



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 AM UTC

PDB ID : 7EU9 / pdb_00007eu9
Title : Crystal structure of the selenomethionine(SeMet)-derived Cas12i1 R-loop complex before target DNA cleavage
Authors : Zhang, B.; Luo, D.Y.; Li, Y.; OuYang, S.Y.
Deposited on : 2021-05-16
Resolution : 2.35 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

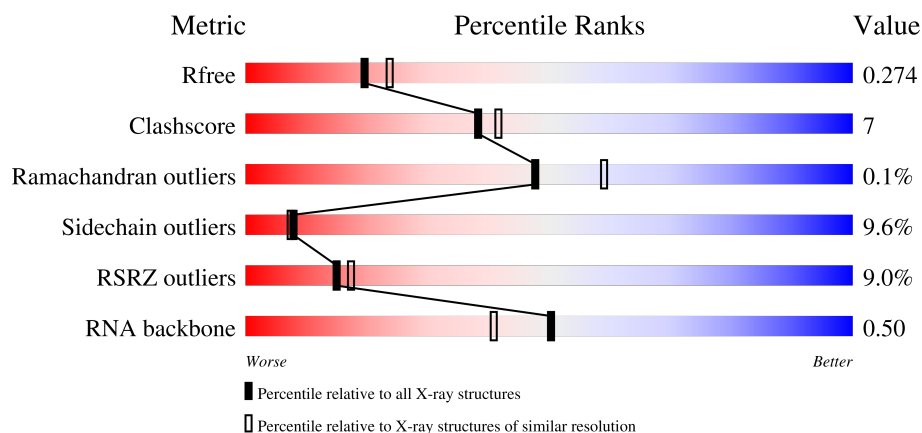
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)
RNA backbone	3983	1027 (2.66-2.06)

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	1101	9% 77% 17% • •
2	B	43	60% 26% 14%
3	C	40	5% 50% 25% • 22%
4	D	40	15% 38% 22% 40%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10849 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 Cas12i1 D647A mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1078	Total	C	N	O	S	Se	0	0	0
			8720	5549	1508	1623	14	26			

- Molecule 2 is a RNA chain called RNA (43-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	43	Total	C	N	O	P	0	0	0
			914	409	158	304	43			

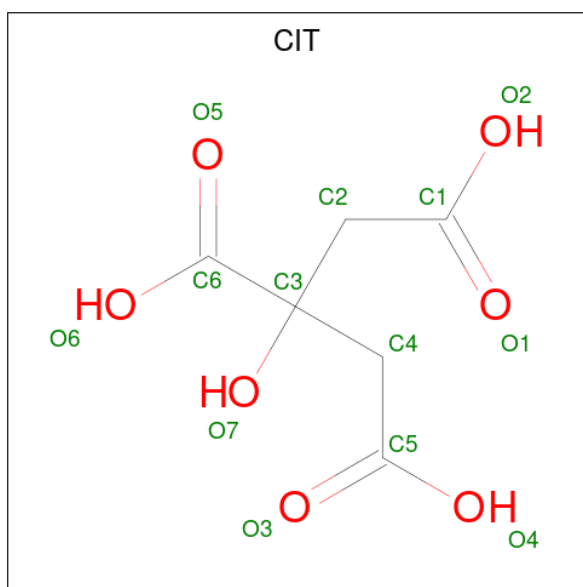
- Molecule 3 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	P	0	0	0
			629	303	108	187	31			

- Molecule 4 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	24	Total	C	N	O	P	0	0	0
			494	235	89	146	24			

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is water.

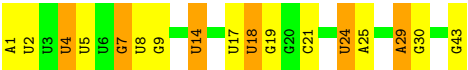
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	69	Total	O	0	0
			69	69		
6	B	3	Total	O	0	0
			3	3		
6	C	3	Total	O	0	0
			3	3		
6	D	4	Total	O	0	0
			4	4		

Chain B:

60%

26%

14%



● Molecule 3: DNA (31-MER)

Chain C:

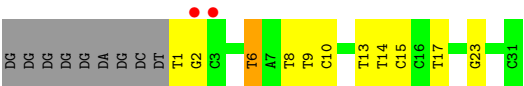
5%

50%

25%

•

22%



● Molecule 4: DNA (24-MER)

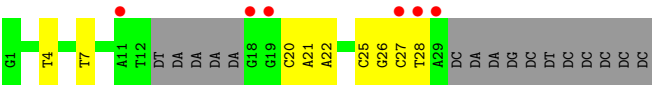
Chain D:

15%

38%

22%

40%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.06Å 141.58Å 208.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.63 – 2.35 58.63 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.63-2.35) 99.6 (58.63-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.228 , 0.268 0.237 , 0.274	Depositor DCC
R_{free} test set	3923 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10849	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: CIT

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	0.83	2/8872 (0.0%)	1.11	11/11896 (0.1%)
2	B	0.78	1/1021 (0.1%)	0.94	2/1588 (0.1%)
3	C	0.68	1/703 (0.1%)	0.94	3/1081 (0.3%)
4	D	0.48	0/552	0.97	2/848 (0.2%)
All	All	0.81	4/11148 (0.0%)	1.07	18/15413 (0.1%)

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	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ILE	C-O	-7.02	1.16	1.24
3	C	15	DC	O3'-P	-5.66	1.52	1.61
2	B	29	A	O3'-P	-5.54	1.52	1.61
1	A	464	GLN	C-O	-5.38	1.17	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	ASN	N-CA-C	8.56	122.86	110.10
1	A	727	MSE	N-CA-C	7.55	120.49	110.53
1	A	1089	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	149	MSE	N-CA-C	-6.80	103.80	111.14
3	C	23	DG	C2'-C3'-O3'	-6.55	101.68	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	722	TYR	CA-C-N	6.24	128.55	120.44
1	A	722	TYR	C-N-CA	6.24	128.55	120.44
2	B	21	C	C4'-C3'-O3'	-6.17	103.74	113.00
3	C	6	DT	C2'-C3'-O3'	5.88	120.33	111.50
2	B	4	U	C1'-C2'-O2'	-5.74	103.20	111.80
4	D	4	DT	C4'-C3'-O3'	-5.56	101.66	110.00
1	A	156	MSE	N-CA-C	-5.54	105.33	111.36
4	D	22	DA	C4'-C3'-O3'	-5.50	101.76	110.00
1	A	370	GLU	CB-CA-C	-5.39	110.34	116.54
3	C	10	DC	C4'-C3'-O3'	5.25	117.88	110.00
1	A	316	THR	CB-CA-C	5.16	118.97	110.88
1	A	690	VAL	N-CA-C	-5.14	98.60	107.24
1	A	944	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	57	ARG	Sidechain
1	A	606	ARG	Sidechain
1	A	723	ARG	Sidechain
1	A	918	ARG	Sidechain
1	A	962	ARG	Sidechain
1	A	976	ARG	Sidechain

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	8720	0	8784	123	0
2	B	914	0	459	10	0
3	C	629	0	353	8	0
4	D	494	0	273	8	0
5	A	13	0	5	3	0
6	A	69	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	4	0	0	0	0
All	All	10849	0	9874	142	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 7.

All (142) 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:574:GLN:HG2	1:A:593:MSE:HE2	1.52	0.90
1:A:966:CYS:SG	1:A:971:LEU:CD2	2.60	0.90
3:C:6:DT:H5''	3:C:6:DT:H6	1.38	0.89
1:A:483:LYS:NZ	1:A:614:ASN:HD22	1.75	0.83
1:A:225:ARG:O	1:A:229:ILE:HD12	1.80	0.81
1:A:966:CYS:SG	1:A:971:LEU:HD22	2.20	0.81
1:A:849:MSE:CE	1:A:852:LEU:HD23	2.13	0.78
1:A:593:MSE:HE3	1:A:593:MSE:HA	1.68	0.75
1:A:693:LYS:HD3	1:A:695:TYR:OH	1.86	0.74
5:A:1201:CIT:O1	5:A:1201:CIT:O7	2.04	0.74
1:A:849:MSE:HE1	1:A:852:LEU:HD23	1.68	0.74
1:A:483:LYS:HZ2	1:A:614:ASN:HD22	1.35	0.73
1:A:240:ILE:HG23	1:A:241:LEU:HD12	1.71	0.72
2:B:18:U:O2'	2:B:19:G:H5''	1.90	0.71
1:A:1025:ILE:O	1:A:1029:ILE:HD12	1.91	0.71
1:A:228:ARG:HH21	1:A:237:THR:HG22	1.53	0.71
3:C:6:DT:H6	3:C:6:DT:C5'	2.05	0.69
1:A:946:HIS:HE1	1:A:996:TYR:OH	1.74	0.69
1:A:941:PRO:O	1:A:944:THR:HB	1.92	0.68
1:A:689:GLN:NE2	1:A:694:SER:HB3	2.08	0.68
3:C:13:DT:H2''	3:C:14:DT:H5'	1.77	0.67
1:A:49:ASN:HB3	1:A:131:MSE:CE	2.26	0.65
1:A:73:LEU:HG	1:A:112:GLN:HB3	1.77	0.65
1:A:834:ALA:N	1:A:835:PRO:CD	2.60	0.65
1:A:399:LYS:H	1:A:399:LYS:HE2	1.63	0.64
1:A:772:SER:HB2	1:A:820:HIS:ND1	2.12	0.64
1:A:470:ILE:HG13	2:B:29:A:H5'	1.79	0.64
4:D:25:DC:H5''	4:D:25:DC:C6	2.32	0.63
1:A:727:MSE:HG3	1:A:737:ILE:HG13	1.81	0.63
1:A:834:ALA:N	1:A:835:PRO:HD2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASN:C	1:A:664:ASN:HD22	2.09	0.60
1:A:36:TYR:CE1	1:A:522:MSE:HE1	2.36	0.60
1:A:727:MSE:HG3	1:A:737:ILE:CG1	2.31	0.60
1:A:689:GLN:HE21	1:A:694:SER:HB3	1.67	0.59
4:D:27:DC:H3'	4:D:28:DT:H5''	1.84	0.59
1:A:691:ARG:HH11	2:B:14:U:H3	1.50	0.59
1:A:948:ASP:OD2	1:A:960:ARG:NH2	2.34	0.57
4:D:25:DC:H5''	4:D:25:DC:H6	1.68	0.57
1:A:412:GLN:HA	1:A:412:GLN:OE1	2.05	0.57
1:A:528:HIS:HD2	5:A:1201:CIT:O1	1.88	0.56
1:A:966:CYS:SG	1:A:971:LEU:HD21	2.43	0.56
1:A:547:GLU:OE1	1:A:548:ASN:N	2.36	0.56
1:A:33:PHE:CD2	1:A:516:VAL:HG22	2.41	0.56
1:A:727:MSE:CG	1:A:737:ILE:HG13	2.36	0.55
1:A:347:PHE:CZ	1:A:353:PHE:HB2	2.40	0.55
1:A:973:GLU:CD	1:A:976:ARG:HH22	2.14	0.55
4:D:25:DC:C6	4:D:25:DC:C5'	2.89	0.55
1:A:691:ARG:NH1	2:B:14:U:H3	2.06	0.54
1:A:849:MSE:HA	1:A:849:MSE:HE3	1.88	0.54
1:A:660:GLU:HB2	1:A:679:ILE:HD11	1.90	0.53
4:D:20:DC:H2'	4:D:21:DA:C8	2.44	0.53
1:A:928:VAL:HG13	1:A:934:LEU:HB3	1.92	0.52
1:A:238:PRO:HG2	1:A:241:LEU:HD13	1.91	0.52
1:A:546:SER:HB3	1:A:602:ASN:HD22	1.75	0.51
1:A:849:MSE:HE2	1:A:852:LEU:HD23	1.91	0.51
1:A:748:ASP:HB2	1:A:751:THR:CG2	2.40	0.51
1:A:715:ARG:NE	1:A:781:GLU:OE2	2.37	0.51
1:A:786:LEU:O	1:A:794:LEU:HB2	2.11	0.51
1:A:170:HIS:HE1	4:D:7:DT:O4	1.93	0.51
1:A:1085:ASP:HB3	1:A:1088:LYS:HD3	1.92	0.51
1:A:295:PRO:HD2	1:A:522:MSE:HE3	1.92	0.51
1:A:477:ASN:HB3	1:A:614:ASN:HD21	1.76	0.50
1:A:724:ASN:OD1	1:A:724:ASN:N	2.31	0.50
1:A:946:HIS:CE1	1:A:996:TYR:OH	2.61	0.50
1:A:276:GLU:O	1:A:277:CYS:HB2	2.11	0.50
1:A:483:LYS:HZ3	1:A:614:ASN:HD22	1.56	0.50
1:A:38:MSE:HG2	1:A:474:PRO:HG2	1.93	0.50
1:A:701:ASN:O	1:A:752:SER:HB3	2.12	0.50
1:A:764:LEU:O	1:A:768:ILE:HG13	2.11	0.50
1:A:60:ILE:O	1:A:63:THR:HG22	2.11	0.49
1:A:344:VAL:HG11	1:A:452:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ARG:HB2	2:B:7:G:C6	2.47	0.49
1:A:748:ASP:HB2	1:A:751:THR:HG23	1.95	0.49
3:C:6:DT:C5'	3:C:6:DT:C6	2.92	0.49
1:A:344:VAL:HG12	1:A:363:LEU:HD13	1.95	0.49
1:A:483:LYS:NZ	1:A:614:ASN:ND2	2.52	0.49
1:A:390:ASP:HA	1:A:394:LEU:HB2	1.95	0.48
1:A:643:VAL:CG1	1:A:892:LYS:HD3	2.43	0.48
1:A:149:MSE:HE2	1:A:153:LEU:HD13	1.95	0.48
1:A:646:TYR:CE1	1:A:875:ILE:HD11	2.48	0.48
1:A:727:MSE:O	1:A:728:LYS:C	2.56	0.48
1:A:338:GLU:N	1:A:339:PRO:CD	2.77	0.48
1:A:593:MSE:HA	1:A:593:MSE:CE	2.42	0.48
1:A:149:MSE:HE3	1:A:152:ASP:HB2	1.95	0.48
1:A:709:LYS:N	1:A:710:PRO:CD	2.77	0.47
1:A:634:LYS:NZ	1:A:934:LEU:O	2.41	0.47
1:A:896:ILE:O	1:A:918:ARG:HD3	2.15	0.47
1:A:49:ASN:HB3	1:A:131:MSE:HE1	1.95	0.47
3:C:6:DT:H5''	3:C:6:DT:C6	2.30	0.47
1:A:546:SER:CB	1:A:602:ASN:HD22	2.28	0.47
2:B:8:U:H2'	2:B:9:G:O4'	2.15	0.46
1:A:20:ILE:HD11	1:A:532:SER:HB3	1.97	0.46
1:A:34:MSE:HE2	1:A:617:ILE:HG22	1.98	0.46
1:A:947:GLN:HB2	1:A:1080:ASN:ND2	2.30	0.46
1:A:250:GLY:HA2	1:A:253:HIS:CD2	2.51	0.46
1:A:250:GLY:HA2	1:A:253:HIS:NE2	2.31	0.46
4:D:26:DG:H2''	4:D:27:DC:H5''	1.98	0.46
1:A:41:THR:HB	1:A:42:PRO:HD3	1.97	0.45
1:A:549:PRO:HA	1:A:602:ASN:HD21	1.81	0.45
1:A:63:THR:HG23	1:A:65:ASN:HD22	1.82	0.45
1:A:364:HIS:ND1	1:A:456:SER:OG	2.44	0.45
2:B:30:G:N2	3:C:17:DT:C2	2.85	0.45
1:A:399:LYS:HE2	1:A:399:LYS:N	2.28	0.45
1:A:333:ILE:CD1	1:A:461:VAL:HG11	2.47	0.44
1:A:12:ARG:HA	1:A:630:THR:O	2.18	0.44
1:A:636:LYS:HB3	1:A:636:LYS:HE3	1.82	0.44
1:A:570:LEU:HG	2:B:18:U:N3	2.32	0.44
1:A:825:PRO:O	1:A:826:LYS:C	2.59	0.44
1:A:387:TYR:OH	1:A:403:ILE:HD11	2.17	0.44
1:A:727:MSE:HG3	1:A:737:ILE:HD11	1.99	0.44
1:A:1062:ASN:HD21	1:A:1065:GLY:HA2	1.82	0.44
3:C:8:DT:H2'	3:C:9:DT:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG23	1:A:65:ASN:ND2	2.33	0.43
3:C:1:DT:H2''	3:C:2:DG:H5'	2.00	0.43
1:A:235:GLY:HA2	4:D:7:DT:O2	2.19	0.43
1:A:892:LYS:HE3	1:A:939:VAL:HG11	2.00	0.43
1:A:527:HIS:ND1	5:A:1201:CIT:H22	2.34	0.43
1:A:782:ILE:HG21	1:A:849:MSE:SE	2.69	0.42
1:A:948:ASP:CG	1:A:960:ARG:NH2	2.77	0.42
1:A:88:LYS:N	1:A:89:PRO:CD	2.82	0.42
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.90	0.42
1:A:733:ASN:OD1	1:A:734:ASN:N	2.52	0.42
1:A:356:ASP:C	1:A:358:ASN:H	2.26	0.42
1:A:727:MSE:HG3	1:A:737:ILE:CD1	2.49	0.42
1:A:314:GLY:C	1:A:315:MSE:HE2	2.45	0.41
1:A:992:THR:HA	1:A:995:TYR:CD2	2.55	0.41
1:A:38:MSE:HE2	1:A:38:MSE:HB3	1.94	0.41
1:A:276:GLU:O	1:A:277:CYS:CB	2.68	0.41
1:A:574:GLN:HG2	1:A:593:MSE:CE	2.38	0.41
1:A:742:ASP:HB3	1:A:763:LEU:HD21	2.01	0.41
1:A:333:ILE:HD11	1:A:461:VAL:HG11	2.02	0.41
1:A:353:PHE:C	1:A:353:PHE:CD1	2.98	0.41
1:A:258:ASN:OD1	1:A:260:PRO:HD2	2.21	0.41
1:A:695:TYR:CD1	1:A:695:TYR:N	2.89	0.41
1:A:111:ILE:HD12	1:A:111:ILE:H	1.85	0.41
1:A:131:MSE:O	1:A:134:GLU:HB2	2.21	0.41
2:B:24:U:O2	2:B:25:A:C8	2.74	0.41
1:A:779:ARG:HD2	1:A:846:ASP:OD2	2.20	0.41
1:A:672:ASN:OD1	1:A:953:LYS:O	2.39	0.40
1:A:933:GLY:O	1:A:934:LEU:HD12	2.21	0.40
1:A:82:VAL:HG21	1:A:466:ILE:HG21	2.02	0.40
2:B:1:A:O5'	2:B:1:A:N3	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1074/1101 (98%)	1025 (95%)	48 (4%)	1 (0%)	48 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	666	ASP

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
1	A	959/956 (100%)	867 (90%)	92 (10%)	8 7

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	57	ARG
1	A	65	ASN
1	A	66	LYS
1	A	73	LEU
1	A	96	ASN
1	A	111	ILE
1	A	123	THR
1	A	153	LEU
1	A	155	LEU
1	A	166	LEU
1	A	186	GLN
1	A	198	LEU
1	A	214	ILE
1	A	222	ASP
1	A	229	ILE
1	A	233	ARG
1	A	237	THR

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Mol	Chain	Res	Type
1	A	256	GLU
1	A	266	LEU
1	A	270	LEU
1	A	277	CYS
1	A	324	LEU
1	A	325	LYS
1	A	370	GLU
1	A	387	TYR
1	A	391	ILE
1	A	397	ASP
1	A	398	LYS
1	A	399	LYS
1	A	401	LYS
1	A	403	ILE
1	A	404	LYS
1	A	419	GLU
1	A	429	LEU
1	A	440	LYS
1	A	452	ILE
1	A	505	GLN
1	A	516	VAL
1	A	523	ARG
1	A	537	LEU
1	A	547	GLU
1	A	561	THR
1	A	593	MSE
1	A	595	LEU
1	A	638	LYS
1	A	641	LYS
1	A	664	ASN
1	A	666	ASP
1	A	704	LYS
1	A	705	LEU
1	A	712	VAL
1	A	714	SER
1	A	715	ARG
1	A	719	LEU
1	A	723	ARG
1	A	724	ASN
1	A	726	THR
1	A	727	MSE
1	A	735	ILE

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Mol	Chain	Res	Type
1	A	737	ILE
1	A	740	MSE
1	A	751	THR
1	A	781	GLU
1	A	785	LEU
1	A	794	LEU
1	A	811	LYS
1	A	826	LYS
1	A	840	GLU
1	A	843	GLN
1	A	849	MSE
1	A	885	LYS
1	A	901	LYS
1	A	913	MSE
1	A	930	MSE
1	A	944	THR
1	A	969	SER
1	A	971	LEU
1	A	976	ARG
1	A	985	ASP
1	A	986	LYS
1	A	988	SER
1	A	1010	LYS
1	A	1017	VAL
1	A	1018	SER
1	A	1021	LYS
1	A	1029	ILE
1	A	1030	LEU
1	A	1038	LEU
1	A	1046	MSE
1	A	1049	LEU
1	A	1089	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	65	ASN
1	A	170	HIS
1	A	186	GLN
1	A	307	ASN
1	A	358	ASN

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Mol	Chain	Res	Type
1	A	381	ASN
1	A	384	HIS
1	A	407	GLN
1	A	505	GLN
1	A	528	HIS
1	A	577	GLN
1	A	602	ASN
1	A	614	ASN
1	A	616	ASN
1	A	622	ASN
1	A	649	ASN
1	A	662	HIS
1	A	664	ASN
1	A	672	ASN
1	A	689	GLN
1	A	711	HIS
1	A	843	GLN
1	A	946	HIS
1	A	1024	GLN
1	A	1028	ASN
1	A	1062	ASN
1	A	1080	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	42/43 (97%)	9 (21%)	2 (4%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	4	U
2	B	5	U
2	B	7	G
2	B	14	U
2	B	17	U
2	B	18	U
2	B	24	U
2	B	43	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	4	U
2	B	14	U

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CIT	A	1201	-	12,12,12	1.97	4 (33%)	17,17,17	2.58	7 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	A	1201	-	-	6/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1201	CIT	C3-C6	4.26	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1201	CIT	C2-C3	-3.21	1.50	1.54
5	A	1201	CIT	O1-C1	2.21	1.29	1.22
5	A	1201	CIT	O2-C1	-2.07	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1201	CIT	O6-C6-C3	6.59	125.78	113.14
5	A	1201	CIT	C4-C3-C6	4.58	120.16	110.03
5	A	1201	CIT	C3-C2-C1	-3.94	103.14	113.92
5	A	1201	CIT	O7-C3-C2	-2.82	102.95	109.38
5	A	1201	CIT	O6-C6-O5	-2.71	115.18	123.86
5	A	1201	CIT	O4-C5-C4	2.31	121.67	114.35
5	A	1201	CIT	O4-C5-O3	-2.20	117.68	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1201	CIT	C2-C3-C6-O5
5	A	1201	CIT	C2-C3-C6-O6
5	A	1201	CIT	O7-C3-C6-O5
5	A	1201	CIT	O7-C3-C6-O6
5	A	1201	CIT	C3-C4-C5-O4
5	A	1201	CIT	C3-C4-C5-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	CIT	3	0

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	1052/1101 (95%)	0.79	96 (9%) 15 17	31, 54, 100, 166	0
2	B	43/43 (100%)	-0.18	0 100 100	38, 50, 81, 140	0
3	C	31/40 (77%)	0.21	2 (6%) 25 28	39, 50, 175, 187	0
4	D	24/40 (60%)	0.98	6 (25%) 2 1	40, 73, 151, 173	0
All	All	1150/1224 (93%)	0.74	104 (9%) 15 17	31, 54, 104, 187	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	LEU	6.3
1	A	587	LYS	5.9
1	A	66	LYS	5.1
1	A	834	ALA	4.9
1	A	555	ALA	4.8
1	A	730	ASN	4.8
1	A	361	TRP	4.7
1	A	735	ILE	4.4
1	A	733	ASN	4.3
1	A	64	ALA	4.2
1	A	359	VAL	4.1
1	A	737	ILE	4.1
1	A	690	VAL	4.1
1	A	695	TYR	4.0
1	A	62	GLY	4.0
1	A	689	GLN	4.0
1	A	724	ASN	4.0
1	A	693	LYS	3.9
1	A	403	ILE	3.6
1	A	1076	VAL	3.6
1	A	825	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	688	SER	3.6
1	A	7	ASN	3.6
1	A	398	LYS	3.5
1	A	356	ASP	3.5
1	A	729	ASP	3.5
1	A	399	LYS	3.5
1	A	745	ALA	3.4
1	A	65	ASN	3.4
1	A	8	ALA	3.3
1	A	583	VAL	3.3
1	A	1017	VAL	3.3
1	A	778	TYR	3.3
1	A	397	ASP	3.3
3	C	2	DG	3.3
1	A	1010	LYS	3.2
1	A	694	SER	3.2
1	A	691	ARG	3.2
3	C	3	DC	3.2
1	A	760	TYR	3.2
1	A	898	ASP	3.2
1	A	732	GLY	3.0
1	A	728	LYS	3.0
1	A	826	LYS	3.0
1	A	275	TYR	3.0
4	D	29	DA	2.9
1	A	836	PRO	2.9
1	A	370	GLU	2.9
1	A	357	THR	2.9
1	A	726	THR	2.8
1	A	1049	LEU	2.8
1	A	739	PHE	2.7
1	A	234	LYS	2.7
1	A	1038	LEU	2.7
1	A	835	PRO	2.6
4	D	28	DT	2.6
1	A	406	TYR	2.6
1	A	1015	LEU	2.6
1	A	546	SER	2.6
1	A	638	LYS	2.6
1	A	392	ALA	2.5
1	A	391	ILE	2.5
1	A	473	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1033	ARG	2.5
1	A	375	THR	2.5
1	A	776	LYS	2.4
1	A	824	LYS	2.4
1	A	734	ASN	2.4
1	A	393	SER	2.4
1	A	718	PHE	2.4
4	D	19	DG	2.4
1	A	1021	LYS	2.4
1	A	1091	LYS	2.4
1	A	861	LEU	2.4
1	A	1019	LEU	2.4
1	A	790	LYS	2.3
1	A	80	PHE	2.3
1	A	1039	LEU	2.3
1	A	353	PHE	2.3
1	A	943	PHE	2.3
1	A	822	LEU	2.3
1	A	542	TYR	2.3
1	A	837	ILE	2.3
4	D	11	DA	2.2
1	A	1016	GLY	2.2
1	A	374	LYS	2.2
1	A	500	LYS	2.2
1	A	272	ARG	2.2
1	A	111	ILE	2.2
1	A	764	LEU	2.2
1	A	67	ASP	2.2
1	A	354	GLU	2.2
1	A	590	LYS	2.2
1	A	731	ARG	2.1
4	D	18	DG	2.1
1	A	646	TYR	2.1
1	A	1011	LYS	2.1
1	A	547	GLU	2.1
1	A	1014	VAL	2.1
1	A	425	ALA	2.1
4	D	27	DC	2.1
1	A	410	VAL	2.1
1	A	771	HIS	2.0
1	A	548	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CIT	A	1201	13/13	0.83	0.13	42,65,76,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.