Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 10:13 PM JST

PDB ID	:	6K57
Title	:	Crystal structure of dCas9 in complex with sgRNA and DNA (CGA PAM)
Authors	:	Chen, W.; Zhang, H.; Zhang, Y.; Wang, Y.; Gan, J.; Ji, Q.
Deposited on	:	2019-05-28
Resolution	:	2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

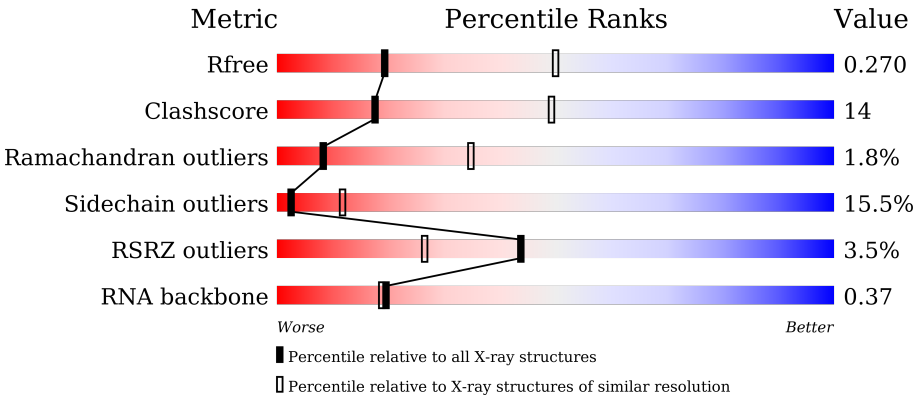
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	83	36% 34% 25%
2	B	1368	4% 62% 29% 5%
3	C	28	4% 46% 43% 11%
4	D	12	25% 50% 17% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13302 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 sgRNA.

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
			10754	6856	1865	2011	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 target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			569	277	95	170	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
			225	109	44	62	10			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		

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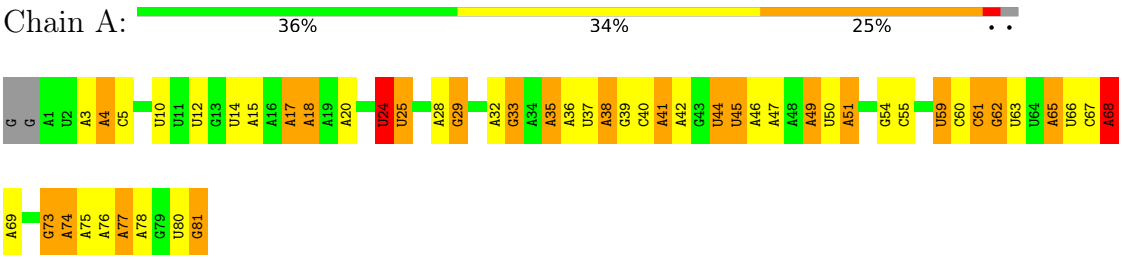
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	19	Total O 19 19	0	0
5	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

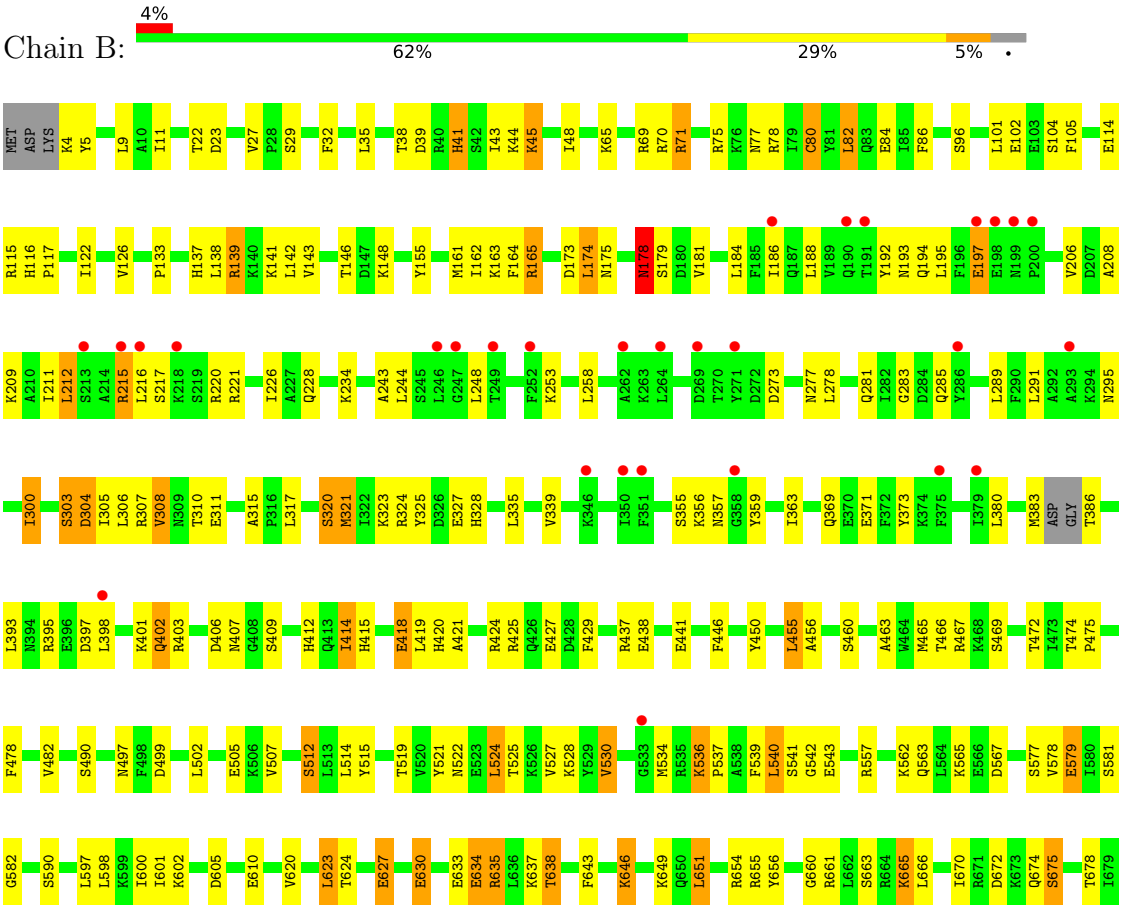
• Molecule 1: sgRNA

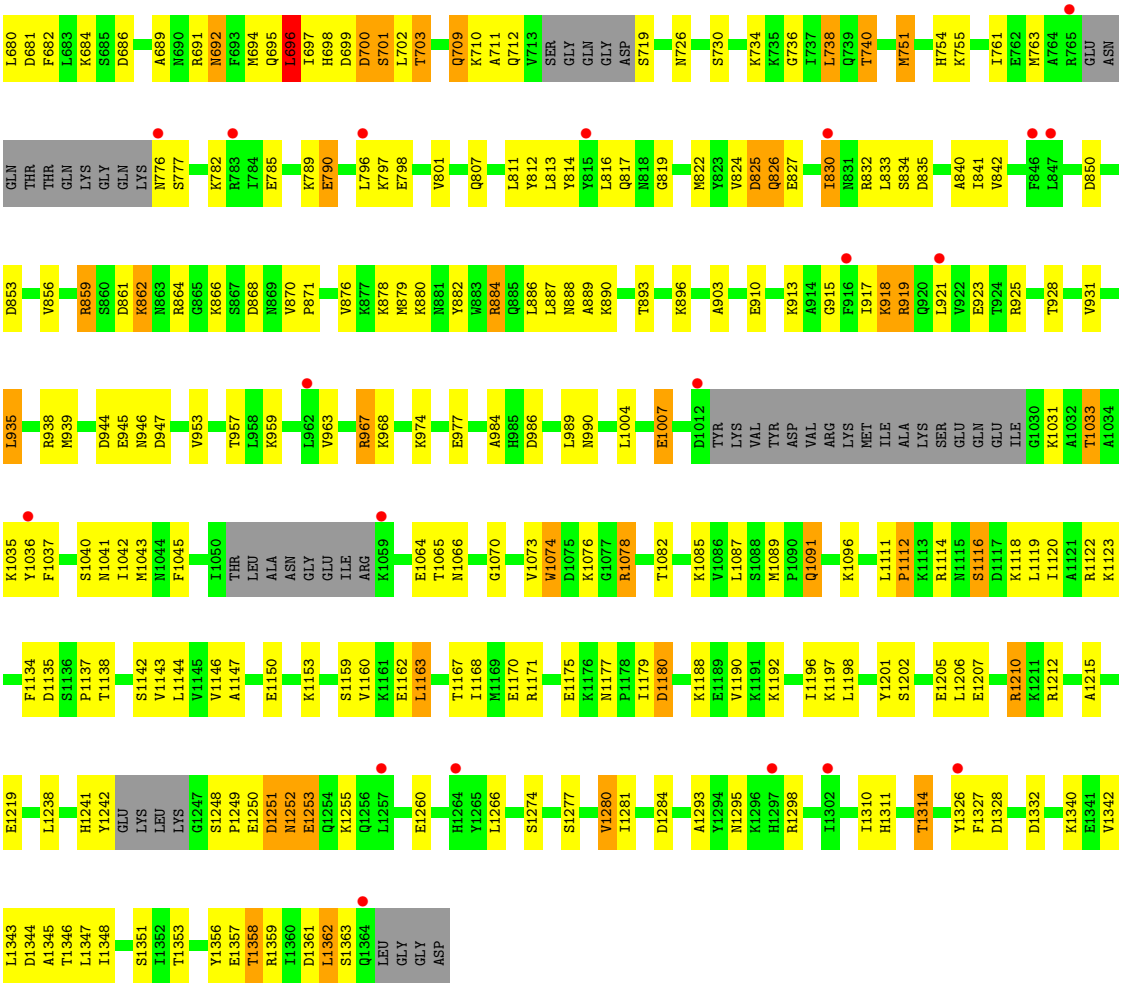
Chain A:



• Molecule 2: CRISPR-associated endonuclease Cas9

Chain B:





• Molecule 3: target DNA

• Molecule 4: non-target DNA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.96Å 69.14Å 189.24Å 90.00° 110.34° 90.00°	Depositor
Resolution (Å)	48.89 – 2.98 48.85 – 2.98	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.89-2.98) 92.0 (48.85-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.197 , 0.274 0.204 , 0.270	Depositor DCC
R_{free} test set	2073 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13302	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.15	19/1942 (1.0%)	0.91	0/3023
2	B	0.74	0/10943	0.95	0/14703
3	C	1.03	4/636 (0.6%)	0.96	0/980
4	D	1.27	3/253 (1.2%)	0.96	0/389
All	All	0.84	26/13774 (0.2%)	0.94	0/19095

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	DT	O3'-P	-9.21	1.50	1.61
4	D	7	DA	O3'-P	-8.71	1.50	1.61
1	A	15	A	O3'-P	-7.98	1.51	1.61
1	A	5	C	O3'-P	-7.85	1.51	1.61
1	A	68	A	O3'-P	-7.76	1.51	1.61
3	C	14	DT	O3'-P	-7.75	1.51	1.61
1	A	24	U	O3'-P	-7.56	1.52	1.61
1	A	14	U	O3'-P	-7.51	1.52	1.61
3	C	12	DT	O3'-P	-7.38	1.52	1.61
1	A	61	C	O3'-P	-7.29	1.52	1.61
1	A	65	A	O3'-P	-7.27	1.52	1.61
1	A	49	A	O3'-P	-7.08	1.52	1.61
1	A	62	G	O3'-P	-6.98	1.52	1.61
3	C	19	DA	O3'-P	-6.97	1.52	1.61
1	A	69	A	O3'-P	-6.83	1.52	1.61
1	A	51	A	O3'-P	-6.73	1.53	1.61
1	A	25	U	O3'-P	-6.68	1.53	1.61
1	A	12	U	O3'-P	-6.49	1.53	1.61
1	A	17	A	O3'-P	-6.47	1.53	1.61
1	A	67	C	O3'-P	-6.41	1.53	1.61
1	A	29	G	O3'-P	-6.35	1.53	1.61
3	C	3	DA	O3'-P	-6.17	1.53	1.61
4	D	6	DG	O3'-P	-5.94	1.54	1.61
1	A	18	A	O3'-P	-5.61	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	A	O3'-P	-5.60	1.54	1.61
1	A	66	U	O3'-P	-5.15	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 (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	50	0
2	B	10754	0	10917	281	0
3	C	569	0	323	26	0
4	D	225	0	126	17	0
5	A	2	0	0	0	0
5	B	19	0	0	0	0
5	C	1	0	0	0	0
All	All	13302	0	12235	347	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 14.

All (347) 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:B:317:LEU:HD22	2:B:414:ILE:CD1	1.45	1.42
2:B:317:LEU:CD2	2:B:414:ILE:HD11	1.56	1.34
3:C:19:DA:H5"	3:C:19:DA:H8	1.14	1.13
3:C:19:DA:H5"	3:C:19:DA:C8	1.92	1.03
2:B:882:TYR:CZ	2:B:886:LEU:HD11	2.00	0.96
1:A:32:A:N6	1:A:33:G:C6	2.34	0.96
3:C:11:DT:C2'	3:C:12:DT:H5"	1.97	0.94
3:C:11:DT:H2"	3:C:12:DT:H5"	1.52	0.92
4:D:8:DT:H2"	4:D:9:DA:O5'	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LEU:HD22	2:B:281:GLN:OE1	1.70	0.90
2:B:380:LEU:O	2:B:386:THR:HG21	1.74	0.87
2:B:321:MET:HE1	2:B:324:ARG:CZ	2.06	0.86
2:B:882:TYR:CE2	2:B:886:LEU:HD11	2.12	0.85
2:B:178:ASN:HD21	2:B:310:THR:H	1.25	0.82
2:B:424:ARG:NH1	2:B:437:ARG:NH1	2.27	0.82
3:C:5:DA:C2	4:D:9:DA:C2	2.67	0.82
2:B:813:LEU:O	2:B:817:GLN:HG3	1.78	0.81
2:B:1248:SER:HB2	2:B:1249:PRO:HD2	1.62	0.81
2:B:317:LEU:CD2	2:B:414:ILE:CD1	2.31	0.80
2:B:502:LEU:HD21	2:B:670:ILE:HD11	1.66	0.77
2:B:420:HIS:CD2	2:B:441:GLU:OE1	2.38	0.75
2:B:217:SER:OG	2:B:220:ARG:HG2	1.86	0.75
2:B:870:VAL:HG13	2:B:871:PRO:HD2	1.68	0.75
1:A:76:A:H2'	1:A:77:A:O4'	1.87	0.75
2:B:317:LEU:HB2	2:B:414:ILE:HD13	1.68	0.74
1:A:18:A:OP2	2:B:71:ARG:NH1	2.21	0.74
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.68	0.74
2:B:35:LEU:HB2	2:B:1358:THR:HB	1.68	0.73
2:B:623:LEU:HG	2:B:654:ARG:O	1.89	0.73
3:C:11:DT:H2'	3:C:12:DT:H5"	1.72	0.72
1:A:32:A:C6	1:A:33:G:C6	2.79	0.70
2:B:1162:GLU:HA	2:B:1343:LEU:HD11	1.73	0.70
2:B:709:GLN:O	2:B:709:GLN:NE2	2.23	0.70
2:B:122:ILE:O	2:B:126:VAL:HG23	1.91	0.70
2:B:1210:ARG:HG3	2:B:1280:VAL:HA	1.72	0.69
2:B:1311:HIS:O	2:B:1314:THR:HG23	1.92	0.69
1:A:18:A:OP1	2:B:165:ARG:HD3	1.92	0.69
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.25	0.68
2:B:736:GLY:O	2:B:740:THR:HG22	1.93	0.68
3:C:2:DA:H2"	3:C:3:DA:OP2	1.94	0.67
1:A:75:A:H2'	1:A:76:A:C8	2.30	0.67
2:B:143:VAL:HG11	2:B:315:ALA:HB2	1.77	0.67
2:B:1205:GLU:HB2	2:B:1348:ILE:HD11	1.77	0.67
2:B:635:ARG:CG	2:B:635:ARG:HH11	2.07	0.66
2:B:1295:ASN:HA	2:B:1298:ARG:CD	2.26	0.66
2:B:165:ARG:O	2:B:412:HIS:HA	1.96	0.65
2:B:424:ARG:HH11	2:B:437:ARG:NH1	1.92	0.65
2:B:627:GLU:O	2:B:655:ARG:NH1	2.29	0.65
2:B:507:VAL:HG11	2:B:660:GLY:O	1.97	0.64
2:B:893:THR:HG23	2:B:896:LYS:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ASN:HD21	3:C:19:DA:P	2.20	0.64
2:B:777:SER:OG	2:B:807:GLN:NE2	2.30	0.64
3:C:19:DA:H2"	3:C:20:DT:O5'	1.97	0.64
2:B:307:ARG:O	2:B:308:VAL:HG23	1.98	0.64
2:B:672:ASP:OD2	2:B:674:GLN:HB3	1.97	0.64
2:B:414:ILE:C	2:B:414:ILE:HD12	2.17	0.63
2:B:691:ARG:HB3	2:B:696:LEU:HD13	1.80	0.63
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.80	0.63
2:B:678:THR:O	2:B:681:ASP:HB2	1.99	0.62
2:B:1295:ASN:HA	2:B:1298:ARG:HD3	1.81	0.62
2:B:82:LEU:HD13	2:B:155:TYR:CE1	2.34	0.62
2:B:824:VAL:O	2:B:825:ASP:HB3	2.00	0.62
2:B:208:ALA:O	2:B:212:LEU:HB2	1.98	0.62
3:C:2:DA:H61	4:D:11:DT:H3	1.46	0.62
2:B:1144:LEU:HD22	2:B:1196:ILE:HD12	1.82	0.61
1:A:73:G:H5"	1:A:74:A:OP2	1.99	0.61
2:B:114:GLU:CD	2:B:116:HIS:HD1	2.04	0.61
2:B:1344:ASP:HA	2:B:1362:LEU:O	2.00	0.61
3:C:12:DT:C5'	3:C:12:DT:H6	2.13	0.60
2:B:86:PHE:CE2	2:B:155:TYR:HB2	2.35	0.60
2:B:22:THR:HG22	2:B:23:ASP:H	1.67	0.60
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.84	0.60
2:B:686:ASP:OD2	2:B:691:ARG:HB2	2.01	0.59
2:B:680:LEU:HG	2:B:684:LYS:HE2	1.83	0.59
1:A:33:G:O2'	1:A:35:A:N6	2.31	0.59
2:B:420:HIS:HD2	2:B:441:GLU:OE1	1.85	0.59
2:B:884:ARG:O	2:B:888:ASN:ND2	2.35	0.59
2:B:165:ARG:NH2	2:B:446:PHE:O	2.34	0.59
2:B:217:SER:O	2:B:221:ARG:HG3	2.02	0.59
2:B:178:ASN:ND2	2:B:310:THR:OG1	2.36	0.58
2:B:505:GLU:CD	2:B:665:LYS:HD3	2.24	0.58
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.84	0.58
2:B:876:VAL:O	2:B:880:LYS:HB2	2.04	0.58
2:B:317:LEU:CB	2:B:414:ILE:HD13	2.33	0.58
1:A:24:U:O2	2:B:105:PHE:CD1	2.57	0.58
4:D:7:DA:H2"	4:D:8:DT:C5'	2.34	0.58
1:A:75:A:C6	1:A:76:A:C6	2.92	0.58
2:B:1248:SER:O	2:B:1252:ASN:HB2	2.04	0.57
3:C:2:DA:N6	4:D:11:DT:H3	2.01	0.57
3:C:2:DA:N1	4:D:11:DT:O2	2.37	0.57
1:A:20:A:OP1	2:B:403:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:TYR:CG	2:B:155:TYR:O	2.57	0.57
1:A:32:A:C6	1:A:33:G:C5	2.93	0.57
2:B:212:LEU:O	2:B:221:ARG:NE	2.38	0.56
1:A:25:U:H1'	2:B:104:SER:O	2.05	0.56
2:B:450:TYR:OH	2:B:627:GLU:CG	2.54	0.56
2:B:181:VAL:CG1	2:B:300:ILE:HD11	2.36	0.56
2:B:682:PHE:CE1	2:B:702:LEU:HD11	2.41	0.56
4:D:7:DA:H2"	4:D:8:DT:H5"	1.87	0.56
4:D:8:DT:C2'	4:D:9:DA:O5'	2.49	0.56
2:B:418:GLU:O	2:B:419:LEU:C	2.42	0.56
2:B:1361:ASP:O	2:B:1363:SER:N	2.37	0.56
1:A:32:A:N6	1:A:33:G:N1	2.52	0.56
2:B:373:TYR:CE1	2:B:398:LEU:HB3	2.40	0.56
2:B:1138:THR:HB	2:B:1168:ILE:HD12	1.88	0.56
1:A:68:A:H2	2:B:1358:THR:HG23	1.71	0.55
2:B:646:LYS:HE3	2:B:649:LYS:HD3	1.87	0.55
2:B:1277:SER:HA	2:B:1281:ILE:HB	1.87	0.55
1:A:44:U:C4	2:B:328:HIS:CD2	2.95	0.55
2:B:692:ASN:C	2:B:692:ASN:HD22	2.10	0.55
4:D:8:DT:H2"	4:D:9:DA:C5'	2.36	0.55
2:B:307:ARG:NH2	2:B:397:ASP:OD2	2.23	0.55
1:A:54:G:C6	1:A:55:C:N4	2.75	0.55
1:A:74:A:H2'	1:A:75:A:O4'	2.07	0.55
2:B:77:ASN:HA	2:B:80:CYS:HB2	1.89	0.55
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.40	0.55
2:B:78:ARG:NH1	2:B:162:ILE:O	2.40	0.54
2:B:116:HIS:CE1	2:B:122:ILE:HG12	2.42	0.54
2:B:700:ASP:N	2:B:700:ASP:OD1	2.36	0.54
2:B:1167:THR:OG1	2:B:1170:GLU:HG3	2.08	0.54
2:B:730:SER:O	2:B:734:LYS:HG3	2.08	0.54
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.08	0.54
3:C:10:DT:H2"	3:C:11:DT:H5'	1.90	0.54
2:B:939:MET:HB3	2:B:953:VAL:HG21	1.90	0.53
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.40	0.53
2:B:321:MET:CE	2:B:324:ARG:NE	2.72	0.53
1:A:32:A:C5	1:A:33:G:C5	2.96	0.53
2:B:155:TYR:O	2:B:155:TYR:CD2	2.61	0.53
2:B:944:ASP:OD1	2:B:947:ASP:N	2.41	0.53
2:B:1248:SER:CB	2:B:1249:PRO:HD2	2.37	0.53
2:B:563:GLN:O	2:B:567:ASP:HB2	2.09	0.53
2:B:1250:GLU:O	2:B:1253:GLU:HB3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:672:ASP:HA	2:B:703:THR:HB	1.92	0.52
2:B:910:GLU:HG2	2:B:1033:THR:HG23	1.92	0.52
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.45	0.52
2:B:450:TYR:OH	2:B:627:GLU:HG2	2.09	0.52
1:A:46:A:H2'	1:A:47:A:C8	2.45	0.52
2:B:303:SER:OG	2:B:304:ASP:N	2.42	0.52
1:A:33:G:HO2'	1:A:35:A:H62	1.52	0.52
2:B:824:VAL:O	2:B:825:ASP:CB	2.56	0.52
1:A:62:G:C5	2:B:69:ARG:HD3	2.45	0.52
2:B:870:VAL:CG1	2:B:871:PRO:HD2	2.39	0.52
2:B:635:ARG:HH11	2:B:635:ARG:HG2	1.73	0.52
3:C:18:DA:C2'	3:C:19:DA:O5'	2.57	0.52
2:B:143:VAL:HG21	2:B:418:GLU:HB3	1.90	0.51
2:B:826:GLN:NE2	2:B:859:ARG:HD3	2.24	0.51
2:B:1340:LYS:O	2:B:1343:LEU:HB2	2.11	0.51
2:B:686:ASP:O	2:B:689:ALA:O	2.28	0.51
2:B:22:THR:HG22	2:B:23:ASP:N	2.25	0.51
2:B:161:MET:CE	2:B:419:LEU:HA	2.40	0.51
2:B:1163:LEU:HD21	2:B:1198:LEU:HD12	1.93	0.51
2:B:321:MET:HE2	2:B:321:MET:HA	1.93	0.51
2:B:323:LYS:O	2:B:327:GLU:HG3	2.11	0.51
2:B:317:LEU:HD21	2:B:415:HIS:CD2	2.45	0.51
2:B:524:LEU:HD22	2:B:540:LEU:HD23	1.93	0.51
2:B:630:GLU:O	2:B:633:GLU:HB3	2.11	0.51
2:B:512:SER:HB3	2:B:515:TYR:HB2	1.92	0.50
2:B:635:ARG:HG2	2:B:635:ARG:NH1	2.25	0.50
2:B:41:HIS:ND1	2:B:41:HIS:N	2.60	0.50
2:B:672:ASP:OD1	2:B:703:THR:HB	2.10	0.50
2:B:812:TYR:CZ	2:B:816:LEU:HD11	2.46	0.50
3:C:12:DT:H6	3:C:12:DT:H5'	1.76	0.50
2:B:335:LEU:O	2:B:339:VAL:HG23	2.11	0.50
2:B:161:MET:HE1	2:B:419:LEU:HA	1.92	0.50
2:B:373:TYR:CZ	2:B:398:LEU:HB3	2.46	0.50
2:B:181:VAL:HB	2:B:209:LYS:HE2	1.94	0.50
1:A:65:A:O5'	1:A:65:A:H8	1.93	0.50
2:B:155:TYR:CD2	2:B:155:TYR:C	2.85	0.50
1:A:20:A:P	2:B:403:ARG:NH1	2.85	0.49
1:A:73:G:C5'	1:A:74:A:OP2	2.60	0.49
2:B:1066:ASN:O	2:B:1070:GLY:N	2.43	0.49
2:B:497:ASN:ND2	3:C:18:DA:O3'	2.43	0.49
2:B:527:VAL:HA	2:B:582:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1078:ARG:O	2:B:1082:THR:HG23	2.13	0.49
2:B:184:LEU:HD22	2:B:295:ASN:HB3	1.95	0.49
2:B:1215:ALA:HB3	2:B:1219:GLU:O	2.12	0.49
2:B:1250:GLU:HA	2:B:1250:GLU:OE1	2.12	0.49
1:A:47:A:O5'	1:A:47:A:H8	1.95	0.49
2:B:402:GLN:NE2	2:B:402:GLN:N	2.60	0.49
2:B:977:GLU:CG	2:B:1310:ILE:HG23	2.41	0.49
2:B:1114:ARG:HD3	2:B:1116:SER:CB	2.42	0.49
2:B:1171:ARG:O	2:B:1175:GLU:HG3	2.13	0.49
2:B:1357:GLU:O	2:B:1358:THR:HG22	2.13	0.49
1:A:41:A:H8	1:A:41:A:OP2	1.95	0.49
2:B:306:LEU:O	2:B:320:SER:HB2	2.13	0.49
2:B:424:ARG:O	2:B:427:GLU:HG2	2.13	0.49
2:B:600:ILE:HG21	2:B:651:LEU:HD23	1.94	0.49
2:B:181:VAL:HG13	2:B:300:ILE:HD11	1.95	0.48
2:B:181:VAL:HG22	2:B:300:ILE:HD12	1.94	0.48
2:B:1114:ARG:HD3	2:B:1116:SER:HB2	1.94	0.48
4:D:7:DA:C2'	4:D:8:DT:H5"	2.43	0.48
2:B:963:VAL:HG13	2:B:989:LEU:HB3	1.94	0.48
3:C:19:DA:H2"	3:C:20:DT:C5'	2.43	0.48
2:B:1120:ILE:HD11	2:B:1137:PRO:HD3	1.96	0.48
2:B:317:LEU:CD2	2:B:415:HIS:CD2	2.97	0.48
2:B:505:GLU:OE2	2:B:665:LYS:HD3	2.13	0.48
2:B:192:TYR:O	2:B:194:GLN:N	2.47	0.48
2:B:45:LYS:HA	2:B:1091:GLN:OE1	2.14	0.48
2:B:635:ARG:CG	2:B:635:ARG:NH1	2.72	0.48
3:C:17:DA:H2"	3:C:18:DA:H5'	1.95	0.48
2:B:624:THR:HA	2:B:656:TYR:O	2.14	0.47
2:B:380:LEU:O	2:B:383:MET:HB2	2.14	0.47
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.44	0.47
2:B:86:PHE:CD2	2:B:155:TYR:HB2	2.50	0.47
2:B:840:ALA:O	2:B:864:ARG:NH2	2.47	0.47
2:B:1210:ARG:HA	2:B:1280:VAL:HG22	1.97	0.47
2:B:1238:LEU:O	2:B:1241:HIS:N	2.41	0.47
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.97	0.47
2:B:499:ASP:OD2	2:B:663:SER:N	2.48	0.47
2:B:814:TYR:CZ	2:B:830:ILE:HG23	2.50	0.47
2:B:317:LEU:HD22	2:B:414:ILE:HD11	0.60	0.46
2:B:321:MET:CE	2:B:324:ARG:CZ	2.86	0.46
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.60	0.46
2:B:507:VAL:CG1	2:B:660:GLY:C	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:LEU:O	2:B:601:ILE:HG13	2.15	0.46
2:B:1150:GLU:OE2	2:B:1188:LYS:NZ	2.31	0.46
2:B:1251:ASP:C	2:B:1253:GLU:H	2.19	0.46
1:A:45:U:O2'	1:A:46:A:H5'	2.16	0.46
2:B:637:LYS:O	2:B:638:THR:C	2.54	0.46
1:A:35:A:H2'	1:A:36:A:C8	2.50	0.46
2:B:273:ASP:O	2:B:277:ASN:OD1	2.33	0.46
2:B:186:ILE:CG2	2:B:186:ILE:O	2.63	0.46
1:A:40:C:H2'	1:A:41:A:O4'	2.15	0.46
3:C:8:DG:C6	4:D:4:DA:N6	2.84	0.46
1:A:81:G:N1	2:B:1356:TYR:HB3	2.31	0.46
2:B:1293:ALA:HB1	2:B:1326:TYR:CD2	2.51	0.46
2:B:1045:PHE:O	2:B:1064:GLU:HG3	2.15	0.46
2:B:186:ILE:O	2:B:186:ILE:HG22	2.16	0.46
2:B:817:GLN:O	2:B:882:TYR:OH	2.28	0.46
2:B:822:MET:CB	2:B:856:VAL:HG13	2.46	0.46
4:D:11:DT:H2"	4:D:12:DG:C8	2.51	0.46
1:A:38:A:H8	1:A:38:A:H5"	1.80	0.45
1:A:73:G:O2'	1:A:75:A:N7	2.27	0.45
2:B:1179:ILE:HD11	2:B:1192:LYS:HD3	1.98	0.45
1:A:38:A:H5"	1:A:38:A:C8	2.52	0.45
2:B:181:VAL:HG13	2:B:300:ILE:CD1	2.47	0.45
3:C:1:DC:H5"	3:C:1:DC:H6	1.81	0.45
2:B:853:ASP:OD1	2:B:893:THR:HG21	2.16	0.45
2:B:357:ASN:ND2	2:B:371:GLU:HB3	2.32	0.45
2:B:133:PRO:HG2	2:B:137:HIS:CE1	2.52	0.45
2:B:356:LYS:HD2	2:B:356:LYS:N	2.32	0.45
2:B:672:ASP:OD2	2:B:675:SER:OG	2.31	0.45
2:B:1351:SER:OG	2:B:1356:TYR:HB2	2.17	0.45
4:D:3:DA:H2"	4:D:4:DA:C8	2.52	0.45
2:B:853:ASP:CG	2:B:893:THR:HG21	2.37	0.45
2:B:871:PRO:O	2:B:903:ALA:HB2	2.17	0.45
1:A:33:G:HO2'	1:A:35:A:N6	2.11	0.45
2:B:139:ARG:HH22	2:B:415:HIS:CD2	2.35	0.45
2:B:335:LEU:O	2:B:335:LEU:HG	2.16	0.45
1:A:60:C:OP1	2:B:455:LEU:HB2	2.17	0.44
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.98	0.44
2:B:832:ARG:O	2:B:833:LEU:C	2.56	0.44
2:B:1120:ILE:N	2:B:1134:PHE:O	2.49	0.44
2:B:278:LEU:O	2:B:281:GLN:N	2.44	0.44
2:B:565:LYS:HG2	2:B:578:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:LEU:O	2:B:1112:PRO:O	2.35	0.44
2:B:206:VAL:HG22	2:B:228:GLN:HB3	1.99	0.44
1:A:33:G:N2	1:A:36:A:OP2	2.51	0.44
2:B:918:LYS:HE2	2:B:1007:GLU:OE2	2.18	0.44
4:D:11:DT:C2'	4:D:12:DG:C8	3.01	0.44
1:A:76:A:H2'	1:A:77:A:C4'	2.47	0.44
2:B:915:GLY:O	2:B:919:ARG:NH1	2.48	0.44
2:B:1073:VAL:O	2:B:1074:TRP:HB2	2.17	0.44
2:B:305:ILE:HG22	2:B:306:LEU:HD23	1.99	0.44
2:B:923:GLU:OE1	2:B:925:ARG:NH1	2.51	0.44
2:B:138:LEU:HG	2:B:142:LEU:HD12	1.99	0.43
2:B:211:ILE:O	2:B:221:ARG:HD2	2.18	0.43
2:B:215:ARG:O	2:B:216:LEU:HD23	2.17	0.43
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.54	0.43
2:B:692:ASN:O	2:B:695:GLN:HB2	2.18	0.43
2:B:738:LEU:HD23	2:B:738:LEU:HA	1.82	0.43
2:B:1118:LYS:HD3	2:B:1118:LYS:HA	1.81	0.43
2:B:450:TYR:OH	2:B:627:GLU:HG3	2.19	0.43
1:A:44:U:N3	2:B:328:HIS:CD2	2.87	0.43
2:B:507:VAL:HG13	2:B:660:GLY:C	2.39	0.43
2:B:692:ASN:O	2:B:695:GLN:N	2.52	0.43
2:B:736:GLY:O	2:B:740:THR:CG2	2.65	0.43
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.53	0.43
1:A:49:A:H2'	1:A:50:U:O4'	2.18	0.43
2:B:651:LEU:HD23	2:B:651:LEU:HA	1.62	0.43
2:B:675:SER:H	2:B:675:SER:HG	1.55	0.43
2:B:5:TYR:CE1	2:B:751:MET:HG3	2.54	0.43
2:B:143:VAL:HG22	2:B:421:ALA:HB3	2.01	0.43
2:B:826:GLN:O	2:B:826:GLN:HG3	2.18	0.43
2:B:116:HIS:CE1	2:B:122:ILE:CG1	3.02	0.43
2:B:755:LYS:HG2	2:B:939:MET:CE	2.49	0.42
2:B:817:GLN:C	2:B:882:TYR:HH	2.21	0.42
3:C:9:DT:H2"	3:C:10:DT:O5'	2.19	0.42
2:B:324:ARG:NH1	2:B:401:LYS:O	2.51	0.42
2:B:861:ASP:O	2:B:864:ARG:HD2	2.19	0.42
2:B:1177:ASN:ND2	2:B:1180:ASP:CG	2.73	0.42
3:C:16:DC:H2'	3:C:17:DA:C8	2.54	0.42
2:B:868:ASP:OD1	2:B:868:ASP:O	2.36	0.42
2:B:1004:LEU:HD11	2:B:1042:ILE:CD1	2.50	0.42
2:B:1251:ASP:O	2:B:1255:LYS:HG2	2.19	0.42
2:B:324:ARG:HH22	2:B:407:ASN:HD21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:646:LYS:HD2	2:B:646:LYS:HA	1.90	0.42
2:B:817:GLN:C	2:B:882:TYR:OH	2.58	0.42
2:B:695:GLN:O	2:B:698:HIS:N	2.48	0.42
3:C:2:DA:N1	4:D:11:DT:C2	2.87	0.42
3:C:18:DA:H2"	3:C:19:DA:O5'	2.18	0.42
1:A:47:A:O2'	2:B:101:LEU:O	2.38	0.42
2:B:22:THR:CG2	2:B:23:ASP:H	2.32	0.42
2:B:163:LYS:HD3	2:B:164:PHE:CE2	2.55	0.42
2:B:32:PHE:HD1	2:B:45:LYS:HG3	1.85	0.42
2:B:48:ILE:HG12	2:B:984:ALA:HB1	2.02	0.42
2:B:460:SER:HB3	2:B:463:ALA:CB	2.50	0.42
2:B:620:VAL:O	2:B:624:THR:OG1	2.30	0.41
2:B:862:LYS:O	2:B:864:ARG:N	2.53	0.41
2:B:43:ILE:HG22	2:B:45:LYS:HG2	2.02	0.41
2:B:283:GLY:HA3	2:B:285:GLN:OE1	2.20	0.41
2:B:359:TYR:O	2:B:363:ILE:HG12	2.20	0.41
2:B:699:ASP:OD1	2:B:701:SER:HB3	2.20	0.41
2:B:935:LEU:HD12	2:B:935:LEU:HA	1.86	0.41
1:A:59:U:OP1	2:B:467:ARG:NH2	2.54	0.41
2:B:634:GLU:OE2	2:B:637:LYS:HE2	2.20	0.41
2:B:692:ASN:C	2:B:692:ASN:ND2	2.73	0.41
2:B:178:ASN:HD21	2:B:310:THR:N	2.06	0.41
2:B:530:VAL:HG22	2:B:537:PRO:HB3	2.02	0.41
2:B:536:LYS:HG2	2:B:537:PRO:HD2	2.03	0.41
2:B:928:THR:O	2:B:931:VAL:HB	2.21	0.41
4:D:7:DA:H2"	4:D:8:DT:H5'	2.02	0.41
2:B:796:LEU:C	2:B:798:GLU:H	2.23	0.41
1:A:59:U:O4	2:B:475:PRO:HG3	2.20	0.41
2:B:530:VAL:HG23	2:B:579:GLU:HB3	2.02	0.41
1:A:60:C:H4'	2:B:456:ALA:HA	2.03	0.41
2:B:243:ALA:O	2:B:248:LEU:HB2	2.20	0.41
4:D:11:DT:H2"	4:D:12:DG:O4'	2.21	0.41
1:A:35:A:H2'	1:A:36:A:N9	2.36	0.41
1:A:61:C:OP2	2:B:70:ARG:HD3	2.21	0.41
1:A:81:G:C2	2:B:1356:TYR:HB3	2.56	0.41
2:B:11:ILE:HB	2:B:763:MET:HG2	2.03	0.41
2:B:192:TYR:O	2:B:195:LEU:N	2.54	0.41
2:B:879:MET:O	2:B:882:TYR:N	2.52	0.41
2:B:1206:LEU:CD2	2:B:1345:ALA:HB2	2.51	0.41
1:A:24:U:C2	2:B:105:PHE:CD1	3.09	0.40
2:B:181:VAL:HG11	2:B:300:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:DA:H2'	3:C:19:DA:C8	2.57	0.40
1:A:3:A:H2'	1:A:4:A:C8	2.56	0.40
2:B:148:LYS:HG3	2:B:429:PHE:CG	2.57	0.40
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.92	0.40
2:B:369:GLN:HG2	2:B:373:TYR:CE2	2.57	0.40
2:B:1037:PHE:O	2:B:1041:ASN:HB2	2.21	0.40
1:A:75:A:C5	1:A:76:A:C6	3.10	0.40
2:B:393:LEU:O	2:B:393:LEU:HD23	2.22	0.40
2:B:521:TYR:O	2:B:522:ASN:C	2.60	0.40
2:B:1241:HIS:O	2:B:1242:TYR:C	2.60	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%)	1125 (86%)	153 (12%)	23 (2%)	8 35

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	197	GLU
2	B	826	GLN
2	B	696	LEU
2	B	825	ASP
2	B	1036	TYR
2	B	1074	TRP
2	B	1112	PRO
2	B	1252	ASN
2	B	1362	LEU
2	B	178	ASN
2	B	193	ASN

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Mol	Chain	Res	Type
2	B	542	GLY
2	B	711	ALA
2	B	789	LYS
2	B	1116	SER
2	B	1201	TYR
2	B	797	LYS
2	B	1284	ASP
2	B	325	TYR
2	B	1202	SER
2	B	179	SER
2	B	841	ILE
2	B	1253	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	1180/1225 (96%)	997 (84%)	183 (16%)	2 12

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	4	LYS
2	B	27	VAL
2	B	29	SER
2	B	38	THR
2	B	39	ASP
2	B	41	HIS
2	B	44	LYS
2	B	45	LYS
2	B	65	LYS
2	B	71	ARG
2	B	75	ARG
2	B	80	CYS
2	B	82	LEU
2	B	84	GLU

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Mol	Chain	Res	Type
2	B	96	SER
2	B	102	GLU
2	B	115	ARG
2	B	117	PRO
2	B	139	ARG
2	B	141	LYS
2	B	146	THR
2	B	165	ARG
2	B	173	ASP
2	B	174	LEU
2	B	175	ASN
2	B	178	ASN
2	B	188	LEU
2	B	197	GLU
2	B	212	LEU
2	B	215	ARG
2	B	226	ILE
2	B	234	LYS
2	B	244	LEU
2	B	253	LYS
2	B	291	LEU
2	B	300	ILE
2	B	303	SER
2	B	304	ASP
2	B	308	VAL
2	B	311	GLU
2	B	320	SER
2	B	321	MET
2	B	355	SER
2	B	395	ARG
2	B	402	GLN
2	B	406	ASP
2	B	409	SER
2	B	414	ILE
2	B	418	GLU
2	B	425	ARG
2	B	438	GLU
2	B	455	LEU
2	B	465	MET
2	B	466	THR
2	B	469	SER
2	B	472	THR

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Mol	Chain	Res	Type
2	B	474	THR
2	B	490	SER
2	B	512	SER
2	B	514	LEU
2	B	519	THR
2	B	524	LEU
2	B	525	THR
2	B	530	VAL
2	B	534	MET
2	B	536	LYS
2	B	540	LEU
2	B	541	SER
2	B	543	GLU
2	B	557	ARG
2	B	562	LYS
2	B	577	SER
2	B	579	GLU
2	B	581	SER
2	B	590	SER
2	B	598	LEU
2	B	602	LYS
2	B	605	ASP
2	B	610	GLU
2	B	623	LEU
2	B	627	GLU
2	B	630	GLU
2	B	634	GLU
2	B	635	ARG
2	B	638	THR
2	B	643	PHE
2	B	646	LYS
2	B	651	LEU
2	B	661	ARG
2	B	665	LYS
2	B	666	LEU
2	B	675	SER
2	B	692	ASN
2	B	694	MET
2	B	696	LEU
2	B	697	ILE
2	B	700	ASP
2	B	701	SER

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Mol	Chain	Res	Type
2	B	703	THR
2	B	709	GLN
2	B	710	LYS
2	B	712	GLN
2	B	719	SER
2	B	726	ASN
2	B	738	LEU
2	B	740	THR
2	B	751	MET
2	B	754	HIS
2	B	776	ASN
2	B	782	LYS
2	B	785	GLU
2	B	790	GLU
2	B	801	VAL
2	B	811	LEU
2	B	827	GLU
2	B	830	ILE
2	B	834	SER
2	B	835	ASP
2	B	842	VAL
2	B	850	ASP
2	B	859	ARG
2	B	862	LYS
2	B	866	LYS
2	B	878	LYS
2	B	884	ARG
2	B	887	LEU
2	B	890	LYS
2	B	913	LYS
2	B	917	ILE
2	B	918	LYS
2	B	919	ARG
2	B	921	LEU
2	B	935	LEU
2	B	938	ARG
2	B	945	GLU
2	B	946	ASN
2	B	957	THR
2	B	959	LYS
2	B	967	ARG
2	B	968	LYS

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Mol	Chain	Res	Type
2	B	974	LYS
2	B	1007	GLU
2	B	1031	LYS
2	B	1033	THR
2	B	1035	LYS
2	B	1040	SER
2	B	1065	THR
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	1096	LYS
2	B	1119	LEU
2	B	1122	ARG
2	B	1123	LYS
2	B	1135	ASP
2	B	1142	SER
2	B	1143	VAL
2	B	1146	VAL
2	B	1153	LYS
2	B	1159	SER
2	B	1160	VAL
2	B	1163	LEU
2	B	1180	ASP
2	B	1197	LYS
2	B	1207	GLU
2	B	1210	ARG
2	B	1251	ASP
2	B	1260	GLU
2	B	1266	LEU
2	B	1274	SER
2	B	1280	VAL
2	B	1314	THR
2	B	1327	PHE
2	B	1328	ASP
2	B	1332	ASP
2	B	1342	VAL
2	B	1346	THR
2	B	1347	LEU
2	B	1353	THR

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Mol	Chain	Res	Type
2	B	1358	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	113	HIS
2	B	178	ASN
2	B	341	GLN
2	B	394	ASN
2	B	407	ASN
2	B	415	HIS
2	B	420	HIS
2	B	563	GLN
2	B	692	ASN
2	B	698	HIS
2	B	709	GLN
2	B	712	GLN
2	B	726	ASN
2	B	807	GLN
2	B	817	GLN
2	B	826	GLN
2	B	926	GLN
2	B	946	ASN
2	B	1364	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	24 (30%)	1 (1%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	17	A
1	A	24	U
1	A	28	A
1	A	29	G
1	A	33	G
1	A	35	A

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Mol	Chain	Res	Type
1	A	37	U
1	A	38	A
1	A	39	G
1	A	41	A
1	A	42	A
1	A	44	U
1	A	45	U
1	A	51	A
1	A	59	U
1	A	63	U
1	A	68	A
1	A	73	G
1	A	74	A
1	A	77	A
1	A	78	A
1	A	80	U
1	A	81	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	38	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 monosaccharides 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	81/83 (97%)	-0.43	0 100 100	25, 45, 101, 110	0
2	B	1315/1368 (96%)	0.11	49 (3%) 41 25	28, 60, 101, 134	0
3	C	28/28 (100%)	-0.44	1 (3%) 42 26	31, 49, 80, 113	0
4	D	11/12 (91%)	-0.22	0 100 100	38, 63, 106, 127	0
All	All	1435/1491 (96%)	0.07	50 (3%) 44 26	25, 59, 101, 134	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	DC	5.3
2	B	350	ILE	4.1
2	B	200	PRO	3.8
2	B	346	LYS	3.5
2	B	198	GLU	3.3
2	B	846	PHE	3.3
2	B	197	GLU	3.1
2	B	776	ASN	3.1
2	B	247	GLY	3.0
2	B	358	GLY	3.0
2	B	199	ASN	2.9
2	B	190	GLN	2.7
2	B	1059	LYS	2.7
2	B	398	LEU	2.6
2	B	1257	LEU	2.6
2	B	264	LEU	2.6
2	B	191	THR	2.6
2	B	213	SER	2.6
2	B	1364	GLN	2.6
2	B	293	ALA	2.6
2	B	286	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	815	TYR	2.5
2	B	783	ARG	2.5
2	B	1264	HIS	2.5
2	B	533	GLY	2.5
2	B	271	TYR	2.4
2	B	216	LEU	2.4
2	B	765	ARG	2.4
2	B	830	ILE	2.4
2	B	1326	TYR	2.3
2	B	962	LEU	2.3
2	B	262	ALA	2.2
2	B	916	PHE	2.2
2	B	186	ILE	2.2
2	B	921	LEU	2.2
2	B	252	PHE	2.2
2	B	249	THR	2.1
2	B	246	LEU	2.1
2	B	269	ASP	2.1
2	B	351	PHE	2.1
2	B	1302	ILE	2.1
2	B	375	PHE	2.1
2	B	379	ILE	2.1
2	B	218	LYS	2.1
2	B	1036	TYR	2.0
2	B	1012	ASP	2.0
2	B	1297	HIS	2.0
2	B	215	ARG	2.0
2	B	796	LEU	2.0
2	B	847	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.