Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 06:05 PM JST

PDB ID	:	7D3J
Title	:	Crystal structure of the Cas12i1 R-loop complex after target DNA cleavage
Authors	:	Zhang, B.; Luo, D.Y.; Li, Y.; OuYang, S.Y.
Deposited on	:	2020-09-19
Resolution	:	2.45 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 (i) 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 (i)) were used in the production of this report:

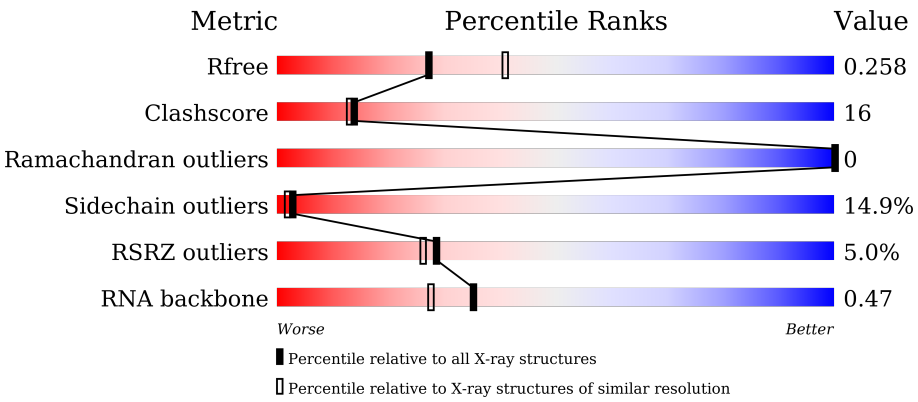
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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	1101	5%; 64%, 27%, 7%, •
2	B	43	9%; 28%, 56%, 14%, •
3	C	40	42%, 28%, 30%
4	D	40	5%; 20%, 28%, 10%, 42%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10727 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 12i1-WT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1077	8717	5545	1507	1625	40	0	0	0

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

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

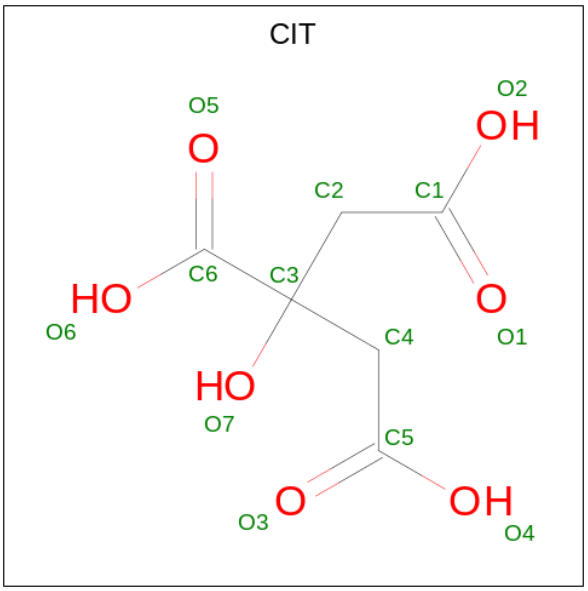
- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	28	568	274	98	168	28	0	0	0

- Molecule 4 is a DNA chain called DNA (23-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	23	475	227	88	137	23	0	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 6 is water.

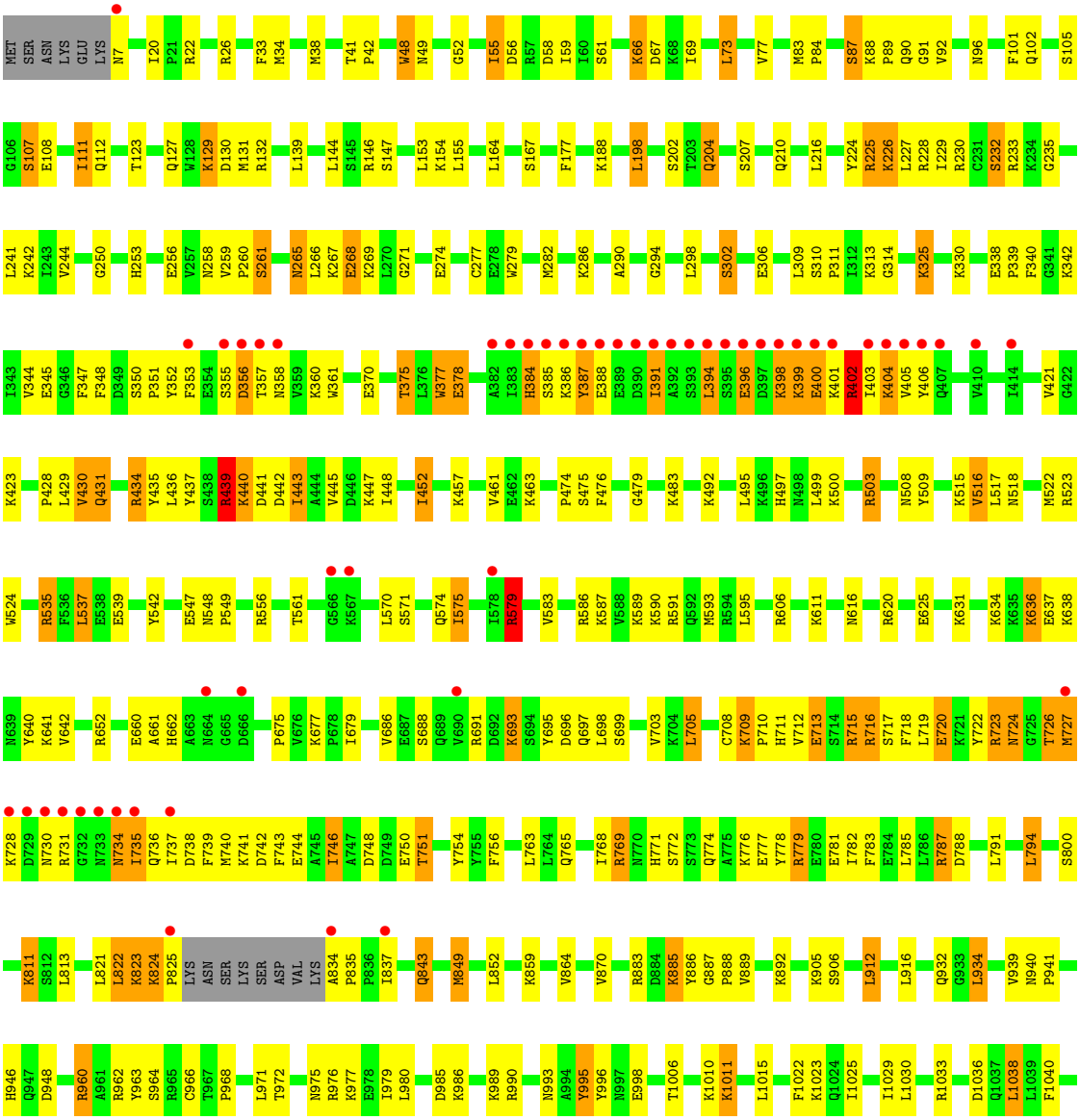
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	33	Total O 33 33	0	0
6	B	1	Total O 1 1	0	0
6	C	5	Total O 5 5	0	0
6	D	1	Total O 1 1	0	0

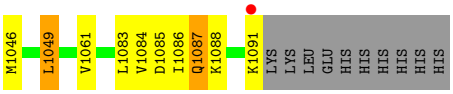
3 Residue-property plots (i)

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: 12i1-WT

Chain A:





• Molecule 2: RNA (43-MER)

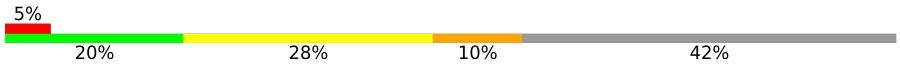
Chain B:

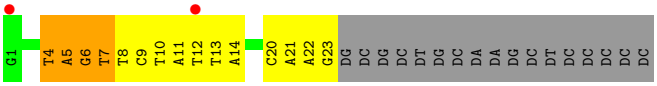
• Molecule 3: DNA (28-MER)

Chain C:

• Molecule 4: DNA (23-MER)

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	129.80Å 141.97Å 208.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.73 – 2.45 58.66 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.73-2.45) 99.9 (58.66-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.220 , 0.257 0.220 , 0.258	Depositor DCC
R_{free} test set	3545 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10727	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 2.70% 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: 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	0.72	0/8895	0.74	0/11971
2	B	1.37	21/1021 (2.1%)	0.82	0/1588
3	C	0.71	1/635 (0.2%)	0.91	0/976
4	D	1.15	7/533 (1.3%)	0.79	0/821
All	All	0.83	29/11084 (0.3%)	0.76	0/15356

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	23

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	G	O3'-P	-8.24	1.51	1.61
2	B	29	A	O3'-P	-7.80	1.51	1.61
2	B	25	A	O3'-P	-7.47	1.52	1.61
2	B	26	U	O3'-P	-7.45	1.52	1.61
2	B	19	G	O3'-P	-7.42	1.52	1.61
2	B	30	G	O3'-P	-6.96	1.52	1.61
2	B	20	G	O3'-P	-6.77	1.53	1.61
2	B	21	C	O3'-P	-6.70	1.53	1.61
2	B	33	A	O3'-P	-6.63	1.53	1.61
4	D	4	DT	O3'-P	-6.54	1.53	1.61
2	B	28	A	O3'-P	-6.36	1.53	1.61
2	B	8	U	O3'-P	-6.27	1.53	1.61
2	B	5	U	O3'-P	-6.27	1.53	1.61
2	B	23	C	O3'-P	-6.25	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	DT	O3'-P	-6.02	1.53	1.61
2	B	34	U	O3'-P	-6.02	1.53	1.61
2	B	22	A	O3'-P	-6.00	1.53	1.61
4	D	5	DA	O3'-P	-5.91	1.54	1.61
4	D	6	DG	O3'-P	-5.91	1.54	1.61
2	B	2	U	O3'-P	-5.90	1.54	1.61
4	D	20	DC	O3'-P	-5.89	1.54	1.61
2	B	31	G	O3'-P	-5.87	1.54	1.61
4	D	9	DC	O3'-P	-5.84	1.54	1.61
2	B	4	U	O3'-P	-5.61	1.54	1.61
2	B	35	G	O3'-P	-5.19	1.54	1.61
2	B	27	U	O3'-P	-5.18	1.54	1.61
4	D	21	DA	O3'-P	-5.17	1.54	1.61
4	D	7	DT	O3'-P	-5.14	1.54	1.61
2	B	6	U	O3'-P	-5.08	1.55	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	ARG	Sidechain
1	A	132	ARG	Sidechain
1	A	22	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	402	ARG	Sidechain
1	A	434	ARG	Sidechain
1	A	439	ARG	Sidechain
1	A	523	ARG	Sidechain
1	A	535	ARG	Sidechain
1	A	579	ARG	Sidechain
1	A	586	ARG	Sidechain
1	A	591	ARG	Sidechain
1	A	652	ARG	Sidechain
1	A	716	ARG	Sidechain
1	A	769	ARG	Sidechain
1	A	779	ARG	Sidechain
1	A	787	ARG	Sidechain
1	A	960	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	962	ARG	Sidechain
1	A	976	ARG	Sidechain
1	A	990	ARG	Sidechain

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	8717	0	8774	301	0
2	B	914	0	459	13	0
3	C	568	0	319	11	0
4	D	475	0	261	20	0
5	A	13	0	5	2	0
6	A	33	0	0	0	0
6	B	1	0	0	0	0
6	C	5	0	0	0	0
6	D	1	0	0	0	0
All	All	10727	0	9818	324	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 16.

All (324) 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:824:LYS:HE3	1:A:825:PRO:CD	1.59	1.31
1:A:575:ILE:HD11	1:A:579:ARG:NH2	1.48	1.27
1:A:824:LYS:CE	1:A:825:PRO:HD3	1.66	1.22
1:A:387:TYR:HB2	1:A:402:ARG:NH1	1.53	1.22
1:A:574:GLN:HG2	1:A:593:MET:CE	1.72	1.19
1:A:574:GLN:HG2	1:A:593:MET:HE2	1.20	1.16
1:A:394:LEU:HD22	1:A:396:GLU:OE2	1.51	1.08
1:A:720:GLU:HA	1:A:740:MET:HE3	1.28	1.06
1:A:824:LYS:CE	1:A:825:PRO:CD	2.30	1.04
4:D:11:DA:H5"	4:D:11:DA:H8	1.28	0.99
1:A:783:PHE:HE1	1:A:849:MET:HE3	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:HD2	1:A:524:TRP:HB3	1.46	0.97
1:A:111:ILE:HD12	1:A:111:ILE:H	1.25	0.97
1:A:384:HIS:HB2	1:A:406:TYR:OH	1.64	0.96
1:A:574:GLN:CG	1:A:593:MET:CE	2.43	0.95
1:A:49:ASN:HB3	1:A:131:MET:CE	1.96	0.95
1:A:387:TYR:HB2	1:A:402:ARG:HH12	1.26	0.94
1:A:748:ASP:HB3	1:A:751:THR:HG22	1.49	0.94
1:A:972:THR:H	1:A:975:ASN:HD22	0.94	0.94
1:A:824:LYS:HD3	1:A:825:PRO:HD2	1.49	0.93
1:A:972:THR:H	1:A:975:ASN:ND2	1.67	0.93
1:A:89:PRO:HB2	1:A:129:LYS:HG2	1.51	0.92
4:D:11:DA:H5"	4:D:11:DA:C8	2.04	0.92
1:A:575:ILE:HD11	1:A:579:ARG:HH22	1.34	0.91
1:A:387:TYR:CB	1:A:402:ARG:NH1	2.34	0.91
1:A:720:GLU:CA	1:A:740:MET:HE3	2.01	0.90
1:A:824:LYS:HD3	1:A:825:PRO:CD	2.02	0.90
1:A:571:SER:O	1:A:575:ILE:HG23	1.71	0.89
1:A:574:GLN:CG	1:A:593:MET:HE2	2.00	0.88
1:A:972:THR:N	1:A:975:ASN:HD22	1.73	0.86
1:A:720:GLU:N	1:A:740:MET:CE	2.39	0.86
1:A:1011:LYS:NZ	1:A:1011:LYS:HB3	1.91	0.85
1:A:824:LYS:CD	1:A:825:PRO:CD	2.55	0.84
1:A:727:MET:O	1:A:734:ASN:HB3	1.78	0.84
1:A:52:GLY:O	1:A:55:ILE:CG1	2.26	0.83
1:A:387:TYR:HB2	1:A:402:ARG:HH11	1.42	0.83
1:A:384:HIS:HA	1:A:406:TYR:HE1	1.44	0.83
1:A:748:ASP:O	1:A:751:THR:HG23	1.79	0.83
1:A:824:LYS:CD	1:A:825:PRO:HD2	2.08	0.83
1:A:402:ARG:O	1:A:402:ARG:HD3	1.80	0.81
1:A:575:ILE:CD1	1:A:579:ARG:NH2	2.39	0.81
1:A:849:MET:CE	1:A:849:MET:HA	2.10	0.81
1:A:356:ASP:OD1	1:A:356:ASP:N	2.10	0.81
1:A:394:LEU:HD13	1:A:399:LYS:HG2	1.64	0.79
1:A:33:PHE:CD2	1:A:516:VAL:HG22	2.18	0.79
1:A:348:PHE:HD1	1:A:353:PHE:CE2	2.00	0.79
1:A:724:ASN:O	1:A:771:HIS:CE1	2.35	0.78
1:A:52:GLY:O	1:A:55:ILE:HG12	1.83	0.78
1:A:387:TYR:CB	1:A:402:ARG:HH12	1.96	0.78
1:A:783:PHE:HE1	1:A:849:MET:CE	1.96	0.78
3:C:3:DT:H5"	3:C:3:DT:H6	1.48	0.78
1:A:402:ARG:HD3	1:A:402:ARG:C	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:GLU:CA	1:A:740:MET:CE	2.63	0.77
1:A:824:LYS:CE	1:A:825:PRO:HD2	2.14	0.77
1:A:394:LEU:CD1	1:A:399:LYS:HG2	2.16	0.76
1:A:737:ILE:HG22	1:A:738:ASP:H	1.51	0.76
1:A:403:ILE:HG13	1:A:404:LYS:HD3	1.68	0.76
1:A:724:ASN:O	1:A:771:HIS:HE1	1.67	0.76
1:A:720:GLU:HA	1:A:740:MET:CE	2.12	0.75
1:A:724:ASN:ND2	1:A:724:ASN:H	1.84	0.75
1:A:495:LEU:O	1:A:499:LEU:HD23	1.85	0.75
1:A:783:PHE:CE1	1:A:849:MET:HE3	2.19	0.75
1:A:384:HIS:HA	1:A:406:TYR:CE1	2.22	0.74
1:A:824:LYS:HE3	1:A:825:PRO:HD3	0.78	0.73
1:A:1087:GLN:H	1:A:1087:GLN:NE2	1.86	0.73
1:A:727:MET:O	1:A:734:ASN:CB	2.37	0.72
1:A:225:ARG:O	1:A:229:ILE:HD12	1.89	0.72
1:A:774:GLN:HB3	1:A:777:GLU:OE1	1.90	0.72
1:A:52:GLY:O	1:A:55:ILE:HG13	1.89	0.71
1:A:892:LYS:NZ	1:A:1084:VAL:O	2.24	0.70
1:A:338:GLU:N	1:A:339:PRO:HD2	2.07	0.70
1:A:772:SER:OG	1:A:823:LYS:NZ	2.24	0.70
1:A:719:LEU:C	1:A:740:MET:HE2	2.12	0.70
1:A:111:ILE:HD12	1:A:111:ILE:N	2.05	0.70
1:A:575:ILE:HD12	1:A:575:ILE:O	1.92	0.69
1:A:298:LEU:O	1:A:302:SER:HB3	1.92	0.69
1:A:719:LEU:HG	1:A:740:MET:HE2	1.73	0.69
4:D:4:DT:H2"	4:D:5:DA:C8	2.28	0.69
1:A:268:GLU:CD	4:D:12:DT:O2	2.29	0.69
1:A:720:GLU:N	1:A:740:MET:HE1	2.06	0.69
1:A:834:ALA:N	1:A:835:PRO:HD2	2.08	0.69
1:A:849:MET:HA	1:A:849:MET:HE2	1.75	0.68
1:A:387:TYR:CG	1:A:406:TYR:CD1	2.81	0.68
1:A:821:LEU:C	1:A:822:LEU:HD13	2.14	0.67
1:A:843:GLN:O	1:A:843:GLN:NE2	2.27	0.67
4:D:12:DT:OP2	4:D:12:DT:H3'	1.94	0.67
4:D:11:DA:H8	4:D:11:DA:C5'	2.06	0.66
1:A:574:GLN:CG	1:A:593:MET:HE1	2.26	0.66
1:A:768:ILE:HG13	1:A:778:TYR:CE2	2.31	0.66
1:A:177:PHE:HB3	1:A:286:LYS:HD3	1.77	0.65
1:A:859:LYS:NZ	2:B:11:C:OP2	2.28	0.65
1:A:429:LEU:HD21	3:C:3:DT:H2"	1.78	0.65
1:A:719:LEU:C	1:A:740:MET:CE	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:CD2	1:A:396:GLU:OE2	2.39	0.64
1:A:849:MET:HE3	1:A:849:MET:HA	1.80	0.64
1:A:258:ASN:ND2	1:A:261:SER:HB2	2.13	0.64
1:A:575:ILE:HD12	1:A:575:ILE:C	2.17	0.64
1:A:693:LYS:HD2	1:A:695:TYR:OH	1.97	0.64
1:A:479:GLY:HA3	1:A:483:LYS:HE3	1.79	0.64
1:A:391:ILE:HD12	1:A:391:ILE:O	1.97	0.64
1:A:344:VAL:HG11	1:A:452:ILE:HG13	1.81	0.62
1:A:570:LEU:HB3	1:A:575:ILE:HG22	1.82	0.62
1:A:350:SER:HB2	1:A:351:PRO:HD2	1.82	0.61
4:D:22:DA:H1'	4:D:23:DG:H5'	1.83	0.61
1:A:34:MET:O	1:A:38:MET:HG3	2.01	0.61
1:A:431:GLN:HE21	1:A:431:GLN:HA	1.66	0.60
1:A:400:GLU:HA	1:A:403:ILE:HD11	1.83	0.60
1:A:636:LYS:HE2	1:A:638:LYS:HB2	1.83	0.60
1:A:972:THR:N	1:A:975:ASN:ND2	2.40	0.60
1:A:763:LEU:N	1:A:763:LEU:HD23	2.16	0.60
1:A:748:ASP:O	1:A:751:THR:CG2	2.49	0.59
1:A:535:ARG:O	1:A:539:GLU:HG3	2.03	0.59
1:A:590:LYS:NZ	2:B:20:G:OP2	2.35	0.59
1:A:637:GLU:OE1	1:A:932:GLN:NE2	2.37	0.58
1:A:102:GLN:HG3	1:A:108:GLU:HG2	1.85	0.58
1:A:87:SER:HB3	1:A:89:PRO:HD2	1.85	0.58
1:A:574:GLN:HG3	1:A:593:MET:HE1	1.86	0.58
1:A:49:ASN:HB3	1:A:131:MET:HE2	1.82	0.58
1:A:693:LYS:HD2	1:A:695:TYR:CZ	2.39	0.58
1:A:268:GLU:OE2	4:D:12:DT:O2	2.22	0.57
1:A:90:GLN:HE21	1:A:91:GLY:H	1.53	0.57
1:A:620:ARG:HD2	1:A:625:GLU:OE1	2.05	0.57
1:A:822:LEU:HD13	1:A:822:LEU:N	2.18	0.57
1:A:352:TYR:CE2	1:A:435:TYR:HA	2.39	0.57
1:A:716:ARG:HB2	1:A:743:PHE:CZ	2.40	0.57
1:A:49:ASN:HB3	1:A:131:MET:HE3	1.84	0.57
1:A:348:PHE:HA	1:A:353:PHE:CD2	2.40	0.56
1:A:503:ARG:HD3	2:B:2:U:O2'	2.05	0.56
1:A:783:PHE:CE1	1:A:849:MET:CE	2.83	0.56
1:A:1011:LYS:HB3	1:A:1011:LYS:HZ2	1.68	0.56
1:A:696:ASP:OD2	1:A:699:SER:OG	2.21	0.56
1:A:697:GLN:NE2	2:B:10:C:O2'	2.39	0.56
1:A:26:ARG:NH1	5:A:1201:CIT:O2	2.39	0.56
1:A:350:SER:HB3	1:A:435:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:LEU:HD13	1:A:1022:PHE:CE2	2.41	0.56
1:A:734:ASN:OD1	1:A:734:ASN:N	2.34	0.56
1:A:207:SER:OG	1:A:210:GLN:HG3	2.06	0.55
1:A:355:SER:HB3	1:A:358:ASN:HA	1.87	0.55
1:A:310:SER:HB3	3:C:17:DA:H2"	1.89	0.55
1:A:387:TYR:CA	1:A:402:ARG:HH12	2.18	0.55
1:A:66:LYS:HG2	1:A:164:LEU:HD12	1.88	0.54
1:A:387:TYR:CB	1:A:406:TYR:CD1	2.90	0.54
1:A:388:GLU:O	1:A:388:GLU:HG2	2.07	0.54
1:A:571:SER:O	1:A:575:ILE:CG2	2.52	0.54
1:A:111:ILE:H	1:A:111:ILE:CD1	1.96	0.54
1:A:83:MET:HB2	1:A:129:LYS:HD3	1.90	0.54
1:A:361:TRP:CE2	3:C:4:DA:H4'	2.43	0.54
1:A:883:ARG:HA	1:A:887:GLY:O	2.08	0.54
3:C:7:DC:H2'	3:C:8:DC:C6	2.44	0.53
4:D:12:DT:H3'	4:D:12:DT:P	2.49	0.53
1:A:885:LYS:HD3	1:A:886:TYR:CE1	2.43	0.53
1:A:774:GLN:HG2	1:A:777:GLU:OE1	2.09	0.53
1:A:946:HIS:HE1	1:A:996:TYR:OH	1.90	0.53
1:A:267:LYS:NZ	4:D:14:DA:N3	2.53	0.53
1:A:708:CYS:O	1:A:712:VAL:HG23	2.09	0.53
1:A:235:GLY:HA2	4:D:7:DT:O2	2.09	0.53
1:A:722:TYR:OH	1:A:777:GLU:HB3	2.09	0.53
1:A:101:PHE:O	1:A:105:SER:HB3	2.09	0.52
1:A:724:ASN:H	1:A:724:ASN:HD22	1.58	0.52
1:A:58:ASP:OD2	1:A:154:LYS:HE2	2.09	0.52
1:A:92:VAL:HG21	1:A:130:ASP:HB2	1.92	0.52
1:A:268:GLU:OE1	4:D:13:DT:H2'	2.10	0.52
1:A:998:GLU:OE2	1:A:998:GLU:HA	2.09	0.52
4:D:11:DA:C8	4:D:11:DA:C5'	2.85	0.52
1:A:439:ARG:HB3	1:A:442:ASP:HB2	1.91	0.52
3:C:3:DT:H6	3:C:3:DT:C5'	2.19	0.52
1:A:517:LEU:HD13	1:A:524:TRP:CE2	2.45	0.52
1:A:968:PRO:O	1:A:1023:LYS:HD3	2.09	0.52
1:A:483:LYS:NZ	3:C:20:DG:OP2	2.44	0.51
1:A:963:TYR:CE2	1:A:1049:LEU:HD22	2.45	0.51
1:A:338:GLU:N	1:A:339:PRO:CD	2.72	0.51
1:A:84:PRO:O	1:A:87:SER:HB2	2.11	0.51
1:A:620:ARG:HG2	1:A:620:ARG:HH11	1.76	0.51
1:A:948:ASP:OD2	1:A:960:ARG:NH2	2.43	0.51
1:A:271:GLY:O	1:A:274:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:C:H5"	2:B:21:C:H6	1.76	0.51
1:A:431:GLN:OE1	2:B:42:A:H4'	2.11	0.51
1:A:634:LYS:NZ	1:A:934:LEU:O	2.44	0.50
1:A:641:LYS:NZ	1:A:661:ALA:O	2.44	0.50
1:A:377:TRP:CD1	1:A:445:VAL:HB	2.46	0.50
1:A:718:PHE:CD1	1:A:718:PHE:C	2.85	0.50
1:A:1011:LYS:HB3	1:A:1011:LYS:HZ1	1.72	0.50
1:A:662:HIS:HA	1:A:675:PRO:HG2	1.93	0.50
1:A:350:SER:HB3	1:A:435:TYR:HE1	1.76	0.50
1:A:966:CYS:SG	1:A:971:LEU:HD23	2.52	0.50
1:A:279:TRP:HB3	1:A:282:MET:HG2	1.94	0.49
1:A:730:ASN:HB2	1:A:735:ILE:HG22	1.93	0.49
1:A:387:TYR:HD2	1:A:402:ARG:HD2	1.77	0.49
1:A:754:TYR:OH	2:B:12:C:OP1	2.25	0.49
1:A:787:ARG:NH1	1:A:788:ASP:OD2	2.45	0.49
1:A:404:LYS:CD	1:A:404:LYS:N	2.75	0.49
1:A:737:ILE:HG22	1:A:738:ASP:N	2.22	0.49
1:A:822:LEU:HB3	1:A:837:ILE:HD12	1.95	0.49
1:A:852:LEU:HD12	1:A:852:LEU:O	2.13	0.49
1:A:330:LYS:HG3	1:A:461:VAL:HG11	1.94	0.49
1:A:642:VAL:HB	1:A:889:VAL:HG22	1.95	0.49
1:A:843:GLN:HE21	1:A:843:GLN:C	2.16	0.49
1:A:387:TYR:CD2	1:A:402:ARG:HD2	2.48	0.48
1:A:430:VAL:O	1:A:434:ARG:HG3	2.14	0.48
1:A:709:LYS:N	1:A:710:PRO:CD	2.76	0.48
1:A:823:LYS:HE3	2:B:38:A:OP1	2.13	0.48
1:A:739:PHE:O	1:A:742:ASP:HB2	2.13	0.48
1:A:447:LYS:HA	1:A:447:LYS:HD3	1.61	0.48
1:A:772:SER:CB	1:A:823:LYS:NZ	2.77	0.48
1:A:892:LYS:HD3	1:A:939:VAL:HG11	1.94	0.48
1:A:660:GLU:HB2	1:A:679:ILE:HD11	1.96	0.48
1:A:548:ASN:N	1:A:549:PRO:CD	2.77	0.48
1:A:834:ALA:N	1:A:835:PRO:CD	2.76	0.48
2:B:37:A:H2'	2:B:38:A:O4'	2.14	0.47
1:A:765:GLN:O	1:A:769:ARG:HG3	2.14	0.47
2:B:18:U:O2'	2:B:19:G:H5"	2.14	0.47
1:A:348:PHE:CD1	1:A:353:PHE:CE2	2.92	0.47
1:A:693:LYS:CD	1:A:695:TYR:OH	2.63	0.47
1:A:711:HIS:O	1:A:715:ARG:HG2	2.15	0.47
1:A:979:ILE:HD11	1:A:1040:PHE:CD2	2.49	0.47
1:A:73:LEU:HG	1:A:112:GLN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ASN:HA	1:A:537:LEU:HD21	1.96	0.47
1:A:743:PHE:CD1	1:A:743:PHE:C	2.87	0.47
1:A:774:GLN:CB	1:A:777:GLU:OE1	2.62	0.47
4:D:6:DG:H2'	4:D:7:DT:C6	2.49	0.47
1:A:768:ILE:HG13	1:A:778:TYR:CD2	2.50	0.47
1:A:1030:LEU:HD11	1:A:1038:LEU:HB3	1.97	0.47
1:A:631:LYS:NZ	3:C:21:DA:OP1	2.45	0.46
1:A:698:LEU:O	1:A:800:SER:HA	2.15	0.46
1:A:340:PHE:O	1:A:344:VAL:HG23	2.15	0.46
1:A:387:TYR:CD2	1:A:406:TYR:HB2	2.51	0.46
1:A:509:TYR:HB2	2:B:3:U:O4	2.16	0.46
1:A:794:LEU:HD12	1:A:794:LEU:HA	1.73	0.46
1:A:347:PHE:CZ	1:A:353:PHE:HB2	2.50	0.46
1:A:127:GLN:OE1	1:A:129:LYS:NZ	2.48	0.46
1:A:400:GLU:O	1:A:400:GLU:HG2	2.16	0.46
1:A:139:LEU:HA	1:A:144:LEU:HB2	1.98	0.45
1:A:748:ASP:HB3	1:A:751:THR:CG2	2.35	0.45
3:C:1:DT:H5"	3:C:1:DT:H6	1.80	0.45
4:D:12:DT:OP2	4:D:12:DT:H2'	2.15	0.45
1:A:258:ASN:CG	1:A:261:SER:HB2	2.37	0.45
1:A:268:GLU:OE1	4:D:13:DT:C2'	2.65	0.45
1:A:394:LEU:HD23	1:A:394:LEU:HA	1.76	0.45
1:A:774:GLN:CG	1:A:777:GLU:OE1	2.65	0.45
1:A:387:TYR:HA	1:A:402:ARG:NH1	2.32	0.45
1:A:726:THR:HA	1:A:736:GLN:HA	1.97	0.45
1:A:400:GLU:OE2	1:A:400:GLU:N	2.49	0.45
1:A:640:TYR:HA	1:A:888:PRO:HB2	1.98	0.45
3:C:6:DT:H2'	3:C:7:DC:C6	2.52	0.45
1:A:48:TRP:CD1	1:A:309:LEU:HD21	2.52	0.45
1:A:258:ASN:OD1	1:A:260:PRO:HD2	2.17	0.45
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.82	0.45
1:A:718:PHE:CE2	1:A:781:GLU:HB2	2.52	0.45
1:A:1083:LEU:HD23	1:A:1086:ILE:HD13	1.98	0.45
1:A:1025:ILE:O	1:A:1029:ILE:HG13	2.17	0.45
4:D:10:DT:H6	4:D:10:DT:H2'	1.51	0.45
4:D:11:DA:H8	4:D:11:DA:OP2	1.99	0.45
4:D:11:DA:C8	4:D:11:DA:OP2	2.70	0.45
1:A:443:ILE:HD11	1:A:447:LYS:HB3	1.99	0.44
1:A:535:ARG:HB2	2:B:7:G:C6	2.51	0.44
1:A:400:GLU:HA	1:A:403:ILE:CD1	2.46	0.44
1:A:713:GLU:HA	1:A:716:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LYS:HE3	1:A:325:LYS:HB2	1.49	0.44
1:A:437:TYR:CE2	1:A:440:LYS:HE2	2.52	0.44
1:A:518:ASN:O	1:A:522:MET:N	2.51	0.44
1:A:724:ASN:ND2	1:A:724:ASN:N	2.59	0.44
1:A:26:ARG:HH11	5:A:1201:CIT:C1	2.31	0.44
1:A:73:LEU:HD22	1:A:77:VAL:HG13	1.98	0.44
1:A:226:LYS:HB2	1:A:226:LYS:HE2	1.64	0.44
1:A:606:ARG:HH11	1:A:606:ARG:HG2	1.83	0.44
1:A:746:ILE:HG13	1:A:756:PHE:HD1	1.83	0.44
1:A:387:TYR:CA	1:A:402:ARG:NH1	2.78	0.44
1:A:782:ILE:HG12	1:A:813:LEU:HD21	2.00	0.44
1:A:940:ASN:OD1	1:A:941:PRO:HD2	2.17	0.44
1:A:1085:ASP:HB3	1:A:1088:LYS:HG3	2.00	0.44
1:A:497:HIS:CD2	1:A:503:ARG:NH2	2.86	0.44
1:A:439:ARG:HB3	1:A:439:ARG:HE	1.43	0.43
1:A:399:LYS:HB2	1:A:399:LYS:HE3	1.79	0.43
1:A:394:LEU:HD12	1:A:399:LYS:HG2	1.96	0.43
1:A:980:LEU:HD11	1:A:1015:LEU:HA	1.99	0.43
1:A:265:ASN:O	1:A:269:LYS:HG3	2.19	0.43
1:A:20:ILE:HG13	1:A:509:TYR:CE1	2.53	0.43
1:A:387:TYR:HA	1:A:402:ARG:HH12	1.82	0.43
1:A:705:LEU:HD12	1:A:705:LEU:HA	1.74	0.43
1:A:204:GLN:HE21	1:A:204:GLN:HB2	1.55	0.43
1:A:375:THR:HA	1:A:378:GLU:HG3	2.01	0.43
1:A:843:GLN:NE2	1:A:843:GLN:C	2.72	0.43
4:D:7:DT:H2'	4:D:8:DT:C6	2.54	0.43
1:A:224:TYR:HB2	1:A:244:VAL:HG12	2.01	0.43
1:A:720:GLU:O	1:A:723:ARG:HG2	2.19	0.42
1:A:67:ASP:O	1:A:69:ILE:HG13	2.20	0.42
1:A:290:ALA:HA	1:A:294:GLY:O	2.19	0.42
1:A:686:VAL:HG21	1:A:870:VAL:CG2	2.49	0.42
1:A:708:CYS:HB3	1:A:791:LEU:CD1	2.49	0.42
1:A:403:ILE:HG13	1:A:404:LYS:CD	2.44	0.42
1:A:575:ILE:HD12	1:A:579:ARG:HG3	2.02	0.42
1:A:864:VAL:HG13	1:A:916:LEU:HD21	2.00	0.42
1:A:811:LYS:HB3	1:A:811:LYS:HE2	1.79	0.42
1:A:912:LEU:HD12	1:A:912:LEU:HA	1.83	0.42
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.79	0.42
1:A:995:TYR:CD1	1:A:995:TYR:N	2.86	0.42
1:A:188:LYS:HZ1	1:A:232:SER:HG	1.60	0.42
1:A:230:ARG:NH1	1:A:230:ARG:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:VAL:HG11	1:A:428:PRO:CG	2.50	0.42
1:A:475:SER:HB2	1:A:616:ASN:HD21	1.85	0.42
1:A:394:LEU:O	1:A:396:GLU:HG3	2.20	0.41
1:A:980:LEU:HD23	1:A:980:LEU:HA	1.89	0.41
1:A:314:GLY:CA	3:C:16:DA:H2"	2.50	0.41
1:A:436:LEU:HD13	1:A:448:ILE:HG21	2.02	0.41
1:A:774:GLN:O	1:A:777:GLU:HB2	2.20	0.41
1:A:474:PRO:HB2	1:A:476:PHE:CZ	2.55	0.41
1:A:259:VAL:N	1:A:260:PRO:CD	2.84	0.41
1:A:746:ILE:HG13	1:A:756:PHE:CD1	2.56	0.41
2:B:27:U:H2'	2:B:28:A:O4'	2.21	0.41
1:A:41:THR:HB	1:A:42:PRO:HD3	2.02	0.41
1:A:56:ASP:OD1	1:A:59:ILE:HD12	2.21	0.41
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.86	0.41
1:A:822:LEU:N	1:A:822:LEU:CD1	2.81	0.41
1:A:310:SER:HB2	1:A:311:PRO:HD3	2.03	0.41
1:A:398:LYS:HB2	1:A:398:LYS:HE3	1.44	0.41
1:A:548:ASN:N	1:A:549:PRO:HD3	2.37	0.40
1:A:102:GLN:HA	1:A:107:SER:O	2.21	0.40
1:A:250:GLY:HA2	1:A:253:HIS:NE2	2.36	0.40
1:A:849:MET:CE	1:A:849:MET:CA	2.87	0.40
1:A:400:GLU:HA	1:A:403:ILE:CG1	2.52	0.40
1:A:350:SER:CB	1:A:435:TYR:CE1	3.04	0.40
1:A:352:TYR:CD2	1:A:435:TYR:HB2	2.56	0.40
1:A:421:VAL:HG12	1:A:428:PRO:HD3	2.03	0.40
1:A:722:TYR:OH	1:A:777:GLU:CG	2.69	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	1073/1101 (98%)	1047 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	960/984 (98%)	817 (85%)	143 (15%)	3	2

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	48	TRP
1	A	55	ILE
1	A	61	SER
1	A	66	LYS
1	A	73	LEU
1	A	87	SER
1	A	88	LYS
1	A	96	ASN
1	A	107	SER
1	A	111	ILE
1	A	123	THR
1	A	129	LYS
1	A	146	ARG
1	A	147	SER
1	A	153	LEU
1	A	155	LEU
1	A	167	SER
1	A	198	LEU
1	A	202	SER
1	A	204	GLN
1	A	216	LEU
1	A	226	LYS

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	232	SER
1	A	241	LEU
1	A	242	LYS
1	A	256	GLU
1	A	261	SER
1	A	265	ASN
1	A	266	LEU
1	A	268	GLU
1	A	277	CYS
1	A	302	SER
1	A	306	GLU
1	A	313	LYS
1	A	325	LYS
1	A	342	LYS
1	A	345	GLU
1	A	356	ASP
1	A	357	THR
1	A	360	LYS
1	A	370	GLU
1	A	375	THR
1	A	377	TRP
1	A	378	GLU
1	A	384	HIS
1	A	385	SER
1	A	386	LYS
1	A	387	TYR
1	A	391	ILE
1	A	394	LEU
1	A	396	GLU
1	A	398	LYS
1	A	399	LYS
1	A	400	GLU
1	A	401	LYS
1	A	402	ARG
1	A	404	LYS
1	A	405	VAL
1	A	423	LYS
1	A	430	VAL
1	A	431	GLN
1	A	439	ARG
1	A	440	LYS

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Mol	Chain	Res	Type
1	A	441	ASP
1	A	443	ILE
1	A	452	ILE
1	A	457	LYS
1	A	463	LYS
1	A	492	LYS
1	A	500	LYS
1	A	503	ARG
1	A	516	VAL
1	A	537	LEU
1	A	542	TYR
1	A	547	GLU
1	A	556	ARG
1	A	561	THR
1	A	575	ILE
1	A	579	ARG
1	A	583	VAL
1	A	587	LYS
1	A	589	LYS
1	A	595	LEU
1	A	611	LYS
1	A	636	LYS
1	A	677	LYS
1	A	688	SER
1	A	691	ARG
1	A	693	LYS
1	A	703	VAL
1	A	705	LEU
1	A	709	LYS
1	A	713	GLU
1	A	715	ARG
1	A	717	SER
1	A	720	GLU
1	A	723	ARG
1	A	724	ASN
1	A	726	THR
1	A	727	MET
1	A	728	LYS
1	A	731	ARG
1	A	734	ASN
1	A	735	ILE
1	A	741	LYS

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Mol	Chain	Res	Type
1	A	744	GLU
1	A	746	ILE
1	A	750	GLU
1	A	751	THR
1	A	776	LYS
1	A	779	ARG
1	A	785	LEU
1	A	794	LEU
1	A	811	LYS
1	A	822	LEU
1	A	823	LYS
1	A	824	LYS
1	A	843	GLN
1	A	849	MET
1	A	885	LYS
1	A	905	LYS
1	A	906	SER
1	A	912	LEU
1	A	934	LEU
1	A	964	SER
1	A	977	LYS
1	A	985	ASP
1	A	986	LYS
1	A	989	LYS
1	A	993	ASN
1	A	995	TYR
1	A	1006	THR
1	A	1010	LYS
1	A	1011	LYS
1	A	1036	ASP
1	A	1038	LEU
1	A	1046	MET
1	A	1049	LEU
1	A	1061	VAL
1	A	1087	GLN
1	A	1091	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	90	GLN

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	204	GLN
1	A	265	ASN
1	A	358	ASN
1	A	381	ASN
1	A	505	GLN
1	A	672	ASN
1	A	697	GLN
1	A	724	ASN
1	A	736	GLN
1	A	843	GLN
1	A	922	ASN
1	A	942	ASN
1	A	946	HIS
1	A	975	ASN
1	A	993	ASN
1	A	997	ASN
1	A	1087	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	42/43 (97%)	3 (7%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	17	U
2	B	24	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 monosaccharides 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	1.25	1 (8%)	17,17,17	1.73	2 (11%)

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	-	-	5/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1201	CIT	C4-C3	2.14	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1201	CIT	O6-C6-C3	4.58	121.00	113.05
5	A	1201	CIT	O4-C5-C4	2.51	122.41	114.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1201	CIT	C2-C3-C4-C5
5	A	1201	CIT	O7-C3-C4-C5
5	A	1201	CIT	C6-C3-C4-C5
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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	CIT	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	1077/1101 (97%)	0.37	53 (4%) 29 27	31, 56, 108, 162	0
2	B	43/43 (100%)	0.04	4 (9%) 8 5	37, 49, 92, 130	2 (4%)
3	C	28/40 (70%)	0.09	0 100 100	35, 47, 97, 128	0
4	D	23/40 (57%)	0.32	2 (8%) 10 7	40, 61, 130, 158	3 (13%)
All	All	1171/1224 (95%)	0.35	59 (5%) 28 26	31, 56, 110, 162	5 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	ALA	7.7
1	A	403	ILE	7.0
1	A	393	SER	5.6
1	A	405	VAL	5.3
1	A	395	SER	5.1
1	A	732	GLY	4.9
1	A	733	ASN	4.9
1	A	357	THR	4.8
1	A	391	ILE	4.7
1	A	397	ASP	4.6
1	A	356	ASP	4.5
1	A	729	ASP	4.4
1	A	386	LYS	4.4
1	A	730	ASN	4.3
1	A	735	ILE	4.3
1	A	734	ASN	4.1
2	B	43	G	4.0
1	A	834	ALA	3.9
1	A	728	LYS	3.6
4	D	1	DG	3.6
1	A	382	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	389	GLU	3.5
1	A	355	SER	3.4
1	A	666	ASP	3.4
1	A	399	LYS	3.4
1	A	358	ASN	3.4
1	A	390	ASP	3.4
1	A	731	ARG	3.3
1	A	737	ILE	3.3
1	A	825	PRO	3.1
1	A	387	TYR	3.1
1	A	394	LEU	3.1
1	A	566	GLY	3.0
1	A	410	VAL	2.9
1	A	385	SER	2.9
1	A	7	ASN	2.9
1	A	567	LYS	2.8
1	A	400	GLU	2.7
1	A	1091	LYS	2.7
1	A	727	MET	2.7
1	A	383	ILE	2.7
1	A	837	ILE	2.7
1	A	407	GLN	2.6
2	B	42	A	2.6
1	A	398	LYS	2.6
1	A	404	LYS	2.6
4	D	12	DT	2.6
1	A	353	PHE	2.5
1	A	401	LYS	2.5
1	A	406	TYR	2.3
1	A	388	GLU	2.3
2	B	40	A	2.2
1	A	396	GLU	2.2
1	A	690	VAL	2.1
1	A	664	ASN	2.0
2	B	41	U	2.0
1	A	414	ILE	2.0
1	A	384	HIS	2.0
1	A	578	ILE	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, 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(Å^2)	Q<0.9
5	CIT	A	1201	13/13	0.91	0.14	51,62,87,89	0

6.5 Other polymers (i)

There are no such residues in this entry.