



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:18 pm BST

PDB ID : 1NZB  
Title : Crystal structure of wild type Cre recombinase-loxP synapse  
Authors : Ennifar, E.; Meyer, J.E.W.; Buchholz, F.; Stewart, A.F.; Suck, D.  
Deposited on : 2003-02-17  
Resolution : 3.10 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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

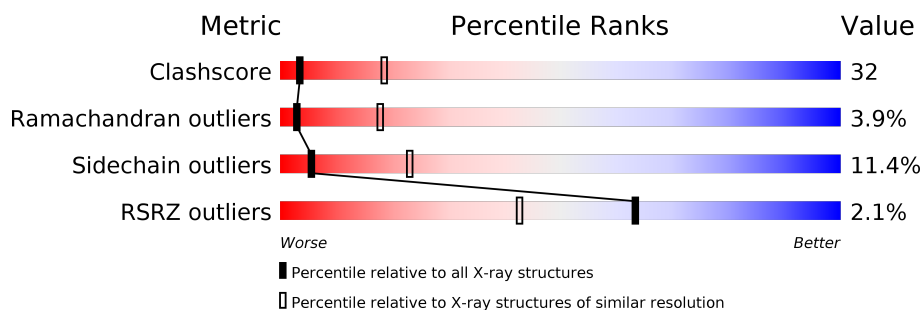
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	C	37	
1	G	37	
2	D	37	
2	H	37	
3	A	343	
3	B	343	
3	E	343	

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Mol	Chain	Length	Quality of chain
3	F	343	<div> <div>%</div> <div> <div></div> <div>48%</div> <div>38%</div> <div>7%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	F	5307	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13299 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 DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	37	Total	C	N	O	P	0	0	0
			754	363	134	221	36			
1	G	37	Total	C	N	O	P	0	0	0
			754	363	134	221	36			

- Molecule 2 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	37	Total	C	N	O	P	0	0	0
			756	364	137	219	36			
2	H	37	Total	C	N	O	P	0	0	0
			756	364	137	219	36			

- Molecule 3 is a protein called Cre recombinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	332	Total	C	N	O	S	0	0	0
			2620	1629	497	479	15			
3	B	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			
3	E	321	Total	C	N	O	S	0	0	0
			2544	1581	485	463	15			
3	F	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Mg 3	0	0
4	C	1	Total 1	Mg 1	0	0
4	F	2	Total 2	Mg 2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	I 1	0	0
5	F	1	Total 1	I 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0

### 3 Residue-property plots [i](#)

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

#### • Molecule 1: loxP DNA

Chain C: 



#### • Molecule 1: loxP DNA

Chain G: 



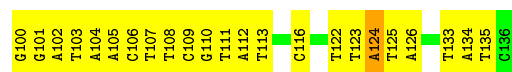
#### • Molecule 2: loxP DNA

Chain D: 



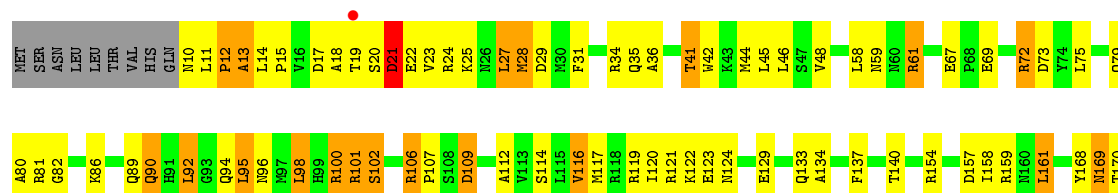
#### • Molecule 2: loxP DNA

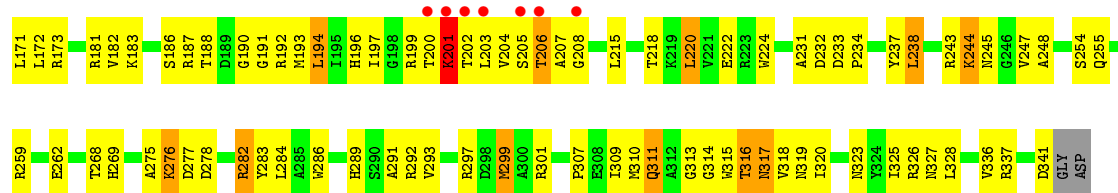
Chain H: 



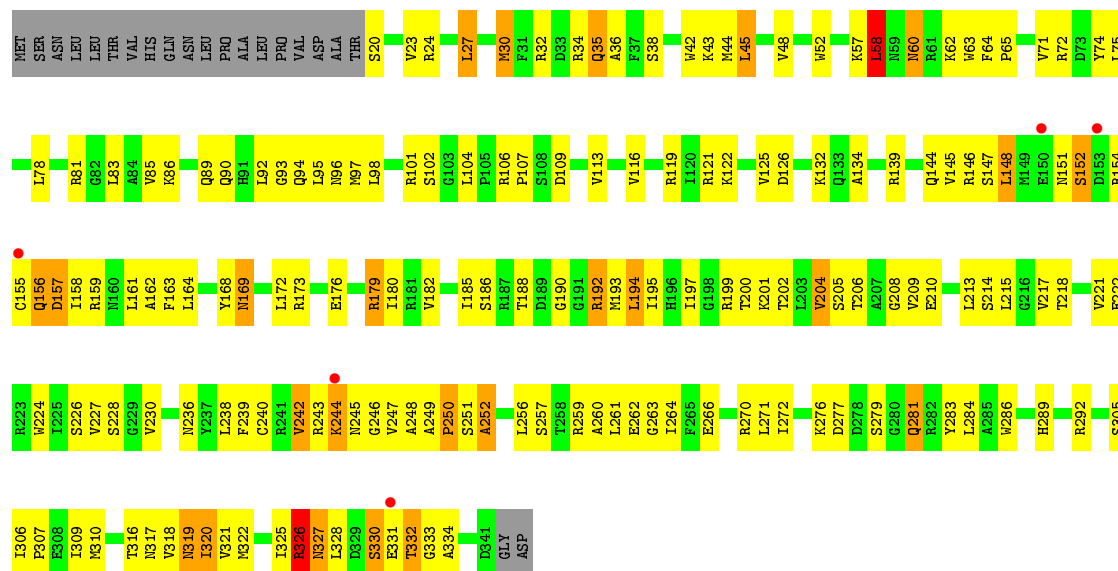
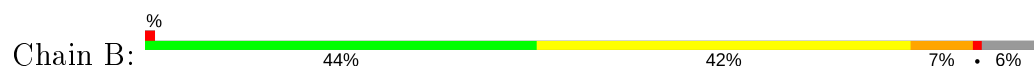
#### • Molecule 3: Cre recombinase

Chain A: 

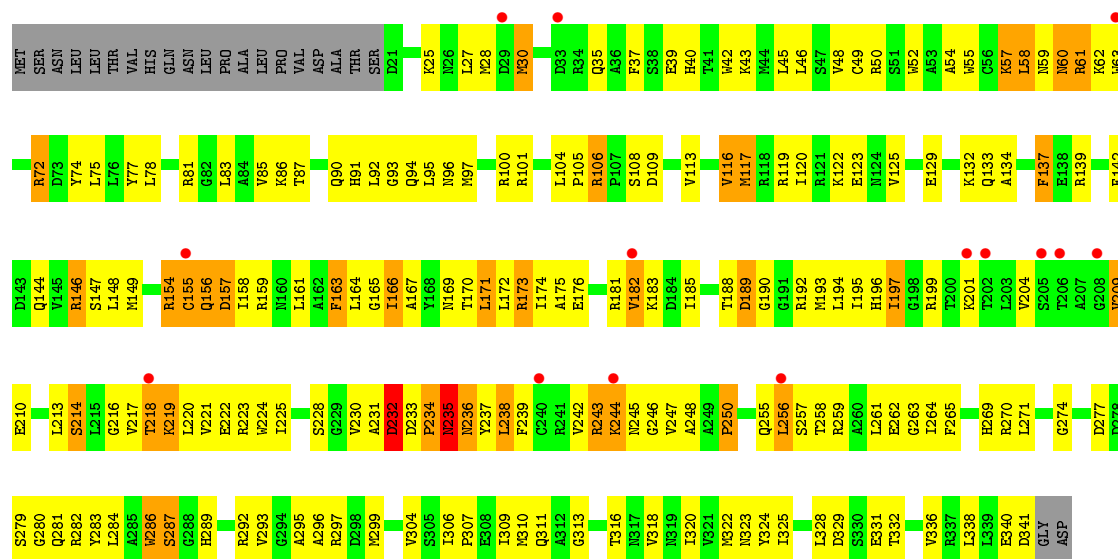




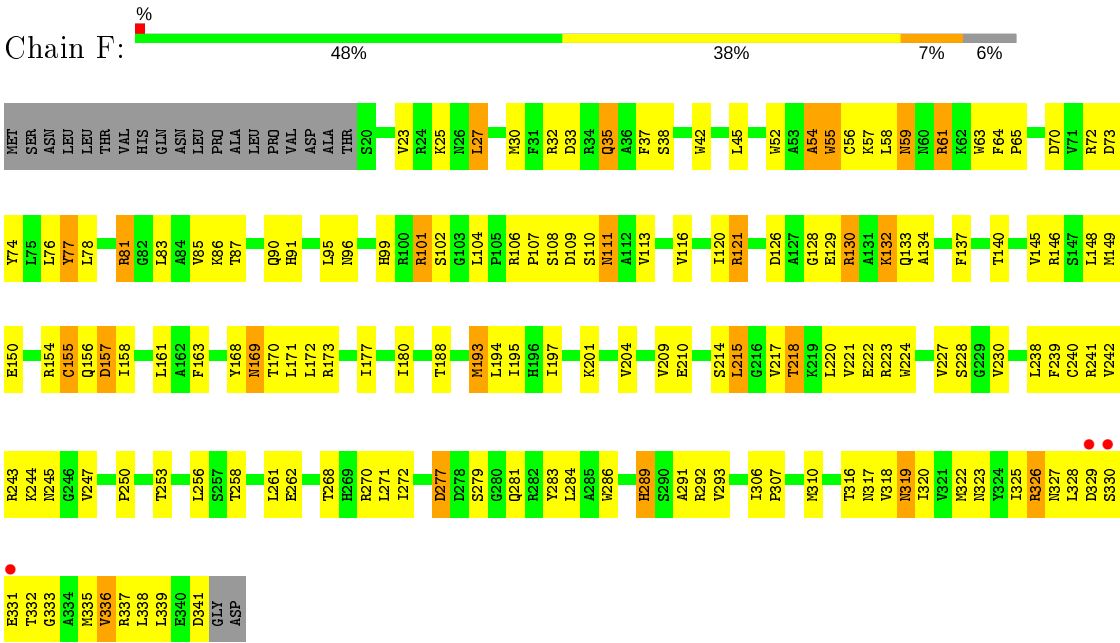
• Molecule 3: Cre recombinase



• Molecule 3: Cre recombinase



• Molecule 3: Cre recombinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.89Å 163.53Å 195.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10 49.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (8.00-3.10) 98.3 (49.95-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.257 0.209 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.8	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 77.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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

### 5.1 Standard geometry

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

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	C	0.50	0/823	0.81	0/1266
1	G	0.45	0/823	0.77	0/1266
2	D	0.51	0/848	0.81	0/1307
2	H	0.41	0/848	0.76	0/1307
3	A	0.45	0/2663	0.69	0/3595
3	B	0.37	0/2591	0.64	2/3493 (0.1%)
3	E	0.37	0/2585	0.63	0/3485
3	F	0.38	0/2591	0.63	1/3493 (0.0%)
All	All	0.42	0/13772	0.69	3/19212 (0.0%)

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	C	0	1
1	G	0	2
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	137	PHE	N-CA-C	-5.68	95.66	111.00
3	B	326	ARG	N-CA-C	-5.41	96.38	111.00
3	B	58	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	DT	Sidechain
1	G	106	DC	Sidechain
1	G	115	DA	Sidechain
2	H	124	DA	Sidechain

## 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	C	754	0	420	32	0
1	G	754	0	420	22	0
2	D	756	0	421	56	0
2	H	756	0	421	39	0
3	A	2620	0	2643	164	0
3	B	2550	0	2571	181	0
3	E	2544	0	2566	258	0
3	F	2550	0	2571	165	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
5	B	1	0	0	1	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	F	1	0	0	0	0
All	All	13299	0	12033	812	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 32.

All (812) 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:E:166:ILE:HD13	3:E:213:LEU:HD11	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:332:THR:HG22	3:B:333:GLY:H	1.17	1.04
3:E:188:THR:HB	3:E:192:ARG:H	1.21	1.04
3:A:72:ARG:HG3	3:A:116:VAL:HG21	1.37	1.03
3:A:276:LYS:HG2	3:A:277:ASP:H	1.18	1.02
2:D:122:DT:H5''	3:B:97:MET:HE2	1.43	1.00
2:D:132:DT:H2''	2:D:133:DT:H5''	1.41	1.00
2:D:135:DT:H1'	3:B:244:LYS:HD2	1.46	0.97
3:A:193:MET:HG3	3:A:218:THR:HG23	1.49	0.95
2:H:105:DA:H2''	2:H:106:DC:H5''	1.50	0.94
3:A:15:PRO:HB2	3:A:18:ALA:HB3	1.50	0.93
1:G:122:DC:H2''	1:G:123:DT:H5'	1.48	0.93
3:E:146:ARG:HH21	3:E:220:LEU:HD11	1.33	0.92
1:C:124:DA:OP1	3:A:201:LYS:HD2	1.72	0.89
3:A:206:THR:HG21	3:A:316:THR:HG23	1.54	0.88
1:C:105:DA:H2''	1:C:106:DC:H5''	1.56	0.88
3:F:214:SER:O	3:F:218:THR:HG22	1.72	0.88
3:B:90:GLN:HE21	3:B:94:GLN:HG2	1.37	0.87
3:F:317:ASN:ND2	3:F:319:ASN:H	1.71	0.86
2:H:116:DC:C5'	3:E:173:ARG:HH21	1.88	0.86
3:E:243:ARG:HG3	3:E:243:ARG:HH11	1.40	0.85
1:C:119:DA:H2''	1:C:120:DT:H5'	1.58	0.85
3:A:310:MET:SD	3:A:318:VAL:HG12	2.17	0.85
3:E:209:VAL:HB	3:F:326:ARG:CZ	2.07	0.84
3:B:319:ASN:HD22	3:B:320:ILE:H	1.24	0.84
3:F:333:GLY:HA2	3:F:337:ARG:HG3	1.59	0.84
1:G:105:DA:H2''	1:G:106:DC:H5''	1.59	0.84
2:D:129:DA:H2''	2:D:130:DA:H5''	1.58	0.83
3:E:154:ARG:HB2	3:E:157:ASP:HB2	1.60	0.83
3:B:75:LEU:HD11	3:B:92:LEU:HD13	1.61	0.83
3:E:195:ILE:HD11	3:E:213:LEU:HD21	1.60	0.82
2:D:108:DT:H2''	2:D:109:DC:H5'	1.62	0.82
3:F:72:ARG:HG3	3:F:116:VAL:HG11	1.62	0.82
3:B:332:THR:HG22	3:B:333:GLY:N	1.94	0.81
3:E:92:LEU:HD23	3:E:96:ASN:HD21	1.45	0.81
3:E:245:ASN:OD1	3:E:247:VAL:HG23	1.80	0.81
3:F:328:LEU:HB3	3:F:332:THR:HA	1.62	0.81
3:E:154:ARG:HB3	3:E:154:ARG:HH11	1.47	0.80
3:E:210:GLU:CG	3:F:326:ARG:HH21	1.94	0.80
2:H:106:DC:H2'	2:H:107:DT:H72	1.62	0.80
3:F:332:THR:HG22	3:F:333:GLY:H	1.46	0.79
3:E:230:VAL:HG12	3:E:236:ASN:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:306:ILE:O	3:B:310:MET:HG2	1.83	0.78
2:H:134:DA:H2"	2:H:135:DT:C5'	2.14	0.78
2:D:117:DA:H3'	3:A:202:THR:HG23	1.66	0.78
3:B:154:ARG:O	3:B:158:ILE:HG12	1.83	0.78
1:G:122:DC:H2"	1:G:123:DT:C5'	2.13	0.77
3:E:159:ARG:HB2	3:E:224:TRP:CZ3	2.19	0.77
3:E:90:GLN:HE21	3:E:94:GLN:HG2	1.49	0.77
3:A:11:LEU:HD23	3:A:12:PRO:HD2	1.67	0.76
3:B:236:ASN:ND2	3:B:250:PRO:HB3	1.98	0.76
3:F:121:ARG:HG3	3:F:121:ARG:HH11	1.47	0.76
1:G:131:DG:H2"	1:G:132:DT:C5'	2.16	0.76
3:A:19:THR:HG22	3:A:24:ARG:HG2	1.67	0.75
3:F:328:LEU:CB	3:F:332:THR:HA	2.15	0.75
3:A:10:ASN:HD22	3:A:31:PHE:HE2	1.35	0.75
3:E:48:VAL:HG11	3:E:94:GLN:HB3	1.65	0.75
3:E:75:LEU:HA	3:E:78:LEU:HD23	1.69	0.75
3:F:55:TRP:O	3:F:59:ASN:HB2	1.87	0.75
3:A:276:LYS:CG	3:A:277:ASP:H	1.98	0.74
3:F:193:MET:HE3	3:F:221:VAL:HG11	1.69	0.74
3:B:262:GLU:O	3:B:266:GLU:HG3	1.86	0.74
3:B:319:ASN:O	3:B:320:ILE:HB	1.87	0.74
3:A:96:ASN:OD1	3:A:107:PRO:HD2	1.86	0.74
3:B:259:ARG:HH11	3:B:259:ARG:HG3	1.52	0.74
3:A:27:LEU:HD13	3:A:102:SER:HB2	1.68	0.74
3:B:58:LEU:O	3:B:58:LEU:HD12	1.87	0.74
3:B:113:VAL:O	3:B:116:VAL:HG12	1.87	0.73
3:A:276:LYS:HG2	3:A:277:ASP:N	2.01	0.73
3:E:188:THR:HG22	3:E:190:GLY:H	1.52	0.73
2:D:132:DT:C2'	2:D:133:DT:H5"	2.16	0.73
3:E:188:THR:HB	3:E:192:ARG:N	2.01	0.73
3:F:146:ARG:O	3:F:150:GLU:HB2	1.87	0.73
3:E:72:ARG:HD2	3:E:116:VAL:CG2	2.19	0.73
3:B:45:LEU:HD21	3:B:98:LEU:HD13	1.71	0.73
3:E:169:ASN:ND2	3:E:213:LEU:HA	2.03	0.73
3:E:217:VAL:O	3:E:221:VAL:HG23	1.88	0.73
3:B:332:THR:CG2	3:B:333:GLY:H	1.98	0.73
3:F:317:ASN:HD22	3:F:319:ASN:H	1.35	0.73
3:B:159:ARG:HB2	3:B:224:TRP:CZ3	2.24	0.73
2:H:105:DA:C2'	2:H:106:DC:H5"	2.18	0.72
2:H:108:DT:H2"	2:H:109:DC:H5'	1.70	0.72
2:H:124:DA:H5'	3:F:201:LYS:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:154:ARG:NH1	3:E:154:ARG:HB3	2.04	0.72
3:A:12:PRO:O	3:A:13:ALA:HB2	1.88	0.72
3:B:182:VAL:HG23	3:B:236:ASN:O	1.89	0.72
1:C:112:DA:H62	3:B:44:MET:CE	2.02	0.72
3:E:199:ARG:HA	3:F:130:ARG:NH2	2.05	0.72
2:H:102:DA:H2"	2:H:103:DT:O5'	1.89	0.72
2:H:134:DA:H2"	2:H:135:DT:H5"	1.69	0.72
3:E:122:LYS:O	3:E:125:VAL:HG12	1.90	0.72
3:E:222:GLU:HA	3:E:225:ILE:HD12	1.70	0.72
3:E:292:ARG:O	3:E:295:ALA:HB3	1.89	0.72
2:H:116:DC:H5"	3:E:173:ARG:HH21	1.52	0.72
2:D:119:DA:OP1	3:B:121:ARG:NH1	2.24	0.71
3:A:192:ARG:HB3	3:A:215:LEU:HD23	1.72	0.71
3:A:15:PRO:CB	3:A:18:ALA:HB3	2.19	0.70
3:E:243:ARG:CG	3:E:243:ARG:HH11	2.03	0.70
3:B:85:VAL:O	3:B:89:GLN:HG3	1.91	0.70
2:H:106:DC:H2'	2:H:107:DT:C7	2.21	0.70
3:F:158:ILE:HG12	3:F:223:ARG:NH1	2.06	0.70
3:E:237:TYR:CD1	3:E:255:GLN:HB3	2.27	0.70
2:H:133:DT:H2"	2:H:134:DA:C8	2.27	0.70
3:F:134:ALA:HA	3:F:283:TYR:CD2	2.27	0.70
3:A:307:PRO:HG3	3:B:306:ILE:CD1	2.22	0.70
2:H:116:DC:H5'	3:E:173:ARG:HH21	1.57	0.70
3:E:270:ARG:HA	3:E:274:GLY:O	1.92	0.69
3:B:236:ASN:HA	3:B:251:SER:O	1.93	0.69
3:E:210:GLU:HG3	3:F:326:ARG:HH21	1.57	0.69
3:A:168:TYR:HA	3:A:291:ALA:HB1	1.75	0.69
3:E:221:VAL:O	3:E:225:ILE:HG13	1.91	0.69
3:F:277:ASP:OD2	3:F:279:SER:HB2	1.93	0.69
1:C:103:DT:H2"	1:C:104:DA:C8	2.27	0.69
3:E:181:ARG:CZ	3:E:237:TYR:HE2	2.06	0.69
3:E:139:ARG:HH11	3:F:339:LEU:HD23	1.57	0.69
3:F:180:ILE:HD13	3:F:195:ILE:HG21	1.74	0.69
3:B:319:ASN:ND2	3:B:320:ILE:H	1.91	0.69
3:E:139:ARG:HH12	3:F:339:LEU:HA	1.58	0.69
3:E:188:THR:HG22	3:E:190:GLY:N	2.08	0.69
3:F:230:VAL:HG12	3:F:250:PRO:HB3	1.73	0.68
3:E:163:PHE:CE2	3:E:261:LEU:HD22	2.28	0.68
3:E:219:LYS:HA	3:E:222:GLU:OE1	1.92	0.68
3:B:319:ASN:HD22	3:B:320:ILE:N	1.90	0.68
3:F:332:THR:HG22	3:F:333:GLY:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:DA:H2''	2:D:130:DA:C5'	2.23	0.68
3:E:156:GLN:HB2	3:E:242:VAL:HG11	1.76	0.68
3:E:93:GLY:HA2	3:E:96:ASN:HD22	1.57	0.68
1:G:133:DT:H2''	1:G:134:DA:C8	2.29	0.68
3:E:134:ALA:HA	3:E:283:TYR:CD2	2.29	0.67
3:F:193:MET:CE	3:F:221:VAL:HG11	2.24	0.67
3:A:72:ARG:CG	3:A:116:VAL:HG21	2.20	0.67
3:A:197:ILE:O	3:A:197:ILE:HG13	1.93	0.67
3:E:171:LEU:HD22	3:E:295:ALA:CB	2.25	0.67
2:H:103:DT:H2''	2:H:104:DA:C8	2.29	0.67
3:A:243:ARG:HG2	3:A:243:ARG:HH11	1.58	0.67
3:B:204:VAL:O	3:B:204:VAL:HG13	1.94	0.67
3:B:57:LYS:NZ	3:B:57:LYS:HB3	2.09	0.66
3:E:169:ASN:HD22	3:E:213:LEU:HD13	1.60	0.66
1:C:100:DC:H2''	1:C:101:DG:C8	2.30	0.66
3:E:72:ARG:HD2	3:E:116:VAL:HG21	1.77	0.66
1:G:131:DG:H2''	1:G:132:DT:H5''	1.76	0.66
3:A:299:MET:HE3	3:A:309:ILE:HA	1.77	0.66
3:A:11:LEU:CD2	3:A:12:PRO:HD2	2.24	0.66
3:E:52:TRP:HZ3	3:E:74:TYR:HB2	1.61	0.66
3:B:169:ASN:C	3:B:169:ASN:HD22	1.99	0.65
3:F:23:VAL:HG21	3:F:104:LEU:HD21	1.78	0.65
3:A:14:LEU:HB3	3:A:19:THR:OG1	1.95	0.65
3:B:317:ASN:ND2	3:B:319:ASN:HB2	2.11	0.65
3:E:139:ARG:NH1	3:F:339:LEU:HA	2.11	0.65
3:F:91:HIS:O	3:F:95:LEU:HD23	1.96	0.65
3:F:204:VAL:O	3:F:204:VAL:HG13	1.97	0.65
3:A:12:PRO:O	3:A:13:ALA:CB	2.45	0.65
3:B:215:LEU:O	3:B:218:THR:HG22	1.97	0.65
2:D:124:DA:H2'	2:D:125:DT:H72	1.79	0.65
3:A:121:ARG:HH11	3:A:121:ARG:HG2	1.61	0.64
2:D:116:DC:H2''	2:D:117:DA:C8	2.32	0.64
3:E:222:GLU:HA	3:E:225:ILE:CD1	2.27	0.64
1:G:128:DG:H1	2:H:109:DC:H42	1.46	0.64
3:E:144:GLN:O	3:E:148:LEU:HG	1.97	0.64
2:D:134:DA:H2''	2:D:135:DT:O5'	1.98	0.64
3:A:14:LEU:HG	3:A:27:LEU:CD2	2.26	0.64
3:B:188:THR:HG23	3:B:194:LEU:HD21	1.80	0.64
3:E:92:LEU:HD21	3:E:108:SER:OG	1.96	0.64
3:F:317:ASN:CG	3:F:318:VAL:H	2.00	0.64
1:G:131:DG:H2''	1:G:132:DT:H5'	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:PRO:HB2	3:A:18:ALA:CB	2.26	0.64
3:B:20:SER:O	3:B:24:ARG:HG3	1.97	0.64
3:E:158:ILE:HD11	3:E:223:ARG:HH21	1.63	0.64
3:E:92:LEU:HD23	3:E:96:ASN:ND2	2.13	0.64
2:D:135:DT:H2''	2:D:136:DC:C6	2.33	0.64
3:A:14:LEU:HG	3:A:27:LEU:HD23	1.79	0.63
3:B:156:GLN:HB3	3:B:242:VAL:HG11	1.79	0.63
3:E:183:LYS:HG2	3:E:183:LYS:O	1.97	0.63
3:E:139:ARG:NH1	3:F:339:LEU:HD23	2.14	0.63
3:E:210:GLU:HB2	3:F:326:ARG:HE	1.62	0.63
3:B:146:ARG:O	3:B:148:LEU:N	2.29	0.63
3:E:182:VAL:HG23	3:E:236:ASN:O	1.99	0.63
3:A:116:VAL:O	3:A:120:ILE:HG13	1.98	0.63
3:A:207:ALA:HA	3:A:314:GLY:HA2	1.80	0.63
3:F:243:ARG:HG2	3:F:243:ARG:HH11	1.64	0.63
3:E:216:GLY:O	3:E:220:LEU:HG	1.99	0.62
3:B:259:ARG:HG3	3:B:259:ARG:NH1	2.08	0.62
3:A:207:ALA:HA	3:A:314:GLY:CA	2.29	0.62
3:E:62:LYS:H	3:E:62:LYS:HD2	1.64	0.62
3:F:271:LEU:HD13	3:F:271:LEU:O	1.99	0.62
2:H:134:DA:H2''	2:H:135:DT:H5'	1.80	0.62
3:A:19:THR:CG2	3:A:24:ARG:HG2	2.30	0.62
3:B:218:THR:O	3:B:222:GLU:HG3	2.00	0.62
3:E:119:ARG:O	3:E:123:GLU:HB2	1.99	0.62
3:B:58:LEU:HD12	3:B:58:LEU:C	2.19	0.62
3:E:137:PHE:CD1	3:E:265:PHE:HE1	2.18	0.62
3:E:185:ILE:HG21	3:E:193:MET:HE1	1.82	0.61
3:A:202:THR:HG22	3:A:204:VAL:H	1.66	0.61
3:B:163:PHE:CE1	3:B:261:LEU:HD22	2.35	0.61
1:C:100:DC:O2	1:C:100:DC:H2'	2.01	0.61
3:E:92:LEU:CD2	3:E:96:ASN:HD21	2.14	0.61
3:F:37:PHE:HD1	3:F:42:TRP:HE1	1.47	0.61
3:B:317:ASN:HD22	3:B:319:ASN:CB	2.13	0.61
2:D:113:DT:H2''	2:D:114:DA:C8	2.35	0.61
2:D:128:DG:H2''	2:D:129:DA:C5'	2.30	0.61
3:E:318:VAL:O	3:E:322:MET:HG2	2.00	0.61
3:E:209:VAL:HB	3:F:326:ARG:NH1	2.14	0.61
3:E:271:LEU:HD23	3:E:271:LEU:O	2.00	0.61
3:E:48:VAL:HG11	3:E:94:GLN:CB	2.29	0.61
3:B:199:ARG:HG3	3:B:204:VAL:HG23	1.82	0.61
3:B:306:ILE:N	3:B:307:PRO:HD2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:297:ARG:HH12	3:A:327:ASN:HD21	1.49	0.61
3:A:208:GLY:HA2	3:B:326:ARG:HG2	1.81	0.61
1:C:112:DA:H62	3:B:44:MET:HE3	1.64	0.61
3:F:148:LEU:HD23	3:F:148:LEU:O	2.01	0.61
3:F:99:HIS:O	3:F:102:SER:HB2	2.01	0.61
3:E:204:VAL:HG13	3:F:323:ASN:ND2	2.16	0.60
3:A:72:ARG:NH1	3:F:33:ASP:OD2	2.34	0.60
3:E:113:VAL:O	3:E:116:VAL:HG23	2.01	0.60
3:E:258:THR:O	3:E:262:GLU:HG3	2.02	0.60
1:C:119:DA:H2''	1:C:120:DT:C5'	2.29	0.60
3:E:201:LYS:HE2	3:F:126:ASP:OD1	2.01	0.60
3:A:23:VAL:O	3:A:27:LEU:HB2	2.01	0.60
3:A:42:TRP:O	3:A:46:LEU:HG	2.02	0.60
3:B:251:SER:OG	3:B:252:ALA:N	2.33	0.60
3:E:146:ARG:CG	3:E:147:SER:N	2.65	0.60
3:B:90:GLN:NE2	3:B:94:GLN:HG2	2.13	0.60
3:E:230:VAL:HG13	3:E:236:ASN:HD22	1.67	0.60
3:F:30:MET:SD	3:F:101:ARG:HG2	2.42	0.60
3:A:208:GLY:HA2	3:B:326:ARG:CG	2.32	0.60
3:B:193:MET:HG3	3:B:218:THR:OG1	2.02	0.60
2:H:116:DC:H5'	3:E:173:ARG:NH2	2.17	0.60
3:F:317:ASN:ND2	3:F:318:VAL:H	2.00	0.60
3:B:236:ASN:HD22	3:B:250:PRO:HB3	1.67	0.59
3:B:185:ILE:HG21	3:B:193:MET:CE	2.32	0.59
3:B:240:CYS:SG	3:B:248:ALA:HB1	2.43	0.59
3:A:188:THR:HG23	3:B:330:SER:HB2	1.83	0.59
3:E:279:SER:O	3:E:281:GLN:N	2.30	0.59
2:D:117:DA:H3'	3:A:202:THR:CG2	2.33	0.59
3:B:94:GLN:HA	3:B:94:GLN:OE1	2.02	0.59
3:E:158:ILE:HG22	3:E:159:ARG:N	2.17	0.59
3:E:218:THR:O	3:E:222:GLU:HG3	2.01	0.59
3:A:181:ARG:HA	3:A:237:TYR:HA	1.85	0.59
3:E:195:ILE:CD1	3:E:213:LEU:HD21	2.29	0.59
3:F:172:LEU:HD21	3:F:197:ILE:HG13	1.83	0.59
2:D:103:DT:O2	3:A:244:LYS:HE3	2.03	0.59
3:A:112:ALA:O	3:A:116:VAL:HG23	2.02	0.59
3:E:245:ASN:OD1	3:E:246:GLY:N	2.36	0.59
3:F:154:ARG:HB2	3:F:157:ASP:HB2	1.85	0.58
3:F:158:ILE:HG12	3:F:223:ARG:HH12	1.66	0.58
3:E:172:LEU:HD23	3:E:176:GLU:OE2	2.02	0.58
3:A:277:ASP:HB3	3:A:284:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:DT:H2"	2:D:109:DC:C5'	2.30	0.58
1:C:106:DC:H2"	1:C:107:UMP:O5'	2.04	0.58
3:A:277:ASP:HB3	3:A:284:LEU:CD1	2.33	0.58
3:E:297:ARG:HG2	3:E:324:TYR:O	2.03	0.58
3:E:72:ARG:HG2	3:E:72:ARG:HH11	1.69	0.58
3:E:48:VAL:HG21	3:E:91:HIS:HA	1.86	0.58
3:F:242:VAL:O	3:F:242:VAL:HG23	2.03	0.58
2:D:128:DG:H2"	2:D:129:DA:H5"	1.86	0.58
3:E:94:GLN:HA	3:E:94:GLN:NE2	2.18	0.58
1:G:133:DT:H2"	1:G:134:DA:N7	2.19	0.58
3:A:154:ARG:O	3:A:158:ILE:HG13	2.04	0.58
2:D:117:DA:H2"	2:D:118:DT:H71	1.85	0.58
3:B:30:MET:SD	3:B:101:ARG:HG2	2.43	0.57
3:F:72:ARG:HG3	3:F:116:VAL:CG1	2.32	0.57
1:C:116:DT:H5'	3:B:201:LYS:HE3	1.86	0.57
3:B:245:ASN:OD1	3:B:246:GLY:N	2.37	0.57
3:E:210:GLU:CB	3:F:326:ARG:HH21	2.16	0.57
3:E:237:TYR:CE1	3:E:255:GLN:HB3	2.38	0.57
3:F:218:THR:O	3:F:222:GLU:HG3	2.04	0.57
3:A:14:LEU:HB3	3:A:19:THR:HG21	1.85	0.57
3:B:180:ILE:HD13	3:B:195:ILE:HG21	1.84	0.57
1:C:124:DA:H8	1:C:124:DA:H5"	1.70	0.57
3:E:234:PRO:C	3:E:236:ASN:H	2.06	0.57
3:F:161:LEU:HG	3:F:220:LEU:HD13	1.87	0.57
2:H:126:DA:OP2	3:F:262:GLU:OE2	2.23	0.57
3:B:172:LEU:HD21	3:B:197:ILE:HG13	1.87	0.57
2:D:100:DG:H2"	2:D:101:DG:O5'	2.05	0.57
3:E:146:ARG:HG2	3:E:147:SER:N	2.20	0.57
3:E:238:LEU:HD23	3:E:238:LEU:C	2.25	0.57
3:F:78:LEU:HD22	3:F:83:LEU:HD12	1.85	0.57
3:B:243:ARG:HH11	3:B:243:ARG:HG2	1.70	0.57
3:A:307:PRO:HG3	3:B:306:ILE:HD13	1.86	0.57
3:B:316:THR:HG22	3:B:316:THR:O	2.04	0.57
3:F:272:ILE:HG22	3:F:272:ILE:O	2.03	0.57
3:E:146:ARG:HA	3:E:161:LEU:HD11	1.86	0.56
3:F:209:VAL:HG22	3:F:210:GLU:N	2.20	0.56
3:A:171:LEU:O	3:A:292:ARG:NH1	2.39	0.56
3:F:59:ASN:O	3:F:61:ARG:HD3	2.06	0.56
3:A:336:VAL:HG13	3:F:214:SER:HA	1.87	0.56
3:E:85:VAL:HG23	3:E:129:GLU:OE2	2.05	0.56
3:E:174:ILE:HG13	3:E:175:ALA:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:230:VAL:CG1	3:E:236:ASN:HD22	2.18	0.56
1:G:114:DA:C8	3:F:86:LYS:HD3	2.40	0.56
1:C:105:DA:C2'	1:C:106:DC:H5''	2.33	0.56
3:B:209:VAL:HG22	3:B:210:GLU:N	2.20	0.56
3:E:163:PHE:C	3:E:165:GLY:H	2.09	0.56
3:E:117:MET:HA	3:E:117:MET:HE3	1.87	0.56
3:E:248:ALA:C	3:E:250:PRO:HD3	2.27	0.56
3:F:96:ASN:OD1	3:F:107:PRO:HD2	2.06	0.56
1:G:126:DA:OP1	3:E:287:SER:HB2	2.06	0.56
3:B:192:ARG:HH11	3:B:192:ARG:HG2	1.70	0.56
2:D:128:DG:O6	3:B:259:ARG:NE	2.36	0.56
3:F:224:TRP:CZ3	3:F:228:SER:HB3	2.40	0.56
3:B:163:PHE:CD2	3:B:164:LEU:HD23	2.42	0.55
3:E:171:LEU:HD23	3:E:171:LEU:N	2.21	0.55
3:F:163:PHE:CE1	3:F:261:LEU:HD22	2.41	0.55
1:C:126:DA:OP2	3:A:262:GLU:OE1	2.25	0.55
3:A:15:PRO:CG	3:A:18:ALA:HB3	2.36	0.55
3:B:321:VAL:O	3:B:325:ILE:HG13	2.05	0.55
3:E:45:LEU:O	3:E:48:VAL:HG12	2.07	0.55
3:A:20:SER:O	3:A:21:ASP:HB2	2.06	0.55
2:D:107:DT:H2''	2:D:108:DT:H5'	1.89	0.55
2:D:124:DA:H2'	2:D:125:DT:C7	2.36	0.55
3:A:35:GLN:HB2	3:B:119:ARG:HD2	1.89	0.55
3:F:155:CYS:SG	3:F:227:VAL:HG12	2.46	0.55
3:F:87:THR:O	3:F:91:HIS:HD2	1.89	0.55
3:B:27:LEU:HD22	3:B:102:SER:HB3	1.88	0.55
3:E:116:VAL:O	3:E:120:ILE:HG13	2.07	0.55
3:E:171:LEU:HD22	3:E:295:ALA:HB1	1.88	0.55
3:E:27:LEU:HA	3:E:30:MET:HB3	1.87	0.55
3:E:35:GLN:C	3:E:37:PHE:H	2.10	0.55
3:F:332:THR:CG2	3:F:333:GLY:H	2.19	0.55
2:H:111:DT:H73	3:E:43:LYS:HE3	1.88	0.55
2:D:129:DA:C2'	2:D:130:DA:H5''	2.32	0.54
3:F:326:ARG:NH1	3:F:326:ARG:HG2	2.22	0.54
2:D:117:DA:H5''	3:A:202:THR:OG1	2.07	0.54
3:A:326:ARG:HD3	3:F:210:GLU:HG3	1.90	0.54
3:A:27:LEU:CD1	3:A:102:SER:HB2	2.37	0.54
3:A:268:THR:HG22	3:A:286:TRP:HZ3	1.72	0.54
3:B:188:THR:C	3:B:190:GLY:H	2.11	0.54
2:D:132:DT:H2''	2:D:133:DT:C5'	2.27	0.54
3:E:142:PHE:O	3:E:146:ARG:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:318:VAL:O	3:F:322:MET:HG2	2.08	0.54
3:F:328:LEU:HB2	3:F:332:THR:HA	1.90	0.54
3:B:188:THR:HG23	3:B:194:LEU:CD2	2.38	0.54
2:D:108:DT:H1'	2:D:109:DC:H5''	1.90	0.54
2:D:118:DT:H2''	2:D:119:DA:N7	2.23	0.54
3:E:281:GLN:HB2	3:E:284:LEU:HD11	1.90	0.54
3:E:39:GLU:HG3	3:E:40:HIS:N	2.22	0.54
3:E:137:PHE:HD2	3:E:137:PHE:C	2.11	0.54
3:E:155:CYS:SG	3:E:156:GLN:N	2.81	0.54
3:F:325:ILE:HG22	3:F:326:ARG:N	2.22	0.54
3:B:260:ALA:HA	5:B:344:IOD:I	2.79	0.53
3:B:319:ASN:ND2	3:B:320:ILE:N	2.54	0.53
3:A:119:ARG:O	3:A:123:GLU:HG3	2.07	0.53
3:E:97:MET:O	3:E:101:ARG:HB2	2.08	0.53
3:E:85:VAL:HG23	3:E:129:GLU:CD	2.28	0.53
3:A:106:ARG:O	3:A:109:ASP:HB2	2.09	0.53
2:D:112:DA:OP1	3:A:81:ARG:NH2	2.40	0.53
3:B:242:VAL:HG12	3:B:242:VAL:O	2.07	0.53
1:G:128:DG:H1	2:H:109:DC:N4	2.07	0.53
3:A:277:ASP:CB	3:A:284:LEU:HD13	2.38	0.53
2:D:135:DT:C1'	3:B:244:LYS:HD2	2.31	0.53
3:A:243:ARG:NH1	3:A:243:ARG:HG2	2.23	0.53
3:B:161:LEU:HG	3:B:161:LEU:O	2.08	0.53
1:G:113:DT:H71	3:F:87:THR:HG23	1.90	0.53
3:B:204:VAL:CG2	3:E:125:VAL:HG11	2.39	0.53
2:D:106:DC:H2''	2:D:107:DT:H5'	1.90	0.53
3:E:234:PRO:HG2	3:E:235:ASN:H	1.72	0.53
1:G:106:DC:H2''	1:G:107:UMP:O5'	2.09	0.53
3:A:44:MET:O	3:A:48:VAL:HG23	2.09	0.53
3:B:158:ILE:HG22	3:B:224:TRP:HB2	1.91	0.53
3:E:137:PHE:CD2	3:E:137:PHE:C	2.82	0.53
3:E:166:ILE:CD1	3:E:213:LEU:HD11	2.24	0.53
3:B:35:GLN:HB3	3:E:119:ARG:HG3	1.91	0.52
1:C:102:DA:H2''	1:C:103:DT:C5'	2.39	0.52
2:D:105:DA:H2''	2:D:106:DC:O5'	2.08	0.52
3:E:171:LEU:HD12	3:E:313:GLY:CA	2.40	0.52
3:E:185:ILE:HG21	3:E:193:MET:CE	2.38	0.52
3:E:213:LEU:HD12	3:E:217:VAL:CG1	2.40	0.52
3:E:256:LEU:HD13	3:E:261:LEU:HD21	1.91	0.52
2:H:135:DT:H1'	3:F:244:LYS:HD2	1.92	0.52
3:F:326:ARG:O	3:F:326:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:ALA:O	3:F:57:LYS:N	2.37	0.52
3:E:166:ILE:O	3:E:170:THR:HG23	2.10	0.52
3:E:75:LEU:HD21	3:E:92:LEU:HB2	1.92	0.52
3:A:14:LEU:HB3	3:A:19:THR:CG2	2.40	0.52
3:E:72:ARG:HD2	3:E:116:VAL:HG22	1.92	0.52
3:E:228:SER:OG	3:E:230:VAL:HG23	2.10	0.52
3:E:94:GLN:HA	3:E:94:GLN:HE21	1.74	0.52
3:F:78:LEU:HD22	3:F:83:LEU:CD1	2.40	0.52
3:B:317:ASN:ND2	3:B:319:ASN:CB	2.72	0.52
3:E:94:GLN:CA	3:E:94:GLN:HE21	2.23	0.52
3:F:121:ARG:CG	3:F:121:ARG:HH11	2.17	0.52
1:C:123:DT:H71	3:A:41:THR:CG2	2.40	0.52
3:B:34:ARG:HB2	3:B:42:TRP:CE2	2.44	0.52
1:G:105:DA:C2'	1:G:106:DC:H5''	2.35	0.52
3:A:161:LEU:HD13	3:A:220:LEU:HD13	1.92	0.51
3:E:25:LYS:O	3:E:28:MET:HB2	2.10	0.51
1:G:128:DG:O6	3:E:259:ARG:NE	2.39	0.51
1:G:135:DT:H2''	1:G:136:DC:C6	2.45	0.51
3:A:13:ALA:O	3:A:14:LEU:C	2.48	0.51
3:E:238:LEU:HD22	3:E:239:PHE:CD1	2.46	0.51
3:E:75:LEU:HD11	3:E:92:LEU:HD12	1.92	0.51
3:F:335:MET:HE3	3:F:335:MET:HA	1.91	0.51
3:E:171:LEU:HB2	3:E:313:GLY:HA2	1.91	0.51
3:E:171:LEU:CD2	3:E:295:ALA:HB1	2.40	0.51
3:A:282:ARG:O	3:A:283:TYR:HB2	2.11	0.51
3:A:192:ARG:HH11	3:B:331:GLU:HA	1.76	0.51
2:D:122:DT:C6	2:D:123:DT:H72	2.45	0.51
3:B:259:ARG:HH11	3:B:259:ARG:CG	2.21	0.50
3:B:279:SER:HB3	3:B:281:GLN:HG3	1.92	0.50
3:E:233:ASP:O	3:E:236:ASN:HB2	2.12	0.50
3:E:90:GLN:NE2	3:E:94:GLN:HG2	2.23	0.50
1:C:133:DT:H2''	1:C:134:DA:C8	2.46	0.50
3:E:146:ARG:HG2	3:E:147:SER:H	1.77	0.50
3:E:92:LEU:HA	3:E:95:LEU:HD23	1.93	0.50
3:B:102:SER:O	3:B:104:LEU:HG	2.12	0.50
3:B:64:PHE:HA	3:B:65:PRO:C	2.32	0.50
3:E:170:THR:OG1	3:E:172:LEU:HD12	2.11	0.50
3:F:23:VAL:CG2	3:F:104:LEU:HD21	2.42	0.50
3:B:72:ARG:HG3	3:B:116:VAL:HG11	1.94	0.50
3:F:227:VAL:O	3:F:227:VAL:HG12	2.10	0.50
3:F:227:VAL:CG1	3:F:227:VAL:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:DC:H2"	2:H:110:DG:C8	2.46	0.50
3:A:14:LEU:CD2	3:A:14:LEU:H	2.25	0.50
3:E:296:ALA:HA	3:E:299:MET:HE3	1.94	0.50
3:F:238:LEU:HD23	3:F:239:PHE:CE1	2.47	0.50
3:E:209:VAL:HB	3:F:326:ARG:NH2	2.26	0.50
3:F:169:ASN:ND2	3:F:169:ASN:O	2.45	0.50
3:B:188:THR:C	3:B:190:GLY:N	2.64	0.49
2:D:113:DT:H2"	2:D:114:DA:H8	1.77	0.49
3:E:306:ILE:N	3:E:307:PRO:HD2	2.27	0.49
3:E:310:MET:HE1	3:E:318:VAL:HG12	1.94	0.49
3:E:92:LEU:HD23	3:E:92:LEU:C	2.32	0.49
3:A:206:THR:CG2	3:A:316:THR:HG23	2.36	0.49
3:B:151:ASN:O	3:B:152:SER:C	2.50	0.49
3:B:209:VAL:HG22	3:B:210:GLU:H	1.77	0.49
3:E:169:ASN:HD22	3:E:213:LEU:HA	1.77	0.49
3:F:258:THR:O	3:F:262:GLU:HG3	2.12	0.49
3:F:168:TYR:HA	3:F:291:ALA:HB1	1.93	0.49
3:F:317:ASN:CG	3:F:318:VAL:N	2.66	0.49
3:A:11:LEU:HD23	3:A:12:PRO:CD	2.40	0.49
3:B:97:MET:O	3:B:101:ARG:HB2	2.12	0.49
3:B:326:ARG:O	3:B:327:ASN:O	2.30	0.49
3:B:52:TRP:HZ3	3:B:74:TYR:HB2	1.77	0.49
3:E:57:LYS:HD3	3:E:57:LYS:N	2.28	0.49
3:F:240:CYS:O	3:F:256:LEU:HD22	2.13	0.49
3:F:277:ASP:HB3	3:F:284:LEU:HD13	1.95	0.49
2:H:134:DA:C2'	2:H:135:DT:H5"	2.41	0.49
3:A:59:ASN:O	3:A:61:ARG:HD3	2.13	0.49
3:F:145:VAL:O	3:F:145:VAL:HG12	2.13	0.49
3:F:170:THR:O	3:F:171:LEU:HB2	2.13	0.49
3:B:159:ARG:HB2	3:B:224:TRP:CE3	2.47	0.49
3:A:14:LEU:CB	3:A:19:THR:OG1	2.60	0.49
3:B:57:LYS:HB3	3:B:57:LYS:HZ2	1.77	0.49
3:E:85:VAL:N	3:E:129:GLU:OE2	2.38	0.49
3:E:163:PHE:C	3:E:165:GLY:N	2.67	0.49
3:E:74:TYR:CZ	3:E:78:LEU:HD21	2.48	0.49
3:B:276:LYS:HD2	3:B:284:LEU:HB2	1.95	0.48
3:E:78:LEU:HB3	3:E:83:LEU:HD12	1.95	0.48
2:H:126:DA:OP1	3:F:289:HIS:N	2.34	0.48
3:A:188:THR:HG22	3:A:190:GLY:H	1.78	0.48
1:C:135:DT:H4'	3:A:245:ASN:HD22	1.78	0.48
3:E:181:ARG:C	3:E:183:LYS:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:DA:OP1	3:E:81:ARG:NH2	2.46	0.48
3:F:61:ARG:HG3	3:F:70:ASP:OD2	2.12	0.48
2:H:122:DT:C6	2:H:123:DT:H72	2.49	0.48
3:A:14:LEU:H	3:A:14:LEU:HD22	1.78	0.48
3:A:169:ASN:HD22	3:A:169:ASN:C	2.13	0.48
3:A:59:ASN:HB3	3:A:61:ARG:HH11	1.78	0.48
2:H:113:DT:H72	3:E:87:THR:HA	1.94	0.48
3:A:183:LYS:HB3	3:A:234:PRO:O	2.13	0.48
3:B:144:GLN:OE1	3:B:272:ILE:HG21	2.14	0.48
3:B:38:SER:HA	3:E:122:LYS:NZ	2.28	0.48
3:B:245:ASN:OD1	3:B:247:VAL:HG23	2.13	0.48
3:B:317:ASN:HD22	3:B:319:ASN:H	1.60	0.48
3:E:248:ALA:O	3:E:250:PRO:HD3	2.13	0.48
3:A:14:LEU:CA	3:A:19:THR:OG1	2.60	0.48
3:A:61:ARG:NH2	3:A:73:ASP:OD1	2.46	0.48
3:E:169:ASN:HD21	3:E:213:LEU:HA	1.77	0.48
3:E:234:PRO:O	3:E:236:ASN:N	2.47	0.48
3:E:75:LEU:CD1	3:E:92:LEU:HD12	2.43	0.48
3:F:332:THR:CG2	3:F:333:GLY:N	2.77	0.48
2:D:107:DT:H1'	2:D:108:DT:H5''	1.94	0.48
3:E:117:MET:HA	3:E:117:MET:CE	2.44	0.48
3:E:306:ILE:O	3:E:310:MET:HG3	2.13	0.48
3:F:326:ARG:HH11	3:F:326:ARG:HG2	1.77	0.48
2:D:117:DA:H2''	2:D:118:DT:C7	2.44	0.48
3:E:230:VAL:CG1	3:E:236:ASN:HB3	2.42	0.48
3:E:311:GLN:HG2	3:F:325:ILE:HG21	1.96	0.48
3:E:42:TRP:O	3:E:46:LEU:HG	2.14	0.48
3:F:129:GLU:C	3:F:130:ARG:HG2	2.34	0.47
3:A:245:ASN:OD1	3:A:247:VAL:HG23	2.14	0.47
3:A:317:ASN:N	3:A:317:ASN:ND2	2.62	0.47
1:G:100:DC:H2''	1:G:101:DG:O5'	2.14	0.47
3:B:32:ARG:CZ	3:E:72:ARG:NH1	2.78	0.47
2:D:128:DG:H2''	2:D:129:DA:H5'	1.97	0.47
3:E:243:ARG:NH1	3:E:243:ARG:CG	2.68	0.47
2:H:103:DT:O2	3:E:244:LYS:NZ	2.45	0.47
1:C:108:DT:H2''	1:C:109:DC:H5'	1.96	0.47
3:E:325:ILE:HB	3:E:328:LEU:HD12	1.96	0.47
3:A:204:VAL:O	3:A:204:VAL:HG13	2.14	0.47
2:D:117:DA:H5''	3:A:201:LYS:HE2	1.95	0.47
3:E:188:THR:CG2	3:E:189:ASP:N	2.78	0.47
3:A:187:ARG:NH1	3:A:191:GLY:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:159:ARG:O	3:B:162:ALA:HB3	2.14	0.47
1:C:116:DT:H4'	3:B:202:THR:HG22	1.97	0.47
3:E:262:GLU:O	3:E:265:PHE:HB2	2.15	0.47
1:C:114:DA:C8	3:B:86:LYS:HG2	2.50	0.47
1:C:102:DA:H2''	1:C:103:DT:H5'	1.95	0.47
3:F:113:VAL:O	3:F:116:VAL:HG12	2.15	0.47
3:F:268:THR:HG22	3:F:286:TRP:HZ3	1.78	0.47
3:B:154:ARG:HB2	3:B:157:ASP:HB2	1.95	0.47
3:B:227:VAL:HG12	3:B:227:VAL:O	2.15	0.47
3:B:238:LEU:HD23	3:B:239:PHE:CE1	2.50	0.47
3:E:182:VAL:HG21	3:E:230:VAL:HG12	1.97	0.47
3:E:194:LEU:HD11	3:E:210:GLU:HB3	1.96	0.47
3:B:106:ARG:NH1	3:B:109:ASP:OD2	2.48	0.47
3:B:271:LEU:HD13	3:B:271:LEU:O	2.15	0.47
3:E:193:MET:HG3	3:E:218:THR:OG1	2.14	0.47
3:F:335:MET:CE	3:F:335:MET:HA	2.44	0.47
3:E:310:MET:CE	3:E:318:VAL:HG12	2.44	0.47
3:F:270:ARG:HH11	3:F:270:ARG:HG3	1.80	0.47
3:A:14:LEU:N	3:A:14:LEU:HD22	2.30	0.46
3:E:169:ASN:OD1	3:F:339:LEU:HD12	2.15	0.46
3:A:301:ARG:HG2	3:A:328:LEU:HD13	1.97	0.46
3:B:176:GLU:OE2	3:B:200:THR:HB	2.15	0.46
2:D:134:DA:H2'	2:D:135:DT:H71	1.97	0.46
3:E:149:MET:HB2	3:E:161:LEU:HD22	1.97	0.46
3:E:35:GLN:HE21	3:E:35:GLN:HA	1.79	0.46
3:E:60:ASN:O	3:E:61:ARG:HD2	2.15	0.46
1:G:113:DT:C7	3:F:87:THR:HG23	2.45	0.46
3:E:320:ILE:O	3:E:323:ASN:HB2	2.15	0.46
3:F:54:ALA:O	3:F:55:TRP:C	2.52	0.46
3:E:234:PRO:C	3:E:236:ASN:N	2.68	0.46
3:E:48:VAL:CG1	3:E:49:CYS:N	2.78	0.46
3:F:209:VAL:CG2	3:F:210:GLU:N	2.79	0.46
3:B:188:THR:CG2	3:B:194:LEU:HD21	2.44	0.46
3:B:243:ARG:NH1	3:B:243:ARG:HG2	2.30	0.46
3:B:325:ILE:O	3:B:326:ARG:HD2	2.14	0.46
3:A:100:ARG:C	3:A:102:SER:H	2.19	0.46
3:B:185:ILE:HG21	3:B:193:MET:HE1	1.97	0.46
2:D:130:DA:H5'	2:D:130:DA:H8	1.79	0.46
3:E:336:VAL:O	3:E:340:GLU:HG3	2.16	0.46
3:B:271:LEU:HD13	3:B:271:LEU:C	2.36	0.46
3:B:132:LYS:HB3	3:B:283:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:DT:C7	3:E:43:LYS:HE3	2.46	0.46
3:A:21:ASP:HB3	3:A:22:GLU:H	1.50	0.46
3:A:317:ASN:H	3:A:317:ASN:ND2	2.13	0.46
3:B:204:VAL:HG23	3:E:125:VAL:HG11	1.98	0.46
3:B:317:ASN:ND2	3:B:319:ASN:H	2.13	0.46
3:B:319:ASN:O	3:B:320:ILE:CB	2.62	0.46
2:D:135:DT:C2'	2:D:136:DC:C6	2.98	0.46
3:E:101:ARG:CA	3:F:111:ASN:HD21	2.29	0.46
3:E:106:ARG:H	3:E:106:ARG:HG2	1.56	0.46
3:E:137:PHE:HE1	3:E:164:LEU:HD22	1.80	0.46
3:E:72:ARG:HG2	3:E:72:ARG:NH1	2.31	0.46
3:E:214:SER:OG	3:E:217:VAL:HG23	2.15	0.46
3:F:146:ARG:O	3:F:150:GLU:N	2.43	0.46
3:B:132:LYS:N	3:B:132:LYS:HD2	2.30	0.46
3:B:134:ALA:HA	3:B:283:TYR:CD2	2.51	0.46
3:B:310:MET:HE3	3:B:316:THR:C	2.36	0.46
1:C:124:DA:OP1	3:A:201:LYS:CD	2.56	0.46
1:C:128:DG:N7	3:A:259:ARG:NH2	2.59	0.46
3:E:329:ASP:O	3:E:332:THR:HG23	2.16	0.46
3:E:97:MET:O	3:E:97:MET:HG2	2.15	0.46
3:B:106:ARG:HH11	3:B:109:ASP:CG	2.20	0.45
3:F:81:ARG:HH11	3:F:81:ARG:HG3	1.80	0.45
3:F:27:LEU:HD11	3:F:102:SER:OG	2.16	0.45
3:F:242:VAL:O	3:F:242:VAL:CG2	2.64	0.45
3:E:158:ILE:HG22	3:E:224:TRP:HE3	1.80	0.45
3:E:55:TRP:O	3:E:59:ASN:ND2	2.47	0.45
1:G:117:DG:H5'	3:F:316:THR:HB	1.99	0.45
3:A:92:LEU:HD12	3:A:117:MET:HG2	1.98	0.45
3:A:137:PHE:HD1	3:A:286:TRP:CE2	2.35	0.45
3:A:86:LYS:HD3	3:A:86:LYS:O	2.16	0.45
3:B:179:ARG:CZ	3:B:199:ARG:HH21	2.30	0.45
3:E:62:LYS:N	3:E:62:LYS:HD2	2.30	0.45
3:A:161:LEU:HD22	3:A:220:LEU:CD1	2.46	0.45
3:B:248:ALA:C	3:B:250:PRO:HD3	2.36	0.45
3:B:289:HIS:CD2	3:B:292:ARG:HD3	2.52	0.45
3:F:325:ILE:HG22	3:F:326:ARG:H	1.82	0.45
3:F:52:TRP:HZ3	3:F:74:TYR:HB2	1.81	0.45
3:F:85:VAL:HG23	3:F:129:GLU:OE2	2.17	0.45
3:B:188:THR:O	3:B:190:GLY:N	2.50	0.45
2:D:135:DT:H1'	3:B:244:LYS:CD	2.33	0.45
3:E:137:PHE:HD1	3:E:265:PHE:HE1	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:339:LEU:C	3:F:341:ASP:H	2.20	0.45
3:A:15:PRO:O	3:A:19:THR:HB	2.16	0.45
3:A:79:GLN:NE2	3:A:120:ILE:HG23	2.32	0.45
3:B:139:ARG:HG2	3:B:139:ARG:NH1	2.31	0.45
3:B:249:ALA:N	3:B:250:PRO:HD3	2.32	0.45
3:B:306:ILE:CG2	3:B:318:VAL:HG22	2.46	0.45
3:E:204:VAL:CG1	3:F:323:ASN:ND2	2.79	0.45
3:F:116:VAL:O	3:F:120:ILE:HG13	2.16	0.45
3:A:121:ARG:NH1	3:F:204:VAL:HG13	2.31	0.45
3:A:247:VAL:HG12	3:A:248:ALA:O	2.17	0.45
3:B:78:LEU:HB3	3:B:83:LEU:HD12	1.98	0.45
3:E:106:ARG:O	3:E:109:ASP:HB2	2.16	0.45
3:F:61:ARG:NH1	3:F:70:ASP:OD1	2.50	0.45
2:D:124:DA:H2"	2:D:125:DT:H6	1.82	0.45
3:E:163:PHE:C	3:E:163:PHE:CD1	2.91	0.45
1:C:102:DA:H1'	1:C:103:DT:H5"	1.99	0.45
2:D:124:DA:H2"	2:D:125:DT:C6	2.52	0.45
3:E:173:ARG:CG	3:E:173:ARG:HH11	2.30	0.45
3:B:36:ALA:HA	3:E:119:ARG:HA	1.99	0.44
3:A:194:LEU:HD23	3:A:196:HIS:CE1	2.52	0.44
3:A:203:LEU:HD23	3:A:203:LEU:O	2.18	0.44
3:E:204:VAL:HG12	3:E:204:VAL:O	2.17	0.44
3:E:182:VAL:HG21	3:E:230:VAL:CG1	2.47	0.44
3:E:48:VAL:HG13	3:E:49:CYS:N	2.33	0.44
3:F:121:ARG:NH1	3:F:121:ARG:HG3	2.24	0.44
2:D:135:DT:H2"	2:D:136:DC:H6	1.80	0.44
3:E:116:VAL:O	3:E:119:ARG:HB3	2.18	0.44
3:E:101:ARG:HA	3:F:111:ASN:HD21	1.82	0.44
3:F:331:GLU:O	3:F:336:VAL:HG11	2.17	0.44
3:B:318:VAL:O	3:B:322:MET:HG2	2.17	0.44
2:D:116:DC:H5"	3:A:173:ARG:HH21	1.83	0.44
3:E:197:ILE:CG1	3:E:197:ILE:O	2.65	0.44
3:F:156:GLN:HB2	3:F:242:VAL:HG21	1.98	0.44
3:A:90:GLN:HE21	3:A:90:GLN:HA	1.83	0.44
3:E:173:ARG:HH11	3:E:173:ARG:HB3	1.82	0.44
3:F:54:ALA:O	3:F:56:CYS:N	2.51	0.44
3:A:75:LEU:HD11	3:A:92:LEU:HG	1.99	0.44
3:B:62:LYS:HB2	3:B:62:LYS:HE3	1.87	0.44
2:D:128:DG:C2'	2:D:129:DA:H5"	2.46	0.44
3:B:192:ARG:HB3	3:B:213:LEU:O	2.17	0.44
2:D:107:DT:H2"	2:D:108:DT:C5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:DT:H4'	3:B:289:HIS:CE1	2.53	0.44
3:E:196:HIS:ND1	3:E:197:ILE:N	2.66	0.44
3:E:199:ARG:HA	3:F:130:ARG:HH21	1.80	0.44
3:E:210:GLU:HG3	3:F:326:ARG:NH2	2.30	0.44
3:F:245:ASN:OD1	3:F:247:VAL:HB	2.18	0.44
3:A:107:PRO:C	3:A:109:ASP:H	2.21	0.44
3:E:243:ARG:H	3:E:243:ARG:HD2	1.83	0.44
3:A:187:ARG:NH2	3:A:222:GLU:OE2	2.51	0.44
3:A:317:ASN:H	3:A:317:ASN:HD22	1.65	0.44
3:B:186:SER:OG	3:B:194:LEU:HB2	2.18	0.44
3:B:71:VAL:O	3:B:75:LEU:HG	2.18	0.44
3:E:269:HIS:HB2	3:E:286:TRP:CE3	2.53	0.44
3:F:243:ARG:HG2	3:F:243:ARG:NH1	2.30	0.44
3:F:64:PHE:HA	3:F:65:PRO:C	2.39	0.44
3:B:305:SER:O	3:B:309:ILE:HG13	2.18	0.43
3:B:44:MET:O	3:B:48:VAL:HG23	2.18	0.43
3:E:55:TRP:CD1	3:E:77:TYR:CD2	3.06	0.43
3:A:186:SER:OG	3:A:196:HIS:HE1	2.00	0.43
3:A:25:LYS:HD2	3:A:29:ASP:OD2	2.17	0.43
1:C:119:DA:H1'	1:C:120:DT:H5"	1.99	0.43
3:E:58:LEU:HD12	3:E:58:LEU:O	2.18	0.43
3:A:269:HIS:HB2	3:A:286:TRP:CE3	2.53	0.43
3:A:311:GLN:HB3	3:A:311:GLN:HE21	1.59	0.43
3:B:261:LEU:HD23	3:B:264:ILE:HD12	2.00	0.43
3:F:245:ASN:OD1	3:F:247:VAL:N	2.51	0.43
2:H:112:DA:H2	3:E:282:ARG:HH22	1.66	0.43
3:A:101:ARG:HD3	3:A:101:ARG:HA	1.64	0.43
3:A:80:ALA:C	3:A:82:GLY:N	2.72	0.43
3:B:318:VAL:HG12	3:B:318:VAL:O	2.18	0.43
3:B:60:ASN:HA	3:B:60:ASN:HD22	1.64	0.43
3:F:106:ARG:NH1	3:F:109:ASP:OD2	2.51	0.43
3:B:332:THR:CG2	3:B:333:GLY:N	2.65	0.43
3:F:128:GLY:HA2	3:F:130:ARG:NH2	2.33	0.43
3:F:173:ARG:CZ	3:F:201:LYS:HB3	2.48	0.43
2:H:122:DT:OP2	3:F:101:ARG:NH1	2.51	0.43
3:A:24:ARG:O	3:A:28:MET:HB2	2.19	0.43
3:A:311:GLN:HG3	3:B:325:ILE:HG22	2.01	0.43
3:B:226:SER:OG	3:B:227:VAL:N	2.50	0.43
3:E:92:LEU:HD13	3:E:117:MET:SD	2.59	0.43
3:F:154:ARG:O	3:F:158:ILE:HG13	2.18	0.43
3:A:201:LYS:O	3:B:125:VAL:HG11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:ILE:HG23	3:E:193:MET:HB3	2.01	0.43
3:E:235:ASN:HD22	3:E:235:ASN:N	2.15	0.43
3:F:320:ILE:HD12	3:F:320:ILE:H	1.83	0.43
3:A:95:LEU:HD12	3:A:95:LEU:HA	1.81	0.43
3:E:52:TRP:HD1	3:E:63:TRP:HE3	1.66	0.43
3:F:27:LEU:HD12	3:F:27:LEU:HA	1.77	0.43
3:F:317:ASN:ND2	3:F:319:ASN:HB2	2.34	0.43
3:E:204:VAL:HG13	3:F:323:ASN:HD21	1.83	0.43
3:A:122:LYS:O	3:A:123:GLU:C	2.56	0.43
3:A:159:ARG:HB2	3:A:224:TRP:CZ3	2.53	0.43
3:A:34:ARG:C	3:A:36:ALA:H	2.23	0.43
3:B:327:ASN:HB3	3:B:328:LEU:H	1.43	0.43
2:D:122:DT:C5'	3:B:97:MET:HE2	2.32	0.43
3:E:137:PHE:HD1	3:E:265:PHE:CE1	2.37	0.43
3:E:340:GLU:O	3:E:341:ASP:HB2	2.19	0.43
3:F:329:ASP:O	3:F:332:THR:OG1	2.37	0.43
3:F:77:TYR:C	3:F:77:TYR:CD1	2.92	0.43
3:A:11:LEU:HA	3:A:12:PRO:HD3	1.90	0.43
1:C:123:DT:H71	3:A:41:THR:HG23	2.01	0.43
3:F:25:LYS:HD3	3:F:25:LYS:O	2.18	0.43
3:A:154:ARG:HB2	3:A:157:ASP:HB2	2.00	0.42
3:A:208:GLY:HA2	3:B:326:ARG:HG3	2.01	0.42
3:A:307:PRO:HG3	3:B:306:ILE:HD11	1.98	0.42
3:E:243:ARG:N	3:E:243:ARG:HD2	2.33	0.42
3:F:261:LEU:HA	3:F:261:LEU:HD23	1.79	0.42
3:F:317:ASN:HD22	3:F:319:ASN:HB2	1.83	0.42
3:A:170:THR:OG1	3:A:172:LEU:HG	2.20	0.42
3:E:62:LYS:H	3:E:62:LYS:CD	2.29	0.42
3:E:78:LEU:HD22	3:E:78:LEU:H	1.84	0.42
3:A:133:GLN:HG2	3:A:134:ALA:N	2.34	0.42
3:A:207:ALA:HA	3:A:314:GLY:HA3	1.99	0.42
3:A:293:VAL:O	3:A:297:ARG:HG3	2.19	0.42
3:A:69:GLU:OE1	3:F:32:ARG:NH1	2.47	0.42
3:B:284:LEU:HA	3:B:284:LEU:HD23	1.74	0.42
3:E:113:VAL:HA	3:E:116:VAL:HG23	2.01	0.42
3:B:93:GLY:O	3:B:96:ASN:HB2	2.19	0.42
3:F:132:LYS:HZ3	3:F:132:LYS:HA	1.84	0.42
3:E:35:GLN:C	3:E:37:PHE:N	2.72	0.42
3:E:74:TYR:O	3:E:78:LEU:CD2	2.67	0.42
3:F:171:LEU:O	3:F:292:ARG:NH1	2.50	0.42
3:F:172:LEU:HB2	3:F:177:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:188:THR:HG22	3:F:194:LEU:HD11	2.01	0.42
3:E:231:ALA:O	3:E:232:ASP:C	2.57	0.42
3:F:145:VAL:HG12	3:F:149:MET:HE2	2.02	0.42
3:A:19:THR:HG22	3:A:24:ARG:CG	2.41	0.42
3:A:277:ASP:CG	3:A:278:ASP:H	2.23	0.42
3:E:210:GLU:HB2	3:F:326:ARG:NE	2.32	0.42
3:E:304:VAL:HG12	3:E:309:ILE:HG13	2.01	0.42
3:F:55:TRP:CE3	3:F:77:TYR:CD2	3.07	0.42
3:A:72:ARG:HD2	3:A:116:VAL:CG2	2.50	0.42
3:B:74:TYR:CE2	3:B:78:LEU:HD11	2.55	0.42
2:D:124:DA:H5'	2:D:124:DA:H8	1.84	0.42
3:E:100:ARG:NH1	3:E:106:ARG:NE	2.68	0.42
3:E:166:ILE:HG22	3:E:167:ALA:N	2.34	0.42
3:B:42:TRP:O	3:B:43:LYS:C	2.55	0.42
2:D:117:DA:C5'	3:A:201:LYS:HE2	2.49	0.42
3:F:214:SER:OG	3:F:217:VAL:HG23	2.20	0.42
3:F:76:LEU:HD23	3:F:76:LEU:HA	1.92	0.42
3:B:155:CYS:O	3:B:158:ILE:HB	2.20	0.42
3:B:276:LYS:HD2	3:B:284:LEU:CB	2.50	0.42
3:B:310:MET:HE3	3:B:316:THR:HA	2.01	0.42
3:E:304:VAL:CG1	3:E:309:ILE:HG13	2.50	0.42
3:F:81:ARG:NH1	3:F:81:ARG:HG3	2.35	0.42
3:B:214:SER:O	3:B:218:THR:HB	2.20	0.41
1:C:133:DT:H2''	1:C:134:DA:N7	2.35	0.41
2:D:106:DC:H2'	2:D:107:DT:C7	2.50	0.41
3:A:231:ALA:O	3:A:233:ASP:N	2.53	0.41
1:C:107:UMP:OP2	3:B:256:LEU:HD12	2.20	0.41
3:E:27:LEU:CA	3:E:30:MET:HB3	2.50	0.41
2:H:108:DT:H2''	2:H:109:DC:C5'	2.45	0.41
3:B:58:LEU:C	3:B:58:LEU:CD1	2.88	0.41
3:E:197:ILE:HG13	3:E:197:ILE:O	2.20	0.41
3:F:132:LYS:HA	3:F:132:LYS:NZ	2.34	0.41
2:H:100:DG:H2''	2:H:101:DG:C8	2.56	0.41
3:A:319:ASN:OD1	3:A:320:ILE:HG12	2.20	0.41
1:C:124:DA:C8	1:C:124:DA:H5''	2.54	0.41
3:E:74:TYR:CE1	3:E:78:LEU:HD21	2.55	0.41
3:F:215:LEU:O	3:F:218:THR:HG23	2.21	0.41
1:G:135:DT:H2''	1:G:136:DC:H6	1.84	0.41
3:A:45:LEU:N	3:A:94:GLN:HE21	2.17	0.41
3:B:228:SER:OG	3:B:230:VAL:HG22	2.21	0.41
3:E:104:LEU:HB3	3:E:105:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:220:LEU:HD23	3:E:220:LEU:N	2.34	0.41
3:E:74:TYR:O	3:E:78:LEU:HD22	2.21	0.41
3:A:72:ARG:HG3	3:A:116:VAL:CG2	2.27	0.41
3:E:52:TRP:CD1	3:E:63:TRP:HE3	2.38	0.41
3:E:74:TYR:O	3:E:77:TYR:HB3	2.20	0.41
3:F:35:GLN:HE21	3:F:35:GLN:H	1.68	0.41
1:G:115:DA:H2''	1:G:116:DT:H5'	2.02	0.41
3:A:35:GLN:O	3:B:122:LYS:HD3	2.20	0.41
3:B:217:VAL:O	3:B:221:VAL:HG23	2.20	0.41
3:B:261:LEU:HD23	3:B:261:LEU:HA	1.89	0.41
3:E:318:VAL:O	3:E:318:VAL:HG23	2.20	0.41
2:H:111:DT:OP2	3:E:50:ARG:NH2	2.40	0.41
3:A:337:ARG:O	3:A:341:ASP:N	2.54	0.41
3:B:205:SER:OG	3:B:206:THR:N	2.54	0.41
3:B:270:ARG:HG3	3:B:270:ARG:HH11	1.86	0.41
3:E:158:ILE:CG2	3:E:159:ARG:N	2.84	0.41
3:E:170:THR:OG1	3:E:172:LEU:HB2	2.21	0.41
3:E:210:GLU:HB2	3:F:326:ARG:HH21	1.83	0.41
3:A:14:LEU:HB3	3:A:19:THR:CB	2.50	0.41
3:B:57:LYS:HB3	3:B:57:LYS:HZ3	1.85	0.41
1:C:123:DT:H71	3:A:41:THR:HG22	2.03	0.41
3:E:238:LEU:C	3:E:238:LEU:CD2	2.88	0.41
3:F:306:ILE:N	3:F:307:PRO:HD2	2.35	0.41
2:H:106:DC:H2''	2:H:107:DT:O5'	2.21	0.41
3:A:200:THR:HB	3:A:201:LYS:H	1.60	0.41
3:A:243:ARG:O	3:A:245:ASN:N	2.53	0.41
3:B:173:ARG:HB2	3:B:176:GLU:HG3	2.02	0.41
3:E:242:VAL:HG22	3:E:248:ALA:HA	2.03	0.41
3:E:57:LYS:HD3	3:E:57:LYS:H	1.85	0.41
3:E:91:HIS:O	3:E:95:LEU:HD22	2.21	0.41
3:A:22:GLU:HA	3:A:25:LYS:HB3	2.03	0.41
3:A:34:ARG:C	3:A:36:ALA:N	2.75	0.41
3:E:42:TRP:CE3	3:E:45:LEU:HD23	2.56	0.41
3:F:306:ILE:HG22	3:F:310:MET:CE	2.51	0.41
3:A:238:LEU:HD23	3:A:238:LEU:HA	1.89	0.40
3:A:325:ILE:HG13	3:A:325:ILE:O	2.21	0.40
3:A:80:ALA:C	3:A:82:GLY:H	2.23	0.40
3:B:107:PRO:O	3:B:113:VAL:HB	2.21	0.40
3:B:144:GLN:O	3:B:145:VAL:C	2.58	0.40
1:C:112:DA:OP1	3:B:81:ARG:NH2	2.54	0.40
3:E:165:GLY:O	3:E:166:ILE:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:279:SER:OG	3:F:281:GLN:HG3	2.20	0.40
2:H:123:DT:H3'	3:F:38:SER:HB2	2.02	0.40
3:B:263:GLY:O	3:B:264:ILE:C	2.58	0.40
3:E:78:LEU:HD12	3:E:83:LEU:CD1	2.51	0.40
3:F:52:TRP:HD1	3:F:63:TRP:HE3	1.69	0.40
3:A:173:ARG:HH11	3:A:173:ARG:HG3	1.86	0.40
3:B:30:MET:HG3	3:B:101:ARG:CG	2.51	0.40
3:B:23:VAL:HG21	3:B:104:LEU:HD21	2.03	0.40
3:B:306:ILE:N	3:B:307:PRO:CD	2.82	0.40
3:B:318:VAL:HG12	3:B:322:MET:HG2	2.03	0.40
2:D:116:DC:H5''	3:A:173:ARG:NH2	2.36	0.40
3:E:171:LEU:HD12	3:E:313:GLY:N	2.37	0.40
2:H:104:DA:H1'	3:E:244:LYS:HB3	2.03	0.40
2:H:124:DA:H2''	2:H:125:DT:C6	2.56	0.40
3:A:313:GLY:HA3	3:A:315:TRP:CZ3	2.57	0.40
3:A:72:ARG:HD2	3:A:116:VAL:HG22	2.01	0.40
3:B:44:MET:O	3:B:45:LEU:C	2.59	0.40
3:B:75:LEU:HA	3:B:78:LEU:HD12	2.02	0.40
2:D:123:DT:C2	2:D:124:DA:C8	3.10	0.40
3:E:329:ASP:HA	3:E:332:THR:CG2	2.52	0.40
3:A:124:ASN:ND2	3:A:129:GLU:OE2	2.50	0.40
3:A:231:ALA:C	3:A:233:ASP:N	2.74	0.40
3:A:59:ASN:HB3	3:A:61:ARG:NH1	2.35	0.40
3:B:139:ARG:HB2	3:B:168:TYR:OH	2.21	0.40
3:B:213:LEU:N	3:B:213:LEU:HD23	2.36	0.40
3:E:181:ARG:O	3:E:183:LYS:N	2.55	0.40
3:E:193:MET:HG3	3:E:218:THR:HG23	2.04	0.40
3:E:263:GLY:O	3:E:264:ILE:C	2.59	0.40
3:E:289:HIS:HD2	3:E:292:ARG:HG3	1.87	0.40
3:F:163:PHE:HE1	3:F:261:LEU:HD13	1.86	0.40
3:F:204:VAL:O	3:F:204:VAL:CG1	2.68	0.40
2:H:112:DA:H2''	2:H:113:DT:C5'	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	330/343 (96%)	286 (87%)	34 (10%)	10 (3%)	4	23
3	B	320/343 (93%)	256 (80%)	48 (15%)	16 (5%)	2	13
3	E	319/343 (93%)	253 (79%)	50 (16%)	16 (5%)	2	13
3	F	320/343 (93%)	269 (84%)	43 (13%)	8 (2%)	5	27
All	All	1289/1372 (94%)	1064 (82%)	175 (14%)	50 (4%)	3	18

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	13	ALA
3	A	182	VAL
3	B	327	ASN
3	B	332	THR
3	E	280	GLY
3	F	54	ALA
3	F	277	ASP
3	F	326	ARG
3	F	327	ASN
3	F	330	SER
3	A	21	ASP
3	A	201	LYS
3	A	244	LYS
3	A	276	LYS
3	B	152	SER
3	B	179	ARG
3	B	208	GLY
3	B	244	LYS
3	B	286	TRP
3	B	326	ARG
3	B	330	SER
3	E	182	VAL
3	E	235	ASN
3	E	238	LEU
3	E	244	LYS
3	E	257	SER
3	E	286	TRP
3	F	55	TRP

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Mol	Chain	Res	Type
3	F	319	ASN
3	A	232	ASP
3	A	275	ALA
3	B	277	ASP
3	E	54	ALA
3	E	58	LEU
3	E	232	ASP
3	A	98	LEU
3	A	199	ARG
3	B	147	SER
3	B	252	ALA
3	B	334	ALA
3	E	234	PRO
3	E	219	LYS
3	B	320	ILE
3	E	250	PRO
3	E	293	VAL
3	B	204	VAL
3	F	336	VAL
3	B	250	PRO
3	E	209	VAL
3	E	166	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	277/287 (96%)	237 (86%)	40 (14%)	3	14
3	B	269/287 (94%)	250 (93%)	19 (7%)	14	44
3	E	268/287 (93%)	234 (87%)	34 (13%)	4	18
3	F	269/287 (94%)	239 (89%)	30 (11%)	6	24
All	All	1083/1148 (94%)	960 (89%)	123 (11%)	5	23

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	12	PRO
3	A	17	ASP
3	A	21	ASP
3	A	27	LEU
3	A	28	MET
3	A	41	THR
3	A	58	LEU
3	A	61	ARG
3	A	67	GLU
3	A	72	ARG
3	A	89	GLN
3	A	90	GLN
3	A	92	LEU
3	A	95	LEU
3	A	98	LEU
3	A	100	ARG
3	A	101	ARG
3	A	102	SER
3	A	106	ARG
3	A	109	ASP
3	A	114	SER
3	A	116	VAL
3	A	140	THR
3	A	161	LEU
3	A	169	ASN
3	A	194	LEU
3	A	201	LYS
3	A	205	SER
3	A	206	THR
3	A	220	LEU
3	A	238	LEU
3	A	254	SER
3	A	255	GLN
3	A	282	ARG
3	A	289	HIS
3	A	299	MET
3	A	311	GLN
3	A	316	THR
3	A	317	ASN
3	A	323	ASN
3	B	27	LEU
3	B	30	MET
3	B	35	GLN

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Mol	Chain	Res	Type
3	B	45	LEU
3	B	58	LEU
3	B	60	ASN
3	B	63	TRP
3	B	95	LEU
3	B	126	ASP
3	B	148	LEU
3	B	156	GLN
3	B	157	ASP
3	B	169	ASN
3	B	192	ARG
3	B	194	LEU
3	B	242	VAL
3	B	257	SER
3	B	281	GLN
3	B	319	ASN
3	E	30	MET
3	E	57	LYS
3	E	60	ASN
3	E	61	ARG
3	E	72	ARG
3	E	86	LYS
3	E	106	ARG
3	E	116	VAL
3	E	117	MET
3	E	132	LYS
3	E	133	GLN
3	E	137	PHE
3	E	146	ARG
3	E	154	ARG
3	E	155	CYS
3	E	156	GLN
3	E	157	ASP
3	E	163	PHE
3	E	171	LEU
3	E	173	ARG
3	E	189	ASP
3	E	197	ILE
3	E	214	SER
3	E	218	THR
3	E	232	ASP
3	E	235	ASN

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Mol	Chain	Res	Type
3	E	236	ASN
3	E	243	ARG
3	E	256	LEU
3	E	277	ASP
3	E	287	SER
3	E	316	THR
3	E	331	GLU
3	E	338	LEU
3	F	27	LEU
3	F	35	GLN
3	F	45	LEU
3	F	58	LEU
3	F	59	ASN
3	F	61	ARG
3	F	73	ASP
3	F	77	TYR
3	F	81	ARG
3	F	90	GLN
3	F	101	ARG
3	F	108	SER
3	F	110	SER
3	F	111	ASN
3	F	121	ARG
3	F	130	ARG
3	F	132	LYS
3	F	133	GLN
3	F	140	THR
3	F	155	CYS
3	F	157	ASP
3	F	169	ASN
3	F	193	MET
3	F	215	LEU
3	F	218	THR
3	F	241	ARG
3	F	253	THR
3	F	289	HIS
3	F	293	VAL
3	F	338	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	10	ASN
3	A	40	HIS
3	A	79	GLN
3	A	90	GLN
3	A	94	GLN
3	A	196	HIS
3	A	311	GLN
3	A	317	ASN
3	B	35	GLN
3	B	60	ASN
3	B	90	GLN
3	B	156	GLN
3	B	235	ASN
3	B	236	ASN
3	B	255	GLN
3	B	289	HIS
3	B	317	ASN
3	B	319	ASN
3	B	327	ASN
3	E	35	GLN
3	E	79	GLN
3	E	90	GLN
3	E	94	GLN
3	E	96	ASN
3	E	169	ASN
3	E	235	ASN
3	E	236	ASN
3	E	323	ASN
3	F	35	GLN
3	F	90	GLN
3	F	94	GLN
3	F	111	ASN
3	F	133	GLN
3	F	144	GLN
3	F	156	GLN
3	F	281	GLN
3	F	317	ASN
3	F	319	ASN
3	F	323	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UMP	G	107	1,2	14,20,21	1.06	1 (7%)	14,28,31	1.15	1 (7%)
1	UMP	C	107	1,2	14,20,21	1.11	1 (7%)	14,28,31	1.16	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UMP	G	107	1,2	-	1/4/21/22	0/2/2/2
1	UMP	C	107	1,2	-	0/4/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	UMP	C4-N3	2.89	1.38	1.33
1	G	107	UMP	C4-N3	2.64	1.37	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	UMP	C5-C4-N3	-3.89	114.75	123.31
1	G	107	UMP	C5-C4-N3	-3.88	114.77	123.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	107	UMP	O4'-C1'-N1-C6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	107	UMP	1	0
1	C	107	UMP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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](#)

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<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	C	36/37 (97%)	-0.17	0 100 100	32, 53, 86, 95	0
1	G	36/37 (97%)	-0.14	0 100 100	39, 69, 96, 147	0
2	D	37/37 (100%)	-0.14	1 (2%) 54 31	33, 50, 85, 93	0
2	H	37/37 (100%)	-0.01	0 100 100	39, 72, 96, 114	0
3	A	332/343 (96%)	-0.09	8 (2%) 59 37	17, 48, 94, 149	0
3	B	322/343 (93%)	-0.03	5 (1%) 72 51	27, 62, 98, 142	0
3	E	321/343 (93%)	0.15	14 (4%) 34 17	38, 71, 109, 156	0
3	F	322/343 (93%)	-0.15	3 (0%) 84 69	31, 57, 95, 138	0
All	All	1443/1520 (94%)	-0.04	31 (2%) 63 43	17, 61, 99, 156	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	202	THR	5.8
3	E	208	GLY	4.8
3	F	331	GLU	4.6
3	A	201	LYS	4.3
3	F	330	SER	4.2
3	E	206	THR	4.0
3	B	331	GLU	3.6
3	E	244	LYS	3.4
3	E	155	CYS	3.2
3	E	205	SER	3.0
3	E	29	ASP	2.9
3	A	200	THR	2.9
3	E	201	LYS	2.8
3	B	244	LYS	2.7
3	E	202	THR	2.7
3	A	203	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	218	THR	2.6
3	E	240	CYS	2.5
3	B	155	CYS	2.4
3	B	153	ASP	2.4
3	A	208	GLY	2.4
3	A	205	SER	2.4
3	A	19	THR	2.3
3	E	63	TRP	2.3
3	A	206	THR	2.2
3	B	150	GLU	2.2
3	F	329	ASP	2.2
3	E	33	ASP	2.0
3	E	256	LEU	2.0
2	D	100	DG	2.0
3	E	182	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	UMP	C	107	19/20	0.95	0.14	43,57,72,74	0
1	UMP	G	107	19/20	0.97	0.20	54,58,65,71	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å <sup>2</sup> )	Q<0.9
4	MG	D	5310	1/1	0.60	0.36	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	F	5307	1/1	0.66	1.07	62,62,62,62	1
4	MG	C	5308	1/1	0.78	0.35	49,49,49,49	0
4	MG	F	5309	1/1	0.84	0.63	44,44,44,44	1
4	MG	G	5306	1/1	0.85	0.37	69,69,69,69	0
4	MG	A	5301	1/1	0.86	0.49	70,70,70,70	0
4	MG	D	5305	1/1	0.87	0.40	42,42,42,42	0
4	MG	D	5304	1/1	0.87	0.36	53,53,53,53	0
4	MG	A	5302	1/1	0.94	0.28	44,44,44,44	0
4	MG	A	5303	1/1	0.95	0.54	44,44,44,44	0
5	IOD	B	344	1/1	0.97	0.17	69,69,69,69	1
5	IOD	F	344	1/1	0.98	0.11	64,64,64,64	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.