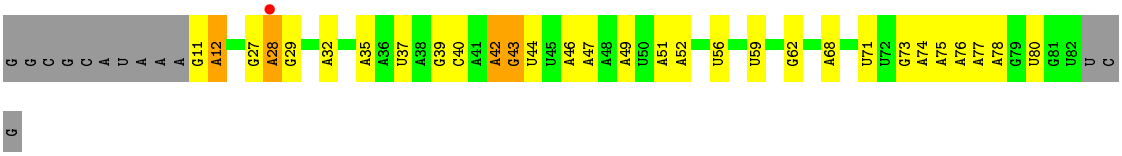
Chain C:





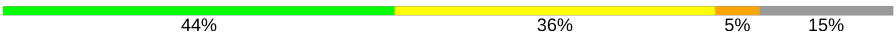
- Molecule 2: single-guide RNA

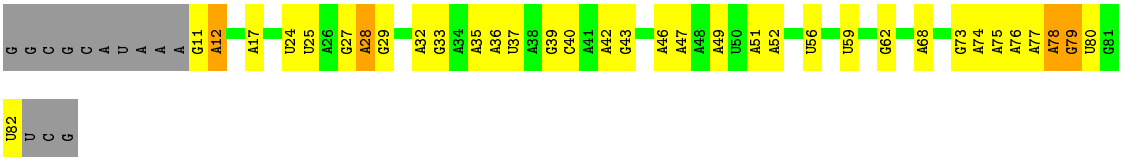
Chain B:



- Molecule 2: single-guide RNA

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.24Å 143.00Å 294.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.90 102.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.15-2.90) 99.5 (102.66-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.264 0.245 , 0.268	Depositor DCC
R_{free} test set	4812 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.8	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	0.92	EDS
Total number of atoms	23790	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8491e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.25	0/10825	0.37	0/14614
1	C	0.26	0/10200	0.38	0/13759
2	B	0.17	0/1732	0.70	0/2698
2	D	0.17	0/1732	0.70	0/2698
All	All	0.24	0/24489	0.44	0/33769

There are no bond length outliers.

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	A	10654	0	10330	92	0
1	C	10046	0	9673	84	0
2	B	1545	0	774	15	0
2	D	1545	0	774	13	0
All	All	23790	0	21551	199	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 4.

All (199) 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:C:1120:ILE:HD11	1:C:1137:PRO:HG3	1.66	0.78
2:B:32:A:H61	2:B:37:U:H3	1.31	0.77
1:C:1122:ARG:NH2	2:D:49:A:N3	2.35	0.74
1:A:218:LYS:HG3	1:A:248:LEU:HD21	1.70	0.73
1:A:762:GLU:OE1	1:A:990:ASN:ND2	2.21	0.73
1:C:78:ARG:NH1	1:C:162:ILE:O	2.22	0.72
1:C:116:HIS:HB3	1:C:125:GLU:HG3	1.74	0.70
2:D:27:G:H5"	2:D:28:A:H5'	1.74	0.69
1:C:100:ARG:NH1	1:C:117:PRO:O	2.27	0.68
2:D:33:G:N2	2:D:36:A:OP2	2.27	0.68
1:A:1122:ARG:NH2	2:B:49:A:N3	2.41	0.67
1:A:761:ILE:HD11	1:A:935:LEU:HD12	1.77	0.67
1:C:79:ILE:HD11	1:C:163:LYS:HB2	1.77	0.66
1:A:1304:GLU:O	1:A:1308:ASN:ND2	2.29	0.66
1:A:116:HIS:HB3	1:A:125:GLU:HG3	1.78	0.65
1:C:762:GLU:OE1	1:C:990:ASN:ND2	2.24	0.64
1:A:869:ASN:HD21	1:A:908:LEU:H	1.44	0.63
2:B:27:G:H5"	2:B:28:A:H5'	1.80	0.62
1:A:1205:GLU:OE1	1:A:1359:ARG:NH2	2.30	0.62
1:A:212:LEU:HD21	1:A:225:LEU:HD22	1.83	0.61
2:B:27:G:N2	2:B:44:U:OP2	2.33	0.61
1:C:1212:ARG:NH2	1:C:1280:VAL:O	2.34	0.61
1:A:817:GLN:HG2	1:A:822:MSE:HE2	1.81	0.60
1:A:100:ARG:NH1	1:A:117:PRO:O	2.35	0.60
1:C:822:MSE:HG3	1:C:883:TRP:HE1	1.66	0.60
1:C:343:LEU:HB2	1:C:383:MSE:HE2	1.84	0.60
1:C:971:GLN:O	1:C:1234:ASN:ND2	2.34	0.59
1:A:479:GLU:OE1	1:A:484:LYS:NZ	2.34	0.58
1:A:1105:PHE:HB3	1:A:1169:MSE:HE2	1.84	0.58
1:A:1008:PHE:HD2	1:A:1009:VAL:HG23	1.69	0.58
1:C:1148:LYS:HG2	1:C:1159:SER:HA	1.86	0.57
1:A:1280:VAL:HG23	1:A:1281:ILE:HD12	1.88	0.56
1:A:1048:THR:HG22	1:A:1076:LYS:HD3	1.87	0.56
1:A:923:GLU:OE1	1:A:925:ARG:NH1	2.39	0.56
1:A:94:ASP:OD2	1:A:152:ARG:NH1	2.38	0.56
1:A:307:ARG:O	1:A:309:ASN:N	2.39	0.55
1:A:78:ARG:NH1	1:A:162:ILE:O	2.39	0.55
2:B:52:A:OP2	2:B:62:G:N2	2.38	0.55
1:A:560:THR:HG23	1:A:563:GLN:H	1.72	0.55
1:C:253:LYS:HB2	1:C:261:ASP:HA	1.88	0.55
1:A:251:ASN:HD21	1:A:261:ASP:HB2	1.72	0.55
1:C:158:LEU:HA	1:C:161:MSE:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:HG22	1:C:383:MSE:HE1	1.89	0.54
1:A:776:ASN:OD1	1:A:777:SER:N	2.41	0.54
1:A:324:ARG:NH1	1:A:401:LYS:O	2.40	0.54
1:A:790:GLU:HG2	1:A:889:ALA:HA	1.89	0.53
1:C:161:MSE:HE1	1:C:422:ILE:HD12	1.90	0.53
1:C:1232:TYR:OH	1:C:1268:GLU:OE2	2.20	0.53
1:A:878:LYS:HG3	1:A:879:MSE:HE2	1.90	0.53
1:A:1065:THR:HG22	1:A:1072:ILE:HG22	1.90	0.53
1:C:1105:PHE:HB3	1:C:1169:MSE:HE2	1.91	0.53
1:C:1215:ALA:HB2	1:C:1221:GLN:HG3	1.91	0.53
2:D:27:G:C5'	2:D:28:A:H5'	2.38	0.53
1:A:108:GLU:OE2	1:A:115:ARG:NH2	2.36	0.52
1:A:201:ILE:HD11	1:A:229:LEU:HD22	1.90	0.52
1:C:138:LEU:HD11	1:C:153:LEU:HB3	1.92	0.52
1:A:266:LEU:HD22	1:A:294:LYS:HD3	1.92	0.52
1:C:501:ASN:HB3	1:C:708:ILE:HD11	1.91	0.52
1:C:811:LEU:H	1:C:811:LEU:HD23	1.75	0.52
1:C:278:LEU:O	1:C:282:ILE:HG13	2.10	0.52
1:A:79:ILE:HD11	1:A:163:LYS:HB2	1.92	0.52
1:A:1000:LYS:HD3	1:A:1073:VAL:HG21	1.92	0.51
1:A:428:ASP:OD1	1:A:428:ASP:N	2.41	0.51
1:A:27:VAL:HG22	1:A:1086:VAL:HG22	1.93	0.51
1:C:761:ILE:HD11	1:C:935:LEU:HD12	1.91	0.51
1:A:492:ILE:HG12	1:A:625:LEU:HD13	1.92	0.51
1:C:465:MSE:HE1	1:C:467:ARG:HG2	1.93	0.50
1:C:465:MSE:HE3	1:C:482:VAL:HG22	1.93	0.50
1:C:633:GLU:HG2	1:C:652:LYS:HD3	1.92	0.50
1:C:1101:GLN:HB2	1:C:1140:ALA:HA	1.94	0.50
1:A:644:ASP:OD1	1:A:645:ASP:N	2.45	0.50
1:C:184:LEU:HD12	1:C:299:ALA:HB2	1.93	0.50
1:C:282:ILE:HD13	1:C:286:TYR:HD2	1.77	0.50
1:C:1066:ASN:HD22	1:C:1069:THR:HG22	1.76	0.50
2:B:42:A:O2'	2:B:43:G:OP1	2.27	0.49
1:C:644:ASP:OD1	1:C:645:ASP:N	2.44	0.49
2:D:78:A:O2'	2:D:79:G:OP1	2.26	0.49
1:C:313:THR:O	1:C:315:ALA:N	2.41	0.49
1:C:201:ILE:HD11	1:C:229:LEU:HD22	1.95	0.49
1:C:282:ILE:HD13	1:C:286:TYR:CD2	2.47	0.49
1:A:1212:ARG:NH2	1:A:1280:VAL:O	2.45	0.48
1:A:925:ARG:HG2	1:A:927:ILE:HG22	1.95	0.48
1:A:893:THR:HG23	1:A:896:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:LEU:HB3	1:A:1196:ILE:HB	1.95	0.48
1:A:780:ARG:HG3	1:A:806:LEU:HD23	1.95	0.48
1:C:1241:HIS:O	1:C:1243:GLU:N	2.47	0.48
1:C:822:MSE:HG3	1:C:883:TRP:NE1	2.28	0.48
1:C:823:TYR:HD2	1:C:858:THR:HG21	1.79	0.48
1:A:817:GLN:O	1:A:882:TYR:OH	2.31	0.48
1:C:111:LYS:NZ	2:D:25:U:O2'	2.35	0.48
1:A:693:PHE:CZ	1:A:697:ILE:HD11	2.49	0.48
1:C:821:ASP:OD1	1:C:822:MSE:N	2.47	0.48
1:A:278:LEU:O	1:A:282:ILE:HG12	2.14	0.47
1:A:596:ASP:O	1:A:600:ILE:HG12	2.14	0.47
2:B:27:G:H3'	2:B:28:A:H5'	1.95	0.47
1:C:525:THR:HA	1:C:545:LYS:HE2	1.97	0.47
1:C:527:VAL:HA	1:C:582:GLY:HA3	1.96	0.47
1:C:137:HIS:HA	1:C:322:ILE:HD11	1.97	0.47
1:A:654:ARG:HH21	1:A:656:TYR:HE1	1.61	0.47
1:C:492:ILE:HG12	1:C:625:LEU:HD13	1.97	0.47
1:A:116:HIS:HA	1:A:117:PRO:HD3	1.74	0.47
1:C:795:ILE:HD13	1:C:818:ASN:HA	1.96	0.47
1:A:600:ILE:HD12	1:A:650:GLN:HG2	1.96	0.46
1:A:870:VAL:HB	1:A:871:PRO:HD2	1.97	0.46
1:C:1266:LEU:HD11	1:C:1302:ILE:HG23	1.97	0.46
1:C:560:THR:HG23	1:C:563:GLN:H	1.80	0.46
1:A:1207:GLU:OE1	1:A:1210:ARG:NH1	2.48	0.46
1:A:34:VAL:HG21	1:A:43:ILE:HG13	1.97	0.46
2:B:73:G:H21	2:B:76:A:H2	1.61	0.46
1:C:106:LEU:O	1:C:111:LYS:HE3	2.16	0.46
1:C:1000:LYS:HG2	1:C:1073:VAL:HG21	1.96	0.46
1:C:968:LYS:NZ	1:C:1237:TYR:OH	2.48	0.46
2:D:46:A:H2'	2:D:47:A:C8	2.50	0.46
1:A:1323:ALA:N	1:A:1333:ARG:HG2	2.31	0.46
1:A:525:THR:HA	1:A:545:LYS:HE2	1.97	0.46
1:A:531:THR:HG22	1:A:534:MSE:SE	2.66	0.46
1:C:700:ASP:C	1:C:702:LEU:H	2.18	0.46
1:A:780:ARG:HB2	1:A:812:TYR:CE1	2.50	0.46
1:C:967:ARG:NH1	1:C:986:ASP:OD1	2.49	0.46
1:A:1008:PHE:CD2	1:A:1009:VAL:HG23	2.50	0.46
1:A:535:ARG:HD2	1:A:535:ARG:HA	1.77	0.46
1:A:830:ILE:HD12	1:A:830:ILE:H	1.80	0.46
1:A:978:ILE:HG12	1:A:1313:PHE:CE2	2.52	0.45
1:C:212:LEU:HD21	1:C:225:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1120:ILE:HG21	1:C:1169:MSE:HE1	1.97	0.45
1:C:1292:SER:O	1:C:1296:LYS:HG2	2.17	0.45
1:A:1213:MSE:HE3	1:A:1318:LEU:HD11	1.97	0.45
1:A:305:ILE:HD11	1:A:321:MSE:SE	2.66	0.45
1:A:527:VAL:HA	1:A:582:GLY:HA3	1.99	0.45
1:A:241:LEU:HD11	1:A:289:LEU:HD21	1.98	0.45
1:C:783:ARG:NH2	1:C:812:TYR:OH	2.32	0.44
1:A:750:VAL:HG12	1:A:751:MSE:HE3	1.99	0.44
2:D:11:G:O2'	2:D:12:A:O5'	2.35	0.44
1:A:131:LYS:HG2	1:A:132:TYR:CZ	2.52	0.44
1:A:775:LYS:O	1:A:779:GLU:HG2	2.18	0.44
1:A:788:ILE:HG13	1:A:796:LEU:HD13	2.00	0.44
1:C:220:ARG:HA	1:C:220:ARG:HD2	1.73	0.44
2:D:32:A:H61	2:D:37:U:H3	1.66	0.44
1:A:48:ILE:HG12	1:A:984:ALA:HB1	1.99	0.44
1:C:575:PHE:O	1:C:577:SER:N	2.46	0.44
1:C:893:THR:HG23	1:C:896:LYS:H	1.83	0.43
1:A:783:ARG:NH2	1:A:890:LYS:O	2.51	0.43
2:D:52:A:OP2	2:D:62:G:N2	2.45	0.43
1:C:251:ASN:HD21	1:C:261:ASP:HB2	1.84	0.43
1:C:873:GLU:O	1:C:874:GLU:HB3	2.17	0.43
1:A:708:ILE:O	1:A:712:GLN:HG2	2.18	0.43
1:A:751:MSE:HE2	1:A:751:MSE:HA	2.01	0.43
1:C:1207:GLU:OE1	1:C:1210:ARG:NH1	2.52	0.43
1:C:1213:MSE:HE3	1:C:1318:LEU:HD11	2.01	0.43
1:C:478:PHE:CE1	1:C:482:VAL:HG21	2.54	0.43
1:C:133:PRO:HD2	1:C:137:HIS:CG	2.54	0.43
1:A:225:LEU:HD23	1:A:242:ILE:HG21	2.01	0.43
1:C:1267:ASP:OD1	1:C:1294:TYR:OH	2.28	0.43
1:A:1120:ILE:HG21	1:A:1169:MSE:HE1	1.99	0.43
1:C:609:ASN:C	1:C:611:GLU:H	2.23	0.43
2:B:71:U:H3	2:B:78:A:H61	1.66	0.42
2:B:46:A:H2'	2:B:47:A:C8	2.54	0.42
1:C:305:ILE:HG22	1:C:306:LEU:H	1.84	0.42
1:A:913:LYS:HB2	1:A:1022:ILE:HD13	2.01	0.42
1:A:1277:SER:HA	1:A:1281:ILE:HD13	2.01	0.42
1:A:1292:SER:O	1:A:1296:LYS:HG3	2.19	0.42
1:C:1163:LEU:HD11	1:C:1198:LEU:HD12	2.01	0.42
1:A:530:VAL:HG22	1:A:537:PRO:HA	2.02	0.42
1:C:269:ASP:OD1	1:C:269:ASP:N	2.51	0.42
1:A:75:ARG:HD3	1:A:163:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TYR:CE1	1:A:684:LYS:HG2	2.55	0.42
2:D:74:A:H2'	2:D:75:A:O4'	2.19	0.42
1:A:118:ILE:N	1:A:125:GLU:OE2	2.53	0.42
1:A:586:ARG:NH1	1:A:587:PHE:O	2.53	0.42
1:A:869:ASN:OD1	1:A:870:VAL:N	2.47	0.42
1:A:116:HIS:NE2	2:B:27:G:OP1	2.52	0.41
1:C:467:ARG:HH12	1:C:473:ILE:HG13	1.86	0.41
1:A:38:THR:HG22	1:A:1361:ASP:HB2	2.02	0.41
2:B:74:A:H2'	2:B:75:A:O4'	2.20	0.41
1:C:241:LEU:HD11	1:C:289:LEU:HD21	2.03	0.41
1:C:684:LYS:HB2	1:C:684:LYS:HE3	1.85	0.41
1:A:1042:ILE:HG13	1:A:1043:MSE:HG2	2.02	0.41
1:A:332:LEU:O	1:A:336:LYS:HG3	2.20	0.41
1:C:1066:ASN:ND2	1:C:1069:THR:HG22	2.34	0.41
1:C:1314:THR:HA	1:C:1317:ASN:ND2	2.35	0.41
1:C:468:LYS:HB3	1:C:483:ASP:HB2	2.02	0.41
1:C:502:LEU:HA	1:C:503:PRO:HD2	1.97	0.41
1:A:745:ASP:OD2	1:A:938:ARG:NH1	2.53	0.41
2:B:27:G:H3'	2:B:28:A:C5'	2.51	0.41
1:C:788:ILE:HG13	1:C:796:LEU:HD23	2.03	0.41
1:C:782:LYS:HB2	1:C:782:LYS:HE2	1.83	0.41
1:C:615:ILE:O	1:C:619:ILE:HG13	2.21	0.41
2:B:42:A:HO2'	2:B:43:G:P	2.43	0.41
1:A:827:GLU:O	1:A:859:ARG:NH2	2.38	0.41
1:A:448:ILE:HA	1:A:449:PRO:HD3	1.92	0.41
1:C:447:ARG:HG3	2:D:17:A:H5'	2.03	0.41
1:C:60:GLU:HG3	1:C:63:ARG:HH22	1.84	0.41
2:D:73:G:H21	2:D:76:A:H2	1.68	0.40
1:A:63:ARG:HG3	1:A:66:ARG:NH2	2.36	0.40
1:A:769:THR:C	1:A:771:GLN:H	2.25	0.40
2:B:11:G:O2'	2:B:12:A:O5'	2.37	0.40
1:C:48:ILE:HG12	1:C:984:ALA:HB1	2.04	0.40
1:C:986:ASP:O	1:C:990:ASN:ND2	2.40	0.40
1:A:184:LEU:HD22	1:A:299:ALA:HB2	2.03	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	1362/1369 (100%)	1301 (96%)	59 (4%)	2 (0%)	51 82
1	C	1276/1369 (93%)	1216 (95%)	51 (4%)	9 (1%)	22 54
All	All	2638/2738 (96%)	2517 (95%)	110 (4%)	11 (0%)	34 66

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	VAL
1	C	874	GLU
1	C	688	PHE
1	C	1242	TYR
1	C	692	ASN
1	C	860	SER
1	C	908	LEU
1	C	693	PHE
1	C	701	SER
1	A	1029	ILE
1	C	610	GLU

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	1106/1206 (92%)	1094 (99%)	12 (1%)	73 92
1	C	1031/1206 (86%)	1015 (98%)	16 (2%)	62 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2137/2412 (89%)	2109 (99%)	28 (1%)	69 90

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

Mol	Chain	Res	Type
1	A	174	LEU
1	A	198	GLU
1	A	218	LYS
1	A	288	ASP
1	A	343	LEU
1	A	627	GLU
1	A	642	LEU
1	A	643	PHE
1	A	709	GLN
1	A	798	GLU
1	A	1008	PHE
1	A	1156	LYS
1	C	288	ASP
1	C	530	VAL
1	C	609	ASN
1	C	642	LEU
1	C	643	PHE
1	C	782	LYS
1	C	786	GLU
1	C	791	LEU
1	C	794	GLN
1	C	811	LEU
1	C	829	ASP
1	C	874	GLU
1	C	879	MSE
1	C	998	ILE
1	C	1242	TYR
1	C	1260	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	71/85 (83%)	14 (19%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	71/85 (83%)	16 (22%)	2 (2%)
All	All	142/170 (83%)	30 (21%)	3 (2%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	A
2	B	28	A
2	B	29	G
2	B	35	A
2	B	39	G
2	B	40	C
2	B	42	A
2	B	43	G
2	B	51	A
2	B	56	U
2	B	59	U
2	B	68	A
2	B	77	A
2	B	80	U
2	D	12	A
2	D	24	U
2	D	28	A
2	D	29	G
2	D	35	A
2	D	39	G
2	D	40	C
2	D	43	G
2	D	51	A
2	D	56	U
2	D	59	U
2	D	68	A
2	D	77	A
2	D	79	G
2	D	80	U
2	D	82	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	42	A
2	D	42	A

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Mol	Chain	Res	Type
2	D	78	A

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 carbohydrates 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	1343/1369 (98%)	0.22	51 (3%) 40 36	37, 97, 152, 216	0
1	C	1276/1369 (93%)	0.36	77 (6%) 21 18	39, 93, 181, 232	0
2	B	72/85 (84%)	0.06	1 (1%) 75 75	46, 78, 221, 260	0
2	D	72/85 (84%)	0.09	0 100 100	47, 65, 156, 194	0
All	All	2763/2908 (95%)	0.28	129 (4%) 31 28	37, 94, 170, 260	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	GLN	8.5
1	C	811	LEU	7.1
1	C	856	VAL	7.0
1	C	835	ASP	6.7
1	A	767	ASN	6.6
1	C	912	ASP	5.9
1	A	715	GLY	5.3
1	C	852	ILE	5.3
1	C	857	LEU	5.0
1	C	838	VAL	4.9
1	C	814	TYR	4.8
1	C	954	LYS	4.8
1	C	823	TYR	4.5
1	C	532	GLU	4.5
1	C	815	TYR	4.2
1	C	861	ASP	4.2
1	C	854	ASN	4.1
1	C	1014	LYS	3.9
1	C	855	LYS	3.8
1	C	834	SER	3.8
1	C	782	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	881	ASN	3.7
1	C	818	ASN	3.7
1	C	809	GLU	3.6
1	A	517	TYR	3.5
1	C	784	ILE	3.5
1	C	778	ARG	3.4
1	A	376	ILE	3.4
1	A	771	GLN	3.4
1	A	379	ILE	3.3
1	A	128	TYR	3.3
1	A	561	VAL	3.2
1	A	389	LEU	3.2
1	C	788	ILE	3.2
1	A	685	SER	3.1
1	C	935	LEU	3.1
1	C	953	VAL	3.1
1	C	899	ASN	3.1
1	A	759	ILE	3.1
1	C	1154	SER	3.0
1	C	841	ILE	3.0
1	C	958	LEU	3.0
1	C	801	VAL	3.0
1	A	338	LEU	2.9
1	C	794	GLN	2.9
1	C	524	LEU	2.9
2	B	28	A	2.9
1	C	1009	VAL	2.9
1	A	772	LYS	2.9
1	C	748	VAL	2.9
1	C	851	SER	2.9
1	C	831	ASN	2.9
1	C	955	VAL	2.9
1	C	956	ILE	2.9
1	C	1073	VAL	2.8
1	C	551	LEU	2.8
1	A	755	LYS	2.8
1	C	581	SER	2.8
1	A	806	LEU	2.8
1	C	533	GLY	2.8
1	A	135	ILE	2.8
1	A	717	GLY	2.7
1	C	913	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	322	ILE	2.7
1	C	812	TYR	2.7
1	C	758	ASN	2.7
1	A	945	GLU	2.6
1	A	1217	ALA	2.6
1	A	651	LEU	2.6
1	C	1145	VAL	2.5
1	A	124	ASP	2.5
1	C	1247	GLY	2.5
1	A	686	ASP	2.5
1	A	952	GLU	2.5
1	C	189	VAL	2.4
1	C	580	ILE	2.4
1	C	693	PHE	2.4
1	C	1240	SER	2.4
1	C	761	ILE	2.4
1	C	810	LYS	2.4
1	A	954	LYS	2.4
1	C	557	ARG	2.3
1	A	802	GLU	2.3
1	C	916	PHE	2.3
1	C	936	ASP	2.3
1	A	521	TYR	2.3
1	A	158	LEU	2.3
1	A	85	ILE	2.3
1	A	129	HIS	2.3
1	A	502	LEU	2.3
1	A	1245	LEU	2.3
1	C	785	GLU	2.3
1	A	919	ARG	2.2
1	A	308	VAL	2.2
1	C	690	ASN	2.2
1	C	1120	ILE	2.2
1	A	693	PHE	2.2
1	A	132	TYR	2.2
1	A	529	TYR	2.2
1	C	925	ARG	2.1
1	A	683	LEU	2.1
1	C	997	LEU	2.1
1	C	883	TRP	2.1
1	A	1247	GLY	2.1
1	C	942	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	311	GLU	2.1
1	A	372	PHE	2.1
1	C	1312	LEU	2.1
1	A	1251	ASP	2.1
1	A	697	ILE	2.1
1	A	837	ASP	2.1
1	A	936	ASP	2.1
1	A	796	LEU	2.1
1	C	536	LYS	2.1
1	C	853	ASP	2.1
1	C	600	ILE	2.0
1	C	892	ILE	2.0
1	A	636	LEU	2.0
1	C	273	ASP	2.0
1	A	438	GLU	2.0
1	C	760	VAL	2.0
1	A	195	LEU	2.0
1	A	681	ASP	2.0
1	C	376	ILE	2.0
1	C	858	THR	2.0
1	C	941	THR	2.0
1	C	896	LYS	2.0
1	C	999	LYS	2.0
1	C	1286	ASN	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.