



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:22 PM UTC

PDB ID : 5FQ5 / pdb_00005fq5
Title : Crystal structure of Cas9-sgRNA-DNA complex solved by native SAD phasing
Authors : Olieric, V.; Weinert, T.; Finke, A.; Anders, C.; Jinek, M.; Wang, M.
Deposited on : 2015-12-07
Resolution : 2.14 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

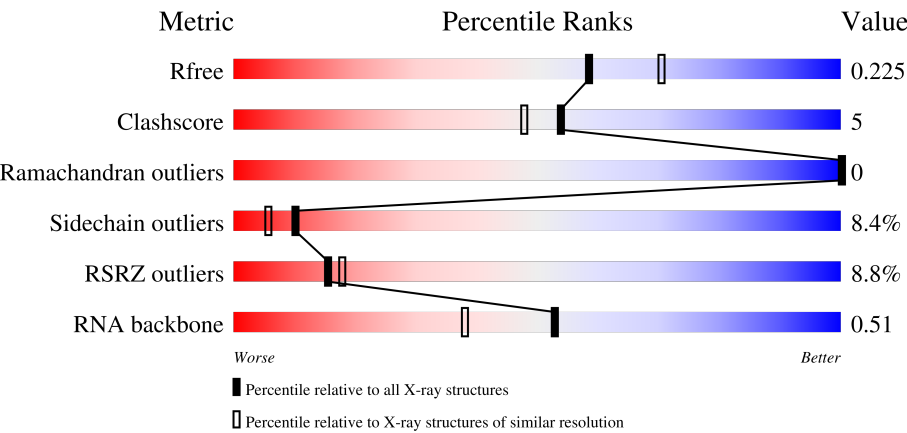
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)
RNA backbone	3983	1030 (2.48-1.80)

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	70%24%5%•
2	B	1372	9% 81%14%••
3	C	11	27% 36%45%18%
4	D	11	9% 64%27%9%

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Mol	Chain	Length	Quality of chain
5	E	17	 88% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26622 atoms, of which 12243 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	83	Total	C	H	N	O	P	0	0	1
			2605	778	868	318	559	82			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	1318	Total	C	H	N	O	S	0	2	0
			21749	6877	10959	1874	2017	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	H	N	O	P	0	0	0
			279	86	102	34	49	8			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	10	Total	C	H	N	O	P	0	0	0
			323	100	117	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	H	N	O	P	0	0	0
			543	169	197	59	102	16			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	K	0	0
			3	3		
7	B	9	Total	K	0	0
			9	9		
7	D	1	Total	K	0	0
			1	1		

- Molecule 8 is water.

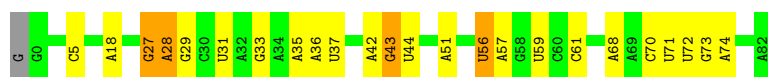
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	301	Total	O	0	0
			301	301		
8	B	744	Total	O	0	0
			744	744		
8	C	6	Total	O	0	0
			6	6		
8	D	10	Total	O	0	0
			10	10		
8	E	47	Total	O	0	0
			47	47		

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.

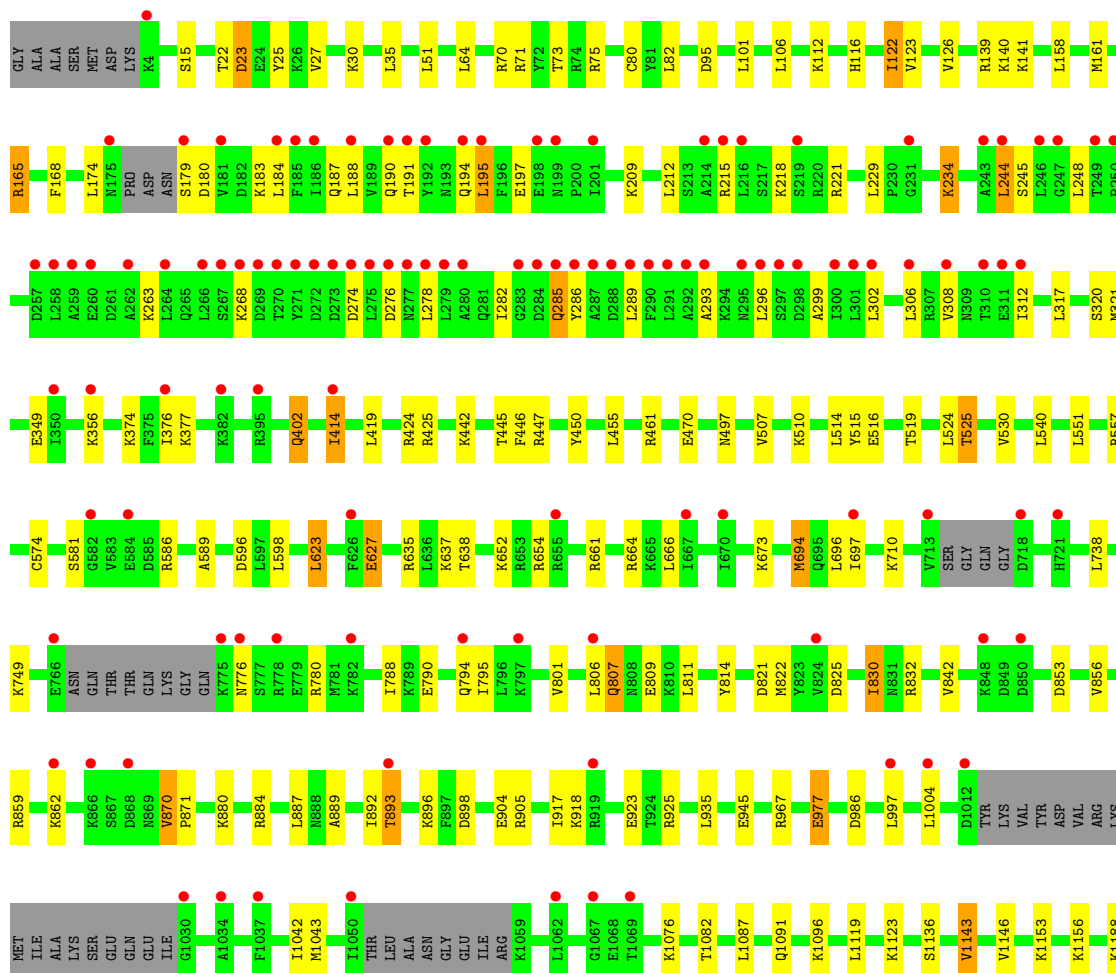
• Molecule 1: SGRNA

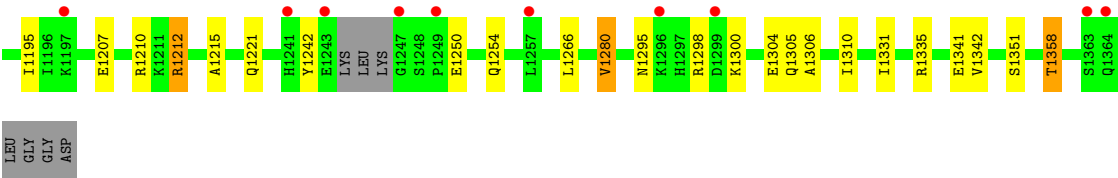
Chain A: 



• Molecule 2: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1

Chain B: 





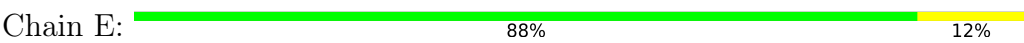
● Molecule 3: TARGET DNA STRAND PROXIMAL FRAGMENT



● Molecule 4: NON-TARGET DNA STRAND



● Molecule 5: TARGET DNA STRAND DISTAL FRAGMENT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.74Å 67.57Å 188.19Å 90.00° 111.31° 90.00°	Depositor
Resolution (Å)	47.91 – 2.14 47.91 – 2.14	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.91-2.14) 97.8 (47.91-2.14)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.191 , 0.225 0.193 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26622	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.15	0/1947	0.38	0/3033
2	B	0.16	0/10984	0.35	0/14754
3	C	0.27	0/198	0.53	0/302
4	D	0.26	0/230	0.56	0/355
5	E	0.23	0/387	0.50	0/596
All	All	0.16	0/13746	0.37	0/19040

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 [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	1737	868	868	15	0
2	B	10790	10959	10957	105	0
3	C	177	102	102	4	0
4	D	206	117	117	5	0
5	E	346	197	197	1	0
6	A	2	0	0	0	0
7	A	3	0	0	0	0
7	B	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
8	A	301	0	0	6	0
8	B	744	0	0	47	2
8	C	6	0	0	0	0
8	D	10	0	0	0	0
8	E	47	0	0	0	0
All	All	14379	12243	12241	123	2

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 (123) 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:248:LEU:O	8:B:3181:HOH:O	1.75	1.01
2:B:229:LEU:O	8:B:3174:HOH:O	1.78	0.99
2:B:825:ASP:N	8:B:3473:HOH:O	2.05	0.89
2:B:321:MET:SD	8:B:3205:HOH:O	2.31	0.86
2:B:306:LEU:O	2:B:320:SER:OG	1.92	0.86
2:B:574:CYS:SG	8:B:3350:HOH:O	2.32	0.85
2:B:652:LYS:O	8:B:3388:HOH:O	1.93	0.85
2:B:285:GLN:O	8:B:3191:HOH:O	1.94	0.84
7:B:2369:K:K	8:B:3174:HOH:O	1.86	0.84
2:B:581:SER:O	8:B:3355:HOH:O	1.96	0.84
2:B:80:CYS:SG	8:B:3074:HOH:O	2.35	0.82
2:B:282:ILE:O	8:B:3189:HOH:O	1.97	0.81
2:B:276:ASP:O	8:B:3186:HOH:O	2.01	0.78
1:A:27:G:H5'	1:A:28:A:H5''	1.66	0.77
2:B:116:HIS:ND1	8:B:3115:HOH:O	2.19	0.75
3:C:9:DC:O2	4:D:4:DG:N2	2.23	0.71
2:B:190:GLN:OE1	8:B:3166:HOH:O	2.09	0.70
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.25	0.69
2:B:180:ASP:OD2	2:B:209:LYS:NZ	2.25	0.69
1:A:56:U:OP2	8:A:3217:HOH:O	2.10	0.68
1:A:33:G:N2	1:A:36:A:OP2	2.26	0.68
2:B:859:ARG:NH1	8:B:3480:HOH:O	2.22	0.65
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.30	0.65
1:A:27:G:H5'	1:A:28:A:C5'	2.26	0.64
2:B:139:ARG:NH2	8:B:3132:HOH:O	2.30	0.64
1:A:44:U:O2'	2:B:402:GLN:OE1	2.10	0.63
2:B:1335:ARG:NH2	4:D:7:DG:O6	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:ARG:NH1	2:B:806:LEU:O	2.32	0.61
2:B:809:GLU:OE2	8:B:3463:HOH:O	2.16	0.61
2:B:1295:ASN:OD1	2:B:1298:ARG:NH2	2.31	0.61
2:B:299:ALA:HB3	8:B:3154:HOH:O	2.02	0.59
2:B:286:TYR:HA	8:B:3191:HOH:O	2.04	0.57
1:A:27:G:H4'	1:A:28:A:OP2	2.05	0.56
2:B:516:GLU:HA	2:B:519:THR:HG22	1.87	0.54
4:D:3:DT:H2''	4:D:4:DG:H5'	1.89	0.54
2:B:967:ARG:NH2	8:B:3545:HOH:O	2.32	0.54
8:A:3084:HOH:O	2:B:71:ARG:NH2	2.41	0.53
2:B:187:GLN:HG3	8:B:3163:HOH:O	2.09	0.53
2:B:557:ARG:NH1	8:B:3336:HOH:O	2.35	0.52
2:B:1156:LYS:NZ	8:B:3635:HOH:O	2.35	0.52
3:C:2:DA:H2'	3:C:3:DA:C8	2.44	0.52
2:B:191:THR:HG23	2:B:289:LEU:HD12	1.92	0.52
1:A:43:G:OP1	8:A:3150:HOH:O	2.19	0.52
4:D:3:DT:H2''	4:D:4:DG:C8	2.45	0.52
1:A:57:A:N1	8:A:3223:HOH:O	2.33	0.51
2:B:1082:THR:HB	8:B:3024:HOH:O	2.11	0.51
2:B:1210:ARG:NH2	8:B:3676:HOH:O	2.43	0.51
2:B:195:LEU:HG	8:B:3191:HOH:O	2.11	0.51
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.94	0.50
2:B:116:HIS:CE1	2:B:122:ILE:HG23	2.46	0.50
2:B:184:LEU:HB2	8:B:3154:HOH:O	2.11	0.50
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.94	0.49
2:B:187:GLN:O	2:B:191:THR:HG22	2.12	0.49
2:B:245:SER:N	8:B:3178:HOH:O	2.46	0.48
2:B:141:LYS:NZ	8:B:3135:HOH:O	2.45	0.48
2:B:450:TYR:OH	2:B:627:GLU:HG2	2.13	0.48
2:B:497:ASN:ND2	8:B:3290:HOH:O	2.46	0.48
2:B:519:THR:HG23	2:B:589:ALA:HB1	1.96	0.48
2:B:140:LYS:NZ	8:B:3133:HOH:O	2.46	0.47
2:B:898:ASP:O	2:B:905:ARG:NH2	2.47	0.47
2:B:977:GLU:OE2	2:B:1242:TYR:OH	2.26	0.47
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.48	0.47
2:B:821:ASP:HB3	8:B:3473:HOH:O	2.14	0.47
2:B:870:VAL:HG22	2:B:871:PRO:HD2	1.97	0.47
3:C:3:DA:H1'	3:C:4:DT:H5'	1.98	0.46
2:B:25:TYR:C	8:B:3024:HOH:O	2.59	0.46
2:B:880:LYS:NZ	2:B:904:GLU:OE2	2.42	0.45
2:B:293:ALA:HB1	8:B:3178:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:GLU:HG3	2:B:1310:ILE:CG2	2.46	0.45
2:B:35:LEU:HB2	2:B:1358:THR:HB	1.98	0.45
2:B:862:LYS:HE3	8:B:3503:HOH:O	2.18	0.45
2:B:244:LEU:HD21	8:B:3182:HOH:O	2.17	0.44
2:B:296:LEU:HA	8:B:3154:HOH:O	2.17	0.44
2:B:349:GLU:HG3	2:B:356:LYS:HD3	1.98	0.44
2:B:1210:ARG:HA	2:B:1280:VAL:HG22	2.00	0.44
2:B:30:LYS:NZ	8:B:3025:HOH:O	2.49	0.44
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.99	0.44
2:B:195:LEU:HD11	2:B:285:GLN:HB2	1.99	0.44
2:B:807:GLN:HE21	2:B:807:GLN:HA	1.83	0.44
1:A:28:A:OP2	2:B:126:VAL:HG22	2.18	0.44
2:B:661:ARG:NH1	8:B:3407:HOH:O	2.37	0.44
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.18	0.44
2:B:168:PHE:CG	2:B:447:ARG:HD2	2.52	0.43
2:B:1300:LYS:O	2:B:1305:GLN:NE2	2.50	0.43
3:C:4:DT:H4'	3:C:5:DA:OP1	2.18	0.43
2:B:442:LYS:NZ	8:B:3252:HOH:O	2.47	0.43
2:B:278:LEU:HG	8:B:3188:HOH:O	2.17	0.43
2:B:317:LEU:HD22	2:B:414:ILE:HD11	2.01	0.43
2:B:461[B]:ARG:HD2	8:B:3267:HOH:O	2.19	0.43
2:B:814:TYR:CE2	2:B:830:ILE:HG23	2.54	0.43
2:B:525:THR:HG21	8:B:3417:HOH:O	2.17	0.43
2:B:623:LEU:HG	2:B:654:ARG:O	2.19	0.43
1:A:28:A:N6	8:A:3139:HOH:O	2.52	0.43
1:A:61:C:OP2	2:B:70:ARG:HD3	2.19	0.43
8:A:3297:HOH:O	2:B:749:LYS:NZ	2.50	0.42
2:B:1153:LYS:O	8:B:3633:HOH:O	2.21	0.42
2:B:218:LYS:HG3	2:B:248:LEU:HD21	2.02	0.42
2:B:694:MET:HE2	2:B:694:MET:HA	2.00	0.42
2:B:1096:LYS:NZ	8:B:3590:HOH:O	2.44	0.42
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	2.02	0.42
1:A:18:A:OP1	2:B:165:ARG:HD3	2.19	0.42
2:B:180:ASP:HB3	2:B:183:LYS:HG2	2.02	0.42
5:E:17:DA:H2'	5:E:18:DA:C8	2.54	0.42
1:A:5:C:OP1	2:B:515:TYR:OH	2.29	0.42
2:B:15:SER:HA	2:B:51:LEU:O	2.19	0.41
2:B:673:LYS:HE3	2:B:673:LYS:HB2	1.96	0.41
2:B:893:THR:HG22	2:B:896:LYS:H	1.84	0.41
2:B:234:LYS:HE3	2:B:234:LYS:HB3	1.93	0.41
2:B:516:GLU:O	2:B:519:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:ARG:HH22	2:B:1341:GLU:CD	2.29	0.41
2:B:165:ARG:NH2	2:B:446:PHE:O	2.54	0.41
1:A:71:U:H2'	1:A:72:U:O4'	2.20	0.41
2:B:158:LEU:HA	2:B:161:MET:HE3	2.01	0.41
2:B:22:THR:OG1	2:B:23:ASP:N	2.53	0.41
2:B:795:ILE:HG12	8:B:3465:HOH:O	2.21	0.41
2:B:1250:GLU:O	2:B:1254:GLN:HG3	2.20	0.41
2:B:221:ARG:NH2	8:B:3172:HOH:O	2.54	0.41
2:B:923:GLU:OE1	2:B:925:ARG:HD3	2.21	0.41
2:B:822:MET:HE1	2:B:892:ILE:HG21	2.03	0.40
2:B:514:LEU:CD2	2:B:664:ARG:HG3	2.52	0.40
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	2.02	0.40
1:A:70:C:H2'	1:A:71:U:C6	2.57	0.40
2:B:1136:SER:HA	4:D:7:DG:O3'	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:3346:HOH:O	8:B:3398:HOH:O[4_546]	2.14	0.06
8:B:3169:HOH:O	8:B:3419:HOH:O[4_546]	2.18	0.02

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	1306/1372 (95%)	1267 (97%)	39 (3%)	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	1183/1226 (96%)	1084 (92%)	99 (8%)	10 6

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	23	ASP
2	B	27	VAL
2	B	64	LEU
2	B	73	THR
2	B	75	ARG
2	B	82	LEU
2	B	95	ASP
2	B	101	LEU
2	B	106	LEU
2	B	112	LYS
2	B	122	ILE
2	B	123	VAL
2	B	165	ARG
2	B	174	LEU
2	B	179	SER
2	B	188	LEU
2	B	194	GLN
2	B	195	LEU
2	B	197	GLU
2	B	212	LEU
2	B	215	ARG
2	B	234	LYS
2	B	244	LEU
2	B	263	LYS
2	B	268	LYS
2	B	274	ASP
2	B	285	GLN
2	B	302	LEU
2	B	308	VAL
2	B	312	ILE

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Mol	Chain	Res	Type
2	B	374	LYS
2	B	376	ILE
2	B	377	LYS
2	B	402	GLN
2	B	414	ILE
2	B	419	LEU
2	B	424	ARG
2	B	425	ARG
2	B	445	THR
2	B	455	LEU
2	B	470	GLU
2	B	507	VAL
2	B	510	LYS
2	B	524	LEU
2	B	525	THR
2	B	530	VAL
2	B	540	LEU
2	B	551	LEU
2	B	586	ARG
2	B	598	LEU
2	B	623	LEU
2	B	627	GLU
2	B	635	ARG
2	B	637	LYS
2	B	638	THR
2	B	666	LEU
2	B	694	MET
2	B	696	LEU
2	B	697	ILE
2	B	710	LYS
2	B	738	LEU
2	B	776	ASN
2	B	788	ILE
2	B	794	GLN
2	B	801	VAL
2	B	807	GLN
2	B	811	LEU
2	B	830	ILE
2	B	832	ARG
2	B	842	VAL
2	B	853	ASP
2	B	856	VAL

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Mol	Chain	Res	Type
2	B	870	VAL
2	B	884	ARG
2	B	887	LEU
2	B	893	THR
2	B	917	ILE
2	B	918	LYS
2	B	935	LEU
2	B	945	GLU
2	B	977	GLU
2	B	997	LEU
2	B	1076	LYS
2	B	1087	LEU
2	B	1091	GLN
2	B	1119	LEU
2	B	1123	LYS
2	B	1143	VAL
2	B	1146	VAL
2	B	1188	LYS
2	B	1207	GLU
2	B	1212	ARG
2	B	1266	LEU
2	B	1280	VAL
2	B	1304	GLU
2	B	1331	ILE
2	B	1342	VAL
2	B	1351	SER
2	B	1358	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	199	ASN
2	B	394	ASN
2	B	650	GLN
2	B	885	GLN
2	B	980	ASN
2	B	983	HIS
2	B	1264	HIS
2	B	1350	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/84 (95%)	12 (15%)	2 (2%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	28	A
1	A	29	G
1	A	31	U
1	A	35	A
1	A	37	U
1	A	43	G
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	73	G
1	A	74	A

All (2) RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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, 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	83/84 (98%)	-0.65	0 100 100	28, 44, 145, 192	0
2	B	1318/1372 (96%)	0.44	123 (9%) 14 16	20, 54, 104, 151	2 (0%)
3	C	9/11 (81%)	1.17	3 (33%) 1 1	50, 73, 122, 140	0
4	D	10/11 (90%)	0.27	1 (10%) 12 14	38, 63, 115, 135	0
5	E	17/17 (100%)	-0.62	0 100 100	37, 42, 50, 61	0
All	All	1437/1495 (96%)	0.36	127 (8%) 15 18	20, 54, 107, 192	2 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	775	LYS	6.2
2	B	293	ALA	5.8
2	B	264	LEU	5.3
2	B	713	VAL	5.1
2	B	291	LEU	5.1
2	B	1364	GLN	4.8
2	B	1247	GLY	4.8
2	B	191	THR	4.7
2	B	271	TYR	4.6
2	B	1030	GLY	4.5
2	B	296	LEU	4.3
2	B	290	PHE	4.2
2	B	278	LEU	4.2
2	B	286	TYR	4.1
2	B	312	ILE	4.1
2	B	1050	ILE	4.0
2	B	259	ALA	4.0
2	B	1243	GLU	4.0
2	B	175	ASN	3.9
2	B	184	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	280	ALA	3.9
2	B	4	LYS	3.8
2	B	297	SER	3.7
2	B	300	ILE	3.7
2	B	188	LEU	3.6
2	B	776	ASN	3.6
2	B	850	ASP	3.5
2	B	272	ASP	3.5
2	B	356	LYS	3.5
2	B	262	ALA	3.5
2	B	306	LEU	3.5
2	B	269	ASP	3.5
2	B	250	PRO	3.4
2	B	287	ALA	3.4
2	B	179	SER	3.4
2	B	1037	PHE	3.4
2	B	1257	LEU	3.3
2	B	214	ALA	3.2
2	B	186	ILE	3.2
2	B	267	SER	3.2
2	B	249	THR	3.2
2	B	285	GLN	3.2
2	B	270	THR	3.2
2	B	195	LEU	3.1
2	B	298	ASP	3.1
2	B	997	LEU	3.1
2	B	697	ILE	3.1
2	B	295	ASN	3.0
2	B	862	LYS	3.0
2	B	258	LEU	2.9
2	B	275	LEU	2.9
3	C	9	DC	2.9
2	B	310	THR	2.9
2	B	1296	LYS	2.9
2	B	279	LEU	2.9
2	B	192	TYR	2.9
2	B	276	ASP	2.8
2	B	766	GLU	2.8
2	B	219	SER	2.8
2	B	302	LEU	2.8
2	B	1012	ASP	2.7
2	B	284	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	670	ILE	2.7
2	B	778	ARG	2.7
2	B	246	LEU	2.6
2	B	1299	ASP	2.6
2	B	582	GLY	2.6
2	B	376	ILE	2.6
2	B	289	LEU	2.6
2	B	667	ILE	2.5
2	B	273	ASP	2.5
3	C	1	DC	2.5
2	B	231	GLY	2.5
2	B	257	ASP	2.4
2	B	181	VAL	2.4
2	B	311	GLU	2.4
2	B	824	VAL	2.4
2	B	244	LEU	2.4
2	B	266	LEU	2.4
2	B	260	GLU	2.3
2	B	655	ARG	2.3
2	B	1249	PRO	2.3
4	D	3	DT	2.3
2	B	308	VAL	2.3
2	B	1034	ALA	2.3
2	B	215	ARG	2.3
2	B	185	PHE	2.3
2	B	201	ILE	2.3
2	B	277	ASN	2.3
2	B	866	LYS	2.3
2	B	868	ASP	2.3
2	B	283	GLY	2.3
2	B	806	LEU	2.3
2	B	1004	LEU	2.3
2	B	848	LYS	2.2
2	B	1197	LYS	2.2
2	B	721	HIS	2.2
2	B	199	ASN	2.2
2	B	414	ILE	2.2
2	B	797	LYS	2.2
2	B	893	THR	2.2
2	B	243	ALA	2.2
2	B	1363	SER	2.2
2	B	288	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	718	ASP	2.2
3	C	2	DA	2.2
2	B	1241	HIS	2.2
2	B	1062	LEU	2.2
2	B	268	LYS	2.2
2	B	198	GLU	2.1
2	B	626	PHE	2.1
2	B	395	ARG	2.1
2	B	919	ARG	2.1
2	B	782	LYS	2.1
2	B	194	GLN	2.1
2	B	382	LYS	2.1
2	B	216	LEU	2.1
2	B	794	GLN	2.1
2	B	1069	THR	2.1
2	B	247	GLY	2.1
2	B	1067	GLY	2.1
2	B	350	ILE	2.1
2	B	292	ALA	2.1
2	B	584	GLU	2.0
2	B	190	GLN	2.0
2	B	301	LEU	2.0
2	B	274	ASP	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	K	D	1013	1/1	0.75	0.25	121,121,121,121	0
7	K	B	2372	1/1	0.92	0.10	92,92,92,92	0
7	K	B	2370	1/1	0.92	0.11	83,83,83,83	0
7	K	B	2369	1/1	0.93	0.10	58,58,58,58	1
7	K	B	2371	1/1	0.95	0.06	62,62,62,62	0
7	K	B	2365	1/1	0.95	0.06	32,32,32,32	1
7	K	B	2366	1/1	0.95	0.06	38,38,38,38	1
7	K	B	2373	1/1	0.96	0.10	69,69,69,69	1
7	K	B	2368	1/1	0.96	0.06	53,53,53,53	0
7	K	A	1085	1/1	0.97	0.06	49,49,49,49	1
7	K	A	2083	1/1	0.98	0.04	30,30,30,30	1
6	MG	A	1084	1/1	0.98	0.05	29,29,29,29	0
7	K	A	2084	1/1	0.99	0.03	40,40,40,40	1
7	K	B	2367	1/1	0.99	0.04	34,34,34,34	1
6	MG	A	1083	1/1	0.99	0.04	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.