Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2024 – 04:13 PM JST

PDB ID	:	8Y05
Title	:	Crystal structure of LbCas12a in complex with crRNA and 9nt target DNA
Authors	:	Lin, X.; Chen, J.; Liu, L.
Deposited on	:	2024-01-22
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

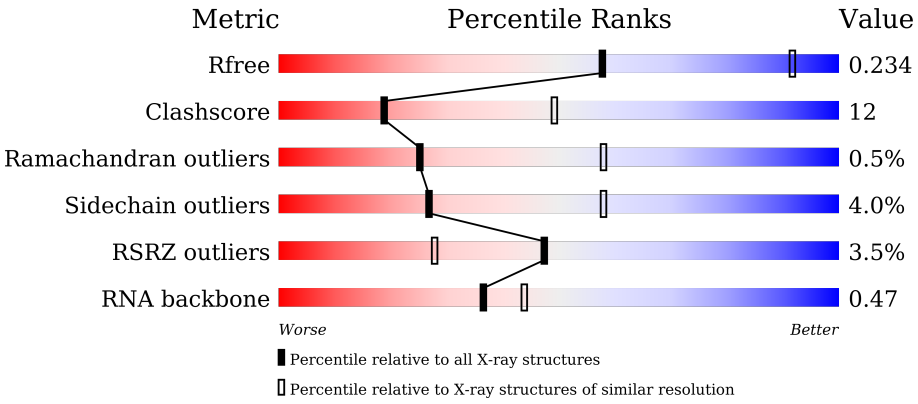
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1228	4% 71% 26%
2	B	40	25% 38% 10% 28%
3	C	18	6% 61% 22% 17%
4	D	11	27% 55% 18%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11051 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
			Total	C	N	O	S			
1	A	1202	9841	6333	1608	1871	29	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	18	376	177	75	106	18	0	0	0

- 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
			Total	C	N	O	P			
4	D	11	217	107	31	69	10	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

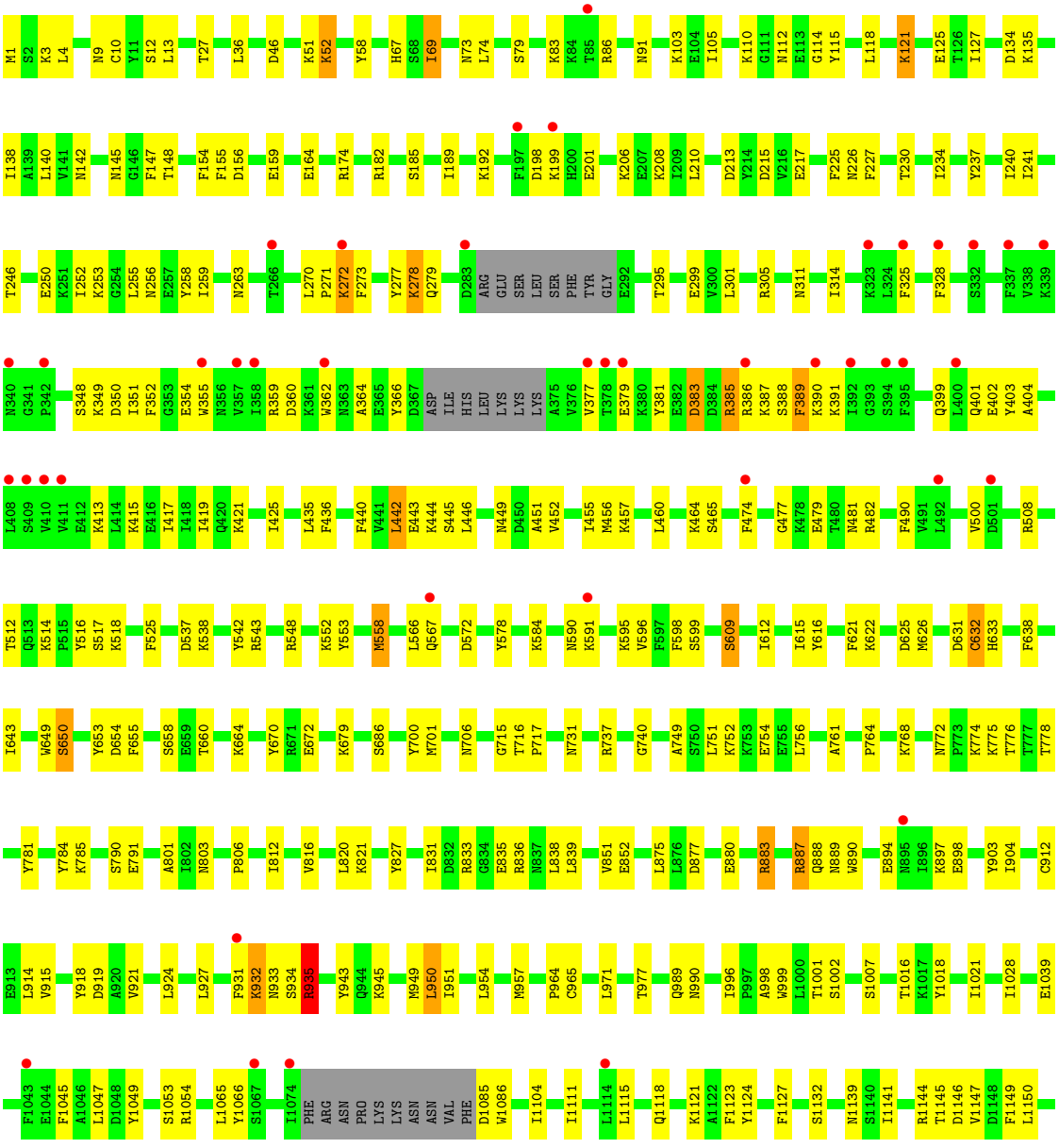
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

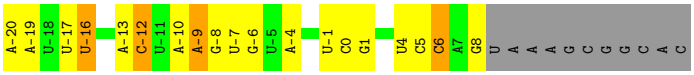
- Molecule 1: LbCas12a

Chain A:



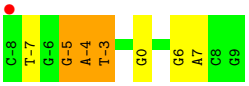
• Molecule 2: RNA (29-MER)

Chain B:



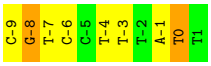
• Molecule 3: DNA (5’-D(P*CP*TP*GP*GP*AP*TP*GP*CP*GP*TP*AP*AP*AP*GP*GP*AP*CP*G)-3’)

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.76Å 154.76Å 210.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 3.10 49.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.4 (49.01-3.10) 85.4 (49.01-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.197 , 0.234 0.199 , 0.234	Depositor DCC
R_{free} test set	2637 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11051	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.52	2/10046 (0.0%)	0.69	3/13514 (0.0%)
2	B	0.98	0/681	1.66	17/1058 (1.6%)
3	C	1.40	1/423 (0.2%)	1.39	4/652 (0.6%)
4	D	1.44	2/240 (0.8%)	1.46	2/368 (0.5%)
All	All	0.65	5/11390 (0.0%)	0.86	26/15592 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	-8	DG	C3'-O3'	-7.75	1.33	1.44
3	C	6	DG	C3'-O3'	-7.38	1.34	1.44
1	A	912	CYS	CB-SG	-5.43	1.73	1.81
4	D	0	DT	C3'-O3'	-5.21	1.37	1.44
1	A	10	CYS	CB-SG	-5.05	1.73	1.81

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	-9	A	N1-C6-N6	9.36	124.21	118.60
3	C	-4	DA	O5'-P-OP1	-8.88	97.71	105.70
2	B	-9	A	C5-N7-C8	-8.03	99.88	103.90
2	B	-9	A	C4-C5-N7	7.74	114.57	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	-9	A	O5'-P-OP1	-7.09	99.32	105.70
1	A	69	ILE	CG1-CB-CG2	-6.68	96.71	111.40
2	B	-1	U	C5-C6-N1	6.58	125.99	122.70
2	B	-12	C	C6-N1-C2	6.46	122.88	120.30
1	A	36	LEU	CB-CG-CD2	-6.39	100.14	111.00
2	B	-1	U	N3-C4-O4	6.17	123.72	119.40
3	C	-5	DG	O4'-C4'-C3'	-6.03	102.09	104.50
3	C	-3	DT	N3-C4-O4	5.96	123.48	119.90
2	B	-9	A	C6-C5-N7	-5.88	128.18	132.30
3	C	7	DA	O4'-C1'-N9	-5.83	103.92	108.00
2	B	1	G	O5'-P-OP1	-5.78	100.49	105.70
2	B	-9	A	C5-C6-N6	-5.75	119.10	123.70
2	B	6	C	C6-N1-C2	-5.71	118.02	120.30
4	D	-6	DC	O5'-P-OP1	-5.36	100.88	105.70
2	B	-16	U	C5-C4-O4	-5.34	122.69	125.90
2	B	-12	C	N3-C4-C5	5.34	124.03	121.90
4	D	-7	DT	C5-C4-O4	-5.25	121.23	124.90
1	A	935	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	B	0	C	O4'-C1'-N1	5.17	112.34	108.20
2	B	-1	U	C5-C4-O4	-5.11	122.83	125.90
2	B	-9	A	N7-C8-N9	5.10	116.35	113.80
2	B	6	C	OP2-P-O3'	5.03	116.26	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	715	GLY	Peptide
1	A	73	ASN	Peptide

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	9841	0	9681	227	0
2	B	610	0	312	11	0
3	C	376	0	202	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	217	0	129	11	0
5	A	1	0	0	0	0
6	A	6	0	0	1	0
All	All	11051	0	10324	247	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 12.

All (247) 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:NH2	1:A:435:LEU:O	1.73	1.22
1:A:381:TYR:HE2	1:A:385:ARG:NH1	1.40	1.15
1:A:381:TYR:CE2	1:A:385:ARG:NH1	2.15	1.11
1:A:752:LYS:NZ	1:A:754:GLU:OE2	1.94	1.00
1:A:263:ASN:HD21	1:A:270:LEU:HB2	1.27	0.99
1:A:305:ARG:CZ	1:A:435:LEU:O	2.09	0.98
1:A:996:ILE:HD11	1:A:1191:VAL:HG23	1.46	0.95
1:A:835:GLU:HG2	1:A:935:ARG:HB2	1.50	0.90
1:A:305:ARG:NH2	1:A:435:LEU:C	2.27	0.88
1:A:774:LYS:NZ	2:B:-8:G:O6	2.07	0.87
1:A:887:ARG:NH1	1:A:889:ASN:OD1	2.07	0.86
1:A:525:PHE:O	1:A:543:ARG:NH2	2.10	0.85
1:A:142:ASN:O	1:A:145:ASN:ND2	2.14	0.81
1:A:1016:THR:HG1	1:A:1132:SER:HG	1.20	0.81
1:A:1194:ALA:HB1	1:A:1211:ILE:HD12	1.64	0.78
1:A:1007:SER:O	1:A:1226:VAL:HG21	1.82	0.78
1:A:591:LYS:HG2	4:D:0:DT:H1'	1.65	0.77
1:A:377:VAL:CG2	1:A:385:ARG:HH22	1.97	0.76
1:A:351:ILE:HG22	1:A:413:LYS:HG3	1.66	0.76
1:A:543:ARG:HG2	1:A:558:MET:HB2	1.67	0.76
1:A:836:ARG:HD2	1:A:1145:THR:HG23	1.69	0.74
1:A:74:LEU:HD21	1:A:225:PHE:HB3	1.70	0.73
1:A:83:LYS:HG2	1:A:86:ARG:HG2	1.71	0.71
1:A:1115:LEU:HD12	1:A:1123:PHE:HZ	1.55	0.71
1:A:351:ILE:HG22	1:A:413:LYS:CG	2.20	0.70
1:A:210:LEU:HD21	1:A:240:ILE:HD11	1.72	0.70
1:A:12:SER:HB3	1:A:803:ASN:O	1.94	0.68
1:A:389:PHE:H	1:A:389:PHE:HD1	1.41	0.67
1:A:295:THR:HG22	1:A:299:GLU:OE1	1.95	0.67
1:A:305:ARG:HH12	1:A:440:PHE:HD2	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ASP:OD1	1:A:625:ASP:N	2.28	0.67
1:A:820:LEU:HD11	1:A:921:VAL:HG21	1.77	0.66
1:A:633:HIS:HD2	1:A:660:THR:HG22	1.60	0.66
1:A:821:LYS:NZ	1:A:1201:ALA:O	2.29	0.65
1:A:305:ARG:HH21	1:A:436:PHE:CA	2.08	0.65
1:A:263:ASN:ND2	1:A:270:LEU:HB2	2.06	0.64
1:A:377:VAL:HG11	1:A:1054:ARG:HH21	1.61	0.64
1:A:835:GLU:HG2	1:A:935:ARG:CB	2.25	0.63
1:A:1039:GLU:N	1:A:1039:GLU:OE2	2.29	0.63
1:A:1198:PHE:CZ	1:A:1211:ILE:HD11	2.33	0.63
1:A:3:LYS:NZ	1:A:919:ASP:O	2.32	0.62
1:A:443:GLU:HG3	1:A:444:LYS:HG3	1.80	0.62
1:A:377:VAL:O	1:A:1053:SER:HB2	2.00	0.62
1:A:477:GLY:HA3	1:A:479:GLU:HB2	1.81	0.62
1:A:9:ASN:OD1	1:A:806:PRO:HA	2.00	0.61
1:A:155:PHE:O	1:A:159:GLU:HG3	2.00	0.61
1:A:621:PHE:HA	1:A:632:CYS:HB2	1.82	0.61
1:A:52:LYS:HD2	1:A:52:LYS:N	2.16	0.61
1:A:349:LYS:HB2	1:A:355:TRP:HD1	1.64	0.61
1:A:1115:LEU:HD12	1:A:1123:PHE:CZ	2.37	0.59
1:A:121:LYS:HA	1:A:148:THR:HG21	1.84	0.59
1:A:377:VAL:HG21	1:A:385:ARG:HH22	1.68	0.58
3:C:-4:DA:H2"	3:C:-3:DT:C5'	2.32	0.58
3:C:-3:DT:H5'	3:C:-3:DT:H6	1.68	0.58
1:A:1198:PHE:CE1	1:A:1211:ILE:HD11	2.38	0.58
1:A:246:THR:OG1	1:A:250:GLU:HG3	2.04	0.58
1:A:1150:LEU:HD22	1:A:1162:TYR:HE2	1.68	0.58
1:A:474:PHE:HE1	1:A:490:PHE:HE2	1.52	0.58
1:A:415:LYS:HG2	1:A:419:ILE:HD12	1.86	0.57
1:A:27:THR:HG23	1:A:700:TYR:HB3	1.87	0.57
1:A:350:ASP:HB3	1:A:417:ILE:HD13	1.86	0.56
1:A:836:ARG:NH2	1:A:1147:VAL:O	2.37	0.56
1:A:954:LEU:HG	1:A:957:MET:HE3	1.88	0.56
4:D:-9:DC:H2'	4:D:-8:DG:C8	2.40	0.56
1:A:206:LYS:HA	1:A:210:LEU:HB2	1.88	0.55
1:A:208:LYS:HG3	1:A:252:ILE:HD12	1.88	0.54
3:C:-7:DT:OP2	3:C:-7:DT:H2'	2.07	0.54
1:A:381:TYR:CD2	1:A:385:ARG:NH1	2.72	0.54
1:A:442:LEU:HD11	1:A:446:LEU:CD1	2.37	0.54
1:A:595:LYS:HB3	4:D:-1:DA:O4'	2.06	0.54
1:A:51:LYS:HE2	1:A:154:PHE:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:HB3	1:A:258:TYR:CE2	2.43	0.54
1:A:595:LYS:HG3	1:A:596:VAL:N	2.23	0.54
1:A:838:LEU:O	1:A:839:LEU:HD12	2.07	0.54
1:A:377:VAL:CG1	1:A:385:ARG:HH22	2.21	0.53
1:A:596:VAL:HG21	1:A:649:TRP:CH2	2.43	0.53
1:A:737:ARG:HB2	1:A:801:ALA:HB3	1.90	0.53
1:A:1021:ILE:HD11	1:A:1121:LYS:HB3	1.89	0.53
3:C:-4:DA:H2"	3:C:-3:DT:H5"	1.89	0.53
1:A:360:ASP:O	1:A:364:ALA:N	2.42	0.52
1:A:362:TRP:HB2	1:A:403:TYR:OH	2.09	0.52
1:A:740:GLY:O	3:C:0:DG:H2"	2.09	0.52
1:A:474:PHE:CE1	1:A:490:PHE:HE2	2.27	0.52
1:A:508:ARG:HG3	1:A:890:TRP:CD1	2.44	0.52
1:A:479:GLU:HB3	1:A:482:ARG:HD2	1.92	0.52
1:A:894:GLU:O	1:A:898:GLU:HG3	2.10	0.51
1:A:362:TRP:CH2	1:A:389:PHE:HA	2.46	0.51
1:A:460:LEU:O	1:A:464:LYS:HB2	2.11	0.51
3:C:-5:DG:C3'	3:C:-4:DA:H5"	2.41	0.51
1:A:598:PHE:CE1	1:A:638:PHE:HE2	2.27	0.51
1:A:325:PHE:O	1:A:415:LYS:HG3	2.11	0.51
1:A:1104:ILE:HD11	1:A:1118:GLN:HG3	1.93	0.51
3:C:-5:DG:C2'	3:C:-4:DA:H5"	2.41	0.51
1:A:189:ILE:HG23	1:A:271:PRO:HG2	1.92	0.50
1:A:255:LEU:O	1:A:259:ILE:HG13	2.10	0.50
1:A:833:ARG:HH22	1:A:932:LYS:HG3	1.75	0.50
3:C:-5:DG:H2'	3:C:-4:DA:H5"	1.92	0.50
4:D:0:DT:H5"	4:D:0:DT:H6	1.76	0.50
1:A:756:LEU:HD11	1:A:790:SER:HB3	1.94	0.50
1:A:1186:ASN:OD1	1:A:1189:ARG:NH1	2.44	0.50
1:A:998:ALA:O	1:A:1001:THR:OG1	2.28	0.50
1:A:643:ILE:O	1:A:650:SER:HB3	2.12	0.49
1:A:653:TYR:O	1:A:655:PHE:N	2.45	0.49
1:A:514:LYS:HD2	1:A:516:TYR:CZ	2.48	0.49
1:A:615:ILE:HG12	1:A:631:ASP:HB3	1.95	0.49
1:A:784:TYR:O	2:B:-19:A:H5'	2.13	0.49
1:A:1039:GLU:H	1:A:1039:GLU:CD	2.14	0.49
1:A:305:ARG:HH21	1:A:436:PHE:HA	1.76	0.49
1:A:127:ILE:HD12	1:A:127:ILE:H	1.78	0.48
1:A:1111:ILE:HG22	1:A:1115:LEU:HD22	1.94	0.48
2:B:5:C:H2'	2:B:6:C:H6	1.78	0.48
1:A:596:VAL:O	1:A:599:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:ASN:O	1:A:775:LYS:HE2	2.13	0.48
1:A:932:LYS:HD2	1:A:932:LYS:N	2.28	0.48
1:A:301:LEU:O	1:A:305:ARG:HG3	2.14	0.48
1:A:217:GLU:HG2	1:A:217:GLU:O	2.13	0.48
1:A:314:ILE:HD13	1:A:500:VAL:HG12	1.95	0.48
1:A:512:THR:HB	1:A:894:GLU:HG3	1.95	0.48
1:A:421:LYS:O	1:A:425:ILE:HG13	2.14	0.48
1:A:880:GLU:HG2	1:A:883:ARG:HH12	1.79	0.48
1:A:1066:TYR:CE1	1:A:1155:LYS:HE3	2.49	0.47
1:A:351:ILE:HD12	1:A:352:PHE:H	1.78	0.47
1:A:548:ARG:HD3	1:A:553:TYR:CZ	2.48	0.47
1:A:103:LYS:HG2	1:A:164:GLU:OE1	2.13	0.47
1:A:377:VAL:HG11	1:A:1054:ARG:NH2	2.29	0.47
1:A:609:SER:OG	1:A:612:ILE:HG13	2.14	0.47
1:A:989:GLN:HG2	1:A:990:ASN:N	2.28	0.47
1:A:572:ASP:HB2	1:A:686:SER:HB2	1.97	0.47
1:A:4:LEU:HD11	1:A:915:VAL:HG12	1.96	0.47
1:A:125:GLU:HG2	1:A:145:ASN:OD1	2.14	0.47
1:A:349:LYS:HB2	1:A:355:TRP:CD1	2.47	0.47
2:B:4:U:H2'	2:B:5:C:C6	2.50	0.47
1:A:383:ASP:O	1:A:387:LYS:N	2.46	0.47
1:A:401:GLN:OE1	1:A:404:ALA:HB3	2.14	0.47
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.74	0.47
3:C:-4:DA:H2"	3:C:-3:DT:H5'	1.96	0.47
1:A:278:LYS:HG3	1:A:279:GLN:O	2.15	0.47
2:B:8:G:O5'	2:B:8:G:H8	1.98	0.47
1:A:616:TYR:OH	4:D:0:DT:OP1	2.32	0.46
1:A:827:TYR:HE1	1:A:851:VAL:HG21	1.80	0.46
1:A:764:PRO:HB2	1:A:776:THR:CG2	2.46	0.46
1:A:887:ARG:CG	1:A:888:GLN:H	2.28	0.46
1:A:457:LYS:HZ2	1:A:888:GLN:HG3	1.79	0.46
1:A:1018:TYR:HE1	1:A:1124:TYR:HB2	1.80	0.46
1:A:1028:ILE:HG12	1:A:1127:PHE:CE2	2.50	0.46
4:D:-4:DT:H1'	4:D:-3:DT:H5'	1.98	0.46
1:A:964:PRO:O	1:A:971:LEU:HB2	2.15	0.46
1:A:390:LYS:O	1:A:390:LYS:NZ	2.32	0.46
1:A:86:ARG:HH21	1:A:91:ASN:ND2	2.14	0.45
1:A:451:ALA:O	1:A:455:ILE:HG12	2.16	0.45
1:A:69:ILE:HD11	1:A:105:ILE:HA	1.97	0.45
1:A:875:LEU:HD23	1:A:875:LEU:HA	1.62	0.45
1:A:112:ASN:HB3	1:A:114:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:O	1:A:201:GLU:N	2.50	0.45
1:A:366:TYR:CE2	1:A:385:ARG:HG3	2.51	0.45
1:A:706:ASN:HB2	2:B:-17:U:OP1	2.16	0.45
1:A:134:ASP:OD1	1:A:135:LYS:N	2.50	0.45
1:A:256:ASN:OD1	1:A:272:LYS:HB2	2.17	0.45
1:A:225:PHE:O	1:A:227:PHE:N	2.51	0.45
1:A:1045:PHE:HB2	1:A:1065:LEU:HB2	1.99	0.45
1:A:1146:ASP:OD1	1:A:1146:ASP:N	2.43	0.45
1:A:305:ARG:HH21	1:A:436:PHE:C	2.21	0.44
1:A:951:ILE:O	1:A:977:THR:HG21	2.16	0.44
1:A:74:LEU:HD12	1:A:74:LEU:HA	1.77	0.44
1:A:633:HIS:NE2	1:A:660:THR:O	2.50	0.44
4:D:-9:DC:H5"	4:D:-9:DC:H6	1.82	0.44
1:A:852:GLU:OE1	1:A:918:TYR:OH	2.24	0.44
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.64	0.44
1:A:13:LEU:N	1:A:13:LEU:HD23	2.33	0.44
1:A:156:ASP:OD1	6:A:1401:HOH:O	2.21	0.44
1:A:241:ILE:HD13	1:A:273:PHE:HB3	2.00	0.44
1:A:812:ILE:O	1:A:816:VAL:HG23	2.18	0.44
1:A:110:LYS:HG2	1:A:115:TYR:CZ	2.52	0.44
1:A:820:LEU:HD23	1:A:820:LEU:HA	1.76	0.44
1:A:566:LEU:HD23	1:A:566:LEU:HA	1.67	0.44
1:A:927:LEU:HD11	1:A:943:TYR:HD2	1.82	0.43
1:A:399:GLN:O	1:A:402:GLU:HB2	2.19	0.43
1:A:633:HIS:CD2	1:A:660:THR:O	2.71	0.43
1:A:142:ASN:HA	1:A:145:ASN:HD21	1.83	0.43
1:A:716:THR:HA	1:A:717:PRO:HD3	1.85	0.43
1:A:951:ILE:HG23	1:A:977:THR:CG2	2.48	0.43
1:A:377:VAL:HG22	1:A:385:ARG:HH22	1.77	0.43
1:A:518:LYS:HE2	2:B:-16:U:O3'	2.19	0.43
1:A:435:LEU:HD13	1:A:455:ILE:HG21	2.01	0.43
1:A:590:ASN:OD1	1:A:591:LYS:HE2	2.18	0.43
1:A:134:ASP:O	1:A:138:ILE:HG13	2.19	0.43
1:A:359:ARG:HH12	1:A:389:PHE:HE2	1.66	0.43
1:A:1141:ILE:HB	1:A:1144:ARG:HB2	2.00	0.43
1:A:452:VAL:O	1:A:456:MET:HG3	2.18	0.43
1:A:996:ILE:CG2	1:A:1190:LYS:HD2	2.48	0.43
1:A:756:LEU:HD23	1:A:756:LEU:HA	1.80	0.43
1:A:121:LYS:HB3	4:D:-3:DT:OP1	2.19	0.42
1:A:590:ASN:ND2	4:D:0:DT:H2"	2.34	0.42
1:A:595:LYS:HG3	1:A:596:VAL:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:SER:OG	1:A:672:GLU:OE1	2.37	0.42
1:A:558:MET:CE	1:A:566:LEU:HD12	2.49	0.42
1:A:751:LEU:O	1:A:790:SER:HA	2.20	0.42
1:A:445:SER:O	1:A:449:ASN:N	2.53	0.42
1:A:508:ARG:HG3	1:A:890:TRP:CG	2.54	0.42
1:A:612:ILE:HG13	1:A:612:ILE:H	1.55	0.42
1:A:1045:PHE:CD1	1:A:1045:PHE:N	2.87	0.42
1:A:403:TYR:N	1:A:403:TYR:CD1	2.87	0.42
1:A:749:ALA:HB2	1:A:791:GLU:C	2.39	0.42
1:A:904:ILE:HG21	1:A:904:ILE:HD13	1.79	0.42
1:A:237:TYR:CE1	1:A:241:ILE:HD11	2.55	0.42
1:A:537:ASP:OD2	1:A:584:LYS:NZ	2.49	0.42
1:A:945:LYS:O	1:A:949:MET:HG3	2.20	0.42
1:A:827:TYR:CE1	1:A:851:VAL:HG21	2.53	0.42
1:A:933:ASN:O	1:A:934:SER:HB2	2.20	0.42
3:C:-5:DG:C6	3:C:-4:DA:C5	3.07	0.42
4:D:0:DT:H6	4:D:0:DT:C5'	2.32	0.42
1:A:598:PHE:HE2	1:A:616:TYR:CD1	2.37	0.42
1:A:731:ASN:HB3	1:A:965:CYS:SG	2.59	0.42
1:A:764:PRO:HB3	1:A:778:THR:OG1	2.19	0.42
1:A:1141:ILE:HG13	1:A:1147:VAL:HG11	2.01	0.42
1:A:538:LYS:HB3	1:A:542:TYR:CE2	2.54	0.42
1:A:761:ALA:HB2	1:A:781:TYR:C	2.41	0.41
1:A:831:ILE:HD12	1:A:924:LEU:HD21	2.01	0.41
1:A:1211:ILE:HD13	1:A:1211:ILE:HA	1.63	0.41
1:A:67:HIS:ND1	1:A:230:THR:HG21	2.36	0.41
1:A:999:TRP:CD1	1:A:999:TRP:N	2.87	0.41
2:B:-8:G:H4'	2:B:-7:U:OP1	2.20	0.41
1:A:46:ASP:HB3	1:A:140:LEU:HD11	2.02	0.41
1:A:348:SER:OG	1:A:354:GLU:O	2.25	0.41
1:A:362:TRP:HB2	1:A:403:TYR:CZ	2.55	0.41
1:A:388:SER:O	1:A:391:LYS:HB3	2.21	0.41
1:A:590:ASN:HA	1:A:670:TYR:CE2	2.56	0.41
1:A:621:PHE:CE1	1:A:622:LYS:HG3	2.54	0.41
1:A:1111:ILE:O	1:A:1115:LEU:HD22	2.21	0.41
1:A:887:ARG:NH1	1:A:889:ASN:CG	2.73	0.41
1:A:58:TYR:HE1	1:A:118:LEU:HB3	1.85	0.41
1:A:305:ARG:HH11	1:A:305:ARG:HD2	1.76	0.41
1:A:1185:TYR:CZ	1:A:1189:ARG:HD2	2.56	0.41
2:B:-13:A:N1	2:B:-4:A:C6	2.89	0.41
1:A:379:GLU:HG2	1:A:1054:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:HD23	1:A:903:TYR:CZ	2.56	0.41
1:A:514:LYS:HD2	1:A:516:TYR:OH	2.21	0.40
1:A:1085:ASP:HB3	1:A:1086:TRP:H	1.70	0.40
1:A:914:LEU:HD23	1:A:914:LEU:HA	1.91	0.40
1:A:225:PHE:O	1:A:226:ASN:C	2.60	0.40
1:A:234:ILE:HD13	1:A:277:TYR:O	2.22	0.40
1:A:591:LYS:O	4:D:-1:DA:H1'	2.21	0.40
1:A:785:LYS:HB2	2:B:-20:A:H5"	2.03	0.40
2:B:-17:U:C4	2:B:-16:U:C4	3.09	0.40
1:A:121:LYS:O	1:A:121:LYS:HG2	2.21	0.40
1:A:578:TYR:CZ	1:A:701:MET:HE1	2.56	0.40
1:A:1139:ASN:HB2	1:A:1149:PHE:CZ	2.56	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%)	1135 (95%)	53 (4%)	6 (0%)	25 58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	385	ARG
1	A	389	PHE
1	A	654	ASP
1	A	199	LYS
1	A	481	ASN
1	A	386	ARG

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	1068/1115 (96%)	1025 (96%)	43 (4%)	27 58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	52	LYS
1	A	79	SER
1	A	121	LYS
1	A	147	PHE
1	A	174	ARG
1	A	182	ARG
1	A	185	SER
1	A	192	LYS
1	A	213	ASP
1	A	215	ASP
1	A	253	LYS
1	A	272	LYS
1	A	278	LYS
1	A	311	ASN
1	A	328	PHE
1	A	383	ASP
1	A	442	LEU
1	A	465	SER
1	A	517	SER
1	A	552	LYS
1	A	558	MET
1	A	567	GLN
1	A	609	SER
1	A	626	MET
1	A	632	CYS
1	A	650	SER
1	A	664	LYS
1	A	679	LYS
1	A	768	LYS

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Mol	Chain	Res	Type
1	A	877	ASP
1	A	883	ARG
1	A	887	ARG
1	A	897	LYS
1	A	931	PHE
1	A	932	LYS
1	A	935	ARG
1	A	950	LEU
1	A	1002	SER
1	A	1047	LEU
1	A	1049	TYR
1	A	1157	SER
1	A	1207	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	862	ASN
1	A	888	GLN

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1202/1228 (97%)	-0.10	43 (3%) 46 27	26, 56, 157, 177	0
2	B	29/40 (72%)	-0.96	0 100 100	32, 38, 53, 83	0
3	C	18/18 (100%)	-0.58	1 (5%) 31 19	31, 43, 95, 111	0
4	D	11/11 (100%)	-1.18	0 100 100	37, 39, 54, 60	0
All	All	1260/1297 (97%)	-0.13	44 (3%) 47 28	26, 55, 157, 177	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1227	LYS	4.1
1	A	1043	PHE	3.8
1	A	378	THR	3.6
1	A	386	ARG	3.6
1	A	392	ILE	3.5
1	A	408	LEU	3.4
1	A	895	ASN	3.1
1	A	328	PHE	3.1
1	A	355	TRP	3.1
1	A	400	LEU	3.0
1	A	339	LYS	2.9
1	A	266	THR	2.9
1	A	342	PRO	2.8
1	A	931	PHE	2.8
1	A	1067	SER	2.7
1	A	340	ASN	2.7
1	A	325	PHE	2.7
1	A	395	PHE	2.6
1	A	410	VAL	2.6
1	A	501	ASP	2.6
1	A	411	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	197	PHE	2.5
1	A	362	TRP	2.4
1	A	377	VAL	2.4
1	A	1074	ILE	2.3
1	A	283	ASP	2.3
1	A	567	GLN	2.3
1	A	272	LYS	2.3
1	A	591	LYS	2.3
1	A	390	LYS	2.2
1	A	474	PHE	2.1
3	C	-8	DC	2.1
1	A	199	LYS	2.1
1	A	379	GLU	2.1
1	A	332	SER	2.1
1	A	394	SER	2.1
1	A	409	SER	2.1
1	A	492	LEU	2.1
1	A	323	LYS	2.0
1	A	357	VAL	2.0
1	A	358	ILE	2.0
1	A	85	THR	2.0
1	A	337	PHE	2.0
1	A	1114	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1301	1/1	0.97	0.24	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.