



# Full wwPDB X-ray Structure Validation Report i

Dec 23, 2024 – 04:08 PM JST

PDB ID : 8Y0D  
Title : Crystal structure of SauCas9 in complex with sgRNA and 20nt ssDNA target  
Authors : Chen, Y.; Chen, J.; Liu, L.  
Deposited on : 2024-01-22  
Resolution : 3.92 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](mailto: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 i symbol.

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

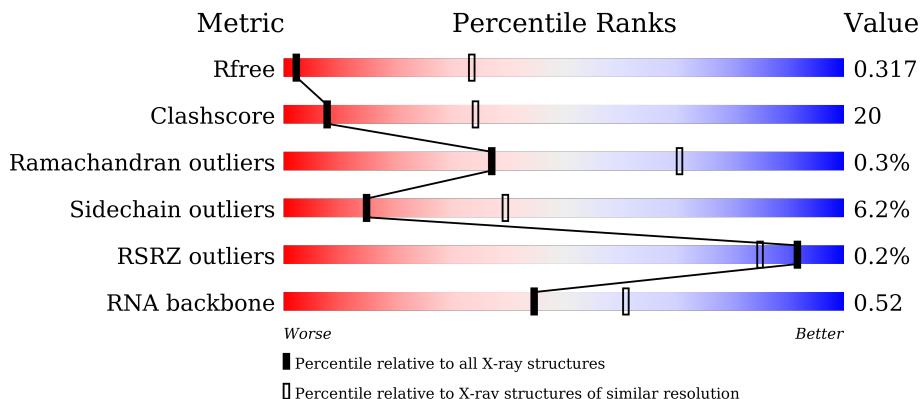
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1175 (4.14-3.70)
Clashscore	180529	1045 (4.12-3.72)
Ramachandran outliers	177936	1006 (4.12-3.72)
Sidechain outliers	177891	1185 (4.14-3.70)
RSRZ outliers	164620	1175 (4.14-3.70)
RNA backbone	3690	1136 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	74	19%	53%	23%	..	..
2	C	20	30%	50%	15%	5%	
3	A	1053	56%	37%	.	.	.

## 2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 10023 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 (73-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	73	1530	684	265	508	73	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*TP\*AP\*AP\*AP\*GP\*TP\*TP\*AP\*AP\*AP\*TP\*AP\*GP\*CP\*AP\*GP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	19	395	188	79	109	19	0	0	0

- Molecule 3 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1009	8093	5154	1376	1550	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ASN	conflict	UNP J7RUA5
A	946	ALA	CYS	conflict	UNP J7RUA5

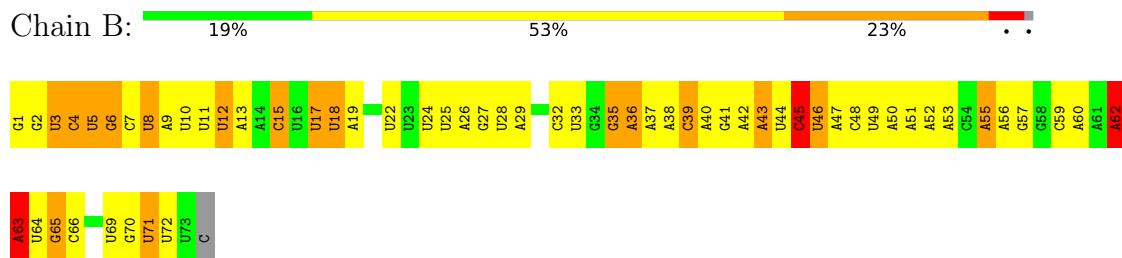
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
			Total	O	
4	B	1	1	1	0
4	A	4	4	4	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.

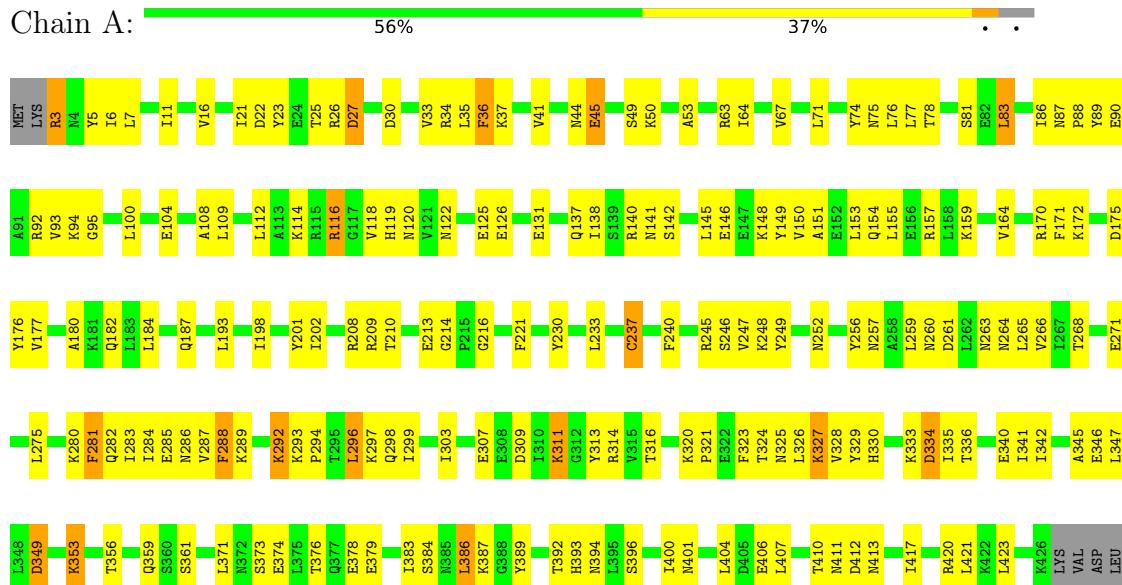
- Molecule 1: RNA (73-MER)

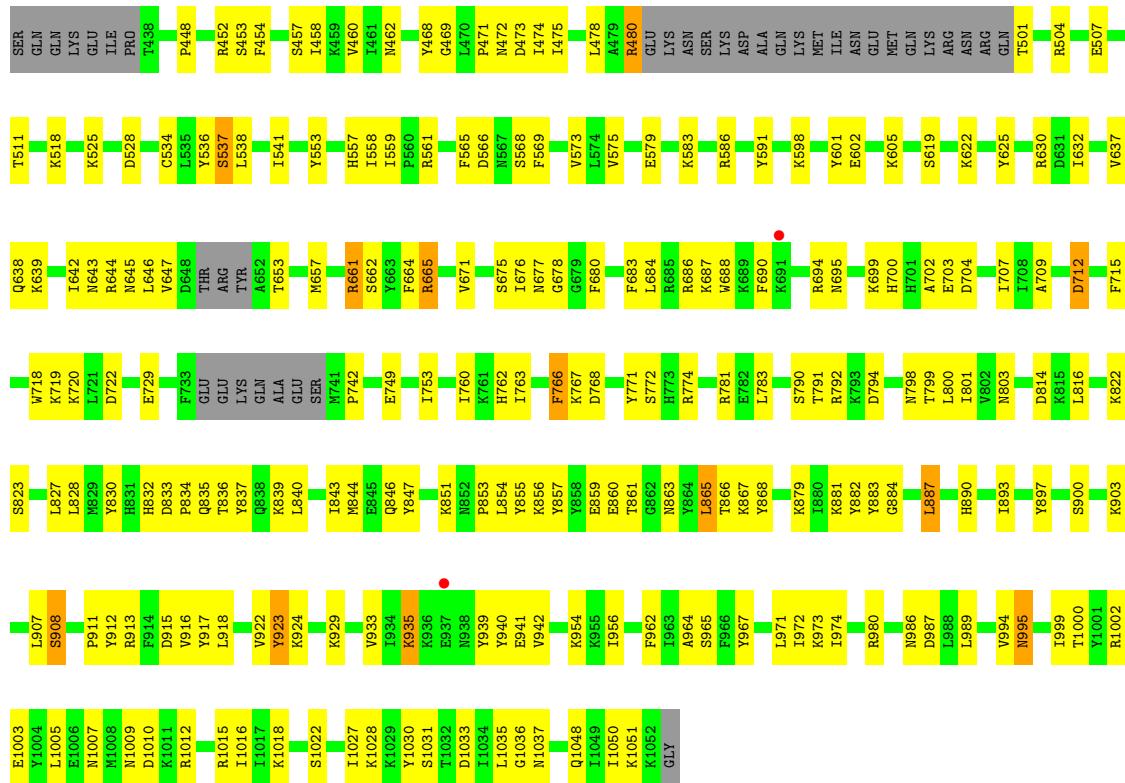


- Molecule 2: DNA (5'-D(P\*GP\*TP\*AP\*AP\*AP\*GP\*TP\*TP\*AP\*AP\*AP\*TP\*AP\*GP\*CP\*A P\*GP\*AP\*C)-3')



- Molecule 3: CRISPR-associated endonuclease Cas9





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.96 Å    145.57 Å    97.53 Å 90.00°    93.99°    90.00°	Depositor
Resolution (Å)	48.65 – 3.92 48.65 – 3.92	Depositor EDS
% Data completeness (in resolution range)	77.0 (48.65-3.92) 74.5 (48.65-3.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.86 (at 3.88 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
$R$ , $R_{free}$	0.286 , 0.318 0.286 , 0.317	Depositor DCC
$R_{free}$ test set	11962 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-1.3	Xtriage
Anisotropy	6.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.10 , 0.0	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.38$ , $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	10023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.63	9/1709 (0.5%)	0.97	7/2657 (0.3%)
2	C	0.98	3/445 (0.7%)	0.90	0/685
3	A	0.30	0/8231	0.50	0/11115
All	All	0.42	12/10385 (0.1%)	0.64	7/14457 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	G	OP3-P	-10.65	1.48	1.61
1	B	12	U	C1'-N1	6.68	1.58	1.48
1	B	5	U	C1'-N1	6.39	1.58	1.48
1	B	18	U	C1'-N1	6.37	1.58	1.48
1	B	8	U	C1'-N1	6.15	1.57	1.48
1	B	6	G	C1'-N9	-6.12	1.38	1.46
2	C	24	DA	C1'-N9	-6.04	1.38	1.47
1	B	3	U	C1'-N1	6.04	1.57	1.48
1	B	10	U	C1'-N1	6.04	1.57	1.48
1	B	4	C	C1'-N1	5.89	1.57	1.48
2	C	16	DT	C1'-N1	5.85	1.56	1.49
2	C	19	DA	C1'-N9	-5.09	1.40	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	C	C2-N1-C1'	8.17	127.79	118.80
1	B	15	C	O5'-P-OP1	-6.64	99.72	105.70
1	B	45	C	C6-N1-C1'	-5.74	113.91	120.80
1	B	63	A	O4'-C1'-N9	5.66	112.72	108.20
1	B	62	A	P-O3'-C3'	5.23	125.97	119.70
1	B	45	C	C5-C6-N1	5.20	123.60	121.00
1	B	45	C	C6-N1-C2	-5.05	118.28	120.30

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	1530	0	769	72	0
2	C	395	0	214	26	0
3	A	8093	0	7933	310	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
All	All	10023	0	8916	369	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 20.

All (369) 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)
3:A:907:LEU:HD13	3:A:908:SER:H	1.34	0.92
3:A:284:ILE:HA	3:A:288:PHE:HB2	1.51	0.90
1:B:45:C:OP2	3:A:792:ARG:NH1	2.07	0.88
3:A:911:PRO:HA	3:A:929:LYS:HA	1.57	0.87
3:A:3:ARG:HG3	3:A:22:ASP:OD2	1.77	0.84
3:A:3:ARG:HE	3:A:22:ASP:HB2	1.43	0.84
3:A:94:LYS:HD3	3:A:100:LEU:HD21	1.59	0.84
3:A:836:THR:HG22	3:A:868:TYR:H	1.42	0.83
1:B:32:C:H5'	3:A:835:GLN:HE22	1.45	0.82
3:A:1010:ASP:OD2	3:A:1012:ARG:NE	2.10	0.81
3:A:44:ASN:CB	3:A:44:ASN:C	2.49	0.81
3:A:37:LYS:O	3:A:452:ARG:NH1	2.14	0.81
3:A:766:PHE:HE2	3:A:768:ASP:HB3	1.44	0.81
2:C:17:DA:H2'	2:C:18:DA:C8	2.19	0.78
3:A:44:ASN:CB	3:A:44:ASN:N	2.47	0.76
3:A:137:GLN:NE2	3:A:141:ASN:OD1	2.18	0.76
3:A:954:LYS:NZ	3:A:987:ASP:O	2.18	0.76
3:A:507:GLU:O	3:A:511:THR:OG1	2.03	0.76
1:B:28:U:H2'	1:B:29:A:H8	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:A:C2	2:C:21:DA:C2	2.75	0.75
3:A:3:ARG:NH1	3:A:27:ASP:HB3	2.02	0.73
3:A:138:ILE:HD11	3:A:170:ARG:HB3	1.71	0.72
3:A:263:ASN:ND2	3:A:412:ASP:O	2.23	0.72
3:A:566:ASP:OD1	3:A:568:SER:OG	2.07	0.72
3:A:49:SER:O	3:A:53:ALA:N	2.22	0.72
3:A:95:GLY:HA2	3:A:100:LEU:HD12	1.70	0.72
3:A:252:ASN:ND2	3:A:401:ASN:OD1	2.23	0.72
3:A:833:ASP:OD2	3:A:867:LYS:NZ	2.23	0.71
3:A:1005:LEU:O	3:A:1009:ASN:N	2.24	0.70
2:C:18:DA:OP1	3:A:392:THR:OG1	2.07	0.70
1:B:4:C:OP1	3:A:394:ASN:ND2	2.17	0.70
1:B:56:A:H61	3:A:935:LYS:HG2	1.56	0.69
3:A:92:ARG:NH1	3:A:154:GLN:OE1	2.25	0.69
3:A:3:ARG:HH12	3:A:27:ASP:HB3	1.57	0.69
3:A:7:LEU:HB3	3:A:474:ILE:HG12	1.74	0.69
3:A:695:ASN:OD1	3:A:1007:ASN:ND2	2.20	0.68
3:A:942:VAL:HB	3:A:1048:GLN:HB2	1.74	0.68
3:A:814:ASP:HB3	3:A:851:LYS:HG2	1.76	0.68
1:B:39:C:H2'	1:B:40:A:H8	1.59	0.68
3:A:907:LEU:HD13	3:A:908:SER:N	2.09	0.68
3:A:44:ASN:C	3:A:44:ASN:N	2.47	0.68
3:A:5:TYR:OH	3:A:469:GLY:O	2.07	0.67
1:B:7:C:H42	2:C:22:DG:H1	1.42	0.67
3:A:625:TYR:OH	3:A:645:ASN:ND2	2.28	0.67
3:A:453:SER:O	3:A:457:SER:OG	2.13	0.67
1:B:2:G:C6	1:B:3:U:O4	2.48	0.66
3:A:642:ILE:HG23	3:A:646:LEU:HD23	1.77	0.66
3:A:282:GLN:O	3:A:286:ASN:N	2.17	0.66
3:A:602:GLU:OE1	3:A:602:GLU:N	2.28	0.65
3:A:261:ASP:HB3	3:A:323:PHE:HD1	1.62	0.65
1:B:11:U:H2'	1:B:12:U:C6	2.32	0.65
1:B:5:U:O2'	3:A:314:ARG:NH2	2.31	0.64
1:B:11:U:H2'	1:B:12:U:H6	1.63	0.64
3:A:50:LYS:HA	3:A:53:ALA:HB3	1.79	0.64
3:A:828:LEU:HD12	3:A:881:LYS:HB2	1.80	0.64
3:A:847:TYR:HB2	3:A:853:PRO:HB3	1.78	0.64
3:A:1005:LEU:HD22	3:A:1010:ASP:HB3	1.80	0.64
3:A:406:GLU:OE1	3:A:420:ARG:NH1	2.26	0.64
2:C:11:DA:H2'	2:C:12:DA:C8	2.34	0.63
3:A:376:THR:HG22	3:A:378:GLU:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:677:ASN:OD1	3:A:678:GLY:N	2.31	0.63
3:A:803:ASN:HB2	3:A:882:TYR:CE1	2.33	0.63
3:A:336:THR:HG21	3:A:341:ILE:HD11	1.81	0.62
3:A:800:LEU:HD22	3:A:883:TYR:HD1	1.65	0.62
2:C:15:DT:H2'	2:C:16:DT:C6	2.34	0.62
3:A:119:HIS:CD2	3:A:208:ARG:HD2	2.35	0.62
3:A:119:HIS:NE2	3:A:208:ARG:HD2	2.15	0.61
3:A:275:LEU:O	3:A:411:ASN:ND2	2.33	0.61
1:B:41:G:H2'	1:B:42:A:H8	1.65	0.61
3:A:261:ASP:OD1	3:A:314:ARG:NH1	2.34	0.61
3:A:285:GLU:HA	3:A:289:LYS:HG3	1.82	0.61
3:A:22:ASP:OD1	3:A:25:THR:N	2.26	0.60
1:B:8:U:H2'	1:B:9:A:H8	1.66	0.60
3:A:292:LYS:HA	3:A:330:HIS:CD2	2.36	0.60
1:B:50:A:H2'	1:B:51:A:C8	2.37	0.60
3:A:283:ILE:HG21	3:A:299:ILE:HG23	1.84	0.59
1:B:32:C:H5'	3:A:835:GLN:NE2	2.15	0.59
1:B:2:G:H2'	1:B:3:U:C6	2.38	0.59
3:A:328:VAL:HA	3:A:389:TYR:OH	2.02	0.59
1:B:66:C:H5"	3:A:216:GLY:H	1.66	0.59
3:A:78:THR:O	3:A:81:SER:OG	2.21	0.58
3:A:249:TYR:CD1	3:A:327:LYS:HD2	2.38	0.58
1:B:28:U:H2'	1:B:29:A:C8	2.36	0.58
3:A:801:ILE:O	3:A:884:GLY:N	2.37	0.58
3:A:3:ARG:NE	3:A:22:ASP:HB2	2.17	0.58
3:A:95:GLY:O	3:A:187:GLN:NE2	2.36	0.58
3:A:131:GLU:O	3:A:140:ARG:NH1	2.37	0.58
3:A:149:TYR:HE2	3:A:182:GLN:HG2	1.69	0.58
3:A:565:PHE:CD2	3:A:646:LEU:HD22	2.38	0.58
3:A:558:ILE:HG21	3:A:625:TYR:HB3	1.86	0.57
3:A:924:LYS:HB2	3:A:956:ILE:HD11	1.87	0.57
1:B:64:U:H5"	1:B:65:G:H5"	1.85	0.57
3:A:240:PHE:HE2	3:A:423:LEU:HD13	1.70	0.57
3:A:676:ILE:HD11	3:A:680:PHE:CG	2.40	0.57
3:A:268:THR:N	3:A:309:ASP:OD1	2.38	0.57
1:B:55:A:H2	1:B:56:A:H62	1.52	0.57
3:A:333:LYS:HA	3:A:336:THR:O	2.04	0.57
3:A:93:VAL:HG21	3:A:155:LEU:HD22	1.87	0.56
3:A:148:LYS:HD2	3:A:153:LEU:HD13	1.88	0.56
3:A:33:VAL:HG12	3:A:35:LEU:CD1	2.36	0.56
3:A:92:ARG:HG2	3:A:108:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:92:ARG:NH2	3:A:151:ALA:HB2	2.20	0.56
3:A:210:THR:N	3:A:213:GLU:OE2	2.33	0.56
3:A:861:THR:HG23	3:A:863:ASN:H	1.71	0.56
3:A:257:ASN:O	3:A:324:THR:OG1	2.22	0.56
3:A:646:LEU:HD11	3:A:680:PHE:HA	1.89	0.55
3:A:695:ASN:HB2	3:A:1003:GLU:OE2	2.07	0.55
3:A:791:THR:O	3:A:792:ARG:NH2	2.36	0.55
3:A:541:ILE:HG23	3:A:553:TYR:CE2	2.41	0.55
1:B:39:C:H2'	1:B:40:A:C8	2.41	0.55
3:A:92:ARG:NH2	3:A:112:LEU:HD21	2.22	0.55
1:B:47:A:H2'	1:B:48:C:C6	2.42	0.54
1:B:56:A:N6	3:A:935:LYS:HZ3	2.05	0.54
3:A:280:LYS:O	3:A:284:ILE:HG12	2.07	0.54
3:A:379:GLU:O	3:A:383:ILE:N	2.39	0.54
3:A:601:TYR:O	3:A:605:LYS:N	2.31	0.54
3:A:833:ASP:N	3:A:834:PRO:HD3	2.23	0.54
1:B:33:U:O2	1:B:41:G:N2	2.41	0.53
1:B:9:A:N3	2:C:21:DA:C2	2.76	0.53
3:A:245:ARG:NH1	3:A:394:ASN:OD1	2.41	0.53
3:A:266:VAL:N	3:A:311:LYS:O	2.28	0.53
3:A:404:LEU:HA	3:A:407:LEU:HD12	1.90	0.53
3:A:971:LEU:HB2	3:A:1030:TYR:O	2.08	0.53
1:B:17:U:OP1	3:A:208:ARG:HB2	2.08	0.53
3:A:296:LEU:HB3	3:A:321:PRO:HG3	1.91	0.53
3:A:839:LYS:NZ	3:A:866:THR:O	2.30	0.53
1:B:51:A:H2'	1:B:52:A:C8	2.44	0.53
3:A:88:PRO:O	3:A:92:ARG:HG3	2.08	0.53
3:A:501:THR:HG21	3:A:525:LYS:HD2	1.91	0.53
3:A:41:VAL:HB	3:A:448:PRO:HG2	1.89	0.53
3:A:265:LEU:HD21	3:A:313:TYR:HB3	1.90	0.53
1:B:8:U:H2'	1:B:9:A:C8	2.43	0.52
3:A:341:ILE:HG22	3:A:347:LEU:HD12	1.91	0.52
3:A:766:PHE:HD2	3:A:767:LYS:N	2.07	0.52
1:B:15:C:OP1	3:A:221:PHE:HD1	1.91	0.52
3:A:184:LEU:HD13	3:A:198:ILE:HG13	1.92	0.52
3:A:534:CYS:HB2	3:A:541:ILE:HD11	1.92	0.52
3:A:688:TRP:CE3	3:A:760:ILE:HG21	2.45	0.52
3:A:632:ILE:O	3:A:638:GLN:NE2	2.43	0.52
3:A:480:ARG:NH1	3:A:677:ASN:HD21	2.08	0.52
3:A:150:VAL:HG11	3:A:176:TYR:CE1	2.45	0.51
3:A:855:TYR:O	3:A:859:GLU:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:HIS:O	3:A:334:ASP:HB2	2.10	0.51
3:A:839:LYS:HZ1	3:A:868:TYR:N	2.07	0.51
3:A:986:ASN:OD1	3:A:989:LEU:N	2.40	0.51
3:A:63:ARG:O	3:A:67:VAL:HG23	2.10	0.51
1:B:56:A:H61	3:A:935:LYS:HZ3	1.57	0.51
3:A:5:TYR:CE2	3:A:471:PRO:HB3	2.45	0.51
3:A:287:VAL:HB	3:A:298:GLN:OE1	2.11	0.51
3:A:1033:ASP:OD2	3:A:1037:ASN:ND2	2.42	0.51
3:A:33:VAL:HG12	3:A:35:LEU:HD12	1.93	0.50
3:A:630:ARG:NH1	3:A:637:VAL:HG13	2.26	0.50
1:B:5:U:H3	2:C:24:DA:H61	1.59	0.50
1:B:29:A:H2	1:B:46:U:O2	1.93	0.50
3:A:142:SER:O	3:A:146:GLU:N	2.44	0.50
1:B:6:G:C2	2:C:24:DA:N3	2.79	0.50
3:A:122:ASN:HA	3:A:172:LYS:NZ	2.27	0.50
3:A:293:LYS:HG2	3:A:325:ASN:HD21	1.76	0.50
3:A:939:TYR:HA	3:A:1051:LYS:HA	1.92	0.50
3:A:699:LYS:HB3	3:A:771:TYR:OH	2.11	0.50
1:B:13:A:OP1	3:A:44:ASN:ND2	2.45	0.50
1:B:35:G:N2	1:B:37:A:O5'	2.44	0.50
3:A:64:ILE:HD11	3:A:114:LYS:CA	2.42	0.50
3:A:916:VAL:HG11	3:A:1027:ILE:HD12	1.94	0.50
3:A:145:LEU:HD12	3:A:171:PHE:CE1	2.47	0.50
3:A:653:THR:O	3:A:657:MET:HE2	2.12	0.50
3:A:664:PHE:CE2	3:A:671:VAL:HB	2.47	0.50
3:A:791:THR:OG1	3:A:903:LYS:O	2.25	0.50
3:A:918:LEU:HB2	3:A:923:TYR:HE1	1.77	0.50
1:B:66:C:C5'	3:A:216:GLY:H	2.23	0.49
3:A:684:LEU:HD22	3:A:688:TRP:CZ2	2.47	0.49
1:B:37:A:H2'	1:B:38:A:C8	2.47	0.49
3:A:153:LEU:O	3:A:157:ARG:N	2.38	0.49
3:A:694:ARG:HD2	3:A:700:HIS:CG	2.47	0.49
1:B:46:U:H2'	1:B:47:A:H8	1.77	0.49
3:A:643:ASN:HA	3:A:647:VAL:HG12	1.94	0.49
3:A:840:LEU:O	3:A:844:MET:HG2	2.13	0.49
3:A:1033:ASP:OD1	3:A:1037:ASN:N	2.46	0.49
3:A:413:ASN:O	3:A:417:ILE:HG13	2.12	0.49
3:A:536:TYR:CD2	3:A:575:VAL:HG11	2.47	0.49
3:A:712:ASP:HA	3:A:715:PHE:HD1	1.77	0.49
1:B:2:G:C4	1:B:3:U:C5	3.00	0.49
1:B:52:A:H2'	1:B:53:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:917:TYR:HD2	3:A:962:PHE:HA	1.78	0.49
1:B:41:G:H2'	1:B:42:A:C8	2.47	0.49
3:A:34:ARG:HD3	3:A:772:SER:OG	2.12	0.49
1:B:2:G:H1	2:C:27:DC:H42	1.58	0.49
1:B:6:G:C2	2:C:24:DA:C2	3.00	0.49
3:A:248:LYS:HG3	3:A:393:HIS:HA	1.95	0.49
3:A:586:ARG:HH21	3:A:591:TYR:HD1	1.61	0.49
3:A:601:TYR:CE2	3:A:605:LYS:HD3	2.48	0.48
3:A:177:VAL:HG13	3:A:202:ILE:HD11	1.95	0.48
3:A:284:ILE:HA	3:A:288:PHE:CB	2.34	0.48
3:A:454:PHE:O	3:A:458:ILE:HG13	2.14	0.48
3:A:718:TRP:NE1	3:A:753:ILE:HG23	2.28	0.48
3:A:999:ILE:HD11	3:A:1003:GLU:HG3	1.96	0.48
3:A:209:ARG:NH1	3:A:214:GLY:O	2.46	0.48
3:A:45:GLU:O	3:A:49:SER:HB3	2.14	0.48
3:A:537:SER:HB3	3:A:579:GLU:HG3	1.96	0.48
1:B:13:A:H61	2:C:16:DT:H3	1.61	0.48
3:A:347:LEU:HD11	3:A:373:SER:OG	2.13	0.48
3:A:356:THR:O	3:A:359:GLN:NE2	2.47	0.47
1:B:43:A:H2'	1:B:44:U:H5'	1.96	0.47
3:A:912:TYR:CD2	3:A:933:VAL:HG21	2.49	0.47
3:A:980:ARG:HG2	3:A:995:ASN:O	2.14	0.47
3:A:240:PHE:CE2	3:A:423:LEU:HD13	2.49	0.47
3:A:704:ASP:HA	3:A:707:ILE:HD12	1.94	0.47
3:A:345:ALA:O	3:A:349:ASP:N	2.41	0.47
3:A:565:PHE:HB3	3:A:646:LEU:HD13	1.97	0.47
1:B:55:A:C6	3:A:783:LEU:HG	2.49	0.47
2:C:19:DA:OP1	3:A:245:ARG:NH2	2.34	0.47
3:A:36:PHE:HB3	3:A:774:ARG:HB3	1.96	0.47
1:B:62:A:H4'	1:B:63:A:O5'	2.14	0.47
3:A:247:VAL:HG21	3:A:353:LYS:HA	1.96	0.47
3:A:311:LYS:HD2	3:A:313:TYR:HE2	1.78	0.46
3:A:887:LEU:HG	3:A:890:HIS:HD2	1.79	0.46
1:B:19:A:O4'	3:A:170:ARG:HG3	2.14	0.46
3:A:119:HIS:CE1	3:A:120:ASN:OD1	2.69	0.46
3:A:237:CYS:HB3	3:A:240:PHE:H	1.79	0.46
3:A:261:ASP:HB3	3:A:323:PHE:CD1	2.46	0.46
3:A:940:TYR:N	3:A:1050:ILE:O	2.31	0.46
1:B:37:A:H2'	1:B:38:A:H8	1.81	0.46
2:C:11:DA:H2'	2:C:12:DA:H8	1.79	0.46
3:A:396:SER:O	3:A:400:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:C:H2'	1:B:60:A:O4'	2.16	0.46
2:C:13:DA:N3	3:A:120:ASN:ND2	2.63	0.46
3:A:149:TYR:CE2	3:A:182:GLN:HG2	2.51	0.46
3:A:313:TYR:CD1	3:A:321:PRO:HB3	2.50	0.46
3:A:822:LYS:O	3:A:823:SER:OG	2.32	0.46
1:B:45:C:P	3:A:792:ARG:HH11	2.39	0.46
1:B:2:G:H1	2:C:27:DC:N4	2.14	0.46
3:A:118:VAL:HG22	3:A:171:PHE:O	2.16	0.46
3:A:558:ILE:HD11	3:A:573:VAL:HG13	1.98	0.46
3:A:760:ILE:HB	3:A:763:ILE:HD12	1.98	0.46
1:B:62:A:H4'	1:B:63:A:C5'	2.46	0.46
3:A:639:LYS:HB3	3:A:639:LYS:HE2	1.77	0.46
3:A:89:TYR:CE1	3:A:164:VAL:HG11	2.51	0.45
3:A:373:SER:OG	3:A:374:GLU:N	2.49	0.45
3:A:119:HIS:ND1	3:A:120:ASN:OD1	2.48	0.45
1:B:46:U:H2'	1:B:47:A:C8	2.51	0.45
3:A:541:ILE:HG23	3:A:553:TYR:HE2	1.82	0.45
1:B:18:U:H4'	3:A:118:VAL:CG1	2.46	0.45
3:A:87:ASN:O	3:A:89:TYR:N	2.50	0.45
3:A:237:CYS:SG	3:A:396:SER:N	2.73	0.45
3:A:664:PHE:CD2	3:A:671:VAL:HB	2.51	0.45
3:A:800:LEU:HD21	3:A:884:GLY:O	2.16	0.45
1:B:22:U:H5"	3:A:879:LYS:HZ1	1.81	0.45
1:B:27:G:H2'	1:B:28:U:C6	2.52	0.45
1:B:47:A:H2'	1:B:48:C:H6	1.81	0.45
3:A:857:TYR:O	3:A:861:THR:HG22	2.17	0.45
3:A:248:LYS:HB2	3:A:392:THR:C	2.37	0.45
3:A:971:LEU:HD23	3:A:980:ARG:HA	1.98	0.45
3:A:109:LEU:HD22	3:A:201:TYR:CZ	2.51	0.45
3:A:504:ARG:NE	3:A:528:ASP:OD2	2.50	0.45
3:A:657:MET:SD	3:A:675:SER:HB2	2.57	0.45
3:A:856:LYS:O	3:A:860:GLU:HG2	2.17	0.45
1:B:49:U:H2'	1:B:50:A:C8	2.52	0.44
3:A:6:ILE:HG12	3:A:473:ASP:HB2	1.98	0.44
3:A:125:GLU:O	3:A:126:GLU:HG2	2.17	0.44
3:A:558:ILE:HG22	3:A:559:ILE:HG12	1.98	0.44
3:A:676:ILE:HD11	3:A:680:PHE:CD1	2.51	0.44
1:B:3:U:H3	2:C:26:DA:H61	1.65	0.44
1:B:50:A:H2'	1:B:51:A:H8	1.82	0.44
3:A:292:LYS:HA	3:A:330:HIS:NE2	2.31	0.44
3:A:843:ILE:HG22	3:A:846:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1018:LYS:HA	3:A:1018:LYS:HD2	1.83	0.44
3:A:64:ILE:HD11	3:A:114:LYS:N	2.32	0.44
3:A:361:SER:HA	3:A:384:SER:HB3	1.99	0.44
3:A:565:PHE:CB	3:A:646:LEU:HD13	2.48	0.44
1:B:70:G:OP2	3:A:781:ARG:HA	2.16	0.44
3:A:83:LEU:O	3:A:86:ILE:HG13	2.18	0.44
3:A:297:LYS:HG2	3:A:307:GLU:HG3	2.00	0.44
3:A:303:ILE:HD12	3:A:303:ILE:HA	1.87	0.44
3:A:662:SER:HA	3:A:665:ARG:HG2	2.00	0.44
2:C:21:DA:H2'	2:C:22:DG:C8	2.53	0.44
3:A:720:LYS:HA	3:A:742:PRO:HB2	1.99	0.44
3:A:259:LEU:O	3:A:263:ASN:HB2	2.18	0.44
3:A:475:ILE:HD12	3:A:712:ASP:HB2	1.99	0.44
3:A:21:ILE:HG22	3:A:709:ALA:HB1	2.00	0.43
3:A:90:GLU:OE1	3:A:155:LEU:HD11	2.18	0.43
3:A:557:HIS:CD2	3:A:561:ARG:HD3	2.53	0.43
3:A:688:TRP:N	3:A:688:TRP:CD1	2.85	0.43
3:A:794:ASP:OD2	3:A:798:ASN:HB2	2.18	0.43
3:A:854:LEU:HD11	3:A:865:LEU:HD12	2.00	0.43
3:A:683:PHE:O	3:A:686:ARG:N	2.49	0.43
3:A:794:ASP:OD1	3:A:798:ASN:N	2.52	0.43
1:B:2:G:H2'	1:B:3:U:C5	2.53	0.43
2:C:18:DA:O5'	2:C:18:DA:H8	2.01	0.43
3:A:830:TYR:HD1	3:A:837:TYR:CZ	2.36	0.43
3:A:972:ILE:HD11	3:A:974:ILE:HD11	2.00	0.43
3:A:386:LEU:C	3:A:387:LYS:HD3	2.38	0.43
3:A:703:GLU:O	3:A:707:ILE:HG13	2.18	0.43
3:A:336:THR:O	3:A:342:ILE:HD11	2.18	0.43
3:A:749:GLU:O	3:A:753:ILE:HG13	2.18	0.43
3:A:100:LEU:HD22	3:A:104:GLU:CB	2.48	0.43
3:A:687:LYS:HD2	3:A:687:LYS:HA	1.85	0.43
3:A:854:LEU:HD23	3:A:854:LEU:HA	1.71	0.43
1:B:18:U:H2'	1:B:19:A:C8	2.54	0.43
2:C:21:DA:H2'	2:C:22:DG:H8	1.84	0.43
3:A:316:THR:HG22	3:A:320:LYS:O	2.19	0.43
3:A:941:GLU:HA	3:A:1048:GLN:O	2.19	0.43
3:A:76:LEU:O	3:A:77:LEU:HD23	2.19	0.42
3:A:280:LYS:NZ	3:A:410:THR:O	2.51	0.42
3:A:772:SER:HB3	3:A:1036:GLY:HA2	2.00	0.42
3:A:917:TYR:CD2	3:A:962:PHE:HA	2.53	0.42
2:C:17:DA:H2"	3:A:233:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:766:PHE:HD2	3:A:768:ASP:H	1.67	0.42
3:A:71:LEU:O	3:A:75:ASN:N	2.52	0.42
3:A:122:ASN:HA	3:A:172:LYS:HZ2	1.83	0.42
3:A:371:LEU:C	3:A:373:SER:H	2.23	0.42
3:A:781:ARG:HA	3:A:781:ARG:HD3	1.91	0.42
1:B:71:U:OP2	3:A:781:ARG:NH1	2.53	0.42
3:A:923:TYR:CE2	3:A:1027:ILE:HG13	2.54	0.42
3:A:973:LYS:HB2	3:A:1028:LYS:HB2	2.01	0.42
3:A:994:VAL:O	3:A:1016:ILE:HB	2.20	0.42
3:A:986:ASN:HB3	3:A:989:LEU:HB2	2.01	0.42
3:A:646:LEU:HG	3:A:680:PHE:HD1	1.84	0.42
3:A:915:ASP:OD1	3:A:965:SER:HB3	2.20	0.42
1:B:72:U:OP1	3:A:452:ARG:HG3	2.20	0.42
3:A:417:ILE:O	3:A:421:LEU:N	2.53	0.42
3:A:534:CYS:O	3:A:538:LEU:N	2.38	0.42
3:A:893:ILE:HD12	3:A:897:TYR:HE2	1.85	0.42
3:A:719:LYS:HD3	3:A:719:LYS:HA	1.77	0.42
1:B:36:A:H2'	1:B:36:A:N3	2.35	0.41
2:C:26:DA:H1'	3:A:264:ASN:ND2	2.35	0.41
3:A:116:ARG:HH21	3:A:208:ARG:NE	2.18	0.41
3:A:583:LYS:HA	3:A:591:TYR:CD1	2.55	0.41
3:A:800:LEU:HD23	3:A:801:ILE:N	2.35	0.41
3:A:1000:THR:HG23	3:A:1003:GLU:HB3	2.01	0.41
2:C:16:DT:H73	2:C:16:DT:OP2	2.20	0.41
3:A:246:SER:H	3:A:396:SER:HA	1.84	0.41
3:A:3:ARG:HE	3:A:22:ASP:CB	2.21	0.41
3:A:281:PHE:CD1	3:A:285:GLU:HG3	2.55	0.41
3:A:664:PHE:CD1	3:A:664:PHE:N	2.89	0.41
3:A:1035:LEU:HB2	3:A:1037:ASN:ND2	2.35	0.41
1:B:25:U:H2'	1:B:26:A:H8	1.84	0.41
3:A:781:ARG:O	3:A:783:LEU:HD23	2.21	0.41
3:A:23:TYR:CB	3:A:472:ASN:HD21	2.34	0.41
3:A:289:LYS:HZ3	3:A:326:LEU:HD13	1.86	0.41
3:A:661:ARG:HH21	3:A:729:GLU:HA	1.86	0.41
3:A:619:SER:HB3	3:A:622:LYS:HB2	2.03	0.41
3:A:922:VAL:HG13	3:A:1022:SER:HA	2.02	0.41
3:A:986:ASN:ND2	3:A:989:LEU:HD22	2.35	0.41
3:A:100:LEU:HD22	3:A:104:GLU:HB2	2.02	0.41
3:A:412:ASP:OD2	3:A:420:ARG:NH2	2.33	0.41
1:B:9:A:C4	2:C:21:DA:C2	3.09	0.41
3:A:16:VAL:HG11	3:A:460:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:472:ASN:OD1	3:A:472:ASN:N	2.48	0.41
3:A:834:PRO:O	3:A:837:TYR:HB3	2.21	0.41
3:A:839:LYS:HB3	3:A:839:LYS:HE3	1.78	0.41
2:C:16:DT:H6	2:C:16:DT:O5'	2.04	0.41
3:A:5:TYR:CE1	3:A:468:TYR:HB3	2.56	0.41
3:A:95:GLY:CA	3:A:100:LEU:HD12	2.46	0.40
3:A:149:TYR:N	3:A:149:TYR:CD1	2.89	0.40
3:A:268:THR:OG1	3:A:309:ASP:OD2	2.38	0.40
3:A:294:PRO:HB2	3:A:299:ILE:HD11	2.03	0.40
3:A:843:ILE:HD12	3:A:854:LEU:HD21	2.03	0.40
1:B:6:G:N2	2:C:24:DA:C4	2.89	0.40
3:A:33:VAL:HG22	3:A:702:ALA:HB2	2.04	0.40
3:A:346:GLU:HA	3:A:349:ASP:HB2	2.02	0.40
3:A:799:THR:HB	3:A:887:LEU:HD21	2.04	0.40
3:A:176:TYR:O	3:A:180:ALA:N	2.48	0.40
3:A:335:ILE:HD11	3:A:383:ILE:HG12	2.03	0.40
3:A:816:LEU:HD11	3:A:840:LEU:HD11	2.03	0.40
1:B:24:U:H4'	3:A:900:SER:HB2	2.03	0.40
3:A:827:LEU:HA	3:A:827:LEU:HD23	1.86	0.40
3:A:11:ILE:HB	3:A:478:LEU:HD12	2.03	0.40
3:A:638:GLN:O	3:A:642:ILE:HD12	2.22	0.40
3:A:843:ILE:HD11	3:A:865:LEU:HD11	2.04	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
3	A	998/1053 (95%)	938 (94%)	57 (6%)	3 (0%)	37 70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	292	LYS
3	A	908	SER
3	A	964	ALA

### 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
3	A	864/970 (89%)	810 (94%)	54 (6%)	15   39

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	26	ARG
3	A	27	ASP
3	A	30	ASP
3	A	36	PHE
3	A	45	GLU
3	A	74	TYR
3	A	83	LEU
3	A	116	ARG
3	A	159	LYS
3	A	175	ASP
3	A	193	LEU
3	A	230	TYR
3	A	237	CYS
3	A	256	TYR
3	A	260	ASN
3	A	271	GLU
3	A	281	PHE
3	A	288	PHE
3	A	296	LEU
3	A	311	LYS
3	A	327	LYS
3	A	329	TYR
3	A	334	ASP

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Mol	Chain	Res	Type
3	A	340	GLU
3	A	349	ASP
3	A	353	LYS
3	A	386	LEU
3	A	462	ASN
3	A	480	ARG
3	A	518	LYS
3	A	537	SER
3	A	569	PHE
3	A	598	LYS
3	A	644	ARG
3	A	661	ARG
3	A	665	ARG
3	A	690	PHE
3	A	712	ASP
3	A	722	ASP
3	A	762	HIS
3	A	766	PHE
3	A	790	SER
3	A	832	HIS
3	A	865	LEU
3	A	887	LEU
3	A	913	ARG
3	A	923	TYR
3	A	935	LYS
3	A	967	TYR
3	A	995	ASN
3	A	1002	ARG
3	A	1015	ARG
3	A	1031	SER

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

Mol	Chain	Res	Type
3	A	137	GLN
3	A	141	ASN
3	A	330	HIS
3	A	557	HIS
3	A	645	ASN
3	A	835	GLN
3	A	846	GLN
3	A	1037	ASN

### 5.3.3 RNA [\(i\)](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	71/74 (95%)	13 (18%)	2 (2%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	17	U
1	B	36	A
1	B	39	C
1	B	43	A
1	B	45	C
1	B	46	U
1	B	55	A
1	B	57	G
1	B	62	A
1	B	63	A
1	B	65	G
1	B	69	U
1	B	71	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	35	G
1	B	62	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 [\(i\)](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	73/74 (98%)	-1.42	0   100   100	19, 39, 90, 115	0
2	C	19/20 (95%)	-1.06	0   100   100	21, 34, 50, 52	0
3	A	1009/1053 (95%)	-1.18	2 (0%)   92   85	16, 39, 60, 149	0
All	All	1101/1147 (95%)	-1.19	2 (0%)   92   85	16, 39, 62, 149	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	937	GLU	3.1
3	A	691	LYS	2.1

### 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.