



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:24 am BST

PDB ID : 6K4U
Title : Crystal structure of xCas9 in complex with sgRNA and DNA (TGA PAM)
Authors : Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.
Deposited on : 2019-05-27
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

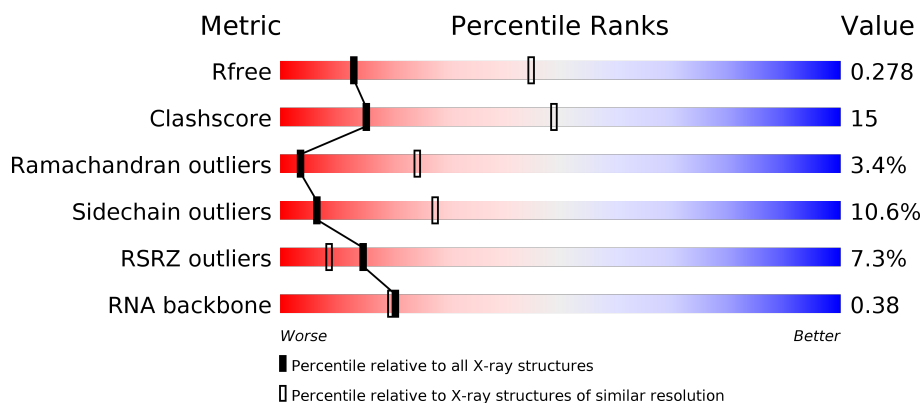
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 on 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	
2	A	83	
3	C	28	
4	D	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12814 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1312	Total	C	N	O	S	0	0	0
			10326	6583	1785	1941	17			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	262	THR	ALA	engineered mutation	UNP Q99ZW2
B	324	LEU	ARG	engineered mutation	UNP Q99ZW2
B	409	ILE	SER	engineered mutation	UNP Q99ZW2
B	480	LYS	GLU	engineered mutation	UNP Q99ZW2
B	543	ASP	GLU	engineered mutation	UNP Q99ZW2
B	694	ILE	MET	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1219	VAL	GLU	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	80	Total	C	N	O	P	0	0	0
			1710	768	313	549	80			

- Molecule 3 is a DNA chain called target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	27	Total	C	N	O	P	0	0	0
			552	268	92	165	27			

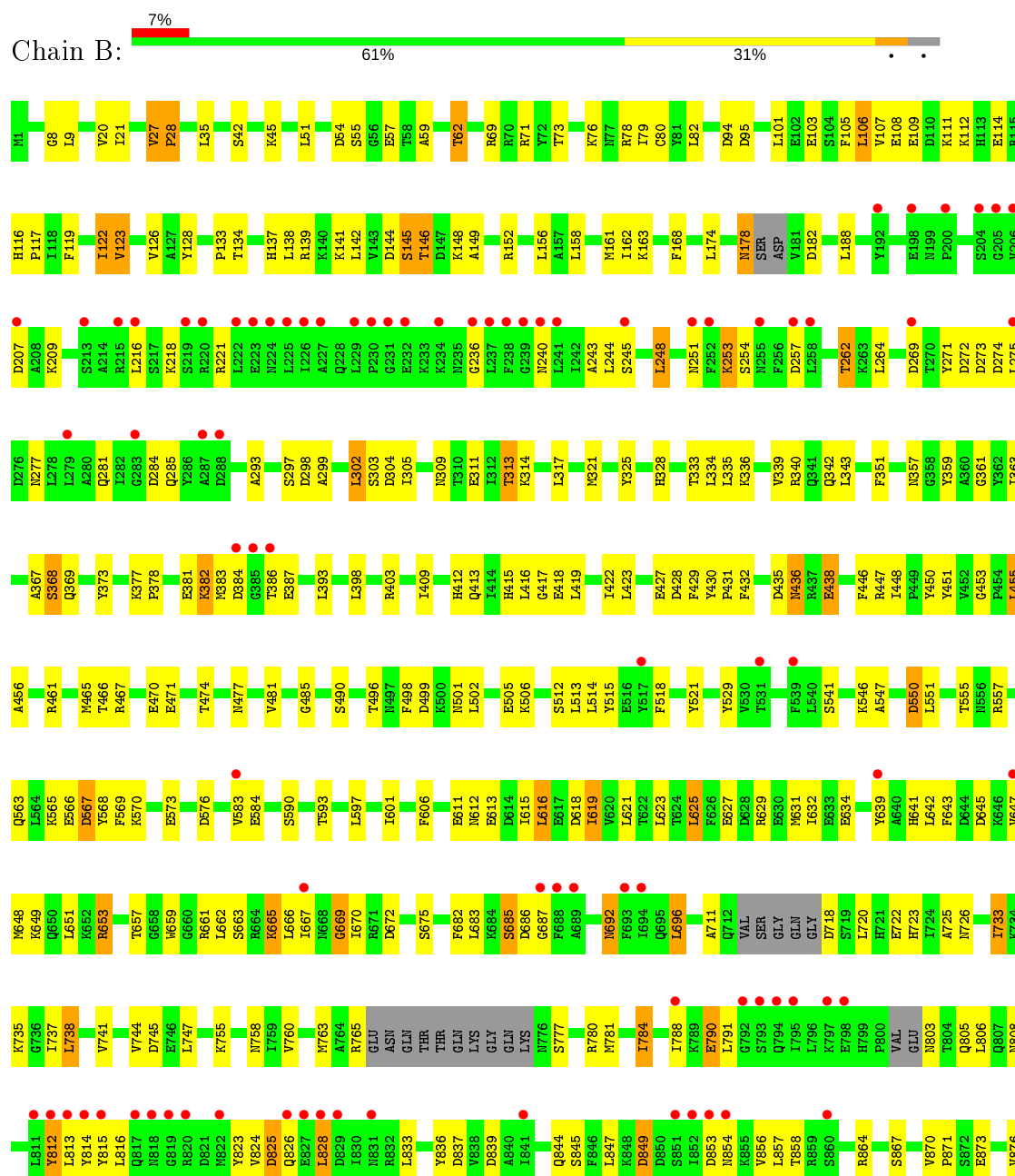
- Molecule 4 is a DNA chain called non-target DNA.

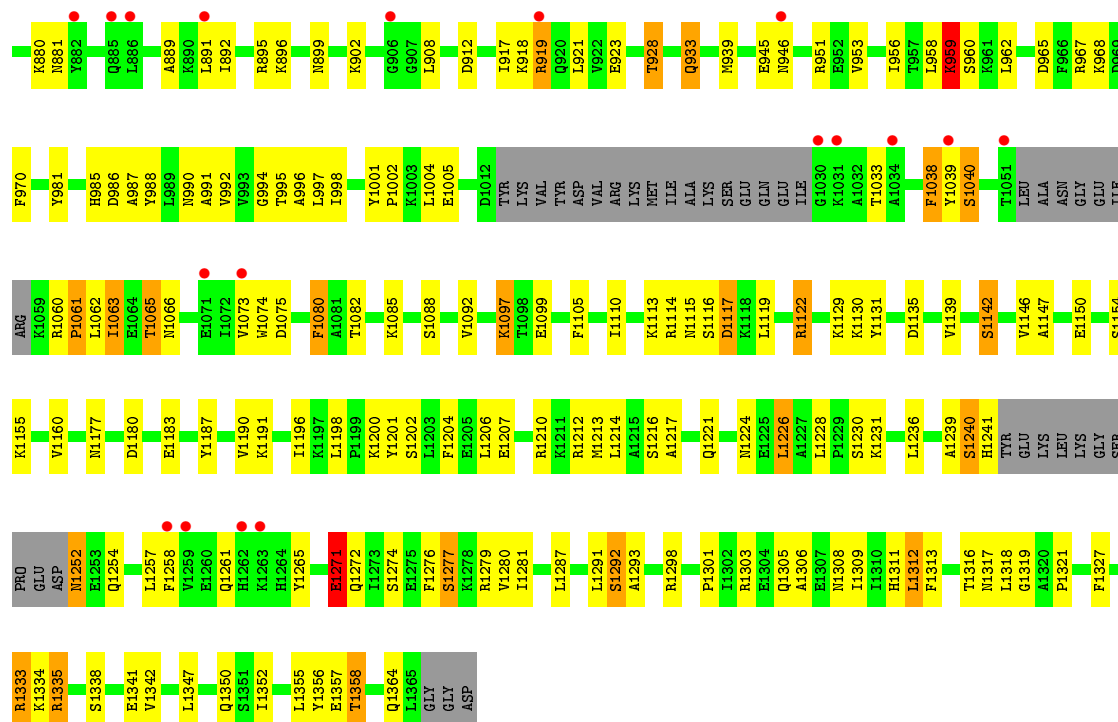
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			226	110	43	63	10			

3 Residue-property plots

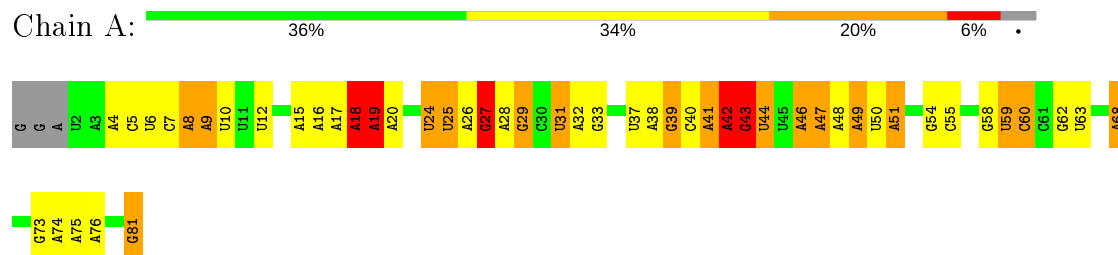
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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





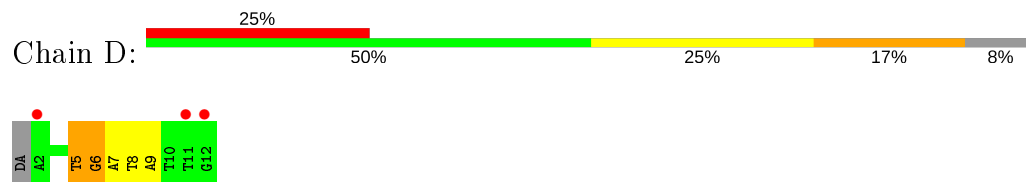
• Molecule 2: sgRNA



• Molecule 3: target DNA



• Molecule 4: non-target DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.00Å 70.31Å 190.08Å 90.00° 110.34° 90.00°	Depositor
Resolution (Å)	49.38 – 3.20 49.34 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.8 (49.38-3.20) 81.9 (49.34-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.220 , 0.282 0.221 , 0.278	Depositor DCC
R_{free} test set	1566 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12814	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.74	0/10504	0.90	0/14169
2	A	1.02	17/1917 (0.9%)	0.95	0/2984
3	C	0.70	1/617 (0.2%)	0.88	0/950
4	D	1.19	2/254 (0.8%)	0.87	0/391
All	All	0.80	20/13292 (0.2%)	0.91	0/18494

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	DG	O3'-P	-10.46	1.48	1.61
2	A	18	A	O3'-P	-9.44	1.49	1.61
2	A	49	A	O3'-P	-9.16	1.50	1.61
2	A	12	U	O3'-P	-8.95	1.50	1.61
4	D	5	DT	O3'-P	-8.53	1.50	1.61
2	A	47	A	O3'-P	-7.92	1.51	1.61
2	A	25	U	O3'-P	-7.68	1.51	1.61
2	A	60	C	O3'-P	-7.14	1.52	1.61
2	A	19	A	O3'-P	-6.88	1.52	1.61
2	A	41	A	O3'-P	-6.80	1.52	1.61
2	A	59	U	O3'-P	-6.40	1.53	1.61
2	A	48	A	O3'-P	-6.38	1.53	1.61
2	A	50	U	O3'-P	-6.18	1.53	1.61
2	A	28	A	O3'-P	-6.11	1.53	1.61
2	A	43	G	O3'-P	-6.09	1.53	1.61
2	A	46	A	O3'-P	-5.54	1.54	1.61
2	A	24	U	O3'-P	-5.54	1.54	1.61
2	A	42	A	O3'-P	-5.49	1.54	1.61
2	A	27	G	O3'-P	-5.48	1.54	1.61
3	C	10	DT	O3'-P	-5.32	1.54	1.61

There are no bond angle outliers.

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	10326	0	10134	301	0
2	A	1710	0	858	65	0
3	C	552	0	311	12	0
4	D	226	0	127	6	0
All	All	12814	0	11430	359	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 15.

All (359) 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)
2:A:18:A:H8	2:A:18:A:H5'	1.11	1.15
2:A:37:U:C2	2:A:38:A:C8	2.48	1.00
2:A:18:A:C8	2:A:18:A:H5'	1.98	0.99
1:B:615:ILE:HD12	1:B:615:ILE:H	1.27	0.98
2:A:42:A:O2'	2:A:43:G:OP1	1.87	0.93
2:A:37:U:O2	2:A:38:A:C8	2.30	0.85
1:B:71:ARG:NH1	2:A:18:A:H62	1.75	0.84
2:A:17:A:H2'	2:A:18:A:H5''	1.57	0.84
3:C:19:DA:H5''	3:C:19:DA:H8	1.43	0.83
1:B:870:VAL:HG22	1:B:871:PRO:HD2	1.60	0.83
3:C:19:DA:H5''	3:C:19:DA:C8	2.15	0.80
1:B:923:GLU:HG2	1:B:928:THR:HG21	1.64	0.78
1:B:1214:LEU:HD12	1:B:1214:LEU:O	1.83	0.77
1:B:616:LEU:HA	1:B:619:ILE:HG13	1.66	0.76
1:B:758:ASN:HD22	1:B:956:ILE:HD11	1.49	0.76
1:B:71:ARG:HH12	2:A:18:A:H62	1.33	0.75
2:A:42:A:HO2'	2:A:43:G:P	2.09	0.75
1:B:302:LEU:O	1:B:304:ASP:N	2.20	0.74
1:B:1226:LEU:HD12	1:B:1226:LEU:C	2.08	0.74
2:A:17:A:C2'	2:A:18:A:H5''	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:37:U:N3	2:A:38:A:N7	2.37	0.72
1:B:615:ILE:N	1:B:615:ILE:HD12	2.02	0.71
1:B:499:ASP:OD2	1:B:663:SER:HB2	1.90	0.71
1:B:615:ILE:CD1	1:B:615:ILE:H	2.04	0.71
1:B:805:GLN:O	1:B:808:ASN:ND2	2.24	0.71
1:B:1277:SER:HA	1:B:1281:ILE:HB	1.73	0.70
1:B:1335:ARG:HH11	1:B:1335:ARG:CG	2.04	0.70
1:B:448:ILE:HG12	1:B:455:LEU:HD21	1.73	0.69
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.14	0.67
1:B:1082:THR:O	1:B:1085:LYS:HB3	1.94	0.67
1:B:51:LEU:HD22	1:B:1352:ILE:HG13	1.76	0.67
1:B:615:ILE:HG23	1:B:639:TYR:CE1	2.29	0.67
1:B:1321:PRO:HG2	1:B:1335:ARG:HA	1.77	0.67
1:B:755:LYS:HE2	1:B:939:MET:O	1.94	0.67
2:A:58:G:C2	2:A:60:C:O2	2.49	0.66
2:A:37:U:C2	2:A:38:A:H8	2.09	0.65
1:B:557:ARG:O	1:B:590:SER:HB2	1.97	0.65
1:B:1216:SER:OG	1:B:1217:ALA:N	2.27	0.65
1:B:970:PHE:CD1	1:B:1080:PHE:HZ	2.15	0.64
1:B:182:ASP:HB3	1:B:209:LYS:H	1.62	0.64
2:A:46:A:H2'	2:A:47:A:C8	2.33	0.64
1:B:377:LYS:HB3	1:B:378:PRO:HD3	1.79	0.64
1:B:813:LEU:HD22	1:B:857:LEU:HB3	1.79	0.63
1:B:1001:TYR:HB2	1:B:1004:LEU:HD12	1.80	0.63
2:A:8:A:O2'	2:A:9:A:OP1	2.15	0.63
2:A:18:A:H8	2:A:18:A:C5'	2.01	0.63
2:A:19:A:H2'	2:A:20:A:O4'	1.98	0.63
1:B:967:ARG:NH1	1:B:986:ASP:OD1	2.33	0.62
3:C:18:DA:H2''	3:C:19:DA:H5''	1.81	0.62
1:B:1147:ALA:HB2	1:B:1190:VAL:HA	1.82	0.62
2:A:18:A:O2'	2:A:19:A:H5'	2.00	0.61
1:B:111:LYS:NZ	2:A:25:U:O2'	2.26	0.61
1:B:568:TYR:O	1:B:573:GLU:N	2.28	0.61
1:B:1065:THR:OG1	1:B:1066:ASN:N	2.33	0.61
1:B:1239:ALA:O	1:B:1303:ARG:HA	2.01	0.60
2:A:37:U:N3	2:A:38:A:C8	2.68	0.60
1:B:499:ASP:OD2	1:B:663:SER:CB	2.49	0.60
1:B:8:GLY:HA3	1:B:987:ALA:O	2.01	0.60
1:B:342:GLN:NE2	1:B:384:ASP:O	2.34	0.60
1:B:1204:PHE:CD2	1:B:1342:VAL:HG13	2.37	0.60
1:B:1114:ARG:NH1	4:D:9:DA:OP1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1335:ARG:HH11	1:B:1335:ARG:HG2	1.66	0.59
1:B:1356:TYR:HB3	2:A:81:G:N1	2.17	0.59
1:B:133:PRO:HG2	1:B:137:HIS:CE1	2.38	0.58
1:B:1258:PHE:O	1:B:1261:GLN:O	2.20	0.58
1:B:615:ILE:CG2	1:B:639:TYR:CE1	2.85	0.58
1:B:243:ALA:O	1:B:248:LEU:HB2	2.03	0.58
1:B:448:ILE:O	2:A:16:A:H4'	2.03	0.58
1:B:615:ILE:HG23	1:B:639:TYR:HE1	1.67	0.58
1:B:828:LEU:HD21	1:B:836:TYR:CD2	2.38	0.58
1:B:139:ARG:NH1	1:B:418:GLU:OE1	2.36	0.58
1:B:450:TYR:CD1	1:B:451:TYR:N	2.72	0.58
2:A:29:G:N2	2:A:41:A:H1'	2.19	0.58
1:B:1139:VAL:HG11	1:B:1216:SER:OG	2.04	0.58
1:B:615:ILE:CG2	1:B:639:TYR:CD1	2.87	0.57
1:B:207:ASP:OD1	1:B:207:ASP:O	2.23	0.57
1:B:518:PHE:CG	1:B:667:ILE:HD12	2.40	0.57
2:A:18:A:C2'	2:A:19:A:H5'	2.33	0.57
1:B:293:ALA:O	1:B:297:SER:N	2.34	0.57
1:B:499:ASP:OD2	1:B:663:SER:N	2.36	0.57
1:B:918:LYS:HB3	1:B:1039:TYR:CD2	2.40	0.57
1:B:69:ARG:HD2	2:A:62:G:N7	2.19	0.57
1:B:111:LYS:HZ1	2:A:25:U:HO2'	1.51	0.57
1:B:718:ASP:HA	1:B:722:GLU:OE1	2.05	0.57
1:B:995:THR:O	1:B:998:ILE:HG22	2.04	0.57
2:A:32:A:N6	2:A:38:A:N6	2.53	0.57
2:A:31:U:H3	2:A:38:A:H61	1.51	0.57
1:B:648:MET:HA	1:B:651:LEU:HD12	1.86	0.57
1:B:1113:LYS:HB2	1:B:1129:LYS:O	2.05	0.56
1:B:685:SER:C	1:B:687:GLY:H	2.09	0.56
1:B:412:HIS:CE1	1:B:413:GLN:HE22	2.24	0.56
1:B:597:LEU:O	1:B:601:ILE:HG13	2.06	0.56
1:B:35:LEU:HB2	1:B:1358:THR:HB	1.87	0.56
1:B:1210:ARG:NH2	1:B:1341:GLU:OE1	2.39	0.56
1:B:816:LEU:HD23	1:B:816:LEU:O	2.05	0.56
1:B:146:THR:OG1	1:B:146:THR:O	2.23	0.56
1:B:236:GLY:O	1:B:240:ASN:ND2	2.38	0.56
1:B:876:VAL:O	1:B:880:LYS:CB	2.54	0.56
1:B:791:LEU:CD1	1:B:889:ALA:HB2	2.35	0.56
1:B:1309:ILE:O	1:B:1312:LEU:N	2.36	0.55
1:B:784:ILE:HD11	1:B:812:TYR:CE1	2.41	0.55
1:B:216:LEU:O	1:B:221:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HG22	1:B:126:VAL:CG2	2.36	0.55
1:B:981:TYR:CD2	1:B:1092:VAL:HG21	2.42	0.55
1:B:933:GLN:O	1:B:933:GLN:NE2	2.40	0.55
1:B:921:LEU:HD22	1:B:962:LEU:CD2	2.36	0.55
1:B:178:ASN:HD22	1:B:178:ASN:C	2.11	0.54
1:B:71:ARG:HH12	2:A:18:A:N6	2.04	0.54
1:B:921:LEU:HD22	1:B:962:LEU:HD23	1.90	0.54
1:B:1001:TYR:CB	1:B:1004:LEU:HD12	2.37	0.54
1:B:382:LYS:HG3	1:B:383:MET:N	2.22	0.54
1:B:158:LEU:HA	1:B:161:MET:HE3	1.90	0.54
1:B:450:TYR:CD1	1:B:450:TYR:C	2.81	0.54
1:B:919:ARG:O	1:B:959:LYS:NZ	2.37	0.53
1:B:951:ARG:HH11	1:B:951:ARG:HB2	1.73	0.53
1:B:1236:LEU:O	1:B:1240:SER:OG	2.24	0.53
3:C:11:DT:C5	3:C:12:DT:H73	2.44	0.53
1:B:513:LEU:HG	1:B:593:THR:HG21	1.91	0.53
1:B:521:TYR:HB3	1:B:683:LEU:O	2.09	0.53
2:A:42:A:N3	2:A:42:A:C5'	2.72	0.53
1:B:264:LEU:CD2	1:B:274:ASP:HB3	2.39	0.53
1:B:178:ASN:OD1	1:B:299:ALA:HB1	2.09	0.53
2:A:18:A:C5'	2:A:18:A:C8	2.83	0.53
4:D:8:DT:H2''	4:D:9:DA:O4'	2.09	0.53
1:B:119:PHE:HE2	1:B:128:TYR:HB2	1.74	0.52
1:B:547:ALA:HA	1:B:550:ASP:HB2	1.91	0.52
1:B:54:ASP:O	1:B:735:LYS:NZ	2.38	0.52
1:B:837:ASP:N	1:B:837:ASP:OD1	2.42	0.52
1:B:1357:GLU:O	1:B:1358:THR:HG22	2.10	0.52
1:B:518:PHE:CD1	1:B:667:ILE:HD12	2.44	0.52
1:B:870:VAL:HG21	1:B:902:LYS:HB3	1.92	0.52
1:B:333:THR:O	1:B:336:LYS:HB2	2.10	0.52
2:A:73:G:H2'	2:A:75:A:N7	2.25	0.52
1:B:970:PHE:CG	1:B:1080:PHE:HZ	2.27	0.52
1:B:917:ILE:HG21	1:B:1040:SER:HB2	1.92	0.51
1:B:1196:ILE:HG22	1:B:1198:LEU:HG	1.90	0.51
1:B:383:MET:O	1:B:386:THR:OG1	2.25	0.51
1:B:1150:GLU:HB2	1:B:1155:LYS:HA	1.92	0.51
1:B:788:ILE:HD11	1:B:815:TYR:O	2.11	0.51
1:B:335:LEU:O	1:B:339:VAL:HG23	2.11	0.51
1:B:615:ILE:HG22	1:B:639:TYR:CD1	2.46	0.51
1:B:760:VAL:HG11	1:B:990:ASN:O	2.11	0.51
3:C:19:DA:H2''	3:C:20:DT:O5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:NH1	1:B:161:MET:HG2	2.26	0.51
1:B:1135:ASP:C	1:B:1135:ASP:OD1	2.49	0.51
1:B:1116:SER:OG	1:B:1117:ASP:N	2.42	0.50
1:B:340:ARG:NH2	2:A:41:A:OP2	2.43	0.50
2:A:54:G:C6	2:A:55:C:N4	2.80	0.50
1:B:114:GLU:OE2	1:B:116:HIS:HB2	2.12	0.50
1:B:1277:SER:HA	1:B:1281:ILE:CB	2.42	0.50
1:B:970:PHE:CG	1:B:1080:PHE:CZ	2.99	0.50
1:B:780:ARG:O	1:B:784:ILE:HB	2.12	0.50
1:B:665:LYS:O	1:B:669:GLY:N	2.45	0.50
1:B:496:THR:HG21	1:B:659:TRP:CE2	2.47	0.49
1:B:1333:ARG:CZ	4:D:5:DT:H72	2.42	0.49
1:B:781:MET:O	1:B:781:MET:CG	2.60	0.49
1:B:381:GLU:HG3	1:B:382:LYS:N	2.27	0.49
1:B:498:PHE:HB3	1:B:505:GLU:O	2.12	0.49
2:A:38:A:N3	2:A:38:A:H2'	2.28	0.49
1:B:1073:VAL:HG23	1:B:1074:TRP:N	2.27	0.49
1:B:1291:LEU:C	1:B:1293:ALA:H	2.16	0.49
2:A:32:A:C6	2:A:38:A:C6	3.01	0.49
1:B:108:GLU:O	1:B:111:LYS:HB2	2.13	0.49
1:B:122:ILE:HG22	1:B:126:VAL:HG23	1.95	0.49
1:B:833:LEU:HD22	1:B:833:LEU:O	2.13	0.49
1:B:117:PRO:HD2	2:A:26:A:O2'	2.13	0.49
1:B:485:GLY:HA2	1:B:631:MET:SD	2.53	0.49
1:B:514:LEU:HD12	1:B:613:GLU:OE1	2.13	0.49
1:B:1216:SER:CB	4:D:7:DA:OP1	2.61	0.49
1:B:1088:SER:OG	1:B:1230:SER:HB2	2.12	0.49
1:B:641:HIS:NE2	1:B:642:LEU:HG	2.28	0.49
1:B:94:ASP:OD2	1:B:152:ARG:NH1	2.45	0.48
1:B:790:GLU:HA	1:B:790:GLU:OE1	2.13	0.48
1:B:1226:LEU:HD12	1:B:1226:LEU:O	2.13	0.48
1:B:427:GLU:O	1:B:428:ASP:C	2.51	0.48
1:B:645:ASP:O	1:B:649:LYS:HB2	2.13	0.48
1:B:1105:PHE:CZ	2:A:51:A:C6	3.01	0.48
1:B:939:MET:HE2	1:B:953:VAL:HG21	1.95	0.48
1:B:328:HIS:NE2	1:B:359:TYR:OH	2.35	0.48
1:B:844:GLN:HA	1:B:847:LEU:O	2.14	0.48
1:B:551:LEU:O	1:B:555:THR:OG1	2.24	0.48
1:B:996:ALA:C	1:B:998:ILE:H	2.17	0.48
2:A:33:G:O5'	2:A:33:G:H8	1.97	0.47
1:B:1240:SER:HB2	1:B:1241:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ASN:HB3	1:B:653:ARG:CZ	2.44	0.47
1:B:760:VAL:HG22	1:B:956:ILE:HB	1.97	0.47
1:B:59:ALA:O	1:B:62:THR:HG23	2.14	0.47
1:B:45:LYS:HD3	1:B:1355:LEU:HA	1.96	0.47
1:B:1206:LEU:HD13	1:B:1210:ARG:CZ	2.45	0.47
1:B:720:LEU:O	1:B:723:HIS:N	2.48	0.47
1:B:824:VAL:O	1:B:826:GLN:N	2.47	0.47
1:B:923:GLU:HG2	1:B:928:THR:CG2	2.42	0.47
1:B:1280:VAL:HG23	1:B:1281:ILE:HD13	1.96	0.46
1:B:1313:PHE:O	1:B:1316:THR:N	2.48	0.46
1:B:78:ARG:NH2	1:B:162:ILE:O	2.34	0.46
1:B:601:ILE:HA	1:B:647:VAL:HG13	1.98	0.46
1:B:985:HIS:O	1:B:988:TYR:HB3	2.16	0.46
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.48	0.46
1:B:343:LEU:HD11	1:B:382:LYS:HD2	1.97	0.46
1:B:806:LEU:O	1:B:812:TYR:HB2	2.15	0.46
1:B:1200:LYS:HE2	1:B:1201:TYR:CZ	2.50	0.46
1:B:1200:LYS:O	1:B:1201:TYR:HB2	2.15	0.46
1:B:1210:ARG:HA	1:B:1280:VAL:HG12	1.97	0.46
1:B:1364:GLN:O	1:B:1364:GLN:HG3	2.15	0.46
1:B:368:SER:OG	1:B:369:GLN:N	2.49	0.46
1:B:956:ILE:HG22	1:B:958:LEU:HD21	1.97	0.46
1:B:363:ILE:HD12	2:A:44:U:H5'	1.98	0.46
1:B:1350:GLN:O	2:A:68:A:N3	2.49	0.46
1:B:823:TYR:CE2	1:B:864:ARG:HB3	2.51	0.46
1:B:849:ASP:HB2	1:B:854:ASN:HD22	1.81	0.46
1:B:996:ALA:O	1:B:998:ILE:N	2.49	0.45
1:B:895:ARG:O	1:B:899:ASN:ND2	2.49	0.45
1:B:1271:GLU:O	1:B:1274:SER:N	2.49	0.45
1:B:251:ASN:HD21	1:B:253:LYS:HG2	1.82	0.45
1:B:629:ARG:O	1:B:632:ILE:HB	2.17	0.45
1:B:1060:ARG:O	1:B:1061:PRO:O	2.34	0.45
1:B:1204:PHE:CE2	1:B:1342:VAL:HG13	2.51	0.45
1:B:1214:LEU:HD13	1:B:1216:SER:O	2.16	0.45
1:B:435:ASP:HB2	1:B:436:ASN:HD22	1.80	0.45
1:B:79:ILE:HD11	1:B:163:LYS:HB2	1.99	0.45
1:B:1110:ILE:HG12	1:B:1122:ARG:HD2	1.98	0.45
1:B:141:LYS:HD2	1:B:145:SER:HB3	1.98	0.45
1:B:335:LEU:O	1:B:335:LEU:HD23	2.17	0.45
1:B:69:ARG:O	1:B:73:THR:HG23	2.16	0.45
1:B:1114:ARG:HD2	1:B:1116:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LEU:HD21	1:B:415:HIS:HE2	1.82	0.45
1:B:21:ILE:CD1	1:B:991:ALA:HB1	2.47	0.45
1:B:839:ASP:N	1:B:856:VAL:O	2.50	0.45
1:B:566:GLU:O	1:B:570:LYS:CB	2.65	0.45
1:B:685:SER:C	1:B:687:GLY:N	2.70	0.45
1:B:1214:LEU:CD1	1:B:1214:LEU:C	2.85	0.45
1:B:1291:LEU:O	1:B:1293:ALA:N	2.50	0.45
1:B:1207:GLU:HG2	1:B:1207:GLU:O	2.12	0.44
1:B:138:LEU:HG	1:B:142:LEU:HD12	1.98	0.44
1:B:430:TYR:HA	1:B:431:PRO:HD3	1.88	0.44
1:B:965:ASP:HA	1:B:968:LYS:HB2	1.98	0.44
3:C:19:DA:C5'	3:C:19:DA:C8	2.95	0.44
2:A:54:G:H2'	2:A:55:C:C6	2.53	0.44
1:B:373:TYR:CE1	1:B:398:LEU:HB3	2.53	0.44
1:B:621:LEU:HG	1:B:625:LEU:HD22	1.98	0.44
1:B:76:LYS:HD3	2:A:49:A:OP1	2.17	0.44
1:B:1308:ASN:OD1	1:B:1327:PHE:N	2.46	0.44
1:B:393:LEU:HB2	1:B:398:LEU:HD22	2.00	0.44
1:B:309:ASN:HB3	1:B:311:GLU:HG2	2.00	0.44
1:B:892:ILE:HG21	1:B:896:LYS:HE2	1.99	0.44
1:B:1062:LEU:HD23	1:B:1063:ILE:N	2.32	0.44
1:B:148:LYS:HE3	1:B:430:TYR:CZ	2.53	0.44
1:B:313:THR:OG1	1:B:314:LYS:N	2.50	0.44
1:B:403:ARG:HH11	2:A:20:A:P	2.40	0.44
1:B:168:PHE:HB3	1:B:447:ARG:NH1	2.33	0.44
1:B:450:TYR:O	2:A:15:A:O2'	2.31	0.44
1:B:565:LYS:O	1:B:569:PHE:CB	2.66	0.44
1:B:733:ILE:HD11	1:B:763:MET:HE3	2.00	0.44
2:A:75:A:H2'	2:A:76:A:C8	2.53	0.44
1:B:1356:TYR:HD2	2:A:81:G:C4	2.36	0.44
1:B:1001:TYR:N	1:B:1002:PRO:HD3	2.32	0.44
1:B:116:HIS:CE1	1:B:122:ILE:HD12	2.53	0.44
1:B:1298:ARG:HA	1:B:1305:GLN:OE1	2.17	0.44
1:B:747:LEU:HD23	1:B:747:LEU:HA	1.87	0.44
1:B:474:THR:N	1:B:477:ASN:OD1	2.51	0.44
2:A:73:G:HO2'	2:A:75:A:H62	1.66	0.43
1:B:264:LEU:HD22	1:B:274:ASP:HB3	1.99	0.43
1:B:814:TYR:HE1	1:B:828:LEU:HB3	1.83	0.43
1:B:870:VAL:HG22	1:B:871:PRO:CD	2.40	0.43
2:A:4:A:C6	2:A:5:C:C4	3.06	0.43
2:A:26:A:H5'	2:A:27:G:OP2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:OE1	1:B:1130:LYS:HE2	2.19	0.43
4:D:6:DG:H2''	4:D:7:DA:H5'	1.99	0.43
2:A:6:U:H2'	2:A:7:C:C6	2.54	0.43
1:B:864:ARG:NH2	1:B:867:SER:HA	2.33	0.43
1:B:958:LEU:HD11	1:B:994:GLY:HA2	2.00	0.43
1:B:1142:SER:OG	1:B:1216:SER:O	2.36	0.43
1:B:446:PHE:CG	1:B:447:ARG:N	2.87	0.43
1:B:616:LEU:HD23	1:B:616:LEU:O	2.18	0.43
1:B:1280:VAL:HG23	1:B:1281:ILE:CD1	2.49	0.43
1:B:271:TYR:O	1:B:275:LEU:N	2.52	0.43
1:B:889:ALA:HB3	1:B:891:LEU:HD12	2.00	0.43
3:C:11:DT:C6	3:C:12:DT:H71	2.53	0.43
1:B:107:VAL:HG22	1:B:1131:TYR:OH	2.19	0.43
1:B:1221:GLN:HB2	1:B:1319:GLY:O	2.19	0.43
1:B:302:LEU:O	1:B:305:ILE:N	2.39	0.43
2:A:18:A:H2'	2:A:19:A:H5'	2.00	0.43
1:B:1201:TYR:HA	1:B:1213:MET:HB3	2.00	0.43
1:B:737:ILE:O	1:B:741:VAL:HG23	2.19	0.43
1:B:1082:THR:O	1:B:1085:LYS:N	2.52	0.43
1:B:1252:ASN:N	1:B:1254:GLN:OE1	2.50	0.43
1:B:149:ALA:O	1:B:430:TYR:OH	2.32	0.43
1:B:361:GLY:O	1:B:367:ALA:HB3	2.19	0.43
1:B:188:LEU:HD23	1:B:188:LEU:O	2.18	0.42
1:B:423:LEU:O	1:B:427:GLU:HG2	2.19	0.42
1:B:512:SER:O	1:B:515:TYR:N	2.51	0.42
1:B:784:ILE:HD12	1:B:806:LEU:HD13	2.01	0.42
1:B:1216:SER:OG	4:D:7:DA:OP1	2.25	0.42
1:B:692:ASN:O	1:B:696:LEU:HD22	2.19	0.42
1:B:917:ILE:HG21	1:B:1040:SER:CB	2.50	0.42
3:C:11:DT:C5	3:C:12:DT:C7	3.02	0.42
2:A:32:A:N1	2:A:38:A:C5	2.87	0.42
1:B:1183:GLU:HA	1:B:1187:TYR:O	2.19	0.42
1:B:1226:LEU:C	1:B:1226:LEU:CD1	2.80	0.42
1:B:20:VAL:O	1:B:27:VAL:HA	2.19	0.42
1:B:1254:GLN:O	1:B:1257:LEU:HB2	2.19	0.42
1:B:1224:ASN:OD1	1:B:1280:VAL:HB	2.19	0.42
1:B:122:ILE:O	1:B:123:VAL:C	2.58	0.42
1:B:643:PHE:HB3	1:B:647:VAL:HB	2.01	0.42
1:B:1277:SER:HB2	1:B:1287:LEU:HD22	2.01	0.42
1:B:456:ALA:O	1:B:467:ARG:NH1	2.52	0.42
1:B:1226:LEU:HB3	1:B:1276:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:PHE:O	1:B:606:PHE:CG	2.72	0.42
1:B:722:GLU:O	1:B:725:ALA:HB3	2.20	0.42
1:B:106:LEU:O	1:B:111:LYS:NZ	2.35	0.42
1:B:450:TYR:CE1	1:B:451:TYR:HB3	2.55	0.42
3:C:18:DA:H2''	3:C:19:DA:C5'	2.48	0.42
1:B:105:PHE:CE1	2:A:24:U:H1'	2.55	0.42
1:B:142:LEU:HB3	1:B:422:ILE:HG12	2.02	0.42
1:B:297:SER:OG	1:B:298:ASP:N	2.53	0.42
1:B:738:LEU:O	1:B:738:LEU:HD22	2.19	0.41
3:C:19:DA:C4	3:C:20:DT:C5	3.07	0.41
1:B:1097:LYS:HE3	1:B:1099:GLU:OE2	2.19	0.41
1:B:1228:LEU:HD12	1:B:1228:LEU:HA	1.97	0.41
1:B:1279:ARG:HG2	1:B:1280:VAL:HG13	2.02	0.41
1:B:253:LYS:HG3	1:B:254:SER:N	2.35	0.41
1:B:601:ILE:HG22	1:B:647:VAL:CG1	2.49	0.41
1:B:814:TYR:CE1	1:B:828:LEU:HB3	2.55	0.41
1:B:144:ASP:O	1:B:145:SER:C	2.58	0.41
3:C:16:DC:H2'	3:C:17:DA:C8	2.55	0.41
1:B:1177:ASN:ND2	1:B:1180:ASP:OD2	2.53	0.41
1:B:777:SER:HB3	1:B:803:ASN:O	2.20	0.41
1:B:813:LEU:O	1:B:813:LEU:HD23	2.21	0.41
2:A:29:G:C2	2:A:41:A:N3	2.88	0.41
2:A:32:A:C6	2:A:38:A:N6	2.89	0.41
1:B:1303:ARG:O	1:B:1306:ALA:N	2.54	0.41
1:B:27:VAL:O	1:B:28:PRO:O	2.38	0.41
1:B:501:ASN:HB2	1:B:666:LEU:HD22	2.02	0.41
1:B:51:LEU:HD22	1:B:1352:ILE:CG1	2.49	0.41
1:B:828:LEU:CD2	1:B:836:TYR:CE2	3.03	0.41
2:A:6:U:O5'	2:A:6:U:H6	2.03	0.41
1:B:156:LEU:HA	1:B:156:LEU:HD23	1.87	0.41
1:B:302:LEU:C	1:B:304:ASP:N	2.74	0.41
2:A:39:G:C6	2:A:40:C:C4	3.09	0.41
2:A:47:A:H8	2:A:47:A:O5'	2.03	0.41
2:A:54:G:C5	2:A:55:C:N4	2.89	0.41
2:A:58:G:C6	2:A:60:C:N3	2.88	0.41
1:B:76:LYS:HD2	1:B:76:LYS:HA	1.88	0.41
1:B:325:TYR:CD1	2:A:44:U:C2	3.09	0.41
1:B:9:LEU:HD11	1:B:744:VAL:CG2	2.51	0.41
1:B:563:GLN:O	1:B:567:ASP:HB2	2.21	0.40
1:B:1075:ASP:O	1:B:1075:ASP:OD1	2.40	0.40
1:B:262:THR:HG21	1:B:281:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD22	1:B:351:PHE:HZ	1.86	0.40
1:B:148:LYS:HD2	1:B:429:PHE:HB3	2.02	0.40
1:B:945:GLU:HG2	1:B:946:ASN:OD1	2.21	0.40
1:B:453:GLY:HA2	2:A:16:A:H5'	2.02	0.40
1:B:662:LEU:HD11	2:A:4:A:H4'	2.04	0.40
1:B:755:LYS:CE	1:B:939:MET:O	2.67	0.40
1:B:758:ASN:ND2	1:B:956:ILE:HD11	2.27	0.40
2:A:25:U:H6	2:A:25:U:O5'	2.05	0.40
1:B:1287:LEU:O	1:B:1291:LEU:HG	2.21	0.40
3:C:6:DT:C2	3:C:7:DC:C6	3.09	0.40
1:B:416:LEU:HA	1:B:416:LEU:HD12	1.93	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	B	1296/1368 (95%)	1077 (83%)	175 (14%)	44 (3%)	3	24

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	SER
1	B	584	GLU
1	B	653	ARG
1	B	670	ILE
1	B	685	SER
1	B	1061	PRO
1	B	262	THR
1	B	417	GLY
1	B	506	LYS
1	B	825	ASP

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Mol	Chain	Res	Type
1	B	959	LYS
1	B	992	VAL
1	B	997	LEU
1	B	1005	GLU
1	B	1231	LYS
1	B	1292	SER
1	B	28	PRO
1	B	145	SER
1	B	438	GLU
1	B	455	LEU
1	B	541	SER
1	B	675	SER
1	B	908	LEU
1	B	95	ASP
1	B	461	ARG
1	B	546	LYS
1	B	634	GLU
1	B	665	LYS
1	B	686	ASP
1	B	711	ALA
1	B	1038	PHE
1	B	1277	SER
1	B	218	LYS
1	B	257	ASP
1	B	302	LEU
1	B	576	ASP
1	B	611	GLU
1	B	1301	PRO
1	B	784	ILE
1	B	1271	GLU
1	B	1063	ILE
1	B	123	VAL
1	B	502	LEU
1	B	669	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1074/1226 (88%)	960 (89%)	114 (11%)	6	27

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	42	SER
1	B	55	SER
1	B	57	GLU
1	B	62	THR
1	B	80	CYS
1	B	82	LEU
1	B	101	LEU
1	B	103	GLU
1	B	106	LEU
1	B	112	LYS
1	B	122	ILE
1	B	134	THR
1	B	146	THR
1	B	174	LEU
1	B	178	ASN
1	B	244	LEU
1	B	245	SER
1	B	248	LEU
1	B	253	LYS
1	B	269	ASP
1	B	272	ASP
1	B	273	ASP
1	B	284	ASP
1	B	285	GLN
1	B	313	THR
1	B	321	MET
1	B	334	LEU
1	B	357	ASN
1	B	368	SER
1	B	382	LYS
1	B	387	GLU
1	B	409	ILE
1	B	419	LEU
1	B	432	PHE
1	B	436	ASN
1	B	438	GLU
1	B	465	MET

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Mol	Chain	Res	Type
1	B	466	THR
1	B	470	GLU
1	B	471	GLU
1	B	481	VAL
1	B	490	SER
1	B	529	TYR
1	B	550	ASP
1	B	567	ASP
1	B	583	VAL
1	B	612	ASN
1	B	616	LEU
1	B	618	ASP
1	B	619	ILE
1	B	623	LEU
1	B	625	LEU
1	B	627	GLU
1	B	657	THR
1	B	661	ARG
1	B	672	ASP
1	B	682	PHE
1	B	692	ASN
1	B	696	LEU
1	B	726	ASN
1	B	733	ILE
1	B	738	LEU
1	B	745	ASP
1	B	765	ARG
1	B	790	GLU
1	B	812	TYR
1	B	825	ASP
1	B	828	LEU
1	B	845	SER
1	B	849	ASP
1	B	853	ASP
1	B	858	THR
1	B	873	GLU
1	B	881	ASN
1	B	912	ASP
1	B	919	ARG
1	B	928	THR
1	B	933	GLN
1	B	959	LYS

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Mol	Chain	Res	Type
1	B	960	SER
1	B	1033	THR
1	B	1038	PHE
1	B	1040	SER
1	B	1065	THR
1	B	1080	PHE
1	B	1097	LYS
1	B	1115	ASN
1	B	1117	ASP
1	B	1119	LEU
1	B	1122	ARG
1	B	1142	SER
1	B	1146	VAL
1	B	1154	SER
1	B	1160	VAL
1	B	1191	LYS
1	B	1202	SER
1	B	1226	LEU
1	B	1240	SER
1	B	1252	ASN
1	B	1265	TYR
1	B	1271	GLU
1	B	1272	GLN
1	B	1292	SER
1	B	1311	HIS
1	B	1312	LEU
1	B	1317	ASN
1	B	1318	LEU
1	B	1333	ARG
1	B	1334	LYS
1	B	1335	ARG
1	B	1338	SER
1	B	1347	LEU
1	B	1358	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	ASN
1	B	251	ASN
1	B	277	ASN
1	B	413	GLN

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Mol	Chain	Res	Type
1	B	436	ASN
1	B	504	ASN
1	B	726	ASN
1	B	1066	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	79/83 (95%)	17 (21%)	4 (5%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	9	A
2	A	10	U
2	A	18	A
2	A	19	A
2	A	27	G
2	A	29	G
2	A	31	U
2	A	39	G
2	A	42	A
2	A	43	G
2	A	44	U
2	A	51	A
2	A	59	U
2	A	63	U
2	A	68	A
2	A	74	A
2	A	81	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	8	A
2	A	9	A
2	A	18	A
2	A	42	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 carbohydrates 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1312/1368 (95%)	0.24	102 (7%) 13 7	24, 83, 157, 224	0
2	A	80/83 (96%)	-0.22	0 100 100	23, 50, 125, 143	0
3	C	27/28 (96%)	0.04	0 100 100	46, 67, 130, 155	0
4	D	11/12 (91%)	0.72	3 (27%) 0 0	49, 76, 162, 168	0
All	All	1430/1491 (95%)	0.21	105 (7%) 15 9	23, 82, 155, 224	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	LEU	9.2
1	B	252	PHE	7.5
1	B	1030	GLY	7.2
1	B	229	LEU	7.0
1	B	237	LEU	6.3
1	B	818	ASN	6.0
1	B	788	ILE	5.9
1	B	241	LEU	5.8
1	B	251	ASN	5.6
1	B	238	PHE	5.2
1	B	817	GLN	4.9
1	B	814	TYR	4.9
1	B	269	ASP	4.8
1	B	688	PHE	4.8
1	B	257	ASP	4.6
1	B	841	ILE	4.4
1	B	198	GLU	4.3
1	B	216	LEU	4.2
1	B	822	MET	4.2
1	B	854	ASN	4.2
1	B	287	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	240	ASN	4.1
1	B	853	ASP	4.1
1	B	815	TYR	4.0
1	B	215	ARG	4.0
1	B	200	PRO	3.9
1	B	205	GLY	3.9
1	B	829	ASP	3.9
1	B	222	LEU	3.8
1	B	288	ASP	3.8
1	B	239	GLY	3.8
1	B	828	LEU	3.8
1	B	851	SER	3.7
4	D	12	DG	3.7
1	B	236	GLY	3.6
1	B	385	GLY	3.6
1	B	794	GLN	3.6
1	B	1031	LYS	3.5
1	B	1259	VAL	3.4
1	B	795	ILE	3.4
1	B	793	SER	3.4
1	B	226	ILE	3.3
1	B	283	GLY	3.3
1	B	223	GLU	3.3
1	B	798	GLU	3.3
1	B	220	ARG	3.3
1	B	224	ASN	3.2
1	B	204	SER	3.1
1	B	231	GLY	3.1
1	B	819	GLY	3.1
1	B	1051	THR	3.0
1	B	517	TYR	2.9
1	B	230	PRO	2.9
1	B	275	LEU	2.9
1	B	687	GLY	2.9
1	B	539	PHE	2.9
1	B	531	THR	2.8
1	B	891	LEU	2.8
1	B	852	ILE	2.7
1	B	234	LYS	2.7
1	B	206	VAL	2.7
1	B	219	SER	2.7
1	B	885	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	882	TYR	2.7
1	B	192	TYR	2.7
1	B	227	ALA	2.7
1	B	1262	HIS	2.6
1	B	946	ASN	2.6
1	B	245	SER	2.6
1	B	258	LEU	2.6
1	B	792	GLY	2.6
1	B	906	GLY	2.6
1	B	255	ASN	2.6
1	B	919	ARG	2.6
1	B	279	LEU	2.6
1	B	860	SER	2.6
1	B	232	GLU	2.5
1	B	207	ASP	2.5
1	B	812	TYR	2.5
1	B	667	ILE	2.5
1	B	831	ASN	2.5
1	B	886	LEU	2.5
1	B	689	ALA	2.5
1	B	1258	PHE	2.5
1	B	639	TYR	2.4
1	B	813	LEU	2.4
1	B	647	VAL	2.4
1	B	1263	LYS	2.3
1	B	826	GLN	2.3
1	B	1034	ALA	2.3
4	D	2	DA	2.3
1	B	386	THR	2.3
4	D	11	DT	2.3
1	B	1071	GLU	2.2
1	B	797	LYS	2.2
1	B	583	VAL	2.2
1	B	694	ILE	2.1
1	B	213	SER	2.1
1	B	1073	VAL	2.1
1	B	820	ARG	2.1
1	B	811	LEU	2.1
1	B	693	PHE	2.1
1	B	1039	TYR	2.0
1	B	827	GLU	2.0
1	B	384	ASP	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 carbohydrates 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.