



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:50 AM UTC

PDB ID : 8Y04 / pdb_00008y04
Title : Crystal structure of LbCas12a in complex with crRNA and 6nt target DNA
Authors : Lin, X.; Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 3.71 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

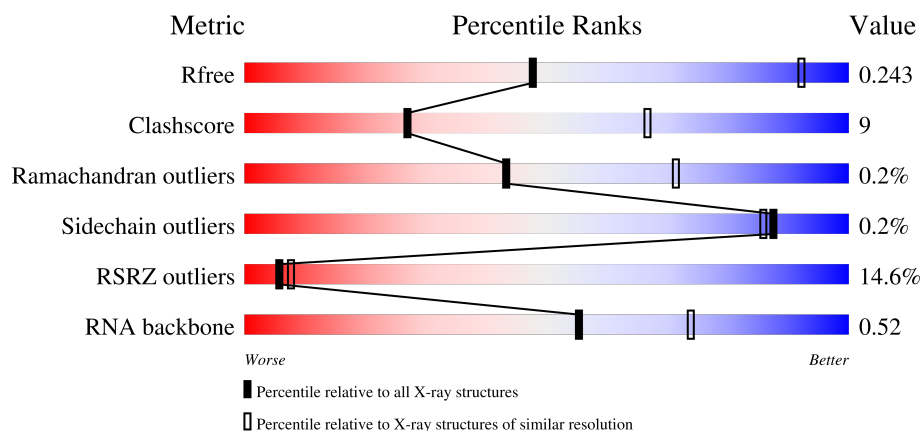
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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	1228	15% 76% 21% .
2	B	40	2% 42% 25% 5% 28%
3	C	15	67% 33%
4	D	11	73% 27%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10967 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LbCas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1202	Total	C	N	O	S	0	0	0
			9824	6318	1607	1870	29			

- Molecule 2 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	29	Total	C	N	O	P	0	0	0
			610	275	106	201	28			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	0	0
			315	148	65	87	15			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			217	107	31	69	10			

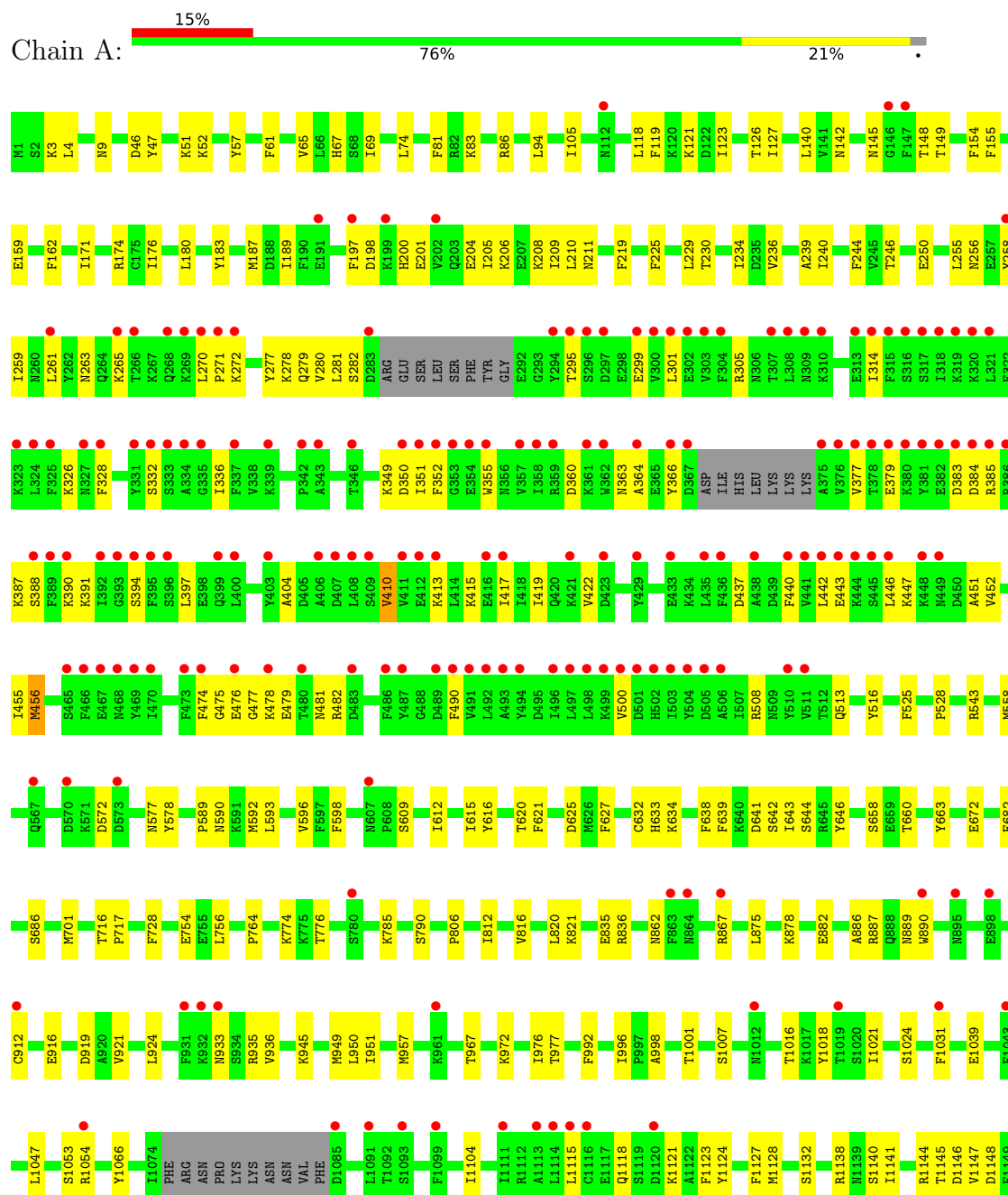
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

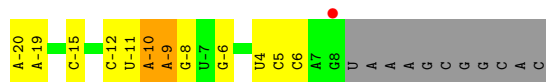
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LbCas12a

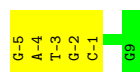




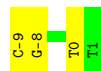
- Molecule 2: RNA (29-MER)



- Molecule 3: DNA (5'-D(P*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3')



- Molecule 4: DNA (5'-D(*CP*GP*TP*CP*CP*TP*TP*TP*AP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.80Å 154.80Å 210.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 3.71 49.27 – 3.71	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.27-3.71) 95.5 (49.27-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.247 0.216 , 0.243	Depositor DCC
R_{free} test set	1453 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10967	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

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	0.15	0/10027	0.37	0/13490
2	B	0.15	0/681	0.36	0/1058
3	C	0.20	0/355	0.35	0/547
4	D	0.23	0/240	0.55	0/368
All	All	0.15	0/11303	0.38	0/15463

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9824	0	9656	185	0
2	B	610	0	312	9	0
3	C	315	0	168	3	0
4	D	217	0	129	3	0
5	A	1	0	0	0	0
All	All	10967	0	10265	194	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 9.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HH12	1:A:440:PHE:HD2	1.07	0.98
1:A:1016:THR:HG1	1:A:1132:SER:HG	1.12	0.89
1:A:835:GLU:HG2	1:A:935:ARG:HB2	1.54	0.88
1:A:774:LYS:NZ	2:B:-8:G:O6	2.07	0.88
1:A:121:LYS:HA	1:A:148:THR:HG21	1.58	0.86
3:C:-4:DA:H2"	3:C:-3:DT:H5"	1.60	0.84
1:A:996:ILE:HD11	1:A:1191:VAL:HG23	1.61	0.83
1:A:263:ASN:HD21	1:A:270:LEU:HB2	1.45	0.82
1:A:83:LYS:HG2	1:A:86:ARG:HG2	1.62	0.81
1:A:442:LEU:HD11	1:A:446:LEU:HD11	1.63	0.81
1:A:305:ARG:NH2	1:A:437:ASP:O	2.15	0.80
1:A:836:ARG:NH2	1:A:1147:VAL:O	2.18	0.76
1:A:74:LEU:HD21	1:A:225:PHE:HB3	1.68	0.75
1:A:305:ARG:NH1	1:A:440:PHE:HD2	1.84	0.75
1:A:142:ASN:O	1:A:145:ASN:ND2	2.20	0.74
1:A:616:TYR:OH	4:D:0:DT:OP1	2.05	0.72
1:A:349:LYS:HB2	1:A:355:TRP:HD1	1.55	0.72
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.72	0.71
1:A:821:LYS:NZ	1:A:1201:ALA:O	2.25	0.70
1:A:383:ASP:O	1:A:387:LYS:N	2.21	0.69
1:A:206:LYS:HA	1:A:210:LEU:HB2	1.74	0.69
1:A:835:GLU:OE2	1:A:1138:ARG:NH1	2.26	0.68
1:A:360:ASP:HA	1:A:363:ASN:HB2	1.76	0.68
1:A:452:VAL:O	1:A:456:MET:HG2	1.95	0.67
1:A:349:LYS:HB2	1:A:355:TRP:CD1	2.30	0.67
1:A:442:LEU:HD11	1:A:446:LEU:CD1	2.25	0.66
1:A:477:GLY:HA3	1:A:479:GLU:HB2	1.78	0.65
1:A:887:ARG:NH1	1:A:889:ASN:OD1	2.30	0.65
1:A:350:ASP:HB3	1:A:417:ILE:HD13	1.80	0.64
1:A:525:PHE:O	1:A:543:ARG:NH2	2.30	0.63
1:A:1115:LEU:HD12	1:A:1123:PHE:HZ	1.63	0.63
1:A:508:ARG:HG3	1:A:890:TRP:CD1	2.34	0.62
1:A:1198:PHE:CZ	1:A:1211:ILE:HD11	2.35	0.62
1:A:174:ARG:HH21	1:A:277:TYR:HB3	1.65	0.61
1:A:377:VAL:HG13	1:A:385:ARG:HH12	1.65	0.61
1:A:360:ASP:O	1:A:364:ALA:N	2.33	0.59
1:A:474:PHE:HE1	1:A:490:PHE:HE2	1.49	0.59
1:A:351:ILE:HD12	1:A:352:PHE:H	1.66	0.59
1:A:51:LYS:HE2	1:A:154:PHE:CD1	2.39	0.58
1:A:835:GLU:HG2	1:A:935:ARG:CB	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:-20:A:O2'	2:B:-11:U:O4	2.15	0.57
1:A:785:LYS:HB2	2:B:-20:A:H5''	1.86	0.57
1:A:263:ASN:CG	1:A:270:LEU:H	2.14	0.56
1:A:543:ARG:HG2	1:A:558:MET:HB2	1.88	0.56
1:A:205:ILE:HG23	1:A:209:ILE:HD12	1.85	0.56
1:A:756:LEU:HD11	1:A:790:SER:HB3	1.88	0.56
1:A:351:ILE:HG22	1:A:413:LYS:CG	2.36	0.56
1:A:377:VAL:HG11	1:A:1054:ARG:HH21	1.70	0.56
1:A:1007:SER:O	1:A:1226:VAL:HG21	2.05	0.55
3:C:-5:DG:H2''	3:C:-4:DA:H5''	1.89	0.55
1:A:951:ILE:HA	1:A:977:THR:HG21	1.89	0.54
1:A:1024:SER:HB3	1:A:1128:MET:HE3	1.90	0.54
1:A:377:VAL:O	1:A:1053:SER:HB2	2.07	0.54
2:B:-10:A:H5'	2:B:-9:A:C2	2.42	0.54
1:A:384:ASP:O	1:A:388:SER:OG	2.19	0.54
1:A:836:ARG:HD2	1:A:1145:THR:HG23	1.90	0.53
1:A:189:ILE:HG23	1:A:271:PRO:HG2	1.89	0.53
1:A:1185:TYR:CZ	1:A:1189:ARG:HD2	2.44	0.53
1:A:46:ASP:HB3	1:A:140:LEU:HD11	1.90	0.53
1:A:351:ILE:HD12	1:A:352:PHE:N	2.22	0.53
1:A:663:TYR:OH	1:A:672:GLU:OE2	2.24	0.53
1:A:836:ARG:NH2	1:A:1144:ARG:O	2.42	0.53
1:A:1194:ALA:HB1	1:A:1211:ILE:HD12	1.91	0.52
1:A:1039:GLU:H	1:A:1039:GLU:CD	2.15	0.52
1:A:1141:ILE:HB	1:A:1144:ARG:HB2	1.91	0.52
1:A:572:ASP:O	1:A:577:ASN:ND2	2.28	0.52
1:A:9:ASN:OD1	1:A:806:PRO:HA	2.09	0.52
1:A:1115:LEU:HD12	1:A:1123:PHE:CZ	2.45	0.52
2:B:-20:A:O2'	2:B:-19:A:OP2	2.28	0.52
2:B:4:U:H2'	2:B:5:C:C6	2.44	0.52
4:D:-9:DC:H2'	4:D:-8:DG:C8	2.44	0.52
1:A:474:PHE:CE1	1:A:490:PHE:HE2	2.28	0.52
1:A:945:LYS:O	1:A:949:MET:HG3	2.09	0.52
1:A:155:PHE:O	1:A:159:GLU:HG3	2.09	0.52
1:A:912:CYS:SG	1:A:957:MET:HE2	2.50	0.52
1:A:366:TYR:CE2	1:A:385:ARG:HG3	2.45	0.51
1:A:263:ASN:ND2	1:A:270:LEU:HB2	2.20	0.51
1:A:620:THR:O	1:A:627:PHE:HA	2.10	0.51
1:A:326:LYS:HD3	1:A:419:ILE:HD11	1.92	0.51
1:A:967:THR:HA	1:A:972:LYS:HB3	1.92	0.51
1:A:764:PRO:HB2	1:A:776:THR:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:MET:O	1:A:596:VAL:HG23	2.10	0.50
1:A:415:LYS:HG2	1:A:419:ILE:HD12	1.93	0.50
1:A:1039:GLU:OE2	1:A:1039:GLU:N	2.35	0.50
1:A:1140:SER:OG	1:A:1148:ASP:OD1	2.30	0.50
1:A:625:ASP:OD1	1:A:625:ASP:N	2.39	0.49
1:A:171:ILE:HG12	1:A:280:VAL:HG21	1.94	0.49
1:A:394:SER:HB3	1:A:475:GLY:HA2	1.95	0.49
1:A:314:ILE:HD13	1:A:500:VAL:HG12	1.95	0.49
1:A:836:ARG:NE	1:A:1145:THR:HA	2.27	0.49
1:A:1018:TYR:HE1	1:A:1124:TYR:HB2	1.76	0.49
1:A:682:PHE:HE1	1:A:728:PHE:HB3	1.78	0.49
1:A:754:GLU:H	1:A:754:GLU:CD	2.21	0.49
1:A:255:LEU:O	1:A:259:ILE:HG13	2.13	0.48
1:A:1031:PHE:CE2	1:A:1047:LEU:HD23	2.48	0.48
1:A:351:ILE:HG22	1:A:413:LYS:HG3	1.96	0.48
1:A:820:LEU:HD11	1:A:921:VAL:HG21	1.95	0.48
1:A:836:ARG:HE	1:A:1145:THR:HA	1.79	0.48
1:A:301:LEU:O	1:A:305:ARG:HG3	2.14	0.48
1:A:3:LYS:NZ	1:A:919:ASP:O	2.32	0.48
1:A:198:ASP:OD1	1:A:200:HIS:N	2.42	0.48
1:A:197:PHE:CZ	1:A:255:LEU:HB3	2.49	0.48
1:A:119:PHE:HZ	1:A:162:PHE:HE2	1.60	0.47
1:A:812:ILE:O	1:A:816:VAL:HG23	2.14	0.47
1:A:1021:ILE:HD11	1:A:1121:LYS:HB3	1.97	0.47
1:A:598:PHE:CE1	1:A:638:PHE:HE2	2.33	0.47
1:A:183:TYR:O	1:A:187:MET:HG3	2.15	0.47
1:A:641:ASP:O	1:A:644:SER:OG	2.27	0.47
1:A:1127:PHE:HD2	1:A:1128:MET:HE2	1.80	0.47
1:A:211:ASN:O	1:A:211:ASN:ND2	2.47	0.47
1:A:61:PHE:O	1:A:65:VAL:HG23	2.14	0.47
1:A:621:PHE:HA	1:A:632:CYS:HB2	1.97	0.46
1:A:615:ILE:HD11	1:A:634:LYS:NZ	2.30	0.46
1:A:404:ALA:HB2	1:A:410:VAL:HG23	1.97	0.46
1:A:118:LEU:HA	1:A:123:ILE:HD13	1.98	0.46
1:A:149:THR:HB	1:A:528:PRO:HB2	1.98	0.46
1:A:204:GLU:HG2	1:A:208:LYS:HG3	1.97	0.46
1:A:886:ALA:O	1:A:887:ARG:HG2	2.15	0.46
1:A:508:ARG:HG3	1:A:890:TRP:CG	2.51	0.46
1:A:589:PRO:O	1:A:593:LEU:HB2	2.16	0.46
3:C:-2:DG:H2'	3:C:-1:DC:C6	2.51	0.46
1:A:69:ILE:HG21	1:A:229:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:GLU:HB3	1:A:482:ARG:HD2	1.98	0.46
1:A:278:LYS:NZ	1:A:282:SER:O	2.46	0.45
1:A:1104:ILE:HD11	1:A:1118:GLN:HG3	1.99	0.45
1:A:52:LYS:N	1:A:52:LYS:HD2	2.31	0.45
1:A:81:PHE:HD2	1:A:94:LEU:HD21	1.81	0.45
1:A:609:SER:OG	1:A:612:ILE:HG13	2.16	0.45
1:A:127:ILE:HD12	1:A:127:ILE:H	1.81	0.45
1:A:176:ILE:O	1:A:180:LEU:HB3	2.17	0.45
1:A:633:HIS:HD2	1:A:660:THR:HG22	1.81	0.45
1:A:590:ASN:OD1	4:D:0:DT:H2''	2.16	0.45
1:A:219:PHE:HE2	1:A:236:VAL:HG12	1.82	0.45
1:A:201:GLU:HB3	1:A:258:TYR:CE2	2.52	0.44
1:A:366:TYR:HE2	1:A:385:ARG:HG3	1.81	0.44
1:A:379:GLU:HG2	1:A:1054:ARG:HG2	1.99	0.44
1:A:67:HIS:CE1	1:A:230:THR:HG21	2.53	0.44
1:A:976:ILE:HB	1:A:992:PHE:CD2	2.52	0.44
1:A:230:THR:O	1:A:234:ILE:HG13	2.17	0.44
1:A:261:LEU:O	1:A:265:LYS:HG2	2.18	0.44
1:A:263:ASN:OD1	1:A:270:LEU:N	2.29	0.44
1:A:240:ILE:HG22	1:A:255:LEU:HG	2.00	0.44
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.83	0.44
1:A:1146:ASP:OD1	1:A:1146:ASP:N	2.43	0.44
1:A:578:TYR:CZ	1:A:701:MET:HE1	2.53	0.43
1:A:642:SER:O	1:A:646:TYR:N	2.51	0.43
1:A:4:LEU:HD12	1:A:916:GLU:HA	2.00	0.43
1:A:385:ARG:HH22	1:A:1054:ARG:HH21	1.65	0.43
1:A:377:VAL:HG11	1:A:1054:ARG:NH2	2.32	0.43
1:A:1150:LEU:HD22	1:A:1162:TYR:HE2	1.83	0.43
1:A:390:LYS:O	1:A:390:LYS:NZ	2.32	0.43
1:A:210:LEU:HD11	1:A:219:PHE:CZ	2.54	0.43
1:A:246:THR:OG1	1:A:250:GLU:HG3	2.19	0.43
1:A:451:ALA:O	1:A:455:ILE:HG12	2.18	0.43
1:A:174:ARG:NH2	1:A:277:TYR:HB3	2.33	0.43
1:A:477:GLY:HA2	1:A:478:LYS:C	2.43	0.43
1:A:998:ALA:O	1:A:1001:THR:OG1	2.31	0.43
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.90	0.42
1:A:377:VAL:CG1	1:A:385:ARG:HH12	2.32	0.42
1:A:225:PHE:CE2	1:A:229:LEU:HD21	2.54	0.42
2:B:-10:A:H4'	2:B:-9:A:H5''	2.01	0.42
1:A:391:LYS:HE3	1:A:391:LYS:HB2	1.87	0.42
1:A:875:LEU:HD23	1:A:875:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PHE:CZ	1:A:397:LEU:HD11	2.53	0.42
1:A:639:PHE:O	1:A:643:ILE:HG13	2.19	0.42
1:A:47:TYR:CZ	1:A:51:LYS:HE3	2.55	0.42
1:A:332:SER:O	1:A:336:ILE:HG12	2.19	0.42
1:A:658:SER:OG	1:A:672:GLU:OE1	2.37	0.42
1:A:716:THR:HA	1:A:717:PRO:HD3	1.89	0.42
1:A:862:ASN:ND2	1:A:867:ARG:HG2	2.35	0.42
1:A:878:LYS:O	1:A:882:GLU:HG3	2.20	0.42
1:A:456:MET:HG2	1:A:456:MET:H	1.49	0.42
1:A:516:TYR:OH	2:B:-15:C:OP1	2.30	0.42
1:A:1211:ILE:HA	1:A:1211:ILE:HD13	1.78	0.42
1:A:57:TYR:HE2	1:A:118:LEU:HD22	1.85	0.41
1:A:349:LYS:HD3	1:A:355:TRP:CD1	2.55	0.41
1:A:1066:TYR:CE1	1:A:1155:LYS:HE3	2.56	0.41
1:A:615:ILE:HD11	1:A:634:LYS:HZ2	1.86	0.41
1:A:69:ILE:HD11	1:A:105:ILE:HA	2.01	0.41
1:A:924:LEU:HD11	1:A:950:LEU:HD12	2.03	0.41
1:A:933:ASN:HD21	1:A:936:VAL:HG13	1.85	0.41
1:A:967:THR:HA	1:A:972:LYS:CB	2.50	0.41
1:A:443:GLU:H	1:A:443:GLU:HG2	1.67	0.41
1:A:126:THR:OG1	1:A:127:ILE:HD12	2.21	0.41
1:A:171:ILE:HG23	1:A:279:GLN:HE22	1.86	0.41
1:A:239:ALA:HB1	1:A:244:PHE:HD2	1.86	0.41
1:A:447:LYS:HZ3	1:A:513:GLN:C	2.29	0.41
1:A:1156:ASN:CG	1:A:1160:ILE:HG22	2.46	0.41
1:A:174:ARG:NH1	2:B:6:C:H4'	2.35	0.40
1:A:295:THR:HG22	1:A:299:GLU:OE1	2.21	0.40
1:A:764:PRO:HB2	1:A:776:THR:HG21	2.03	0.40
1:A:419:ILE:O	1:A:422:VAL:HG22	2.22	0.40
1:A:572:ASP:HB2	1:A:686:SER:HB2	2.04	0.40
1:A:256:ASN:HD21	1:A:272:LYS:HE3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1194/1228 (97%)	1154 (97%)	38 (3%)	2 (0%)	43 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	A	476	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1065/1115 (96%)	1063 (100%)	2 (0%)	87 86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	VAL
1	A	456	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	203	GLN
1	A	399	GLN
1	A	613	GLN
1	A	862	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	28/40 (70%)	4 (14%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-12	C
2	B	-10	A
2	B	-9	A
2	B	-6	G

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 1 ligands modelled in this entry, 1 is 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	A	1202/1228 (97%)	0.77	182 (15%) 5 7	2, 31, 148, 165	0
2	B	29/40 (72%)	0.27	1 (3%) 48 30	5, 13, 29, 95	0
3	C	15/15 (100%)	0.51	0 100 100	5, 18, 35, 42	0
4	D	11/11 (100%)	0.23	0 100 100	12, 14, 31, 35	0
All	All	1257/1294 (97%)	0.75	183 (14%) 6 8	2, 30, 148, 165	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	GLU	5.4
1	A	314	ILE	5.4
1	A	494	TYR	5.3
1	A	362	TRP	5.2
1	A	346	THR	5.1
1	A	377	VAL	5.1
1	A	895	ASN	4.6
1	A	376	VAL	4.5
1	A	497	LEU	4.5
1	A	307	THR	4.5
1	A	500	VAL	4.4
1	A	501	ASP	4.4
1	A	357	VAL	4.4
1	A	474	PHE	4.3
1	A	294	TYR	4.3
1	A	392	ILE	4.3
1	A	355	TRP	4.2
1	A	379	GLU	4.2
1	A	408	LEU	4.1
1	A	383	ASP	4.1
1	A	499	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	386	ARG	4.1
1	A	318	ILE	4.1
1	A	413	LYS	4.0
1	A	313	GLU	4.0
1	A	343	ALA	3.9
1	A	498	LEU	3.8
1	A	466	PHE	3.8
1	A	502	HIS	3.8
1	A	1227	LYS	3.8
1	A	490	PHE	3.8
1	A	342	PRO	3.8
1	A	496	ILE	3.8
1	A	304	PHE	3.8
1	A	492	LEU	3.7
2	B	8	G	3.7
1	A	339	LYS	3.7
1	A	400	LEU	3.7
1	A	378	THR	3.6
1	A	465	SER	3.6
1	A	272	LYS	3.6
1	A	266	THR	3.4
1	A	440	PHE	3.4
1	A	324	LEU	3.3
1	A	503	ILE	3.3
1	A	380	LYS	3.2
1	A	269	LYS	3.2
1	A	390	LYS	3.2
1	A	441	VAL	3.2
1	A	470	ILE	3.1
1	A	350	ASP	3.1
1	A	327	ASN	3.1
1	A	333	SER	3.1
1	A	931	PHE	3.1
1	A	323	LYS	3.1
1	A	480	THR	3.1
1	A	303	VAL	3.0
1	A	438	ALA	3.0
1	A	308	LEU	3.0
1	A	932	LYS	3.0
1	A	493	ALA	3.0
1	A	1116	CYS	3.0
1	A	467	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	395	PHE	3.0
1	A	364	ALA	3.0
1	A	444	LYS	2.9
1	A	478	LYS	2.9
1	A	487	TYR	2.9
1	A	375	ALA	2.9
1	A	1114	LEU	2.8
1	A	320	LYS	2.8
1	A	864	ASN	2.8
1	A	1091	LEU	2.8
1	A	328	PHE	2.8
1	A	270	LEU	2.8
1	A	491	VAL	2.8
1	A	382	GLU	2.8
1	A	436	PHE	2.8
1	A	890	TRP	2.8
1	A	412	GLU	2.8
1	A	367	ASP	2.7
1	A	302	GLU	2.7
1	A	321	LEU	2.7
1	A	1115	LEU	2.7
1	A	361	LYS	2.7
1	A	268	GLN	2.7
1	A	394	SER	2.7
1	A	407	ASP	2.7
1	A	334	ALA	2.7
1	A	301	LEU	2.7
1	A	1012	ASN	2.7
1	A	366	TYR	2.6
1	A	468	ASN	2.6
1	A	352	PHE	2.6
1	A	300	VAL	2.6
1	A	423	ASP	2.6
1	A	393	GLY	2.6
1	A	403	TYR	2.6
1	A	261	LEU	2.6
1	A	442	LEU	2.6
1	A	389	PHE	2.6
1	A	486	PHE	2.6
1	A	199	LYS	2.5
1	A	448	LYS	2.5
1	A	317	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	197	PHE	2.5
1	A	961	LYS	2.5
1	A	511	VAL	2.5
1	A	573	ASP	2.5
1	A	353	GLY	2.5
1	A	381	TYR	2.5
1	A	435	LEU	2.5
1	A	325	PHE	2.4
1	A	473	PHE	2.4
1	A	867	ARG	2.4
1	A	489	ASP	2.4
1	A	505	ASP	2.4
1	A	429	TYR	2.4
1	A	469	TYR	2.4
1	A	112	ASN	2.4
1	A	332	SER	2.4
1	A	504	TYR	2.4
1	A	567	GLN	2.4
1	A	271	PRO	2.4
1	A	1093	SER	2.4
1	A	351	ILE	2.4
1	A	446	LEU	2.4
1	A	354	GLU	2.4
1	A	310	LYS	2.4
1	A	296	SER	2.3
1	A	607	ASN	2.3
1	A	297	ASP	2.3
1	A	933	ASN	2.3
1	A	1043	PHE	2.3
1	A	385	ARG	2.3
1	A	331	TYR	2.3
1	A	1120	ASP	2.3
1	A	258	TYR	2.3
1	A	299	GLU	2.3
1	A	409	SER	2.3
1	A	265	LYS	2.3
1	A	506	ALA	2.2
1	A	510	TYR	2.2
1	A	319	LYS	2.2
1	A	1113	ALA	2.2
1	A	315	PHE	2.2
1	A	316	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	399	GLN	2.2
1	A	358	ILE	2.2
1	A	483	ASP	2.2
1	A	570	ASP	2.2
1	A	898	GLU	2.2
1	A	1031	PHE	2.2
1	A	406	ALA	2.1
1	A	283	ASP	2.1
1	A	202	VAL	2.1
1	A	191	GLU	2.1
1	A	912	CYS	2.1
1	A	147	PHE	2.1
1	A	1085	ASP	2.1
1	A	146	GLY	2.1
1	A	1054	ARG	2.1
1	A	388	SER	2.1
1	A	335	GLY	2.1
1	A	417	ILE	2.1
1	A	863	PHE	2.1
1	A	1099	PHE	2.1
1	A	309	ASN	2.1
1	A	295	THR	2.0
1	A	1019	THR	2.0
1	A	1111	ILE	2.0
1	A	337	PHE	2.0
1	A	449	ASN	2.0
1	A	384	ASP	2.0
1	A	416	GLU	2.0
1	A	445	SER	2.0
1	A	780	SER	2.0
1	A	411	VAL	2.0
1	A	359	ARG	2.0
1	A	421	LYS	2.0
1	A	443	GLU	2.0
1	A	476	GLU	2.0
1	A	396	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
5	MG	A	1301	1/1	0.85	0.32	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.