



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:48 PM JST

PDB ID : 8KAG / pdb_00008kag
Title : Crystal structure of SpyCas9 in complex with sgRNA and target RNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.88 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)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

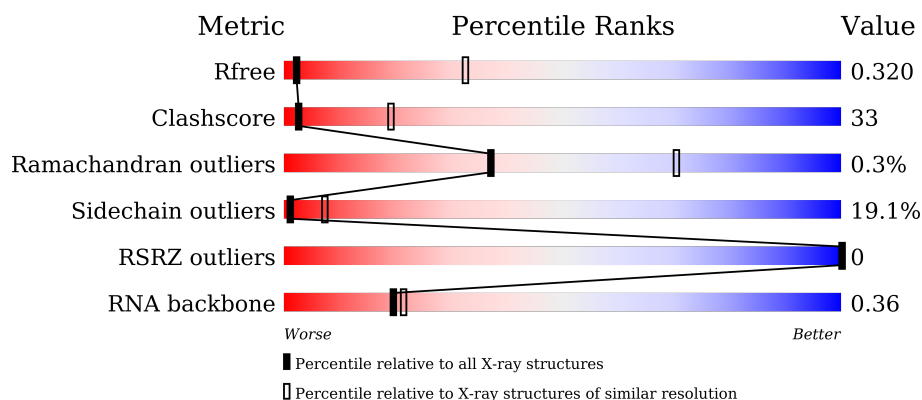
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


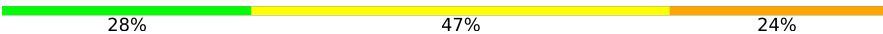
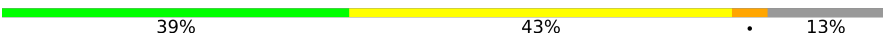
The reported resolution of this entry is 3.88 Å.

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	1075 (4.06-3.70)
Clashscore	180529	1137 (4.06-3.70)
Ramachandran outliers	177936	1094 (4.06-3.70)
Sidechain outliers	177891	1087 (4.06-3.70)
RSRZ outliers	164620	1075 (4.06-3.70)
RNA backbone	3690	1135 (4.76-3.00)

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	B	1368	 40% 46% 11% .
2	A	98	 28% 47% 24% .
3	C	23	 39% 43% . 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13444 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1346	Total	C	N	O	S	0	0	0
			10926	6963	1889	2051	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called RNA (98-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	98	Total	C	N	O	P	0	0	0
			2095	937	377	683	98			

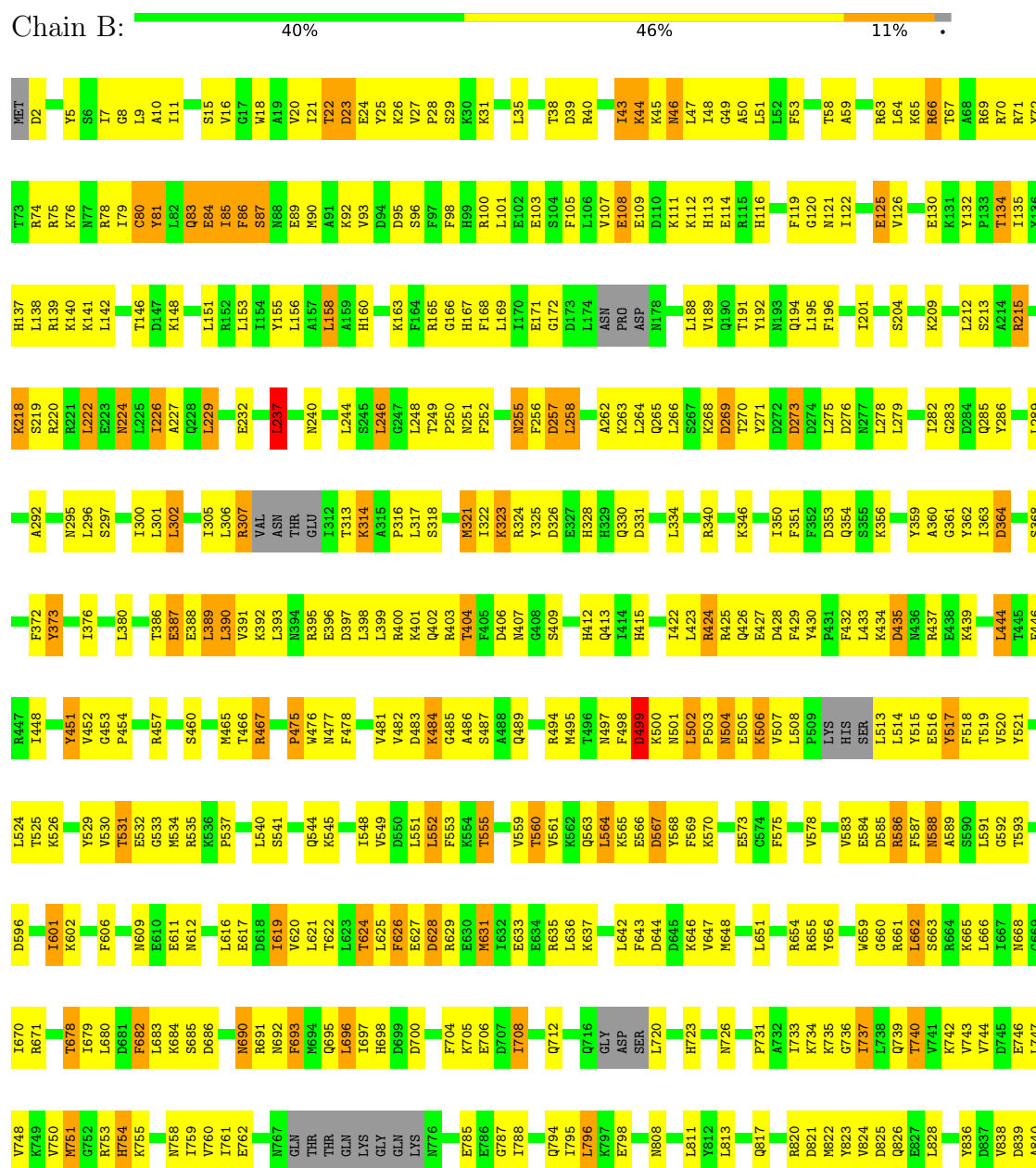
- Molecule 3 is a RNA chain called RNA (5'-R(*CP*CP*AP*CP*UP*UP*CP*AP*AP*UP*UP*AP*GP*AP*AP*CP*AP*CP*GP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	P	0	0	0
			423	190	76	137	20			

3 Residue-property plots

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

• Molecule 1: CRISPR-associated endonuclease Cas9/Csn1





A68	A69	U72	G73	A74	A75	A76	A77	G81	G82	C83	A84	C85	C86	G87	A88	G89	U90	C91	G92	G93	U94	G95	C96	U97	C98
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- Molecule 3: RNA (5'-R(*CP*CP*AP*CP*UP*UP*CP*AP*AP*UP*UP*AP*GP*AP*AP*CP*AP*CP*GP*GP*AP*CP*C)-3')

C	C	A	C1	U2	U3	C4	A5	A6	U7	U8	A9	G10	A11	A12	C13	C20
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.68Å 185.68Å 137.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.92 – 3.88 49.92 – 3.88	Depositor EDS
% Data completeness (in resolution range)	79.6 (49.92-3.88) 79.6 (49.92-3.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.303 , 0.320 0.303 , 0.320	Depositor DCC
R_{free} test set	958 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.927	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.189 for -h,-k,l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	13444	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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

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	B	0.38	0/11116	0.61	4/14945 (0.0%)
2	A	0.41	0/2345	1.02	9/3653 (0.2%)
3	C	0.34	0/472	0.99	1/732 (0.1%)
All	All	0.39	0/13933	0.72	14/19330 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1303	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	A	62	G	N3-C4-C5	6.23	131.71	128.60
2	A	89	G	C5-C6-O6	-6.22	124.87	128.60
2	A	89	G	N9-C4-C5	-6.06	102.97	105.40
2	A	89	G	C6-C5-N7	-5.87	126.88	130.40
3	C	2	U	C5-C6-N1	5.79	125.60	122.70
2	A	89	G	N1-C6-O6	5.59	123.25	119.90
2	A	62	G	N3-C4-N9	-5.53	122.68	126.00
2	A	89	G	C4-C5-N7	5.45	112.98	110.80
1	B	237	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	499	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	A	89	G	N3-C4-N9	5.13	129.08	126.00
2	A	10	U	C5-C6-N1	5.09	125.25	122.70
1	B	1122	ARG	NE-CZ-NH2	5.05	122.82	120.30

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	B	10926	0	11019	789	1
2	A	2095	0	1052	106	0
3	C	423	0	217	13	0
All	All	13444	0	12288	843	1

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 33.

All (843) 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:B:1218:GLY:HA2	1:B:1339:THR:N	1.68	1.08
1:B:1218:GLY:H	1:B:1339:THR:HG23	1.19	1.01
1:B:1142:SER:OG	1:B:1214:LEU:HD11	1.58	1.01
1:B:668:ASN:HA	1:B:678:THR:HG21	1.45	0.98
1:B:748:VAL:HB	1:B:753:ARG:HA	1.45	0.94
1:B:861:ASP:OD1	1:B:861:ASP:N	2.01	0.93
1:B:1218:GLY:HA2	1:B:1338:SER:C	1.88	0.93
1:B:1045:PHE:O	1:B:1076:LYS:NZ	2.03	0.92
1:B:876:VAL:HG11	1:B:904:GLU:HB2	1.52	0.92
1:B:400:ARG:NH2	1:B:406:ASP:OD2	2.03	0.91
1:B:83:GLN:NE2	1:B:155:TYR:OH	2.03	0.91
1:B:865:GLY:HA3	1:B:872:SER:HB3	1.50	0.91
1:B:1074:TRP:HE1	1:B:1080:PHE:HE1	1.15	0.90
1:B:1215:ALA:HB3	1:B:1219:GLU:O	1.74	0.87
1:B:917:ILE:HB	1:B:921:LEU:HD12	1.56	0.87
1:B:460:SER:HB2	2:A:61:C:H5'	1.56	0.86
1:B:1218:GLY:N	1:B:1339:THR:HG23	1.90	0.86
1:B:1218:GLY:HA2	1:B:1338:SER:CA	2.07	0.85
1:B:988:TYR:CE2	1:B:1086:VAL:HG11	2.11	0.85
1:B:1000:LYS:HB2	1:B:1073:VAL:HG11	1.59	0.85
1:B:172:GLY:O	1:B:413:GLN:NE2	2.09	0.84
1:B:373:TYR:OH	1:B:398:LEU:O	1.93	0.84
1:B:508:LEU:HD12	1:B:515:TYR:HB2	1.60	0.84
1:B:1110:ILE:HD12	1:B:1122:ARG:HE	1.42	0.84
1:B:391:VAL:HG12	1:B:395:ARG:HH22	1.44	0.82
1:B:917:ILE:O	1:B:921:LEU:N	2.12	0.82
1:B:682:PHE:HD2	1:B:696:LEU:HD11	1.43	0.82
1:B:1123:LYS:HG2	2:A:52:A:H5''	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:NH1	2:A:40:C:OP1	2.13	0.81
1:B:362:TYR:HB2	1:B:372:PHE:HB2	1.63	0.81
1:B:507:VAL:HG21	1:B:659:TRP:HB3	1.62	0.81
1:B:1218:GLY:CA	1:B:1338:SER:HA	2.10	0.81
1:B:218:LYS:HB3	1:B:246:LEU:HD13	1.62	0.80
1:B:700:ASP:OD1	1:B:705:LYS:NZ	2.15	0.79
1:B:305:ILE:HD11	1:B:324:ARG:HH21	1.46	0.79
1:B:1120:ILE:HD11	1:B:1137:PRO:HB3	1.62	0.79
1:B:499:ASP:HB3	1:B:502:LEU:H	1.48	0.79
1:B:1140:ALA:HB3	1:B:1171:ARG:HD2	1.64	0.78
1:B:1281:ILE:HG12	1:B:1283:ALA:H	1.47	0.78
1:B:1101:GLN:HB2	1:B:1140:ALA:HA	1.64	0.78
1:B:1062:LEU:O	1:B:1076:LYS:HG2	1.84	0.78
1:B:1094:ILE:HG13	1:B:1225:GLU:OE1	1.84	0.78
1:B:1268:GLU:O	1:B:1272:GLN:N	2.15	0.78
1:B:1269:ILE:HA	1:B:1272:GLN:HB2	1.65	0.78
1:B:1218:GLY:HA2	1:B:1339:THR:H	1.46	0.77
1:B:201:ILE:HG23	1:B:229:LEU:HD11	1.64	0.77
1:B:914:ALA:HA	1:B:917:ILE:HD11	1.66	0.77
1:B:1353:THR:HG23	1:B:1355:LEU:H	1.48	0.77
1:B:842:VAL:H	1:B:854:ASN:HD21	1.30	0.77
1:B:38:THR:HG21	1:B:1359:ARG:HG2	1.67	0.77
1:B:551:LEU:O	1:B:555:THR:OG1	2.02	0.76
1:B:1218:GLY:CA	1:B:1338:SER:CA	2.63	0.76
1:B:720:LEU:HD21	1:B:938:ARG:HD2	1.68	0.76
1:B:404:THR:N	1:B:407:ASN:OD1	2.16	0.76
1:B:843:PRO:HB3	1:B:1053:ALA:HA	1.66	0.76
1:B:934:ILE:O	1:B:938:ARG:N	2.19	0.76
1:B:516:GLU:O	1:B:520:VAL:HG23	1.86	0.76
1:B:1215:ALA:HB1	1:B:1219:GLU:HB3	1.68	0.75
1:B:83:GLN:O	1:B:87:SER:N	2.20	0.75
1:B:1250:GLU:O	1:B:1254:GLN:NE2	2.20	0.75
1:B:50:ALA:HB2	1:B:984:ALA:HB2	1.69	0.74
1:B:1232:TYR:CG	1:B:1269:ILE:HD11	2.20	0.74
1:B:1272:GLN:NE2	2:A:89:G:O6	2.20	0.74
1:B:1269:ILE:O	1:B:1273:ILE:N	2.18	0.74
1:B:966:PHE:HB2	1:B:1043:MET:SD	2.28	0.74
1:B:583:VAL:HG11	1:B:587:PHE:HE1	1.52	0.74
1:B:20:VAL:HB	1:B:47:LEU:HD23	1.70	0.74
1:B:1218:GLY:O	1:B:1337:THR:C	2.27	0.73
1:B:1206:LEU:HG	1:B:1345:ALA:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1222:LYS:NZ	1:B:1317:ASN:O	2.16	0.73
1:B:148:LYS:HD2	1:B:429:PHE:CD1	2.23	0.73
1:B:1297:HIS:O	1:B:1305:GLN:NE2	2.22	0.73
1:B:1074:TRP:NE1	1:B:1080:PHE:HE1	1.87	0.73
1:B:116:HIS:HE2	1:B:122:ILE:HD12	1.52	0.72
1:B:1298:ARG:HH21	1:B:1299:ASP:HA	1.55	0.72
1:B:1215:ALA:CB	1:B:1219:GLU:HB3	2.19	0.72
1:B:137:HIS:O	1:B:141:LYS:HG2	1.89	0.72
1:B:1089:MET:SD	2:A:88:A:N6	2.62	0.71
1:B:1225:GLU:HG2	1:B:1318:LEU:HD11	1.70	0.71
1:B:75:ARG:HD3	1:B:163:LYS:HE3	1.72	0.71
1:B:1241:HIS:O	1:B:1245:LEU:HD11	1.90	0.71
1:B:331:ASP:HB2	1:B:399:LEU:HD21	1.71	0.71
1:B:1347:LEU:HD12	1:B:1362:LEU:HD11	1.70	0.71
1:B:1091:GLN:OE1	2:A:91:C:H5''	1.91	0.71
1:B:46:ASN:OD1	2:A:91:C:N4	2.24	0.71
3:C:4:C:H2'	3:C:5:A:H8	1.56	0.71
1:B:967:ARG:NH2	1:B:973:TYR:O	2.22	0.71
1:B:973:TYR:CD2	1:B:1237:TYR:HB3	2.25	0.71
1:B:364:ASP:OD1	1:B:364:ASP:N	2.24	0.70
1:B:103:GLU:HB3	1:B:111:LYS:HG3	1.73	0.70
1:B:508:LEU:O	1:B:660:GLY:N	2.19	0.70
1:B:44:LYS:HD3	2:A:91:C:C4	2.27	0.70
1:B:505:GLU:OE2	1:B:665:LYS:N	2.25	0.70
1:B:134:THR:HB	2:A:45:U:H4'	1.73	0.70
1:B:160:HIS:NE2	2:A:46:A:OP1	2.23	0.70
1:B:307:ARG:HB2	1:B:323:LYS:HE2	1.72	0.70
1:B:746:GLU:HG2	1:B:1353:THR:HB	1.74	0.70
1:B:403:ARG:NH2	2:A:20:G:OP2	2.24	0.70
1:B:588:ASN:OD1	1:B:588:ASN:N	2.19	0.70
1:B:911:LEU:O	1:B:915:GLY:N	2.25	0.70
1:B:1218:GLY:HA3	1:B:1338:SER:HA	1.73	0.69
1:B:1210:ARG:HA	1:B:1224:ASN:HD21	1.57	0.69
1:B:626:PHE:HZ	1:B:635:ARG:HD2	1.57	0.69
2:A:7:U:H2'	2:A:8:G:C8	2.27	0.69
1:B:992:VAL:O	1:B:995:THR:OG1	2.10	0.69
1:B:305:ILE:HD11	1:B:324:ARG:NH2	2.08	0.69
1:B:911:LEU:HA	1:B:914:ALA:HB3	1.75	0.69
1:B:977:GLU:N	1:B:977:GLU:OE1	2.25	0.69
1:B:909:SER:OG	1:B:912:ASP:N	2.20	0.69
1:B:848:LYS:HD3	1:B:1041:ASN:HD21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:ARG:NH2	1:B:1116:SER:OG	2.26	0.68
1:B:1139:VAL:HA	1:B:1167:THR:HA	1.74	0.68
1:B:977:GLU:O	1:B:1317:ASN:ND2	2.26	0.68
1:B:132:TYR:HB3	1:B:137:HIS:HB2	1.75	0.68
1:B:1300:LYS:O	1:B:1305:GLN:NE2	2.26	0.68
1:B:762:GLU:HB3	1:B:990:ASN:OD1	1.92	0.68
1:B:15:SER:HG	1:B:983:HIS:CE1	2.10	0.68
1:B:380:LEU:HD12	1:B:390:LEU:HD22	1.75	0.68
1:B:519:THR:HG23	1:B:589:ALA:HB1	1.76	0.68
1:B:525:THR:HG22	1:B:690:ASN:HB3	1.75	0.67
1:B:746:GLU:O	1:B:750:VAL:HG23	1.93	0.67
1:B:1215:ALA:HB3	1:B:1219:GLU:C	2.14	0.67
1:B:628:ASP:HB3	1:B:631:MET:HB2	1.77	0.67
1:B:735:LYS:NZ	1:B:1099:GLU:OE2	2.26	0.67
1:B:561:VAL:N	1:B:585:ASP:O	2.27	0.67
1:B:867:SER:HB2	1:B:1053:ALA:HB3	1.76	0.67
1:B:116:HIS:HD2	1:B:125:GLU:HB3	1.59	0.67
1:B:808:ASN:ND2	1:B:1243:GLU:OE2	2.28	0.67
1:B:215:ARG:O	1:B:395:ARG:HD3	1.95	0.67
1:B:354:GLN:HA	1:B:361:GLY:HA2	1.76	0.67
1:B:901:THR:O	1:B:905:ARG:N	2.24	0.67
1:B:1179:ILE:HG22	1:B:1190:VAL:HG21	1.76	0.66
1:B:1349:HIS:HB2	1:B:1358:THR:HB	1.77	0.66
1:B:1127:ASP:H	1:B:1131:TYR:HD2	1.43	0.66
1:B:191:THR:O	1:B:195:LEU:N	2.23	0.66
1:B:897:PHE:HA	1:B:900:LEU:HD12	1.78	0.66
1:B:1120:ILE:HD13	1:B:1169:MET:HE1	1.76	0.66
1:B:40:ARG:HE	1:B:43:ILE:HD12	1.61	0.66
1:B:9:LEU:HD12	1:B:761:ILE:HG22	1.78	0.66
1:B:148:LYS:HB2	1:B:429:PHE:CD2	2.31	0.66
1:B:165:ARG:NH1	1:B:444:LEU:O	2.29	0.66
1:B:817:GLN:O	1:B:882:TYR:OH	2.13	0.65
1:B:1218:GLY:HA2	1:B:1338:SER:HA	1.71	0.65
1:B:1318:LEU:HD22	1:B:1318:LEU:H	1.62	0.65
1:B:869:ASN:OD1	1:B:870:VAL:N	2.29	0.65
1:B:59:ALA:N	2:A:13:A:OP1	2.30	0.65
1:B:314:LYS:O	1:B:316:PRO:HD3	1.97	0.65
1:B:853:ASP:N	1:B:853:ASP:OD1	2.28	0.65
1:B:898:ASP:OD1	1:B:902:LYS:NZ	2.27	0.65
1:B:125:GLU:OE2	2:A:26:A:O2'	2.13	0.64
1:B:788:ILE:HG21	1:B:796:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:ASN:ND2	1:B:611:GLU:OE1	2.30	0.64
1:B:81:TYR:CE2	1:B:475:PRO:HD3	2.32	0.64
1:B:237:LEU:HA	1:B:255:ASN:HD21	1.60	0.64
1:B:7:ILE:HG12	1:B:20:VAL:HA	1.80	0.64
1:B:1253:GLU:HA	1:B:1256:GLN:HB2	1.79	0.64
1:B:448:ILE:HB	2:A:16:U:O3'	1.98	0.63
1:B:897:PHE:HA	1:B:900:LEU:CD1	2.27	0.63
1:B:71:ARG:HH22	2:A:18:A:H62	1.45	0.63
1:B:1099:GLU:O	1:B:1101:GLN:NE2	2.32	0.63
1:B:89:GLU:OE1	1:B:92:LYS:NZ	2.27	0.63
1:B:848:LYS:NZ	1:B:969:ASP:OD2	2.32	0.63
1:B:1003:LYS:HE2	1:B:1020:LYS:HE3	1.81	0.63
1:B:679:ILE:HG13	1:B:704:PHE:CE2	2.33	0.63
1:B:63:ARG:O	1:B:67:THR:HG23	1.99	0.63
1:B:1174:PHE:HE1	1:B:1178:PRO:HB3	1.62	0.63
1:B:736:GLY:O	1:B:740:THR:OG1	2.17	0.63
1:B:1060:ARG:HB3	1:B:1064:GLU:OE2	1.99	0.62
3:C:10:G:H2'	3:C:11:A:H8	1.64	0.62
1:B:135:ILE:HD12	1:B:138:LEU:HB3	1.79	0.62
1:B:1326:TYR:O	1:B:1329:THR:OG1	2.16	0.62
3:C:4:C:H2'	3:C:5:A:C8	2.33	0.62
1:B:1308:ASN:HB3	1:B:1326:TYR:CE1	2.34	0.62
2:A:87:G:H2'	2:A:88:A:C8	2.34	0.62
1:B:648:MET:HA	1:B:651:LEU:HD12	1.82	0.62
1:B:1045:PHE:HA	1:B:1060:ARG:HD2	1.81	0.62
1:B:515:TYR:HE1	1:B:662:LEU:HB2	1.63	0.62
1:B:516:GLU:OE1	1:B:593:THR:N	2.30	0.62
1:B:380:LEU:O	1:B:386:THR:HG21	2.00	0.62
1:B:531:THR:HG22	1:B:534:MET:HG2	1.81	0.62
1:B:23:ASP:OD1	1:B:24:GLU:N	2.33	0.61
1:B:883:TRP:CE3	1:B:900:LEU:HD13	2.35	0.61
1:B:191:THR:HA	1:B:194:GLN:HB3	1.82	0.61
1:B:351:PHE:HB3	2:A:43:G:H1	1.65	0.61
1:B:1066:ASN:OD1	1:B:1069:THR:N	2.29	0.61
1:B:69:ARG:NH2	2:A:62:G:H3'	2.16	0.61
1:B:545:LYS:NZ	1:B:683:LEU:O	2.33	0.61
1:B:1219:GLU:C	1:B:1220:LEU:HG	2.21	0.61
1:B:1266:LEU:H	1:B:1266:LEU:HD23	1.65	0.61
1:B:532:GLU:HG2	1:B:533:GLY:N	2.15	0.61
1:B:507:VAL:HB	1:B:660:GLY:O	2.01	0.61
1:B:1206:LEU:HG	1:B:1345:ALA:CB	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1214:LEU:HD22	1:B:1215:ALA:N	2.15	0.61
1:B:166:GLY:C	2:A:18:A:H4'	2.21	0.60
1:B:1225:GLU:HA	1:B:1318:LEU:HD11	1.82	0.60
1:B:1228:LEU:HD23	1:B:1233:VAL:HG22	1.83	0.60
1:B:516:GLU:OE1	1:B:592:GLY:N	2.32	0.60
1:B:1030:GLY:HA2	1:B:1033:THR:HG23	1.82	0.60
1:B:1276:PHE:O	1:B:1280:VAL:HG22	2.01	0.60
1:B:460:SER:CB	2:A:61:C:H5'	2.28	0.60
1:B:1014:LYS:HB2	1:B:1016:TYR:CE1	2.37	0.60
1:B:1140:ALA:CB	1:B:1171:ARG:HD2	2.32	0.60
1:B:215:ARG:HG2	1:B:307:ARG:HH11	1.66	0.60
1:B:787:GLY:HA3	1:B:891:LEU:HD21	1.83	0.60
1:B:913:LYS:HA	1:B:916:PHE:CD2	2.37	0.60
1:B:1266:LEU:O	1:B:1270:ILE:N	2.23	0.60
1:B:29:SER:HB2	1:B:44:LYS:HE3	1.83	0.60
1:B:49:GLY:HA3	1:B:1093:ASN:HB2	1.84	0.60
3:C:10:G:H2'	3:C:11:A:C8	2.37	0.60
1:B:397:ASP:HA	1:B:400:ARG:HD3	1.83	0.60
1:B:1045:PHE:HA	1:B:1060:ARG:CD	2.32	0.59
1:B:1099:GLU:HG2	2:A:67:C:N4	2.17	0.59
2:A:54:G:H1	2:A:60:C:H42	1.49	0.59
1:B:116:HIS:O	1:B:120:GLY:N	2.32	0.59
1:B:973:TYR:CD2	1:B:1234:ASN:HA	2.37	0.59
1:B:1082:THR:O	1:B:1086:VAL:N	2.31	0.59
1:B:1122:ARG:HD3	1:B:1126:TRP:CZ3	2.37	0.59
1:B:116:HIS:CD2	1:B:122:ILE:HA	2.38	0.59
1:B:871:PRO:O	1:B:903:ALA:HB1	2.02	0.59
1:B:1096:LYS:HG2	1:B:1201:TYR:CD1	2.38	0.59
1:B:1218:GLY:O	1:B:1338:SER:N	2.36	0.59
2:A:40:C:H2'	2:A:41:A:H8	1.67	0.59
1:B:760:VAL:HG11	1:B:990:ASN:O	2.02	0.59
1:B:981:TYR:HE1	1:B:1225:GLU:OE1	1.86	0.59
1:B:1095:VAL:HG21	1:B:1354:GLY:HA3	1.84	0.58
1:B:220:ARG:O	1:B:224:ASN:N	2.35	0.58
1:B:485:GLY:O	1:B:489:GLN:HB2	2.02	0.58
1:B:351:PHE:O	2:A:43:G:N2	2.24	0.58
1:B:733:ILE:O	1:B:737:ILE:HG13	2.04	0.58
1:B:1287:LEU:HD23	1:B:1288:ASP:N	2.18	0.58
1:B:569:PHE:CE2	1:B:578:VAL:HG21	2.38	0.58
1:B:823:TYR:CE2	1:B:864:ARG:HB3	2.38	0.58
1:B:256:PHE:HB2	1:B:258:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:SER:O	1:B:322:ILE:HG13	2.03	0.58
1:B:864:ARG:HD3	1:B:1054:ASN:ND2	2.18	0.58
1:B:7:ILE:HD11	1:B:20:VAL:HG13	1.85	0.58
1:B:116:HIS:NE2	1:B:122:ILE:HA	2.18	0.58
1:B:296:LEU:O	1:B:300:ILE:N	2.37	0.58
1:B:498:PHE:HD1	1:B:506:LYS:HG3	1.69	0.58
1:B:1206:LEU:N	1:B:1210:ARG:O	2.30	0.58
1:B:616:LEU:O	1:B:619:ILE:HG22	2.04	0.58
1:B:1001:TYR:CD1	1:B:1036:TYR:HD2	2.21	0.58
1:B:750:VAL:HG11	1:B:1355:LEU:HD13	1.85	0.58
1:B:192:TYR:CZ	1:B:196:PHE:HE2	2.21	0.58
1:B:914:ALA:O	1:B:917:ILE:HG12	2.04	0.58
1:B:1218:GLY:HA3	1:B:1337:THR:O	2.04	0.58
1:B:1237:TYR:HA	1:B:1240:SER:HB3	1.84	0.58
1:B:44:LYS:HD2	2:A:92:G:N7	2.19	0.57
1:B:515:TYR:CE1	1:B:662:LEU:HB2	2.38	0.57
1:B:1297:HIS:CE1	1:B:1300:LYS:HG3	2.39	0.57
1:B:1036:TYR:OH	1:B:1066:ASN:ND2	2.37	0.57
1:B:1315:LEU:HB2	1:B:1324:PHE:CE1	2.39	0.57
1:B:40:ARG:HE	1:B:43:ILE:CD1	2.18	0.57
1:B:531:THR:CG2	1:B:534:MET:HG2	2.34	0.57
1:B:876:VAL:O	1:B:880:LYS:HB2	2.04	0.57
1:B:1170:GLU:HB3	1:B:1181:PHE:CZ	2.39	0.57
1:B:453:GLY:HA2	2:A:15:U:O2'	2.05	0.57
1:B:867:SER:HB2	1:B:1054:ASN:H	1.69	0.57
1:B:1145:VAL:HG11	1:B:1182:LEU:HD11	1.85	0.57
1:B:1157:LEU:HD22	1:B:1188:LYS:HE3	1.86	0.57
1:B:237:LEU:HA	1:B:255:ASN:ND2	2.19	0.57
1:B:362:TYR:HB2	1:B:372:PHE:CB	2.35	0.57
1:B:606:PHE:O	1:B:612:ASN:ND2	2.37	0.57
1:B:1232:TYR:HE1	1:B:1265:TYR:HB3	1.69	0.57
1:B:1241:HIS:C	1:B:1245:LEU:HD11	2.24	0.57
1:B:209:LYS:O	1:B:213:SER:OG	2.19	0.57
1:B:516:GLU:CD	1:B:593:THR:H	2.08	0.57
1:B:565:LYS:HA	1:B:569:PHE:HB2	1.87	0.57
1:B:823:TYR:CZ	1:B:864:ARG:HB3	2.40	0.57
1:B:979:ASN:N	1:B:979:ASN:OD1	2.38	0.57
1:B:670:ILE:O	1:B:678:THR:HG23	2.05	0.56
1:B:1276:PHE:CE2	1:B:1280:VAL:HG21	2.40	0.56
1:B:297:SER:HA	1:B:300:ILE:HD12	1.87	0.56
1:B:31:LYS:HA	1:B:43:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HD21	1:B:279:LEU:HD13	1.87	0.56
1:B:451:TYR:CE1	1:B:452:VAL:HG23	2.40	0.56
1:B:359:TYR:CZ	1:B:363:ILE:HG13	2.40	0.56
1:B:742:LYS:NZ	2:A:68:A:OP2	2.38	0.56
1:B:981:TYR:OH	2:A:90:U:N3	2.38	0.56
1:B:551:LEU:HB3	1:B:552:LEU:HD23	1.88	0.56
1:B:1110:ILE:HG23	1:B:1133:GLY:HA2	1.88	0.56
1:B:257:ASP:OD1	1:B:257:ASP:N	2.38	0.56
1:B:841:ILE:N	1:B:854:ASN:HD22	2.02	0.56
1:B:1037:PHE:CE2	1:B:1044:ASN:HB2	2.40	0.56
1:B:1294:TYR:O	1:B:1298:ARG:N	2.39	0.56
1:B:1303:ARG:HH11	1:B:1303:ARG:CG	2.18	0.56
1:B:949:LEU:HD12	1:B:950:ILE:N	2.21	0.56
1:B:990:ASN:N	1:B:990:ASN:HD22	2.04	0.56
1:B:1218:GLY:O	1:B:1336:TYR:O	2.23	0.56
1:B:530:VAL:HG13	1:B:534:MET:HB2	1.88	0.56
1:B:563:GLN:O	1:B:567:ASP:HB2	2.06	0.56
1:B:48:ILE:O	1:B:1093:ASN:ND2	2.38	0.55
1:B:165:ARG:O	1:B:412:HIS:HA	2.06	0.55
1:B:116:HIS:CD2	1:B:125:GLU:HB3	2.40	0.55
1:B:402:GLN:N	2:A:45:U:OP1	2.39	0.55
1:B:870:VAL:HG23	1:B:903:ALA:HB2	1.88	0.55
2:A:20:G:C2'	2:A:21:G:H5'	2.36	0.55
1:B:446:PHE:HE1	1:B:448:ILE:HG13	1.70	0.55
1:B:1000:LYS:O	1:B:1066:ASN:HB2	2.06	0.55
1:B:498:PHE:CD1	1:B:506:LYS:HG3	2.40	0.55
1:B:514:LEU:O	1:B:518:PHE:N	2.25	0.55
1:B:758:ASN:HD22	1:B:995:THR:HG22	1.71	0.55
1:B:1148:LYS:HD2	1:B:1157:LEU:HB3	1.87	0.55
1:B:132:TYR:CE1	1:B:141:LYS:HG3	2.41	0.55
1:B:167:HIS:HB2	1:B:169:LEU:HG	1.87	0.55
1:B:275:LEU:O	1:B:278:LEU:N	2.36	0.55
1:B:395:ARG:HH11	1:B:395:ARG:HG3	1.71	0.55
1:B:620:VAL:O	1:B:624:THR:OG1	2.25	0.55
1:B:760:VAL:HG22	1:B:994:GLY:HA3	1.88	0.55
1:B:1146:VAL:O	1:B:1191:LYS:HG2	2.07	0.55
1:B:540:LEU:HD12	1:B:544:GLN:HB3	1.89	0.55
1:B:1258:PHE:HE1	1:B:1262:HIS:ND1	2.05	0.55
1:B:853:ASP:O	1:B:896:LYS:HD2	2.06	0.55
1:B:5:TYR:OH	1:B:754:HIS:O	2.20	0.55
1:B:866:LYS:HD3	1:B:867:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:GLU:HA	1:B:519:THR:HG22	1.89	0.55
1:B:135:ILE:HG21	1:B:160:HIS:CD2	2.42	0.54
1:B:359:TYR:CE1	1:B:363:ILE:HG13	2.43	0.54
1:B:624:THR:HA	1:B:656:TYR:O	2.07	0.54
1:B:633:GLU:O	1:B:637:LYS:HG3	2.07	0.54
1:B:841:ILE:H	1:B:854:ASN:HD22	1.56	0.54
1:B:1064:GLU:CG	1:B:1076:LYS:HE2	2.38	0.54
1:B:354:GLN:HA	1:B:361:GLY:CA	2.38	0.54
1:B:986:ASP:HA	1:B:989:LEU:HD12	1.89	0.54
1:B:813:LEU:HD11	1:B:855:LYS:HB3	1.89	0.54
1:B:1167:THR:O	1:B:1170:GLU:N	2.29	0.54
1:B:435:ASP:OD1	1:B:435:ASP:N	2.40	0.54
1:B:742:LYS:HG2	1:B:1352:ILE:HD12	1.89	0.54
1:B:531:THR:HB	1:B:575:PHE:CD2	2.43	0.54
1:B:919:ARG:HH11	1:B:919:ARG:HB3	1.72	0.54
1:B:1232:TYR:CD2	1:B:1269:ILE:HD11	2.43	0.54
1:B:1267:ASP:O	1:B:1271:GLU:N	2.37	0.54
1:B:252:PHE:HA	1:B:255:ASN:HB2	1.90	0.54
1:B:750:VAL:HA	1:B:1356:TYR:OH	2.07	0.54
1:B:917:ILE:HB	1:B:921:LEU:CD1	2.34	0.54
2:A:58:G:H2'	2:A:60:C:H5'	1.88	0.54
1:B:836:TYR:CD1	1:B:859:ARG:HA	2.42	0.53
1:B:965:ASP:O	1:B:969:ASP:N	2.29	0.53
1:B:1170:GLU:HB3	1:B:1181:PHE:CE1	2.43	0.53
1:B:585:ASP:OD1	1:B:586:ARG:N	2.39	0.53
2:A:95:G:H2'	2:A:96:C:C6	2.42	0.53
1:B:93:VAL:HG21	1:B:151:LEU:HD23	1.89	0.53
1:B:192:TYR:HA	1:B:289:LEU:HD21	1.89	0.53
1:B:981:TYR:HB3	1:B:985:HIS:NE2	2.23	0.53
1:B:18:TRP:CH2	1:B:1355:LEU:HD11	2.44	0.53
1:B:251:ASN:HA	1:B:262:ALA:O	2.08	0.53
1:B:478:PHE:CE1	1:B:482:VAL:HG21	2.44	0.53
1:B:629:ARG:HB2	1:B:655:ARG:NH2	2.23	0.53
1:B:839:ASP:OD1	1:B:1054:ASN:ND2	2.41	0.53
2:A:20:G:H2'	2:A:21:G:H5'	1.89	0.53
1:B:1060:ARG:HD3	1:B:1064:GLU:OE2	2.09	0.53
1:B:373:TYR:O	1:B:376:ILE:HG22	2.09	0.53
1:B:1313:PHE:O	1:B:1317:ASN:N	2.42	0.53
1:B:21:ILE:HG22	1:B:22:THR:O	2.09	0.53
1:B:1020:LYS:O	1:B:1035:LYS:HB3	2.09	0.53
1:B:1147:ALA:HB1	1:B:1188:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1227:ALA:N	2:A:90:U:O4	2.42	0.53
2:A:87:G:H2'	2:A:88:A:H8	1.74	0.53
1:B:451:TYR:CD1	1:B:452:VAL:HG23	2.44	0.52
1:B:483:ASP:OD1	1:B:486:ALA:N	2.42	0.52
1:B:499:ASP:OD2	1:B:663:SER:N	2.41	0.52
1:B:520:VAL:HG21	1:B:591:LEU:HG	1.91	0.52
1:B:148:LYS:HA	1:B:426:GLN:OE1	2.10	0.52
1:B:936:ASP:OD1	1:B:949:LEU:HD21	2.10	0.52
1:B:986:ASP:O	1:B:990:ASN:ND2	2.42	0.52
1:B:1086:VAL:HA	1:B:1089:MET:HE2	1.92	0.52
2:A:60:C:H2'	2:A:61:C:C6	2.43	0.52
1:B:886:LEU:HB3	1:B:891:LEU:HD12	1.90	0.52
1:B:1019:ARG:HD2	1:B:1019:ARG:O	2.09	0.52
1:B:351:PHE:O	1:B:360:ALA:HB2	2.09	0.52
1:B:1052:LEU:HD23	1:B:1056:GLU:HB2	1.91	0.52
1:B:647:VAL:O	1:B:651:LEU:N	2.42	0.52
1:B:966:PHE:HA	1:B:969:ASP:HB2	1.91	0.52
1:B:108:GLU:N	1:B:108:GLU:OE1	2.43	0.52
1:B:478:PHE:HE1	1:B:482:VAL:HG21	1.74	0.52
1:B:521:TYR:CZ	1:B:549:VAL:HG21	2.45	0.52
1:B:917:ILE:CG2	1:B:1042:ILE:HD11	2.40	0.52
1:B:1090:PRO:HG3	2:A:88:A:O2'	2.09	0.52
1:B:158:LEU:HD21	1:B:422:ILE:HG21	1.91	0.52
1:B:363:ILE:HG23	2:A:44:U:H5'	1.92	0.52
1:B:531:THR:OG1	1:B:532:GLU:N	2.42	0.52
1:B:821:ASP:HA	1:B:828:LEU:HD21	1.92	0.52
1:B:1086:VAL:O	1:B:1089:MET:HB2	2.10	0.52
2:A:40:C:H2'	2:A:41:A:C8	2.45	0.52
1:B:330:GLN:O	1:B:334:LEU:HB2	2.10	0.52
1:B:346:LYS:O	1:B:350:ILE:HG12	2.09	0.52
1:B:525:THR:HG23	1:B:690:ASN:OD1	2.08	0.52
1:B:981:TYR:CD1	1:B:981:TYR:N	2.78	0.52
1:B:1214:LEU:CD2	1:B:1215:ALA:N	2.73	0.52
1:B:844:GLN:HG2	1:B:848:LYS:HA	1.92	0.52
1:B:853:ASP:HB3	1:B:896:LYS:HB2	1.92	0.52
1:B:1117:ASP:OD1	1:B:1117:ASP:N	2.41	0.52
1:B:1205:GLU:O	1:B:1345:ALA:HB1	2.08	0.52
1:B:105:PHE:HA	2:A:24:U:O2	2.10	0.52
1:B:1106:SER:CB	1:B:1134:PHE:HB3	2.40	0.52
1:B:26:LYS:HG3	1:B:27:VAL:N	2.25	0.51
1:B:75:ARG:HA	1:B:78:ARG:HH21	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:SER:O	1:B:301:LEU:HG	2.10	0.51
1:B:970:PHE:CE2	1:B:1080:PHE:CE2	2.98	0.51
1:B:305:ILE:HG22	1:B:305:ILE:O	2.11	0.51
1:B:328:HIS:ND1	2:A:44:U:O2	2.44	0.51
1:B:893:THR:HG23	1:B:896:LYS:H	1.75	0.51
1:B:465:MET:CE	1:B:467:ARG:HG3	2.41	0.51
1:B:1157:LEU:CD2	1:B:1188:LYS:HE3	2.41	0.51
1:B:531:THR:HA	1:B:578:VAL:HG23	1.93	0.51
1:B:1004:LEU:O	1:B:1007:GLU:HG2	2.10	0.51
1:B:44:LYS:HE2	2:A:87:G:N2	2.26	0.51
1:B:981:TYR:N	1:B:981:TYR:HD1	2.09	0.51
1:B:1080:PHE:CD1	1:B:1080:PHE:N	2.78	0.51
1:B:1300:LYS:HE2	1:B:1301:PRO:HD3	1.93	0.51
1:B:126:VAL:O	1:B:130:GLU:HG2	2.10	0.51
1:B:460:SER:HB3	2:A:60:C:O2'	2.11	0.51
1:B:475:PRO:HG3	2:A:59:U:O4	2.10	0.51
1:B:564:LEU:HG	1:B:569:PHE:HE1	1.75	0.51
1:B:1003:LYS:HE3	1:B:1016:TYR:HE2	1.74	0.51
2:A:83:C:H2'	2:A:84:A:C8	2.46	0.51
1:B:391:VAL:CG1	1:B:395:ARG:HH22	2.22	0.51
1:B:1152:GLY:O	1:B:1155:LYS:N	2.42	0.51
1:B:1258:PHE:HE1	1:B:1262:HIS:CG	2.29	0.51
1:B:626:PHE:CZ	1:B:635:ARG:HD2	2.43	0.51
1:B:919:ARG:HB3	1:B:919:ARG:NH1	2.26	0.51
1:B:970:PHE:CE2	1:B:1080:PHE:HE2	2.29	0.51
1:B:305:ILE:O	1:B:306:LEU:HD12	2.11	0.50
1:B:560:THR:HA	1:B:586:ARG:HA	1.92	0.50
1:B:995:THR:O	1:B:998:ILE:HG12	2.10	0.50
1:B:1239:ALA:HB1	1:B:1303:ARG:HA	1.92	0.50
1:B:265:GLN:O	1:B:271:TYR:HB2	2.10	0.50
1:B:821:ASP:CA	1:B:828:LEU:HD21	2.41	0.50
1:B:915:GLY:HA3	1:B:919:ARG:NH2	2.26	0.50
1:B:165:ARG:C	1:B:415:HIS:HD2	2.15	0.50
1:B:250:PRO:HD2	1:B:264:LEU:O	2.12	0.50
1:B:387:GLU:O	1:B:391:VAL:HG23	2.11	0.50
1:B:1202:SER:O	1:B:1213:MET:HA	2.11	0.50
1:B:1219:GLU:O	1:B:1220:LEU:HD23	2.12	0.50
1:B:1357:GLU:OE1	1:B:1359:ARG:NH1	2.40	0.50
1:B:28:PRO:HD2	1:B:47:LEU:HD22	1.92	0.50
1:B:84:GLU:OE1	1:B:85:ILE:HG23	2.12	0.50
1:B:86:PHE:CE1	1:B:433:LEU:HD21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:GLN:OE1	1:B:1097:LYS:HD2	2.11	0.50
1:B:363:ILE:CG2	2:A:44:U:H5'	2.42	0.50
1:B:875:VAL:O	1:B:878:LYS:O	2.29	0.50
1:B:956:ILE:HD11	1:B:998:ILE:HD13	1.94	0.50
1:B:1006:SER:HB3	1:B:1013:TYR:C	2.32	0.50
1:B:1258:PHE:HA	1:B:1261:GLN:HB2	1.94	0.50
1:B:1347:LEU:HD23	1:B:1348:ILE:N	2.26	0.50
1:B:386:THR:HG23	1:B:387:GLU:N	2.27	0.50
1:B:841:ILE:HG23	1:B:871:PRO:CG	2.41	0.50
1:B:881:ASN:O	1:B:885:GLN:N	2.41	0.50
1:B:1105:PHE:CE1	1:B:1169:MET:HA	2.47	0.50
1:B:1218:GLY:O	1:B:1337:THR:CA	2.59	0.50
1:B:389:LEU:H	1:B:389:LEU:HD22	1.76	0.50
1:B:1168:ILE:HG23	1:B:1171:ARG:HD3	1.94	0.50
1:B:1235:PHE:CZ	1:B:1266:LEU:HD22	2.47	0.50
1:B:1196:ILE:HB	1:B:1198:LEU:HD21	1.93	0.49
2:A:54:G:H1	2:A:60:C:N4	2.10	0.49
1:B:514:LEU:HD23	1:B:617:GLU:HG3	1.94	0.49
1:B:876:VAL:O	1:B:880:LYS:CB	2.60	0.49
1:B:1037:PHE:HE2	1:B:1044:ASN:HB2	1.77	0.49
1:B:1181:PHE:CZ	1:B:1185:LYS:HE2	2.48	0.49
1:B:1225:GLU:HG2	1:B:1318:LEU:CD1	2.39	0.49
1:B:1263:LYS:HD2	1:B:1302:ILE:HD11	1.94	0.49
2:A:20:G:O2'	2:A:21:G:OP1	2.22	0.49
1:B:601:ILE:HG13	1:B:602:LYS:N	2.26	0.49
1:B:708:ILE:HG23	1:B:712:GLN:HG3	1.93	0.49
1:B:898:ASP:O	1:B:902:LYS:NZ	2.35	0.49
2:A:45:U:H2'	2:A:46:A:H8	1.77	0.49
1:B:11:ILE:HB	1:B:762:GLU:O	2.12	0.49
1:B:276:ASP:OD2	2:A:9:U:H5''	2.12	0.49
1:B:282:ILE:HG21	1:B:286:TYR:CE2	2.48	0.49
1:B:391:VAL:HG12	1:B:395:ARG:NH2	2.22	0.49
1:B:1141:TYR:OH	1:B:1175:GLU:HG2	2.13	0.49
1:B:192:TYR:CZ	1:B:196:PHE:CE2	3.00	0.49
1:B:1066:ASN:OD1	1:B:1068:GLU:N	2.46	0.49
1:B:548:ILE:HD11	1:B:568:TYR:CD2	2.47	0.49
1:B:916:PHE:HA	1:B:919:ARG:HG2	1.93	0.49
1:B:1171:ARG:O	1:B:1175:GLU:HG3	2.13	0.49
1:B:1308:ASN:O	1:B:1312:LEU:HG	2.13	0.49
2:A:9:U:H2'	2:A:10:U:C6	2.48	0.49
1:B:237:LEU:CA	1:B:255:ASN:HD21	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ALA:HA	1:B:295:ASN:HB2	1.95	0.49
1:B:686:ASP:OD2	1:B:691:ARG:HB2	2.13	0.49
1:B:680:LEU:O	1:B:684:LYS:HG2	2.13	0.49
1:B:1203:LEU:O	1:B:1348:ILE:HB	2.13	0.49
1:B:114:GLU:HB2	1:B:120:GLY:HA2	1.95	0.48
1:B:849:ASP:OD1	1:B:851:SER:N	2.46	0.48
1:B:1292:SER:HA	1:B:1295:ASN:OD1	2.13	0.48
2:A:31:U:H2'	2:A:32:A:C8	2.48	0.48
1:B:916:PHE:HD1	1:B:919:ARG:HE	1.61	0.48
1:B:1052:LEU:HD23	1:B:1056:GLU:HG3	1.96	0.48
2:A:23:U:O5'	2:A:23:U:H6	1.96	0.48
1:B:29:SER:O	1:B:29:SER:OG	2.25	0.48
1:B:75:ARG:O	1:B:79:ILE:HG12	2.13	0.48
1:B:424:ARG:HA	1:B:427:GLU:CD	2.33	0.48
1:B:514:LEU:HD23	1:B:617:GLU:CG	2.44	0.48
1:B:1052:LEU:HB2	1:B:1058:ARG:HG2	1.95	0.48
1:B:1093:ASN:ND2	1:B:1093:ASN:H	2.12	0.48
1:B:2:ASP:HB2	2:A:84:A:OP1	2.14	0.48
1:B:39:ASP:OD1	1:B:39:ASP:N	2.44	0.48
1:B:553:PHE:HZ	1:B:587:PHE:HD2	1.62	0.48
1:B:857:LEU:HD12	1:B:858:THR:N	2.28	0.48
1:B:1266:LEU:O	1:B:1269:ILE:HB	2.14	0.48
1:B:393:LEU:O	1:B:396:GLU:N	2.45	0.48
1:B:457:ARG:HD3	1:B:467:ARG:NH2	2.29	0.48
1:B:501:ASN:O	1:B:712:GLN:NE2	2.44	0.48
1:B:10:ALA:HB2	1:B:987:ALA:N	2.29	0.48
1:B:1277:SER:OG	1:B:1287:LEU:HD12	2.14	0.48
2:A:38:A:H8	2:A:38:A:OP2	1.97	0.48
1:B:1293:ALA:HB1	1:B:1326:TYR:CD2	2.49	0.48
1:B:1315:LEU:HD22	1:B:1324:PHE:HZ	1.78	0.48
1:B:962:LEU:HD21	1:B:1043:MET:HG3	1.95	0.48
1:B:973:TYR:HE2	1:B:1234:ASN:O	1.96	0.48
1:B:1106:SER:OG	1:B:1134:PHE:HB3	2.14	0.48
1:B:1003:LYS:HE3	1:B:1003:LYS:HB3	1.55	0.47
1:B:1212:ARG:HD3	1:B:1221:GLN:O	2.14	0.47
3:C:5:A:H2'	3:C:6:A:H8	1.79	0.47
1:B:864:ARG:O	1:B:872:SER:N	2.47	0.47
1:B:1215:ALA:HB3	1:B:1219:GLU:HB3	1.96	0.47
1:B:1232:TYR:CB	1:B:1269:ILE:HD11	2.44	0.47
1:B:44:LYS:HD3	2:A:91:C:C5	2.49	0.47
1:B:530:VAL:HG12	1:B:531:THR:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:VAL:HA	1:B:563:GLN:OE1	2.13	0.47
1:B:626:PHE:N	1:B:626:PHE:CD1	2.81	0.47
1:B:850:ASP:OD1	1:B:850:ASP:N	2.44	0.47
1:B:936:ASP:CG	1:B:951:ARG:HH12	2.17	0.47
1:B:45:LYS:NZ	1:B:1091:GLN:HE22	2.12	0.47
1:B:1245:LEU:HD12	1:B:1245:LEU:N	2.29	0.47
1:B:1358:THR:HG21	2:A:69:A:O2'	2.14	0.47
1:B:240:ASN:ND2	1:B:255:ASN:OD1	2.26	0.47
1:B:1041:ASN:HD22	1:B:1044:ASN:HD21	1.62	0.47
1:B:1111:LEU:CD1	1:B:1135:ASP:HB3	2.44	0.47
2:A:86:C:C2	2:A:93:G:N2	2.82	0.47
1:B:351:PHE:HB3	2:A:43:G:N1	2.30	0.47
1:B:820:ARG:NE	1:B:825:ASP:OD1	2.26	0.47
1:B:1006:SER:HB3	1:B:1013:TYR:HB2	1.96	0.47
1:B:1041:ASN:HB3	1:B:1044:ASN:ND2	2.30	0.47
1:B:168:PHE:HA	1:B:412:HIS:HD1	1.78	0.47
1:B:517:TYR:O	1:B:521:TYR:HD2	1.95	0.47
1:B:795:ILE:HA	1:B:798:GLU:HB2	1.97	0.47
1:B:1174:PHE:CE1	1:B:1178:PRO:HB3	2.45	0.47
1:B:1252:ASN:HD22	1:B:1256:GLN:HG2	1.80	0.47
1:B:1257:LEU:O	1:B:1261:GLN:HB2	2.15	0.47
1:B:1266:LEU:HA	1:B:1269:ILE:HB	1.96	0.47
1:B:69:ARG:HG3	2:A:51:A:P	2.55	0.47
1:B:265:GLN:HB2	1:B:268:LYS:HG2	1.97	0.47
1:B:1014:LYS:HB2	1:B:1016:TYR:HE1	1.79	0.47
1:B:1095:VAL:CG2	1:B:1354:GLY:HA3	2.44	0.47
1:B:70:ARG:NH1	2:A:15:U:OP1	2.46	0.47
1:B:1101:GLN:HG2	1:B:1140:ALA:O	2.14	0.47
1:B:1298:ARG:NH2	1:B:1299:ASP:HA	2.26	0.47
1:B:105:PHE:HE2	1:B:1131:TYR:CD1	2.33	0.47
1:B:167:HIS:CG	1:B:169:LEU:HG	2.50	0.47
1:B:644:ASP:HB3	1:B:647:VAL:HG22	1.97	0.47
1:B:1003:LYS:HE3	1:B:1016:TYR:CE2	2.50	0.47
1:B:1165:GLY:C	1:B:1166:ILE:HD13	2.35	0.47
2:A:8:G:H1	3:C:13:C:H42	1.63	0.47
2:A:10:U:H2'	2:A:11:C:C6	2.49	0.47
3:C:5:A:H2'	3:C:6:A:C8	2.50	0.47
1:B:506:LYS:HE3	1:B:506:LYS:H	1.80	0.46
1:B:1000:LYS:HA	1:B:1073:VAL:HG21	1.97	0.46
1:B:1174:PHE:CD1	1:B:1178:PRO:HA	2.50	0.46
1:B:1064:GLU:HG2	1:B:1076:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1200:LYS:O	1:B:1201:TYR:HB2	2.15	0.46
1:B:58:THR:HG22	1:B:731:PRO:HD2	1.98	0.46
1:B:74:ARG:NH2	2:A:16:U:OP1	2.48	0.46
1:B:108:GLU:OE1	1:B:109:GLU:HG2	2.15	0.46
1:B:974:LYS:HG3	1:B:974:LYS:O	2.15	0.46
1:B:1080:PHE:N	1:B:1080:PHE:HD1	2.13	0.46
1:B:116:HIS:NE2	1:B:122:ILE:HD12	2.27	0.46
1:B:321:MET:SD	1:B:402:GLN:HG3	2.56	0.46
1:B:502:LEU:HD23	1:B:502:LEU:HA	1.72	0.46
1:B:692:ASN:OD1	1:B:693:PHE:N	2.49	0.46
1:B:1074:TRP:CH2	1:B:1079:ASP:HB3	2.51	0.46
1:B:746:GLU:OE2	1:B:1351:SER:OG	2.18	0.46
1:B:755:LYS:HD2	1:B:952:GLU:OE2	2.15	0.46
1:B:1020:LYS:HG3	1:B:1035:LYS:HA	1.96	0.46
1:B:532:GLU:N	1:B:532:GLU:OE1	2.39	0.46
1:B:821:ASP:HB3	1:B:825:ASP:H	1.81	0.46
1:B:918:LYS:HA	1:B:921:LEU:HB2	1.97	0.46
1:B:1144:LEU:O	1:B:1195:ILE:HG22	2.16	0.46
1:B:25:TYR:CD1	1:B:25:TYR:N	2.84	0.46
1:B:902:LYS:O	1:B:906:GLY:N	2.43	0.46
1:B:970:PHE:HE2	1:B:1080:PHE:HE2	1.64	0.46
1:B:1347:LEU:CD1	1:B:1362:LEU:HD11	2.44	0.46
1:B:51:LEU:HD12	1:B:1095:VAL:O	2.15	0.46
1:B:1006:SER:OG	1:B:1007:GLU:OE2	2.32	0.46
2:A:27:G:H5''	2:A:28:A:H4'	1.98	0.46
1:B:108:GLU:OE1	1:B:109:GLU:N	2.48	0.46
1:B:591:LEU:HD23	1:B:591:LEU:HA	1.68	0.46
1:B:822:MET:HG3	1:B:883:TRP:HE1	1.80	0.46
1:B:965:ASP:O	1:B:969:ASP:HB2	2.16	0.46
1:B:1268:GLU:O	1:B:1272:GLN:HG2	2.15	0.46
1:B:896:LYS:O	1:B:900:LEU:HG	2.15	0.46
1:B:1280:VAL:HG23	1:B:1281:ILE:N	2.31	0.46
1:B:8:GLY:HA3	1:B:991:ALA:HB2	1.97	0.45
1:B:246:LEU:HD23	1:B:246:LEU:HA	1.65	0.45
1:B:743:VAL:HG22	1:B:1352:ILE:HD11	1.98	0.45
1:B:951:ARG:HG2	1:B:1013:TYR:OH	2.16	0.45
1:B:1099:GLU:HG2	2:A:67:C:H42	1.79	0.45
1:B:1140:ALA:HB2	1:B:1168:ILE:HG12	1.98	0.45
1:B:1312:LEU:HD11	1:B:1326:TYR:CE1	2.50	0.45
1:B:1315:LEU:CD1	1:B:1321:PRO:HB3	2.45	0.45
1:B:679:ILE:HG13	1:B:704:PHE:CZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:SER:O	1:B:1025:SER:OG	2.34	0.45
1:B:1120:ILE:HB	1:B:1134:PHE:HB2	1.97	0.45
1:B:1203:LEU:HD11	1:B:1211:LYS:HB3	1.98	0.45
1:B:824:VAL:HG22	1:B:863:ASN:HD22	1.81	0.45
1:B:165:ARG:HA	1:B:415:HIS:CD2	2.52	0.45
1:B:222:LEU:O	1:B:226:ILE:HG23	2.17	0.45
1:B:451:TYR:OH	1:B:484:LYS:HE3	2.17	0.45
2:A:87:G:H1	2:A:91:C:H42	1.64	0.45
1:B:76:LYS:HD2	2:A:49:A:OP1	2.17	0.45
1:B:380:LEU:HB3	1:B:386:THR:OG1	2.17	0.45
1:B:592:GLY:O	1:B:596:ASP:N	2.50	0.45
2:A:54:G:C6	2:A:55:C:N4	2.85	0.45
1:B:65:LYS:NZ	2:A:63:U:O2	2.36	0.45
1:B:626:PHE:N	1:B:626:PHE:HD1	2.15	0.45
1:B:1315:LEU:HD12	1:B:1321:PRO:HB3	1.98	0.45
1:B:84:GLU:OE1	1:B:85:ILE:N	2.50	0.45
1:B:692:ASN:HB3	1:B:695:GLN:HG3	1.98	0.45
1:B:862:LYS:H	1:B:862:LYS:HG2	1.48	0.45
1:B:1041:ASN:HD22	1:B:1044:ASN:ND2	2.13	0.45
1:B:1219:GLU:O	1:B:1220:LEU:HG	2.17	0.45
1:B:760:VAL:HG13	1:B:958:LEU:HG	1.99	0.45
1:B:961:LYS:HG2	1:B:965:ASP:OD1	2.17	0.45
1:B:1182:LEU:HD23	1:B:1182:LEU:HA	1.68	0.45
3:C:1:C:HO2'	3:C:2:U:H6	1.60	0.45
1:B:148:LYS:HD2	1:B:429:PHE:CG	2.50	0.45
1:B:439:LYS:HB3	1:B:476:TRP:NE1	2.32	0.45
1:B:499:ASP:HA	1:B:507:VAL:HG12	1.99	0.45
1:B:678:THR:O	1:B:682:PHE:N	2.50	0.45
1:B:883:TRP:CZ3	1:B:900:LEU:HD22	2.52	0.45
1:B:1279:ARG:HG2	1:B:1280:VAL:HG13	1.99	0.45
1:B:425:ARG:HA	1:B:425:ARG:HD3	1.74	0.45
1:B:840:ALA:O	1:B:864:ARG:NH1	2.50	0.45
1:B:101:LEU:HA	1:B:101:LEU:HD23	1.75	0.44
1:B:351:PHE:HB3	2:A:43:G:O6	2.17	0.44
2:A:11:C:H2'	2:A:12:U:C6	2.52	0.44
2:A:93:G:C6	2:A:94:U:C4	3.05	0.44
1:B:96:SER:O	1:B:100:ARG:N	2.50	0.44
1:B:363:ILE:O	1:B:401:LYS:NZ	2.41	0.44
1:B:423:LEU:HD13	1:B:437:ARG:HG3	1.99	0.44
1:B:138:LEU:HD11	1:B:153:LEU:HD13	1.98	0.44
1:B:160:HIS:O	1:B:160:HIS:ND1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:VAL:HG11	1:B:1247:GLY:N	2.32	0.44
1:B:1074:TRP:HZ2	1:B:1080:PHE:CD1	2.35	0.44
1:B:1170:GLU:O	1:B:1174:PHE:N	2.49	0.44
1:B:148:LYS:HB2	1:B:429:PHE:CG	2.52	0.44
1:B:148:LYS:HA	1:B:426:GLN:HE22	1.82	0.44
1:B:553:PHE:HZ	1:B:587:PHE:CD2	2.36	0.44
1:B:629:ARG:HB2	1:B:655:ARG:HH21	1.82	0.44
1:B:740:THR:O	1:B:744:VAL:HG23	2.17	0.44
1:B:825:ASP:H	1:B:879:MET:HE1	1.82	0.44
1:B:1099:GLU:O	1:B:1199:PRO:HB3	2.16	0.44
1:B:1142:SER:HG	1:B:1214:LEU:HD11	1.72	0.44
1:B:1347:LEU:HD13	1:B:1362:LEU:HD21	1.99	0.44
1:B:1006:SER:CA	1:B:1013:TYR:HB2	2.48	0.44
1:B:1232:TYR:CE1	1:B:1265:TYR:HB3	2.51	0.44
2:A:8:G:H2'	2:A:9:U:C6	2.53	0.44
1:B:302:LEU:HD12	1:B:306:LEU:HD13	2.00	0.44
1:B:305:ILE:HD12	1:B:305:ILE:HG23	1.73	0.44
1:B:465:MET:HE1	1:B:467:ARG:HG3	2.00	0.44
1:B:685:SER:O	1:B:685:SER:OG	2.34	0.44
1:B:705:LYS:HE2	1:B:705:LYS:HB3	1.35	0.44
1:B:794:GLN:O	1:B:798:GLU:N	2.51	0.44
1:B:531:THR:OG1	1:B:532:GLU:OE1	2.35	0.44
2:A:55:C:H1'	2:A:56:U:C6	2.53	0.44
1:B:142:LEU:H	1:B:142:LEU:HG	1.69	0.44
1:B:160:HIS:HD2	2:A:46:A:H5''	1.83	0.44
1:B:359:TYR:OH	2:A:43:G:O2'	2.13	0.44
1:B:864:ARG:HD3	1:B:1054:ASN:HD21	1.80	0.44
1:B:324:ARG:O	1:B:328:HIS:N	2.46	0.43
1:B:448:ILE:O	2:A:16:U:O2'	2.16	0.43
1:B:452:VAL:HG13	1:B:465:MET:HG3	2.00	0.43
2:A:23:U:H2'	2:A:24:U:C6	2.53	0.43
1:B:29:SER:HB2	2:A:91:C:N4	2.33	0.43
1:B:427:GLU:HB2	1:B:434:LYS:HG3	1.99	0.43
1:B:686:ASP:HB3	1:B:690:ASN:HA	2.00	0.43
1:B:921:LEU:HD23	1:B:1008:PHE:HD1	1.83	0.43
1:B:1014:LYS:H	1:B:1014:LYS:HG2	1.54	0.43
1:B:1121:ALA:HB2	1:B:1128:PRO:HD3	1.99	0.43
2:A:74:A:H2'	2:A:74:A:N3	2.33	0.43
1:B:140:LYS:HB2	1:B:318:SER:HB3	2.00	0.43
1:B:85:ILE:H	1:B:85:ILE:HG12	1.53	0.43
1:B:270:THR:O	1:B:273:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:NH2	2:A:58:G:H5'	2.34	0.43
1:B:16:VAL:HG23	1:B:53:PHE:HE1	1.84	0.43
1:B:135:ILE:O	1:B:139:ARG:N	2.49	0.43
1:B:226:ILE:HG13	1:B:227:ALA:N	2.33	0.43
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.82	0.43
1:B:251:ASN:ND2	1:B:263:LYS:HE2	2.34	0.43
1:B:256:PHE:HB2	1:B:258:LEU:CD2	2.48	0.43
1:B:297:SER:O	1:B:300:ILE:HB	2.18	0.43
1:B:465:MET:SD	1:B:466:THR:N	2.91	0.43
1:B:1266:LEU:HD23	1:B:1266:LEU:N	2.33	0.43
1:B:269:ASP:OD1	1:B:270:THR:N	2.52	0.43
1:B:862:LYS:O	1:B:864:ARG:N	2.52	0.43
1:B:1000:LYS:HD2	1:B:1066:ASN:N	2.34	0.43
1:B:1093:ASN:OD1	1:B:1355:LEU:HD23	2.19	0.43
1:B:90:MET:HG2	1:B:98:PHE:CZ	2.53	0.43
1:B:95:ASP:OD1	1:B:96:SER:OG	2.34	0.43
1:B:430:TYR:O	1:B:433:LEU:HB2	2.18	0.43
1:B:1182:LEU:O	1:B:1187:TYR:HB2	2.18	0.43
1:B:1245:LEU:CD2	1:B:1252:ASN:HD21	2.32	0.43
1:B:20:VAL:CB	1:B:47:LEU:HD23	2.46	0.43
2:A:8:G:N2	3:C:13:C:N3	2.64	0.43
2:A:93:G:C2	2:A:94:U:C2	3.06	0.43
1:B:86:PHE:CE2	1:B:151:LEU:HD11	2.53	0.43
1:B:112:LYS:CB	1:B:113:HIS:HD2	2.31	0.43
1:B:748:VAL:HB	1:B:753:ARG:CA	2.32	0.43
1:B:1215:ALA:HB1	1:B:1219:GLU:CB	2.45	0.43
1:B:1266:LEU:O	1:B:1270:ILE:HG12	2.19	0.43
1:B:16:VAL:HG23	1:B:53:PHE:CE1	2.53	0.43
1:B:35:LEU:HB2	1:B:1358:THR:HA	2.00	0.43
1:B:188:LEU:O	1:B:192:TYR:HB2	2.18	0.43
1:B:503:PRO:HG2	1:B:504:ASN:ND2	2.34	0.43
1:B:967:ARG:HE	1:B:973:TYR:C	2.22	0.43
1:B:973:TYR:CE2	1:B:1237:TYR:HB3	2.54	0.43
1:B:1179:ILE:H	1:B:1179:ILE:HG12	1.24	0.43
1:B:1269:ILE:HD12	1:B:1269:ILE:HG23	1.58	0.43
2:A:29:G:H22	2:A:41:A:H1'	1.84	0.43
1:B:500:LYS:HE3	1:B:661:ARG:HH22	1.84	0.42
1:B:761:ILE:HG12	1:B:956:ILE:O	2.19	0.42
1:B:1294:TYR:HD1	1:B:1295:ASN:ND2	2.16	0.42
2:A:24:U:H2'	2:A:25:U:C6	2.53	0.42
2:A:75:A:H2'	2:A:76:A:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ARG:HG3	1:B:395:ARG:NH1	2.34	0.42
1:B:1041:ASN:HB3	1:B:1044:ASN:OD1	2.20	0.42
1:B:1093:ASN:H	1:B:1093:ASN:HD22	1.67	0.42
1:B:1156:LYS:HG2	1:B:1157:LEU:N	2.34	0.42
1:B:18:TRP:CZ3	1:B:47:LEU:O	2.73	0.42
1:B:218:LYS:H	1:B:218:LYS:HG2	1.44	0.42
1:B:273:ASP:N	1:B:273:ASP:OD1	2.48	0.42
1:B:976:ARG:HA	1:B:982:HIS:CD2	2.54	0.42
1:B:1112:PRO:HA	2:A:23:U:H5''	2.01	0.42
1:B:1179:ILE:CG2	1:B:1190:VAL:HG21	2.46	0.42
1:B:1321:PRO:HB2	1:B:1334:LYS:H	1.85	0.42
1:B:1336:TYR:CD1	1:B:1336:TYR:N	2.88	0.42
1:B:119:PHE:HB3	1:B:121:ASN:ND2	2.35	0.42
1:B:215:ARG:H	1:B:215:ARG:HG3	1.59	0.42
1:B:1163:LEU:HD12	1:B:1339:THR:HB	2.00	0.42
1:B:334:LEU:HD12	1:B:334:LEU:HA	1.82	0.42
1:B:813:LEU:HB3	1:B:857:LEU:HB2	2.02	0.42
1:B:943:TYR:HD1	1:B:943:TYR:HA	1.69	0.42
1:B:1148:LYS:HE3	1:B:1157:LEU:HB3	2.01	0.42
1:B:325:TYR:O	1:B:328:HIS:HB3	2.20	0.42
1:B:723:HIS:HA	1:B:726:ASN:ND2	2.34	0.42
1:B:1232:TYR:HB3	1:B:1269:ILE:HD11	2.01	0.42
2:A:72:U:H2'	2:A:73:G:O4'	2.20	0.42
1:B:967:ARG:CZ	1:B:974:LYS:HB3	2.49	0.42
1:B:1066:ASN:HB3	1:B:1069:THR:OG1	2.20	0.42
1:B:1222:LYS:HZ3	1:B:1317:ASN:C	2.13	0.42
2:A:58:G:C2	2:A:60:C:C2	3.07	0.42
1:B:83:GLN:H	1:B:83:GLN:HG2	1.53	0.42
1:B:388:GLU:HA	1:B:391:VAL:HG23	2.02	0.42
1:B:465:MET:HE3	1:B:467:ARG:HG3	2.02	0.42
1:B:583:VAL:HG13	1:B:584:GLU:O	2.19	0.42
1:B:731:PRO:HA	1:B:734:LYS:HB2	2.01	0.42
1:B:647:VAL:O	1:B:651:LEU:HG	2.20	0.42
1:B:1049:GLU:HB2	1:B:1059:LYS:HA	2.01	0.42
1:B:1265:TYR:HD1	1:B:1265:TYR:HA	1.70	0.42
2:A:8:G:H1	3:C:13:C:N4	2.17	0.42
1:B:63:ARG:HA	1:B:66:ARG:CG	2.50	0.42
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.86	0.42
1:B:392:LYS:HB2	1:B:398:LEU:HD13	2.02	0.42
1:B:481:VAL:HG12	1:B:481:VAL:O	2.20	0.42
1:B:1263:LYS:O	1:B:1266:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1294:TYR:CZ	1:B:1298:ARG:HG3	2.55	0.42
1:B:44:LYS:HE2	2:A:87:G:H22	1.84	0.41
1:B:105:PHE:CE2	1:B:1131:TYR:CD1	3.08	0.41
1:B:251:ASN:HD22	1:B:263:LYS:HE2	1.85	0.41
1:B:328:HIS:ND1	1:B:400:ARG:O	2.49	0.41
1:B:530:VAL:HG22	1:B:537:PRO:HA	2.02	0.41
1:B:553:PHE:CZ	1:B:587:PHE:HD2	2.38	0.41
1:B:910:GLU:O	1:B:914:ALA:N	2.47	0.41
1:B:1064:GLU:HG3	1:B:1076:LYS:HE2	2.01	0.41
1:B:1080:PHE:O	1:B:1083:VAL:N	2.53	0.41
1:B:1257:LEU:HB3	1:B:1261:GLN:OE1	2.19	0.41
2:A:20:G:O2'	2:A:21:G:H5'	2.19	0.41
2:A:45:U:H2'	2:A:46:A:C8	2.55	0.41
1:B:7:ILE:O	1:B:759:ILE:HA	2.20	0.41
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.83	0.41
1:B:69:ARG:HG3	2:A:51:A:OP2	2.20	0.41
1:B:84:GLU:HA	1:B:87:SER:HB2	2.02	0.41
1:B:76:LYS:O	1:B:80:CYS:HB2	2.20	0.41
1:B:307:ARG:CB	1:B:323:LYS:HE2	2.45	0.41
1:B:76:LYS:HA	1:B:79:ILE:HG12	2.01	0.41
1:B:81:TYR:HD1	1:B:81:TYR:HA	1.53	0.41
1:B:980:ASN:ND2	1:B:1318:LEU:HD23	2.35	0.41
1:B:1221:GLN:HB3	1:B:1319:GLY:C	2.40	0.41
3:C:9:A:H2'	3:C:10:G:C8	2.54	0.41
1:B:59:ALA:HB3	2:A:13:A:H5''	2.02	0.41
1:B:402:GLN:HB2	2:A:45:U:C5'	2.51	0.41
1:B:451:TYR:HD1	1:B:452:VAL:N	2.17	0.41
1:B:626:PHE:CD2	1:B:631:MET:HG3	2.55	0.41
1:B:970:PHE:HE2	1:B:1080:PHE:CE2	2.38	0.41
1:B:974:LYS:NZ	1:B:986:ASP:OD2	2.54	0.41
1:B:1242:TYR:CD2	1:B:1303:ARG:HD2	2.56	0.41
1:B:112:LYS:HB2	1:B:113:HIS:HD2	1.85	0.41
1:B:841:ILE:HG23	1:B:871:PRO:HG2	2.03	0.41
1:B:985:HIS:O	1:B:988:TYR:N	2.54	0.41
1:B:1090:PRO:HD2	2:A:88:A:C2	2.56	0.41
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.71	0.41
1:B:560:THR:HG23	1:B:563:GLN:OE1	2.21	0.41
1:B:822:MET:HG3	1:B:883:TRP:NE1	2.35	0.41
1:B:825:ASP:HB2	1:B:879:MET:HE3	2.02	0.41
1:B:1347:LEU:O	1:B:1359:ARG:HG3	2.21	0.41
1:B:67:THR:O	1:B:70:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:O	1:B:224:ASN:HB2	2.20	0.41
1:B:636:LEU:HD11	1:B:648:MET:SD	2.61	0.41
1:B:662:LEU:HD22	1:B:663:SER:H	1.86	0.41
1:B:842:VAL:H	1:B:854:ASN:ND2	2.08	0.41
1:B:1280:VAL:HG23	1:B:1281:ILE:CG2	2.51	0.41
1:B:1315:LEU:HD22	1:B:1324:PHE:CZ	2.54	0.41
2:A:31:U:H3	2:A:38:A:H61	1.68	0.41
2:A:36:A:C5	2:A:37:U:H1'	2.55	0.41
1:B:402:GLN:HB2	2:A:45:U:H5'	2.02	0.41
1:B:531:THR:HB	1:B:575:PHE:CE2	2.56	0.41
1:B:668:ASN:CA	1:B:678:THR:HG21	2.33	0.41
1:B:750:VAL:HG21	1:B:1355:LEU:HD12	2.02	0.41
1:B:750:VAL:HG12	1:B:751:MET:SD	2.61	0.41
1:B:910:GLU:CB	1:B:1022:ILE:HG13	2.51	0.41
1:B:963:VAL:HG11	1:B:990:ASN:ND2	2.36	0.41
1:B:1123:LYS:HE2	2:A:52:A:OP1	2.21	0.41
1:B:188:LEU:O	1:B:188:LEU:HG	2.20	0.40
1:B:189:VAL:HA	1:B:192:TYR:HB3	2.02	0.40
1:B:283:GLY:O	1:B:285:GLN:N	2.52	0.40
1:B:870:VAL:HB	1:B:871:PRO:CD	2.51	0.40
3:C:4:C:C2	3:C:5:A:C8	3.09	0.40
1:B:697:ILE:HG23	1:B:698:HIS:ND1	2.36	0.40
1:B:79:ILE:O	1:B:83:GLN:HG2	2.21	0.40
1:B:448:ILE:O	2:A:16:U:H4'	2.21	0.40
1:B:917:ILE:O	1:B:921:LEU:HB2	2.22	0.40
1:B:1050:ILE:O	1:B:1050:ILE:HG12	2.21	0.40
1:B:1126:TRP:CD1	1:B:1126:TRP:N	2.88	0.40
1:B:1204:PHE:CD2	1:B:1342:VAL:HG11	2.57	0.40
1:B:1250:GLU:HA	1:B:1250:GLU:OE1	2.21	0.40
3:C:7:U:H2'	3:C:8:U:C6	2.56	0.40
1:B:282:ILE:O	1:B:282:ILE:HG22	2.22	0.40
1:B:454:PRO:HD3	2:A:15:U:H4'	2.02	0.40
1:B:1209:GLY:O	1:B:1224:ASN:ND2	2.54	0.40
1:B:353:ASP:OD1	1:B:356:LYS:N	2.54	0.40
1:B:1036:TYR:OH	1:B:1068:GLU:OE1	2.14	0.40
2:A:68:A:H2'	2:A:69:A:O4'	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LYS:O	1:B:532:GLU:O[4_565]	2.11	0.09

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	B	1334/1368 (98%)	1265 (95%)	65 (5%)	4 (0%)	37 70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1052	LEU
1	B	1051	THR
1	B	863	ASN
1	B	870	VAL

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	B	1186/1225 (97%)	960 (81%)	226 (19%)	1 7

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	THR
1	B	23	ASP

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Mol	Chain	Res	Type
1	B	43	ILE
1	B	44	LYS
1	B	46	ASN
1	B	66	ARG
1	B	72	TYR
1	B	80	CYS
1	B	81	TYR
1	B	83	GLN
1	B	84	GLU
1	B	85	ILE
1	B	86	PHE
1	B	87	SER
1	B	107	VAL
1	B	108	GLU
1	B	125	GLU
1	B	134	THR
1	B	146	THR
1	B	156	LEU
1	B	158	LEU
1	B	171	GLU
1	B	204	SER
1	B	212	LEU
1	B	215	ARG
1	B	218	LYS
1	B	219	SER
1	B	222	LEU
1	B	224	ASN
1	B	226	ILE
1	B	229	LEU
1	B	232	GLU
1	B	237	LEU
1	B	244	LEU
1	B	246	LEU
1	B	249	THR
1	B	255	ASN
1	B	257	ASP
1	B	258	LEU
1	B	266	LEU
1	B	269	ASP
1	B	273	ASP
1	B	302	LEU
1	B	307	ARG

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Mol	Chain	Res	Type
1	B	313	THR
1	B	314	LYS
1	B	317	LEU
1	B	321	MET
1	B	323	LYS
1	B	326	ASP
1	B	364	ASP
1	B	368	SER
1	B	373	TYR
1	B	387	GLU
1	B	389	LEU
1	B	390	LEU
1	B	404	THR
1	B	409	SER
1	B	424	ARG
1	B	428	ASP
1	B	432	PHE
1	B	435	ASP
1	B	444	LEU
1	B	451	TYR
1	B	467	ARG
1	B	475	PRO
1	B	477	ASN
1	B	484	LYS
1	B	487	SER
1	B	494	ARG
1	B	495	MET
1	B	497	ASN
1	B	499	ASP
1	B	502	LEU
1	B	504	ASN
1	B	506	LYS
1	B	513	LEU
1	B	517	TYR
1	B	524	LEU
1	B	526	LYS
1	B	529	TYR
1	B	531	THR
1	B	535	ARG
1	B	541	SER
1	B	552	LEU
1	B	555	THR

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Mol	Chain	Res	Type
1	B	560	THR
1	B	564	LEU
1	B	566	GLU
1	B	567	ASP
1	B	570	LYS
1	B	573	GLU
1	B	586	ARG
1	B	588	ASN
1	B	601	ILE
1	B	619	ILE
1	B	621	LEU
1	B	622	THR
1	B	624	THR
1	B	625	LEU
1	B	626	PHE
1	B	627	GLU
1	B	628	ASP
1	B	631	MET
1	B	642	LEU
1	B	643	PHE
1	B	646	LYS
1	B	654	ARG
1	B	662	LEU
1	B	666	LEU
1	B	671	ARG
1	B	678	THR
1	B	682	PHE
1	B	690	ASN
1	B	693	PHE
1	B	696	LEU
1	B	706	GLU
1	B	708	ILE
1	B	737	ILE
1	B	740	THR
1	B	747	LEU
1	B	751	MET
1	B	754	HIS
1	B	785	GLU
1	B	796	LEU
1	B	811	LEU
1	B	826	GLN
1	B	844	GLN

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Mol	Chain	Res	Type
1	B	850	ASP
1	B	853	ASP
1	B	854	ASN
1	B	857	LEU
1	B	859	ARG
1	B	861	ASP
1	B	862	LYS
1	B	866	LYS
1	B	868	ASP
1	B	878	LYS
1	B	900	LEU
1	B	902	LYS
1	B	917	ILE
1	B	918	LYS
1	B	919	ARG
1	B	921	LEU
1	B	933	GLN
1	B	938	ARG
1	B	939	MET
1	B	942	LYS
1	B	943	TYR
1	B	949	LEU
1	B	959	LYS
1	B	960	SER
1	B	961	LYS
1	B	962	LEU
1	B	964	SER
1	B	965	ASP
1	B	969	ASP
1	B	970	PHE
1	B	974	LYS
1	B	976	ARG
1	B	981	TYR
1	B	983	HIS
1	B	988	TYR
1	B	990	ASN
1	B	1008	PHE
1	B	1014	LYS
1	B	1019	ARG
1	B	1020	LYS
1	B	1021	MET
1	B	1024	LYS

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Mol	Chain	Res	Type
1	B	1037	PHE
1	B	1040	SER
1	B	1050	ILE
1	B	1056	GLU
1	B	1060	ARG
1	B	1062	LEU
1	B	1080	PHE
1	B	1113	LYS
1	B	1117	ASP
1	B	1118	LYS
1	B	1127	ASP
1	B	1135	ASP
1	B	1141	TYR
1	B	1142	SER
1	B	1145	VAL
1	B	1169	MET
1	B	1174	PHE
1	B	1179	ILE
1	B	1182	LEU
1	B	1188	LYS
1	B	1191	LYS
1	B	1192	LYS
1	B	1194	LEU
1	B	1198	LEU
1	B	1205	GLU
1	B	1206	LEU
1	B	1214	LEU
1	B	1226	LEU
1	B	1230	SER
1	B	1250	GLU
1	B	1252	ASN
1	B	1254	GLN
1	B	1256	GLN
1	B	1258	PHE
1	B	1261	GLN
1	B	1263	LYS
1	B	1266	LEU
1	B	1281	ILE
1	B	1282	LEU
1	B	1287	LEU
1	B	1289	LYS
1	B	1294	TYR

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Mol	Chain	Res	Type
1	B	1295	ASN
1	B	1296	LYS
1	B	1297	HIS
1	B	1298	ARG
1	B	1299	ASP
1	B	1300	LYS
1	B	1303	ARG
1	B	1314	THR
1	B	1333	ARG
1	B	1337	THR
1	B	1341	GLU
1	B	1342	VAL
1	B	1343	LEU
1	B	1352	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	GLN
1	B	113	HIS
1	B	854	ASN
1	B	920	GLN
1	B	990	ASN
1	B	1027	GLN
1	B	1041	ASN
1	B	1044	ASN
1	B	1091	GLN
1	B	1252	ASN
1	B	1254	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	97/98 (98%)	31 (31%)	1 (1%)
3	C	19/23 (82%)	0	0
All	All	116/121 (95%)	31 (26%)	1 (0%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	9	U
2	A	13	A
2	A	19	A
2	A	20	G
2	A	21	G
2	A	24	U
2	A	27	G
2	A	28	A
2	A	29	G
2	A	30	C
2	A	34	A
2	A	35	A
2	A	37	U
2	A	38	A
2	A	51	A
2	A	56	U
2	A	57	A
2	A	59	U
2	A	63	U
2	A	72	U
2	A	74	A
2	A	75	A
2	A	77	A
2	A	81	G
2	A	82	G
2	A	83	C
2	A	87	G
2	A	89	G
2	A	90	U
2	A	91	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	20	G

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1346/1368 (98%)	-1.22	0 100 100	3, 38, 98, 155	0
2	A	98/98 (100%)	-1.50	0 100 100	10, 69, 178, 219	0
3	C	20/23 (86%)	-1.52	0 100 100	19, 58, 237, 247	0
All	All	1464/1489 (98%)	-1.24	0 100 100	3, 40, 112, 247	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.