



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:52 am BST

PDB ID : 5W1I
Title : Crystal structure of LbaCas13a (C2c2) bound to mature crRNA (20-nt spacer)
Authors : Knott, G.J.; Doudna, J.A.
Deposited on : 2017-06-03
Resolution : 2.20 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 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	:	2.11
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

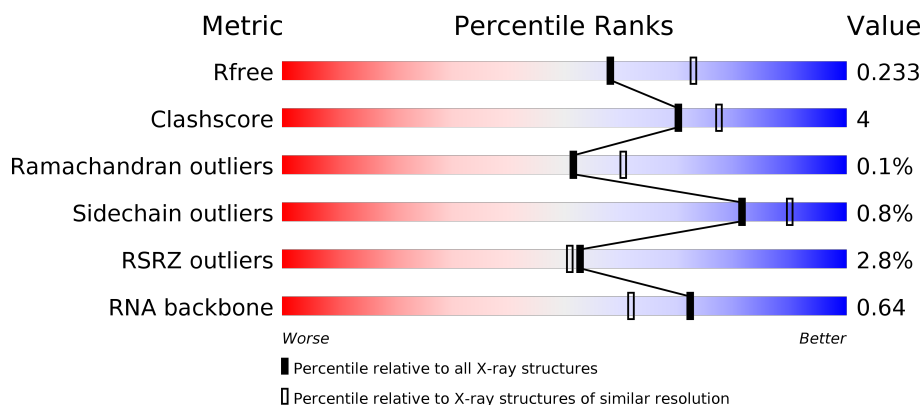
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)
RNA backbone	3102	1032 (2.60-1.80)

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 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 $\leq 5\%$. 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	B	52	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	52	<div> <div>58%</div> <div>17%</div> <div>25%</div> </div>
2	A	1440	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div> </div>
2	C	1440	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	1503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24245 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 mature crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	41	Total	C	N	O	P	0	0	0
			841	377	164	261	39			
1	D	39	Total	C	N	O	P	0	0	0
			801	358	157	248	38			

- Molecule 2 is a protein called LbaCas13a (C2c2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1294	Total	C	N	O	S	0	0	0
			10707	6817	1811	2038	41			
2	C	1298	Total	C	N	O	S	0	0	0
			10737	6834	1817	2045	41			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	I	0	0
			6	6		
3	C	10	Total	I	0	0
			10	10		

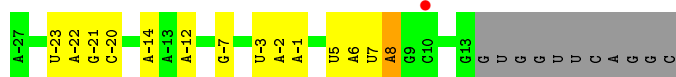
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	77	Total	O	0	0
			77	77		
4	A	428	Total	O	0	0
			428	428		
4	D	99	Total	O	0	0
			99	99		
4	C	539	Total	O	0	0
			539	539		

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.

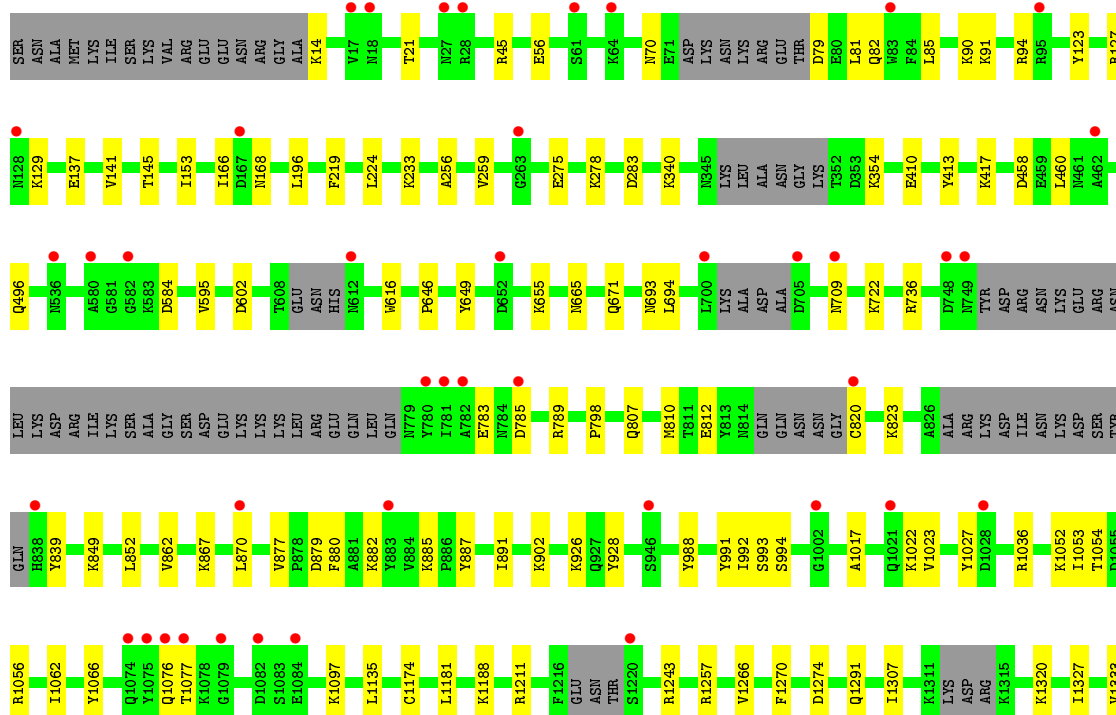
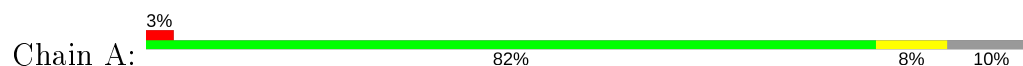
- Molecule 1: mature crRNA

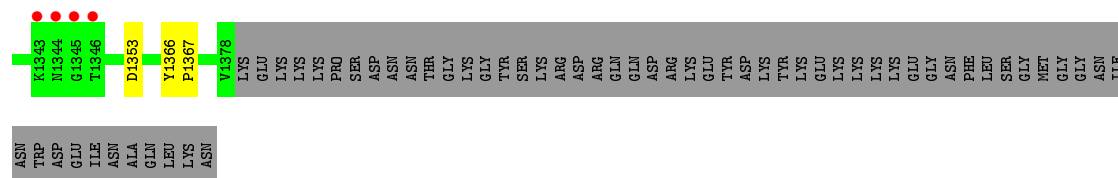


- Molecule 1: mature crRNA

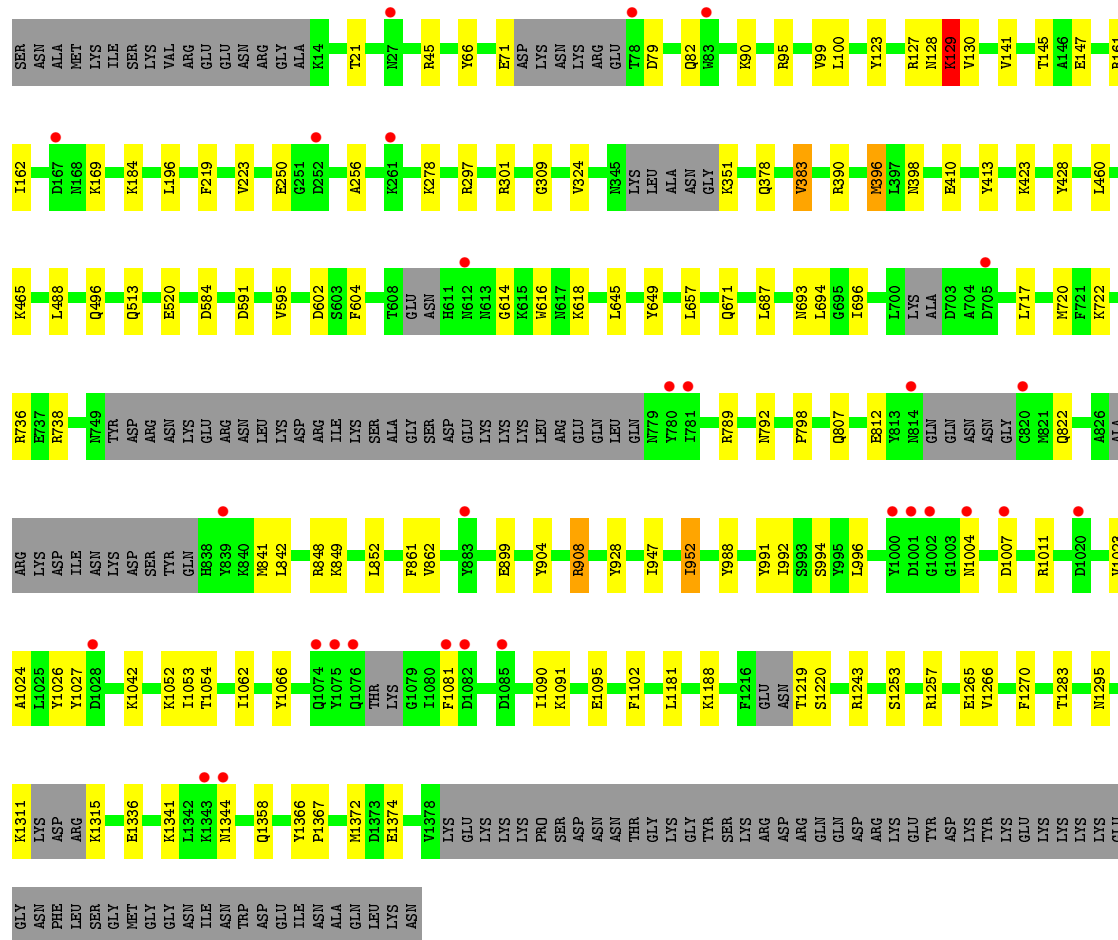
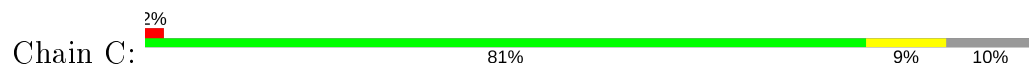


- Molecule 2: LbaCas13a (C2c2)





• Molecule 2: LbaCas13a (C2c2)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	88.78Å 89.21Å 116.31Å 86.14° 86.97° 66.16°	Depositor
Resolution (Å)	48.42 – 2.20 48.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.42-2.20) 89.8 (48.42-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.197 , 0.233 0.197 , 0.233	Depositor DCC
R_{free} test set	2014 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24245	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.16	0/943	0.72	0/1467
1	D	0.16	0/898	0.69	0/1395
2	A	0.24	0/10908	0.38	0/14654
2	C	0.24	0/10938	0.38	0/14694
All	All	0.23	0/23687	0.42	0/32210

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	B	841	0	426	8	0
1	D	801	0	404	7	0
2	A	10707	0	10550	72	0
2	C	10737	0	10572	85	0
3	A	6	0	0	3	0
3	C	10	0	0	2	0
4	A	428	0	0	13	0
4	B	77	0	0	1	0
4	C	539	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	99	0	0	1	0
All	All	24245	0	21952	163	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 (163) 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:A:354:LYS:O	4:A:1601:HOH:O	1.94	0.86
2:C:1253:SER:OG	4:C:1601:HOH:O	2.01	0.77
2:A:91:LYS:NZ	2:A:168:ASN:OD1	2.20	0.74
2:A:283:ASP:OD1	4:A:1602:HOH:O	2.06	0.74
2:A:584:ASP:OD2	4:A:1603:HOH:O	2.07	0.72
2:C:1295:ASN:ND2	2:C:1336:GLU:OE1	2.27	0.68
2:A:785:ASP:OD2	2:A:839:TYR:OH	2.11	0.68
1:D:-4:A:H61	2:C:21:THR:HG23	1.60	0.66
2:A:91:LYS:HE2	2:A:166:ILE:HD13	1.77	0.66
2:A:1274:ASP:OD1	4:A:1604:HOH:O	2.14	0.65
2:A:665:ASN:O	4:A:1606:HOH:O	2.14	0.64
2:A:458:ASP:OD1	4:A:1605:HOH:O	2.14	0.64
2:C:71:GLU:O	2:C:90:LYS:NZ	2.28	0.63
1:D:6:A:OP2	2:C:722:LYS:NZ	2.31	0.63
2:C:95:ARG:HH22	2:C:161:ARG:HH12	1.45	0.63
2:C:693:ASN:HB3	2:C:852:LEU:HD13	1.80	0.62
2:A:1017:ALA:O	4:A:1607:HOH:O	2.16	0.62
1:B:8:A:OP1	2:A:1097:LYS:NZ	2.32	0.62
2:C:591:ASP:OD2	4:C:1602:HOH:O	2.16	0.61
2:A:123:TYR:OH	2:A:127:ARG:NH2	2.33	0.61
2:A:1076:GLN:HG3	2:A:1077:THR:HG23	1.82	0.60
2:C:141:VAL:HG13	2:C:145:THR:HB	1.82	0.60
2:A:123:TYR:CZ	2:A:127:ARG:HD2	2.36	0.59
2:C:513:GLN:OE1	2:C:1042:LYS:NZ	2.36	0.59
2:C:520:GLU:OE2	4:C:1603:HOH:O	2.16	0.58
1:B:6:A:OP2	2:A:722:LYS:NZ	2.36	0.58
2:C:1257:ARG:NH2	2:C:1265:GLU:OE2	2.37	0.58
2:C:1053:ILE:HG13	2:C:1054:THR:HG23	1.86	0.57
2:C:1188:LYS:HE3	3:C:1503:IOD:I	2.75	0.57
2:C:162:ILE:O	4:C:1604:HOH:O	2.17	0.56
2:A:460:LEU:HD22	2:A:1181:LEU:HD21	1.89	0.55
1:D:-7:G:O2'	2:C:21:THR:HG21	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1023:VAL:O	2:A:1066:TYR:OH	2.21	0.55
2:A:14:LYS:N	4:A:1636:HOH:O	2.39	0.54
2:C:614:GLY:O	2:C:618:LYS:NZ	2.39	0.54
2:C:736:ARG:NH1	2:C:798:PRO:O	2.41	0.54
2:A:879:ASP:O	2:A:882:LYS:HG2	2.08	0.53
2:A:1307:ILE:HD11	2:A:1320:LYS:HD2	1.89	0.53
2:A:1053:ILE:HG13	2:A:1054:THR:HG23	1.89	0.53
2:C:250:GLU:OE2	4:C:1605:HOH:O	2.19	0.53
2:C:1311:LYS:O	2:C:1315:LYS:NZ	2.42	0.53
2:A:1023:VAL:HG13	2:A:1062:ILE:HG21	1.91	0.53
2:C:460:LEU:HD22	2:C:1181:LEU:HD21	1.91	0.52
2:A:926:LYS:NZ	4:A:1620:HOH:O	2.31	0.52
1:B:-7:G:H4'	2:A:21:THR:HG21	1.90	0.52
2:A:649:TYR:CE1	2:A:862:VAL:HA	2.46	0.51
2:A:1052:LYS:HD3	2:A:1366:TYR:CE2	2.45	0.51
2:C:657:LEU:HD22	2:C:720:MET:HE3	1.93	0.51
2:C:645:LEU:HD11	2:C:720:MET:HB2	1.92	0.51
2:C:95:ARG:HH21	2:C:99:VAL:HB	1.75	0.51
2:C:822:GLN:HG2	2:C:1283:THR:HG23	1.93	0.50
2:C:496:GLN:NE2	2:C:602:ASP:O	2.44	0.50
2:A:1188:LYS:HE3	3:A:1503:IOD:I	2.82	0.49
2:A:655:LYS:HE2	2:A:877:VAL:HG13	1.93	0.49
2:A:991:TYR:O	2:A:994:SER:OG	2.30	0.49
2:C:147:GLU:OE2	4:C:1606:HOH:O	2.19	0.49
1:D:12:U:H5''	2:C:1341:LYS:HD2	1.95	0.49
2:A:56:GLU:HG2	2:A:233:LYS:HG3	1.94	0.49
2:A:496:GLN:NE2	2:A:602:ASP:O	2.46	0.49
2:C:1052:LYS:HD3	2:C:1366:TYR:CE2	2.48	0.49
2:C:66:TYR:CE2	2:C:184:LYS:HE2	2.48	0.49
2:A:137:GLU:OE1	4:A:1608:HOH:O	2.20	0.49
2:A:823:LYS:NZ	2:A:1291:GLN:OE1	2.40	0.49
2:C:738:ARG:NH2	4:C:1641:HOH:O	2.45	0.48
2:A:45:ARG:HD3	3:C:1506:IOD:I	2.83	0.48
2:A:671:GLN:HB2	2:A:807:GLN:HG2	1.95	0.48
2:A:70:ASN:ND2	4:A:1644:HOH:O	2.44	0.48
2:C:256:ALA:HB1	2:C:278:LYS:HD2	1.94	0.48
2:A:820:CYS:N	4:A:1649:HOH:O	2.46	0.48
2:C:694:LEU:HG	2:C:852:LEU:HD22	1.95	0.48
2:A:595:VAL:HG22	2:A:616:TRP:CD2	2.49	0.47
2:C:671:GLN:HB2	2:C:807:GLN:HG2	1.96	0.47
2:C:1023:VAL:HG13	2:C:1062:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:A:OP2	4:B:101:HOH:O	2.20	0.47
2:A:1257:ARG:NH2	4:A:1652:HOH:O	2.48	0.47
2:C:1091:LYS:NZ	2:C:1095:GLU:OE2	2.37	0.47
2:A:141:VAL:HG13	2:A:145:THR:HB	1.97	0.47
1:D:-4:A:N6	2:C:21:THR:HG23	2.28	0.47
2:C:1081:PHE:CZ	2:C:1090:ILE:HG13	2.49	0.47
2:C:465:LYS:HE2	2:C:465:LYS:HB3	1.80	0.47
2:A:1211:ARG:HG3	3:A:1503:IOD:I	2.85	0.47
2:C:1024:ALA:O	2:C:1026:TYR:N	2.43	0.47
2:C:128:ASN:O	2:C:130:VAL:N	2.48	0.46
2:C:991:TYR:O	2:C:994:SER:OG	2.33	0.46
2:C:996:LEU:HB2	2:C:1102:PHE:HZ	1.79	0.46
2:C:123:TYR:OH	2:C:127:ARG:NH2	2.48	0.46
2:C:789:ARG:NH2	2:C:812:GLU:OE2	2.36	0.46
2:C:1266:VAL:HA	2:C:1270:PHE:HB2	1.96	0.46
2:A:1266:VAL:HA	2:A:1270:PHE:HB2	1.97	0.46
2:C:849:LYS:HD3	2:C:849:LYS:HA	1.71	0.46
2:A:256:ALA:HB1	2:A:278:LYS:HD2	1.98	0.46
2:C:595:VAL:HG22	2:C:616:TRP:CD2	2.51	0.46
2:A:602:ASP:OD2	2:A:902:LYS:NZ	2.46	0.46
2:C:488:LEU:HB3	2:C:947:ILE:HG13	1.96	0.46
2:A:694:LEU:HD13	2:A:852:LEU:HD22	1.98	0.46
2:A:259:VAL:HG11	2:A:275:GLU:HG2	1.98	0.46
2:C:789:ARG:HH12	2:C:792:ASN:HB3	1.81	0.46
2:C:128:ASN:O	2:C:129:LYS:HG2	2.15	0.45
2:A:885:LYS:HA	3:A:1502:IOD:I	2.87	0.45
2:A:646:PRO:HB2	2:A:870:LEU:HD21	1.98	0.45
2:A:90:LYS:O	2:A:94:ARG:HG3	2.17	0.45
2:A:79:ASP:HB3	2:A:82:GLN:HB2	1.99	0.45
2:C:169:LYS:HB3	2:C:169:LYS:HE2	1.81	0.45
2:C:988:TYR:CZ	2:C:992:ILE:HD11	2.52	0.44
2:A:849:LYS:HA	2:A:849:LYS:HD3	1.73	0.44
2:C:45:ARG:NH2	4:C:1635:HOH:O	2.42	0.44
2:C:1366:TYR:CG	2:C:1367:PRO:HA	2.53	0.44
2:C:904:TYR:O	2:C:908:ARG:HB2	2.18	0.44
2:A:870:LEU:HA	2:A:870:LEU:HD23	1.69	0.44
2:C:383:VAL:HG21	2:C:398:ASN:HB3	2.00	0.44
2:C:1023:VAL:O	2:C:1066:TYR:OH	2.26	0.44
2:C:687:LEU:HD21	2:C:848:ARG:HD3	1.99	0.44
2:C:79:ASP:HB3	2:C:82:GLN:HB2	2.00	0.44
2:C:899:GLU:OE1	4:C:1607:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:877:VAL:HG12	2:A:880:PHE:HB2	2.00	0.43
2:C:1219:THR:N	4:C:1658:HOH:O	2.51	0.43
2:C:309:GLY:HA2	2:C:378:GLN:NE2	2.34	0.43
2:C:423:LYS:HG3	2:C:428:TYR:CE2	2.52	0.43
2:A:736:ARG:NH1	2:A:798:PRO:O	2.51	0.43
2:C:396:MET:N	2:C:396:MET:SD	2.92	0.43
2:A:693:ASN:HB3	2:A:852:LEU:HD13	2.00	0.43
2:A:153:ILE:HG21	2:A:224:LEU:HD11	2.01	0.43
2:C:591:ASP:O	2:C:595:VAL:HG23	2.18	0.43
2:C:410:GLU:HA	2:C:413:TYR:CE2	2.54	0.42
2:A:196:LEU:HD13	2:A:219:PHE:CZ	2.55	0.42
2:A:709:ASN:ND2	2:A:867:LYS:HE3	2.34	0.42
2:C:1004:ASN:HD21	2:C:1007:ASP:CG	2.22	0.42
2:C:95:ARG:NE	2:C:95:ARG:HA	2.34	0.42
2:C:351:LYS:HG3	4:C:1949:HOH:O	2.18	0.42
2:A:988:TYR:CZ	2:A:992:ILE:HD11	2.54	0.42
2:C:720:MET:HE1	2:C:861:PHE:CZ	2.55	0.42
2:A:891:ILE:HA	2:A:891:ILE:HD13	1.84	0.42
2:C:196:LEU:HD13	2:C:219:PHE:CZ	2.55	0.42
2:A:887:TYR:O	2:A:891:ILE:HG12	2.19	0.42
2:C:841:MET:HG3	2:C:842:LEU:N	2.35	0.42
1:D:-23:U:H5''	1:D:-22:A:H4'	2.00	0.42
2:C:649:TYR:CE1	2:C:862:VAL:HA	2.55	0.41
2:A:1135:LEU:HD11	2:A:1174:CYS:SG	2.60	0.41
2:A:129:LYS:HE3	2:A:129:LYS:HB2	1.79	0.41
2:C:584:ASP:HB2	4:C:1926:HOH:O	2.19	0.41
2:A:81:LEU:O	2:A:85:LEU:HG	2.21	0.41
2:A:410:GLU:HA	2:A:413:TYR:CE2	2.56	0.41
2:C:378:GLN:HG2	4:C:1749:HOH:O	2.20	0.41
2:A:993:SER:O	2:A:1056:ARG:NH1	2.47	0.41
2:C:696:ILE:HD12	2:C:717:LEU:HD21	2.02	0.41
1:D:-7:G:N7	4:D:105:HOH:O	2.37	0.41
1:B:6:A:O2'	2:A:1036:ARG:NH1	2.52	0.41
2:A:1366:TYR:CG	2:A:1367:PRO:HA	2.55	0.41
2:A:417:LYS:HD2	2:A:417:LYS:H	1.86	0.41
1:B:-2:A:H2'	1:B:-1:A:O4'	2.20	0.41
2:C:100:LEU:HD11	2:C:223:VAL:HG12	2.02	0.41
2:C:129:LYS:HE2	2:C:129:LYS:HB3	1.87	0.41
2:C:297:ARG:HA	2:C:324:VAL:HG11	2.03	0.41
2:C:301:ARG:HD2	2:C:390:ARG:O	2.21	0.41
2:C:604:PHE:CD2	2:C:952:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1327:ILE:HG21	2:A:1333:VAL:HG23	2.02	0.41
1:B:-23:U:H5''	1:B:-22:A:H4'	2.03	0.41
2:C:1358:GLN:HG2	2:C:1372:MET:HE3	2.03	0.41
2:C:789:ARG:NH1	2:C:792:ASN:HB3	2.35	0.41
2:A:1353:ASP:N	2:A:1353:ASP:OD1	2.44	0.40
2:A:789:ARG:HD3	2:A:812:GLU:OE2	2.21	0.40
1:B:-21:G:H2'	1:B:-20:C:C6	2.56	0.40
2:C:100:LEU:HA	2:C:100:LEU:HD23	1.96	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	A	1274/1440 (88%)	1234 (97%)	40 (3%)	0	100	100
2	C	1276/1440 (89%)	1236 (97%)	38 (3%)	2 (0%)	47	55
All	All	2550/2880 (88%)	2470 (97%)	78 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1220	SER
2	C	129	LYS

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	A	1168/1296 (90%)	1161 (99%)	7 (1%)	86	93
2	C	1171/1296 (90%)	1160 (99%)	11 (1%)	78	88
All	All	2339/2592 (90%)	2321 (99%)	18 (1%)	81	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	340	LYS
2	A	783	GLU
2	A	810	MET
2	A	928	TYR
2	A	1022	LYS
2	A	1027	TYR
2	A	1243	ARG
2	C	129	LYS
2	C	383	VAL
2	C	396	MET
2	C	908	ARG
2	C	928	TYR
2	C	952	ILE
2	C	1011	ARG
2	C	1027	TYR
2	C	1243	ARG
2	C	1344	ASN
2	C	1374	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
1	B	37/52 (71%)	6 (16%)	0
1	D	35/52 (67%)	3 (8%)	0
All	All	72/104 (69%)	9 (12%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	-14	A
1	B	-12	A
1	B	-3	U
1	B	5	U
1	B	7	U
1	B	8	A
1	D	-14	A
1	D	-3	U
1	D	5	U

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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 ⓘ

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	B	41/52 (78%)	0.00	1 (2%) 59 56	20, 34, 75, 78	15 (36%)
1	D	39/52 (75%)	-0.04	0 100 100	21, 29, 51, 64	15 (38%)
2	A	1294/1440 (89%)	0.01	46 (3%) 42 41	22, 45, 78, 106	0
2	C	1298/1440 (90%)	-0.13	29 (2%) 62 59	21, 40, 72, 95	0
All	All	2672/2984 (89%)	-0.06	76 (2%) 53 51	20, 42, 75, 106	30 (1%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	883	TYR	6.1
2	A	1077	THR	5.7
2	A	83	TRP	5.7
2	C	83	TRP	5.3
2	A	785	ASP	5.2
2	A	1074	GLN	5.1
2	A	1344	ASN	5.0
2	A	870	LEU	4.9
2	A	167	ASP	4.4
2	C	1001	ASP	4.3
2	C	1343	LYS	4.0
2	C	1075	TYR	3.8
2	A	28	ARG	3.8
2	A	536	ASN	3.7
2	A	1002	GLY	3.7
2	C	1344	ASN	3.6
2	A	1343	LYS	3.6
2	A	1345	GLY	3.5
2	C	820	CYS	3.4
2	C	1002	GLY	3.3
2	A	263	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	1079	GLY	3.3
2	A	780	TYR	3.2
2	C	781	ILE	3.2
2	A	1082	ASP	3.2
2	A	781	ILE	3.1
2	C	1020	ASP	3.1
2	A	652	ASP	3.1
2	A	883	TYR	3.0
2	A	1346	THR	3.0
2	A	1076	GLN	2.9
2	C	78	THR	2.8
2	A	1021	GLN	2.8
1	B	10	C	2.8
2	C	167	ASP	2.8
2	A	612	ASN	2.8
2	C	1004	ASN	2.8
2	C	1082	ASP	2.7
2	A	1075	TYR	2.7
2	A	462	ALA	2.7
2	C	1076	GLN	2.7
2	A	820	CYS	2.6
2	C	252	ASP	2.6
2	A	17	VAL	2.6
2	C	1028	ASP	2.5
2	C	1074	GLN	2.5
2	C	814	ASN	2.5
2	A	61	SER	2.5
2	C	1000	TYR	2.5
2	A	27	ASN	2.5
2	A	748	ASP	2.5
2	C	780	TYR	2.4
2	A	128	ASN	2.4
2	A	582	GLY	2.4
2	C	1085	ASP	2.4
2	A	95	ARG	2.3
2	C	612	ASN	2.3
2	C	1007	ASP	2.3
2	A	580	ALA	2.3
2	A	782	ALA	2.3
2	A	700	LEU	2.2
2	A	705	ASP	2.2
2	A	18	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	1081	PHE	2.2
2	C	705	ASP	2.2
2	A	946	SER	2.2
2	A	838	HIS	2.2
2	A	1220	SER	2.2
2	A	64	LYS	2.1
2	C	261	LYS	2.1
2	A	1084	GLU	2.1
2	C	839	TYR	2.1
2	C	27	ASN	2.1
2	A	749	ASN	2.0
2	A	709	ASN	2.0
2	A	1028	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 carbohydrates 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(\AA^2)	Q<0.9
3	IOD	C	1504	1/1	0.82	0.12	153,153,153,153	1
3	IOD	C	1503	1/1	0.85	0.11	89,89,89,89	1
3	IOD	A	1502	1/1	0.90	0.16	115,115,115,115	1
3	IOD	C	1505	1/1	0.93	0.08	93,93,93,93	1
3	IOD	A	1503	1/1	0.96	0.13	80,80,80,80	1
3	IOD	C	1510	1/1	0.96	0.15	133,133,133,133	1
3	IOD	C	1509	1/1	0.97	0.07	67,67,67,67	1
3	IOD	A	1506	1/1	0.97	0.04	88,88,88,88	1
3	IOD	C	1506	1/1	0.98	0.08	109,109,109,109	1
3	IOD	A	1504	1/1	0.99	0.09	79,79,79,79	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	IOD	C	1507	1/1	0.99	0.05	61,61,61,61	1
3	IOD	C	1502	1/1	0.99	0.10	53,53,53,53	1
3	IOD	C	1508	1/1	1.00	0.11	54,54,54,54	1
3	IOD	A	1505	1/1	1.00	0.13	55,55,55,55	1
3	IOD	C	1501	1/1	1.00	0.11	51,51,51,51	1
3	IOD	A	1501	1/1	1.00	0.10	55,55,55,55	1

6.5 Other polymers [i](#)

There are no such residues in this entry.