



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:44 AM UTC

PDB ID : 8Y03 / pdb_00008y03
Title : Crystal structure of LbCas12a-crRNA complex
Authors : Lin, X.; Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 2.93 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

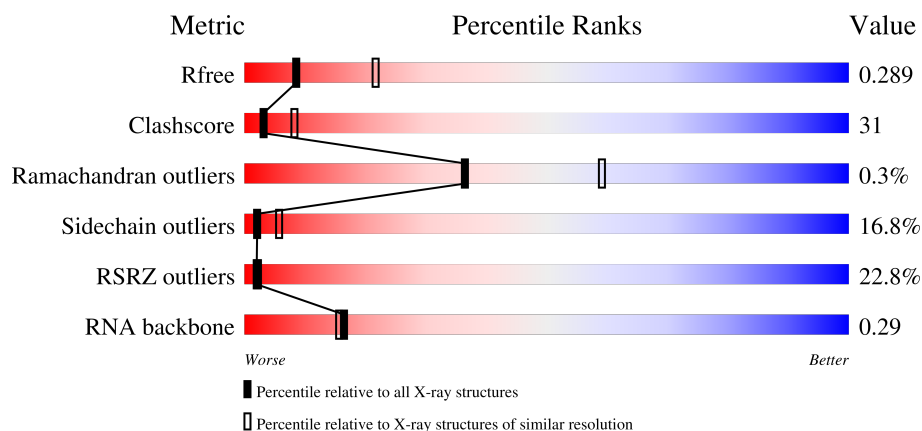
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)
RNA backbone	3983	1018 (3.14-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	1228	
2	G	40	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10770 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called LbCas12a.

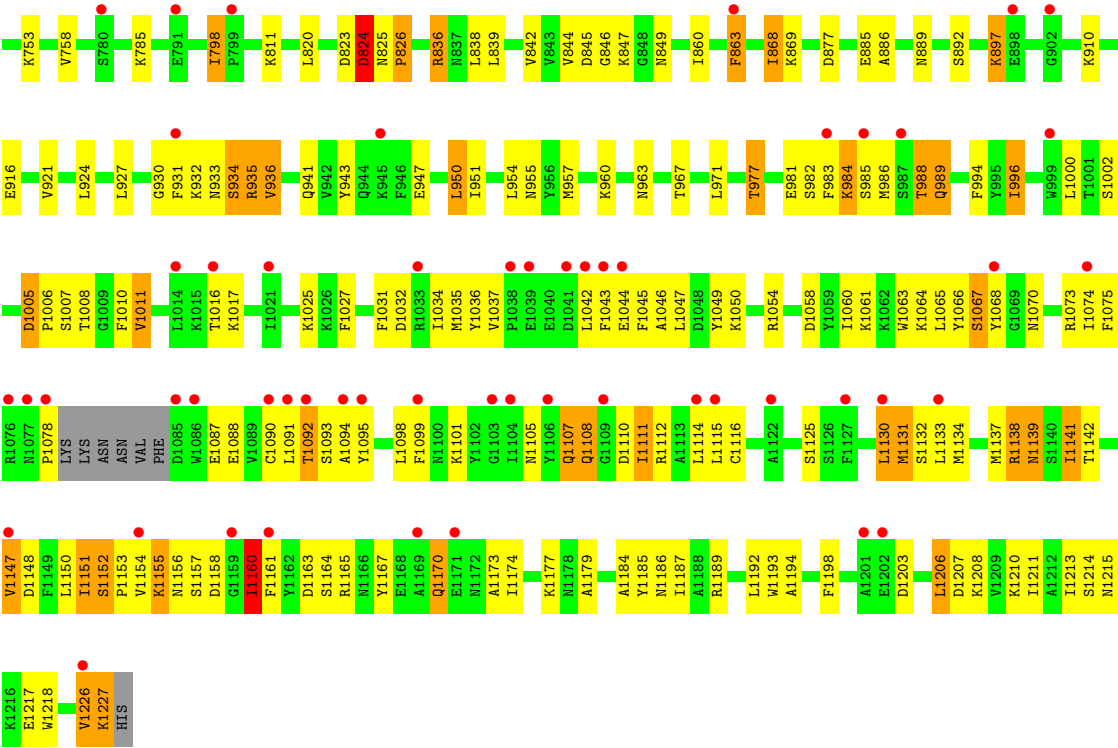
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1208	Total	C	N	O	S	0	0	0
			9918	6383	1628	1879	28			

- Molecule 2 is a RNA chain called RNA (41-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	40	Total	C	N	O	P	0	0	0
			850	381	152	277	40			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	1	0
			1	1		
3	G	1	Total	Mg	1	0
			1	1		



● Molecule 2: RNA (41-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.26Å 83.22Å 124.30Å 90.00° 106.21° 90.00°	Depositor
Resolution (Å)	49.66 – 2.93 49.66 – 2.93	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.66-2.93) 98.9 (49.66-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.269 , 0.289 0.269 , 0.289	Depositor DCC
R_{free} test set	1734 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10770	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	6/10122 (0.1%)	1.02	42/13600 (0.3%)
2	G	0.53	0/950	0.77	1/1477 (0.1%)
All	All	0.62	6/11072 (0.1%)	1.00	43/15077 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	825	ASN	C-N	5.83	1.41	1.33
1	A	1005	ASP	C-N	5.50	1.40	1.34
1	A	607	ASN	C-N	5.49	1.40	1.33
1	A	1006	PRO	N-CD	5.31	1.55	1.47
1	A	826	PRO	N-CD	5.27	1.55	1.47
1	A	608	PRO	N-CD	5.08	1.54	1.47

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	VAL	N-CA-C	19.47	128.83	110.53
1	A	267	LYS	N-CA-C	-17.61	89.50	112.93
1	A	203	GLN	N-CA-C	-12.64	97.63	113.55
1	A	202	VAL	CB-CA-C	-9.67	99.35	112.02
1	A	592	MET	N-CA-C	7.70	119.75	111.36
1	A	266	THR	CB-CA-C	-7.11	100.27	111.51
1	A	607	ASN	CA-C-N	-7.05	112.71	119.76
1	A	607	ASN	C-N-CA	-7.05	112.71	119.76
1	A	824	ASP	N-CA-C	7.05	119.04	111.36
1	A	1141	ILE	N-CA-C	7.02	117.81	110.72
1	A	266	THR	N-CA-C	-6.95	103.34	112.24
1	A	1078	PRO	N-CA-CB	6.91	110.60	103.00
1	A	1174	ILE	N-CA-C	6.57	117.33	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ILE	N-CA-C	6.41	113.39	107.56
1	A	825	ASN	CA-C-N	-6.22	113.27	119.99
1	A	825	ASN	C-N-CA	-6.22	113.27	119.99
1	A	682	PHE	N-CA-C	6.14	118.96	109.07
1	A	646	TYR	CA-C-N	6.14	125.62	119.24
1	A	646	TYR	C-N-CA	6.14	125.62	119.24
1	A	295	THR	N-CA-C	6.08	117.91	111.28
1	A	69	ILE	N-CA-C	6.08	116.68	108.17
1	A	241	ILE	CB-CA-C	-5.98	104.15	111.87
1	A	90	GLU	N-CA-C	-5.84	105.04	111.82
1	A	113	GLU	N-CA-C	5.83	119.62	111.74
1	A	203	GLN	N-CA-CB	5.82	118.84	110.40
1	A	112	ASN	N-CA-C	5.71	116.61	108.74
1	A	173	PHE	N-CA-C	-5.68	105.09	111.28
1	A	576	GLY	N-CA-C	5.66	119.56	110.90
1	A	476	GLU	N-CA-C	-5.60	103.93	111.54
1	A	984	LYS	N-CA-C	-5.51	105.65	112.38
1	A	64	ASP	N-CA-C	-5.46	106.29	113.12
1	A	76	ASN	N-CA-C	-5.46	105.33	111.28
2	G	20	G	C5'-C4'-C3'	-5.45	107.82	116.00
1	A	1147	VAL	N-CA-C	5.41	115.78	107.77
1	A	493	ALA	N-CA-C	5.38	117.23	111.36
1	A	631	ASP	N-CA-C	-5.31	105.49	111.28
1	A	242	GLY	N-CA-C	5.24	119.47	112.77
1	A	1005	ASP	CA-C-N	-5.22	113.16	118.85
1	A	1005	ASP	C-N-CA	-5.22	113.16	118.85
1	A	1160	ILE	N-CA-C	5.15	115.31	108.11
1	A	538	LYS	N-CA-C	-5.13	105.74	112.41
1	A	603	MET	N-CA-C	-5.08	105.74	111.28
1	A	623	LYS	N-CA-C	-5.00	104.26	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9918	0	9825	595	0
2	G	850	0	431	82	0
3	A	1	0	0	0	0
3	G	1	0	0	0	0
All	All	10770	0	10256	654	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 31.

All (654) 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:535:ASP:HA	1:A:583:TYR:CB	1.47	1.40
1:A:1111:ILE:CD1	1:A:1115:LEU:HD21	1.50	1.40
1:A:1111:ILE:HD12	1:A:1115:LEU:CG	1.58	1.33
1:A:1111:ILE:HD12	1:A:1115:LEU:CD2	1.65	1.24
1:A:941:GLN:CB	2:G:29:C:H42	1.50	1.23
1:A:1111:ILE:CD1	1:A:1115:LEU:CD2	2.14	1.23
1:A:746:MET:CE	1:A:748:ARG:HD3	1.69	1.22
1:A:732:ASN:OD1	1:A:971:LEU:CD2	1.87	1.22
1:A:941:GLN:CB	2:G:29:C:N4	2.03	1.21
2:G:27:U:H3'	2:G:28:C:C5'	1.68	1.21
1:A:535:ASP:CA	1:A:583:TYR:CB	2.21	1.18
1:A:1111:ILE:HD12	1:A:1115:LEU:HG	1.21	1.17
2:G:30:A:C2	2:G:33:A:C6	2.33	1.16
2:G:30:A:H2'	2:G:33:A:H61	1.07	1.16
2:G:29:C:C1'	2:G:30:A:H5'	1.76	1.15
1:A:3:LYS:HE3	1:A:823:ASP:OD2	1.47	1.14
1:A:897:LYS:HD3	2:G:28:C:O2	1.47	1.14
1:A:85:THR:O	1:A:86:ARG:NE	1.81	1.13
1:A:1111:ILE:CD1	1:A:1115:LEU:CG	2.26	1.12
1:A:205:ILE:HG21	1:A:252:ILE:HD13	1.26	1.12
1:A:746:MET:CE	1:A:748:ARG:CD	2.29	1.10
2:G:30:A:N3	2:G:33:A:C6	2.20	1.10
1:A:1111:ILE:HD11	1:A:1115:LEU:HD11	1.25	1.10
1:A:198:ASP:HB3	1:A:201:GLU:HB3	1.31	1.09
1:A:1095:TYR:CE1	1:A:1130:LEU:HD22	1.89	1.08
1:A:201:GLU:O	1:A:206:LYS:NZ	1.88	1.07
1:A:746:MET:HE1	1:A:748:ARG:CD	1.85	1.07
1:A:199:LYS:O	1:A:203:GLN:NE2	1.88	1.05
1:A:1108:GLN:OE1	1:A:1108:GLN:N	1.89	1.05
1:A:85:THR:CG2	1:A:86:ARG:H	1.68	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:GLY:HA3	2:G:31:G:N2	1.72	1.04
1:A:1058:ASP:O	1:A:1061:LYS:NZ	1.90	1.02
2:G:27:U:C3'	2:G:28:C:H5''	1.90	1.02
1:A:530:PHE:CE2	1:A:531:MET:HE2	1.94	1.02
1:A:1035:MET:HE2	1:A:1037:VAL:HG12	1.41	1.02
2:G:29:C:H1'	2:G:30:A:H5'	1.02	1.01
1:A:447:LYS:HE3	1:A:511:VAL:O	1.61	1.01
1:A:732:ASN:OD1	1:A:971:LEU:HD22	1.59	1.01
1:A:206:LYS:HE3	1:A:206:LYS:N	1.76	1.01
1:A:535:ASP:CB	1:A:583:TYR:CB	2.39	1.01
1:A:407:ASP:O	1:A:408:LEU:HD12	1.61	1.00
1:A:475:GLY:HA3	1:A:479:GLU:OE2	1.60	1.00
1:A:85:THR:HG23	1:A:86:ARG:N	1.65	1.00
1:A:577:ASN:ND2	1:A:685:ALA:C	2.19	1.00
1:A:246:THR:CG2	1:A:252:ILE:HG22	1.92	0.99
1:A:732:ASN:OD1	1:A:971:LEU:HD21	1.59	0.99
1:A:198:ASP:CB	1:A:201:GLU:HB3	1.93	0.99
1:A:337:PHE:CG	1:A:479:GLU:OE1	2.16	0.99
1:A:607:ASN:OD1	1:A:607:ASN:O	1.78	0.99
1:A:530:PHE:CZ	1:A:531:MET:HE2	1.98	0.99
1:A:101:LEU:HB3	1:A:176:ILE:HD12	1.41	0.98
1:A:1138:ARG:NH1	1:A:1148:ASP:OD2	1.95	0.98
1:A:206:LYS:HE3	1:A:206:LYS:H	1.29	0.98
1:A:1170:GLN:NE2	1:A:1173:ALA:HA	1.79	0.98
1:A:85:THR:HG23	1:A:86:ARG:H	0.82	0.97
2:G:27:U:H3'	2:G:28:C:H5''	0.97	0.97
2:G:34:A:H5'	2:G:34:A:H8	1.26	0.97
1:A:955:ASN:OD1	1:A:977:THR:HG22	1.62	0.97
1:A:951:ILE:HD11	1:A:986:MET:HE3	1.47	0.96
1:A:279:GLN:HG2	1:A:280:VAL:HG13	1.48	0.95
2:G:29:C:H1'	2:G:30:A:C5'	1.95	0.95
1:A:1111:ILE:HD11	1:A:1115:LEU:CD1	1.95	0.95
1:A:1111:ILE:HD13	1:A:1115:LEU:HD21	1.46	0.95
1:A:628:ASN:ND2	1:A:631:ASP:OD2	1.99	0.94
1:A:252:ILE:HD12	1:A:253:LYS:N	1.81	0.94
1:A:447:LYS:CE	1:A:511:VAL:O	2.15	0.94
1:A:622:LYS:O	1:A:627:PHE:HB2	1.68	0.94
1:A:1005:ASP:OD1	1:A:1007:SER:OG	1.85	0.93
1:A:77:TYR:HH	1:A:81:PHE:HE1	1.00	0.93
1:A:746:MET:HE3	1:A:748:ARG:HD3	1.50	0.93
1:A:746:MET:HE1	1:A:748:ARG:HD3	1.42	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:GLN:OE1	1:A:994:PHE:CE2	2.21	0.93
1:A:182:ARG:NH2	1:A:491:VAL:CG1	2.32	0.92
1:A:1111:ILE:CD1	1:A:1115:LEU:HD11	2.00	0.92
1:A:1047:LEU:HD23	1:A:1063:TRP:O	1.70	0.92
1:A:982:SER:HB2	2:G:36:G:OP2	1.70	0.91
2:G:30:A:H2'	2:G:33:A:N6	1.86	0.91
2:G:30:A:C4	2:G:33:A:N1	2.40	0.90
1:A:1110:ASP:OD2	1:A:1112:ARG:NH2	2.05	0.90
2:G:30:A:N3	2:G:33:A:N1	2.20	0.90
1:A:535:ASP:HB3	1:A:583:TYR:CB	2.01	0.90
1:A:1198:PHE:CZ	1:A:1211:ILE:HD11	2.06	0.90
1:A:207:GLU:O	1:A:212:SER:N	2.05	0.89
1:A:1170:GLN:NE2	1:A:1173:ALA:CA	2.36	0.89
1:A:989:GLN:OE1	1:A:994:PHE:CZ	2.26	0.88
1:A:658:SER:HB3	1:A:662:LYS:HE2	1.52	0.88
1:A:1111:ILE:HD11	1:A:1115:LEU:HD21	1.55	0.88
1:A:497:LEU:O	1:A:500:VAL:HG13	1.74	0.88
1:A:74:LEU:O	1:A:77:TYR:HB3	1.74	0.88
1:A:577:ASN:ND2	1:A:686:SER:HA	1.89	0.87
1:A:203:GLN:HE21	1:A:204:GLU:HG2	1.38	0.87
1:A:245:VAL:O	1:A:246:THR:OG1	1.92	0.87
1:A:337:PHE:CD2	1:A:479:GLU:OE1	2.27	0.87
2:G:30:A:N3	2:G:33:A:N6	2.22	0.87
1:A:182:ARG:NH2	1:A:491:VAL:HG11	1.91	0.86
1:A:951:ILE:CD1	1:A:986:MET:HE3	2.05	0.86
1:A:1131:MET:HE3	1:A:1134:MET:CE	2.04	0.86
1:A:1095:TYR:O	1:A:1099:PHE:CD2	2.28	0.86
1:A:746:MET:HE1	1:A:748:ARG:HD2	1.57	0.86
1:A:1111:ILE:CD1	1:A:1115:LEU:CD1	2.52	0.86
1:A:377:VAL:HG11	1:A:1054:ARG:HG2	1.58	0.85
1:A:663:TYR:OH	1:A:672:GLU:OE1	1.93	0.85
1:A:1170:GLN:HE21	1:A:1173:ALA:HB2	1.40	0.85
1:A:3:LYS:HZ2	1:A:820:LEU:HD23	1.40	0.85
1:A:205:ILE:CG2	1:A:252:ILE:HD13	2.04	0.84
1:A:572:ASP:OD2	1:A:574:VAL:HG12	1.78	0.84
1:A:666:ILE:HD12	1:A:670:TYR:CE2	2.12	0.83
2:G:34:A:H5'	2:G:34:A:C8	2.14	0.83
1:A:247:GLU:O	1:A:248:SER:OG	1.96	0.82
1:A:577:ASN:HD21	1:A:686:SER:N	1.77	0.82
1:A:246:THR:HG22	1:A:252:ILE:HG22	1.61	0.82
2:G:30:A:C2'	2:G:33:A:H61	1.89	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:PHE:CE2	1:A:531:MET:CE	2.62	0.82
2:G:20:G:H5''	2:G:20:G:H8	1.43	0.82
1:A:1075:PHE:CD2	1:A:1087:GLU:HB2	2.16	0.81
1:A:1170:GLN:HE22	1:A:1173:ALA:HA	1.43	0.81
1:A:1141:ILE:O	1:A:1142:THR:OG1	1.98	0.81
1:A:173:PHE:HD1	1:A:177:ASN:HD22	1.25	0.81
1:A:1105:ASN:HB3	1:A:1108:GLN:HE22	1.46	0.80
1:A:577:ASN:HD21	1:A:686:SER:HA	1.46	0.80
1:A:982:SER:CB	2:G:36:G:OP2	2.29	0.80
1:A:1110:ASP:CG	1:A:1112:ARG:HH21	1.90	0.80
1:A:1170:GLN:HE21	1:A:1173:ALA:CB	1.95	0.79
1:A:1005:ASP:OD2	1:A:1152:SER:CB	2.31	0.79
1:A:390:LYS:HZ2	2:G:32:U:H4'	1.46	0.79
1:A:263:ASN:HA	1:A:268:GLN:HG2	1.64	0.79
1:A:663:TYR:CE1	1:A:669:PHE:HA	2.18	0.79
2:G:29:C:H4'	2:G:30:A:OP1	1.80	0.79
1:A:78:ILE:O	1:A:82:ARG:HG3	1.82	0.79
1:A:930:GLY:HA3	2:G:31:G:C2	2.17	0.79
1:A:930:GLY:HA3	2:G:31:G:H21	1.47	0.79
1:A:897:LYS:HD3	2:G:28:C:C2	2.18	0.79
2:G:39:G:H5''	2:G:40:C:OP2	1.82	0.78
1:A:231:GLN:HB2	1:A:278:LYS:HZ2	1.48	0.78
1:A:184:ILE:HA	1:A:187:MET:HG3	1.64	0.78
1:A:295:THR:HG22	1:A:299:GLU:OE1	1.82	0.78
1:A:205:ILE:HG21	1:A:252:ILE:CD1	2.10	0.78
1:A:252:ILE:HD12	1:A:253:LYS:H	1.47	0.78
1:A:1016:THR:OG1	1:A:1132:SER:CB	2.32	0.78
1:A:180:LEU:HD13	1:A:225:PHE:CD1	2.19	0.78
1:A:180:LEU:HA	1:A:225:PHE:CE1	2.19	0.78
2:G:30:A:H2'	2:G:30:A:N3	1.98	0.78
1:A:619:GLY:HA2	1:A:621:PHE:CE2	2.19	0.77
1:A:292:GLU:HA	1:A:506:ALA:CB	2.15	0.77
1:A:205:ILE:HG22	1:A:252:ILE:HG12	1.67	0.77
1:A:951:ILE:O	1:A:977:THR:HG21	1.85	0.76
1:A:1095:TYR:CZ	1:A:1130:LEU:HD22	2.21	0.76
1:A:569:ILE:HG21	1:A:685:ALA:HB1	1.66	0.76
1:A:1111:ILE:CD1	1:A:1115:LEU:HG	2.03	0.76
1:A:439:ASP:OD1	1:A:439:ASP:N	2.17	0.75
1:A:666:ILE:O	1:A:666:ILE:HD13	1.86	0.75
1:A:577:ASN:ND2	1:A:686:SER:CA	2.50	0.75
1:A:1010:PHE:CD2	1:A:1137:MET:HE1	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:CB	1:A:250:GLU:HB3	2.17	0.75
1:A:1016:THR:OG1	1:A:1132:SER:HB2	1.87	0.75
2:G:30:A:C2	2:G:33:A:C5	2.75	0.74
1:A:577:ASN:HD21	1:A:686:SER:CA	1.98	0.74
1:A:1067:SER:HB3	1:A:1092:THR:HG22	1.69	0.74
1:A:198:ASP:O	1:A:202:VAL:HG12	1.87	0.74
1:A:1137:MET:HE2	1:A:1153:PRO:HD2	1.68	0.74
1:A:180:LEU:HD12	1:A:180:LEU:O	1.87	0.73
1:A:1107:GLN:N	1:A:1108:GLN:OE1	2.20	0.73
1:A:535:ASP:HB3	1:A:583:TYR:C	2.12	0.73
1:A:1198:PHE:CE1	1:A:1211:ILE:HD11	2.23	0.73
1:A:603:MET:O	1:A:606:TYR:O	2.07	0.73
2:G:34:A:H8	2:G:34:A:C5'	2.00	0.73
1:A:566:LEU:O	1:A:580:LYS:NZ	2.15	0.73
1:A:577:ASN:ND2	1:A:685:ALA:O	2.17	0.73
2:G:36:G:H8	2:G:36:G:H5''	1.54	0.73
1:A:577:ASN:ND2	1:A:686:SER:N	2.35	0.73
1:A:1107:GLN:C	1:A:1108:GLN:OE1	2.32	0.73
1:A:3:LYS:CE	1:A:823:ASP:HB2	2.19	0.72
1:A:615:ILE:HG12	1:A:631:ASP:OD1	1.89	0.72
1:A:390:LYS:NZ	2:G:32:U:H4'	2.04	0.72
1:A:180:LEU:HD22	1:A:225:PHE:CE2	2.25	0.71
1:A:1163:ASP:OD2	1:A:1165:ARG:NH2	2.22	0.71
1:A:198:ASP:O	1:A:202:VAL:N	2.23	0.71
1:A:182:ARG:NH2	1:A:491:VAL:HG13	2.06	0.71
1:A:1111:ILE:O	1:A:1115:LEU:HG	1.91	0.71
1:A:653:TYR:CE1	1:A:677:GLY:O	2.44	0.71
1:A:85:THR:O	1:A:86:ARG:CG	2.39	0.70
2:G:28:C:OP1	2:G:28:C:O3'	2.08	0.70
1:A:941:GLN:CB	2:G:29:C:C4	2.75	0.70
1:A:180:LEU:HB2	1:A:225:PHE:CZ	2.27	0.69
1:A:1131:MET:HE3	1:A:1134:MET:HE1	1.74	0.69
1:A:27:THR:HG21	1:A:701:MET:H	1.57	0.69
1:A:84:LYS:HE2	1:A:480:THR:HB	1.75	0.69
1:A:85:THR:O	1:A:86:ARG:CB	2.41	0.69
1:A:200:HIS:O	1:A:204:GLU:HB2	1.93	0.69
1:A:272:LYS:NZ	1:A:489:ASP:OD1	2.26	0.69
1:A:606:TYR:HE1	1:A:645:ARG:HE	1.41	0.69
1:A:182:ARG:NH1	1:A:275:PRO:O	2.26	0.69
1:A:1007:SER:O	1:A:1226:VAL:HG21	1.93	0.68
1:A:371:LEU:HD23	1:A:371:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:ILE:HD11	1:A:1218:TRP:HA	1.74	0.68
1:A:1198:PHE:HZ	1:A:1211:ILE:HD11	1.59	0.68
1:A:84:LYS:O	1:A:85:THR:HG22	1.94	0.68
1:A:63:ASN:ND2	1:A:231:GLN:OE1	2.27	0.67
1:A:205:ILE:CG2	1:A:252:ILE:CD1	2.70	0.67
1:A:73:ASN:HD21	1:A:97:LEU:HG	1.60	0.67
1:A:361:LYS:NZ	1:A:403:TYR:O	2.21	0.67
1:A:496:ILE:O	1:A:499:LYS:HB2	1.95	0.67
1:A:406:ALA:O	1:A:407:ASP:HB2	1.92	0.67
1:A:182:ARG:HH22	1:A:491:VAL:CG1	2.08	0.67
1:A:199:LYS:HA	1:A:202:VAL:HG12	1.75	0.66
1:A:534:TRP:HZ2	1:A:742:ALA:CB	2.07	0.66
1:A:3:LYS:HE2	1:A:823:ASP:HB2	1.78	0.66
1:A:377:VAL:CG1	1:A:1054:ARG:HG2	2.26	0.66
1:A:245:VAL:C	1:A:246:THR:HG1	2.00	0.65
1:A:1036:TYR:HB2	1:A:1043:PHE:CE1	2.31	0.65
1:A:200:HIS:HA	1:A:204:GLU:HG3	1.78	0.65
2:G:33:A:C8	2:G:34:A:C8	2.84	0.65
1:A:933:ASN:C	1:A:933:ASN:HD22	2.03	0.65
1:A:1005:ASP:OD2	1:A:1152:SER:OG	2.14	0.65
1:A:933:ASN:HD22	1:A:934:SER:N	1.95	0.65
1:A:85:THR:O	1:A:86:ARG:CD	2.43	0.65
1:A:930:GLY:CA	2:G:31:G:N2	2.56	0.65
1:A:377:VAL:HG23	1:A:381:TYR:CD2	2.31	0.64
1:A:1060:ILE:O	1:A:1063:TRP:NE1	2.31	0.64
1:A:1094:ALA:HB1	1:A:1130:LEU:HD11	1.78	0.64
1:A:1194:ALA:HB1	1:A:1211:ILE:HD12	1.79	0.64
1:A:50:VAL:HG21	1:A:144:PHE:CE2	2.33	0.64
1:A:173:PHE:O	1:A:177:ASN:HB2	1.98	0.64
1:A:933:ASN:HB3	1:A:936:VAL:HG13	1.79	0.63
2:G:33:A:H2'	2:G:34:A:C5'	2.28	0.63
1:A:199:LYS:HA	1:A:202:VAL:CG1	2.28	0.63
1:A:326:LYS:HD3	1:A:419:ILE:HD11	1.79	0.63
1:A:1035:MET:O	1:A:1044:GLU:HG2	1.98	0.63
1:A:1138:ARG:HH11	1:A:1148:ASP:CG	2.06	0.63
1:A:1058:ASP:OD2	1:A:1060:ILE:O	2.16	0.63
1:A:1170:GLN:HE22	1:A:1173:ALA:CA	2.04	0.63
1:A:603:MET:SD	1:A:608:PRO:HG3	2.39	0.63
1:A:27:THR:CG2	1:A:701:MET:H	2.13	0.62
1:A:180:LEU:HD22	1:A:225:PHE:CD2	2.34	0.62
1:A:785:LYS:HB2	2:G:3:A:H5''	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:TYR:HE1	1:A:645:ARG:NE	1.98	0.62
1:A:180:LEU:HD13	1:A:225:PHE:CG	2.34	0.62
2:G:20:G:H5''	2:G:20:G:C8	2.30	0.62
1:A:1186:ASN:OD1	1:A:1189:ARG:NH1	2.31	0.62
2:G:30:A:C2	2:G:33:A:N1	2.61	0.62
1:A:443:GLU:OE2	1:A:444:LYS:HE3	1.99	0.62
1:A:246:THR:OG1	1:A:250:GLU:HB3	2.00	0.62
1:A:199:LYS:CA	1:A:202:VAL:HG12	2.30	0.62
1:A:442:LEU:HD11	1:A:446:LEU:HD13	1.82	0.61
1:A:1010:PHE:HD2	1:A:1137:MET:HE1	1.65	0.61
1:A:1016:THR:OG1	1:A:1132:SER:HB3	1.98	0.61
1:A:203:GLN:HG2	1:A:204:GLU:N	2.16	0.61
1:A:209:ILE:HG21	1:A:252:ILE:HG21	1.82	0.61
1:A:1073:ARG:HB2	1:A:1133:LEU:HD21	1.83	0.61
1:A:951:ILE:HG23	1:A:977:THR:HG23	1.83	0.61
2:G:24:G:H1	2:G:37:C:H42	1.47	0.61
2:G:27:U:C3'	2:G:28:C:C5'	2.58	0.61
1:A:78:ILE:HD13	1:A:187:MET:HE1	1.83	0.61
1:A:184:ILE:HA	1:A:187:MET:HE2	1.83	0.61
1:A:246:THR:HG23	1:A:252:ILE:HG22	1.77	0.60
1:A:531:MET:SD	1:A:534:TRP:CH2	2.94	0.60
1:A:746:MET:HE2	1:A:748:ARG:CD	2.31	0.60
1:A:534:TRP:CZ2	1:A:742:ALA:CB	2.85	0.60
1:A:574:VAL:HG13	1:A:575:ASN:N	2.17	0.60
2:G:33:A:H2'	2:G:34:A:H5'	1.83	0.60
1:A:935:ARG:CG	1:A:935:ARG:HH11	2.15	0.60
1:A:1111:ILE:HD11	1:A:1115:LEU:CD2	2.15	0.60
1:A:1226:VAL:O	1:A:1227:LYS:NZ	2.35	0.60
1:A:620:THR:O	1:A:627:PHE:HA	2.02	0.59
1:A:1067:SER:O	1:A:1091:LEU:HD12	2.02	0.59
1:A:339:LYS:HB2	1:A:474:PHE:O	2.02	0.59
1:A:3:LYS:CE	1:A:823:ASP:CB	2.81	0.59
1:A:3:LYS:NZ	1:A:820:LEU:HD23	2.16	0.59
1:A:1105:ASN:HB3	1:A:1108:GLN:NE2	2.15	0.59
1:A:301:LEU:HD23	1:A:305:ARG:HD2	1.83	0.59
1:A:836:ARG:HH12	1:A:1142:THR:HA	1.68	0.58
1:A:1170:GLN:HE21	1:A:1173:ALA:CA	2.11	0.58
1:A:3:LYS:CE	1:A:823:ASP:OD2	2.36	0.58
1:A:2:SER:N	1:A:5:GLU:HG3	2.18	0.58
1:A:666:ILE:CD1	1:A:670:TYR:CZ	2.86	0.58
1:A:341:GLY:HA2	2:G:32:U:C2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:PHE:HA	1:A:986:MET:HG3	1.85	0.58
1:A:211:ASN:N	1:A:211:ASN:OD1	2.37	0.58
2:G:36:G:H5''	2:G:36:G:C8	2.37	0.58
1:A:246:THR:HG21	1:A:250:GLU:HB3	1.85	0.58
1:A:666:ILE:HD12	1:A:670:TYR:CZ	2.39	0.58
1:A:1138:ARG:NH1	1:A:1148:ASP:CG	2.59	0.58
1:A:1047:LEU:CD2	1:A:1063:TRP:O	2.47	0.57
2:G:33:A:C3'	2:G:34:A:C5'	2.82	0.57
1:A:3:LYS:HE3	1:A:823:ASP:CG	2.27	0.57
2:G:20:G:H2'	2:G:21:A:O4'	2.03	0.57
1:A:34:LYS:NZ	1:A:697:GLY:O	2.37	0.57
1:A:294:TYR:CD1	1:A:294:TYR:N	2.73	0.57
1:A:1047:LEU:HD23	1:A:1047:LEU:H	1.70	0.57
1:A:482:ARG:NH2	1:A:487:TYR:CD2	2.73	0.57
1:A:1067:SER:OG	1:A:1095:TYR:HD2	1.87	0.57
1:A:203:GLN:O	1:A:207:GLU:HB3	2.04	0.57
1:A:256:ASN:HD21	1:A:273:PHE:H	1.50	0.57
1:A:628:ASN:HB3	1:A:631:ASP:HB2	1.86	0.56
1:A:1073:ARG:NH2	1:A:1075:PHE:CE2	2.73	0.56
1:A:377:VAL:HG11	1:A:1054:ARG:CG	2.32	0.56
1:A:443:GLU:HG3	1:A:444:LYS:N	2.19	0.56
1:A:954:LEU:HB3	1:A:977:THR:HB	1.87	0.56
1:A:724:PHE:O	1:A:727:LEU:HB2	2.05	0.56
1:A:1073:ARG:NH2	1:A:1075:PHE:CZ	2.73	0.56
1:A:75:ASN:ND2	1:A:223:GLU:OE2	2.38	0.56
1:A:237:TYR:HA	1:A:240:ILE:HD12	1.87	0.56
1:A:1073:ARG:NH2	1:A:1075:PHE:CD2	2.73	0.56
1:A:63:ASN:OD1	1:A:231:GLN:NE2	2.37	0.56
1:A:951:ILE:HG23	1:A:977:THR:CG2	2.35	0.56
1:A:73:ASN:HB3	1:A:101:LEU:HD13	1.88	0.56
1:A:1073:ARG:NH2	1:A:1075:PHE:CE1	2.73	0.56
1:A:1131:MET:CE	1:A:1134:MET:HE1	2.36	0.56
2:G:14:A:H8	2:G:14:A:H5''	1.71	0.56
1:A:1150:LEU:H	1:A:1164:SER:HB2	1.71	0.56
1:A:120:LYS:O	1:A:123:ILE:HG22	2.06	0.56
1:A:533:GLY:HA3	1:A:536:LYS:HD2	1.86	0.56
1:A:951:ILE:HD11	1:A:986:MET:CE	2.29	0.56
1:A:1131:MET:HE3	1:A:1134:MET:HE2	1.85	0.56
1:A:1185:TYR:CZ	1:A:1189:ARG:HD2	2.41	0.55
1:A:85:THR:CG2	1:A:86:ARG:N	2.38	0.55
1:A:483:ASP:HB3	1:A:486:PHE:HB3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:GLN:O	1:A:1111:ILE:HG22	2.06	0.55
1:A:2:SER:H	1:A:5:GLU:HG3	1.72	0.55
1:A:245:VAL:HG13	1:A:247:GLU:H	1.72	0.55
1:A:182:ARG:HH21	1:A:491:VAL:HG11	1.71	0.55
1:A:1046:ALA:HB2	1:A:1064:LYS:HG2	1.87	0.55
1:A:602:TRP:HH2	1:A:645:ARG:O	1.90	0.55
1:A:16:THR:CG2	2:G:23:C:H1'	2.37	0.55
1:A:74:LEU:O	1:A:77:TYR:CB	2.53	0.55
1:A:897:LYS:CD	2:G:28:C:O2	2.38	0.55
2:G:33:A:C2'	2:G:34:A:C5'	2.85	0.55
1:A:407:ASP:C	1:A:408:LEU:HD12	2.30	0.54
1:A:585:LEU:HD12	1:A:678:TYR:HB2	1.88	0.54
1:A:584:LYS:O	1:A:678:TYR:HA	2.08	0.54
1:A:860:ILE:HG12	1:A:869:LYS:HB3	1.88	0.54
1:A:954:LEU:CD1	1:A:957:MET:CE	2.86	0.54
1:A:244:PHE:HB3	1:A:252:ILE:HG23	1.90	0.54
1:A:658:SER:CB	1:A:662:LYS:HE2	2.32	0.54
2:G:33:A:H8	2:G:34:A:C8	2.24	0.54
1:A:77:TYR:OH	1:A:81:PHE:HE1	1.80	0.54
1:A:1063:TRP:HE3	1:A:1154:VAL:HG11	1.72	0.54
1:A:115:TYR:O	1:A:118:LEU:HB2	2.08	0.54
1:A:955:ASN:OD1	1:A:977:THR:CG2	2.46	0.54
2:G:23:C:H2'	2:G:23:C:O2	2.06	0.54
2:G:33:A:C2'	2:G:34:A:H5''	2.38	0.54
1:A:1105:ASN:CB	1:A:1108:GLN:NE2	2.71	0.54
1:A:198:ASP:HB2	1:A:201:GLU:HB3	1.86	0.54
1:A:245:VAL:HG13	1:A:246:THR:N	2.21	0.54
1:A:246:THR:CG2	1:A:250:GLU:HB3	2.38	0.54
1:A:549:TYR:HB2	1:A:578:TYR:HD1	1.73	0.54
1:A:1198:PHE:CZ	1:A:1211:ILE:CD1	2.87	0.54
1:A:863:PHE:N	1:A:863:PHE:CD1	2.75	0.54
2:G:30:A:C2	2:G:33:A:N6	2.73	0.54
1:A:180:LEU:CB	1:A:225:PHE:CZ	2.91	0.54
1:A:231:GLN:HB2	1:A:278:LYS:NZ	2.21	0.54
1:A:292:GLU:HA	1:A:506:ALA:HB1	1.88	0.54
2:G:14:A:H5''	2:G:14:A:C8	2.43	0.54
1:A:405:ASP:OD1	1:A:405:ASP:N	2.39	0.53
1:A:1031:PHE:O	1:A:1112:ARG:NH1	2.40	0.53
1:A:83:LYS:O	1:A:84:LYS:HB3	2.09	0.53
1:A:85:THR:HG21	1:A:480:THR:CG2	2.38	0.53
1:A:85:THR:HG21	1:A:480:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TYR:CE2	1:A:385:ARG:HB2	2.43	0.53
1:A:508:ARG:O	1:A:512:THR:HB	2.07	0.53
1:A:1073:ARG:NH2	1:A:1075:PHE:CG	2.74	0.53
1:A:85:THR:CG2	1:A:480:THR:HG21	2.39	0.53
1:A:531:MET:SD	1:A:534:TRP:HH2	2.32	0.53
1:A:666:ILE:HD12	1:A:670:TYR:CD2	2.44	0.53
1:A:1214:SER:O	1:A:1215:ASN:C	2.48	0.53
2:G:25:C:O2'	2:G:26:A:H5'	2.09	0.53
1:A:100:ASN:HA	1:A:103:LYS:HB2	1.90	0.52
1:A:85:THR:CG2	1:A:480:THR:CG2	2.87	0.52
1:A:1131:MET:CE	1:A:1134:MET:CE	2.84	0.52
1:A:1046:ALA:CB	1:A:1064:LYS:HG2	2.39	0.52
1:A:182:ARG:HH22	1:A:491:VAL:HG13	1.69	0.52
1:A:534:TRP:CZ2	1:A:742:ALA:HB3	2.45	0.52
1:A:295:THR:HG23	1:A:296:SER:OG	2.10	0.52
1:A:262:TYR:C	1:A:268:GLN:HE21	2.17	0.52
1:A:1032:ASP:HB2	1:A:1046:ALA:O	2.10	0.52
1:A:102:ARG:NH2	1:A:166:ALA:HB2	2.25	0.52
1:A:954:LEU:HG	1:A:957:MET:CE	2.40	0.52
1:A:1063:TRP:CE3	1:A:1154:VAL:HG11	2.45	0.52
1:A:734:GLY:O	1:A:737:ARG:NE	2.43	0.52
1:A:253:LYS:HE2	1:A:258:TYR:HE1	1.74	0.52
2:G:34:A:C8	2:G:34:A:C5'	2.85	0.52
1:A:180:LEU:HD13	1:A:225:PHE:CE1	2.45	0.52
1:A:554:TYR:CG	1:A:701:MET:HE3	2.44	0.52
1:A:930:GLY:CA	2:G:31:G:H21	2.18	0.51
1:A:205:ILE:HG22	1:A:252:ILE:CG1	2.36	0.51
1:A:244:PHE:HB3	1:A:252:ILE:CG2	2.39	0.51
1:A:535:ASP:CB	1:A:583:TYR:C	2.83	0.51
1:A:84:LYS:O	1:A:84:LYS:HD2	2.10	0.51
1:A:209:ILE:CG2	1:A:252:ILE:HG21	2.40	0.51
1:A:1193:TRP:CE3	1:A:1213:ILE:HB	2.46	0.51
1:A:615:ILE:CG1	1:A:631:ASP:OD1	2.58	0.51
1:A:1110:ASP:OD1	1:A:1112:ARG:NE	2.37	0.51
1:A:628:ASN:HB3	1:A:631:ASP:OD2	2.11	0.51
1:A:1067:SER:OG	1:A:1095:TYR:CD2	2.63	0.51
1:A:193:VAL:O	1:A:196:ILE:HG12	2.11	0.50
1:A:666:ILE:HD11	1:A:670:TYR:CE1	2.45	0.50
1:A:1031:PHE:CE1	1:A:1047:LEU:HB3	2.46	0.50
1:A:1010:PHE:CD2	1:A:1137:MET:CE	2.93	0.50
1:A:77:TYR:CE2	1:A:81:PHE:CD1	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG22	1:A:252:ILE:CG2	2.36	0.50
1:A:73:ASN:OD1	1:A:100:ASN:HB2	2.12	0.50
1:A:127:ILE:HA	1:A:130:GLU:OE1	2.11	0.50
1:A:954:LEU:CD1	1:A:957:MET:HE2	2.41	0.50
1:A:74:LEU:CD1	1:A:180:LEU:HD21	2.42	0.50
1:A:174:ARG:O	1:A:179:ASN:HB2	2.11	0.50
1:A:265:LYS:HG2	1:A:267:LYS:H	1.76	0.50
1:A:954:LEU:HG	1:A:957:MET:HE3	1.93	0.50
1:A:252:ILE:HD12	1:A:252:ILE:C	2.37	0.50
1:A:673:VAL:O	1:A:677:GLY:N	2.45	0.50
1:A:117:SER:HB2	1:A:127:ILE:HD11	1.94	0.50
1:A:933:ASN:ND2	1:A:935:ARG:H	2.10	0.50
1:A:935:ARG:CG	1:A:935:ARG:NH1	2.73	0.50
1:A:982:SER:O	1:A:985:SER:HB2	2.12	0.50
1:A:1211:ILE:HG22	1:A:1211:ILE:O	2.10	0.50
1:A:211:ASN:HB2	1:A:213:ASP:H	1.76	0.49
1:A:935:ARG:HH11	1:A:935:ARG:HG3	1.77	0.49
1:A:930:GLY:O	1:A:931:PHE:HD2	1.95	0.49
1:A:328:PHE:HE1	1:A:486:PHE:CE1	2.30	0.49
1:A:96:ASN:O	1:A:100:ASN:ND2	2.45	0.49
1:A:199:LYS:C	1:A:202:VAL:HG12	2.37	0.49
1:A:475:GLY:CA	1:A:479:GLU:OE2	2.48	0.49
1:A:729:ASP:OD2	1:A:731:ASN:N	2.40	0.49
1:A:1139:ASN:N	1:A:1139:ASN:ND2	2.60	0.49
2:G:26:A:C2	2:G:36:G:C6	3.00	0.49
1:A:85:THR:O	1:A:86:ARG:HB2	2.10	0.49
1:A:666:ILE:HD11	1:A:670:TYR:CZ	2.47	0.49
1:A:188:ASP:OD1	1:A:188:ASP:O	2.30	0.49
1:A:464:LYS:CE	1:A:501:ASP:OD1	2.61	0.49
1:A:535:ASP:HA	1:A:583:TYR:CA	2.34	0.49
1:A:180:LEU:O	1:A:184:ILE:HG13	2.13	0.49
1:A:67:HIS:ND1	1:A:230:THR:HG21	2.28	0.48
1:A:475:GLY:O	1:A:476:GLU:C	2.56	0.48
1:A:863:PHE:HZ	1:A:868:ILE:HG13	1.78	0.48
1:A:1066:TYR:HE1	1:A:1155:LYS:HD2	1.77	0.48
1:A:1073:ARG:HE	1:A:1075:PHE:CB	2.27	0.48
1:A:65:VAL:O	1:A:69:ILE:HG12	2.14	0.48
1:A:180:LEU:HA	1:A:225:PHE:CZ	2.47	0.48
1:A:180:LEU:CA	1:A:225:PHE:CZ	2.96	0.48
1:A:401:GLN:HG2	1:A:410:VAL:HB	1.96	0.48
1:A:746:MET:CE	1:A:748:ARG:HD2	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:33:A:H2'	2:G:34:A:H5''	1.95	0.48
1:A:445:SER:O	1:A:449:ASN:N	2.46	0.48
1:A:1025:LYS:HE2	1:A:1116:CYS:O	2.13	0.48
1:A:545:THR:OG1	1:A:581:ILE:HG22	2.14	0.48
1:A:951:ILE:HD12	1:A:986:MET:HE3	1.92	0.48
1:A:161:MET:CE	1:A:280:VAL:HG12	2.43	0.48
1:A:103:LYS:HB3	1:A:103:LYS:HE2	1.57	0.48
1:A:92:LYS:HA	1:A:95:GLU:OE1	2.14	0.48
1:A:407:ASP:O	1:A:408:LEU:CD1	2.46	0.48
1:A:606:TYR:O	1:A:608:PRO:HD3	2.14	0.48
1:A:545:THR:OG1	1:A:581:ILE:CG2	2.62	0.48
1:A:616:TYR:HA	1:A:621:PHE:CE2	2.49	0.48
1:A:183:TYR:CZ	1:A:219:PHE:O	2.67	0.47
1:A:390:LYS:HZ2	2:G:33:A:P	2.37	0.47
1:A:1070:ASN:OD1	1:A:1070:ASN:N	2.45	0.47
1:A:1170:GLN:HB3	1:A:1173:ALA:HB2	1.95	0.47
1:A:331:TYR:HB3	1:A:483:ASP:OD1	2.13	0.47
1:A:183:TYR:CE2	1:A:219:PHE:O	2.67	0.47
1:A:184:ILE:CA	1:A:187:MET:HG3	2.40	0.47
1:A:205:ILE:CG2	1:A:252:ILE:CG1	2.92	0.47
1:A:1031:PHE:CD1	1:A:1047:LEU:HB3	2.50	0.47
1:A:47:TYR:CZ	1:A:51:LYS:HD2	2.48	0.47
1:A:574:VAL:CG1	1:A:575:ASN:N	2.77	0.47
1:A:595:LYS:HE3	1:A:595:LYS:HB2	1.66	0.47
2:G:33:A:C2'	2:G:34:A:H5'	2.44	0.47
1:A:842:VAL:HG23	1:A:1184:ALA:HB3	1.96	0.47
1:A:16:THR:HG23	2:G:23:C:O2'	2.15	0.47
1:A:196:ILE:HD12	1:A:262:TYR:CE1	2.50	0.47
1:A:230:THR:O	1:A:234:ILE:HG13	2.14	0.47
1:A:494:TYR:C	1:A:494:TYR:CD2	2.92	0.47
1:A:538:LYS:HE3	1:A:538:LYS:HB3	1.66	0.47
1:A:826:PRO:HD2	1:A:846:GLY:HA3	1.96	0.47
1:A:202:VAL:HG13	1:A:203:GLN:N	2.30	0.47
1:A:84:LYS:HD2	1:A:84:LYS:C	2.40	0.47
1:A:182:ARG:HH21	1:A:491:VAL:CG1	2.20	0.47
1:A:361:LYS:HZ3	1:A:403:TYR:HB3	1.80	0.47
1:A:3:LYS:NZ	1:A:823:ASP:CB	2.78	0.46
1:A:50:VAL:HG21	1:A:144:PHE:CD2	2.49	0.46
1:A:666:ILE:HD13	1:A:666:ILE:C	2.39	0.46
1:A:960:LYS:NZ	2:G:20:G:OP2	2.42	0.46
1:A:337:PHE:CD1	1:A:479:GLU:OE1	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LEU:HD22	1:A:1011:VAL:HG21	1.97	0.46
1:A:85:THR:C	1:A:86:ARG:HG3	2.39	0.46
1:A:442:LEU:HD22	1:A:444:LYS:O	2.16	0.46
1:A:572:ASP:CG	1:A:574:VAL:HG12	2.39	0.46
1:A:1047:LEU:HD23	1:A:1047:LEU:N	2.30	0.46
1:A:1107:GLN:CA	1:A:1108:GLN:OE1	2.63	0.46
1:A:578:TYR:HE2	1:A:690:VAL:HG22	1.80	0.46
1:A:798:ILE:O	1:A:798:ILE:HG13	2.14	0.46
1:A:2:SER:OG	1:A:5:GLU:HG2	2.15	0.46
1:A:117:SER:HB2	1:A:127:ILE:CD1	2.45	0.46
1:A:328:PHE:CE1	1:A:486:PHE:CE1	3.04	0.46
1:A:197:PHE:HB3	1:A:202:VAL:HB	1.98	0.46
1:A:266:THR:HG22	1:A:266:THR:O	2.15	0.46
2:G:28:C:O2	2:G:28:C:H2'	2.15	0.46
1:A:206:LYS:HE2	1:A:252:ILE:HD11	1.97	0.45
1:A:566:LEU:HD23	1:A:566:LEU:HA	1.77	0.45
1:A:1137:MET:HG2	1:A:1151:ILE:O	2.17	0.45
1:A:1167:TYR:O	1:A:1177:LYS:HG2	2.16	0.45
1:A:102:ARG:CZ	1:A:166:ALA:HB2	2.46	0.45
1:A:927:LEU:HD21	1:A:943:TYR:HD2	1.82	0.45
2:G:33:A:C3'	2:G:34:A:H5'	2.46	0.45
1:A:1170:GLN:HE22	1:A:1173:ALA:N	2.15	0.45
1:A:567:GLN:HB3	1:A:568:LYS:HD3	1.98	0.45
1:A:924:LEU:HD23	1:A:924:LEU:HA	1.77	0.45
1:A:933:ASN:HB3	1:A:936:VAL:CG1	2.46	0.45
1:A:247:GLU:C	1:A:248:SER:HG	2.06	0.45
1:A:414:LEU:HD12	1:A:414:LEU:HA	1.87	0.45
1:A:571:LYS:HB3	1:A:684:SER:HB3	1.97	0.45
2:G:29:C:C1'	2:G:30:A:C5'	2.69	0.45
1:A:174:ARG:HG2	1:A:279:GLN:HB3	1.97	0.45
1:A:183:TYR:O	1:A:187:MET:HG2	2.16	0.45
1:A:1042:LEU:CD2	1:A:1068:TYR:HB2	2.47	0.45
1:A:1156:ASN:HD21	1:A:1158:ASP:HB2	1.82	0.45
1:A:180:LEU:HB2	1:A:225:PHE:CE2	2.51	0.45
1:A:203:GLN:O	1:A:207:GLU:N	2.34	0.45
1:A:686:SER:OG	1:A:688:LYS:HG3	2.17	0.45
1:A:845:ASP:C	1:A:847:LYS:H	2.25	0.45
1:A:36:LEU:HD13	1:A:525:PHE:HD1	1.82	0.45
1:A:161:MET:O	1:A:171:ILE:HG13	2.16	0.45
1:A:183:TYR:OH	1:A:224:PHE:HB3	2.17	0.45
1:A:951:ILE:CD1	1:A:986:MET:CE	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:GLU:HG3	1:A:1044:GLU:O	2.16	0.45
1:A:80:LEU:HA	1:A:83:LYS:HB2	1.99	0.45
1:A:184:ILE:HA	1:A:187:MET:CE	2.46	0.45
1:A:1037:VAL:HG22	1:A:1042:LEU:O	2.17	0.45
1:A:1075:PHE:O	1:A:1075:PHE:CD1	2.70	0.45
1:A:16:THR:HG23	2:G:23:C:H1'	1.98	0.44
1:A:123:ILE:HG23	1:A:124:ILE:HG23	2.00	0.44
1:A:171:ILE:O	1:A:175:CYS:N	2.43	0.44
1:A:1067:SER:O	1:A:1091:LEU:HB2	2.17	0.44
1:A:988:THR:HB	1:A:989:GLN:H	1.61	0.44
1:A:1005:ASP:OD2	1:A:1152:SER:HB3	2.16	0.44
1:A:74:LEU:HD13	1:A:180:LEU:HD21	1.99	0.44
1:A:85:THR:C	1:A:86:ARG:CG	2.89	0.44
1:A:294:TYR:O	1:A:510:TYR:HE1	1.99	0.44
1:A:627:PHE:CZ	1:A:629:LEU:HA	2.53	0.44
2:G:34:A:H2'	2:G:35:A:O5'	2.18	0.44
1:A:1137:MET:O	1:A:1139:ASN:ND2	2.51	0.44
1:A:1170:GLN:NE2	1:A:1173:ALA:N	2.65	0.44
1:A:27:THR:HG23	1:A:694:VAL:HG13	1.98	0.44
1:A:1090:CYS:SG	1:A:1091:LEU:N	2.90	0.44
1:A:1090:CYS:SG	1:A:1093:SER:HB3	2.57	0.44
1:A:171:ILE:O	1:A:174:ARG:HB3	2.18	0.44
1:A:466:PHE:O	1:A:470:ILE:HB	2.18	0.44
1:A:1170:GLN:NE2	1:A:1173:ALA:HB2	2.21	0.44
1:A:581:ILE:HG23	1:A:581:ILE:O	2.17	0.44
1:A:596:VAL:O	1:A:599:SER:CB	2.66	0.44
1:A:824:ASP:OD1	1:A:824:ASP:N	2.46	0.44
1:A:1170:GLN:NE2	1:A:1173:ALA:CB	2.66	0.44
1:A:294:TYR:O	1:A:510:TYR:CE1	2.71	0.43
1:A:596:VAL:O	1:A:599:SER:HB3	2.18	0.43
1:A:597:PHE:CE2	1:A:642:SER:HB3	2.53	0.43
1:A:27:THR:HG22	1:A:700:TYR:HA	2.00	0.43
1:A:399:GLN:O	1:A:402:GLU:HB2	2.19	0.43
1:A:621:PHE:H	1:A:621:PHE:HD2	1.66	0.43
1:A:1010:PHE:HD2	1:A:1137:MET:CE	2.28	0.43
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.83	0.43
1:A:354:GLU:HB2	1:A:357:VAL:HG23	1.99	0.43
1:A:158:ARG:O	1:A:161:MET:HB2	2.17	0.43
1:A:328:PHE:HD1	1:A:328:PHE:HA	1.73	0.43
1:A:599:SER:O	1:A:603:MET:HB2	2.19	0.43
1:A:746:MET:HE2	1:A:748:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ASP:OD2	1:A:849:ASN:HB2	2.18	0.43
1:A:1160:ILE:HD12	1:A:1161:PHE:H	1.82	0.43
1:A:180:LEU:HD12	1:A:180:LEU:C	2.42	0.43
1:A:207:GLU:O	1:A:212:SER:CA	2.66	0.43
1:A:535:ASP:HB3	1:A:583:TYR:CA	2.48	0.43
1:A:78:ILE:CD1	1:A:222:GLY:CA	2.97	0.43
1:A:245:VAL:CG1	1:A:246:THR:N	2.82	0.43
1:A:294:TYR:N	1:A:294:TYR:HD1	2.17	0.43
1:A:1067:SER:O	1:A:1091:LEU:CD1	2.67	0.43
1:A:297:ASP:OD1	1:A:510:TYR:OH	2.33	0.43
1:A:933:ASN:C	1:A:933:ASN:ND2	2.73	0.43
1:A:443:GLU:HG3	1:A:444:LYS:HG3	2.00	0.43
1:A:619:GLY:HA2	1:A:621:PHE:HE2	1.80	0.43
1:A:623:LYS:H	1:A:623:LYS:HG2	1.64	0.43
1:A:636:ILE:HD11	1:A:666:ILE:HA	2.01	0.43
1:A:1131:MET:HB3	1:A:1131:MET:HE2	1.75	0.43
1:A:1138:ARG:NH1	1:A:1179:ALA:HB3	2.33	0.43
1:A:58:TYR:O	1:A:62:ILE:HG13	2.19	0.42
1:A:1203:ASP:HA	1:A:1206:LEU:HD22	2.01	0.42
2:G:37:C:H2'	2:G:38:G:O5'	2.18	0.42
2:G:30:A:C4	2:G:33:A:C2	3.07	0.42
1:A:3:LYS:HZ3	1:A:823:ASP:HB3	1.82	0.42
1:A:206:LYS:O	1:A:210:LEU:HB2	2.18	0.42
1:A:451:ALA:O	1:A:455:ILE:HG12	2.20	0.42
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.95	0.42
1:A:161:MET:HE1	1:A:280:VAL:HB	2.02	0.42
1:A:183:TYR:O	1:A:187:MET:CG	2.68	0.42
1:A:354:GLU:HB2	1:A:357:VAL:CG2	2.49	0.42
1:A:374:LYS:HG3	1:A:375:ALA:N	2.34	0.42
2:G:30:A:N3	2:G:30:A:C2'	2.77	0.42
1:A:123:ILE:HD12	1:A:127:ILE:HB	2.01	0.42
1:A:197:PHE:CZ	1:A:255:LEU:HG	2.54	0.42
1:A:237:TYR:CD2	1:A:276:LEU:HD22	2.54	0.42
1:A:351:ILE:HD13	1:A:410:VAL:HG22	2.01	0.42
1:A:1207:ASP:OD2	1:A:1208:LYS:NZ	2.53	0.42
1:A:586:LEU:HD12	1:A:587:PRO:HD2	2.02	0.42
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.71	0.42
1:A:144:PHE:O	1:A:147:PHE:HB2	2.19	0.42
1:A:86:ARG:HB2	1:A:86:ARG:CZ	2.48	0.42
1:A:179:ASN:OD1	1:A:276:LEU:HG	2.20	0.42
1:A:279:GLN:O	1:A:280:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HB3	1:A:323:LYS:HE2	1.83	0.42
1:A:947:GLU:HB3	1:A:986:MET:HE1	2.02	0.41
1:A:1192:LEU:HD23	1:A:1192:LEU:HA	1.78	0.41
1:A:202:VAL:C	1:A:206:LYS:HZ2	2.28	0.41
1:A:1042:LEU:HD21	1:A:1068:TYR:HB2	2.01	0.41
1:A:640:LYS:HE2	1:A:657:PHE:HB3	2.01	0.41
1:A:121:LYS:HD3	1:A:125:GLU:OE2	2.20	0.41
1:A:209:ILE:HG21	1:A:246:THR:HG22	2.03	0.41
1:A:836:ARG:NH1	1:A:1142:THR:HA	2.35	0.41
1:A:1034:ILE:HG12	1:A:1045:PHE:HD1	1.84	0.41
2:G:28:C:OP1	2:G:29:C:P	2.79	0.41
1:A:102:ARG:HD3	1:A:177:ASN:HD21	1.85	0.41
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.85	0.41
2:G:39:G:H3'	2:G:40:C:H6	1.85	0.41
1:A:84:LYS:CE	1:A:480:THR:HB	2.48	0.41
1:A:161:MET:HE1	1:A:280:VAL:CG1	2.51	0.41
1:A:198:ASP:HB2	1:A:201:GLU:CD	2.46	0.41
1:A:203:GLN:NE2	1:A:204:GLU:HG2	2.18	0.41
1:A:886:ALA:HB1	1:A:889:ASN:ND2	2.35	0.41
1:A:1214:SER:N	1:A:1217:GLU:OE1	2.51	0.41
2:G:23:C:C6	2:G:23:C:H5''	2.56	0.41
2:G:25:C:C2'	2:G:26:A:H5'	2.51	0.41
1:A:66:LEU:HB3	1:A:230:THR:HG22	2.03	0.41
1:A:78:ILE:HD12	1:A:222:GLY:HA3	2.02	0.41
1:A:580:LYS:HB3	1:A:683:GLU:HB3	2.03	0.41
1:A:663:TYR:CE1	1:A:669:PHE:CA	2.97	0.41
1:A:1005:ASP:OD1	1:A:1007:SER:N	2.54	0.41
1:A:1160:ILE:O	1:A:1160:ILE:HG23	2.20	0.41
1:A:1206:LEU:HD12	1:A:1206:LEU:HA	1.78	0.41
1:A:210:LEU:HD13	1:A:210:LEU:HA	1.83	0.41
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.90	0.41
1:A:377:VAL:CG2	1:A:381:TYR:CD2	3.04	0.41
1:A:390:LYS:NZ	2:G:33:A:OP1	2.54	0.41
1:A:407:ASP:C	1:A:408:LEU:CD1	2.94	0.41
1:A:424:GLU:O	1:A:428:VAL:HG23	2.21	0.41
1:A:41:GLU:O	1:A:44:ALA:HB3	2.21	0.40
1:A:446:LEU:HA	1:A:446:LEU:HD12	1.80	0.40
1:A:910:LYS:HA	1:A:910:LYS:HD3	1.82	0.40
1:A:1075:PHE:O	1:A:1075:PHE:HD1	2.04	0.40
2:G:29:C:O2	2:G:29:C:C2'	2.69	0.40
1:A:122:ASP:HA	1:A:125:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:LEU:HD12	1:A:1098:LEU:HA	1.82	0.40
1:A:1208:LYS:HA	1:A:1208:LYS:HD3	1.87	0.40
1:A:125:GLU:HG2	1:A:145:ASN:OD1	2.21	0.40
1:A:663:TYR:HE1	1:A:669:PHE:HA	1.81	0.40
1:A:712:LYS:HA	1:A:714:HIS:CE1	2.56	0.40
1:A:811:LYS:HB3	1:A:811:LYS:HE2	1.78	0.40
1:A:1027:PHE:CE2	1:A:1031:PHE:HE2	2.40	0.40
1:A:43:ARG:HG2	1:A:144:PHE:CE1	2.57	0.40
2:G:28:C:O2	2:G:28:C:C2'	2.70	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	1200/1228 (98%)	1164 (97%)	32 (3%)	4 (0%)	36 59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	TYR
1	A	248	SER
1	A	607	ASN
1	A	86	ARG

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1080/1115 (97%)	899 (83%)	181 (17%)	2 6

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	13	LEU
1	A	16	THR
1	A	18	ARG
1	A	35	ARG
1	A	37	LEU
1	A	69	ILE
1	A	71	LEU
1	A	72	LYS
1	A	73	ASN
1	A	81	PHE
1	A	86	ARG
1	A	88	GLU
1	A	94	LEU
1	A	97	LEU
1	A	101	LEU
1	A	116	LYS
1	A	117	SER
1	A	118	LEU
1	A	122	ASP
1	A	124	ILE
1	A	126	THR
1	A	130	GLU
1	A	143	SER
1	A	161	MET
1	A	165	GLU
1	A	175	CYS
1	A	176	ILE
1	A	180	LEU
1	A	182	ARG
1	A	187	MET
1	A	198	ASP
1	A	206	LYS
1	A	211	ASN
1	A	226	ASN
1	A	228	VAL

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Mol	Chain	Res	Type
1	A	244	PHE
1	A	247	GLU
1	A	251	LYS
1	A	252	ILE
1	A	253	LYS
1	A	255	LEU
1	A	260	ASN
1	A	265	LYS
1	A	268	GLN
1	A	276	LEU
1	A	278	LYS
1	A	279	GLN
1	A	280	VAL
1	A	292	GLU
1	A	294	TYR
1	A	295	THR
1	A	296	SER
1	A	301	LEU
1	A	311	ASN
1	A	323	LYS
1	A	328	PHE
1	A	371	LEU
1	A	374	LYS
1	A	383	ASP
1	A	401	GLN
1	A	405	ASP
1	A	410	VAL
1	A	414	LEU
1	A	419	ILE
1	A	422	VAL
1	A	432	SER
1	A	439	ASP
1	A	441	VAL
1	A	442	LEU
1	A	443	GLU
1	A	445	SER
1	A	446	LEU
1	A	447	LYS
1	A	450	ASP
1	A	464	LYS
1	A	465	SER
1	A	470	ILE

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Mol	Chain	Res	Type
1	A	480	THR
1	A	485	SER
1	A	498	LEU
1	A	500	VAL
1	A	512	THR
1	A	531	MET
1	A	535	ASP
1	A	536	LYS
1	A	538	LYS
1	A	540	THR
1	A	548	ARG
1	A	558	MET
1	A	567	GLN
1	A	568	LYS
1	A	570	ASP
1	A	571	LYS
1	A	573	ASP
1	A	577	ASN
1	A	603	MET
1	A	605	TYR
1	A	606	TYR
1	A	609	SER
1	A	611	ASP
1	A	612	ILE
1	A	622	LYS
1	A	623	LYS
1	A	629	LEU
1	A	664	LYS
1	A	665	ASP
1	A	666	ILE
1	A	678	TYR
1	A	680	VAL
1	A	681	SER
1	A	683	GLU
1	A	684	SER
1	A	690	VAL
1	A	691	ASP
1	A	727	LEU
1	A	730	GLU
1	A	738	LEU
1	A	748	ARG
1	A	753	LYS

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Mol	Chain	Res	Type
1	A	758	VAL
1	A	798	ILE
1	A	824	ASP
1	A	836	ARG
1	A	838	LEU
1	A	839	LEU
1	A	844	VAL
1	A	863	PHE
1	A	868	ILE
1	A	877	ASP
1	A	885	GLU
1	A	892	SER
1	A	897	LYS
1	A	916	GLU
1	A	921	VAL
1	A	932	LYS
1	A	934	SER
1	A	935	ARG
1	A	936	VAL
1	A	950	LEU
1	A	963	ASN
1	A	967	THR
1	A	977	THR
1	A	981	GLU
1	A	984	LYS
1	A	988	THR
1	A	989	GLN
1	A	996	ILE
1	A	1002	SER
1	A	1008	THR
1	A	1011	VAL
1	A	1017	LYS
1	A	1049	TYR
1	A	1050	LYS
1	A	1065	LEU
1	A	1067	SER
1	A	1074	ILE
1	A	1088	GLU
1	A	1092	THR
1	A	1101	LYS
1	A	1107	GLN
1	A	1108	GLN

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Mol	Chain	Res	Type
1	A	1111	ILE
1	A	1114	LEU
1	A	1125	SER
1	A	1130	LEU
1	A	1131	MET
1	A	1138	ARG
1	A	1139	ASN
1	A	1147	VAL
1	A	1151	ILE
1	A	1152	SER
1	A	1155	LYS
1	A	1157	SER
1	A	1160	ILE
1	A	1170	GLN
1	A	1187	ILE
1	A	1206	LEU
1	A	1210	LYS
1	A	1226	VAL
1	A	1227	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	28	GLN
1	A	33	ASN
1	A	73	ASN
1	A	157	ASN
1	A	177	ASN
1	A	203	GLN
1	A	256	ASN
1	A	401	GLN
1	A	449	ASN
1	A	577	ASN
1	A	607	ASN
1	A	630	ASN
1	A	861	ASN
1	A	888	GLN
1	A	906	GLN
1	A	933	ASN
1	A	1107	GLN
1	A	1139	ASN
1	A	1170	GLN

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Mol	Chain	Res	Type
1	A	1172	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	39/40 (97%)	15 (38%)	3 (7%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	13	A
2	G	14	A
2	G	16	U
2	G	17	G
2	G	20	G
2	G	23	C
2	G	27	U
2	G	28	C
2	G	29	C
2	G	30	A
2	G	31	G
2	G	32	U
2	G	34	A
2	G	35	A
2	G	36	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	28	C
2	G	29	C
2	G	34	A

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1208/1228 (98%)	1.32	282 (23%) 2 2	8, 57, 99, 141	0
2	G	40/40 (100%)	0.28	3 (7%) 20 17	12, 33, 97, 99	0
All	All	1248/1268 (98%)	1.29	285 (22%) 2 2	8, 56, 99, 141	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	VAL	8.4
1	A	228	VAL	7.6
1	A	229	LEU	7.6
1	A	166	ALA	6.4
1	A	216	VAL	6.3
1	A	62	ILE	5.9
1	A	280	VAL	5.7
1	A	1130	LEU	5.7
1	A	74	LEU	5.6
1	A	69	ILE	5.6
1	A	1099	PHE	5.4
1	A	101	LEU	5.4
1	A	1078	PRO	5.2
1	A	71	LEU	5.1
1	A	214	TYR	4.8
1	A	1044	GLU	4.7
1	A	222	GLY	4.7
1	A	1095	TYR	4.6
1	A	1068	TYR	4.5
1	A	66	LEU	4.4
1	A	534	TRP	4.4
1	A	173	PHE	4.4
1	A	102	ARG	4.3
1	A	236	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1085	ASP	4.3
1	A	1091	LEU	4.1
1	A	225	PHE	4.0
1	A	355	TRP	4.0
1	A	73	ASN	4.0
1	A	233	GLY	3.9
2	G	28	C	3.9
1	A	105	ILE	3.9
1	A	61	PHE	3.9
1	A	88	GLU	3.9
1	A	197	PHE	3.9
1	A	54	LEU	3.9
1	A	1077	ASN	3.8
1	A	474	PHE	3.8
1	A	127	ILE	3.8
1	A	279	GLN	3.8
1	A	131	PHE	3.8
1	A	172	ALA	3.7
1	A	226	ASN	3.7
1	A	275	PRO	3.7
1	A	368	ASP	3.7
1	A	219	PHE	3.7
1	A	148	THR	3.6
1	A	343	ALA	3.6
1	A	240	ILE	3.6
1	A	249	GLY	3.6
1	A	212	SER	3.5
1	A	193	VAL	3.5
1	A	1	MET	3.5
1	A	999	TRP	3.5
1	A	68	SER	3.5
1	A	163	SER	3.5
1	A	85	THR	3.5
1	A	607	ASN	3.4
1	A	177	ASN	3.4
1	A	641	ASP	3.4
1	A	256	ASN	3.4
1	A	1074	ILE	3.4
1	A	605	TYR	3.4
1	A	1147	VAL	3.3
1	A	152	THR	3.3
1	A	57	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	945	LYS	3.3
1	A	124	ILE	3.3
1	A	168	SER	3.3
1	A	276	LEU	3.2
1	A	87	THR	3.2
1	A	81	PHE	3.2
1	A	198	ASP	3.2
1	A	178	GLU	3.2
1	A	123	ILE	3.2
1	A	704	ILE	3.2
1	A	118	LEU	3.1
1	A	132	LEU	3.1
1	A	211	ASN	3.1
1	A	210	LEU	3.1
1	A	476	GLU	3.1
1	A	1092	THR	3.1
1	A	1171	GLU	3.1
1	A	109	PHE	3.1
1	A	160	ASN	3.1
1	A	204	GLU	3.1
1	A	192	LYS	3.1
1	A	146	GLY	3.1
1	A	113	GLU	3.1
1	A	273	PHE	3.0
1	A	140	LEU	3.0
1	A	58	TYR	3.0
1	A	115	TYR	3.0
1	A	654	ASP	3.0
1	A	686	SER	3.0
1	A	1043	PHE	3.0
1	A	536	LYS	3.0
1	A	213	ASP	3.0
1	A	566	LEU	3.0
1	A	36	LEU	3.0
1	A	95	GLU	3.0
1	A	235	ASP	2.9
1	A	684	SER	2.9
1	A	98	GLU	2.9
1	A	644	SER	2.9
1	A	1021	ILE	2.9
1	A	164	GLU	2.9
1	A	122	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	170	SER	2.9
1	A	38	VAL	2.9
1	A	585	LEU	2.9
1	A	353	GLY	2.9
1	A	709	PHE	2.8
1	A	138	ILE	2.8
1	A	1109	GLY	2.8
1	A	237	TYR	2.8
1	A	863	PHE	2.8
1	A	277	TYR	2.8
1	A	1033	ARG	2.8
1	A	1122	ALA	2.8
1	A	59	LEU	2.8
1	A	590	ASN	2.8
1	A	693	LEU	2.8
1	A	16	THR	2.8
1	A	248	SER	2.8
1	A	739	SER	2.8
1	A	119	PHE	2.7
1	A	126	THR	2.7
1	A	221	GLU	2.7
1	A	65	VAL	2.7
1	A	155	PHE	2.7
1	A	525	PHE	2.7
1	A	174	ARG	2.7
1	A	271	PRO	2.7
1	A	1076	ARG	2.7
1	A	171	ILE	2.7
1	A	255	LEU	2.7
1	A	112	ASN	2.7
1	A	537	ASP	2.7
1	A	128	LEU	2.7
1	A	524	TYR	2.7
1	A	181	THR	2.7
1	A	740	GLY	2.7
1	A	159	GLU	2.7
1	A	1114	LEU	2.7
1	A	114	GLY	2.6
1	A	94	LEU	2.6
1	A	217	GLU	2.6
1	A	1127	PHE	2.6
1	A	548	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	147	PHE	2.6
1	A	1106	TYR	2.6
1	A	194	ASP	2.6
1	A	478	LYS	2.6
1	A	562	TYR	2.6
1	A	1103	GLY	2.6
1	A	435	LEU	2.6
1	A	165	GLU	2.6
1	A	156	ASP	2.6
1	A	677	GLY	2.5
1	A	1042	LEU	2.5
1	A	245	VAL	2.5
1	A	612	ILE	2.5
1	A	86	ARG	2.5
1	A	84	LYS	2.5
1	A	480	THR	2.5
1	A	179	ASN	2.5
1	A	218	ASP	2.5
1	A	411	VAL	2.5
1	A	657	PHE	2.5
1	A	427	LYS	2.5
1	A	188	ASP	2.5
1	A	161	MET	2.5
1	A	111	GLY	2.5
1	A	153	GLY	2.5
1	A	1014	LEU	2.4
1	A	931	PHE	2.4
1	A	121	LYS	2.4
1	A	64	ASP	2.4
1	A	643	ILE	2.4
1	A	568	LYS	2.4
1	A	77	TYR	2.4
1	A	576	GLY	2.4
1	A	1094	ALA	2.4
1	A	135	LYS	2.4
1	A	39	GLU	2.4
1	A	96	ASN	2.3
1	A	175	CYS	2.3
1	A	224	PHE	2.3
1	A	625	ASP	2.3
2	G	29	C	2.3
1	A	985	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	687	LYS	2.3
1	A	533	GLY	2.3
1	A	227	PHE	2.3
1	A	400	LEU	2.3
1	A	649	TRP	2.3
1	A	100	ASN	2.3
1	A	436	PHE	2.3
1	A	983	PHE	2.3
1	A	406	ALA	2.3
1	A	492	LEU	2.3
1	A	145	ASN	2.3
1	A	151	PHE	2.3
1	A	220	PHE	2.3
1	A	45	GLU	2.3
1	A	1169	ALA	2.3
1	A	89	LYS	2.3
1	A	200	HIS	2.3
1	A	27	THR	2.3
1	A	799	PRO	2.3
1	A	139	ALA	2.2
1	A	157	ASN	2.2
1	A	732	ASN	2.2
1	A	699	LEU	2.2
1	A	1086	TRP	2.2
1	A	215	ASP	2.2
1	A	594	PRO	2.2
1	A	620	THR	2.2
1	A	1154	VAL	2.2
1	A	403	TYR	2.2
1	A	987	SER	2.2
1	A	349	LYS	2.2
1	A	130	GLU	2.2
1	A	150	ALA	2.2
1	A	1133	LEU	2.2
1	A	18	ARG	2.2
1	A	241	ILE	2.2
1	A	470	ILE	2.2
1	A	190	PHE	2.2
1	A	1115	LEU	2.2
1	A	696	GLU	2.2
1	A	1201	ALA	2.2
1	A	481	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	107	LYS	2.2
1	A	902	GLY	2.2
1	A	1159	GLY	2.2
1	A	162	PHE	2.2
1	A	745	PHE	2.2
1	A	556	ALA	2.2
1	A	356	ASN	2.1
1	A	1226	VAL	2.1
1	A	37	LEU	2.1
1	A	331	TYR	2.1
1	A	90	GLU	2.1
1	A	791	GLU	2.1
1	A	1104	ILE	2.1
1	A	230	THR	2.1
1	A	1016	THR	2.1
1	A	408	LEU	2.1
1	A	652	ALA	2.1
2	G	41	A	2.1
1	A	232	GLU	2.1
1	A	898	GLU	2.1
1	A	526	GLN	2.1
1	A	208	LYS	2.1
1	A	1041	ASP	2.1
1	A	125	GLU	2.1
1	A	234	ILE	2.1
1	A	294	TYR	2.1
1	A	578	TYR	2.1
1	A	626	MET	2.1
1	A	679	LYS	2.1
1	A	342	PRO	2.1
1	A	579	GLU	2.1
1	A	583	TYR	2.1
1	A	609	SER	2.0
1	A	780	SER	2.0
1	A	565	CYS	2.0
1	A	1090	CYS	2.0
1	A	80	LEU	2.0
1	A	1161	PHE	2.0
1	A	259	ILE	2.0
1	A	540	THR	2.0
1	A	563	ALA	2.0
1	A	223	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	267	LYS	2.0
1	A	60	SER	2.0
1	A	117	SER	2.0
1	A	1038	PRO	2.0
1	A	13	LEU	2.0
1	A	209	ILE	2.0
1	A	1039	GLU	2.0
1	A	1202	GLU	2.0
1	A	262	TYR	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
3	MG	A	1301	1/1	-	-	19,19,19,19	1
3	MG	G	101	1/1	-	-	11,11,11,11	1

6.5 Other polymers [i](#)

There are no such residues in this entry.