



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:10 PM UTC

PDB ID : 6K4U / pdb_00006k4u
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 types of validation reports are described at

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

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

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

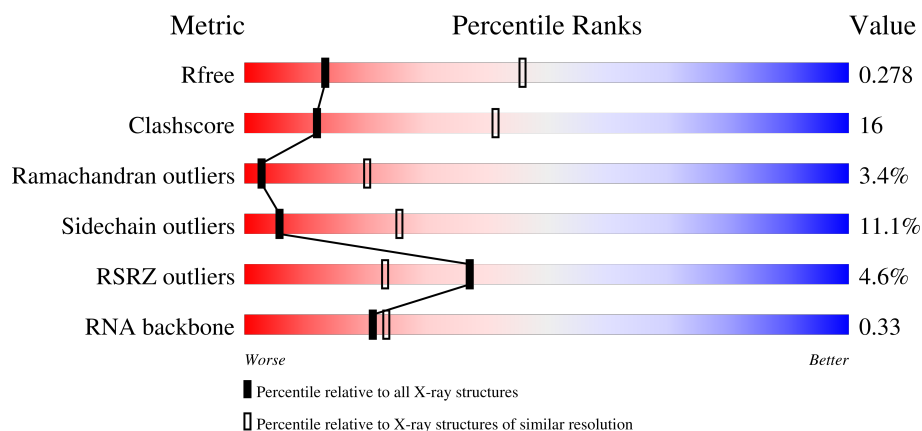
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (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 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	5% 58% 32% 5% .
2	A	83	31% 36% 23% 6% .
3	C	28	64% 32% .
4	D	12	8% 50% 25% 17% 8%

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.

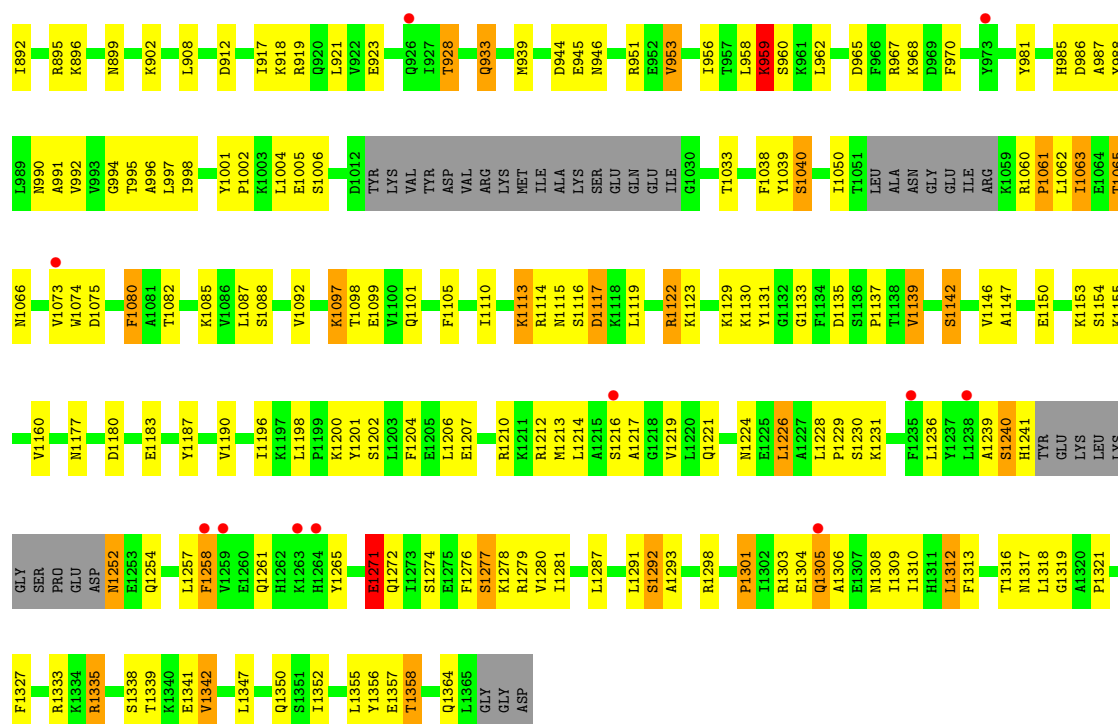
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	80	Total	C	N	O	P	0	0	0
			1710	768	313	549	80			

- Molecule 3 is a DNA chain called target DNA.

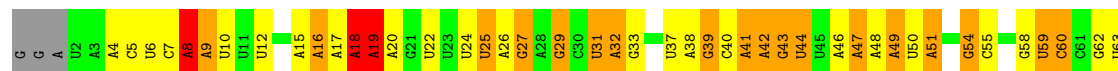
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	27	Total	C	N	O	P	0	0	0
			552	268	92	165	27			

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

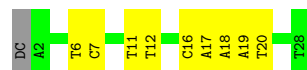
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			226	110	43	63	10			



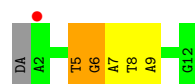
• Molecule 2: sgRNA



• 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 49.38 – 3.20	Depositor EDS
% Data completeness (in resolution range)	81.8 (49.38-3.20) 81.8 (49.38-3.20)	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 0.222 , 0.278	Depositor DCC
R_{free} test set	1566 reflections (4.25%)	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)	0.29 , 64.8	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	0.90	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	1.10	3/10504 (0.0%)	1.55	32/14169 (0.2%)
2	A	0.87	10/1917 (0.5%)	1.16	20/2984 (0.7%)
3	C	0.57	0/617	0.97	0/950
4	D	0.94	2/254 (0.8%)	0.90	0/391
All	All	1.05	15/13292 (0.1%)	1.46	52/18494 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	6	DG	O3'-P	-8.37	1.48	1.61
2	A	18	A	O3'-P	-7.55	1.49	1.61
2	A	49	A	O3'-P	-7.33	1.50	1.61
2	A	12	U	O3'-P	-7.16	1.50	1.61
4	D	5	DT	O3'-P	-6.83	1.50	1.61
1	B	42	SER	C-O	6.74	1.30	1.23
2	A	47	A	O3'-P	-6.33	1.51	1.61
2	A	25	U	O3'-P	-6.14	1.51	1.61
2	A	60	C	O3'-P	-5.71	1.52	1.61
2	A	19	A	O3'-P	-5.50	1.52	1.61
2	A	41	A	O3'-P	-5.44	1.52	1.61
1	B	953	VAL	C-O	5.43	1.30	1.24
1	B	1101	GLN	C-O	5.20	1.30	1.23
2	A	59	U	O3'-P	-5.12	1.53	1.61
2	A	48	A	O3'-P	-5.10	1.53	1.61

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	18	A	C2'-C3'-O3'	-9.51	99.43	113.70
1	B	731	PRO	N-CA-C	-8.83	102.82	113.86
2	A	8	A	C3'-C2'-O2'	7.80	122.41	110.70
2	A	68	A	C3'-C2'-O2'	7.79	122.39	110.70
1	B	1137	PRO	CA-C-O	-7.62	112.65	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	22	U	C3'-C2'-O2'	7.52	121.98	110.70
2	A	49	A	C1'-C2'-O2'	-7.09	97.76	108.40
1	B	207	ASP	CA-CB-CG	6.91	119.51	112.60
2	A	32	A	C3'-C2'-O2'	6.49	120.44	110.70
1	B	837	ASP	CA-C-N	6.35	127.62	121.65
1	B	837	ASP	C-N-CA	6.35	127.62	121.65
1	B	72	TYR	CA-C-O	-6.32	114.18	120.82
1	B	182	ASP	CA-CB-CG	6.10	118.70	112.60
2	A	16	A	C3'-C2'-O2'	6.05	119.78	110.70
2	A	47	A	C4'-C3'-O3'	-5.86	104.22	113.00
1	B	445	THR	CA-CB-OG1	-5.82	100.87	109.60
2	A	73	G	C1'-C2'-O2'	5.75	117.02	108.40
2	A	81	G	C2'-C3'-O3'	5.70	118.05	109.50
1	B	22	THR	CA-C-N	5.56	129.16	120.82
1	B	22	THR	C-N-CA	5.56	129.16	120.82
1	B	865	GLY	CA-C-O	-5.53	118.47	122.45
2	A	66	U	C3'-C2'-O2'	5.52	118.98	110.70
2	A	48	A	C3'-C2'-O2'	5.51	118.96	110.70
2	A	54	G	C4'-C3'-O3'	-5.47	104.79	113.00
2	A	65	A	C1'-C2'-O2'	5.47	116.61	108.40
1	B	407	ASN	N-CA-C	-5.46	106.60	113.20
2	A	47	A	C3'-C2'-O2'	5.40	118.81	110.70
1	B	1133	GLY	CA-C-O	-5.39	116.78	121.04
2	A	50	U	C3'-C2'-O2'	5.39	118.78	110.70
1	B	427	GLU	N-CA-C	-5.37	105.51	111.36
1	B	102	GLU	CB-CG-CD	5.36	121.72	112.60
1	B	838	VAL	CA-C-O	-5.34	117.99	122.63
1	B	67	THR	CA-CB-OG1	-5.30	101.65	109.60
1	B	95	ASP	CA-CB-CG	5.29	117.89	112.60
2	A	67	C	C3'-C2'-O2'	-5.29	102.77	110.70
1	B	861	ASP	CA-CB-CG	5.27	117.87	112.60
2	A	78	A	C3'-C2'-O2'	5.24	118.56	110.70
1	B	1098	THR	CA-CB-OG1	5.16	117.33	109.60
1	B	707	ASP	CA-C-N	5.13	127.12	120.70
1	B	707	ASP	C-N-CA	5.13	127.12	120.70
1	B	944	ASP	CA-C-N	5.13	127.88	120.38
1	B	944	ASP	C-N-CA	5.13	127.88	120.38
2	A	60	C	C1'-C2'-O2'	-5.12	100.71	108.40
2	A	18	A	C3'-C2'-O2'	5.10	118.35	110.70
1	B	254	SER	CA-C-N	5.06	127.07	120.28
1	B	254	SER	C-N-CA	5.06	127.07	120.28
1	B	1153	LYS	CA-C-N	5.04	127.28	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1153	LYS	C-N-CA	5.04	127.28	120.38
1	B	1258	PHE	CA-C-N	5.03	126.85	120.72
1	B	1258	PHE	C-N-CA	5.03	126.85	120.72
1	B	1301	PRO	CA-C-N	5.01	126.83	120.72
1	B	1301	PRO	C-N-CA	5.01	126.83	120.72

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	B	10326	0	10134	322	0
2	A	1710	0	858	64	0
3	C	552	0	311	12	0
4	D	226	0	127	6	0
All	All	12814	0	11430	379	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 (379) 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:H5'	2:A:18:A:H8	1.11	1.15
2:A:37:U:C2	2:A:38:A:C8	2.48	1.00
2:A:18:A:H5'	2:A:18:A:C8	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:923:GLU:HG2	1:B:928:THR:HG21	1.64	0.78
1:B:1226:LEU:C	1:B:1226:LEU:HD12	2.08	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
1:B:302:LEU:O	1:B:304:ASP:N	2.20	0.74
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.14	0.73
2:A:17:A:C2'	2:A:18:A:H5''	2.18	0.73
2:A:37:U:N3	2:A:38:A:N7	2.37	0.72
1:B:615:ILE:HD12	1:B:615:ILE:N	2.02	0.71
1:B:499:ASP:OD2	1:B:663:SER:HB2	1.90	0.71
1:B:615:ILE:H	1:B:615:ILE:CD1	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:CG	1:B:1335:ARG:HH11	2.04	0.70
1:B:448:ILE:HG12	1:B:455:LEU:HD21	1.73	0.69
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:18:A:H8	2:A:18:A:C5'	2.01	0.63
2:A:42:A:HO2'	2:A:43:G:P	2.17	0.63
2:A:19:A:H2'	2:A:20:A:O4'	1.98	0.63
2:A:8:A:O2'	2:A:9:A:OP1	2.15	0.62
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:685:SER:C	1:B:687:GLY:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:LEU:HA	1:B:161:MET:HE3	1.82	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:178:ASN:C	1:B:178:ASN:HD22	2.11	0.59
1:B:1114:ARG:NH1	4:D:9:DA:OP1	2.36	0.59
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:615:ILE:CG2	1:B:639:TYR:CE1	2.85	0.58
1:B:1258:PHE:O	1:B:1261:GLN:O	2.20	0.58
1:B:243:ALA:O	1:B:248:LEU:HB2	2.03	0.58
1:B:450:TYR:CD1	1:B:450:TYR:C	2.81	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
1:B:919:ARG:O	1:B:959:LYS:NZ	2.37	0.58
1:B:1139:VAL:HG11	1:B:1216:SER:OG	2.04	0.58
2:A:29:G:N2	2:A:41:A:H1'	2.19	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'	1.50	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
1:B:648:MET:HA	1:B:651:LEU:HD12	1.86	0.57
2:A:31:U:H3	2:A:38:A:H61	1.51	0.57
2:A:32:A:N6	2:A:38:A:N6	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASP:O	1:B:735:LYS:NZ	2.38	0.56
1:B:412:HIS:CE1	1:B:413:GLN:HE22	2.24	0.56
1:B:1113:LYS:HB2	1:B:1129:LYS:O	2.05	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:816:LEU:HD23	1:B:816:LEU:O	2.05	0.56
1:B:1210:ARG:NH2	1:B:1341:GLU:OE1	2.39	0.56
1:B:146:THR:O	1:B:146:THR:OG1	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:784:ILE:HD11	1:B:812:TYR:CE1	2.41	0.55
1:B:1309:ILE:O	1:B:1312:LEU:N	2.36	0.55
1:B:1135:ASP:C	1:B:1135:ASP:OD1	2.49	0.55
1:B:216:LEU:O	1:B:221:ARG:NH1	2.37	0.55
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:921:LEU:HD22	1:B:962:LEU:CD2	2.36	0.55
1:B:933:GLN:O	1:B:933:GLN:NE2	2.40	0.55
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:1291:LEU:C	1:B:1293:ALA:H	2.16	0.54
1:B:951:ARG:HH11	1:B:951:ARG:HB2	1.73	0.53
1:B:427:GLU:O	1:B:428:ASP:C	2.51	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:178:ASN:OD1	1:B:299:ALA:HB1	2.09	0.53
1:B:264:LEU:CD2	1:B:274:ASP:HB3	2.39	0.53
2:A:18:A:C8	2:A:18:A:C5'	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:837:ASP:OD1	1:B:837:ASP:N	2.42	0.52
1:B:996:ALA:C	1:B:998:ILE:H	2.17	0.52
1:B:518:PHE:CD1	1:B:667:ILE:HD12	2.44	0.52
1:B:1357:GLU:O	1:B:1358:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:ILE:HD11	1:B:763:MET:HE3	1.91	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:788:ILE:HD11	1:B:815:TYR:O	2.11	0.51
1:B:1150:GLU:HB2	1:B:1155:LYS:HA	1.92	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
1:B:139:ARG:NH1	1:B:161:MET:HG2	2.26	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:970:PHE:CG	1:B:1080:PHE:CZ	2.99	0.50
1:B:1277:SER:HA	1:B:1281:ILE:CB	2.42	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:685:SER:C	1:B:687:GLY:N	2.70	0.49
1:B:1333:ARG:CZ	4:D:5:DT:H72	2.42	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
1:B:1073:VAL:HG23	1:B:1074:TRP:N	2.27	0.49
1:B:1214:LEU:C	1:B:1214:LEU:CD1	2.85	0.49
2:A:38:A:H2'	2:A:38:A:N3	2.28	0.49
1:B:108:GLU:O	1:B:111:LYS:HB2	2.13	0.49
2:A:32:A:C6	2:A:38:A:C6	3.01	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:5:TYR:OH	1:B:754:HIS:O	2.23	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:641:HIS:NE2	1:B:642:LEU:HG	2.28	0.49
1:B:1088:SER:OG	1:B:1230:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1226:LEU:C	1:B:1226:LEU:CD1	2.80	0.49
1:B:94:ASP:OD2	1:B:152:ARG:NH1	2.45	0.48
1:B:551:LEU:O	1:B:555:THR:OG1	2.24	0.48
1:B:645:ASP:O	1:B:649:LYS:HB2	2.13	0.48
1:B:1226:LEU:HD12	1:B:1226:LEU:O	2.13	0.48
1:B:781:MET:O	1:B:781:MET:CG	2.60	0.48
1:B:1105:PHE:CZ	2:A:51:A:C6	3.01	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:790:GLU:HA	1:B:790:GLU:OE1	2.13	0.47
1:B:1216:SER:CB	4:D:7:DA:OP1	2.61	0.47
1:B:1240:SER:HB2	1:B:1241:HIS:ND1	2.29	0.47
2:A:33:G:O5'	2:A:33:G:H8	1.97	0.47
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:122:ILE:O	1:B:123:VAL:C	2.58	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:1206:LEU:HD13	1:B:1210:ARG:CZ	2.45	0.47
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: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: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:1212:ARG:NH2	1:B:1280:VAL:O	2.48	0.46
1:B:1200:LYS:HE2	1:B:1201:TYR:CZ	2.50	0.46
1:B:368:SER:OG	1:B:369:GLN:N	2.49	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:HG3	1:B:1364:GLN:O	2.15	0.46
1:B:144:ASP:O	1:B:145:SER:C	2.58	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:823:TYR:CE2	1:B:864:ARG:HB3	2.51	0.46
1:B:1350:GLN:O	2:A:68:A:N3	2.49	0.46
1:B:302:LEU:C	1:B:304:ASP:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1271:GLU:O	1:B:1274:SER:N	2.49	0.45
1:B:79:ILE:HD11	1:B:163:LYS:HB2	1.99	0.45
1:B:435:ASP:HB2	1:B:436:ASN:HD22	1.80	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:69:ARG:O	1:B:73:THR:HG23	2.16	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:1110:ILE:HG12	1:B:1122:ARG:HD2	1.98	0.45
1:B:21:ILE:CD1	1:B:991:ALA:HB1	2.47	0.45
1:B:317:LEU:HD21	1:B:415:HIS:HE2	1.82	0.45
1:B:1114:ARG:HD2	1:B:1116:SER:CB	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:1291:LEU:O	1:B:1293:ALA:N	2.50	0.45
1:B:1309:ILE:O	1:B:1310:ILE:C	2.60	0.45
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
1:B:1207:GLU:O	1:B:1207:GLU:HG2	2.12	0.44
3:C:19:DA:C8	3:C:19:DA:C5'	2.95	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
2:A:54:G:H2'	2:A:55:C:C6	2.53	0.44
1:B:76:LYS:HD3	2:A:49:A:OP1	2.17	0.44
1:B:455:LEU:HA	1:B:465:MET:HE2	1.98	0.44
1:B:939:MET:HE2	1:B:953:VAL:HG21	1.99	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:491:PHE:O	1:B:495:MET:HE3	2.18	0.44
1:B:561:VAL:HG23	1:B:585:ASP:C	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:HH11	2:A:20:A:P	2.40	0.44
1:B:1062:LEU:HD23	1:B:1063:ILE:N	2.32	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:116:HIS:CE1	1:B:122:ILE:HD12	2.53	0.44
1:B:325:TYR:O	1:B:326:ASP:C	2.61	0.44
1:B:747:LEU:HD23	1:B:747:LEU:HA	1.87	0.44
1:B:1001:TYR:N	1:B:1002:PRO:HD3	2.32	0.44
1:B:1298:ARG:HA	1:B:1305:GLN:OE1	2.17	0.44
1:B:1356:TYR:HD2	2:A:81:G:C4	2.36	0.44
2:A:75:A:H2'	2:A:76:A:C8	2.53	0.44
1:B:474:THR:N	1:B:477:ASN:OD1	2.51	0.44
1:B:545:LYS:C	1:B:547:ALA:H	2.26	0.44
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
1:B:1217:ALA:C	1:B:1339:THR:HG21	2.43	0.43
2:A:4:A:C6	2:A:5:C:C4	3.06	0.43
1:B:109:GLU:OE1	1:B:1130:LYS:HE2	2.19	0.43
1:B:1004:LEU:C	1:B:1006:SER:H	2.26	0.43
2:A:26:A:H5'	2:A:27:G:OP2	2.18	0.43
4:D:6:DG:H2''	4:D:7:DA:H5'	1.99	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
2:A:6:U:H2'	2:A:7:C:C6	2.54	0.43
1:B:446:PHE:CG	1:B:447:ARG:N	2.87	0.43
1:B:616:LEU:O	1:B:616:LEU:HD23	2.18	0.43
1:B:1142:SER:OG	1:B:1216:SER:O	2.36	0.43
1:B:271:TYR:O	1:B:275:LEU:N	2.52	0.43
1:B:1280:VAL:HG23	1:B:1281:ILE:CD1	2.49	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:302:LEU:O	1:B:305:ILE:N	2.39	0.43
1:B:1221:GLN:HB2	1:B:1319:GLY:O	2.19	0.43
1:B:737:ILE:O	1:B:741:VAL:HG23	2.19	0.43
1:B:1201:TYR:HA	1:B:1213:MET:HB3	2.00	0.43
2:A:18:A:H2'	2:A:19:A:H5'	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:302:LEU:O	1:B:303:SER:C	2.62	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
1:B:20:VAL:O	1:B:27:VAL:HA	2.19	0.42
1:B:1183:GLU:HA	1:B:1187:TYR:O	2.19	0.42
2:A:32:A:N1	2:A:38:A:C5	2.87	0.42
1:B:1224:ASN:OD1	1:B:1280:VAL:HB	2.19	0.42
1:B:1254:GLN:O	1:B:1257:LEU:HB2	2.19	0.42
1:B:1303:ARG:O	1:B:1304:GLU:C	2.62	0.42
1:B:643:PHE:HB3	1:B:647:VAL:HB	2.01	0.42
1:B:413:GLN:CD	1:B:413:GLN:H	2.27	0.42
1:B:416:LEU:O	1:B:417:GLY:C	2.62	0.42
1:B:456:ALA:O	1:B:467:ARG:NH1	2.52	0.42
1:B:1229:PRO:O	1:B:1230:SER:C	2.63	0.42
1:B:1276:PHE:C	1:B:1278:LYS:H	2.28	0.42
1:B:1277:SER:HB2	1:B:1287:LEU:HD22	2.01	0.42
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:1226:LEU:HB3	1:B:1276:PHE:CZ	2.54	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:996:ALA:C	1:B:998:ILE:N	2.77	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:644:ASP:C	1:B:644:ASP:OD1	2.63	0.41
1:B:763:MET:HB3	1:B:763:MET:HE2	1.75	0.41
1:B:1097:LYS:HE3	1:B:1099:GLU:OE2	2.19	0.41
1:B:60:GLU:O	1:B:61:ALA:C	2.63	0.41
1:B:253:LYS:HG3	1:B:254:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:208:ALA:O	1:B:209:LYS:C	2.63	0.41
3:C:16:DC:H2'	3:C:17:DA:C8	2.55	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
1:B:1177:ASN:ND2	1:B:1180:ASP:OD2	2.53	0.41
1:B:27:VAL:O	1:B:28:PRO:O	2.38	0.41
1:B:51:LEU:HD22	1:B:1352:ILE:CG1	2.49	0.41
1:B:501:ASN:HB2	1:B:666:LEU:HD22	2.02	0.41
1:B:828:LEU:CD2	1:B:836:TYR:CE2	3.03	0.41
1:B:1303:ARG:O	1:B:1306:ALA:N	2.54	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:156:LEU:HD23	1:B:156:LEU:HA	1.87	0.41
2:A:6:U:O5'	2:A:6:U:H6	2.03	0.41
1:B:1210:ARG:NH2	1:B:1341:GLU:CD	2.79	0.41
1:B:76:LYS:HA	1:B:76:LYS:HD2	1.88	0.41
2:A:39:G:C6	2:A:40:C:C4	3.09	0.41
2:A:47:A:O5'	2:A:47:A:H8	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:9:LEU:HD11	1:B:744:VAL:CG2	2.51	0.41
1:B:325:TYR:CD1	2:A:44:U:C2	3.09	0.41
1:B:563:GLN:O	1:B:567:ASP:HB2	2.21	0.40
1:B:148:LYS:HD2	1:B:429:PHE:HB3	2.02	0.40
1:B:262:THR:HG21	1:B:281:GLN:HE22	1.86	0.40
1:B:335:LEU:HD22	1:B:351:PHE:HZ	1.86	0.40
1:B:945:GLU:HG2	1:B:946:ASN:OD1	2.21	0.40
1:B:1075:ASP:OD1	1:B:1075:ASP:O	2.40	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
1:B:1287:LEU:O	1:B:1291:LEU:HG	2.21	0.40
2:A:25:U:O5'	2:A:25:U:H6	2.05	0.40
3:C:6:DT:C2	3:C:7:DC:C6	3.09	0.40
1:B:416:LEU:HD12	1:B:416:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	20

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
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

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Mol	Chain	Res	Type
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%)	955 (89%)	119 (11%)	6 25

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	38	THR
1	B	42	SER
1	B	55	SER
1	B	57	GLU
1	B	62	THR
1	B	79	ILE
1	B	80	CYS
1	B	82	LEU
1	B	101	LEU

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Mol	Chain	Res	Type
1	B	103	GLU
1	B	106	LEU
1	B	112	LYS
1	B	122	ILE
1	B	134	THR
1	B	139	ARG
1	B	146	THR
1	B	174	LEU
1	B	225	LEU
1	B	244	LEU
1	B	245	SER
1	B	248	LEU
1	B	253	LYS
1	B	266	LEU
1	B	267	SER
1	B	269	ASP
1	B	272	ASP
1	B	273	ASP
1	B	284	ASP
1	B	310	THR
1	B	313	THR
1	B	314	LYS
1	B	321	MET
1	B	334	LEU
1	B	338	LEU
1	B	368	SER
1	B	409	ILE
1	B	436	ASN
1	B	438	GLU
1	B	455	LEU
1	B	466	THR
1	B	470	GLU
1	B	471	GLU
1	B	481	VAL
1	B	516	GLU
1	B	550	ASP
1	B	583	VAL
1	B	597	LEU
1	B	615	ILE
1	B	616	LEU
1	B	618	ASP
1	B	619	ILE

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Mol	Chain	Res	Type
1	B	623	LEU
1	B	624	THR
1	B	625	LEU
1	B	627	GLU
1	B	631	MET
1	B	657	THR
1	B	661	ARG
1	B	672	ASP
1	B	692	ASN
1	B	696	LEU
1	B	733	ILE
1	B	738	LEU
1	B	745	ASP
1	B	765	ARG
1	B	790	GLU
1	B	811	LEU
1	B	825	ASP
1	B	828	LEU
1	B	833	LEU
1	B	845	SER
1	B	849	ASP
1	B	853	ASP
1	B	858	THR
1	B	873	GLU
1	B	877	LYS
1	B	881	ASN
1	B	912	ASP
1	B	928	THR
1	B	933	GLN
1	B	959	LYS
1	B	960	SER
1	B	1033	THR
1	B	1040	SER
1	B	1050	ILE
1	B	1065	THR
1	B	1080	PHE
1	B	1087	LEU
1	B	1097	LYS
1	B	1113	LYS
1	B	1115	ASN
1	B	1117	ASP
1	B	1119	LEU

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Mol	Chain	Res	Type
1	B	1122	ARG
1	B	1123	LYS
1	B	1139	VAL
1	B	1142	SER
1	B	1146	VAL
1	B	1154	SER
1	B	1160	VAL
1	B	1202	SER
1	B	1219	VAL
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	1305	GLN
1	B	1312	LEU
1	B	1317	ASN
1	B	1318	LEU
1	B	1335	ARG
1	B	1338	SER
1	B	1342	VAL
1	B	1347	LEU
1	B	1358	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	HIS
1	B	178	ASN
1	B	251	ASN
1	B	277	ASN
1	B	407	ASN
1	B	413	GLN
1	B	436	ASN
1	B	497	ASN
1	B	504	ASN
1	B	612	ASN
1	B	726	ASN
1	B	899	ASN
1	B	980	ASN

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Mol	Chain	Res	Type
1	B	983	HIS
1	B	1066	ASN
1	B	1093	ASN
1	B	1115	ASN
1	B	1177	ASN
1	B	1261	GLN
1	B	1295	ASN
1	B	1297	HIS
1	B	1305	GLN

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

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Mol	Chain	Res	Type
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 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

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%)	0.26	65 (4%) 34 22	24, 83, 157, 224	0
2	A	80/83 (96%)	-0.49	0 100 100	23, 50, 125, 143	0
3	C	27/28 (96%)	-0.09	0 100 100	46, 67, 130, 155	0
4	D	11/12 (91%)	0.18	1 (9%) 15 9	49, 76, 162, 168	0
All	All	1430/1491 (95%)	0.21	66 (4%) 37 23	23, 82, 155, 224	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	LEU	6.4
1	B	853	ASP	5.6
1	B	257	ASP	5.0
1	B	1259	VAL	4.9
1	B	818	ASN	4.7
1	B	287	ALA	4.5
1	B	225	LEU	4.3
1	B	252	PHE	4.3
1	B	237	LEU	3.7
1	B	238	PHE	3.7
1	B	229	LEU	3.4
1	B	239	GLY	3.4
1	B	288	ASP	3.3
1	B	804	THR	3.2
1	B	226	ILE	3.2
1	B	675	SER	3.0
1	B	688	PHE	3.0
1	B	1216	SER	2.9
1	B	817	GLN	2.9
1	B	1263	LYS	2.9
1	B	1258	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	2.9
1	B	651	LEU	2.9
1	B	236	GLY	2.8
1	B	666	LEU	2.7
1	B	248	LEU	2.7
1	B	2	ASP	2.5
1	B	249	THR	2.5
1	B	841	ILE	2.5
1	B	25	TYR	2.5
1	B	291	LEU	2.5
1	B	788	ILE	2.5
1	B	585	ASP	2.5
1	B	240	ASN	2.4
4	D	2	DA	2.4
1	B	200	PRO	2.4
1	B	815	TYR	2.3
1	B	1238	LEU	2.3
1	B	517	TYR	2.3
1	B	973	TYR	2.3
1	B	174	LEU	2.3
1	B	206	VAL	2.3
1	B	268	LYS	2.3
1	B	690	ASN	2.3
1	B	563	GLN	2.2
1	B	926	GLN	2.2
1	B	251	ASN	2.2
1	B	891	LEU	2.2
1	B	704	PHE	2.2
1	B	1235	PHE	2.2
1	B	1073	VAL	2.2
1	B	580	ILE	2.2
1	B	687	GLY	2.2
1	B	852	ILE	2.1
1	B	1305	GLN	2.1
1	B	584	GLU	2.1
1	B	791	LEU	2.1
1	B	295	ASN	2.1
1	B	667	ILE	2.1
1	B	721	HIS	2.1
1	B	703	THR	2.1
1	B	814	TYR	2.1
1	B	211	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1264	HIS	2.1
1	B	586	ARG	2.0
1	B	829	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 oligosaccharides 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.