



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:09 PM UTC

PDB ID : 7OX9 / pdb_00007ox9
Title : Target-bound SpCas9 complex with AAVS1 all-RNA guide
Authors : Pacesa, M.; Donohoue, P.; May, A.P.; Jinek, M.; Cameron, P.
Deposited on : 2021-06-22
Resolution : 2.45 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

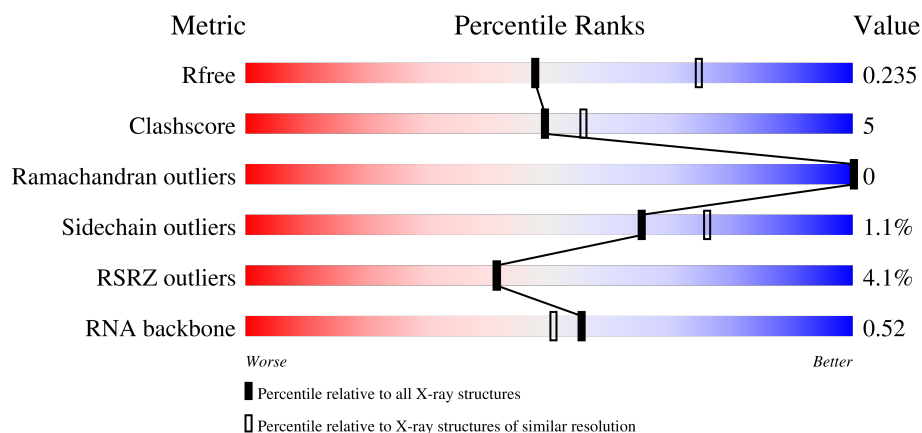
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	84	56% 39% 5%
2	B	1372	4% 84% 13% •
3	C	28	75% 25%
4	D	12	8% 75% 17% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13970 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	84	Total	C	N	O	P	0	0	1
			1772	790	331	568	83			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1338	Total	C	N	O	S	0	0	0
			10930	6962	1898	2048	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 AAVS1 target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			559	268	98	166	27			

- Molecule 4 is a DNA chain called AAVS1 non-target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	1
			209	100	35	64	10			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	K	0	0
			3	3		
6	B	6	Total	K	0	0
			6	6		
6	C	2	Total	K	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	150	Total	O	0	0
			150	150		
7	B	302	Total	O	0	0
			302	302		
7	C	23	Total	O	0	0
			23	23		
7	D	12	Total	O	0	0
			12	12		

3 Residue-property plots

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.

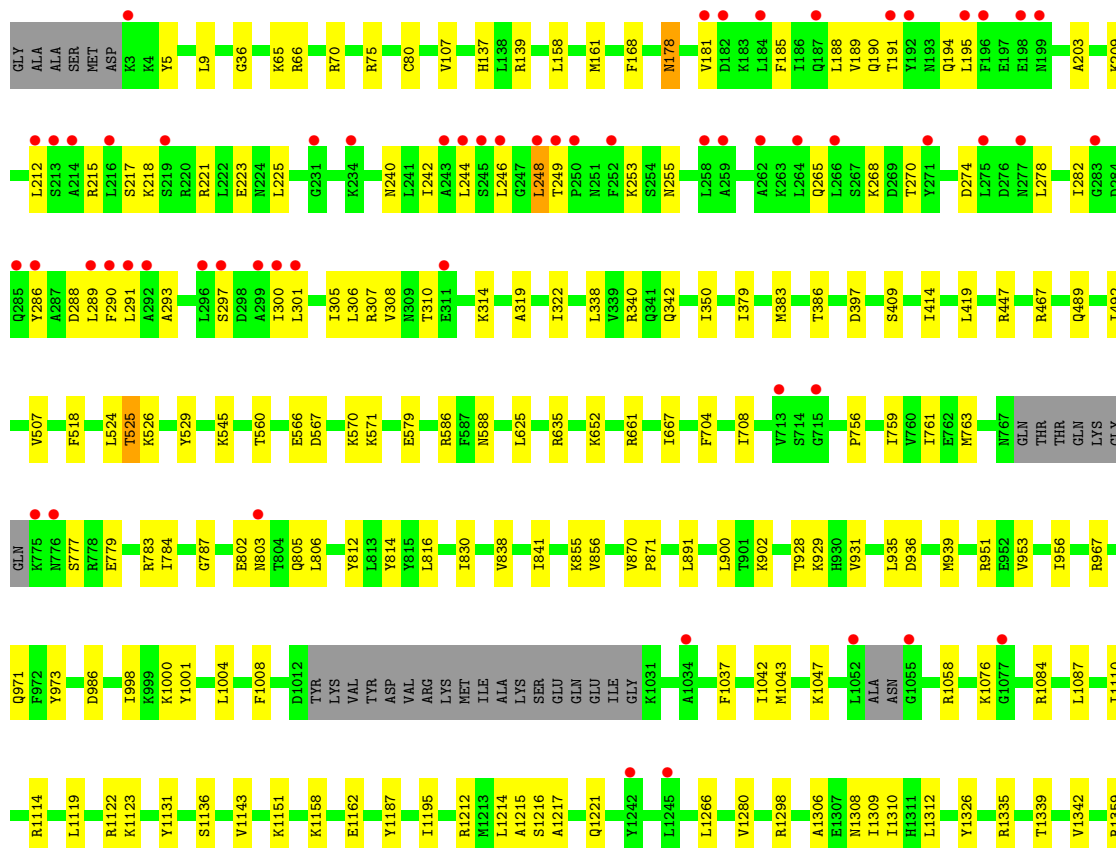
- Molecule 1: sgRNA

Chain A: 



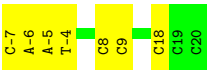
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

Chain B: 

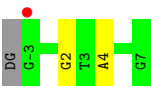
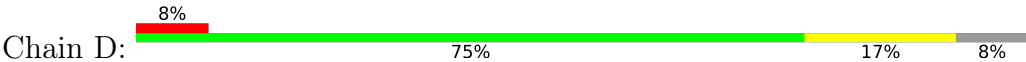




● Molecule 3: AAVS1 target DNA strand



● Molecule 4: AAVS1 non-target DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.08Å 68.20Å 187.77Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	48.16 – 2.45 48.16 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.16-2.45) 99.2 (48.16-2.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.195 , 0.233 0.199 , 0.235	Depositor DCC
R_{free} test set	4373 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13970	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	0.16	0/1987	0.37	0/3100
2	B	0.16	0/11122	0.37	2/14942 (0.0%)
3	C	0.27	0/624	0.51	0/958
4	D	0.28	0/233	0.53	0/360
All	All	0.17	0/13966	0.38	2/19360 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	525	THR	CA-C-N	-5.68	113.22	122.65
2	B	525	THR	C-N-CA	-5.68	113.22	122.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1772	0	883	24	0
2	B	10930	0	11106	117	0
3	C	559	0	316	7	0
4	D	209	0	116	3	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	3	0	0	0	0
6	B	6	0	0	0	0
6	C	2	0	0	0	0
7	A	150	0	0	1	0
7	B	302	0	0	8	0
7	C	23	0	0	0	0
7	D	12	0	0	0	0
All	All	13970	0	12421	139	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 5.

All (139) 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:305:ILE:HD11	2:B:409:SER:HB2	1.64	0.79
2:B:215:ARG:HD2	2:B:307:ARG:HH21	1.56	0.71
2:B:158:LEU:HD22	2:B:419:LEU:HD12	1.74	0.69
2:B:939:MET:HE3	2:B:953:VAL:HG21	1.73	0.69
2:B:80:CYS:SG	7:B:1750:HOH:O	2.51	0.68
1:A:71:U:H2'	1:A:72:U:C6	2.29	0.68
2:B:967:ARG:NH2	7:B:1502:HOH:O	2.25	0.68
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.80	0.63
1:A:22:U:H2'	1:A:23:U:C6	2.35	0.62
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.31	0.62
2:B:1047:LYS:O	2:B:1076:LYS:NZ	2.28	0.62
1:A:59:U:OP1	2:B:467:ARG:NH2	2.32	0.61
2:B:635:ARG:NH1	7:B:1504:HOH:O	2.32	0.61
2:B:870:VAL:HG21	2:B:902:LYS:HB3	1.83	0.61
2:B:240:ASN:ND2	2:B:255:ASN:OD1	2.34	0.60
3:C:-6:DA:H2'	3:C:-5:DA:C8	2.37	0.60
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.84	0.59
2:B:195:LEU:HD21	2:B:286:TYR:CD1	2.37	0.58
1:A:49:A:N3	2:B:1122:ARG:NH2	2.50	0.58
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.37	0.58
1:A:46:A:H2'	1:A:47:A:C8	2.40	0.57
2:B:178:ASN:HD21	2:B:310:THR:HG23	1.70	0.56
2:B:756:PRO:HD2	2:B:939:MET:HE1	1.88	0.56
2:B:181:VAL:HB	2:B:209:LYS:HD2	1.85	0.56
2:B:195:LEU:HD21	2:B:286:TYR:HD1	1.69	0.56
2:B:297:SER:O	2:B:301:LEU:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.40	0.55
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.90	0.54
2:B:181:VAL:HG13	2:B:300:ILE:HD11	1.90	0.54
2:B:779:GLU:O	2:B:783:ARG:HG2	2.08	0.53
2:B:704:PHE:O	2:B:708:ILE:HG12	2.08	0.53
2:B:168:PHE:CG	2:B:447:ARG:HD2	2.44	0.53
2:B:342:GLN:HB2	2:B:383:MET:HE3	1.90	0.53
2:B:248:LEU:HG	2:B:265:GLN:HB2	1.92	0.52
2:B:567:ASP:HA	2:B:571:LYS:HD3	1.92	0.52
2:B:1136:SER:HA	4:D:2:DG:O3'	2.10	0.52
2:B:190:GLN:O	2:B:194:GLN:HG2	2.10	0.51
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.93	0.51
2:B:447:ARG:NH2	7:B:1512:HOH:O	2.44	0.51
2:B:1114:ARG:NH1	4:D:4:DA:OP1	2.44	0.51
2:B:288:ASP:O	2:B:291:LEU:HB3	2.11	0.50
2:B:218:LYS:HB3	2:B:246:LEU:HB3	1.92	0.50
2:B:489:GLN:NE2	7:B:1508:HOH:O	2.42	0.50
3:C:-5:DA:H4'	3:C:-4:DT:OP1	2.11	0.50
1:A:54:G:H2'	1:A:55:C:C6	2.47	0.50
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.94	0.49
2:B:759:ILE:HD11	2:B:939:MET:HE2	1.95	0.49
3:C:-7:DC:H3'	3:C:-6:DA:H8	1.77	0.49
2:B:189:VAL:HG21	2:B:203:ALA:HB2	1.95	0.49
2:B:936:ASP:OD1	2:B:951:ARG:NH1	2.45	0.49
3:C:-7:DC:H2'	3:C:-7:DC:O2	2.12	0.49
1:A:77:A:N7	7:A:204:HOH:O	2.34	0.49
1:A:33:G:H5'	1:A:34:A:OP2	2.13	0.48
2:B:225:LEU:HD23	2:B:242:ILE:HG21	1.96	0.48
1:A:70:C:H2'	1:A:71:U:H6	1.78	0.48
2:B:290:PHE:O	2:B:293:ALA:HB3	2.14	0.48
1:A:63:U:N3	2:B:65:LYS:HD2	2.29	0.47
2:B:529:TYR:HA	2:B:579:GLU:O	2.13	0.47
2:B:956:ILE:HD11	2:B:998:ILE:HD13	1.97	0.47
2:B:518:PHE:CD1	2:B:667:ILE:HD12	2.50	0.47
2:B:586:ARG:NH2	7:B:1518:HOH:O	2.48	0.47
2:B:274:ASP:O	2:B:278:LEU:N	2.46	0.46
2:B:956:ILE:HA	2:B:1008:PHE:O	2.15	0.46
2:B:1212:ARG:NH1	7:B:1506:HOH:O	2.40	0.46
2:B:1151:LYS:HD2	2:B:1158:LYS:HD2	1.97	0.46
2:B:139:ARG:HG2	2:B:161:MET:HE3	1.98	0.45
2:B:812:TYR:CZ	2:B:816:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:814:TYR:CZ	2:B:830:ILE:HG13	2.51	0.45
1:A:4:G:OP1	2:B:661:ARG:HD3	2.17	0.45
2:B:338:LEU:HD13	2:B:386:THR:HG22	1.98	0.45
2:B:526:LYS:HD3	2:B:526:LYS:HA	1.61	0.45
2:B:756:PRO:HD2	2:B:939:MET:CE	2.46	0.45
1:A:3:G:H2'	1:A:4:G:C8	2.51	0.45
2:B:763:MET:HE1	2:B:931:VAL:HG21	1.98	0.45
2:B:217:SER:O	2:B:221:ARG:HG3	2.17	0.45
2:B:268:LYS:HG3	2:B:270:THR:H	1.81	0.45
2:B:107:VAL:HG23	2:B:1131:TYR:CE1	2.51	0.45
2:B:971:GLN:HG2	2:B:973:TYR:OH	2.16	0.45
3:C:-7:DC:H3'	3:C:-6:DA:C8	2.52	0.45
2:B:188:LEU:O	2:B:191:THR:HG22	2.16	0.45
2:B:1162:GLU:OE2	2:B:1187:TYR:OH	2.32	0.45
2:B:350:ILE:HD11	2:B:379:ILE:HD13	1.99	0.44
2:B:178:ASN:ND2	2:B:310:THR:HG23	2.32	0.44
2:B:560:THR:HA	2:B:586:ARG:HA	1.98	0.44
2:B:777:SER:HB2	2:B:803:ASN:HB2	1.98	0.44
2:B:802:GLU:H	2:B:805:GLN:HE21	1.66	0.44
2:B:218:LYS:HD3	2:B:246:LEU:HA	1.99	0.44
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.99	0.44
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.98	0.44
2:B:870:VAL:HG22	2:B:871:PRO:HD2	1.99	0.44
1:A:22:U:H2'	1:A:23:U:H6	1.79	0.43
1:A:74:A:OP1	1:A:74:A:H8	2.00	0.43
2:B:278:LEU:O	2:B:282:ILE:HG12	2.18	0.43
2:B:212:LEU:HD22	2:B:246:LEU:HD11	2.00	0.43
2:B:1339:THR:O	2:B:1342:VAL:HG22	2.17	0.43
1:A:61:C:OP2	2:B:70:ARG:HD3	2.19	0.43
1:A:70:C:H2'	1:A:71:U:C6	2.52	0.43
2:B:763:MET:HE3	2:B:763:MET:HB2	1.89	0.43
1:A:1:G:OP1	2:B:929:LYS:NZ	2.39	0.43
2:B:652:LYS:HB3	2:B:652:LYS:HE2	1.80	0.43
2:B:841:ILE:HD13	2:B:900:LEU:HG	2.00	0.43
2:B:1037:PHE:HZ	2:B:1058:ARG:HH12	1.67	0.43
1:A:41:A:OP2	2:B:340:ARG:NH2	2.51	0.43
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	2.01	0.43
2:B:1216:SER:OG	2:B:1217:ALA:N	2.51	0.42
2:B:1266:LEU:HD22	2:B:1309:ILE:HD12	2.01	0.42
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.19	0.42
2:B:305:ILE:HG22	2:B:306:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:ARG:NH2	2:B:588:ASN:HA	2.35	0.42
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.19	0.42
1:A:74:A:H3'	1:A:75:A:H8	1.84	0.42
2:B:185:PHE:CE1	2:B:225:LEU:HD21	2.54	0.42
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.84	0.42
2:B:314:LYS:HB3	2:B:314:LYS:HE2	1.76	0.42
2:B:838:VAL:HG12	2:B:855:LYS:HE2	2.00	0.42
2:B:137:HIS:HA	2:B:322:ILE:HD11	2.00	0.42
2:B:244:LEU:HA	2:B:249:THR:OG1	2.20	0.42
2:B:524:LEU:HG	2:B:545:LYS:HG2	2.01	0.42
3:C:8:DC:H2'	3:C:9:DC:C6	2.54	0.42
2:B:1308:ASN:HB3	2:B:1326:TYR:CD1	2.55	0.41
2:B:307:ARG:NH2	2:B:397:ASP:OD2	2.46	0.41
2:B:492:ILE:HD13	2:B:492:ILE:HA	1.92	0.41
2:B:1216:SER:OG	7:B:1501:HOH:O	2.22	0.41
1:A:69:A:H2'	1:A:70:C:C6	2.55	0.41
2:B:566:GLU:O	2:B:570:LYS:HB3	2.21	0.41
2:B:784:ILE:HD12	2:B:806:LEU:HD13	2.01	0.41
1:A:15:C:P	2:B:66:ARG:HH11	2.44	0.41
1:A:30:C:H2'	1:A:31:U:C6	2.55	0.41
1:A:32:A:H2'	1:A:33:G:O4'	2.21	0.41
1:A:69:A:H2'	1:A:70:C:H6	1.85	0.41
2:B:526:LYS:HG3	3:C:18:DC:H2''	2.03	0.41
2:B:489:GLN:HG3	2:B:625:LEU:HD21	2.02	0.41
2:B:1119:LEU:HD23	2:B:1119:LEU:HA	1.93	0.41
2:B:1309:ILE:HA	2:B:1312:LEU:HD12	2.03	0.41
2:B:935:LEU:O	2:B:939:MET:HG2	2.21	0.41
2:B:1000:LYS:HG3	2:B:1001:TYR:CE1	2.56	0.41
2:B:306:LEU:HD21	2:B:414:ILE:HD13	2.03	0.40
2:B:5:TYR:OH	2:B:756:PRO:HD3	2.22	0.40
2:B:763:MET:SD	2:B:928:THR:HG22	2.61	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	1330/1372 (97%)	1278 (96%)	52 (4%)	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	
2	B	1199/1226 (98%)	1186 (99%)	13 (1%)	65	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	75	ARG
2	B	178	ASN
2	B	223	GLU
2	B	248	LEU
2	B	253	LYS
2	B	507	VAL
2	B	525	THR
2	B	856	VAL
2	B	1084	ARG
2	B	1087	LEU
2	B	1123	LYS
2	B	1214	LEU
2	B	1298	ARG

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

Mol	Chain	Res	Type
2	B	240	ASN
2	B	255	ASN
2	B	295	ASN

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Mol	Chain	Res	Type
2	B	341	GLN
2	B	436	ASN
2	B	501	ASN
2	B	723	HIS
2	B	799	HIS
2	B	805	GLN
2	B	807	GLN
2	B	826	GLN
2	B	920	GLN
2	B	1041	ASN
2	B	1101	GLN
2	B	1311	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	81/84 (96%)	14 (17%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	C
1	A	11	G
1	A	20	U
1	A	28	A
1	A	29	G
1	A	35	A
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	72	U
1	A	73	G
1	A	75	A
1	A	77	A

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	84/84 (100%)	-0.63	0 100 100	34, 53, 148, 224	0
2	B	1338/1372 (97%)	0.10	59 (4%) 39 38	32, 62, 111, 169	0
3	C	28/28 (100%)	-0.49	0 100 100	38, 54, 123, 135	0
4	D	11/12 (91%)	-0.06	1 (9%) 15 12	43, 66, 120, 131	0
All	All	1461/1496 (97%)	0.04	60 (4%) 41 41	32, 61, 113, 224	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	262	ALA	4.6
2	B	181	VAL	3.9
2	B	246	LEU	3.6
2	B	244	LEU	3.5
2	B	1055	GLY	3.5
2	B	1245	LEU	3.4
2	B	191	THR	3.4
2	B	296	LEU	3.3
2	B	195	LEU	3.2
2	B	775	LYS	3.2
2	B	292	ALA	3.1
2	B	1077	GLY	3.1
2	B	198	GLU	3.0
2	B	264	LEU	3.0
2	B	289	LEU	3.0
2	B	1367	GLY	2.9
2	B	299	ALA	2.9
2	B	283	GLY	2.9
2	B	250	PRO	2.9
2	B	216	LEU	2.9
2	B	245	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	248	LEU	2.8
2	B	277	ASN	2.7
2	B	1034	ALA	2.7
2	B	1052	LEU	2.7
2	B	713	VAL	2.6
2	B	285	GLN	2.6
2	B	187	GLN	2.6
2	B	184	LEU	2.5
2	B	715	GLY	2.5
2	B	266	LEU	2.5
2	B	192	TYR	2.5
2	B	300	ILE	2.5
2	B	249	THR	2.4
2	B	291	LEU	2.4
2	B	3	LYS	2.4
2	B	213	SER	2.4
2	B	182	ASP	2.4
2	B	301	LEU	2.4
2	B	252	PHE	2.3
2	B	803	ASN	2.3
2	B	199	ASN	2.3
2	B	271	TYR	2.3
2	B	776	ASN	2.3
2	B	290	PHE	2.3
2	B	214	ALA	2.2
2	B	1242	TYR	2.3
2	B	275	LEU	2.2
2	B	212	LEU	2.2
4	D	-3	DG	2.2
2	B	196	PHE	2.2
2	B	259	ALA	2.1
2	B	243	ALA	2.1
2	B	297	SER	2.1
2	B	258	LEU	2.1
2	B	234	LYS	2.1
2	B	231	GLY	2.0
2	B	311	GLU	2.0
2	B	286	TYR	2.0
2	B	219	SER	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
6	K	B	1401	1/1	0.63	0.24	123,123,123,123	0
6	K	B	1406	1/1	0.69	0.14	107,107,107,107	0
6	K	C	102	1/1	0.82	0.11	116,116,116,116	0
6	K	A	105	1/1	0.90	0.14	83,83,83,83	0
6	K	B	1402	1/1	0.90	0.12	81,81,81,81	0
6	K	B	1404	1/1	0.92	0.08	91,91,91,91	0
6	K	B	1403	1/1	0.96	0.05	77,77,77,77	0
6	K	C	101	1/1	0.97	0.06	73,73,73,73	0
6	K	B	1405	1/1	0.98	0.04	60,60,60,60	0
5	MG	A	102	1/1	0.99	0.02	35,35,35,35	0
6	K	A	103	1/1	0.99	0.04	39,39,39,39	0
6	K	A	104	1/1	0.99	0.05	53,53,53,53	0
5	MG	A	101	1/1	0.99	0.07	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.