



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:09 PM UTC

PDB ID : 7D2L / pdb_00007d2l
Title : Crystal structure of the Cas12i1 R-loop complex before target DNA cleavage
Authors : Zhang, B.; Luo, D.Y.; Li, Y.; OuYang, S.Y.
Deposited on : 2020-09-16
Resolution : 2.75 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

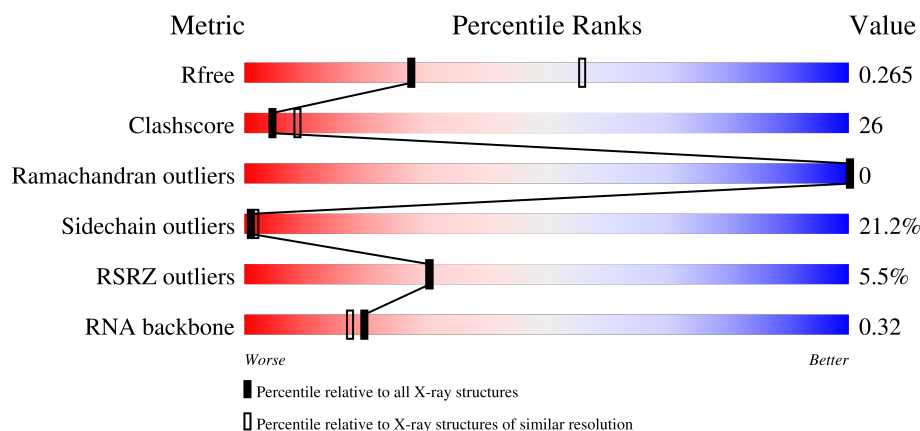
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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	5% 51% 34% 12% ..
2	B	43	33% 37% 26% 5%
3	C	40	5% 55% 20% 25%
4	D	40	12% 32% 30% . 35%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CIT	A	1201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10769 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-D647A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1077	Total	C	N	O	S	0	0	0
			8684	5523	1498	1623	40			

- 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			

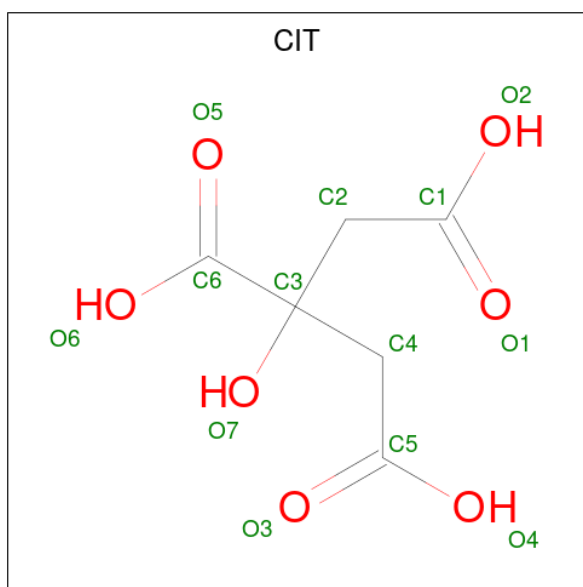
- Molecule 3 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			609	293	106	180	30			

- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	26	Total	C	N	O	P	0	0	0
			537	255	99	157	26			

- 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		

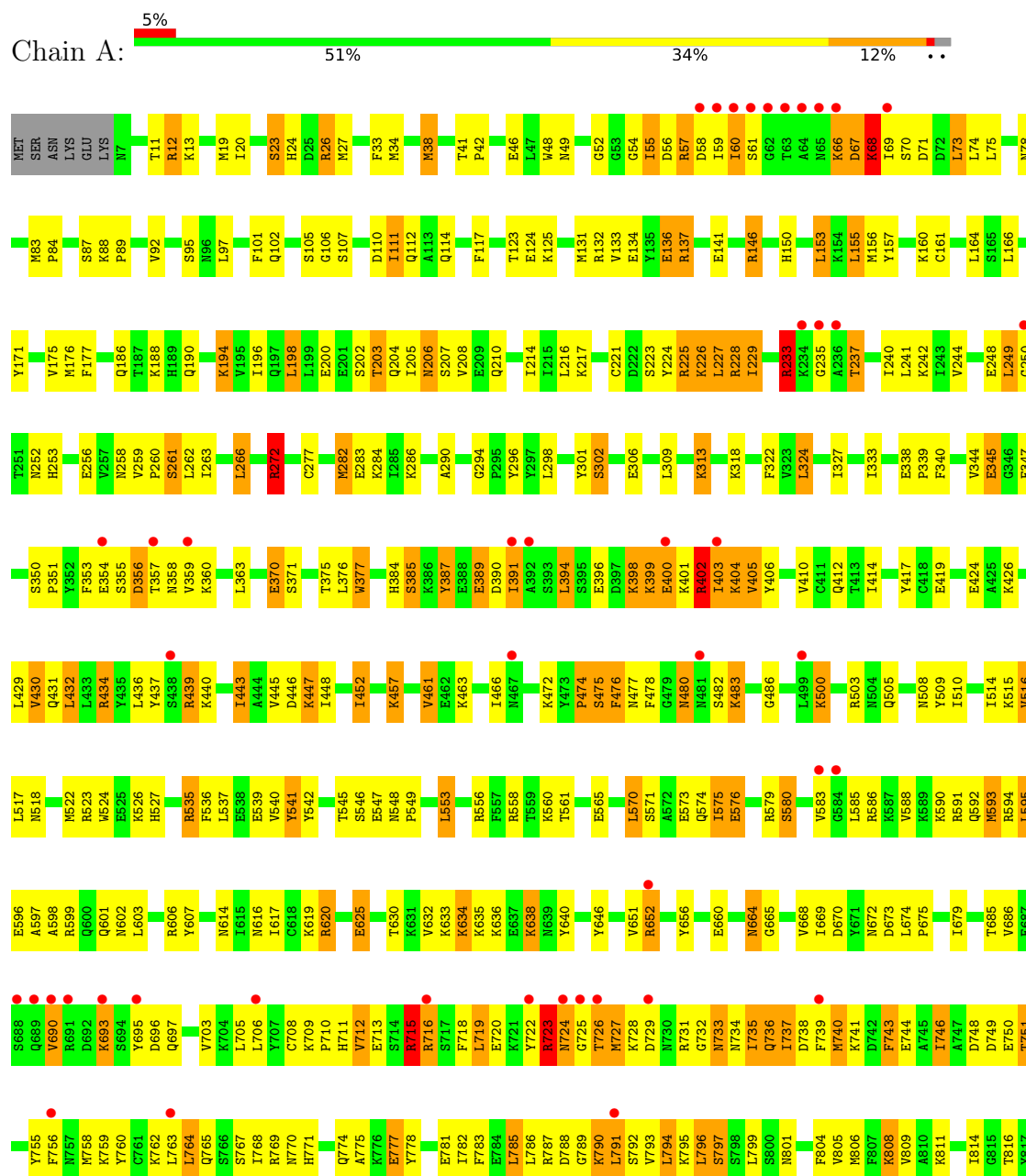
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	2	Total	O	0	0
			2	2		
6	C	1	Total	O	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: 12i1-D647A



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.19Å 142.64Å 209.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.03 – 2.75 59.03 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.03-2.75) 100.0 (59.03-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.213 , 0.264 0.212 , 0.265	Depositor DCC
R_{free} test set	2477 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10769	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.96	0/8862	1.28	10/11936 (0.1%)
2	B	1.07	9/1021 (0.9%)	0.93	5/1588 (0.3%)
3	C	0.78	3/681 (0.4%)	0.85	0/1047
4	D	0.55	0/601	0.85	1/924 (0.1%)
All	All	0.94	12/11165 (0.1%)	1.20	16/15495 (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	30

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	18	DA	O3'-P	-6.28	1.51	1.61
2	B	30	G	O3'-P	-6.14	1.51	1.61
2	B	7	G	O3'-P	-5.94	1.52	1.61
3	C	16	DT	O3'-P	-5.77	1.52	1.61
2	B	29	A	O3'-P	-5.73	1.52	1.61
3	C	19	DA	O3'-P	-5.71	1.52	1.61
2	B	27	U	O3'-P	-5.39	1.53	1.61
2	B	26	U	O3'-P	-5.35	1.53	1.61
2	B	19	G	O3'-P	-5.32	1.53	1.61
2	B	14	U	O3'-P	-5.20	1.53	1.61
2	B	9	G	O3'-P	-5.13	1.53	1.61
2	B	10	C	O3'-P	-5.07	1.53	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	25	DC	C2'-C3'-O3'	-7.99	99.52	111.50
1	A	474	PRO	N-CA-C	7.45	123.23	111.38
1	A	67	ASP	CA-C-N	7.24	132.39	122.19
1	A	67	ASP	C-N-CA	7.24	132.39	122.19
1	A	541	TYR	N-CA-C	5.76	117.56	111.28
2	B	23	C	C1'-C2'-O2'	-5.54	100.10	108.40
1	A	370	GLU	CB-CA-C	-5.48	110.24	116.54
1	A	68	LYS	CA-C-N	5.32	130.11	122.45
1	A	68	LYS	C-N-CA	5.32	130.11	122.45
2	B	9	G	C2'-C3'-O3'	-5.30	105.75	113.70
2	B	24	U	C1'-C2'-O2'	-5.29	103.86	111.80
1	A	476	PHE	CB-CA-C	5.19	119.28	109.37
1	A	835	PRO	N-CA-C	-5.18	105.49	110.47
2	B	31	G	C1'-C2'-O2'	-5.16	100.66	108.40
1	A	764	LEU	N-CA-C	-5.15	105.67	111.28
2	B	22	A	C3'-C2'-O2'	5.01	118.22	110.70

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	137	ARG	Sidechain
1	A	146	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	233	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	272	ARG	Sidechain
1	A	402	ARG	Sidechain
1	A	434	ARG	Sidechain
1	A	439	ARG	Sidechain
1	A	503	ARG	Sidechain
1	A	523	ARG	Sidechain
1	A	535	ARG	Sidechain
1	A	556	ARG	Sidechain
1	A	558	ARG	Sidechain
1	A	57	ARG	Sidechain
1	A	579	ARG	Sidechain
1	A	586	ARG	Sidechain
1	A	591	ARG	Sidechain
1	A	652	ARG	Sidechain
1	A	715	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	716	ARG	Sidechain
1	A	723	ARG	Sidechain
1	A	769	ARG	Sidechain
1	A	860	ARG	Sidechain
1	A	918	ARG	Sidechain
1	A	962	ARG	Sidechain
1	A	965	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	8684	0	8698	502	0
2	B	914	0	459	20	0
3	C	609	0	341	11	0
4	D	537	0	295	27	0
5	A	13	0	5	6	0
6	A	9	0	0	1	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
All	All	10769	0	9798	534	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 26.

All (534) 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:728:LYS:HG3	1:A:733:ASN:ND2	1.37	1.35
1:A:728:LYS:CG	1:A:733:ASN:HD22	1.49	1.23
1:A:632:VAL:HG21	1:A:930:MET:CE	1.75	1.17
1:A:720:GLU:HA	1:A:723:ARG:HG2	1.22	1.15
1:A:782:ILE:HG21	1:A:849:MET:CE	1.78	1.13
1:A:782:ILE:CG2	1:A:849:MET:HE1	1.80	1.12
1:A:632:VAL:HG21	1:A:930:MET:HE1	1.20	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:VAL:HG23	4:D:26:DG:H5''	1.32	1.09
1:A:49:ASN:HB3	1:A:131:MET:CE	1.81	1.09
1:A:570:LEU:HB2	2:B:18:U:C4	1.86	1.09
1:A:1062:ASN:HB2	1:A:1067:GLN:HE22	1.17	1.08
1:A:333:ILE:HD11	1:A:461:VAL:HG11	1.33	1.08
1:A:1062:ASN:HB2	1:A:1067:GLN:NE2	1.70	1.06
1:A:943:PHE:O	1:A:947:GLN:HG3	1.56	1.04
1:A:824:LYS:HD2	1:A:825:PRO:HD3	1.04	1.03
1:A:979:ILE:O	1:A:983:LEU:HD23	1.59	1.02
2:B:13:A:H5''	2:B:13:A:H8	1.15	1.02
1:A:824:LYS:HD2	1:A:825:PRO:CD	1.90	1.00
1:A:824:LYS:CD	1:A:825:PRO:HD3	1.90	1.00
1:A:527:HIS:HD2	5:A:1201:CIT:H41	1.24	1.00
1:A:12:ARG:HG3	1:A:12:ARG:HH11	1.24	1.00
1:A:228:ARG:HH21	1:A:237:THR:HG22	1.25	1.00
2:B:13:A:H5''	2:B:13:A:C8	1.98	0.98
1:A:782:ILE:HG21	1:A:849:MET:HE1	1.01	0.98
1:A:719:LEU:HB3	1:A:740:MET:CE	1.94	0.97
1:A:732:GLY:O	1:A:735:ILE:HG13	1.66	0.96
2:B:1:A:P	2:B:1:A:N3	2.38	0.95
1:A:110:ASP:O	1:A:114:GLN:HG3	1.65	0.95
1:A:1012:ASN:HA	1:A:1015:LEU:HD23	1.47	0.93
1:A:258:ASN:OD1	1:A:261:SER:HB2	1.68	0.93
1:A:176:MET:CE	1:A:282:MET:HE1	2.00	0.92
1:A:720:GLU:CA	1:A:723:ARG:HG2	2.00	0.92
1:A:228:ARG:NH2	1:A:237:THR:HG22	1.86	0.91
1:A:708:CYS:O	1:A:712:VAL:HG12	1.68	0.91
1:A:728:LYS:CG	1:A:733:ASN:ND2	2.21	0.91
1:A:782:ILE:CG2	1:A:849:MET:CE	2.43	0.91
1:A:720:GLU:O	1:A:723:ARG:HG3	1.70	0.90
1:A:570:LEU:HB2	2:B:18:U:O4	1.71	0.89
1:A:480:ASN:HD22	1:A:480:ASN:H	1.18	0.89
1:A:718:PHE:CG	1:A:781:GLU:HG3	2.10	0.87
1:A:720:GLU:O	1:A:723:ARG:CG	2.23	0.87
1:A:60:ILE:HG22	1:A:157:TYR:CZ	2.10	0.86
1:A:527:HIS:HD2	5:A:1201:CIT:C4	1.89	0.86
1:A:664:ASN:O	1:A:664:ASN:ND2	2.10	0.84
1:A:49:ASN:HB3	1:A:131:MET:HE1	1.59	0.84
1:A:344:VAL:HG11	1:A:452:ILE:HG12	1.58	0.83
1:A:333:ILE:HD11	1:A:461:VAL:CG1	2.09	0.83
1:A:602:ASN:ND2	1:A:602:ASN:O	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:HE2	1:A:614:ASN:ND2	1.94	0.83
1:A:774:GLN:O	1:A:777:GLU:HG3	1.78	0.82
3:C:2:DC:H5'	3:C:3:DT:H4'	1.61	0.82
1:A:620:ARG:HG2	1:A:620:ARG:HH11	1.42	0.82
1:A:818:PHE:O	1:A:822:LEU:HD12	1.78	0.82
1:A:34:MET:O	1:A:38:MET:HG3	1.80	0.82
3:C:5:DT:C5'	3:C:5:DT:H6	1.92	0.82
1:A:719:LEU:HB3	1:A:740:MET:HE1	1.62	0.81
1:A:517:LEU:HD13	1:A:524:TRP:CE2	2.15	0.81
1:A:176:MET:HE3	1:A:282:MET:HE1	1.62	0.81
1:A:137:ARG:O	1:A:141:GLU:HG3	1.82	0.80
1:A:176:MET:HE2	1:A:282:MET:CE	2.11	0.80
1:A:33:PHE:CD2	1:A:516:VAL:HG22	2.18	0.79
4:D:26:DG:H2''	4:D:27:DC:OP2	1.82	0.79
1:A:651:VAL:CG2	4:D:26:DG:H4'	2.13	0.79
1:A:943:PHE:O	1:A:947:GLN:CG	2.31	0.78
1:A:651:VAL:HG23	4:D:26:DG:C5'	2.12	0.78
1:A:711:HIS:HB2	1:A:791:LEU:HD13	1.65	0.77
1:A:89:PRO:HA	1:A:134:GLU:OE2	1.85	0.77
1:A:755:TYR:CE1	1:A:759:LYS:HG3	2.20	0.77
1:A:824:LYS:HB3	1:A:825:PRO:HD3	1.67	0.77
1:A:457:LYS:O	1:A:461:VAL:HG12	1.84	0.76
1:A:651:VAL:CG2	4:D:26:DG:C4'	2.64	0.76
1:A:651:VAL:HG21	4:D:26:DG:C4'	2.15	0.76
1:A:176:MET:CE	1:A:282:MET:CE	2.64	0.76
1:A:432:LEU:O	1:A:432:LEU:HD12	1.85	0.76
1:A:225:ARG:O	1:A:229:ILE:HG13	1.85	0.76
1:A:249:LEU:N	1:A:249:LEU:HD23	2.01	0.76
1:A:223:SER:OG	1:A:226:LYS:CD	2.33	0.75
1:A:391:ILE:HA	1:A:394:LEU:HB3	1.67	0.75
1:A:574:GLN:HG2	1:A:593:MET:HG3	1.69	0.75
1:A:722:TYR:HE2	1:A:777:GLU:OE1	1.69	0.75
1:A:250:GLY:HA2	1:A:253:HIS:NE2	2.00	0.74
1:A:711:HIS:CB	1:A:791:LEU:HD13	2.16	0.74
1:A:1029:ILE:O	1:A:1033:ARG:HG3	1.86	0.74
1:A:400:GLU:O	1:A:403:ILE:HD13	1.86	0.74
1:A:97:LEU:HD13	1:A:117:PHE:CD1	2.23	0.74
1:A:553:LEU:N	1:A:553:LEU:HD23	2.03	0.74
1:A:176:MET:HE2	1:A:282:MET:HE1	1.66	0.74
1:A:228:ARG:HH21	1:A:237:THR:CG2	1.98	0.74
1:A:1062:ASN:CB	1:A:1067:GLN:HE22	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:LYS:HB3	1:A:825:PRO:CD	2.18	0.73
1:A:527:HIS:CD2	5:A:1201:CIT:H41	2.15	0.73
1:A:60:ILE:HD11	1:A:75:LEU:HD21	1.69	0.73
2:B:21:C:H5''	2:B:21:C:H6	1.54	0.73
1:A:651:VAL:HG21	4:D:26:DG:H4'	1.70	0.73
1:A:60:ILE:HD11	1:A:75:LEU:CD2	2.19	0.72
1:A:345:GLU:O	1:A:345:GLU:HG3	1.89	0.72
1:A:720:GLU:N	1:A:740:MET:HE1	2.04	0.72
1:A:394:LEU:C	1:A:394:LEU:HD22	2.15	0.72
1:A:808:LYS:NZ	1:A:914:ASP:OD2	2.22	0.72
1:A:1036:ASP:OD1	1:A:1036:ASP:N	2.19	0.72
1:A:685:THR:HG22	1:A:696:ASP:OD2	1.89	0.71
1:A:223:SER:OG	1:A:226:LYS:HD3	1.90	0.71
1:A:1005:ALA:CB	1:A:1064:ASN:OD1	2.39	0.71
1:A:272:ARG:HH11	1:A:272:ARG:HB2	1.56	0.71
1:A:576:GLU:O	1:A:580:SER:HB3	1.91	0.71
1:A:588:VAL:HG21	2:B:6:U:O2	1.91	0.70
3:C:5:DT:H6	3:C:5:DT:H5''	1.55	0.70
1:A:74:LEU:HD13	1:A:164:LEU:HD21	1.73	0.70
1:A:968:PRO:O	1:A:1023:LYS:HG2	1.91	0.70
1:A:651:VAL:CG2	4:D:26:DG:H5''	2.17	0.70
1:A:837:ILE:HD12	1:A:837:ILE:N	2.05	0.70
4:D:28:DT:O3'	4:D:29:DG:O4'	2.11	0.69
4:D:7:DT:H2''	4:D:8:DT:O5'	1.93	0.69
1:A:708:CYS:O	1:A:712:VAL:CG1	2.41	0.69
4:D:16:DA:H2''	4:D:17:DA:H5''	1.75	0.68
1:A:272:ARG:HB2	1:A:272:ARG:NH1	2.07	0.68
1:A:60:ILE:CD1	1:A:75:LEU:HD21	2.24	0.68
1:A:527:HIS:CD2	5:A:1201:CIT:C4	2.73	0.68
1:A:34:MET:HE2	1:A:617:ILE:HG22	1.76	0.68
1:A:1087:GLN:CD	1:A:1087:GLN:H	2.00	0.68
1:A:634:LYS:NZ	1:A:934:LEU:O	2.27	0.67
1:A:693:LYS:HD3	1:A:695:TYR:CZ	2.29	0.67
1:A:355:SER:HB3	1:A:358:ASN:HA	1.76	0.67
1:A:983:LEU:HD21	1:A:1000:ALA:HB1	1.75	0.67
1:A:660:GLU:HB2	1:A:679:ILE:HD11	1.76	0.67
1:A:1022:PHE:HA	1:A:1025:ILE:HD12	1.76	0.67
1:A:1072:ASN:HB3	1:A:1075:LEU:HD12	1.76	0.67
1:A:272:ARG:HH11	1:A:272:ARG:CG	2.08	0.67
1:A:590:LYS:NZ	2:B:20:G:OP2	2.28	0.66
3:C:3:DT:H6	3:C:3:DT:H5'	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:HIS:CG	1:A:791:LEU:HD13	2.30	0.66
1:A:620:ARG:HH11	1:A:620:ARG:CG	2.09	0.66
1:A:196:ILE:O	1:A:200:GLU:HG3	1.95	0.65
1:A:718:PHE:CD2	1:A:781:GLU:HG3	2.31	0.65
1:A:207:SER:HB3	1:A:210:GLN:OE1	1.95	0.65
1:A:896:ILE:O	1:A:918:ARG:HD2	1.96	0.65
3:C:2:DC:N4	4:D:29:DG:N1	2.45	0.65
1:A:632:VAL:CG2	1:A:930:MET:CE	2.64	0.65
1:A:60:ILE:HG22	1:A:157:TYR:CE1	2.30	0.65
1:A:298:LEU:O	1:A:302:SER:HB3	1.96	0.64
1:A:49:ASN:HB3	1:A:131:MET:HE3	1.74	0.64
1:A:997:ASN:O	1:A:1001:MET:HG2	1.97	0.64
1:A:394:LEU:HD22	1:A:394:LEU:O	1.97	0.64
1:A:394:LEU:O	1:A:394:LEU:HD13	1.97	0.64
1:A:975:ASN:N	1:A:975:ASN:HD22	1.93	0.64
1:A:723:ARG:HB3	1:A:740:MET:SD	2.38	0.64
1:A:824:LYS:CB	1:A:825:PRO:CD	2.76	0.64
1:A:632:VAL:HG11	1:A:930:MET:HE2	1.79	0.63
1:A:431:GLN:OE1	1:A:431:GLN:HA	1.97	0.63
1:A:480:ASN:H	1:A:480:ASN:ND2	1.92	0.63
1:A:535:ARG:O	1:A:539:GLU:HG3	1.98	0.63
1:A:824:LYS:CB	1:A:825:PRO:HD3	2.27	0.63
1:A:356:ASP:N	1:A:356:ASP:OD1	2.32	0.63
1:A:722:TYR:CE2	1:A:777:GLU:OE1	2.50	0.63
1:A:518:ASN:O	1:A:522:MET:N	2.32	0.62
1:A:1005:ALA:HB3	1:A:1064:ASN:OD1	1.99	0.62
1:A:57:ARG:NH2	1:A:105:SER:OG	2.30	0.62
1:A:790:LYS:HD2	1:A:790:LYS:O	1.99	0.62
1:A:540:VAL:HG13	1:A:607:TYR:CE2	2.34	0.62
1:A:837:ILE:HD12	1:A:837:ILE:H	1.65	0.62
1:A:87:SER:HB3	1:A:89:PRO:HD2	1.80	0.62
1:A:363:LEU:HB3	1:A:452:ILE:HD11	1.81	0.62
1:A:706:LEU:O	1:A:709:LYS:CG	2.47	0.62
1:A:590:LYS:O	1:A:594:ARG:HG3	2.00	0.61
1:A:60:ILE:CD1	1:A:75:LEU:CD2	2.77	0.61
1:A:979:ILE:O	1:A:983:LEU:CD2	2.43	0.61
1:A:896:ILE:O	1:A:918:ARG:CD	2.49	0.61
1:A:399:LYS:H	1:A:399:LYS:HD2	1.66	0.61
1:A:26:ARG:NH1	5:A:1201:CIT:O6	2.34	0.61
1:A:272:ARG:HH11	1:A:272:ARG:CB	2.14	0.61
1:A:736:GLN:NE2	1:A:736:GLN:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:MET:HE2	1:A:282:MET:HE3	1.82	0.60
1:A:711:HIS:HB2	1:A:791:LEU:CD1	2.30	0.60
1:A:588:VAL:O	1:A:592:GLN:HG3	2.01	0.60
1:A:588:VAL:CG2	2:B:6:U:O2	2.49	0.60
1:A:225:ARG:O	1:A:229:ILE:CG1	2.49	0.60
1:A:679:ILE:HD13	1:A:886:TYR:CZ	2.37	0.60
1:A:596:GLU:OE1	1:A:596:GLU:HA	2.02	0.60
1:A:665:GLY:N	1:A:668:VAL:CG2	2.65	0.60
1:A:227:LEU:O	1:A:227:LEU:HD12	2.02	0.59
1:A:1005:ALA:HB1	1:A:1064:ASN:OD1	2.01	0.59
1:A:224:TYR:HB2	1:A:244:VAL:HG12	1.84	0.59
1:A:272:ARG:HH11	1:A:272:ARG:HG3	1.67	0.58
1:A:399:LYS:O	1:A:402:ARG:N	2.35	0.58
1:A:537:LEU:HD23	1:A:541:TYR:HB3	1.85	0.58
1:A:818:PHE:O	1:A:822:LEU:CD1	2.50	0.58
1:A:883:ARG:HA	1:A:887:GLY:O	2.03	0.58
1:A:1021:LYS:HD2	1:A:1021:LYS:N	2.19	0.58
1:A:1010:LYS:O	1:A:1013:ASP:OD1	2.21	0.58
1:A:240:ILE:HG23	1:A:241:LEU:HD12	1.86	0.58
1:A:720:GLU:C	1:A:723:ARG:CG	2.77	0.58
3:C:29:DA:H2''	3:C:30:DC:OP2	2.04	0.58
1:A:338:GLU:N	1:A:339:PRO:CD	2.67	0.58
1:A:443:ILE:HG12	1:A:448:ILE:HG12	1.85	0.58
1:A:58:ASP:OD2	1:A:150:HIS:NE2	2.34	0.57
1:A:208:VAL:HG21	1:A:252:ASN:O	2.04	0.57
1:A:728:LYS:HE3	1:A:733:ASN:ND2	2.18	0.57
1:A:235:GLY:HA2	4:D:7:DT:O2	2.03	0.57
1:A:226:LYS:HD2	1:A:226:LYS:N	2.18	0.57
1:A:719:LEU:CB	1:A:740:MET:HE1	2.33	0.57
1:A:229:ILE:O	1:A:233:ARG:NH2	2.37	0.57
1:A:347:PHE:O	1:A:350:SER:OG	2.23	0.57
1:A:783:PHE:HE1	1:A:849:MET:HG2	1.69	0.56
1:A:651:VAL:CG2	4:D:26:DG:C5'	2.79	0.56
1:A:706:LEU:O	1:A:709:LYS:HG2	2.05	0.56
1:A:1006:THR:OG1	1:A:1064:ASN:N	2.37	0.56
1:A:1053:LYS:HG3	1:A:1069:TRP:CD2	2.40	0.56
1:A:49:ASN:CB	1:A:131:MET:CE	2.71	0.56
1:A:885:LYS:HD2	1:A:886:TYR:CE1	2.41	0.56
1:A:946:HIS:HE1	1:A:996:TYR:OH	1.89	0.56
1:A:664:ASN:HD22	1:A:664:ASN:C	2.13	0.56
2:B:1:A:P	2:B:1:A:C2	2.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HG3	1:A:12:ARG:NH1	2.05	0.56
1:A:1062:ASN:CB	1:A:1067:GLN:NE2	2.57	0.56
1:A:19:MET:HE3	1:A:27:MET:HE1	1.87	0.56
1:A:223:SER:OG	1:A:226:LYS:HD2	2.05	0.56
1:A:651:VAL:CB	4:D:26:DG:H4'	2.35	0.56
1:A:771:HIS:HD1	1:A:771:HIS:H	1.54	0.56
1:A:651:VAL:HB	4:D:26:DG:H4'	1.87	0.55
1:A:787:ARG:NH2	1:A:788:ASP:OD2	2.38	0.55
1:A:12:ARG:HH11	1:A:12:ARG:CG	2.05	0.55
1:A:483:LYS:HE2	1:A:614:ASN:HD22	1.69	0.55
1:A:743:PHE:CD1	1:A:743:PHE:C	2.84	0.55
1:A:786:LEU:CD2	1:A:793:VAL:HG21	2.37	0.55
1:A:822:LEU:O	1:A:823:LYS:HG3	2.06	0.55
1:A:13:LYS:NZ	1:A:539:GLU:OE1	2.40	0.55
1:A:665:GLY:N	1:A:668:VAL:HG21	2.21	0.55
4:D:7:DT:C2'	4:D:8:DT:O5'	2.54	0.55
1:A:720:GLU:C	1:A:723:ARG:HG3	2.31	0.55
1:A:57:ARG:HH21	1:A:105:SER:HG	1.54	0.55
1:A:248:GLU:C	1:A:249:LEU:HD23	2.31	0.55
3:C:5:DT:C5'	3:C:5:DT:C6	2.82	0.54
3:C:2:DC:N4	4:D:29:DG:H1	2.04	0.54
1:A:646:TYR:CE1	1:A:875:ILE:HD11	2.43	0.54
1:A:797:SER:O	2:B:11:C:H5''	2.07	0.54
1:A:755:TYR:CD1	1:A:755:TYR:C	2.85	0.54
1:A:177:PHE:HB3	1:A:286:LYS:HD3	1.88	0.54
1:A:474:PRO:HB2	1:A:476:PHE:CZ	2.42	0.54
2:B:9:G:C2	2:B:22:A:C2	2.96	0.54
1:A:728:LYS:HG3	1:A:733:ASN:HD22	0.55	0.54
1:A:748:ASP:O	1:A:751:THR:HG23	2.07	0.54
1:A:895:ASN:HB2	1:A:938:GLU:HB3	1.89	0.54
1:A:1012:ASN:HA	1:A:1015:LEU:CD2	2.29	0.54
1:A:333:ILE:CD1	1:A:461:VAL:HG11	2.24	0.53
1:A:1007:TYR:CD2	1:A:1026:MET:HE1	2.43	0.53
1:A:542:TYR:CG	1:A:595:LEU:HD13	2.42	0.53
1:A:782:ILE:HG22	1:A:849:MET:CE	2.34	0.53
1:A:837:ILE:H	1:A:837:ILE:CD1	2.21	0.53
1:A:1019:LEU:HG	1:A:1023:LYS:HD2	1.89	0.53
1:A:210:GLN:O	1:A:214:ILE:HG13	2.08	0.53
1:A:940:ASN:OD1	1:A:941:PRO:HD2	2.08	0.53
1:A:347:PHE:CZ	1:A:353:PHE:HB2	2.43	0.53
1:A:359:VAL:O	1:A:359:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:SER:O	1:A:389:GLU:HG3	2.07	0.53
1:A:216:LEU:HB3	1:A:221:CYS:O	2.08	0.53
1:A:620:ARG:HD2	1:A:625:GLU:OE1	2.07	0.53
1:A:718:PHE:CD2	1:A:781:GLU:CG	2.91	0.53
4:D:3:DC:H2''	4:D:4:DT:OP2	2.09	0.53
4:D:28:DT:H1'	4:D:29:DG:C8	2.44	0.53
1:A:483:LYS:CE	1:A:614:ASN:HD22	2.22	0.52
1:A:719:LEU:HB3	1:A:740:MET:SD	2.49	0.52
1:A:1013:ASP:O	1:A:1017:VAL:HG21	2.09	0.52
2:B:13:A:C8	2:B:13:A:C5'	2.83	0.52
1:A:983:LEU:N	1:A:983:LEU:HD22	2.24	0.52
1:A:102:GLN:O	1:A:106:GLY:N	2.34	0.52
1:A:102:GLN:HA	1:A:107:SER:O	2.08	0.52
1:A:1053:LYS:HG3	1:A:1069:TRP:CE3	2.45	0.52
1:A:585:LEU:HG	1:A:585:LEU:O	2.07	0.52
1:A:801:ASN:O	1:A:805:VAL:HG23	2.09	0.52
1:A:983:LEU:CD2	1:A:983:LEU:N	2.73	0.52
1:A:226:LYS:HD2	1:A:226:LYS:H	1.75	0.52
1:A:789:GLY:O	1:A:792:SER:OG	2.24	0.52
1:A:73:LEU:HG	1:A:112:GLN:HB3	1.92	0.52
1:A:258:ASN:CG	1:A:261:SER:HB2	2.34	0.52
1:A:272:ARG:NH1	1:A:272:ARG:CB	2.73	0.52
1:A:837:ILE:N	1:A:837:ILE:CD1	2.73	0.51
1:A:982:PHE:O	1:A:997:ASN:HB2	2.10	0.51
1:A:1007:TYR:HB2	1:A:1009:LEU:HD12	1.91	0.51
1:A:726:THR:O	1:A:770:ASN:OD1	2.29	0.51
1:A:909:ASN:O	1:A:913:MET:HG3	2.10	0.51
1:A:949:PRO:CG	1:A:1076:VAL:HG13	2.40	0.51
1:A:250:GLY:HA2	1:A:253:HIS:CD2	2.45	0.51
1:A:771:HIS:ND1	1:A:771:HIS:N	2.59	0.51
1:A:483:LYS:NZ	1:A:614:ASN:HD22	2.09	0.51
1:A:719:LEU:HD12	1:A:743:PHE:HD2	1.76	0.51
1:A:720:GLU:CA	1:A:723:ARG:CG	2.82	0.51
1:A:775:ALA:HB3	1:A:821:LEU:HD12	1.93	0.51
1:A:198:LEU:HB3	1:A:214:ILE:HG23	1.93	0.51
1:A:517:LEU:CD1	1:A:524:TRP:CE2	2.90	0.51
1:A:656:TYR:CD1	1:A:656:TYR:C	2.88	0.51
1:A:74:LEU:HD13	1:A:164:LEU:CD2	2.41	0.51
1:A:598:ALA:O	1:A:603:LEU:N	2.35	0.51
1:A:725:GLY:HA3	1:A:739:PHE:CZ	2.46	0.51
1:A:296:TYR:HA	1:A:301:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:HIS:CD2	5:A:1201:CIT:H42	2.47	0.50
2:B:14:U:O2	2:B:14:U:O2'	2.28	0.50
1:A:632:VAL:HG11	1:A:930:MET:CE	2.42	0.50
1:A:690:VAL:O	1:A:693:LYS:CB	2.59	0.50
1:A:48:TRP:CD1	1:A:309:LEU:HD21	2.47	0.50
1:A:767:SER:HG	1:A:778:TYR:HH	1.59	0.50
1:A:156:MET:HE3	1:A:176:MET:CE	2.42	0.50
1:A:720:GLU:O	1:A:723:ARG:CD	2.59	0.50
1:A:767:SER:HG	1:A:778:TYR:HE2	1.59	0.50
1:A:709:LYS:N	1:A:710:PRO:CD	2.75	0.50
1:A:350:SER:HB2	1:A:351:PRO:CD	2.42	0.50
1:A:437:TYR:CE1	1:A:440:LYS:HD2	2.47	0.50
1:A:686:VAL:N	1:A:696:ASP:OD1	2.45	0.50
4:D:11:DA:H2''	4:D:12:DT:C5	2.47	0.50
1:A:52:GLY:O	1:A:78:ASN:HB3	2.12	0.49
1:A:363:LEU:HB3	1:A:452:ILE:CD1	2.43	0.49
1:A:725:GLY:O	1:A:737:ILE:O	2.29	0.49
1:A:483:LYS:CE	1:A:614:ASN:ND2	2.73	0.49
1:A:571:SER:N	1:A:574:GLN:OE1	2.40	0.49
1:A:597:ALA:O	1:A:601:GLN:HG3	2.12	0.49
1:A:728:LYS:HB2	1:A:733:ASN:HA	1.94	0.49
1:A:542:TYR:CD2	1:A:595:LEU:HD13	2.48	0.49
1:A:669:ILE:HD13	1:A:1052:TYR:CZ	2.47	0.49
1:A:797:SER:HB2	1:A:863:LYS:NZ	2.28	0.49
1:A:822:LEU:O	1:A:823:LYS:CG	2.60	0.49
1:A:384:HIS:HA	1:A:406:TYR:HE2	1.78	0.49
1:A:399:LYS:HD2	1:A:399:LYS:C	2.38	0.49
1:A:794:LEU:CD1	1:A:856:LEU:HD23	2.43	0.49
1:A:55:ILE:HG12	1:A:59:ILE:HG21	1.94	0.49
1:A:693:LYS:CE	1:A:695:TYR:OH	2.60	0.49
1:A:399:LYS:C	1:A:399:LYS:CD	2.86	0.48
1:A:768:ILE:HG12	1:A:778:TYR:CE2	2.48	0.48
1:A:171:TYR:CZ	1:A:175:VAL:HG11	2.48	0.48
1:A:259:VAL:O	1:A:263:ILE:HG13	2.13	0.48
1:A:716:ARG:O	1:A:740:MET:CE	2.61	0.48
1:A:83:MET:HB3	1:A:84:PRO:CD	2.43	0.48
1:A:665:GLY:H	1:A:668:VAL:HG21	1.78	0.48
1:A:228:ARG:HH21	1:A:237:THR:CB	2.26	0.48
1:A:693:LYS:CD	1:A:695:TYR:CZ	2.95	0.48
2:B:21:C:H6	2:B:21:C:C5'	2.24	0.48
1:A:588:VAL:HG21	2:B:6:U:H1'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:PHE:O	1:A:860:ARG:NH2	2.46	0.48
1:A:510:ILE:HG12	1:A:541:TYR:CD2	2.49	0.48
1:A:1064:ASN:ND2	1:A:1064:ASN:O	2.46	0.48
1:A:200:GLU:O	1:A:203:THR:HG22	2.13	0.47
1:A:357:THR:HG22	1:A:357:THR:O	2.13	0.47
1:A:399:LYS:O	1:A:399:LYS:HG2	2.13	0.47
1:A:399:LYS:HG2	1:A:402:ARG:HB3	1.96	0.47
1:A:1013:ASP:OD1	1:A:1013:ASP:N	2.46	0.47
3:C:5:DT:H5''	3:C:5:DT:C6	2.44	0.47
1:A:401:LYS:HA	1:A:404:LYS:HB3	1.96	0.47
1:A:517:LEU:HD13	1:A:524:TRP:CZ2	2.48	0.47
1:A:720:GLU:HG3	1:A:740:MET:HE2	1.97	0.47
1:A:1043:ARG:HG2	1:A:1043:ARG:HH11	1.78	0.47
1:A:206:ASN:C	1:A:206:ASN:HD22	2.21	0.47
4:D:25:DC:C6	4:D:25:DC:C5'	2.97	0.47
1:A:430:VAL:O	1:A:434:ARG:HG3	2.14	0.47
1:A:483:LYS:HE2	1:A:614:ASN:HD21	1.76	0.47
1:A:706:LEU:O	1:A:709:LYS:HG3	2.12	0.47
1:A:723:ARG:NH2	1:A:738:ASP:OD2	2.48	0.47
3:C:2:DC:N3	4:D:29:DG:N2	2.60	0.47
1:A:176:MET:HG2	1:A:282:MET:CE	2.44	0.47
1:A:387:TYR:CD1	1:A:387:TYR:C	2.93	0.47
1:A:480:ASN:HD22	1:A:480:ASN:N	1.98	0.47
1:A:719:LEU:HB3	1:A:740:MET:HE3	1.89	0.47
1:A:727:MET:O	1:A:735:ILE:HB	2.15	0.47
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.78	0.47
1:A:718:PHE:CD1	1:A:718:PHE:C	2.93	0.47
1:A:68:LYS:O	1:A:324:LEU:HD21	2.15	0.47
1:A:401:LYS:O	1:A:405:VAL:N	2.39	0.47
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.69	0.47
1:A:736:GLN:NE2	1:A:736:GLN:CA	2.73	0.47
1:A:975:ASN:ND2	1:A:975:ASN:H	2.12	0.47
1:A:705:LEU:HB2	1:A:749:ASP:HA	1.96	0.46
1:A:723:ARG:HG3	1:A:723:ARG:H	1.50	0.46
1:A:816:THR:HG23	1:A:820:HIS:HD2	1.80	0.46
1:A:818:PHE:HB3	1:A:842:LYS:HE2	1.96	0.46
1:A:975:ASN:N	1:A:975:ASN:ND2	2.59	0.46
1:A:709:LYS:HA	1:A:712:VAL:HG13	1.98	0.46
4:D:26:DG:C2'	4:D:27:DC:OP2	2.55	0.46
1:A:88:LYS:N	1:A:89:PRO:CD	2.78	0.46
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:LYS:O	1:A:400:GLU:C	2.58	0.46
1:A:518:ASN:C	1:A:518:ASN:HD22	2.23	0.46
1:A:724:ASN:OD1	1:A:724:ASN:N	2.48	0.46
1:A:785:LEU:O	1:A:785:LEU:HD22	2.15	0.46
1:A:272:ARG:NH1	1:A:272:ARG:CG	2.74	0.46
1:A:716:ARG:O	1:A:740:MET:HE1	2.15	0.46
1:A:651:VAL:HG21	4:D:26:DG:O4'	2.14	0.46
1:A:137:ARG:NH1	1:A:137:ARG:HG2	2.30	0.46
1:A:697:GLN:O	1:A:799:LEU:HB2	2.16	0.46
1:A:290:ALA:HA	1:A:294:GLY:O	2.16	0.46
1:A:705:LEU:HD12	1:A:748:ASP:O	2.16	0.46
1:A:725:GLY:O	1:A:737:ILE:N	2.49	0.46
1:A:706:LEU:HD23	1:A:706:LEU:N	2.31	0.46
1:A:672:ASN:O	1:A:673:ASP:HB2	2.15	0.46
1:A:387:TYR:CD2	1:A:406:TYR:CD2	3.04	0.45
1:A:478:PHE:HB3	1:A:486:GLY:HA3	1.97	0.45
1:A:258:ASN:OD1	1:A:261:SER:N	2.38	0.45
1:A:472:LYS:HG2	2:B:27:U:O2'	2.15	0.45
1:A:926:GLU:HA	1:A:929:MET:HE3	1.99	0.45
3:C:5:DT:H6	3:C:5:DT:H5'	1.78	0.45
1:A:146:ARG:HE	1:A:146:ARG:HB2	1.63	0.45
1:A:399:LYS:HD2	1:A:399:LYS:N	2.26	0.45
1:A:949:PRO:HG2	1:A:1076:VAL:HG13	1.99	0.45
1:A:432:LEU:HD12	1:A:432:LEU:C	2.35	0.45
1:A:640:TYR:HA	1:A:888:PRO:HB2	1.98	0.45
1:A:41:THR:N	1:A:42:PRO:CD	2.80	0.45
1:A:259:VAL:N	1:A:260:PRO:CD	2.80	0.45
1:A:377:TRP:CD1	1:A:445:VAL:HB	2.51	0.45
1:A:475:SER:HB2	1:A:616:ASN:HD21	1.82	0.45
1:A:709:LYS:O	1:A:713:GLU:HG2	2.16	0.45
1:A:445:VAL:HA	1:A:448:ILE:HG13	1.98	0.45
1:A:477:ASN:HB3	1:A:614:ASN:HD21	1.81	0.45
1:A:508:ASN:HA	1:A:537:LEU:HD11	1.99	0.45
1:A:743:PHE:C	1:A:743:PHE:HD1	2.25	0.45
1:A:795:LYS:O	1:A:796:LEU:HD23	2.17	0.45
1:A:976:ARG:O	1:A:980:LEU:HD12	2.17	0.45
1:A:634:LYS:HD2	1:A:931:HIS:O	2.17	0.45
1:A:665:GLY:H	1:A:668:VAL:CG2	2.30	0.45
1:A:786:LEU:HD23	1:A:793:VAL:CG2	2.46	0.45
1:A:867:LYS:O	1:A:871:ILE:HG13	2.16	0.45
1:A:636:LYS:HE3	1:A:638:LYS:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:LYS:HE3	1:A:638:LYS:HG2	1.99	0.44
1:A:665:GLY:N	1:A:668:VAL:HG23	2.31	0.44
1:A:794:LEU:HD13	1:A:856:LEU:HD23	1.97	0.44
1:A:824:LYS:CG	1:A:825:PRO:HD3	2.45	0.44
1:A:83:MET:HB3	1:A:84:PRO:HD2	1.99	0.44
1:A:223:SER:HG	1:A:226:LYS:HD3	1.80	0.44
1:A:966:CYS:SG	1:A:971:LEU:HD13	2.58	0.44
1:A:590:LYS:HD2	1:A:594:ARG:HH21	1.81	0.44
1:A:716:ARG:NH2	1:A:744:GLU:OE2	2.50	0.44
1:A:70:SER:HB3	1:A:112:GLN:OE1	2.18	0.44
1:A:672:ASN:ND2	1:A:953:LYS:O	2.44	0.44
1:A:690:VAL:O	1:A:690:VAL:HG22	2.17	0.44
1:A:728:LYS:CD	1:A:733:ASN:ND2	2.81	0.44
1:A:112:GLN:HA	1:A:327:ILE:HD11	2.00	0.44
1:A:71:ASP:O	1:A:75:LEU:HG	2.18	0.44
1:A:746:ILE:HG13	1:A:756:PHE:CD1	2.53	0.44
1:A:852:LEU:HD12	1:A:852:LEU:O	2.18	0.44
1:A:930:MET:HE2	1:A:930:MET:HB3	1.82	0.44
1:A:309:LEU:HA	1:A:309:LEU:HD23	1.74	0.44
1:A:322:PHE:CD2	1:A:466:ILE:HD12	2.53	0.44
1:A:755:TYR:CD1	1:A:755:TYR:O	2.71	0.44
1:A:401:LYS:O	1:A:405:VAL:HB	2.18	0.44
1:A:715:ARG:HG3	1:A:760:TYR:CE2	2.53	0.44
1:A:720:GLU:HA	1:A:723:ARG:CG	2.15	0.44
4:D:25:DC:H5"	4:D:25:DC:H6	1.82	0.44
1:A:406:TYR:CD1	1:A:406:TYR:C	2.96	0.43
1:A:786:LEU:HD22	1:A:793:VAL:HG21	1.99	0.43
1:A:20:ILE:HG13	1:A:509:TYR:CE1	2.53	0.43
1:A:959:PHE:CB	1:A:995:TYR:CZ	3.02	0.43
1:A:202:SER:O	1:A:202:SER:OG	2.27	0.43
1:A:764:LEU:O	1:A:768:ILE:HG13	2.18	0.43
1:A:768:ILE:HG12	1:A:778:TYR:CD2	2.54	0.43
1:A:54:GLY:HA3	1:A:153:LEU:HD21	2.00	0.43
1:A:432:LEU:O	1:A:436:LEU:HG	2.19	0.43
1:A:746:ILE:HG13	1:A:756:PHE:HD1	1.83	0.43
1:A:313:LYS:HE2	6:A:1302:HOH:O	2.17	0.43
1:A:1002:ALA:HB3	1:A:1063:TRP:HE1	1.82	0.43
1:A:620:ARG:CG	1:A:620:ARG:NH1	2.73	0.43
1:A:725:GLY:HA3	1:A:739:PHE:CE2	2.54	0.43
1:A:60:ILE:O	1:A:60:ILE:HG13	2.19	0.43
1:A:480:ASN:ND2	1:A:480:ASN:N	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:THR:OG1	1:A:599:ARG:NH1	2.42	0.43
1:A:690:VAL:O	1:A:693:LYS:HB3	2.19	0.43
1:A:548:ASN:N	1:A:549:PRO:CD	2.81	0.43
1:A:896:ILE:O	1:A:918:ARG:HD3	2.18	0.43
1:A:971:LEU:HD12	1:A:971:LEU:HA	1.80	0.43
1:A:720:GLU:O	1:A:723:ARG:HD2	2.19	0.42
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.81	0.42
1:A:402:ARG:HD2	1:A:402:ARG:HA	1.63	0.42
1:A:874:LYS:HA	1:A:874:LYS:HD3	1.87	0.42
1:A:398:LYS:HA	1:A:398:LYS:HD3	1.23	0.42
1:A:720:GLU:C	1:A:723:ARG:HG2	2.40	0.42
1:A:818:PHE:CE1	1:A:842:LYS:HB3	2.54	0.42
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.80	0.42
1:A:786:LEU:HD23	1:A:793:VAL:HG23	2.01	0.42
1:A:793:VAL:HG13	1:A:806:MET:HG2	2.01	0.42
1:A:34:MET:HB2	1:A:619:LYS:HD3	2.01	0.42
1:A:111:ILE:HD12	1:A:112:GLN:H	1.85	0.42
1:A:340:PHE:CZ	1:A:447:LYS:HG3	2.54	0.42
1:A:983:LEU:CD2	1:A:1000:ALA:HB1	2.46	0.42
1:A:1051:THR:HG22	1:A:1052:TYR:CD1	2.54	0.42
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.82	0.42
1:A:66:LYS:HB3	1:A:67:ASP:H	1.57	0.42
1:A:227:LEU:HD12	1:A:227:LEU:C	2.42	0.42
1:A:240:ILE:HD13	1:A:266:LEU:CD2	2.50	0.42
1:A:786:LEU:O	1:A:794:LEU:HB2	2.19	0.42
1:A:101:PHE:O	1:A:105:SER:HB3	2.20	0.42
1:A:207:SER:N	1:A:210:GLN:OE1	2.52	0.42
1:A:223:SER:HG	1:A:226:LYS:CD	2.29	0.42
1:A:500:LYS:O	1:A:500:LYS:HG3	2.20	0.42
1:A:785:LEU:O	1:A:792:SER:HA	2.19	0.42
1:A:980:LEU:O	1:A:983:LEU:N	2.47	0.42
1:A:1030:LEU:HD21	1:A:1038:LEU:HB3	2.02	0.42
1:A:57:ARG:O	1:A:61:SER:HB2	2.20	0.42
1:A:156:MET:HB3	1:A:161:CYS:HB2	2.02	0.42
1:A:570:LEU:HD13	1:A:574:GLN:HB3	2.01	0.42
1:A:737:ILE:HD13	1:A:737:ILE:HA	1.75	0.42
1:A:33:PHE:HD2	1:A:516:VAL:HG22	1.76	0.41
1:A:515:LYS:HG3	1:A:526:LYS:HG2	2.03	0.41
1:A:535:ARG:HB2	2:B:7:G:C6	2.55	0.41
1:A:805:VAL:O	1:A:809:VAL:HG22	2.21	0.41
1:A:785:LEU:HD22	1:A:785:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:H	1:A:59:ILE:HB	1.84	0.41
1:A:719:LEU:C	1:A:740:MET:HE1	2.45	0.41
1:A:70:SER:O	1:A:73:LEU:N	2.54	0.41
1:A:652:ARG:HH21	4:D:26:DG:H3'	1.86	0.41
1:A:693:LYS:CD	1:A:695:TYR:OH	2.68	0.41
1:A:720:GLU:N	1:A:740:MET:CE	2.80	0.41
1:A:38:MET:HE3	1:A:38:MET:HB3	1.87	0.41
1:A:194:LYS:HD3	1:A:194:LYS:HA	1.73	0.41
1:A:376:LEU:HB2	1:A:417:TYR:CD1	2.55	0.41
1:A:571:SER:O	1:A:575:ILE:HG13	2.20	0.41
1:A:778:TYR:CD1	1:A:778:TYR:N	2.89	0.41
1:A:786:LEU:CD2	1:A:793:VAL:CG2	2.98	0.41
1:A:949:PRO:HB2	1:A:1054:LEU:HD11	2.03	0.41
1:A:133:VAL:HA	1:A:136:GLU:HG3	2.02	0.41
1:A:510:ILE:HD13	1:A:536:PHE:HD2	1.85	0.41
1:A:908:THR:O	1:A:912:LEU:HG	2.20	0.41
1:A:664:ASN:HA	1:A:668:VAL:HG21	2.03	0.41
2:B:31:G:H2'	2:B:32:A:O4'	2.20	0.41
1:A:370:GLU:HB3	1:A:371:SER:H	1.63	0.41
1:A:783:PHE:N	1:A:783:PHE:CD1	2.87	0.41
1:A:23:SER:O	1:A:26:ARG:N	2.54	0.40
1:A:674:LEU:HA	1:A:675:PRO:HD3	1.93	0.40
1:A:706:LEU:HD23	1:A:706:LEU:H	1.85	0.40
1:A:783:PHE:CE1	1:A:849:MET:HG2	2.55	0.40
1:A:414:ILE:HG22	1:A:430:VAL:HG13	2.03	0.40
1:A:509:TYR:HB2	2:B:3:U:O4	2.21	0.40
1:A:878:LYS:HD3	1:A:878:LYS:HA	1.78	0.40
1:A:23:SER:O	1:A:24:HIS:C	2.65	0.40
1:A:482:SER:C	1:A:483:LYS:HG3	2.46	0.40
1:A:947:GLN:O	1:A:949:PRO:HD3	2.21	0.40
1:A:1030:LEU:HD12	1:A:1030:LEU:HA	1.79	0.40
1:A:399:LYS:C	1:A:401:LYS:N	2.79	0.40
1:A:719:LEU:O	1:A:723:ARG:N	2.55	0.40
1:A:736:GLN:CA	1:A:736:GLN:HE21	2.34	0.40
1:A:794:LEU:HD13	1:A:856:LEU:CD2	2.52	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	1073/1101 (98%)	1053 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	952/983 (97%)	750 (79%)	202 (21%)	1	2

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	23	SER
1	A	38	MET
1	A	46	GLU
1	A	55	ILE
1	A	60	ILE
1	A	66	LYS
1	A	68	LYS
1	A	69	ILE
1	A	73	LEU
1	A	92	VAL
1	A	95	SER
1	A	111	ILE

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Mol	Chain	Res	Type
1	A	123	THR
1	A	124	GLU
1	A	125	LYS
1	A	132	ARG
1	A	136	GLU
1	A	153	LEU
1	A	155	LEU
1	A	160	LYS
1	A	166	LEU
1	A	186	GLN
1	A	188	LYS
1	A	190	GLN
1	A	194	LYS
1	A	198	LEU
1	A	203	THR
1	A	204	GLN
1	A	205	ILE
1	A	206	ASN
1	A	217	LYS
1	A	226	LYS
1	A	227	LEU
1	A	229	ILE
1	A	233	ARG
1	A	237	THR
1	A	242	LYS
1	A	249	LEU
1	A	256	GLU
1	A	261	SER
1	A	262	LEU
1	A	266	LEU
1	A	272	ARG
1	A	277	CYS
1	A	282	MET
1	A	283	GLU
1	A	284	LYS
1	A	302	SER
1	A	306	GLU
1	A	313	LYS
1	A	318	LYS
1	A	324	LEU
1	A	345	GLU
1	A	354	GLU

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Mol	Chain	Res	Type
1	A	356	ASP
1	A	360	LYS
1	A	375	THR
1	A	377	TRP
1	A	385	SER
1	A	387	TYR
1	A	389	GLU
1	A	390	ASP
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	402	ARG
1	A	403	ILE
1	A	404	LYS
1	A	405	VAL
1	A	410	VAL
1	A	412	GLN
1	A	419	GLU
1	A	424	GLU
1	A	426	LYS
1	A	429	LEU
1	A	430	VAL
1	A	432	LEU
1	A	439	ARG
1	A	443	ILE
1	A	446	ASP
1	A	447	LYS
1	A	452	ILE
1	A	457	LYS
1	A	461	VAL
1	A	463	LYS
1	A	475	SER
1	A	480	ASN
1	A	483	LYS
1	A	500	LYS
1	A	505	GLN
1	A	514	ILE
1	A	516	VAL
1	A	546	SER

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Mol	Chain	Res	Type
1	A	547	GLU
1	A	553	LEU
1	A	560	LYS
1	A	561	THR
1	A	565	GLU
1	A	570	LEU
1	A	573	GLU
1	A	575	ILE
1	A	576	GLU
1	A	580	SER
1	A	583	VAL
1	A	593	MET
1	A	595	LEU
1	A	606	ARG
1	A	620	ARG
1	A	625	GLU
1	A	630	THR
1	A	633	LYS
1	A	634	LYS
1	A	635	LYS
1	A	638	LYS
1	A	664	ASN
1	A	670	ASP
1	A	690	VAL
1	A	693	LYS
1	A	703	VAL
1	A	712	VAL
1	A	715	ARG
1	A	719	LEU
1	A	723	ARG
1	A	724	ASN
1	A	726	THR
1	A	727	MET
1	A	729	ASP
1	A	731	ARG
1	A	733	ASN
1	A	734	ASN
1	A	735	ILE
1	A	736	GLN
1	A	737	ILE
1	A	740	MET
1	A	741	LYS

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Mol	Chain	Res	Type
1	A	743	PHE
1	A	746	ILE
1	A	750	GLU
1	A	751	THR
1	A	758	MET
1	A	762	LYS
1	A	763	LEU
1	A	765	GLN
1	A	777	GLU
1	A	785	LEU
1	A	790	LYS
1	A	791	LEU
1	A	794	LEU
1	A	796	LEU
1	A	797	SER
1	A	808	LYS
1	A	811	LYS
1	A	814	ILE
1	A	822	LEU
1	A	824	LYS
1	A	837	ILE
1	A	840	GLU
1	A	843	GLN
1	A	849	MET
1	A	860	ARG
1	A	878	LYS
1	A	885	LYS
1	A	896	ILE
1	A	901	LYS
1	A	906	SER
1	A	907	SER
1	A	916	LEU
1	A	918	ARG
1	A	923	LYS
1	A	930	MET
1	A	932	GLN
1	A	934	LEU
1	A	964	SER
1	A	971	LEU
1	A	975	ASN
1	A	976	ARG
1	A	977	LYS

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Mol	Chain	Res	Type
1	A	980	LEU
1	A	986	LYS
1	A	989	LYS
1	A	997	ASN
1	A	1006	THR
1	A	1013	ASP
1	A	1015	LEU
1	A	1017	VAL
1	A	1021	LYS
1	A	1029	ILE
1	A	1030	LEU
1	A	1032	GLN
1	A	1033	ARG
1	A	1036	ASP
1	A	1038	LEU
1	A	1046	MET
1	A	1049	LEU
1	A	1051	THR
1	A	1062	ASN
1	A	1066	LYS
1	A	1086	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	381	ASN
1	A	415	ASN
1	A	467	ASN
1	A	480	ASN
1	A	505	GLN
1	A	518	ASN
1	A	527	HIS
1	A	614	ASN
1	A	616	ASN
1	A	622	ASN
1	A	733	ASN
1	A	736	GLN
1	A	801	ASN
1	A	820	HIS
1	A	946	HIS
1	A	975	ASN

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Mol	Chain	Res	Type
1	A	1028	ASN
1	A	1067	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	43/43 (100%)	15 (34%)	3 (6%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	U
2	B	4	U
2	B	7	G
2	B	12	C
2	B	13	A
2	B	14	U
2	B	15	C
2	B	16	G
2	B	17	U
2	B	18	U
2	B	19	G
2	B	21	C
2	B	24	U
2	B	29	A
2	B	43	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	A
2	B	13	A
2	B	14	U

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

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	1.45	1 (8%)	17,17,17	1.96	6 (35%)

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	-	-	9/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1201	CIT	C3-C6	2.34	1.55	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1201	CIT	O6-C6-C3	5.16	123.05	113.14
5	A	1201	CIT	C2-C3-C6	3.22	117.15	110.03
5	A	1201	CIT	C4-C3-C6	-2.52	104.47	110.03
5	A	1201	CIT	O6-C6-O5	-2.48	115.92	123.86
5	A	1201	CIT	O2-C1-C2	2.30	121.62	114.35
5	A	1201	CIT	O2-C1-O1	-2.00	118.18	123.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1201	CIT	C1-C2-C3-O7
5	A	1201	CIT	C1-C2-C3-C4
5	A	1201	CIT	C1-C2-C3-C6
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	O7-C3-C4-C5
5	A	1201	CIT	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1201	CIT	6	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	1077/1101 (97%)	0.48	58 (5%) 31 31	41, 73, 120, 166	0
2	B	43/43 (100%)	-0.19	0 100 100	49, 66, 99, 160	0
3	C	30/40 (75%)	-0.04	2 (6%) 24 23	49, 63, 116, 142	2 (6%)
4	D	26/40 (65%)	1.27	5 (19%) 3 2	52, 102, 157, 193	5 (19%)
All	All	1176/1224 (96%)	0.46	65 (5%) 30 30	41, 73, 123, 193	7 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	ILE	5.0
1	A	943	PHE	4.7
1	A	690	VAL	4.4
1	A	729	ASP	4.0
1	A	65	ASN	3.9
1	A	695	TYR	3.8
1	A	61	SER	3.8
1	A	64	ALA	3.8
3	C	1	DG	3.7
1	A	688	SER	3.6
1	A	60	ILE	3.5
1	A	726	THR	3.5
1	A	235	GLY	3.4
1	A	945	SER	3.2
1	A	825	PRO	3.2
1	A	689	GLN	3.2
1	A	791	LEU	3.1
1	A	725	GLY	3.0
1	A	739	PHE	3.0
1	A	942	ASN	3.0
1	A	722	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	2.9
1	A	357	THR	2.9
1	A	63	THR	2.8
1	A	62	GLY	2.8
1	A	236	ALA	2.8
1	A	359	VAL	2.8
1	A	946	HIS	2.8
4	D	16	DA	2.7
1	A	59	ILE	2.7
1	A	391	ILE	2.7
1	A	944	THR	2.7
1	A	250	GLY	2.6
1	A	756	PHE	2.6
1	A	403	ILE	2.5
1	A	691	ARG	2.5
1	A	481	ASN	2.5
4	D	17	DA	2.5
4	D	12	DT	2.5
1	A	835	PRO	2.5
1	A	467	ASN	2.4
1	A	583	VAL	2.4
1	A	716	ARG	2.3
4	D	11	DA	2.3
1	A	763	LEU	2.3
1	A	693	LYS	2.3
1	A	392	ALA	2.3
1	A	438	SER	2.3
3	C	2	DC	2.2
1	A	58	ASP	2.2
1	A	584	GLY	2.2
4	D	29	DG	2.2
1	A	909	ASN	2.2
1	A	499	LEU	2.2
1	A	706	LEU	2.1
1	A	989	LYS	2.1
1	A	652	ARG	2.1
1	A	898	ASP	2.0
1	A	1036	ASP	2.0
1	A	354	GLU	2.0
1	A	234	LYS	2.0
1	A	724	ASN	2.0
1	A	400	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	844	LYS	2.0
1	A	1076	VAL	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	0.84	0.10	68,79,95,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.