



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:34 PM EDT

PDB ID : 5MGA  
Title : Structure of the Cpf1 endonuclease R-loop complex after DNA cleavage  
Authors : Montoya, G.; Stella, S.  
Deposited on : 2016-11-21  
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

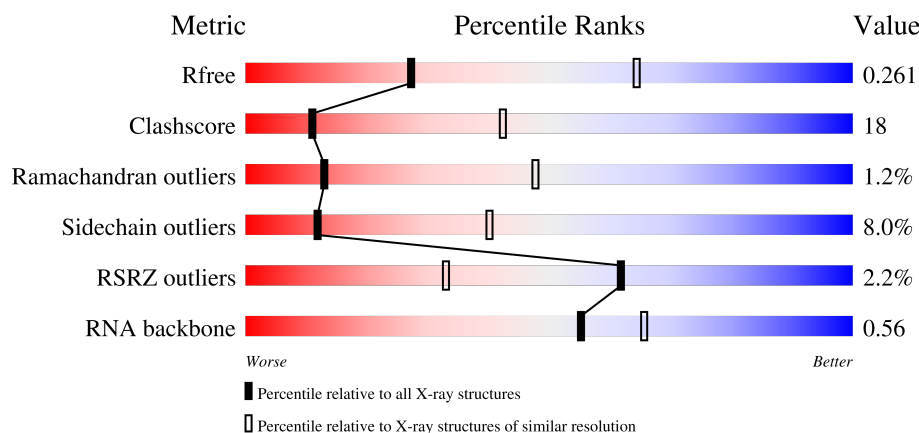
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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  $\geq 3$ , 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	A	1323	<div> <div>2%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>
2	B	40	<div> <div>5%</div> <div>40%</div> <div>50%</div> <div>10%</div> </div>
3	C	26	<div> <div>31%</div> <div>58%</div> <div>12%</div> </div>
4	D	12	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11351 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 Cpf1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9595	6163	1588	1824	20			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ASP	ILE	conflict	UNP A0Q7Q2
A	467	LEU	LYS	conflict	UNP A0Q7Q2
A	842	ILE	THR	conflict	UNP A0Q7Q2
A	1301	GLY	-	expression tag	UNP A0Q7Q2
A	1302	SER	-	expression tag	UNP A0Q7Q2
A	1303	GLU	-	expression tag	UNP A0Q7Q2
A	1304	PHE	-	expression tag	UNP A0Q7Q2
A	1305	GLU	-	expression tag	UNP A0Q7Q2
A	1306	LEU	-	expression tag	UNP A0Q7Q2
A	1307	GLU	-	expression tag	UNP A0Q7Q2
A	1308	ASN	-	expression tag	UNP A0Q7Q2
A	1309	LEU	-	expression tag	UNP A0Q7Q2
A	1310	TYR	-	expression tag	UNP A0Q7Q2
A	1311	PHE	-	expression tag	UNP A0Q7Q2
A	1312	GLN	-	expression tag	UNP A0Q7Q2
A	1313	GLY	-	expression tag	UNP A0Q7Q2
A	1314	GLU	-	expression tag	UNP A0Q7Q2
A	1315	LEU	-	expression tag	UNP A0Q7Q2
A	1316	ARG	-	expression tag	UNP A0Q7Q2
A	1317	ARG	-	expression tag	UNP A0Q7Q2
A	1318	GLN	-	expression tag	UNP A0Q7Q2
A	1319	ALA	-	expression tag	UNP A0Q7Q2
A	1320	SER	-	expression tag	UNP A0Q7Q2
A	1321	ALA	-	expression tag	UNP A0Q7Q2
A	1322	LEU	-	expression tag	UNP A0Q7Q2
A	1323	GLU	-	expression tag	UNP A0Q7Q2

- Molecule 2 is a RNA chain called RNA (40-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	P	0	0	0
			847	381	148	279	39			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	P	0	0	0
			529	254	91	158	26			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*CP\*GP\*TP\*TP\*AP\*GP\*AP\*GP\*AP\*AP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	12	Total	C	N	O	P	0	0	0
			248	119	49	69	11			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		

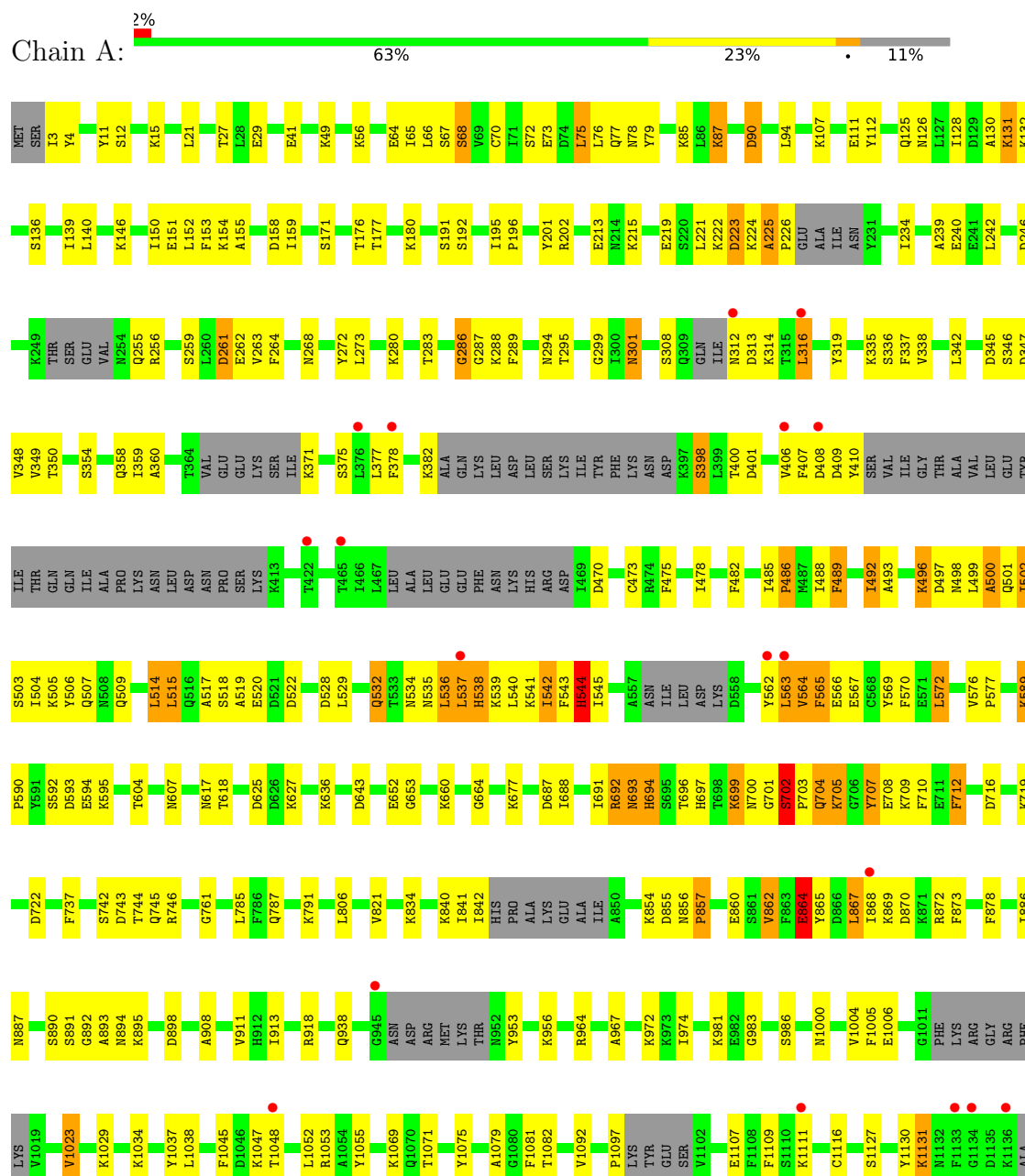
- Molecule 6 is water.

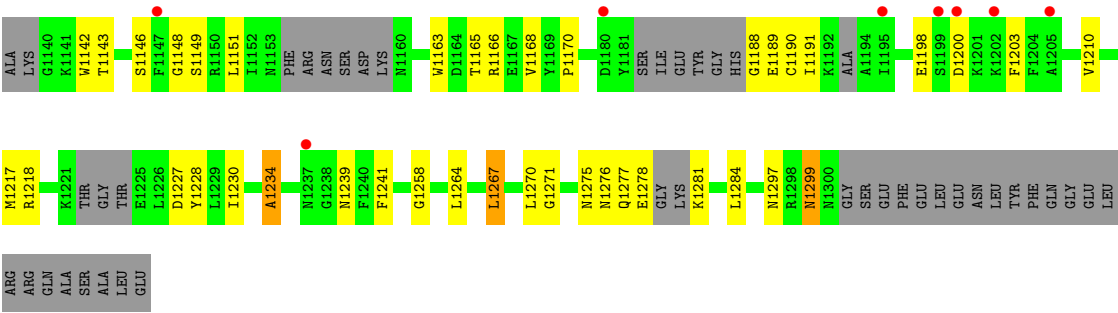
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total	O	0	0
			114	114		
6	B	9	Total	O	0	0
			9	9		
6	C	3	Total	O	0	0
			3	3		
6	D	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

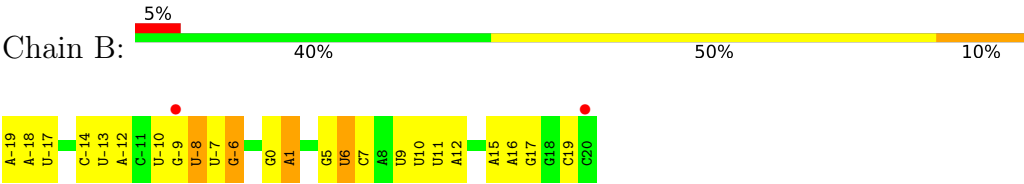
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endonuclease Cpf1





• Molecule 2: RNA (40-MER)



• Molecule 3: DNA (26-MER)



• Molecule 4: DNA (5'-D(P\*CP\*GP\*TP\*TP\*AP\*GP\*AP\*GP\*AP\*AP\*GP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.22Å 137.65Å 320.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 3.00 39.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.58-3.00) 98.3 (39.58-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.242 , 0.265 0.241 , 0.261	Depositor DCC
$R_{free}$ test set	1843 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11351	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.73	2/9763 (0.0%)	0.85	12/13094 (0.1%)
2	B	0.55	1/947 (0.1%)	0.82	4/1473 (0.3%)
3	C	0.75	3/591 (0.5%)	0.85	2/909 (0.2%)
4	D	0.72	0/279	0.88	0/430
All	All	0.72	6/11580 (0.1%)	0.85	18/15906 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	HIS	CA-CB	-9.22	1.33	1.53
2	B	1	A	O3'-P	-5.54	1.54	1.61
1	A	41	GLU	C-O	5.40	1.33	1.23
3	C	3	DA	O3'-P	-5.39	1.54	1.61
3	C	-1	DT	O3'-P	-5.32	1.54	1.61
3	C	-4	DT	O3'-P	-5.25	1.54	1.61

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ALA	C-N-CD	-19.80	77.03	120.60
1	A	702	SER	C-N-CD	-8.85	101.14	120.60
1	A	694	HIS	N-CA-C	8.52	134.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	G	O5'-P-OP1	7.90	120.18	110.70
2	B	5	G	O5'-P-OP2	-6.54	99.82	105.70
1	A	1097	PRO	N-CA-CB	6.43	111.01	103.30
1	A	572	LEU	CB-CG-CD2	6.14	121.44	111.00
1	A	964	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	155	ALA	N-CA-C	-5.84	95.24	111.00
2	B	6	U	O5'-P-OP1	5.80	117.66	110.70
2	B	6	U	O5'-P-OP2	-5.67	100.59	105.70
3	C	-7	DG	O5'-P-OP2	-5.62	100.64	105.70
3	C	2	DA	O5'-P-OP1	5.55	117.36	110.70
1	A	202	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	515	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	864	GLU	N-CA-C	-5.46	96.25	111.00
1	A	746	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	537	LEU	CB-CG-CD2	-5.07	102.39	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	694	HIS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1234	ALA	Peptide
1	A	500	ALA	Peptide
1	A	543	PHE	Peptide
1	A	544	HIS	Peptide
1	A	75	LEU	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9595	0	9345	360	0
2	B	847	0	428	17	0
3	C	529	0	296	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	248	0	137	18	0
5	B	2	0	0	0	0
6	A	114	0	0	1	2
6	B	9	0	0	0	0
6	C	3	0	0	0	0
6	D	4	0	0	0	0
All	All	11351	0	10206	388	2

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 18.

All (388) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LYS:HD2	1:A:544:HIS:CB	1.28	1.64
1:A:694:HIS:N	1:A:705:LYS:HE3	1.35	1.40
1:A:541:LYS:CD	1:A:544:HIS:CB	2.00	1.39
1:A:566:GLU:HB3	1:A:570:PHE:CD1	1.71	1.25
1:A:700:ASN:OD1	1:A:709:LYS:CE	1.91	1.18
1:A:66:LEU:O	1:A:70:CYS:HB3	1.45	1.16
1:A:541:LYS:CG	1:A:544:HIS:CB	2.24	1.15
1:A:700:ASN:OD1	1:A:709:LYS:HE3	1.45	1.14
1:A:493:ALA:O	1:A:496:LYS:HB2	1.48	1.13
1:A:701:GLY:CA	4:D:2:DG:OP1	2.00	1.08
1:A:566:GLU:CB	1:A:570:PHE:HD1	1.67	1.07
1:A:539:LYS:C	1:A:542:ILE:HD11	1.74	1.07
1:A:537:LEU:HD21	1:A:572:LEU:HD22	1.34	1.05
1:A:566:GLU:CB	1:A:570:PHE:CD1	2.40	1.03
1:A:693:ASN:C	1:A:705:LYS:HE3	1.67	1.03
1:A:566:GLU:HB3	1:A:570:PHE:HD1	0.87	1.02
1:A:566:GLU:HG2	1:A:570:PHE:HE1	1.22	1.00
1:A:541:LYS:HA	1:A:544:HIS:CB	1.91	1.00
1:A:542:ILE:HD12	1:A:542:ILE:H	1.26	0.98
1:A:696:THR:HG21	4:D:1:DA:OP1	1.63	0.97
1:A:692:ARG:CZ	1:A:694:HIS:CE1	2.48	0.96
1:A:700:ASN:OD1	1:A:709:LYS:NZ	1.97	0.96
1:A:692:ARG:CA	1:A:705:LYS:HG2	1.95	0.96
1:A:705:LYS:HA	1:A:705:LYS:NZ	1.81	0.96
1:A:692:ARG:N	1:A:705:LYS:HG3	1.82	0.94
1:A:539:LYS:O	1:A:542:ILE:HD11	1.65	0.94
1:A:566:GLU:HG2	1:A:570:PHE:CE1	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ARG:NH2	1:A:694:HIS:HE1	1.65	0.93
1:A:693:ASN:O	1:A:694:HIS:CG	2.22	0.92
1:A:535:ASN:HA	1:A:538:HIS:CE1	2.04	0.91
1:A:693:ASN:C	1:A:705:LYS:CE	2.40	0.91
1:A:496:LYS:O	1:A:501:GLN:CB	2.19	0.90
1:A:222:LYS:NZ	1:A:261:ASP:OD1	2.05	0.90
1:A:692:ARG:N	1:A:705:LYS:CG	2.35	0.89
1:A:66:LEU:O	1:A:70:CYS:CB	2.20	0.89
1:A:701:GLY:N	4:D:2:DG:OP1	2.05	0.88
1:A:840:LYS:O	1:A:868:ILE:HG23	1.74	0.88
1:A:705:LYS:HA	1:A:705:LYS:HZ3	1.39	0.87
1:A:692:ARG:NH1	4:D:0:DG:OP1	2.06	0.86
1:A:541:LYS:HG3	1:A:544:HIS:CB	2.04	0.86
1:A:259:SER:OG	1:A:262:GLU:HG3	1.75	0.86
1:A:517:ALA:HA	1:A:520:GLU:HG3	1.58	0.85
1:A:537:LEU:HD23	1:A:572:LEU:HB3	1.59	0.85
1:A:496:LYS:O	1:A:501:GLN:HA	1.77	0.84
1:A:692:ARG:CA	1:A:705:LYS:CG	2.55	0.84
1:A:694:HIS:N	1:A:705:LYS:CE	2.32	0.83
1:A:537:LEU:HG	1:A:572:LEU:HD13	1.60	0.83
1:A:313:ASP:OD1	1:A:314:LYS:NZ	2.12	0.83
1:A:485:ILE:HG21	1:A:536:LEU:HD21	1.60	0.82
1:A:696:THR:CG2	4:D:1:DA:OP1	2.27	0.82
1:A:535:ASN:OD1	1:A:536:LEU:N	2.13	0.81
1:A:541:LYS:CA	1:A:544:HIS:CB	2.58	0.81
1:A:704:GLN:N	1:A:704:GLN:OE1	2.14	0.81
1:A:539:LYS:O	1:A:542:ILE:CD1	2.28	0.80
1:A:842:ILE:HD13	1:A:860:GLU:OE2	1.82	0.79
1:A:537:LEU:HA	1:A:540:LEU:HD13	1.62	0.79
1:A:496:LYS:O	1:A:501:GLN:CA	2.31	0.78
1:A:87:LYS:NZ	1:A:213:GLU:OE2	2.15	0.78
1:A:694:HIS:H	1:A:705:LYS:HE3	1.44	0.78
1:A:702:SER:N	1:A:703:PRO:CD	2.46	0.77
1:A:537:LEU:HD21	1:A:572:LEU:CD2	2.14	0.77
1:A:702:SER:H	1:A:703:PRO:CD	1.98	0.76
1:A:692:ARG:NH2	1:A:694:HIS:CE1	2.51	0.76
1:A:841:ILE:CB	1:A:868:ILE:HD12	2.16	0.75
1:A:535:ASN:HA	1:A:538:HIS:ND1	2.01	0.75
1:A:701:GLY:HA2	4:D:2:DG:OP1	1.87	0.75
1:A:539:LYS:C	1:A:542:ILE:CD1	2.56	0.74
1:A:493:ALA:O	1:A:496:LYS:CB	2.32	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ILE:O	1:A:503:SER:HB3	1.87	0.73
1:A:701:GLY:HA3	4:D:2:DG:OP1	1.88	0.73
1:A:691:ILE:C	1:A:705:LYS:CG	2.57	0.73
1:A:73:GLU:HG3	1:A:75:LEU:HD13	1.69	0.73
1:A:692:ARG:O	1:A:705:LYS:HE2	1.84	0.73
1:A:75:LEU:O	6:A:1401:HOH:O	2.07	0.72
4:D:-3:DT:H6	4:D:-3:DT:H5'	1.53	0.72
1:A:537:LEU:CD2	1:A:572:LEU:HB3	2.19	0.71
1:A:1271:GLY:O	1:A:1275:ASN:ND2	2.24	0.70
1:A:1218:ARG:NH1	1:A:1227:ASP:OD2	2.24	0.70
1:A:542:ILE:H	1:A:542:ILE:CD1	2.02	0.70
1:A:699:LYS:HB2	1:A:709:LYS:HZ3	1.55	0.70
1:A:240:GLU:HB2	1:A:280:LYS:HG2	1.72	0.70
1:A:699:LYS:CB	1:A:709:LYS:HZ3	2.05	0.70
1:A:308:SER:OG	1:A:316:LEU:HD12	1.91	0.69
1:A:704:GLN:HG3	1:A:709:LYS:HD2	1.75	0.69
1:A:131:LYS:CG	1:A:132:LYS:N	2.56	0.69
1:A:694:HIS:CA	1:A:707:TYR:CE1	2.76	0.68
1:A:541:LYS:CB	1:A:544:HIS:CB	2.71	0.68
1:A:485:ILE:CG2	1:A:536:LEU:HD11	2.23	0.68
1:A:692:ARG:HA	1:A:705:LYS:HG2	1.75	0.68
1:A:566:GLU:CG	1:A:570:PHE:CE1	2.76	0.68
1:A:841:ILE:CB	1:A:868:ILE:CD1	2.72	0.68
1:A:489:PHE:HA	1:A:492:ILE:HB	1.75	0.68
1:A:131:LYS:HG3	1:A:132:LYS:N	2.09	0.67
1:A:485:ILE:HG21	1:A:536:LEU:HD11	1.77	0.67
1:A:1149:SER:CB	1:A:1168:VAL:O	2.42	0.67
1:A:72:SER:CB	1:A:76:LEU:HD11	2.23	0.67
1:A:541:LYS:HE3	1:A:545:ILE:HA	1.77	0.67
1:A:493:ALA:O	1:A:496:LYS:N	2.25	0.67
1:A:308:SER:OG	1:A:316:LEU:CD1	2.44	0.66
1:A:867:LEU:C	1:A:868:ILE:HD13	2.15	0.66
1:A:604:THR:O	1:A:617:ASN:OD1	2.13	0.66
1:A:701:GLY:HA2	4:D:2:DG:P	2.36	0.66
1:A:482:PHE:O	1:A:486:PRO:HD2	1.95	0.66
1:A:221:LEU:O	1:A:225:ALA:O	2.15	0.65
1:A:869:LYS:O	2:B:-18:A:OP1	2.14	0.65
1:A:1149:SER:HB3	1:A:1168:VAL:O	1.97	0.65
1:A:594:GLU:OE2	1:A:834:LYS:N	2.22	0.64
1:A:704:GLN:HB2	1:A:710:PHE:H	1.60	0.64
1:A:485:ILE:HG21	1:A:536:LEU:CD2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:SER:N	1:A:703:PRO:HD2	2.12	0.64
1:A:154:LYS:H	1:A:154:LYS:HD2	1.62	0.64
1:A:154:LYS:HD2	1:A:154:LYS:N	2.13	0.64
1:A:259:SER:OG	1:A:262:GLU:CG	2.45	0.64
1:A:872:ARG:HD3	2:B:-17:U:H2'	1.80	0.63
1:A:692:ARG:N	1:A:705:LYS:HG2	2.09	0.63
1:A:131:LYS:HG3	1:A:132:LYS:H	1.62	0.63
1:A:541:LYS:C	1:A:544:HIS:H	2.01	0.63
1:A:224:LYS:O	1:A:224:LYS:NZ	2.21	0.63
1:A:64:GLU:O	1:A:68:SER:HB2	1.99	0.63
1:A:72:SER:HB3	1:A:76:LEU:CD1	2.29	0.62
1:A:499:LEU:N	1:A:501:GLN:CB	2.62	0.62
1:A:1234:ALA:HA	1:A:1239:ASN:O	1.98	0.62
1:A:263:VAL:HG23	1:A:272:TYR:OH	1.98	0.62
1:A:702:SER:H	1:A:703:PRO:HD3	1.64	0.62
1:A:27:THR:HG21	1:A:785:LEU:H	1.65	0.62
1:A:694:HIS:HB3	1:A:707:TYR:HE1	1.64	0.62
1:A:705:LYS:HA	1:A:705:LYS:HZ2	1.64	0.62
1:A:72:SER:HB3	1:A:76:LEU:HD11	1.83	0.61
1:A:349:VAL:HG11	1:A:506:TYR:CD2	2.36	0.61
1:A:908:ALA:HA	1:A:911:VAL:HG12	1.81	0.61
4:D:3:DA:H2''	4:D:4:DA:OP1	2.00	0.61
1:A:11:TYR:HB3	1:A:893:ALA:HB3	1.83	0.61
1:A:66:LEU:HD13	1:A:273:LEU:HB3	1.83	0.61
1:A:694:HIS:CB	1:A:707:TYR:HE1	2.14	0.61
1:A:146:LYS:CB	1:A:153:PHE:HZ	2.14	0.60
1:A:286:GLY:HA2	1:A:299:GLY:HA3	1.83	0.60
1:A:694:HIS:CB	1:A:707:TYR:CE1	2.84	0.60
1:A:563:LEU:HD12	1:A:563:LEU:O	2.02	0.60
1:A:702:SER:H	1:A:703:PRO:HD2	1.63	0.60
1:A:1069:LYS:HB2	1:A:1284:LEU:HD12	1.83	0.60
1:A:542:ILE:HD12	1:A:542:ILE:N	2.09	0.60
1:A:566:GLU:O	1:A:570:PHE:N	2.21	0.60
1:A:687:ASP:O	1:A:691:ILE:HG13	2.02	0.60
1:A:177:THR:HG22	4:D:-4:DG:H2'	1.84	0.59
1:A:505:LYS:NZ	1:A:522:ASP:OD2	2.35	0.59
1:A:223:ASP:OD1	1:A:223:ASP:N	2.34	0.59
1:A:255:GLN:HG2	1:A:256:ARG:H	1.67	0.59
1:A:700:ASN:H	1:A:709:LYS:NZ	2.01	0.59
1:A:566:GLU:CB	1:A:570:PHE:CE1	2.85	0.59
1:A:72:SER:HB2	1:A:76:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:-3:DT:H5'	4:D:-3:DT:C6	2.36	0.58
1:A:1092:VAL:O	1:A:1130:TYR:OH	2.21	0.58
1:A:700:ASN:ND2	1:A:703:PRO:N	2.52	0.58
1:A:700:ASN:H	1:A:709:LYS:HZ3	1.51	0.58
1:A:694:HIS:CA	1:A:707:TYR:HE1	2.16	0.58
1:A:342:LEU:HD22	1:A:347:ASP:HB3	1.86	0.57
1:A:565:PHE:CD1	1:A:565:PHE:N	2.72	0.57
1:A:691:ILE:C	1:A:705:LYS:HG2	2.25	0.57
2:B:11:U:H2'	2:B:12:A:C8	2.40	0.57
1:A:867:LEU:O	1:A:868:ILE:HD13	2.05	0.57
1:A:691:ILE:C	1:A:705:LYS:HB2	2.25	0.57
1:A:565:PHE:N	1:A:565:PHE:HD1	2.03	0.56
1:A:485:ILE:HG21	1:A:536:LEU:CG	2.36	0.56
1:A:107:LYS:O	1:A:111:GLU:HB2	2.04	0.56
1:A:498:ASN:C	1:A:501:GLN:CB	2.74	0.56
1:A:146:LYS:CB	1:A:153:PHE:CZ	2.89	0.56
1:A:886:ILE:HG21	1:A:1037:TYR:CZ	2.40	0.56
1:A:688:ILE:HA	1:A:691:ILE:HG13	1.87	0.56
1:A:703:PRO:HG2	1:A:712:PHE:CE1	2.41	0.56
1:A:694:HIS:CA	1:A:707:TYR:CD1	2.89	0.55
1:A:699:LYS:HB2	1:A:709:LYS:NZ	2.21	0.55
1:A:913:ILE:HG13	1:A:1267:LEU:HD12	1.87	0.55
1:A:131:LYS:HG2	1:A:132:LYS:O	2.05	0.55
1:A:485:ILE:CB	1:A:536:LEU:HD11	2.36	0.55
1:A:75:LEU:HD12	1:A:75:LEU:N	2.21	0.55
1:A:566:GLU:HB2	1:A:570:PHE:CD1	2.39	0.55
3:C:-11:DA:H2'	3:C:-10:DA:C8	2.41	0.55
1:A:700:ASN:HD21	1:A:704:GLN:N	2.04	0.55
1:A:1277:GLN:HE22	1:A:1281:LYS:N	2.04	0.55
1:A:502:ILE:O	1:A:503:SER:CB	2.53	0.55
1:A:702:SER:N	1:A:703:PRO:HD3	2.20	0.55
1:A:692:ARG:CZ	1:A:694:HIS:NE2	2.70	0.55
1:A:125:GLN:HA	1:A:176:THR:HG21	1.88	0.54
1:A:856:ASN:HB2	1:A:857:PRO:HD2	1.89	0.54
1:A:540:LEU:C	1:A:542:ILE:HD12	2.27	0.54
1:A:1107:GLU:OE2	1:A:1107:GLU:N	2.39	0.54
1:A:1111:LYS:O	1:A:1131:LYS:NZ	2.40	0.54
1:A:345:ASP:HA	1:A:348:VAL:HG22	1.90	0.54
1:A:349:VAL:HG21	1:A:502:ILE:HG23	1.90	0.54
1:A:576:VAL:HG23	1:A:577:PRO:HD3	1.89	0.54
1:A:15:LYS:HE3	2:B:0:G:OP2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:HA	1:A:489:PHE:CD2	2.43	0.54
1:A:514:LEU:O	1:A:515:LEU:HD23	2.07	0.54
1:A:532:GLN:CD	1:A:532:GLN:H	2.11	0.54
1:A:73:GLU:O	1:A:76:LEU:HD13	2.08	0.54
1:A:694:HIS:HB3	1:A:707:TYR:CE1	2.43	0.53
1:A:406:VAL:HG22	1:A:478:ILE:HG21	1.91	0.53
1:A:499:LEU:C	1:A:501:GLN:CB	2.76	0.53
1:A:891:SER:OG	1:A:892:GLY:N	2.42	0.53
1:A:126:ASN:HA	1:A:130:ALA:HA	1.91	0.53
1:A:295:THR:HA	2:B:15:A:H4'	1.91	0.53
1:A:401:ASP:OD1	1:A:401:ASP:N	2.42	0.53
1:A:486:PRO:HA	1:A:489:PHE:CE2	2.44	0.52
1:A:704:GLN:H	1:A:704:GLN:CD	2.10	0.52
1:A:485:ILE:HG21	1:A:536:LEU:CD1	2.40	0.52
1:A:1151:LEU:HD22	1:A:1166:ARG:HB3	1.92	0.52
1:A:1189:GLU:O	1:A:1190:CYS:SG	2.67	0.52
1:A:263:VAL:O	1:A:264:PHE:HB2	2.09	0.51
1:A:693:ASN:O	1:A:694:HIS:CB	2.56	0.51
1:A:842:ILE:O	2:B:-19:A:O5'	2.28	0.51
1:A:1038:LEU:HB3	1:A:1055:TYR:HB2	1.92	0.51
3:C:-1:DT:H2'	3:C:0:DC:C6	2.46	0.51
1:A:313:ASP:N	1:A:314:LYS:HZ3	2.09	0.51
1:A:703:PRO:HG2	1:A:712:PHE:CD1	2.44	0.51
1:A:887:ASN:HB3	1:A:890:SER:OG	2.10	0.51
1:A:485:ILE:HB	1:A:536:LEU:HD11	1.93	0.51
1:A:1198:GLU:HB2	1:A:1203:PHE:CZ	2.46	0.51
1:A:537:LEU:CG	1:A:572:LEU:HD13	2.36	0.50
1:A:1227:ASP:OD1	1:A:1227:ASP:N	2.44	0.50
1:A:400:THR:HB	1:A:410:TYR:OH	2.10	0.50
1:A:136:SER:HB2	1:A:139:ILE:HG12	1.92	0.50
1:A:499:LEU:O	1:A:501:GLN:CB	2.60	0.50
1:A:1228:TYR:CE1	1:A:1230:ILE:HD11	2.47	0.50
1:A:3:ILE:CD1	1:A:4:TYR:H	2.25	0.50
1:A:517:ALA:HB1	1:A:520:GLU:OE2	2.11	0.50
1:A:862:VAL:HG22	1:A:864:GLU:N	2.27	0.50
1:A:592:SER:OG	1:A:593:ASP:HA	2.11	0.50
1:A:66:LEU:HD13	1:A:273:LEU:CB	2.41	0.50
1:A:692:ARG:CA	1:A:705:LYS:HG3	2.36	0.50
1:A:72:SER:CB	1:A:76:LEU:CD1	2.89	0.49
1:A:90:ASP:HB2	1:A:94:LEU:HD22	1.93	0.49
1:A:283:THR:HG23	1:A:287:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:ASP:OD1	1:A:745:GLN:N	2.39	0.49
1:A:842:ILE:CD1	1:A:860:GLU:OE2	2.58	0.49
1:A:49:LYS:HE2	1:A:158:ASP:HB3	1.94	0.49
1:A:1045:PHE:CZ	1:A:1052:LEU:HD13	2.48	0.49
1:A:507:GLN:N	1:A:507:GLN:OE1	2.46	0.49
1:A:722:ASP:OD1	1:A:744:THR:HG21	2.13	0.49
4:D:-4:DG:H1'	4:D:-3:DT:H5''	1.94	0.48
1:A:65:ILE:HD12	1:A:112:TYR:CE2	2.49	0.48
1:A:259:SER:N	1:A:262:GLU:HB2	2.28	0.48
1:A:541:LYS:HD3	1:A:569:TYR:CE1	2.49	0.48
1:A:1276:ASN:OD1	1:A:1277:GLN:N	2.46	0.48
1:A:692:ARG:O	1:A:705:LYS:CE	2.58	0.48
1:A:700:ASN:HD22	1:A:703:PRO:CA	2.26	0.48
1:A:263:VAL:HG22	1:A:264:PHE:N	2.29	0.47
1:A:1188:GLY:C	1:A:1189:GLU:OE1	2.52	0.47
1:A:154:LYS:HG2	1:A:159:ILE:HB	1.95	0.47
1:A:1299:ASN:O	1:A:1299:ASN:ND2	2.47	0.47
1:A:76:LEU:O	1:A:79:TYR:HB3	2.14	0.47
1:A:693:ASN:HB2	1:A:705:LYS:HD3	1.17	0.47
1:A:407:PHE:O	1:A:409:ASP:N	2.47	0.47
1:A:700:ASN:HD22	1:A:703:PRO:N	2.12	0.47
1:A:259:SER:O	1:A:262:GLU:N	2.48	0.47
1:A:576:VAL:CG2	1:A:577:PRO:HD3	2.44	0.47
1:A:692:ARG:O	1:A:693:ASN:O	2.32	0.47
1:A:1127:SER:HA	1:A:1143:THR:HA	1.96	0.47
1:A:77:GLN:O	1:A:78:ASN:C	2.53	0.47
3:C:-14:DA:H8	3:C:-14:DA:H5''	1.80	0.47
1:A:239:ALA:H	1:A:288:LYS:HZ1	1.62	0.47
1:A:504:ILE:HA	1:A:507:GLN:HE22	1.80	0.47
1:A:742:SER:OG	1:A:743:ASP:N	2.48	0.46
4:D:-3:DT:C6	4:D:-3:DT:C5'	2.98	0.46
1:A:85:LYS:HB3	1:A:94:LEU:HD21	1.97	0.46
2:B:0:G:H1'	2:B:1:A:C8	2.51	0.46
1:A:136:SER:O	1:A:140:LEU:HB3	2.15	0.46
1:A:693:ASN:HB3	1:A:705:LYS:CE	2.41	0.46
1:A:737:PHE:CD1	1:A:761:GLY:HA2	2.51	0.46
1:A:377:LEU:CD1	1:A:564:VAL:HG11	2.46	0.46
1:A:1191:ILE:HD12	1:A:1191:ILE:O	2.16	0.46
1:A:259:SER:O	1:A:262:GLU:HB2	2.16	0.46
1:A:359:ILE:HA	1:A:360:ALA:HA	1.58	0.46
1:A:537:LEU:O	1:A:540:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:ILE:C	1:A:705:LYS:CB	2.84	0.46
1:A:1170:PRO:HB3	1:A:1210:VAL:HG22	1.98	0.46
1:A:398:SER:HA	1:A:401:ASP:OD1	2.15	0.46
1:A:607:ASN:HB2	1:A:617:ASN:OD1	2.16	0.46
1:A:382:LYS:HE2	1:A:475:PHE:C	2.36	0.46
1:A:259:SER:H	1:A:262:GLU:HG3	1.82	0.45
1:A:316:LEU:O	1:A:319:TYR:HD1	1.98	0.45
1:A:337:PHE:CG	1:A:337:PHE:O	2.69	0.45
1:A:492:ILE:HG23	1:A:492:ILE:O	2.15	0.45
1:A:532:GLN:H	1:A:532:GLN:NE2	2.13	0.45
1:A:566:GLU:CG	1:A:570:PHE:HE1	2.06	0.45
1:A:75:LEU:HD12	1:A:75:LEU:H	1.79	0.45
3:C:-4:DT:H2'	3:C:-3:DT:H71	1.98	0.45
1:A:225:ALA:H	1:A:226:PRO:HD3	1.59	0.45
1:A:589:LYS:HA	1:A:590:PRO:HD3	1.86	0.45
1:A:1277:GLN:OE1	1:A:1281:LYS:HB2	2.15	0.45
1:A:295:THR:HG23	2:B:15:A:O2'	2.17	0.45
1:A:15:LYS:HG2	2:B:0:G:H5'	1.98	0.45
1:A:196:PRO:HA	1:A:201:TYR:CD1	2.52	0.45
1:A:700:ASN:HD22	1:A:703:PRO:CB	2.29	0.45
1:A:1047:LYS:O	1:A:1053:ARG:HB2	2.17	0.45
3:C:-14:DA:H5''	3:C:-14:DA:C8	2.52	0.45
1:A:27:THR:HG21	1:A:785:LEU:N	2.30	0.45
1:A:618:THR:CG2	1:A:618:THR:O	2.65	0.44
1:A:953:TYR:HA	1:A:956:LYS:HG2	1.98	0.44
1:A:700:ASN:ND2	1:A:704:GLN:N	2.65	0.44
1:A:1006:GLU:HB2	1:A:1079:ALA:HB2	1.99	0.44
1:A:918:ARG:HH12	1:A:1005:PHE:HB3	1.82	0.44
1:A:56:LYS:HD2	1:A:153:PHE:HB3	2.00	0.44
1:A:677:LYS:HE2	3:C:4:DC:OP2	2.18	0.44
1:A:707:TYR:HD1	1:A:707:TYR:HA	1.68	0.44
1:A:704:GLN:HB3	1:A:709:LYS:HE3	2.00	0.44
1:A:938:GLN:O	1:A:938:GLN:HG3	2.17	0.44
2:B:-8:U:HO2'	2:B:-6:G:HO2'	1.48	0.44
3:C:-9:DA:H2'	3:C:-8:DT:C6	2.53	0.44
1:A:870:ASP:HB3	1:A:873:PHE:HD2	1.83	0.44
2:B:-14:C:H2'	2:B:-13:U:C6	2.52	0.44
1:A:3:ILE:HG12	1:A:1000:ASN:OD1	2.18	0.44
2:B:-13:U:H2'	2:B:-12:A:C8	2.53	0.44
1:A:308:SER:OG	1:A:316:LEU:HD13	2.17	0.44
1:A:564:VAL:HB	1:A:565:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:O	1:A:337:PHE:CD2	2.71	0.43
1:A:354:SER:O	1:A:358:GLN:OE1	2.35	0.43
1:A:1277:GLN:HG2	1:A:1278:GLU:N	2.33	0.43
1:A:489:PHE:O	1:A:492:ILE:HG22	2.17	0.43
1:A:73:GLU:CG	1:A:75:LEU:HD13	2.45	0.43
1:A:242:LEU:HA	1:A:256:ARG:O	2.19	0.43
1:A:627:LYS:HD3	1:A:787:GLN:HE21	1.84	0.43
1:A:700:ASN:N	1:A:709:LYS:NZ	2.66	0.43
1:A:1149:SER:HB2	1:A:1168:VAL:O	2.18	0.43
1:A:692:ARG:NH1	1:A:694:HIS:NE2	2.66	0.43
1:A:1071:THR:HG23	1:A:1071:THR:O	2.19	0.43
1:A:1151:LEU:O	1:A:1165:THR:HA	2.19	0.43
4:D:3:DA:H4'	4:D:3:DA:OP1	2.18	0.43
1:A:67:SER:OG	1:A:68:SER:N	2.52	0.42
1:A:541:LYS:HD3	1:A:569:TYR:CZ	2.54	0.42
1:A:563:LEU:HD12	1:A:563:LEU:C	2.39	0.42
1:A:1127:SER:HB3	1:A:1143:THR:HB	2.01	0.42
1:A:541:LYS:N	1:A:542:ILE:HD12	2.33	0.42
1:A:1189:GLU:OE1	1:A:1189:GLU:N	2.52	0.42
1:A:263:VAL:CG2	1:A:264:PHE:N	2.82	0.42
1:A:791:LYS:HG2	2:B:-17:U:H4'	2.00	0.42
1:A:693:ASN:O	1:A:694:HIS:CD2	2.71	0.42
1:A:967:ALA:HA	1:A:972:LYS:HB2	2.01	0.42
1:A:382:LYS:HG2	1:A:475:PHE:O	2.19	0.42
1:A:704:GLN:O	1:A:704:GLN:HG2	2.20	0.42
1:A:894:ASN:OD1	1:A:895:LYS:N	2.50	0.42
3:C:-12:DT:H2'	3:C:-11:DA:C8	2.55	0.42
4:D:-5:DC:H2'	4:D:-4:DG:C8	2.54	0.42
1:A:485:ILE:O	1:A:488:ILE:HG22	2.20	0.42
1:A:691:ILE:O	1:A:705:LYS:HG2	2.19	0.42
1:A:1004:VAL:HG12	1:A:1075:TYR:HB2	2.02	0.42
2:B:6:U:H2'	2:B:7:C:C6	2.55	0.42
4:D:1:DA:H2''	4:D:2:DG:O4'	2.20	0.42
2:B:-10:U:H1'	2:B:-8:U:H5	1.84	0.42
1:A:660:LYS:HD2	1:A:660:LYS:HA	1.95	0.41
1:A:691:ILE:HG23	1:A:716:ASP:HB3	2.01	0.41
1:A:864:GLU:HB3	1:A:865:TYR:H	1.68	0.41
2:B:9:U:H2'	2:B:10:U:H6	1.84	0.41
1:A:301:ASN:HD22	3:C:-14:DA:P	2.43	0.41
1:A:911:VAL:CG1	1:A:1270:LEU:HD11	2.51	0.41
1:A:981:LYS:HG2	1:A:1023:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:-11:DA:H2'	3:C:-10:DA:H8	1.84	0.41
3:C:-6:DA:C4	3:C:-5:DC:C5	3.08	0.41
1:A:313:ASP:OD1	1:A:313:ASP:N	2.52	0.41
1:A:499:LEU:O	1:A:500:ALA:C	2.57	0.41
1:A:349:VAL:HG13	1:A:350:THR:N	2.35	0.41
1:A:313:ASP:O	1:A:314:LYS:NZ	2.39	0.41
1:A:694:HIS:HA	1:A:705:LYS:HE3	2.00	0.41
1:A:21:LEU:HB2	1:A:878:PHE:HB2	2.02	0.41
1:A:177:THR:HG23	4:D:-4:DG:OP2	2.21	0.41
1:A:492:ILE:HG22	1:A:529:LEU:HD23	2.01	0.41
3:C:-13:DT:H2'	3:C:-12:DT:C6	2.55	0.41
1:A:375:SER:HA	1:A:378:PHE:HD2	1.85	0.41
1:A:485:ILE:CG2	1:A:536:LEU:CD1	2.95	0.41
1:A:1230:ILE:HA	1:A:1241:PHE:O	2.21	0.41
1:A:566:GLU:O	1:A:569:TYR:N	2.53	0.41
1:A:1081:PHE:CD1	1:A:1092:VAL:HG21	2.55	0.41
1:A:3:ILE:HG21	1:A:1000:ASN:ND2	2.36	0.41
1:A:191:SER:CB	1:A:195:ILE:HD11	2.51	0.41
1:A:470:ASP:HB2	1:A:473:CYS:HB2	2.03	0.41
1:A:535:ASN:OD1	1:A:536:LEU:HD23	2.21	0.41
1:A:1264:LEU:HD23	1:A:1264:LEU:HA	1.96	0.41
2:B:15:A:H2'	2:B:16:A:C8	2.56	0.41
3:C:1:DT:H2''	3:C:2:DA:N7	2.36	0.41
1:A:1190:CYS:SG	1:A:1190:CYS:O	2.78	0.41
1:A:29:GLU:N	1:A:29:GLU:CD	2.74	0.40
1:A:128:ILE:O	1:A:136:SER:OG	2.31	0.40
1:A:346:SER:HA	1:A:349:VAL:HG12	2.02	0.40
1:A:191:SER:HB3	1:A:195:ILE:HD11	2.03	0.40
1:A:983:GLY:O	1:A:986:SER:OG	2.39	0.40
1:A:1082:THR:O	1:A:1258:GLY:HA2	2.21	0.40
1:A:699:LYS:HD3	1:A:699:LYS:HA	1.70	0.40
1:A:12:SER:HA	1:A:887:ASN:HB2	2.02	0.40
1:A:15:LYS:HB2	1:A:886:ILE:HD11	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1481:HOH:O	6:A:1481:HOH:O[4_555]	1.84	0.36
6:A:1455:HOH:O	6:A:1455:HOH:O[3_554]	2.00	0.20

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1136/1323 (86%)	1028 (90%)	94 (8%)	14 (1%)	13	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ILE
1	A	408	ASP
1	A	693	ASN
1	A	864	GLU
1	A	1148	GLY
1	A	519	ALA
1	A	1023	VAL
1	A	514	LEU
1	A	286	GLY
1	A	702	SER
1	A	234	ILE
1	A	653	GLY
1	A	664	GLY
1	A	857	PRO

### 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	
1	A	1026/1203 (85%)	944 (92%)	82 (8%)	12	40

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	87	LYS
1	A	90	ASP
1	A	131	LYS
1	A	151	GLU
1	A	152	LEU
1	A	171	SER
1	A	180	LYS
1	A	192	SER
1	A	215	LYS
1	A	219	GLU
1	A	223	ASP
1	A	246	ASP
1	A	261	ASP
1	A	268	ASN
1	A	289	PHE
1	A	294	ASN
1	A	301	ASN
1	A	312	ASN
1	A	316	LEU
1	A	335	LYS
1	A	336	SER
1	A	338	VAL
1	A	371	LYS
1	A	398	SER
1	A	486	PRO
1	A	489	PHE
1	A	492	ILE
1	A	496	LYS
1	A	497	ASP
1	A	502	ILE
1	A	509	GLN
1	A	518	SER
1	A	528	ASP
1	A	532	GLN
1	A	534	ASN
1	A	536	LEU
1	A	538	HIS
1	A	542	ILE
1	A	562	TYR
1	A	563	LEU
1	A	564	VAL
1	A	565	PHE

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Mol	Chain	Res	Type
1	A	567	GLU
1	A	589	LYS
1	A	595	LYS
1	A	625	ASP
1	A	636	LYS
1	A	643	ASP
1	A	652	GLU
1	A	692	ARG
1	A	697	HIS
1	A	699	LYS
1	A	704	GLN
1	A	705	LYS
1	A	707	TYR
1	A	708	GLU
1	A	712	PHE
1	A	719	LYS
1	A	806	LEU
1	A	821	VAL
1	A	854	LYS
1	A	855	ASP
1	A	862	VAL
1	A	864	GLU
1	A	867	LEU
1	A	898	ASP
1	A	974	ILE
1	A	1029	LYS
1	A	1034	LYS
1	A	1048	THR
1	A	1109	PHE
1	A	1116	CYS
1	A	1131	LYS
1	A	1142	TRP
1	A	1146	SER
1	A	1163	TRP
1	A	1200	ASP
1	A	1217	MET
1	A	1267	LEU
1	A	1297	ASN
1	A	1299	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	156	ASN
1	A	494	GLN
1	A	495	ASN
1	A	534	ASN
1	A	617	ASN
1	A	694	HIS
1	A	804	HIS
1	A	853	ASN
1	A	1094	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	39/40 (97%)	6 (15%)	1 (2%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-9	G
2	B	-8	U
2	B	-7	U
2	B	-6	G
2	B	17	G
2	B	19	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	-8	U

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	426:ALA	C	459:LYS	N	18.99
1	A	550:GLU	C	555:ASP	N	7.52
1	A	422:THR	C	424:GLU	N	6.96
1	A	556:LYS	C	557:ALA	N	4.69
1	A	548:SER	C	550:GLU	N	3.41
1	A	555:ASP	C	556:LYS	N	3.26



## 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<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	A	1182/1323 (89%)	-0.19	26 (2%) 62 33	38, 91, 183, 234	0
2	B	40/40 (100%)	-0.21	2 (5%) 28 10	39, 79, 163, 202	0
3	C	26/26 (100%)	-0.35	0 100 100	40, 62, 172, 181	0
4	D	12/12 (100%)	-0.27	0 100 100	37, 46, 201, 204	0
All	All	1260/1401 (89%)	-0.20	28 (2%) 62 33	37, 90, 184, 234	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	20	C	4.6
1	A	562	TYR	4.2
1	A	1205	ALA	4.2
1	A	1180	ASP	4.1
1	A	376	LEU	3.9
1	A	563	LEU	3.9
1	A	312	ASN	3.9
1	A	408	ASP	3.7
1	A	1147	PHE	3.1
1	A	1237	ASN	3.1
1	A	1134	GLY	2.9
1	A	1048	THR	2.8
1	A	406	VAL	2.8
1	A	1200	ASP	2.7
1	A	316	LEU	2.7
1	A	378	PHE	2.7
1	A	1136	LYS	2.6
1	A	868	ILE	2.6
1	A	1111	LYS	2.5
1	A	537	LEU	2.4
1	A	422	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	-9	G	2.4
1	A	945	GLY	2.4
1	A	1195	ILE	2.4
1	A	1133	PHE	2.3
1	A	1199	SER	2.2
1	A	465	THR	2.2
1	A	1202	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	102	1/1	0.65	0.21	89,89,89,89	0
5	MG	B	101	1/1	0.73	0.32	68,68,68,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.