



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:05 am BST

PDB ID : 6K3Z
Title : Crystal structure of dCas9 in complex with sgRNA and DNA (TGA PAM)
Authors : Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.
Deposited on : 2019-05-22
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

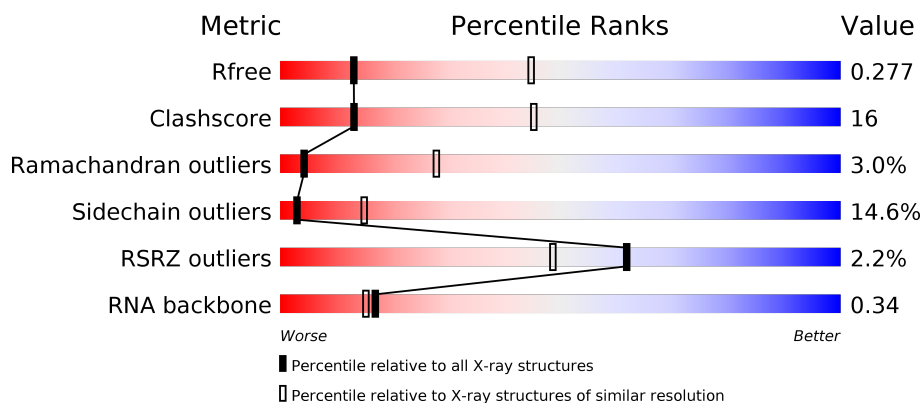
1 Overall quality at a glance

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	A	83	 27% 41% 25% 5%
2	B	1368	 2% 58% 32% 6%
3	C	28	 7% 39% 61%
4	D	12	 8% 33% 58% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13284 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 RNA chain called RNA (81-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	P	0	0	0
			1732	778	318	555	81			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1315	Total	C	N	O	S	0	0	0
			10758	6858	1865	2013	22			

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

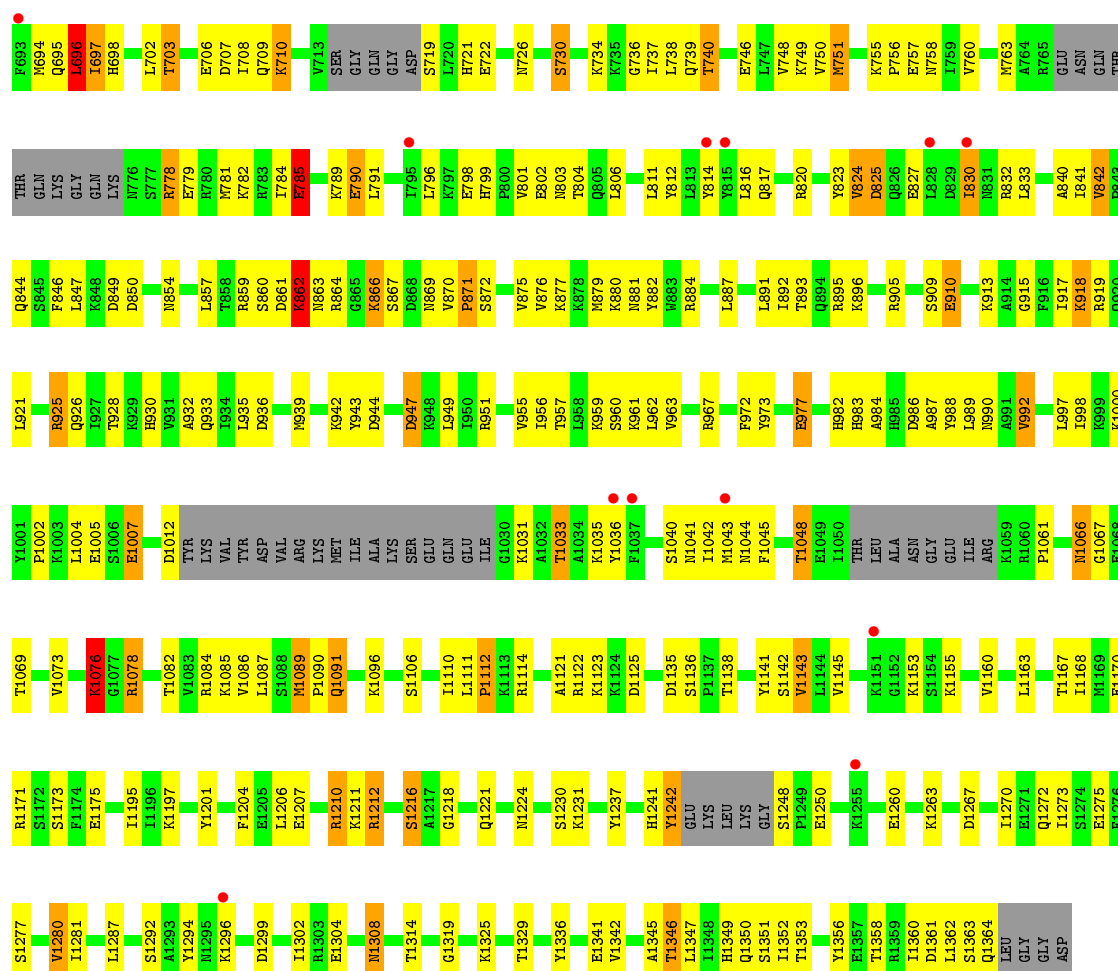
- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			568	277	95	169	27			

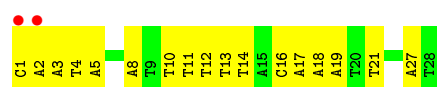
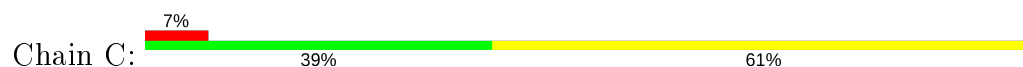
- Molecule 4 is a DNA chain called DNA (5'-D(*AP*AP*AP*TP*GP*AP*TP*AP*TP*TP*G)-3').

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

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 3: DNA (28-MER)



• Molecule 4: DNA (5'-D(*AP*AP*AP*TP*GP*AP*TP*AP*TP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.94Å 69.06Å 190.05Å 90.00° 110.21° 90.00°	Depositor
Resolution (Å)	40.89 – 3.20 48.93 – 3.19	Depositor EDS
% Data completeness (in resolution range)	87.0 (40.89-3.20) 87.1 (48.93-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.197 , 0.276 0.202 , 0.277	Depositor DCC
R_{free} test set	1567 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13284	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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	A	0.85	11/1942 (0.6%)	0.95	0/3023
2	B	0.74	0/10947	0.93	0/14709
3	C	0.69	1/635 (0.2%)	0.99	0/978
4	D	0.70	0/254	0.95	0/391
All	All	0.75	12/13778 (0.1%)	0.94	0/19101

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	U	O3'-P	-7.28	1.52	1.61
1	A	45	U	O3'-P	-7.06	1.52	1.61
1	A	46	A	O3'-P	-6.82	1.52	1.61
1	A	43	G	O3'-P	-6.33	1.53	1.61
1	A	13	G	O3'-P	-5.84	1.54	1.61
3	C	10	DT	O3'-P	-5.60	1.54	1.61
1	A	28	A	O3'-P	-5.41	1.54	1.61
1	A	39	G	O3'-P	-5.29	1.54	1.61
1	A	5	C	O3'-P	-5.29	1.54	1.61
1	A	55	C	O3'-P	-5.14	1.54	1.61
1	A	69	A	O3'-P	-5.12	1.55	1.61
1	A	3	A	O3'-P	-5.04	1.55	1.61

There are no bond angle outliers.

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	1732	0	869	95	0
2	B	10758	0	10918	319	0
3	C	568	0	323	29	0
4	D	226	0	127	9	0
All	All	13284	0	12237	414	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 16.

All (414) 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:41:A:H2'	1:A:42:A:H5''	1.25	1.09
1:A:42:A:H8	1:A:42:A:H5'	1.18	1.07
1:A:81:G:H5'	1:A:81:G:C8	1.91	1.06
1:A:54:G:C6	1:A:55:C:N4	2.25	1.04
1:A:27:G:H5'	1:A:28:A:O5'	1.59	1.02
1:A:41:A:C2'	1:A:42:A:H5''	1.91	1.01
2:B:824:VAL:HG21	2:B:863:ASN:HD22	1.27	0.98
1:A:5:C:H5'	1:A:5:C:H6	1.25	0.97
2:B:672:ASP:HB3	2:B:675:SER:OG	1.68	0.92
1:A:81:G:H5'	1:A:81:G:H8	1.34	0.91
1:A:4:A:C2'	1:A:5:C:H5''	2.02	0.89
2:B:1349:HIS:HB2	2:B:1358:THR:OG1	1.75	0.87
1:A:4:A:H2'	1:A:5:C:H5''	1.57	0.87
1:A:42:A:C8	1:A:42:A:H5'	2.09	0.86
3:C:11:DT:H2'	3:C:12:DT:C6	2.14	0.83
2:B:1210:ARG:HA	2:B:1280:VAL:HG22	1.61	0.83
1:A:5:C:C6	1:A:5:C:H5'	2.13	0.82
1:A:54:G:C5	1:A:55:C:N4	2.47	0.82
2:B:812:TYR:CZ	2:B:816:LEU:HD11	2.15	0.82
1:A:32:A:H3'	1:A:33:G:H8	1.44	0.81
2:B:893:THR:HG23	2:B:896:LYS:H	1.46	0.81
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.64	0.80
2:B:69:ARG:O	2:B:73:THR:HG23	1.82	0.80
1:A:4:A:H2'	1:A:5:C:C5'	2.13	0.77
2:B:397:ASP:O	2:B:397:ASP:OD1	2.04	0.76
2:B:178:ASN:O	2:B:178:ASN:ND2	2.19	0.76
1:A:54:G:H2'	1:A:55:C:C6	2.21	0.74
2:B:1096:LYS:HE3	2:B:1201:TYR:CE1	2.24	0.73
1:A:46:A:H2'	1:A:47:A:C8	2.22	0.73
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1308:ASN:N	2:B:1308:ASN:HD22	1.88	0.71
2:B:1277:SER:HA	2:B:1281:ILE:HB	1.72	0.71
2:B:1210:ARG:HD2	2:B:1280:VAL:HA	1.73	0.70
2:B:303:SER:OG	2:B:304:ASP:N	2.23	0.69
2:B:1352:ILE:HG23	2:B:1353:THR:HG23	1.74	0.69
2:B:817:GLN:HE22	2:B:857:LEU:H	1.40	0.69
2:B:324:ARG:HH22	2:B:407:ASN:HD21	1.40	0.69
1:A:32:A:H3'	1:A:33:G:C8	2.27	0.69
1:A:38:A:H5''	1:A:38:A:H8	1.57	0.69
1:A:44:U:N3	2:B:328:HIS:CD2	2.61	0.69
2:B:335:LEU:O	2:B:339:VAL:HG23	1.93	0.68
1:A:27:G:C5'	1:A:28:A:O5'	2.40	0.68
2:B:114:GLU:HG2	2:B:120:GLY:O	1.94	0.67
2:B:414:ILE:HD12	2:B:414:ILE:C	2.14	0.67
1:A:42:A:H8	1:A:42:A:C5'	2.00	0.67
2:B:86:PHE:CE2	2:B:155:TYR:HB2	2.28	0.67
3:C:11:DT:C4	3:C:12:DT:O4	2.47	0.67
3:C:5:DA:C2	4:D:9:DA:C2	2.83	0.67
3:C:11:DT:H3'	3:C:12:DT:H71	1.77	0.66
2:B:188:LEU:HA	2:B:292:ALA:HB1	1.77	0.66
2:B:450:TYR:OH	2:B:627:GLU:HG2	1.96	0.66
2:B:117:PRO:HD2	2:B:125:GLU:OE2	1.96	0.66
1:A:18:A:OP2	2:B:71:ARG:NH1	2.29	0.66
2:B:736:GLY:O	2:B:740:THR:HG22	1.96	0.65
1:A:24:U:O2	2:B:105:PHE:CD1	2.49	0.65
2:B:324:ARG:NH2	2:B:407:ASN:HD21	1.95	0.65
2:B:357:ASN:ND2	2:B:371:GLU:HB3	2.12	0.65
2:B:812:TYR:CE2	2:B:816:LEU:HD11	2.31	0.65
2:B:1041:ASN:HB3	2:B:1044:ASN:ND2	2.13	0.64
1:A:45:U:H5'	2:B:402:GLN:HG2	1.77	0.64
2:B:179:SER:O	2:B:209:LYS:NZ	2.29	0.64
3:C:12:DT:O5'	3:C:12:DT:H6	1.80	0.64
2:B:1212:ARG:NH1	2:B:1336:TYR:CZ	2.66	0.63
2:B:891:LEU:O	2:B:892:ILE:HG23	1.98	0.63
1:A:75:A:H2'	1:A:76:A:C8	2.34	0.63
2:B:45:LYS:HA	2:B:1091:GLN:OE1	1.99	0.63
2:B:988:TYR:O	2:B:992:VAL:HG23	1.98	0.63
2:B:528:LYS:O	2:B:580:ILE:HA	1.98	0.62
2:B:876:VAL:O	2:B:880:LYS:HB2	1.99	0.62
2:B:48:ILE:HG12	2:B:984:ALA:HB1	1.80	0.62
1:A:38:A:C5'	1:A:38:A:C8	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ARG:O	2:B:73:THR:CG2	2.48	0.61
2:B:719:SER:HB3	2:B:722:GLU:OE2	2.01	0.61
2:B:790:GLU:O	2:B:790:GLU:HG3	1.99	0.61
2:B:1002:PRO:O	2:B:1005:GLU:HG3	2.01	0.61
2:B:243:ALA:O	2:B:248:LEU:HB2	1.99	0.61
1:A:18:A:OP1	2:B:165:ARG:HD3	2.00	0.60
2:B:624:THR:HA	2:B:656:TYR:O	2.01	0.60
2:B:678:THR:O	2:B:681:ASP:HB2	2.01	0.60
2:B:474:THR:HG23	2:B:477:ASN:HD21	1.67	0.60
2:B:599:LYS:O	2:B:602:LYS:HD2	2.02	0.60
2:B:507:VAL:HG11	2:B:660:GLY:O	2.02	0.59
2:B:155:TYR:C	2:B:155:TYR:CD2	2.76	0.59
1:A:18:A:C2	1:A:19:A:C5	2.91	0.59
2:B:114:GLU:HG2	2:B:120:GLY:C	2.23	0.59
2:B:778:ARG:HG2	2:B:779:GLU:H	1.66	0.59
2:B:1210:ARG:CA	2:B:1280:VAL:HG22	2.32	0.59
2:B:870:VAL:HG13	2:B:871:PRO:HD2	1.85	0.58
2:B:212:LEU:O	2:B:221:ARG:NE	2.37	0.58
2:B:450:TYR:OH	2:B:627:GLU:CG	2.52	0.58
2:B:305:ILE:HG22	2:B:306:LEU:HD23	1.86	0.58
2:B:1141:TYR:HE2	2:B:1171:ARG:HD2	1.69	0.58
2:B:373:TYR:CE1	2:B:398:LEU:HB3	2.39	0.58
2:B:847:LEU:HD21	2:B:895:ARG:HH22	1.69	0.58
3:C:12:DT:H71	3:C:12:DT:OP2	2.04	0.57
2:B:789:LYS:C	2:B:791:LEU:H	2.08	0.57
1:A:39:G:H8	1:A:39:G:OP2	1.87	0.57
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.37	0.57
2:B:343:LEU:HD12	2:B:383:MET:SD	2.44	0.57
2:B:748:VAL:O	2:B:749:LYS:C	2.42	0.57
3:C:18:DA:H2'	3:C:19:DA:H8	1.68	0.57
2:B:442:LYS:HA	2:B:445:THR:HB	1.87	0.57
2:B:861:ASP:O	2:B:862:LYS:C	2.42	0.57
2:B:746:GLU:OE1	2:B:1352:ILE:HG22	2.04	0.56
2:B:530:VAL:HG23	2:B:579:GLU:HB3	1.86	0.56
2:B:106:LEU:O	2:B:111:LYS:NZ	2.28	0.56
1:A:17:A:C2	3:C:13:DT:C2	2.92	0.56
1:A:7:C:C2'	1:A:8:A:H5'	2.35	0.56
1:A:47:A:O2'	2:B:101:LEU:O	2.23	0.56
2:B:1111:LEU:O	2:B:1112:PRO:O	2.23	0.56
2:B:525:THR:HG22	2:B:690:ASN:HB3	1.87	0.56
1:A:44:U:C2	2:B:328:HIS:CD2	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:A:C3'	1:A:42:A:H5''	2.35	0.56
2:B:789:LYS:O	2:B:791:LEU:N	2.38	0.56
2:B:529:TYR:HA	2:B:579:GLU:O	2.06	0.56
3:C:11:DT:C4	3:C:12:DT:C4	2.93	0.56
2:B:178:ASN:OD1	2:B:309:ASN:HA	2.06	0.56
2:B:407:ASN:HB3	2:B:410:ILE:HD12	1.87	0.55
2:B:1210:ARG:HG3	2:B:1280:VAL:HG22	1.88	0.55
1:A:69:A:H1'	2:B:1358:THR:HG21	1.88	0.55
1:A:5:C:OP1	2:B:515:TYR:OH	2.25	0.55
2:B:507:VAL:HG11	2:B:660:GLY:C	2.27	0.55
2:B:1078:ARG:O	2:B:1082:THR:HG23	2.06	0.55
2:B:572:ILE:HG22	2:B:572:ILE:O	2.05	0.55
1:A:75:A:C6	1:A:76:A:C6	2.95	0.55
2:B:321:MET:HE1	2:B:324:ARG:CZ	2.37	0.55
1:A:27:G:O2'	2:B:129:HIS:CG	2.60	0.54
2:B:689:ALA:O	2:B:691:ARG:N	2.41	0.54
1:A:18:A:C2	1:A:19:A:C4	2.95	0.54
2:B:1216:SER:C	2:B:1218:GLY:H	2.09	0.54
2:B:672:ASP:CB	2:B:675:SER:OG	2.47	0.54
2:B:866:LYS:N	2:B:866:LYS:HD3	2.22	0.54
2:B:936:ASP:OD2	2:B:951:ARG:NH2	2.32	0.54
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.88	0.54
1:A:5:C:C5'	1:A:5:C:H6	2.08	0.54
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.90	0.54
2:B:539:PHE:HB3	2:B:690:ASN:ND2	2.23	0.54
1:A:16:A:C2	3:C:14:DT:C2	2.96	0.54
3:C:16:DC:H2'	3:C:17:DA:C8	2.42	0.54
2:B:1096:LYS:HE3	2:B:1201:TYR:CD1	2.42	0.53
2:B:165:ARG:O	2:B:412:HIS:HA	2.08	0.53
2:B:305:ILE:HD11	2:B:409:SER:HB3	1.90	0.53
2:B:420:HIS:CD2	2:B:441:GLU:OE1	2.61	0.53
2:B:114:GLU:OE2	2:B:116:HIS:ND1	2.38	0.53
2:B:502:LEU:O	2:B:504:ASN:N	2.41	0.53
2:B:672:ASP:HA	2:B:703:THR:CG2	2.39	0.53
2:B:926:GLN:O	2:B:930:HIS:HD2	1.92	0.53
2:B:317:LEU:O	2:B:320:SER:N	2.42	0.53
2:B:956:ILE:HD11	2:B:998:ILE:HG12	1.90	0.53
2:B:760:VAL:HA	2:B:956:ILE:O	2.09	0.53
2:B:814:TYR:CZ	2:B:830:ILE:HG23	2.44	0.53
3:C:11:DT:N3	3:C:12:DT:C4	2.76	0.53
1:A:47:A:H8	1:A:47:A:O5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:VAL:CG1	2:B:660:GLY:C	2.77	0.52
2:B:278:LEU:O	2:B:281:GLN:N	2.29	0.52
2:B:672:ASP:OD2	2:B:675:SER:OG	2.23	0.52
1:A:63:U:H4'	1:A:64:U:OP2	2.09	0.52
2:B:572:ILE:C	2:B:573:GLU:HG2	2.30	0.52
2:B:1086:VAL:O	2:B:1089:MET:HB2	2.10	0.52
2:B:565:LYS:HG2	2:B:578:VAL:HG13	1.91	0.52
3:C:11:DT:H2'	3:C:12:DT:C5	2.45	0.52
2:B:1304:GLU:O	2:B:1308:ASN:ND2	2.43	0.52
2:B:143:VAL:HG11	2:B:315:ALA:HB2	1.91	0.52
2:B:322:ILE:O	2:B:325:TYR:HB3	2.09	0.52
1:A:7:C:O2'	1:A:8:A:H5'	2.09	0.52
2:B:260:GLU:HA	2:B:260:GLU:OE1	2.10	0.52
2:B:169:LEU:HD21	3:C:13:DT:H1'	1.91	0.52
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.42	0.52
2:B:456:ALA:O	2:B:467:ARG:NH1	2.41	0.51
2:B:763:MET:SD	2:B:928:THR:HG22	2.49	0.51
2:B:305:ILE:HD11	2:B:409:SER:CB	2.40	0.51
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.93	0.51
1:A:38:A:C5'	1:A:38:A:H8	2.21	0.51
2:B:1361:ASP:O	2:B:1363:SER:N	2.42	0.51
2:B:548:ILE:HG23	2:B:552:LEU:HD12	1.92	0.51
3:C:2:DA:C2	4:D:12:DG:N2	2.79	0.51
2:B:1206:LEU:CD2	2:B:1345:ALA:HB2	2.41	0.51
2:B:869:ASN:OD1	2:B:870:VAL:N	2.42	0.51
2:B:1167:THR:O	2:B:1170:GLU:N	2.44	0.50
1:A:35:A:H2'	1:A:36:A:N9	2.26	0.50
3:C:18:DA:H2'	3:C:19:DA:C8	2.45	0.50
2:B:530:VAL:HG13	2:B:537:PRO:HA	1.93	0.50
2:B:670:ILE:O	2:B:678:THR:HG22	2.11	0.50
2:B:1066:ASN:HD22	2:B:1067:GLY:N	2.09	0.50
2:B:672:ASP:OD1	2:B:703:THR:HB	2.11	0.50
2:B:1210:ARG:CB	2:B:1280:VAL:HG22	2.41	0.50
1:A:42:A:C8	1:A:42:A:C5'	2.83	0.50
1:A:4:A:C2'	1:A:5:C:C5'	2.78	0.50
1:A:16:A:H4'	2:B:448:ILE:O	2.12	0.50
1:A:26:A:OP1	2:B:115:ARG:NH1	2.45	0.50
2:B:1048:THR:HG23	2:B:1076:LYS:HG2	1.93	0.50
1:A:44:U:C4	2:B:328:HIS:CD2	3.00	0.49
2:B:1206:LEU:HD23	2:B:1345:ALA:HB2	1.95	0.49
4:D:3:DA:H2''	4:D:4:DA:O5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LYS:CB	2:B:4:LYS:NZ	2.75	0.49
2:B:692:ASN:ND2	3:C:27:DA:O4'	2.45	0.49
1:A:35:A:H2'	1:A:36:A:C1'	2.43	0.49
1:A:73:G:H5''	1:A:74:A:OP2	2.12	0.49
2:B:1221:GLN:HB3	2:B:1319:GLY:C	2.33	0.49
2:B:536:LYS:HG2	2:B:537:PRO:HD2	1.94	0.49
3:C:17:DA:H2''	3:C:18:DA:H5'	1.95	0.49
2:B:373:TYR:CZ	2:B:398:LEU:HB3	2.48	0.48
2:B:485:GLY:O	2:B:488:ALA:N	2.46	0.48
2:B:584:GLU:OE2	2:B:585:ASP:HB2	2.13	0.48
2:B:59:ALA:O	2:B:62:THR:HB	2.14	0.48
1:A:16:A:H5'	2:B:453:GLY:HA2	1.96	0.48
2:B:1066:ASN:HB3	2:B:1069:THR:OG1	2.14	0.48
2:B:184:LEU:HD22	2:B:295:ASN:HB3	1.95	0.48
2:B:1325:LYS:HA	2:B:1329:THR:O	2.13	0.48
2:B:824:VAL:HG21	2:B:863:ASN:ND2	2.11	0.48
3:C:16:DC:H2'	3:C:17:DA:H8	1.78	0.48
1:A:8:A:H2'	1:A:9:A:O5'	2.14	0.48
2:B:348:LYS:O	2:B:352:PHE:HB2	2.14	0.48
2:B:424:ARG:NH2	2:B:437:ARG:NH1	2.61	0.48
2:B:784:ILE:O	2:B:785:GLU:C	2.51	0.48
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.13	0.48
2:B:157:ALA:O	2:B:161:MET:HE2	2.13	0.47
2:B:730:SER:O	2:B:734:LYS:HG3	2.13	0.47
4:D:4:DA:H4'	4:D:5:DT:OP1	2.13	0.47
2:B:177:ASP:O	2:B:299:ALA:HA	2.14	0.47
1:A:25:U:C2'	1:A:26:A:H5'	2.44	0.47
1:A:25:U:H1'	2:B:104:SER:O	2.13	0.47
2:B:409:SER:O	2:B:411:PRO:HD3	2.15	0.47
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.96	0.47
2:B:1078:ARG:HG2	2:B:1078:ARG:O	2.15	0.47
2:B:525:THR:HG23	2:B:545:LYS:NZ	2.30	0.47
2:B:1210:ARG:CD	2:B:1280:VAL:HA	2.43	0.47
1:A:27:G:O2'	2:B:129:HIS:CB	2.63	0.47
2:B:86:PHE:CD2	2:B:155:TYR:HB2	2.49	0.47
2:B:1292:SER:O	2:B:1296:LYS:HG3	2.14	0.47
2:B:204:SER:OG	2:B:204:SER:O	2.26	0.47
3:C:11:DT:C3'	3:C:12:DT:H71	2.43	0.47
2:B:178:ASN:OD1	2:B:308:VAL:O	2.33	0.47
1:A:45:U:C5'	2:B:402:GLN:HG2	2.44	0.47
1:A:4:A:H2'	1:A:5:C:H5'	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1349:HIS:HB2	2:B:1358:THR:HG1	1.78	0.47
2:B:1061:PRO:O	2:B:1076:LYS:HE2	2.15	0.47
2:B:1170:GLU:O	2:B:1173:SER:HB3	2.15	0.47
2:B:1267:ASP:OD1	2:B:1294:TYR:OH	2.21	0.47
2:B:675:SER:HB2	2:B:677:LYS:HB2	1.97	0.47
2:B:963:VAL:HG13	2:B:989:LEU:HB3	1.97	0.47
2:B:209:LYS:O	2:B:213:SER:OG	2.25	0.46
3:C:13:DT:H2'	3:C:14:DT:C6	2.50	0.46
1:A:49:A:N3	2:B:1122:ARG:NH1	2.63	0.46
1:A:60:C:OP1	2:B:455:LEU:HB2	2.15	0.46
1:A:16:A:C6	1:A:17:A:N7	2.84	0.46
2:B:41:HIS:ND1	2:B:41:HIS:N	2.63	0.46
2:B:1210:ARG:HA	2:B:1280:VAL:CG2	2.40	0.46
1:A:76:A:C5	1:A:77:A:H1'	2.51	0.46
2:B:706:GLU:HG3	2:B:707:ASP:N	2.31	0.46
2:B:1346:THR:HA	2:B:1360:ILE:O	2.16	0.46
2:B:599:LYS:O	2:B:602:LYS:CD	2.64	0.46
2:B:879:MET:O	2:B:882:TYR:N	2.42	0.46
1:A:42:A:H2'	1:A:43:G:O5'	2.16	0.46
1:A:4:A:O2'	1:A:5:C:H5''	2.15	0.46
2:B:1141:TYR:CE2	2:B:1171:ARG:HD2	2.49	0.45
2:B:973:TYR:CD1	2:B:1237:TYR:CD1	3.04	0.45
2:B:499:ASP:OD2	2:B:663:SER:N	2.49	0.45
2:B:187:GLN:O	2:B:191:THR:HG23	2.16	0.45
2:B:798:GLU:O	2:B:799:HIS:CD2	2.70	0.45
1:A:35:A:H2'	1:A:36:A:C8	2.52	0.45
2:B:1076:LYS:HD3	2:B:1076:LYS:H	1.82	0.45
2:B:143:VAL:O	2:B:425:ARG:HD3	2.17	0.45
2:B:748:VAL:O	2:B:751:MET:N	2.49	0.45
2:B:846:PHE:CE1	2:B:913:LYS:HG2	2.52	0.45
2:B:872:SER:OG	2:B:875:VAL:HG23	2.16	0.45
2:B:763:MET:HE2	2:B:925:ARG:NH2	2.32	0.45
3:C:8:DA:C5	4:D:4:DA:N6	2.85	0.45
1:A:38:A:C8	1:A:38:A:H5''	2.40	0.45
1:A:54:G:C5	1:A:55:C:C4	3.05	0.45
2:B:1216:SER:C	2:B:1218:GLY:N	2.70	0.45
3:C:1:DC:H2'	3:C:2:DA:C8	2.52	0.45
1:A:18:A:N1	1:A:19:A:C6	2.85	0.45
2:B:8:GLY:O	2:B:987:ALA:HB1	2.17	0.45
2:B:536:LYS:CG	2:B:537:PRO:HD2	2.47	0.44
2:B:1263:LYS:HE3	2:B:1302:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:ILE:CG2	2:B:44:LYS:N	2.80	0.44
2:B:483:ASP:C	2:B:483:ASP:OD1	2.55	0.44
2:B:499:ASP:O	2:B:503:PRO:HA	2.17	0.44
1:A:42:A:C8	1:A:42:A:C4'	3.01	0.44
2:B:1163:LEU:HA	2:B:1163:LEU:HD23	1.83	0.44
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	2.00	0.44
2:B:748:VAL:O	2:B:750:VAL:N	2.51	0.44
1:A:31:U:C4	1:A:32:A:N7	2.86	0.44
1:A:81:G:C2	2:B:1356:TYR:HB3	2.52	0.44
2:B:497:ASN:O	2:B:507:VAL:HG23	2.17	0.44
2:B:667:ILE:O	2:B:679:ILE:HB	2.17	0.44
2:B:796:LEU:C	2:B:798:GLU:H	2.21	0.44
1:A:3:A:C2	1:A:4:A:C5	3.05	0.44
2:B:273:ASP:CG	2:B:653:ARG:NH2	2.70	0.44
2:B:1237:TYR:O	2:B:1241:HIS:ND1	2.46	0.44
2:B:1277:SER:HB2	2:B:1287:LEU:HD22	1.99	0.44
2:B:572:ILE:CG2	2:B:572:ILE:O	2.66	0.44
2:B:812:TYR:CE1	2:B:816:LEU:HD11	2.51	0.44
2:B:977:GLU:H	2:B:977:GLU:HG2	1.54	0.44
3:C:13:DT:H2'	3:C:14:DT:H6	1.83	0.44
1:A:75:A:H2'	1:A:76:A:O4'	2.17	0.44
2:B:515:TYR:O	2:B:519:THR:HB	2.18	0.44
2:B:943:TYR:CD2	2:B:949:LEU:HA	2.53	0.44
2:B:530:VAL:HG13	2:B:537:PRO:CA	2.48	0.44
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.53	0.44
4:D:2:DA:H2''	4:D:3:DA:O5'	2.18	0.44
2:B:696:LEU:HD12	2:B:702:LEU:HD12	2.00	0.43
2:B:778:ARG:HG2	2:B:779:GLU:N	2.30	0.43
2:B:844:GLN:NE2	2:B:850:ASP:HB3	2.33	0.43
2:B:755:LYS:HG2	2:B:939:MET:HE3	1.99	0.43
2:B:1066:ASN:C	2:B:1066:ASN:HD22	2.22	0.43
2:B:209:LYS:O	2:B:213:SER:CB	2.67	0.43
2:B:345:GLU:OE2	2:B:346:LYS:HE2	2.18	0.43
3:C:13:DT:H6	3:C:13:DT:O5'	2.01	0.43
1:A:42:A:C2'	1:A:43:G:O5'	2.67	0.43
2:B:151:LEU:HA	2:B:154:ILE:HD12	2.00	0.43
2:B:393:LEU:HD23	2:B:393:LEU:O	2.17	0.43
2:B:474:THR:HG23	2:B:477:ASN:ND2	2.32	0.43
3:C:3:DA:H2''	3:C:4:DT:O5'	2.18	0.43
1:A:41:A:O5'	1:A:41:A:H8	2.01	0.43
2:B:1242:TYR:CD1	2:B:1242:TYR:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:ILE:CG2	2:B:186:ILE:O	2.67	0.43
2:B:78:ARG:NH1	2:B:162:ILE:O	2.51	0.43
2:B:31:LYS:HE3	2:B:44:LYS:HB3	2.00	0.43
2:B:527:VAL:HA	2:B:582:GLY:HA3	2.00	0.43
2:B:796:LEU:HD23	2:B:796:LEU:HA	1.85	0.43
1:A:67:C:OP1	2:B:739:GLN:NE2	2.47	0.43
2:B:323:LYS:O	2:B:324:ARG:C	2.57	0.43
2:B:802:GLU:O	2:B:803:ASN:C	2.57	0.43
1:A:16:A:C5	1:A:17:A:C8	3.07	0.43
2:B:43:ILE:HG22	2:B:45:LYS:HG2	2.01	0.43
2:B:824:VAL:O	2:B:825:ASP:C	2.56	0.43
2:B:760:VAL:HG11	2:B:990:ASN:O	2.19	0.43
2:B:1000:LYS:C	2:B:1002:PRO:HD3	2.38	0.43
2:B:1145:VAL:HG23	2:B:1145:VAL:O	2.19	0.43
2:B:820:ARG:NH2	2:B:825:ASP:OD1	2.50	0.43
1:A:34:A:N6	1:A:35:A:C2	2.87	0.42
1:A:42:A:C3'	1:A:42:A:C8	3.02	0.42
1:A:68:A:H5''	1:A:68:A:H8	1.84	0.42
2:B:932:ALA:HA	2:B:955:VAL:HG11	2.01	0.42
2:B:961:LYS:O	2:B:962:LEU:C	2.58	0.42
1:A:37:U:H2'	1:A:38:A:H5''	2.01	0.42
2:B:1210:ARG:CG	2:B:1280:VAL:HG22	2.49	0.42
2:B:549:VAL:HA	2:B:553:PHE:HB2	2.00	0.42
2:B:241:LEU:O	2:B:244:LEU:CB	2.68	0.42
2:B:661:ARG:HD2	2:B:661:ARG:HA	1.73	0.42
2:B:781:MET:O	2:B:785:GLU:HB2	2.19	0.42
2:B:241:LEU:O	2:B:244:LEU:HB2	2.18	0.42
2:B:540:LEU:HB3	2:B:545:LYS:HG3	2.01	0.42
1:A:76:A:H2'	1:A:77:A:O4'	2.19	0.42
2:B:1136:SER:HA	4:D:7:DA:O3'	2.20	0.42
1:A:16:A:O4'	2:B:450:TYR:HA	2.20	0.42
2:B:524:LEU:HD22	2:B:540:LEU:HD23	2.01	0.42
2:B:563:GLN:O	2:B:567:ASP:HB2	2.19	0.42
2:B:840:ALA:O	2:B:864:ARG:NH2	2.52	0.42
2:B:982:HIS:O	2:B:983:HIS:C	2.57	0.42
3:C:8:DA:C6	4:D:4:DA:N6	2.87	0.42
2:B:324:ARG:NH1	2:B:401:LYS:O	2.53	0.42
1:A:22:U:O2'	2:B:1110:ILE:HB	2.19	0.42
1:A:69:A:H2'	1:A:70:C:C6	2.55	0.42
2:B:1224:ASN:CB	2:B:1280:VAL:HG11	2.50	0.42
2:B:178:ASN:C	2:B:178:ASN:ND2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:LEU:O	2:B:690:ASN:ND2	2.39	0.42
2:B:516:GLU:OE1	2:B:591:LEU:C	2.58	0.42
2:B:842:VAL:HG13	2:B:854:ASN:OD1	2.20	0.42
2:B:823:TYR:C	2:B:824:VAL:CG2	2.88	0.42
1:A:18:A:N1	1:A:19:A:C5	2.88	0.41
1:A:68:A:C4	2:B:1350:GLN:O	2.73	0.41
2:B:345:GLU:HG2	2:B:346:LYS:HG3	2.02	0.41
2:B:388:GLU:O	2:B:391:VAL:HB	2.19	0.41
2:B:161:MET:CE	2:B:419:LEU:HA	2.50	0.41
1:A:66:U:H5'	2:B:721:HIS:NE2	2.35	0.41
2:B:832:ARG:O	2:B:833:LEU:C	2.59	0.41
1:A:54:G:C4	1:A:55:C:C5	3.08	0.41
2:B:1036:TYR:C	2:B:1036:TYR:CD2	2.93	0.41
2:B:1138:THR:HB	2:B:1168:ILE:HD12	2.02	0.41
1:A:44:U:C2	2:B:325:TYR:CD1	3.08	0.41
2:B:453:GLY:O	2:B:454:PRO:C	2.59	0.41
2:B:695:GLN:C	2:B:697:ILE:H	2.23	0.41
2:B:849:ASP:C	2:B:849:ASP:OD1	2.58	0.41
2:B:944:ASP:O	2:B:947:ASP:N	2.41	0.41
2:B:972:PHE:HE1	2:B:1084:ARG:HD3	1.85	0.41
2:B:910:GLU:HG2	2:B:1033:THR:HG23	2.03	0.41
2:B:143:VAL:HG21	2:B:418:GLU:HB3	2.02	0.41
2:B:219:SER:O	2:B:223:GLU:HG3	2.20	0.41
2:B:155:TYR:CD2	2:B:156:LEU:N	2.88	0.41
2:B:390:LEU:O	2:B:391:VAL:C	2.59	0.41
2:B:790:GLU:O	2:B:790:GLU:CG	2.67	0.41
2:B:918:LYS:HE2	2:B:1007:GLU:OE2	2.21	0.41
1:A:52:A:H5''	2:B:1122:ARG:O	2.21	0.41
2:B:682:PHE:CE1	2:B:702:LEU:HD11	2.56	0.41
3:C:13:DT:H73	3:C:13:DT:OP2	2.20	0.41
2:B:1206:LEU:HD12	2:B:1210:ARG:CZ	2.51	0.41
2:B:737:ILE:HA	2:B:740:THR:CG2	2.51	0.41
2:B:755:LYS:O	2:B:756:PRO:C	2.57	0.41
2:B:925:ARG:HA	3:C:21:DT:OP1	2.21	0.41
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.90	0.41
2:B:1171:ARG:CG	2:B:1175:GLU:OE2	2.69	0.41
2:B:1270:ILE:O	2:B:1273:ILE:HB	2.21	0.41
2:B:697:ILE:HG13	2:B:708:ILE:HD12	2.02	0.41
2:B:1121:ALA:HB1	2:B:1123:LYS:O	2.22	0.40
2:B:1210:ARG:HH22	2:B:1341:GLU:CD	2.24	0.40
2:B:1204:PHE:O	2:B:1211:LYS:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LEU:HB2	2:B:414:ILE:HD13	2.03	0.40
2:B:757:GLU:C	2:B:758:ASN:ND2	2.74	0.40
1:A:54:G:H2'	1:A:55:C:C5	2.55	0.40
2:B:114:GLU:HG2	2:B:120:GLY:CA	2.51	0.40
2:B:695:GLN:O	2:B:697:ILE:N	2.54	0.40
2:B:695:GLN:O	2:B:698:HIS:N	2.45	0.40
2:B:909:SER:O	2:B:910:GLU:C	2.59	0.40
2:B:1171:ARG:O	2:B:1175:GLU:HG3	2.21	0.40
2:B:61:ALA:O	2:B:62:THR:C	2.59	0.40
2:B:695:GLN:C	2:B:697:ILE:N	2.75	0.40
2:B:180:ASP:O	2:B:184:LEU:HD12	2.21	0.40
2:B:378:PRO:O	2:B:382:LYS:HG2	2.22	0.40
2:B:420:HIS:O	2:B:421:ALA:C	2.59	0.40
2:B:806:LEU:O	2:B:812:TYR:HB2	2.22	0.40
2:B:528:LYS:HB2	2:B:581:SER:HB3	2.03	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	
2	B	1301/1368 (95%)	1085 (83%)	177 (14%)	39 (3%)	4	28

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	197	GLU
2	B	304	ASP
2	B	690	ASN
2	B	790	GLU
2	B	862	LYS
2	B	1112	PRO

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Mol	Chain	Res	Type
2	B	341	GLN
2	B	405	PHE
2	B	421	ALA
2	B	660	GLY
2	B	667	ILE
2	B	687	GLY
2	B	696	LEU
2	B	824	VAL
2	B	825	ASP
2	B	841	ILE
2	B	1362	LEU
2	B	247	GLY
2	B	324	ARG
2	B	420	HIS
2	B	710	LYS
2	B	785	GLU
2	B	915	GLY
2	B	1076	LYS
2	B	1216	SER
2	B	613	GLU
2	B	1045	PHE
2	B	28	PRO
2	B	485	GLY
2	B	533	GLY
2	B	619	ILE
2	B	644	ASP
2	B	910	GLU
2	B	46	ASN
2	B	303	SER
2	B	609	ASN
2	B	1155	LYS
2	B	391	VAL
2	B	992	VAL

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
2	B	1181/1225 (96%)	1008 (85%)	173 (15%)	3 15

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	4	LYS
2	B	5	TYR
2	B	13	THR
2	B	22	THR
2	B	27	VAL
2	B	33	LYS
2	B	38	THR
2	B	39	ASP
2	B	41	HIS
2	B	42	SER
2	B	44	LYS
2	B	45	LYS
2	B	55	SER
2	B	58	THR
2	B	65	LYS
2	B	73	THR
2	B	75	ARG
2	B	80	CYS
2	B	82	LEU
2	B	102	GLU
2	B	141	LYS
2	B	146	THR
2	B	158	LEU
2	B	165	ARG
2	B	173	ASP
2	B	174	LEU
2	B	178	ASN
2	B	179	SER
2	B	182	ASP
2	B	186	ILE
2	B	188	LEU
2	B	212	LEU
2	B	234	LYS
2	B	244	LEU
2	B	248	LEU
2	B	253	LYS
2	B	254	SER
2	B	257	ASP

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Mol	Chain	Res	Type
2	B	269	ASP
2	B	300	ILE
2	B	303	SER
2	B	304	ASP
2	B	307	ARG
2	B	311	GLU
2	B	313	THR
2	B	321	MET
2	B	334	LEU
2	B	403	ARG
2	B	409	SER
2	B	414	ILE
2	B	419	LEU
2	B	425	ARG
2	B	455	LEU
2	B	465	MET
2	B	466	THR
2	B	470	GLU
2	B	492	ILE
2	B	504	ASN
2	B	506	LYS
2	B	512	SER
2	B	514	LEU
2	B	519	THR
2	B	525	THR
2	B	530	VAL
2	B	536	LYS
2	B	540	LEU
2	B	541	SER
2	B	573	GLU
2	B	577	SER
2	B	579	GLU
2	B	581	SER
2	B	590	SER
2	B	598	LEU
2	B	599	LYS
2	B	602	LYS
2	B	623	LEU
2	B	627	GLU
2	B	629	ARG
2	B	635	ARG
2	B	643	PHE

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Mol	Chain	Res	Type
2	B	651	LEU
2	B	652	LYS
2	B	661	ARG
2	B	665	LYS
2	B	666	LEU
2	B	694	MET
2	B	696	LEU
2	B	697	ILE
2	B	703	THR
2	B	709	GLN
2	B	710	LYS
2	B	726	ASN
2	B	730	SER
2	B	738	LEU
2	B	740	THR
2	B	751	MET
2	B	778	ARG
2	B	782	LYS
2	B	785	GLU
2	B	801	VAL
2	B	804	THR
2	B	811	LEU
2	B	827	GLU
2	B	830	ILE
2	B	842	VAL
2	B	859	ARG
2	B	860	SER
2	B	862	LYS
2	B	866	LYS
2	B	867	SER
2	B	871	PRO
2	B	877	LYS
2	B	881	ASN
2	B	884	ARG
2	B	887	LEU
2	B	905	ARG
2	B	917	ILE
2	B	918	LYS
2	B	919	ARG
2	B	921	LEU
2	B	925	ARG
2	B	933	GLN

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Mol	Chain	Res	Type
2	B	935	LEU
2	B	942	LYS
2	B	947	ASP
2	B	957	THR
2	B	959	LYS
2	B	960	SER
2	B	977	GLU
2	B	997	LEU
2	B	1007	GLU
2	B	1012	ASP
2	B	1031	LYS
2	B	1033	THR
2	B	1035	LYS
2	B	1040	SER
2	B	1048	THR
2	B	1066	ASN
2	B	1073	VAL
2	B	1076	LYS
2	B	1078	ARG
2	B	1085	LYS
2	B	1087	LEU
2	B	1089	MET
2	B	1091	GLN
2	B	1106	SER
2	B	1125	ASP
2	B	1135	ASP
2	B	1142	SER
2	B	1143	VAL
2	B	1153	LYS
2	B	1160	VAL
2	B	1197	LYS
2	B	1207	GLU
2	B	1210	ARG
2	B	1212	ARG
2	B	1230	SER
2	B	1231	LYS
2	B	1242	TYR
2	B	1248	SER
2	B	1250	GLU
2	B	1260	GLU
2	B	1272	GLN
2	B	1275	GLU

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Mol	Chain	Res	Type
2	B	1280	VAL
2	B	1299	ASP
2	B	1308	ASN
2	B	1314	THR
2	B	1342	VAL
2	B	1346	THR
2	B	1347	LEU
2	B	1351	SER
2	B	1364	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	129	HIS
2	B	190	GLN
2	B	251	ASN
2	B	357	ASN
2	B	407	ASN
2	B	420	HIS
2	B	489	GLN
2	B	563	GLN
2	B	692	ASN
2	B	698	HIS
2	B	709	GLN
2	B	726	ASN
2	B	758	ASN
2	B	799	HIS
2	B	826	GLN
2	B	844	GLN
2	B	863	ASN
2	B	930	HIS
2	B	1066	ASN
2	B	1308	ASN
2	B	1364	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	26 (32%)	3 (3%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	C
1	A	6	U
1	A	8	A
1	A	9	A
1	A	28	A
1	A	29	G
1	A	31	U
1	A	33	G
1	A	34	A
1	A	37	U
1	A	38	A
1	A	39	G
1	A	42	A
1	A	43	G
1	A	51	A
1	A	56	U
1	A	58	G
1	A	59	U
1	A	63	U
1	A	68	A
1	A	71	U
1	A	74	A
1	A	75	A
1	A	77	A
1	A	78	A
1	A	81	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	C
1	A	28	A
1	A	36	A

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

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

5.5 Carbohydrates [i](#)

There are no 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	A	81/83 (97%)	-0.12	0 100 100	40, 61, 131, 174	0
2	B	1315/1368 (96%)	-0.03	28 (2%) 63 49	41, 76, 115, 145	0
3	C	28/28 (100%)	0.16	2 (7%) 16 9	44, 68, 125, 169	0
4	D	11/12 (91%)	-0.00	1 (9%) 9 5	54, 82, 139, 152	0
All	All	1435/1491 (96%)	-0.03	31 (2%) 62 48	40, 75, 116, 174	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	2	DA	5.9
2	B	197	GLU	4.7
2	B	200	PRO	4.6
2	B	199	ASN	4.5
3	C	1	DC	3.9
2	B	815	TYR	3.7
2	B	186	ILE	3.6
2	B	190	GLN	3.4
2	B	194	GLN	3.2
2	B	1151	LYS	3.1
2	B	180	ASP	2.9
2	B	187	GLN	2.8
2	B	795	ILE	2.7
2	B	198	GLU	2.6
2	B	1296	LYS	2.6
2	B	828	LEU	2.5
2	B	246	LEU	2.4
2	B	247	GLY	2.4
2	B	215	ARG	2.4
4	D	12	DG	2.3
2	B	1043	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	193	ASN	2.2
2	B	830	ILE	2.2
2	B	1037	PHE	2.1
2	B	218	LYS	2.1
2	B	814	TYR	2.1
2	B	189	VAL	2.1
2	B	1255	LYS	2.1
2	B	693	PHE	2.0
2	B	252	PHE	2.0
2	B	1036	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.