Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 09:18 pm GMT

PDB ID	:	4UN5
Title	:	Crystal structure of Cas9 bound to PAM-containing DNA target containing mismatches at positions 1-3
Authors	:	Anders, C.; Niewoehner, O.; Duerst, A.; Jinek, M.
Deposited on	:	2014-05-25
Resolution	:	2.40 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:

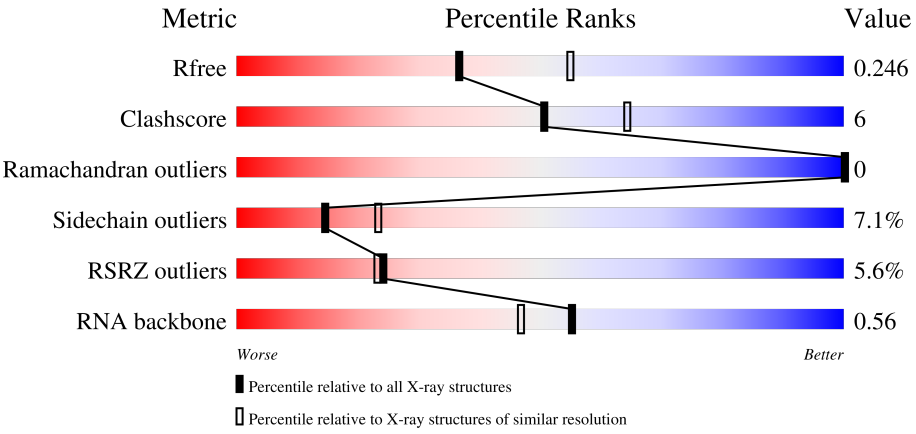
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	83	5% 63% 24% 12% ·
2	B	1372	5% 78% 16% · 5%
3	C	11	9% 55% 18% 9% 18%
4	D	11	9% 64% 27% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	17	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13943 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 SGRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	P	0	0	1
			1733	778	318	556	81			

- Molecule 2 is a protein called CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1310	Total	C	N	O	S	0	0	0
			10716	6832	1860	2002	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q99ZW2
B	-2	ALA	-	expression tag	UNP Q99ZW2
B	-1	ALA	-	expression tag	UNP Q99ZW2
B	0	SER	-	expression tag	UNP Q99ZW2
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called TARGET DNA STRAND PROXIMAL FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			162	77	31	46	8			

- Molecule 4 is a DNA chain called NON-TARGET DNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			206	100	35	62	9			

- Molecule 5 is a DNA chain called TARGET DNA STRAND DISTAL FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	17	Total	C	N	O	P	0	0	0
			346	169	59	102	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Mg	0	0
			4	4		
6	B	4	Total	Mg	0	0
			4	4		

- Molecule 7 is water.

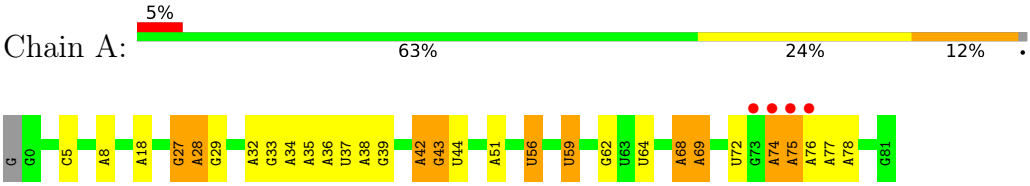
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	233	Total	O	0	0
			233	233		
7	B	491	Total	O	0	0
			491	491		
7	C	6	Total	O	0	0
			6	6		
7	D	15	Total	O	0	0
			15	15		
7	E	27	Total	O	0	0
			27	27		

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.

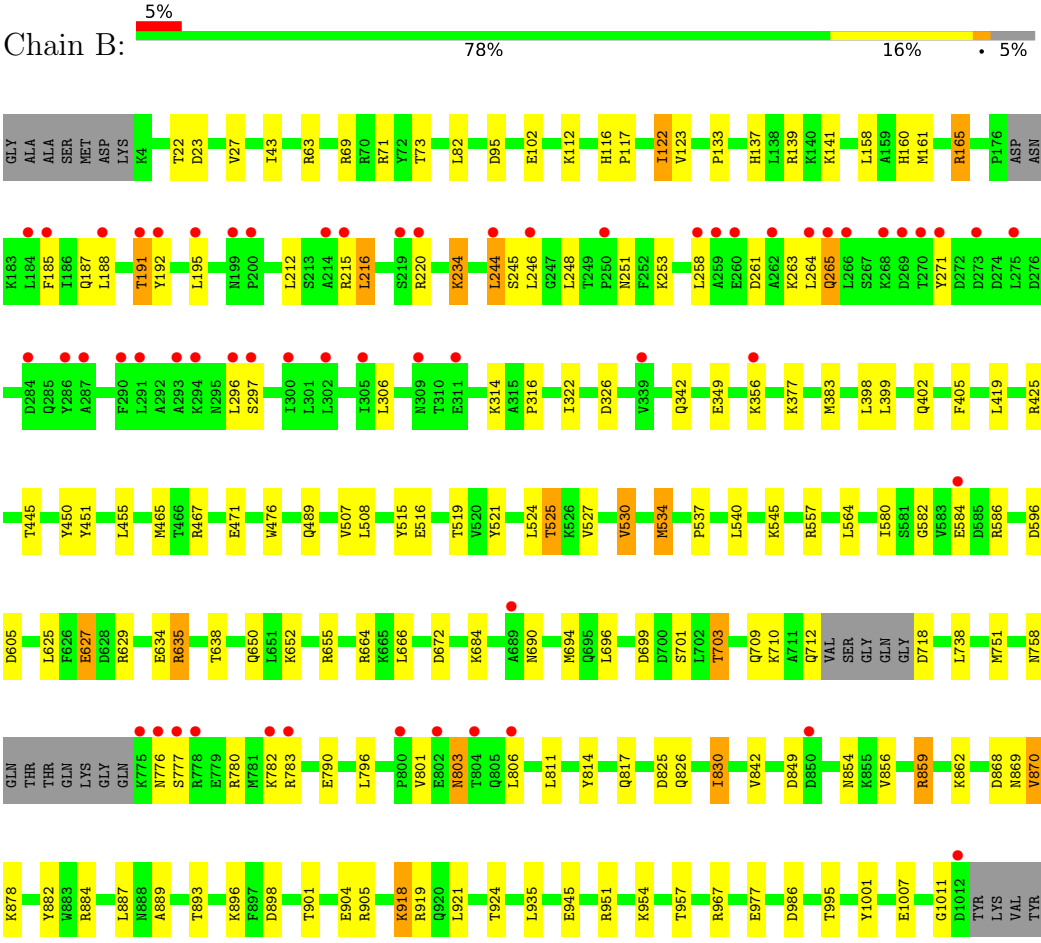
• Molecule 1: SGRNA

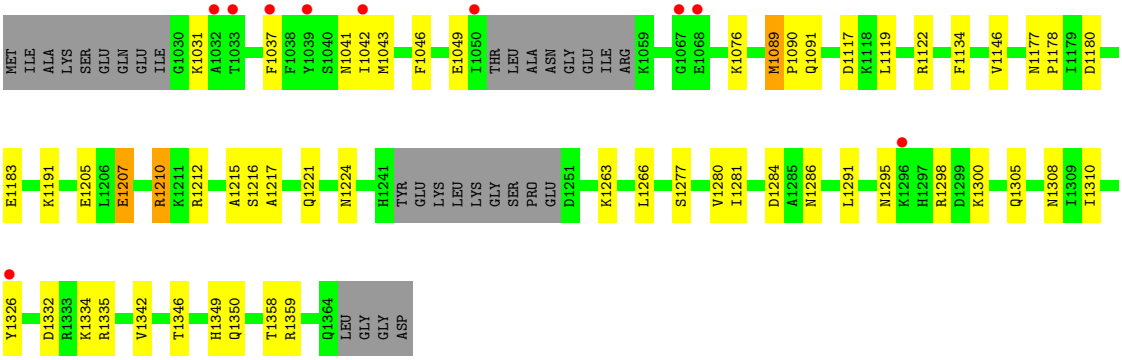
Chain A:



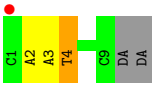
• Molecule 2: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1

Chain B:

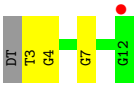




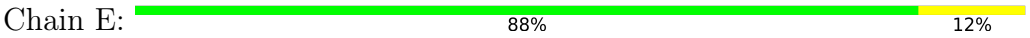
• Molecule 3: TARGET DNA STRAND PROXIMAL FRAGMENT

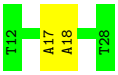


• Molecule 4: NON-TARGET DNA STRAND



• Molecule 5: TARGET DNA STRAND DISTAL FRAGMENT





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.18Å 68.07Å 190.26Å 90.00° 111.37° 90.00°	Depositor
Resolution (Å)	48.35 – 2.40 48.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.35-2.40) 99.9 (48.35-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.246 0.215 , 0.246	Depositor DCC
R_{free} test set	4220 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.5	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	0.93	EDS
Total number of atoms	13943	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 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	A	0.19	0/1943	0.77	0/3026
2	B	0.24	0/10903	0.40	0/14646
3	C	0.48	0/181	1.17	2/277 (0.7%)
4	D	0.46	0/230	1.17	0/355
5	E	0.44	0/387	1.14	0/596
All	All	0.25	0/13644	0.56	2/18900 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	DT	C1'-O4'-C4'	-5.56	104.54	110.10
3	C	4	DT	O4'-C1'-C2'	-5.34	101.63	105.90

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	1733	0	869	19	0
2	B	10716	0	10887	123	0
3	C	162	0	90	3	0
4	D	206	0	117	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	346	0	197	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	233	0	0	10	0
7	B	491	0	0	33	0
7	C	6	0	0	1	0
7	D	15	0	0	0	0
7	E	27	0	0	0	0
All	All	13943	0	12160	143	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 6.

All (143) 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)
2:B:859:ARG:NH1	7:B:3316:HOH:O	2.03	0.89
2:B:1332:ASP:OD2	7:B:3481:HOH:O	1.93	0.87
2:B:437:ARG:NH2	7:B:3169:HOH:O	2.10	0.84
2:B:1212:ARG:NH1	7:B:3443:HOH:O	2.13	0.81
7:A:2187:HOH:O	2:B:69:ARG:NH2	2.15	0.79
2:B:977:GLU:OE2	7:B:3353:HOH:O	2.02	0.78
2:B:251:ASN:O	7:B:3131:HOH:O	2.03	0.77
1:A:27:G:H5'	1:A:28:A:H5"	1.67	0.76
2:B:451:TYR:OH	7:B:3177:HOH:O	2.03	0.75
2:B:1043:MET:O	7:B:3372:HOH:O	2.03	0.75
2:B:1308:ASN:ND2	2:B:1326:TYR:O	2.21	0.73
2:B:234:LYS:O	7:B:3129:HOH:O	2.07	0.73
2:B:1286:ASN:ND2	7:B:3469:HOH:O	2.23	0.71
2:B:783:ARG:NH2	7:B:3308:HOH:O	2.23	0.71
2:B:1183:GLU:OE2	7:B:3430:HOH:O	2.08	0.71
1:A:76:A:H5"	7:A:2228:HOH:O	1.92	0.70
2:B:1049:GLU:OE2	7:B:3373:HOH:O	2.12	0.67
2:B:1335:ARG:NH2	4:D:7:DG:O6	2.28	0.67
3:C:2:DA:N3	7:C:2004:HOH:O	2.27	0.67
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.28	0.66
2:B:1207:GLU:O	7:B:3438:HOH:O	2.13	0.66
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.76	0.66
2:B:261:ASP:O	7:B:3133:HOH:O	2.15	0.65
1:A:64:U:OP1	7:A:2188:HOH:O	2.12	0.65
2:B:245:SER:HB3	2:B:296:LEU:HG	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:849:ASP:HB3	2:B:854:ASN:HD22	1.63	0.64
2:B:141:LYS:NZ	7:B:3099:HOH:O	2.30	0.64
3:C:3:DA:H1'	3:C:4:DT:H5'	1.79	0.64
2:B:248:LEU:O	7:B:3132:HOH:O	2.15	0.63
2:B:898:ASP:O	2:B:905:ARG:NH2	2.31	0.63
7:A:2224:HOH:O	2:B:1358:THR:HG21	1.99	0.61
2:B:185:PHE:N	7:B:3116:HOH:O	2.33	0.61
2:B:758:ASN:OD1	2:B:954:LYS:NZ	2.34	0.60
2:B:874:GLU:HG2	2:B:878:LYS:HE3	1.84	0.60
1:A:33:G:N2	1:A:36:A:OP2	2.34	0.60
2:B:405:PHE:O	7:B:3159:HOH:O	2.16	0.60
2:B:629:ARG:HE	2:B:655:ARG:HD3	1.66	0.59
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.83	0.59
2:B:1295:ASN:OD1	2:B:1298:ARG:NH2	2.34	0.59
2:B:1046:PHE:HB2	7:B:3372:HOH:O	2.03	0.59
7:A:2066:HOH:O	2:B:71:ARG:NH2	2.36	0.58
2:B:635:ARG:NH1	7:B:3259:HOH:O	2.36	0.58
2:B:780:ARG:NH1	2:B:806:LEU:O	2.35	0.58
2:B:1180:ASP:OD1	7:B:3428:HOH:O	2.17	0.58
2:B:349:GLU:HG3	2:B:356:LYS:HD3	1.85	0.58
1:A:59:U:OP1	2:B:467:ARG:NH2	2.36	0.57
2:B:516:GLU:HA	2:B:519:THR:HG22	1.86	0.57
1:A:62:G:OP1	7:A:2183:HOH:O	2.17	0.57
2:B:525:THR:HG22	2:B:690:ASN:HB3	1.87	0.57
1:A:5:C:OP1	2:B:515:TYR:OH	2.22	0.56
2:B:584:GLU:O	2:B:584:GLU:HG3	2.05	0.56
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.86	0.56
2:B:605:ASP:OD1	7:B:3250:HOH:O	2.17	0.56
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.88	0.56
2:B:672:ASP:HA	2:B:703:THR:HG22	1.88	0.56
2:B:442:LYS:HE3	2:B:476:TRP:HA	1.88	0.55
2:B:1300:LYS:O	2:B:1305:GLN:NE2	2.39	0.55
2:B:1037:PHE:O	2:B:1041:ASN:ND2	2.34	0.55
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.89	0.55
2:B:244:LEU:HD11	2:B:264:LEU:HD11	1.88	0.55
2:B:951:ARG:NH1	2:B:1011:GLY:HA3	2.22	0.54
2:B:192:TYR:OH	7:B:3122:HOH:O	2.10	0.54
2:B:139:ARG:HH21	2:B:160:HIS:CE1	2.25	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.42	0.53
2:B:826:GLN:OE1	7:B:3314:HOH:O	2.19	0.53
2:B:326:ASP:OD2	7:B:3146:HOH:O	2.18	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TYR:OH	2:B:627:GLU:HG2	2.08	0.52
2:B:957:THR:HG23	7:B:3343:HOH:O	2.09	0.52
2:B:564:LEU:HD23	2:B:580:ILE:HD13	1.91	0.52
2:B:893:THR:HG23	2:B:896:LYS:H	1.75	0.52
2:B:1350:GLN:NE2	7:B:3035:HOH:O	2.23	0.52
2:B:251:ASN:HB2	2:B:263:LYS:HD2	1.93	0.51
1:A:68:A:HO2'	1:A:69:A:P	2.34	0.51
1:A:27:G:N2	1:A:44:U:OP2	2.44	0.51
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.93	0.50
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.92	0.50
2:B:951:ARG:HH12	2:B:1011:GLY:HA3	1.77	0.50
2:B:1117:ASP:OD1	2:B:1117:ASP:N	2.44	0.50
2:B:825:ASP:HA	7:B:3312:HOH:O	2.10	0.50
2:B:1146:VAL:HG13	2:B:1191:LYS:HB2	1.92	0.50
3:C:2:DA:H2'	3:C:3:DA:C8	2.47	0.49
2:B:253:LYS:HA	2:B:258:LEU:HD12	1.95	0.49
2:B:212:LEU:HD12	2:B:246:LEU:HD21	1.94	0.48
2:B:525:THR:HG23	2:B:545:LYS:HE2	1.95	0.48
2:B:817:GLN:O	2:B:882:TYR:OH	2.32	0.47
2:B:216:LEU:HD22	2:B:220:ARG:HG2	1.96	0.47
2:B:777:SER:HB3	2:B:803:ASN:HB2	1.97	0.47
7:A:2008:HOH:O	2:B:694:MET:HG2	2.14	0.47
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.97	0.47
2:B:862:LYS:HG3	7:B:3325:HOH:O	2.15	0.46
2:B:814:TYR:CZ	2:B:830:ILE:HG23	2.50	0.46
2:B:245:SER:HA	2:B:297:SER:HB3	1.96	0.46
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.98	0.46
4:D:3:DT:H2"	4:D:4:DG:C8	2.51	0.46
2:B:63:ARG:NH2	7:B:3056:HOH:O	2.48	0.46
2:B:133:PRO:HG2	2:B:137:HIS:CE1	2.50	0.46
2:B:758:ASN:HD22	2:B:995:THR:HG22	1.81	0.46
2:B:1216:SER:OG	2:B:1217:ALA:N	2.49	0.45
1:A:42:A:O2'	1:A:43:G:OP1	2.31	0.45
2:B:1001:TYR:OH	7:B:3362:HOH:O	2.13	0.45
2:B:158:LEU:HA	2:B:161:MET:HE3	1.98	0.45
2:B:869:ASN:OD1	2:B:870:VAL:N	2.41	0.45
2:B:527:VAL:HA	2:B:582:GLY:HA3	1.99	0.44
1:A:27:G:H4'	1:A:28:A:OP2	2.17	0.44
1:A:74:A:H3'	1:A:75:A:H8	1.81	0.44
2:B:1277:SER:HA	2:B:1281:ILE:HG12	1.99	0.44
1:A:56:U:OP2	7:A:2166:HOH:O	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.51	0.44
2:B:1349:HIS:HB2	2:B:1358:THR:OG1	2.17	0.44
2:B:265:GLN:O	2:B:271:TYR:HB2	2.18	0.43
2:B:187:GLN:O	2:B:191:THR:HG22	2.18	0.43
2:B:877:LYS:HE3	2:B:877:LYS:HB2	1.74	0.43
1:A:27:G:H2'	7:A:2106:HOH:O	2.18	0.43
1:A:8:A:N7	7:A:2034:HOH:O	2.36	0.43
1:A:68:A:O2'	1:A:69:A:OP1	2.27	0.43
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.82	0.43
2:B:699:ASP:OD1	2:B:701:SER:OG	2.25	0.43
2:B:1122:ARG:HG3	2:B:1134:PHE:CE2	2.54	0.43
2:B:918:LYS:HE3	2:B:918:LYS:HB2	1.80	0.42
2:B:1291:LEU:O	2:B:1295:ASN:ND2	2.50	0.42
1:A:18:A:OP1	2:B:165:ARG:HD3	2.20	0.42
2:B:314:LYS:HB3	2:B:314:LYS:HE2	1.75	0.42
2:B:306:LEU:HD22	2:B:316:PRO:HB2	2.00	0.42
2:B:296:LEU:HD13	7:B:3116:HOH:O	2.18	0.42
2:B:398:LEU:HG	2:B:399:LEU:HG	2.02	0.42
1:A:69:A:H5'	2:B:1349:HIS:CE1	2.55	0.42
2:B:22:THR:OG1	2:B:23:ASP:N	2.52	0.42
5:E:17:DA:H2'	5:E:18:DA:C8	2.55	0.42
2:B:122:ILE:H	2:B:122:ILE:HG12	1.45	0.41
1:A:74:A:H3'	1:A:75:A:C8	2.55	0.41
2:B:342:GLN:HB2	2:B:383:MET:HE3	2.03	0.41
2:B:296:LEU:HD12	2:B:296:LEU:O	2.20	0.41
2:B:652:LYS:HE2	2:B:652:LYS:HB3	1.79	0.41
2:B:521:TYR:O	2:B:525:THR:OG1	2.36	0.41
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.54	0.41
2:B:245:SER:CB	2:B:296:LEU:HG	2.46	0.41
2:B:521:TYR:CE1	2:B:684:LYS:HG2	2.56	0.41
2:B:534:MET:H	2:B:534:MET:HG2	1.61	0.41
2:B:901:THR:O	2:B:904:GLU:HG2	2.21	0.40
2:B:1177:ASN:HA	2:B:1178:PRO:HD2	1.92	0.40
2:B:116:HIS:HA	2:B:117:PRO:HD3	1.82	0.40
2:B:234:LYS:HB3	2:B:234:LYS:HE3	1.81	0.40
2:B:796:LEU:HD23	2:B:796:LEU:HA	1.95	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
2	B	1296/1372 (94%)	1249 (96%)	47 (4%)	0	100 100

There are no Ramachandran outliers to report.

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
2	B	1175/1226 (96%)	1092 (93%)	83 (7%)	14 23

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	27	VAL
2	B	43	ILE
2	B	73	THR
2	B	82	LEU
2	B	95	ASP
2	B	102	GLU
2	B	112	LYS
2	B	122	ILE
2	B	123	VAL
2	B	165	ARG
2	B	182	ASP
2	B	188	LEU
2	B	191	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	195	LEU
2	B	215	ARG
2	B	216	LEU
2	B	234	LYS
2	B	244	LEU
2	B	265	GLN
2	B	377	LYS
2	B	402	GLN
2	B	419	LEU
2	B	425	ARG
2	B	445	THR
2	B	455	LEU
2	B	465	MET
2	B	471	GLU
2	B	507	VAL
2	B	524	LEU
2	B	525	THR
2	B	530	VAL
2	B	534	MET
2	B	540	LEU
2	B	586	ARG
2	B	598	LEU
2	B	599	LYS
2	B	627	GLU
2	B	634	GLU
2	B	635	ARG
2	B	638	THR
2	B	650	GLN
2	B	666	LEU
2	B	696	LEU
2	B	703	THR
2	B	709	GLN
2	B	710	LYS
2	B	712	GLN
2	B	718	ASP
2	B	738	LEU
2	B	751	MET
2	B	776	ASN
2	B	782	LYS
2	B	801	VAL
2	B	803	ASN
2	B	811	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	830	ILE
2	B	842	VAL
2	B	856	VAL
2	B	859	ARG
2	B	868	ASP
2	B	870	VAL
2	B	884	ARG
2	B	887	LEU
2	B	918	LYS
2	B	919	ARG
2	B	921	LEU
2	B	924	THR
2	B	935	LEU
2	B	945	GLU
2	B	1007	GLU
2	B	1031	LYS
2	B	1076	LYS
2	B	1089	MET
2	B	1091	GLN
2	B	1119	LEU
2	B	1207	GLU
2	B	1210	ARG
2	B	1263	LYS
2	B	1266	LEU
2	B	1284	ASP
2	B	1334	LYS
2	B	1342	VAL
2	B	1346	THR

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	20 (25%)	3 (3%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	28	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	29	G
1	A	32	A
1	A	34	A
1	A	35	A
1	A	37	U
1	A	38	A
1	A	39	G
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	69	A
1	A	72	U
1	A	74	A
1	A	75	A
1	A	77	A
1	A	78	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	27	G
1	A	42	A
1	A	68	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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	A	82/83 (98%)	-0.14	4 (4%) 29 28	16, 32, 109, 144	0
2	B	1310/1372 (95%)	0.20	74 (5%) 24 23	14, 37, 75, 132	0
3	C	9/11 (81%)	0.64	1 (11%) 5 4	34, 45, 85, 132	0
4	D	10/11 (90%)	0.34	1 (10%) 7 6	28, 44, 89, 100	0
5	E	17/17 (100%)	-0.67	0 100 100	23, 28, 35, 38	0
All	All	1428/1494 (95%)	0.17	80 (5%) 24 23	14, 36, 77, 144	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ASP	9.2
2	B	293	ALA	7.6
1	A	74	A	4.9
2	B	271	TYR	4.8
2	B	264	LEU	4.8
2	B	1037	PHE	4.7
2	B	297	SER	4.6
3	C	1	DC	4.5
2	B	296	LEU	4.0
2	B	286	TYR	4.0
2	B	290	PHE	4.0
2	B	184	LEU	3.8
2	B	783	ARG	3.7
2	B	278	LEU	3.7
2	B	356	LYS	3.5
2	B	309	ASN	3.4
4	D	12	DG	3.4
1	A	75	A	3.4
2	B	220	ARG	3.4
2	B	275	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	287	ALA	3.3
1	A	76	A	3.3
2	B	259	ALA	3.2
2	B	776	ASN	3.2
2	B	181	VAL	3.1
2	B	270	THR	3.1
2	B	1050	ILE	3.1
2	B	244	LEU	3.1
2	B	800	PRO	3.0
2	B	1033	THR	3.0
2	B	215	ARG	2.9
2	B	291	LEU	2.9
2	B	284	ASP	2.8
2	B	1326	TYR	2.8
2	B	273	ASP	2.8
2	B	191	THR	2.7
2	B	1068	GLU	2.7
2	B	268	LYS	2.7
2	B	802	GLU	2.7
2	B	279	LEU	2.7
2	B	300	ILE	2.6
2	B	280	ALA	2.6
2	B	260	GLU	2.6
2	B	777	SER	2.5
2	B	192	TYR	2.5
2	B	294	LYS	2.5
2	B	246	LEU	2.5
2	B	850	ASP	2.5
2	B	199	ASN	2.5
2	B	219	SER	2.5
1	A	73	G	2.4
2	B	1296	LYS	2.4
2	B	250	PRO	2.4
2	B	689	ALA	2.4
2	B	188	LEU	2.4
2	B	778	ARG	2.4
2	B	258	LEU	2.4
2	B	200	PRO	2.3
2	B	1012	ASP	2.3
2	B	305	ILE	2.3
2	B	266	LEU	2.3
2	B	775	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	214	ALA	2.2
2	B	265	GLN	2.2
2	B	1042	ILE	2.2
2	B	262	ALA	2.1
2	B	1032	ALA	2.1
2	B	195	LEU	2.1
2	B	311	GLU	2.1
2	B	584	GLU	2.1
2	B	339	VAL	2.1
2	B	277	ASN	2.1
2	B	804	THR	2.1
2	B	185	PHE	2.1
2	B	302	LEU	2.0
2	B	1067	GLY	2.0
2	B	182	ASP	2.0
2	B	1039	TYR	2.0
2	B	806	LEU	2.0
2	B	782	LYS	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
6	MG	B	2368	1/1	0.32	0.27	31,31,31,31	0
6	MG	B	2367	1/1	0.77	0.14	43,43,43,43	0
6	MG	A	1084	1/1	0.82	0.34	50,50,50,50	0
6	MG	B	2365	1/1	0.86	0.21	22,22,22,22	0
6	MG	B	2366	1/1	0.88	0.15	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	1082	1/1	0.92	0.15	29,29,29,29	0
6	MG	A	1083	1/1	0.96	0.14	6,6,6,6	0
6	MG	A	1085	1/1	0.96	0.18	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.