Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2024 – 04:12 PM JST

PDB ID	:	8Y03
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:

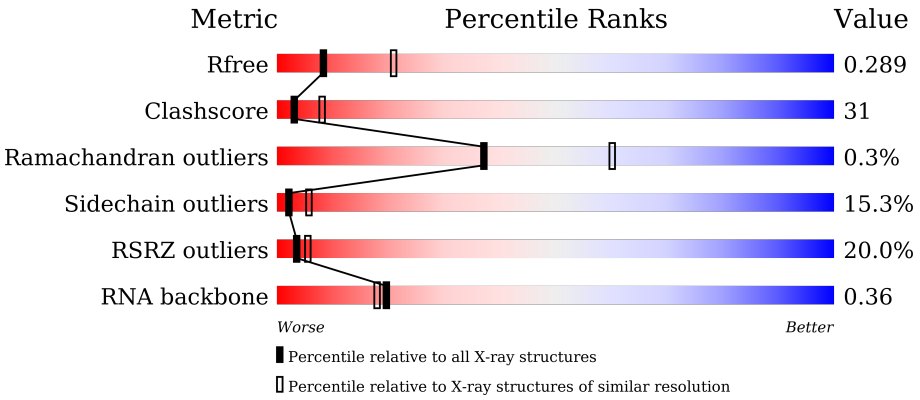
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)
RNA backbone	3690	1105 (3.18-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	1228	20% 58% 32% 8%
2	G	40	8% 28% 42% 22% 8%

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 (three-letter code: MG) (formula: Mg).

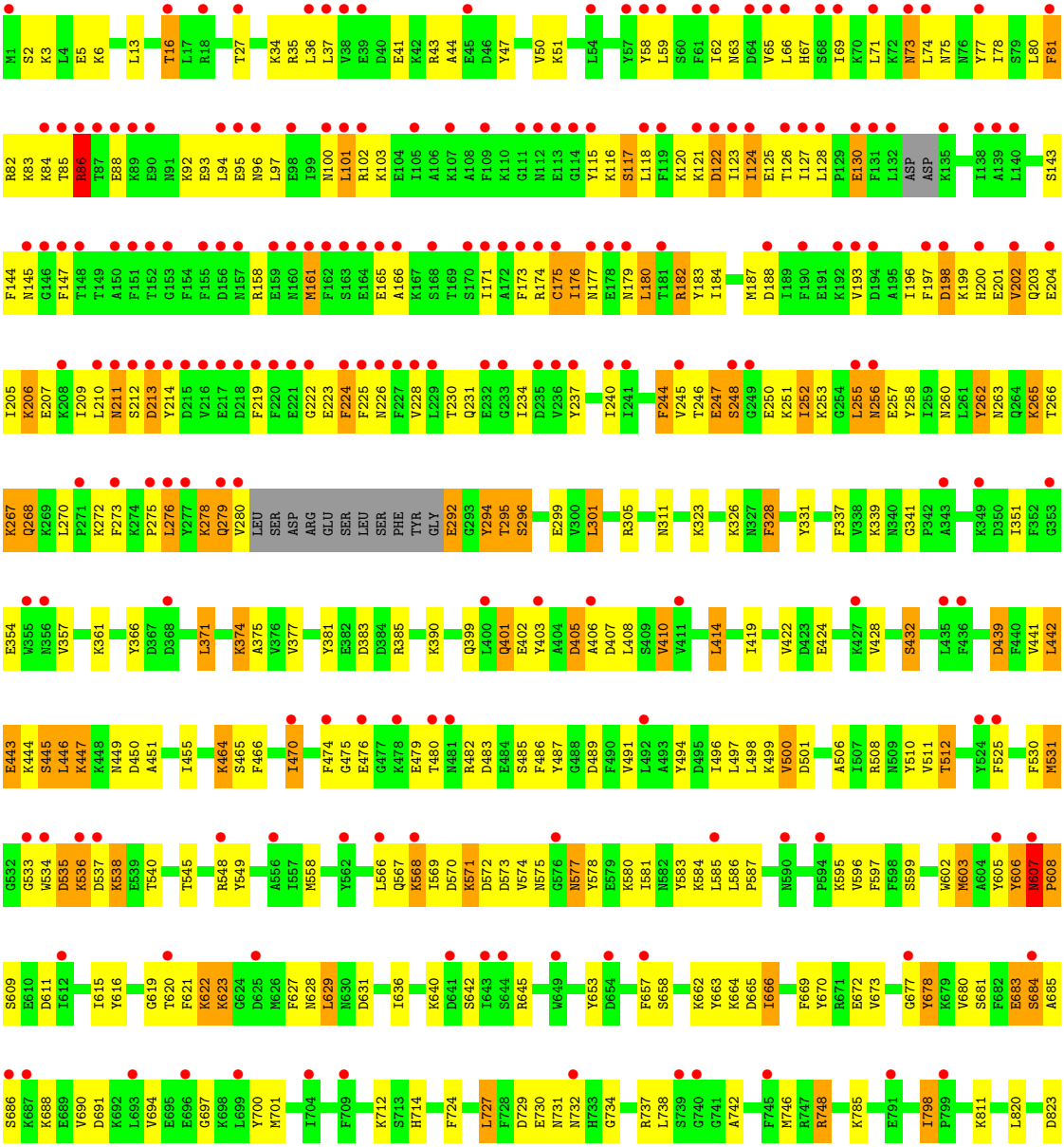
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	1	0
			1	1		
3	G	1	Total	Mg	1	0
			1	1		

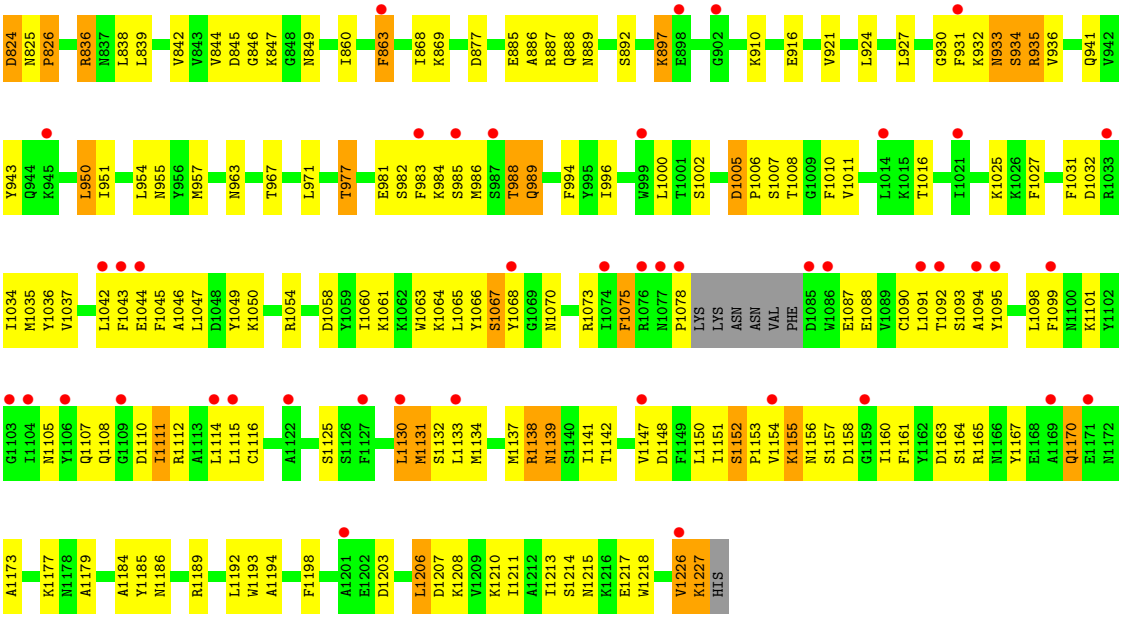
3 Residue-property plots (i)

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

- Molecule 1: LbCas12a

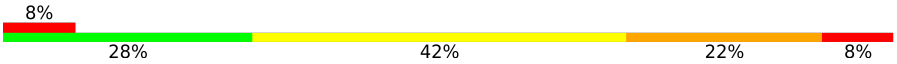
Chain A:

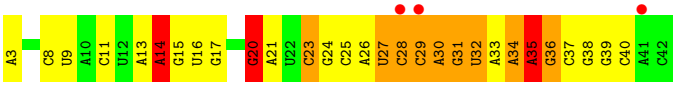




- Molecule 2: RNA (41-MER)

Chain G:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	1752 reflections (4.91%)	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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.48	3/10122 (0.0%)	0.64	7/13600 (0.1%)
2	G	0.82	2/950 (0.2%)	1.33	13/1477 (0.9%)
All	All	0.52	5/11072 (0.0%)	0.74	20/15077 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	14	A	N9-C4	-5.86	1.34	1.37
1	A	1006	PRO	N-CD	5.24	1.55	1.47
1	A	826	PRO	N-CD	5.20	1.55	1.47
2	G	35	A	O3'-P	-5.05	1.55	1.61
1	A	608	PRO	N-CD	5.01	1.54	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	14	A	C2-N3-C4	-8.06	106.57	110.60
1	A	267	LYS	N-CA-C	-7.96	89.50	111.00
2	G	15	G	N1-C6-O6	-7.15	115.61	119.90
2	G	20	G	C8-N9-C4	-7.15	103.54	106.40
2	G	14	A	N1-C6-N6	7.06	122.84	118.60
1	A	202	VAL	N-CA-C	6.61	128.83	111.00
1	A	202	VAL	CB-CA-C	-6.34	99.35	111.40
2	G	20	G	O5'-P-OP1	-6.20	100.12	105.70
2	G	14	A	C5-N7-C8	-6.18	100.81	103.90
1	A	1078	PRO	N-CA-CB	6.08	110.60	103.30
2	G	9	U	C5-C6-N1	-6.07	119.67	122.70
2	G	11	C	O5'-P-OP2	-5.92	100.37	105.70
1	A	607	ASN	C-N-CD	5.79	140.56	128.40
2	G	14	A	C4-C5-N7	5.77	113.58	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	9	U	N1-C2-N3	5.74	118.34	114.90
1	A	825	ASN	C-N-CD	5.59	140.13	128.40
1	A	1005	ASP	C-N-CD	5.43	139.80	128.40
2	G	20	G	N7-C8-N9	5.19	115.70	113.10
2	G	20	G	C5'-C4'-C3'	-5.11	107.82	116.00
2	G	8	C	C5-C4-N4	5.02	123.71	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9918	0	9825	588	0
2	G	850	0	431	81	0
3	A	1	0	0	0	0
3	G	1	0	0	0	0
All	All	10770	0	10256	647	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 (647) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:85:THR:HG23	1:A:86:ARG:N	1.65	1.11
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:746:MET:HE3	1:A:748:ARG:HD3	1.27	1.08
1:A:201:GLU:O	1:A:206:LYS:NZ	1.88	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
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:746:MET:HE1	1:A:748:ARG:CD	1.90	1.01
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:746:MET:HE1	1:A:748:ARG:HD2	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:577:ASN:ND2	1:A:685:ALA:C	2.19	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:530:PHE:CE2	1:A:531:MET:HE2	2.03	0.93
1:A:77:TYR:HH	1:A:81:PHE:HE1	1.00	0.93
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:390:LYS:HZ2	2:G:32:U:H4'	1.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:NH2	1:A:491:VAL:HG11	1.91	0.86
1:A:1095:TYR:O	1:A:1099:PHE:CD2	2.28	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:205:ILE:CG2	1:A:252:ILE:HD13	2.04	0.84
1:A:951:ILE:HD11	1:A:986:MET:HE3	1.58	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:A:H2'	2:G:30:A:N3	1.98	0.78
1:A:577:ASN:ND2	1:A:685:ALA:O	2.17	0.77
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:231:GLN:HB2	1:A:278:LYS:HZ2	1.51	0.75
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:1110:ASP:CG	1:A:1112:ARG:HH21	1.90	0.75
1:A:577:ASN:ND2	1:A:686:SER:N	2.35	0.75
1:A:577:ASN:ND2	1:A:686:SER:CA	2.50	0.75
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: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: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
2:G:36:G:H8	2:G:36:G:H5"	1.54	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:3:LYS:HZ2	1:A:820:LEU:HD23	1.55	0.71
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:1131:MET:HE3	1:A:1134:MET:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ASP:HB3	1:A:583:TYR:C	2.12	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: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:361:LYS:NZ	1:A:403:TYR:O	2.21	0.68
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
1:A:1107:GLN:C	1:A:1108:GLN:OE1	2.32	0.68
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: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:1010:PHE:HD2	1:A:1137:MET:HE2	1.59	0.66
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: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:951:ILE:CD1	1:A:986:MET:HE3	2.26	0.64
1:A:50:VAL:HG21	1:A:144:PHE:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:951:ILE:HD11	1:A:986:MET:CE	2.29	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
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:1010:PHE:CD2	1:A:1137:MET:HE2	2.35	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: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: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: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:3:LYS:NZ	1:A:820:LEU:HD23	2.16	0.60
1:A:530:PHE:CZ	1:A:531:MET:HE2	2.37	0.60
1:A:1035:MET:CE	1:A:1037:VAL:HG12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:933:ASN:HD22	1:A:933:ASN:C	2.03	0.59
1:A:3:LYS:CE	1:A:823:ASP:CB	2.81	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:1138:ARG:HH11	1:A:1148:ASP:CG	2.06	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
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: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:1035:MET:HE2	1:A:1037:VAL:HG12	1.85	0.57
1:A:954:LEU:HG	1:A:957:MET:HE3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:14:A:H8	2:G:14:A:H5"	1.71	0.56
1:A:530:PHE:CZ	1:A:531:MET:CE	2.88	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:245:VAL:HG13	1:A:246:THR:N	2.21	0.56
1:A:533:GLY:HA3	1:A:536:LYS:HD2	1.86	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
1:A:1108:GLN:O	1:A:1111:ILE:HG22	2.06	0.55
1:A:1131:MET:HE3	1:A:1134:MET:HE2	1.88	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
1:A:1131:MET:CE	1:A:1134:MET:CE	2.84	0.55
2:G:33:A:C2'	2:G:34:A:C5'	2.85	0.55
1:A:585:LEU:HD12	1:A:678:TYR:HB2	1.88	0.54
1:A:1067:SER:HG	1:A:1095:TYR:HD2	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:951:ILE:CD1	1:A:986:MET:CE	2.86	0.53
1:A:361:LYS:HZ3	1:A:403:TYR:HB3	1.73	0.53
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:1131:MET:CE	1:A:1134:MET:HE1	2.39	0.53
1:A:1073:ARG:NH2	1:A:1075:PHE:CG	2.74	0.53
1:A:3:LYS:HE3	1:A:823:ASP:CG	2.27	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
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: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:954:LEU:CD1	1:A:957:MET:HE2	2.40	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: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:161:MET:HE2	1:A:280:VAL:HG12	1.91	0.51
1:A:930:GLY:CA	2:G:31:G:H21	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HG22	1:A:252:ILE:CG1	2.36	0.51
1:A:1131:MET:HE1	1:A:1134:MET:HE1	1.92	0.51
1:A:244:PHE:HB3	1:A:252:ILE:CG2	2.39	0.51
1:A:1138:ARG:NH1	1:A:1148:ASP:CG	2.59	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:954:LEU:HG	1:A:957:MET:CE	2.40	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:1010:PHE:CD2	1:A:1137:MET:CE	2.93	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:77:TYR:CE2	1:A:81:PHE:CD1	2.98	0.50
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: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:407:ASP:C	1:A:408:LEU:HD12	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:G:33:A:H2'	2:G:34:A:H5"	1.95	0.48
1:A:184:ILE:HA	1:A:187:MET:HE3	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: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:1070:ASN:OD1	1:A:1070:ASN:N	2.45	0.48
1:A:183:TYR:CZ	1:A:219:PHE:O	2.67	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:1214:SER:O	1:A:1215:ASN:C	2.48	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:161:MET:CE	1:A:280:VAL:HG12	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:C	1:A:246:THR:HG1	1.99	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:954:LEU:HD12	1:A:957:MET:HE2	1.96	0.47
1:A:202:VAL:HG13	1:A:203:GLN:N	2.30	0.47
1:A:262:TYR:C	1:A:268:GLN:HE21	2.17	0.47
1:A:182:ARG:HH21	1:A:491:VAL:CG1	2.20	0.47
1:A:535:ASP:CB	1:A:583:TYR:C	2.83	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:337:PHE:CD1	1:A:479:GLU:OE1	2.66	0.46
1:A:1000:LEU:HD22	1:A:1011:VAL:HG21	1.97	0.46
1:A:442:LEU:HD22	1:A:444:LYS:O	2.16	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:3:LYS:HZ3	1:A:820:LEU:HA	1.81	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:252:ILE:HD12	1:A:252:ILE:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:199:LYS:C	1:A:202:VAL:HG12	2.37	0.45
1:A:1010:PHE:HD2	1:A:1137:MET:CE	2.28	0.45
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: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:202:VAL:C	1:A:206:LYS:HZ2	2.21	0.44
1:A:1035:MET:HE1	1:A:1037:VAL:HG12	2.00	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:475:GLY:O	1:A:476:GLU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:531:MET:HE2	1:A:531:MET:HB2	1.70	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: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:658:SER:OG	1:A:672:GLU:OE2	2.35	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
1:A:428:VAL:O	1:A:432:SER:OG	2.34	0.42
2:G:30:A:C4	2:G:33:A:C2	3.07	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:494:TYR:CD2	1:A:494:TYR:C	2.92	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:84:LYS:HD2	1:A:84:LYS:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:933:ASN:C	1:A:933:ASN:ND2	2.73	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:184:ILE:HG23	1:A:187:MET:HE3	2.02	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
1:A:323:LYS:HB3	1:A:323:LYS:HE2	1.83	0.42
1:A:666:ILE:HD13	1:A:666:ILE:C	2.39	0.42
1:A:572:ASP:CG	1:A:574:VAL:HG12	2.39	0.41
1:A:1192:LEU:HD23	1:A:1192:LEU:HA	1.78	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
1:A:1137:MET:HE2	1:A:1153:PRO:HD2	2.03	0.41
1:A:1160:ILE:HG23	1:A:1160:ILE:O	2.20	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:203:GLN:NE2	1:A:204:GLU:HG2	2.18	0.41
1:A:390:LYS:HZ2	2:G:32:U:C4'	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
1:A:85:THR:C	1:A:86:ARG:HG3	2.39	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:1206:LEU:HD12	1:A:1206:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:845:ASP:C	1:A:847:LYS:H	2.25	0.40
1:A:530:PHE:CE2	1:A:531:MET:HE1	2.51	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%)	37 60

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%)	915 (85%)	165 (15%)	2 6

All (165) 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	35	ARG
1	A	37	LEU
1	A	59	LEU
1	A	71	LEU
1	A	73	ASN
1	A	81	PHE
1	A	86	ARG
1	A	88	GLU
1	A	93	GLU
1	A	94	LEU
1	A	101	LEU
1	A	116	LYS
1	A	117	SER
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

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Mol	Chain	Res	Type
1	A	175	CYS
1	A	176	ILE
1	A	180	LEU
1	A	182	ARG
1	A	198	ASP
1	A	206	LYS
1	A	211	ASN
1	A	213	ASP
1	A	224	PHE
1	A	226	ASN
1	A	228	VAL
1	A	244	PHE
1	A	247	GLU
1	A	251	LYS
1	A	252	ILE
1	A	255	LEU
1	A	256	ASN
1	A	257	GLU
1	A	260	ASN
1	A	262	TYR
1	A	265	LYS
1	A	268	GLN
1	A	276	LEU
1	A	278	LYS
1	A	279	GLN
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	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	422	VAL
1	A	432	SER
1	A	439	ASP

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Mol	Chain	Res	Type
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
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	537	ASP
1	A	538	LYS
1	A	540	THR
1	A	548	ARG
1	A	558	MET
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	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

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Mol	Chain	Res	Type
1	A	684	SER
1	A	691	ASP
1	A	727	LEU
1	A	730	GLU
1	A	738	LEU
1	A	748	ARG
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	877	ASP
1	A	885	GLU
1	A	887	ARG
1	A	888	GLN
1	A	892	SER
1	A	897	LYS
1	A	916	GLU
1	A	921	VAL
1	A	932	LYS
1	A	933	ASN
1	A	934	SER
1	A	935	ARG
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	1002	SER
1	A	1008	THR
1	A	1049	TYR
1	A	1050	LYS
1	A	1065	LEU
1	A	1067	SER
1	A	1075	PHE
1	A	1088	GLU
1	A	1101	LYS

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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	1152	SER
1	A	1155	LYS
1	A	1157	SER
1	A	1170	GLN
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	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	906	GLN
1	A	933	ASN
1	A	989	GLN
1	A	1139	ASN
1	A	1170	GLN
1	A	1172	ASN

5.3.3 RNA (i)

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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1208/1228 (98%)	1.20	247 (20%) 3 5	8, 57, 99, 141	0
2	G	40/40 (100%)	0.33	3 (7%) 22 22	12, 33, 97, 99	0
All	All	1248/1268 (98%)	1.17	250 (20%) 3 5	8, 56, 99, 141	0

All (250) 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	7.5
1	A	166	ALA	6.3
1	A	216	VAL	6.3
1	A	62	ILE	5.8
1	A	280	VAL	5.6
1	A	1130	LEU	5.6
1	A	69	ILE	5.5
1	A	74	LEU	5.5
1	A	1099	PHE	5.3
1	A	101	LEU	5.3
1	A	1078	PRO	5.1
1	A	71	LEU	5.0
1	A	1044	GLU	4.7
1	A	214	TYR	4.7
1	A	222	GLY	4.6
1	A	1095	TYR	4.5
1	A	1068	TYR	4.4
1	A	66	LEU	4.3
1	A	102	ARG	4.3
1	A	236	VAL	4.2
1	A	534	TRP	4.2
1	A	173	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1085	ASP	4.2
2	G	28	C	4.1
1	A	1091	LEU	4.0
1	A	73	ASN	3.9
1	A	88	GLU	3.9
1	A	225	PHE	3.9
1	A	355	TRP	3.9
1	A	105	ILE	3.8
1	A	233	GLY	3.8
1	A	54	LEU	3.8
1	A	1077	ASN	3.8
1	A	61	PHE	3.8
1	A	197	PHE	3.8
1	A	279	GLN	3.7
1	A	127	ILE	3.7
1	A	474	PHE	3.7
1	A	172	ALA	3.7
1	A	226	ASN	3.6
1	A	131	PHE	3.6
1	A	368	ASP	3.6
1	A	275	PRO	3.6
1	A	219	PHE	3.5
1	A	148	THR	3.5
1	A	343	ALA	3.5
1	A	240	ILE	3.5
1	A	212	SER	3.5
1	A	193	VAL	3.4
1	A	249	GLY	3.4
1	A	1	MET	3.4
1	A	68	SER	3.4
1	A	163	SER	3.4
1	A	85	THR	3.4
1	A	999	TRP	3.4
1	A	607	ASN	3.4
1	A	177	ASN	3.3
1	A	256	ASN	3.3
1	A	641	ASP	3.3
1	A	945	LYS	3.3
1	A	1074	ILE	3.3
1	A	1147	VAL	3.3
1	A	152	THR	3.2
1	A	605	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	57	TYR	3.2
1	A	124	ILE	3.2
1	A	168	SER	3.2
1	A	87	THR	3.1
1	A	178	GLU	3.1
1	A	276	LEU	3.1
1	A	198	ASP	3.1
1	A	123	ILE	3.1
1	A	211	ASN	3.1
1	A	81	PHE	3.1
1	A	476	GLU	3.1
1	A	1171	GLU	3.1
1	A	704	ILE	3.1
1	A	204	GLU	3.0
1	A	118	LEU	3.0
1	A	132	LEU	3.0
1	A	192	LYS	3.0
1	A	160	ASN	3.0
1	A	1092	THR	3.0
1	A	113	GLU	3.0
1	A	210	LEU	3.0
1	A	109	PHE	2.9
1	A	146	GLY	2.9
1	A	536	LYS	2.9
1	A	686	SER	2.9
1	A	654	ASP	2.9
1	A	140	LEU	2.9
1	A	95	GLU	2.9
1	A	273	PHE	2.9
1	A	213	ASP	2.9
1	A	58	TYR	2.9
1	A	115	TYR	2.9
1	A	566	LEU	2.9
1	A	98	GLU	2.9
1	A	1043	PHE	2.8
1	A	36	LEU	2.8
1	A	684	SER	2.8
1	A	235	ASP	2.8
1	A	164	GLU	2.8
1	A	644	SER	2.8
1	A	1021	ILE	2.8
1	A	170	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	2.8
1	A	122	ASP	2.8
1	A	585	LEU	2.8
1	A	353	GLY	2.8
1	A	1033	ARG	2.7
1	A	138	ILE	2.7
1	A	1109	GLY	2.7
1	A	590	ASN	2.7
1	A	1122	ALA	2.7
1	A	709	PHE	2.7
1	A	237	TYR	2.7
1	A	59	LEU	2.7
1	A	863	PHE	2.7
1	A	221	GLU	2.7
1	A	248	SER	2.7
1	A	739	SER	2.7
1	A	16	THR	2.7
1	A	277	TYR	2.7
1	A	174	ARG	2.6
1	A	1076	ARG	2.6
1	A	693	LEU	2.6
1	A	126	THR	2.6
1	A	65	VAL	2.6
1	A	119	PHE	2.6
1	A	171	ILE	2.6
1	A	112	ASN	2.6
1	A	159	GLU	2.6
1	A	271	PRO	2.6
1	A	537	ASP	2.6
1	A	255	LEU	2.6
1	A	155	PHE	2.6
1	A	525	PHE	2.6
1	A	217	GLU	2.6
1	A	548	ARG	2.6
1	A	181	THR	2.6
1	A	128	LEU	2.6
1	A	740	GLY	2.5
1	A	524	TYR	2.5
1	A	1114	LEU	2.5
1	A	114	GLY	2.5
1	A	94	LEU	2.5
1	A	478	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLU	2.5
1	A	1127	PHE	2.5
1	A	194	ASP	2.5
1	A	86	ARG	2.5
1	A	147	PHE	2.5
1	A	1106	TYR	2.5
1	A	84	LYS	2.4
1	A	156	ASP	2.4
1	A	1103	GLY	2.4
1	A	435	LEU	2.4
1	A	245	VAL	2.4
1	A	612	ILE	2.4
1	A	562	TYR	2.4
2	G	29	C	2.4
1	A	677	GLY	2.4
1	A	1042	LEU	2.4
1	A	179	ASN	2.4
1	A	427	LYS	2.4
1	A	480	THR	2.4
1	A	218	ASP	2.4
1	A	411	VAL	2.4
1	A	188	ASP	2.4
1	A	121	LYS	2.4
1	A	161	MET	2.3
1	A	111	GLY	2.3
1	A	153	GLY	2.3
1	A	568	LYS	2.3
1	A	657	PHE	2.3
1	A	1014	LEU	2.3
1	A	643	ILE	2.3
1	A	64	ASP	2.3
1	A	135	LYS	2.3
1	A	39	GLU	2.3
1	A	931	PHE	2.3
1	A	1094	ALA	2.3
1	A	77	TYR	2.3
1	A	576	GLY	2.3
1	A	687	LYS	2.3
1	A	96	ASN	2.2
1	A	625	ASP	2.2
1	A	985	SER	2.2
1	A	533	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	100	ASN	2.2
1	A	224	PHE	2.2
1	A	175	CYS	2.2
1	A	406	ALA	2.2
1	A	45	GLU	2.2
1	A	400	LEU	2.2
1	A	89	LYS	2.2
2	G	41	A	2.2
1	A	145	ASN	2.2
1	A	227	PHE	2.2
1	A	1169	ALA	2.2
1	A	492	LEU	2.2
1	A	649	TRP	2.2
1	A	27	THR	2.1
1	A	200	HIS	2.1
1	A	436	PHE	2.1
1	A	983	PHE	2.1
1	A	139	ALA	2.1
1	A	157	ASN	2.1
1	A	732	ASN	2.1
1	A	799	PRO	2.1
1	A	18	ARG	2.1
1	A	151	PHE	2.1
1	A	220	PHE	2.1
1	A	349	LYS	2.1
1	A	699	LEU	2.1
1	A	130	GLU	2.1
1	A	1154	VAL	2.1
1	A	215	ASP	2.1
1	A	620	THR	2.1
1	A	987	SER	2.1
1	A	150	ALA	2.1
1	A	696	GLU	2.1
1	A	594	PRO	2.1
1	A	1086	TRP	2.1
1	A	241	ILE	2.1
1	A	470	ILE	2.1
1	A	107	LYS	2.1
1	A	1133	LEU	2.1
1	A	1201	ALA	2.1
1	A	403	TYR	2.1
1	A	481	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1115	LEU	2.0
1	A	556	ALA	2.0
1	A	90	GLU	2.0
1	A	791	GLU	2.0
1	A	356	ASN	2.0
1	A	1226	VAL	2.0
1	A	190	PHE	2.0
1	A	902	GLY	2.0
1	A	1159	GLY	2.0
1	A	232	GLU	2.0
1	A	898	GLU	2.0
1	A	1104	ILE	2.0
1	A	208	LYS	2.0
1	A	37	LEU	2.0
1	A	162	PHE	2.0
1	A	745	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.