



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:42 AM GMT

PDB ID : 1Q3V
Title : Crystal structure of a wild-type Cre recombinase-loxP synapse: phosphotyrosine covalent intermediate
Authors : Ennifar, E.; Meyer, J.E.W.; Buchholz, F.; Stewart, A.F.; Suck, D.
Deposited on : 2003-08-01
Resolution : 2.91 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

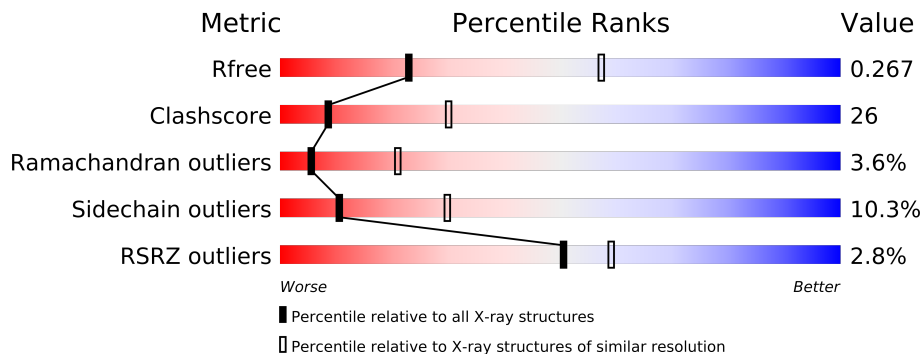
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.91 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}	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	16	
1	G	16	
2	X	21	
2	Y	21	
3	D	37	
3	H	37	
4	A	347	
4	B	347	
4	E	347	
4	F	347	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	IOD	C	200	-	X
6	MG	A	344	-	X
6	MG	A	345	-	X
6	MG	A	346	-	X
6	MG	A	347	-	X
6	MG	D	310	-	X
6	MG	F	345	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13296 atoms, of which 0 are hydrogen and 0 are deuterium.

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	16	Total	C	N	O	P	0	0	0
			326	156	59	95	16			
1	G	16	Total	C	N	O	P	0	0	0
			326	156	59	95	16			

- Molecule 2 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	21	Total	C	N	O	P	0	0	0
			428	207	75	126	20			
2	Y	21	Total	C	N	O	P	0	0	0
			428	207	75	126	20			

- Molecule 3 is a DNA chain called loxP DNA.

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

- Molecule 4 is a protein called Cre recombinase.

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	CLONING ARTIFACT	UNP P06956
A	-2	GLN	-	CLONING ARTIFACT	UNP P06956
A	-1	VAL	-	CLONING ARTIFACT	UNP P06956
A	0	PRO	-	CLONING ARTIFACT	UNP P06956
B	-3	PHE	-	CLONING ARTIFACT	UNP P06956
B	-2	GLN	-	CLONING ARTIFACT	UNP P06956
B	-1	VAL	-	CLONING ARTIFACT	UNP P06956
B	0	PRO	-	CLONING ARTIFACT	UNP P06956
E	-3	PHE	-	CLONING ARTIFACT	UNP P06956
E	-2	GLN	-	CLONING ARTIFACT	UNP P06956
E	-1	VAL	-	CLONING ARTIFACT	UNP P06956
E	0	PRO	-	CLONING ARTIFACT	UNP P06956
F	-3	PHE	-	CLONING ARTIFACT	UNP P06956
F	-2	GLN	-	CLONING ARTIFACT	UNP P06956
F	-1	VAL	-	CLONING ARTIFACT	UNP P06956
F	0	PRO	-	CLONING ARTIFACT	UNP P06956

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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total Mg 5 5	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0

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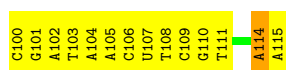
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total 1	O 1	0	0
7	F	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

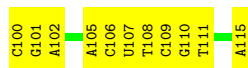
- Molecule 1: loxP DNA

Chain C: 



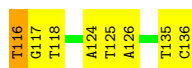
- Molecule 1: loxP DNA

Chain G: 



- Molecule 2: loxP DNA

Chain X: 



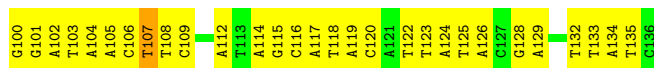
- Molecule 2: loxP DNA

Chain Y: 



- Molecule 3: loxP DNA

Chain D: 



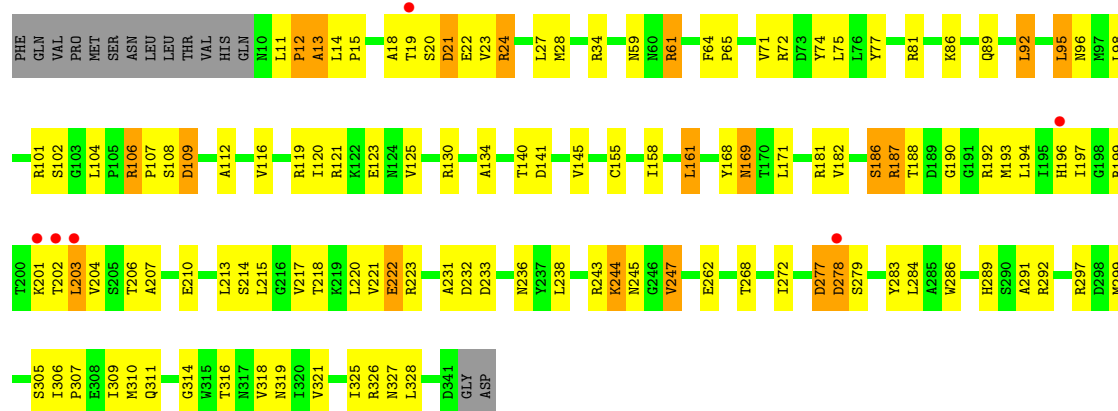
- Molecule 3: loxP DNA

Chain H: 



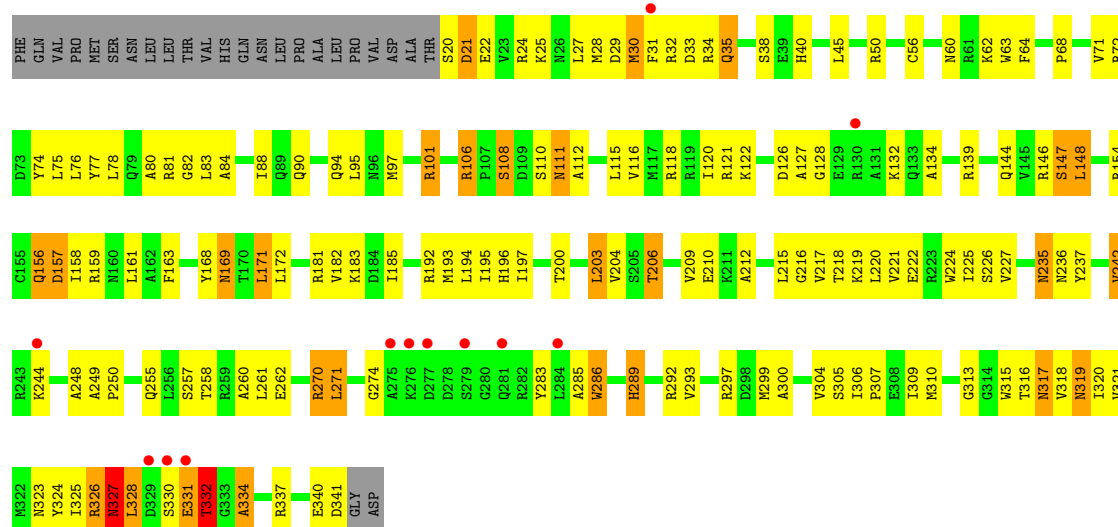
- Molecule 4: Cre recombinase

Chain A:



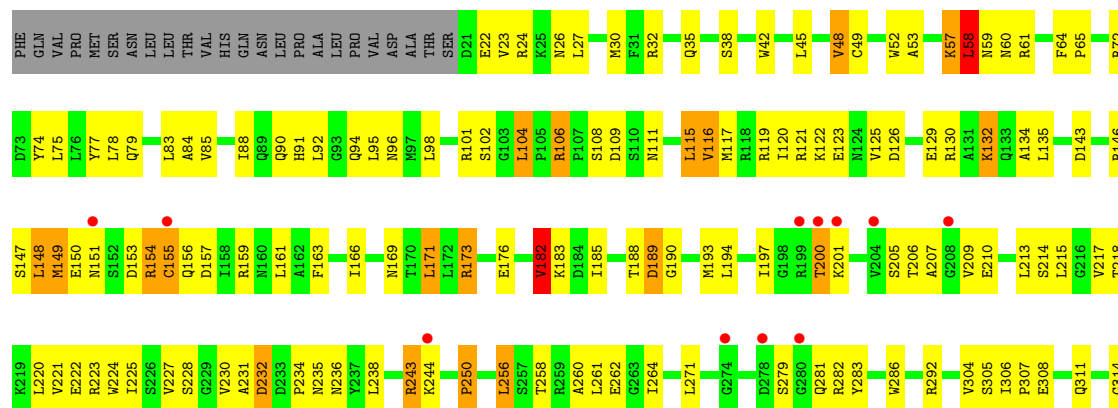
• Molecule 4: Cre recombinase

Chain B:



• Molecule 4: Cre recombinase

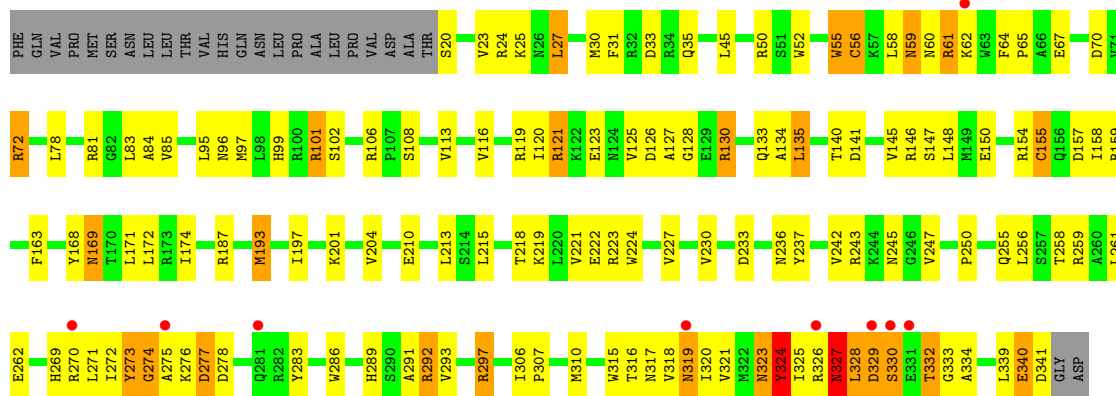
Chain E:





• Molecule 4: Cre recombinase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.94Å 164.16Å 194.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.91 29.92 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.92-2.91) 94.1 (29.92-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.276 0.246 , 0.267	Depositor DCC
R_{free} test set	3694 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	3 of 72511 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13296	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, A3P

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	0.51	0/316	0.85	1/483 (0.2%)
1	G	0.48	0/316	0.78	0/483
2	X	0.81	1/479 (0.2%)	1.18	3/738 (0.4%)
2	Y	0.49	0/479	0.76	0/738
3	D	0.53	0/848	0.79	0/1307
3	H	0.42	0/848	0.76	0/1307
4	A	0.47	0/2663	0.71	0/3595
4	B	0.39	0/2591	0.66	1/3493 (0.0%)
4	E	0.36	0/2585	0.62	0/3485
4	F	0.45	0/2591	0.69	2/3493 (0.1%)
All	All	0.45	1/13716 (0.0%)	0.72	7/19122 (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
3	D	0	2
3	H	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	116	DT	C5-C7	7.33	1.54	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	116	DT	C5'-C4'-O4'	14.52	136.88	109.30
4	F	324	TYR	CB-CG-CD2	7.57	125.54	121.00
2	X	116	DT	O4'-C1'-N1	6.89	112.83	108.00
4	B	327	ASN	N-CA-C	6.23	127.83	111.00
1	C	114	DA	C4'-C3'-C2'	6.16	108.64	103.10
2	X	116	DT	O4'-C1'-C2'	6.00	110.70	105.90
4	F	327	ASN	N-CA-C	5.48	125.79	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	107	DT	Sidechain
3	D	126	DA	Sidechain
3	H	124	DA	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	326	0	178	26	0
1	G	326	0	178	14	0
2	X	428	0	241	24	0
2	Y	428	0	241	25	0
3	D	756	0	421	38	0
3	H	756	0	421	34	0
4	A	2620	0	2643	113	0
4	B	2550	0	2570	170	0
4	E	2544	0	2566	157	0
4	F	2550	0	2570	133	0
5	C	1	0	0	1	0
5	F	1	0	0	0	0
6	A	5	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1	0	0	1	0
7	F	1	0	0	0	0
All	All	13296	0	12029	651	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (651) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:317:ASN:HD21	4:B:320:ILE:HG12	1.08	1.11
4:E:193:MET:HG3	4:E:218:THR:HG23	1.34	1.10
4:B:35:GLN:HA	4:B:35:GLN:HE21	1.10	1.07
1:C:105:DA:H2''	1:C:106:DC:H5''	1.33	1.06
3:H:105:DA:H2''	3:H:106:DC:H5''	1.39	1.04
4:A:72:ARG:HG3	4:A:116:VAL:HG21	1.38	1.02
4:A:15:PRO:HB2	4:A:18:ALA:HB3	1.43	1.00
4:B:315:TRP:HE1	4:B:324:TYR:HE2	1.08	0.97
4:E:200:THR:HG22	4:E:201:LYS:H	1.30	0.97
4:A:188:THR:HG22	4:A:190:GLY:H	1.25	0.96
3:D:132:DT:H2''	3:D:133:DT:H5''	1.46	0.96
4:E:169:ASN:ND2	4:E:213:LEU:HA	1.80	0.95
4:B:315:TRP:NE1	4:B:324:TYR:HE2	1.64	0.94
4:E:154:ARG:HB3	4:E:154:ARG:HH11	1.31	0.94
3:H:134:DA:H2''	3:H:135:DT:H5'	1.50	0.94
4:F:121:ARG:HG3	4:F:121:ARG:HH11	1.34	0.93
4:B:258:THR:HA	4:B:261:LEU:HD12	1.52	0.92
4:E:146:ARG:O	4:E:150:GLU:HB2	1.69	0.91
4:B:317:ASN:HD21	4:B:320:ILE:CG1	1.83	0.90
4:A:181:ARG:HH11	4:A:199:ARG:HH22	1.15	0.90
2:Y:131:DG:H2''	2:Y:132:DT:C5'	2.02	0.89
1:G:105:DA:H2''	1:G:106:DC:H5''	1.55	0.89
4:A:187:ARG:HH11	4:A:187:ARG:HB3	1.39	0.88
1:G:115:A3P:O2P	2:Y:116:DT:H5'	1.75	0.87
4:A:106:ARG:O	4:A:109:ASP:HB2	1.74	0.87
4:A:72:ARG:CG	4:A:116:VAL:HG21	2.05	0.86
2:Y:122:DC:H2''	2:Y:123:DT:H5'	1.57	0.86
4:E:188:THR:HG22	4:E:190:GLY:H	1.41	0.85
1:C:105:DA:C2'	1:C:106:DC:H5''	2.06	0.85
2:X:116:DT:H2''	2:X:117:DG:OP2	1.76	0.84
3:H:105:DA:C2'	3:H:106:DC:H5''	2.06	0.84
4:B:236:ASN:ND2	4:B:250:PRO:HB3	1.93	0.83
3:H:106:DC:H2'	3:H:107:DT:H72	1.61	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:185:ILE:HD13	4:B:193:MET:CE	2.09	0.82
4:B:317:ASN:ND2	4:B:320:ILE:HG12	1.92	0.82
4:F:320:ILE:HD12	4:F:320:ILE:H	1.45	0.82
2:Y:131:DG:H2''	2:Y:132:DT:H5'	1.62	0.81
4:A:59:ASN:O	4:A:61:ARG:HD3	1.79	0.81
4:E:48:VAL:HB	7:E:344:HOH:O	1.79	0.80
4:E:121:ARG:O	4:E:125:VAL:HG12	1.82	0.79
4:E:148:LEU:O	4:E:149:MET:HB2	1.82	0.79
4:E:271:LEU:HD23	4:E:271:LEU:O	1.82	0.79
4:A:15:PRO:CB	4:A:18:ALA:HB3	2.11	0.79
4:E:317:ASN:HD22	4:E:317:ASN:H	1.29	0.79
4:B:35:GLN:HA	4:B:35:GLN:NE2	1.92	0.79
3:D:105:DA:H2''	3:D:106:DC:O5'	1.82	0.79
4:E:173:ARG:HG2	4:E:173:ARG:HH11	1.48	0.79
4:B:154:ARG:HB2	4:B:157:ASP:HB2	1.65	0.78
4:E:316:THR:HG23	4:E:317:ASN:ND2	1.99	0.77
3:H:134:DA:H2''	3:H:135:DT:C5'	2.14	0.77
4:E:169:ASN:HD22	4:E:213:LEU:HA	1.48	0.77
4:E:48:VAL:HG21	4:E:91:HIS:HA	1.66	0.77
4:B:315:TRP:NE1	4:B:324:TYR:CE2	2.51	0.76
4:B:215:LEU:O	4:B:218:THR:HG22	1.86	0.76
4:B:328:LEU:O	4:B:332:THR:HG23	1.86	0.76
4:E:243:ARG:HG2	4:E:243:ARG:HH11	1.52	0.75
4:E:122:LYS:O	4:E:126:ASP:HB2	1.84	0.75
4:E:166:ILE:HG12	4:E:213:LEU:HD11	1.68	0.75
2:Y:131:DG:H2''	2:Y:132:DT:H5''	1.66	0.74
4:B:206:THR:HG22	4:E:130:ARG:HA	1.68	0.74
4:B:134:ALA:HA	4:B:283:TYR:CD2	2.22	0.74
4:E:148:LEU:HD23	4:E:148:LEU:H	1.52	0.74
2:X:117:DG:OP2	4:B:320:ILE:HG13	1.86	0.73
2:X:118:DT:H73	4:B:319:ASN:HB3	1.70	0.73
3:D:122:DT:H5''	4:B:97:MET:HE2	1.70	0.73
3:H:102:DA:H2''	3:H:103:DT:O5'	1.88	0.73
4:A:72:ARG:HD2	4:A:116:VAL:HG21	1.71	0.73
4:E:200:THR:HG21	4:E:205:SER:HB2	1.70	0.73
4:E:193:MET:CG	4:E:218:THR:HG23	2.17	0.73
4:A:72:ARG:CD	4:A:116:VAL:HG21	2.17	0.72
2:X:117:DG:H2''	2:X:118:DT:H5'	1.71	0.72
2:Y:122:DC:H2''	2:Y:123:DT:C5'	2.20	0.72
2:Y:117:DG:H5''	4:F:320:ILE:HD11	1.71	0.72
4:E:171:LEU:HD23	4:E:171:LEU:N	2.05	0.71
4:F:230:VAL:HG12	4:F:250:PRO:HB3	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:117:DG:H5'	4:B:316:THR:OG1	1.89	0.71
4:A:15:PRO:HB2	4:A:18:ALA:CB	2.18	0.71
4:B:315:TRP:CZ2	4:B:324:TYR:CD2	2.78	0.71
4:B:326:ARG:HH11	4:B:326:ARG:HG3	1.55	0.71
4:A:193:MET:HG3	4:A:218:THR:HG23	1.72	0.71
1:C:104:DA:O4'	4:B:244:LYS:HE3	1.91	0.71
4:E:183:LYS:HG2	4:E:234:PRO:HB2	1.72	0.71
4:F:219:LYS:HD3	4:F:222:GLU:OE1	1.91	0.71
2:Y:118:DT:H71	4:F:319:ASN:ND2	2.06	0.70
4:A:307:PRO:HG3	4:B:306:ILE:CD1	2.21	0.70
4:E:209:VAL:O	4:E:210:GLU:HG3	1.91	0.70
4:F:328:LEU:HD12	4:F:328:LEU:H	1.56	0.70
4:A:326:ARG:HD3	4:F:210:GLU:HG3	1.74	0.70
4:B:320:ILE:O	4:B:323:ASN:HB2	1.92	0.69
2:Y:117:DG:H3'	4:F:317:ASN:HB2	1.74	0.69
4:B:325:ILE:O	4:B:326:ARG:HG3	1.91	0.69
4:B:315:TRP:CZ2	4:B:324:TYR:CE2	2.80	0.69
3:H:106:DC:H2'	3:H:107:DT:C7	2.22	0.69
4:E:154:ARG:NH1	4:E:154:ARG:HB3	2.06	0.69
4:E:193:MET:HG3	4:E:218:THR:CG2	2.20	0.69
4:E:305:SER:OG	4:E:308:GLU:HG3	1.91	0.69
4:F:243:ARG:HG2	4:F:243:ARG:HH11	1.58	0.68
4:F:174:ILE:HD12	4:F:258:THR:HB	1.74	0.68
3:D:132:DT:C2'	3:D:133:DT:H5''	2.22	0.68
4:A:297:ARG:HH12	4:A:327:ASN:HD21	1.42	0.68
4:A:194:LEU:HD21	4:A:210:GLU:OE1	1.93	0.68
4:F:245:ASN:OD1	4:F:247:VAL:HG23	1.93	0.68
4:E:182:VAL:HG23	4:E:234:PRO:O	1.94	0.68
4:A:161:LEU:HD22	4:A:220:LEU:CD1	2.23	0.68
1:C:111:DT:P	4:B:50:ARG:HH12	2.17	0.67
4:A:207:ALA:HB2	4:A:314:GLY:HA3	1.76	0.67
4:B:194:LEU:HD13	4:B:212:ALA:HB2	1.74	0.67
4:F:215:LEU:O	4:F:218:THR:HG22	1.93	0.67
4:B:163:PHE:CE1	4:B:261:LEU:HD22	2.30	0.67
4:A:305:SER:HB2	4:A:307:PRO:HD2	1.77	0.67
3:H:108:DT:H2''	3:H:109:DC:C5'	2.25	0.67
4:F:121:ARG:NH1	4:F:121:ARG:HG3	2.10	0.67
4:E:58:LEU:HD12	4:E:58:LEU:O	1.95	0.67
4:E:116:VAL:O	4:E:119:ARG:HB3	1.95	0.67
4:E:74:TYR:CE1	4:E:78:LEU:HD11	2.30	0.66
4:F:121:ARG:CG	4:F:121:ARG:HH11	2.08	0.66
4:E:53:ALA:O	4:E:57:LYS:HD3	1.94	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:130:ARG:HH11	4:F:130:ARG:HB3	1.60	0.66
3:D:116:DC:OP1	3:D:116:DC:H4'	1.96	0.65
4:F:258:THR:O	4:F:262:GLU:HG3	1.95	0.65
4:B:147:SER:O	4:B:148:LEU:HB2	1.95	0.65
4:E:317:ASN:N	4:E:317:ASN:HD22	1.94	0.65
3:D:120:DC:H3'	4:B:106:ARG:HH21	1.59	0.65
1:G:105:DA:C2'	1:G:106:DC:H5''	2.26	0.65
3:D:119:DA:P	4:B:121:ARG:HH12	2.20	0.65
4:E:134:ALA:HA	4:E:283:TYR:CD2	2.33	0.64
4:B:204:VAL:HG22	4:E:125:VAL:HG11	1.78	0.64
4:A:14:LEU:HG	4:A:27:LEU:CD2	2.28	0.64
4:E:117:MET:HE3	4:E:120:ILE:HD12	1.79	0.64
4:B:315:TRP:CE2	4:B:324:TYR:CE2	2.85	0.64
1:C:103:DT:H2''	1:C:104:DA:C8	2.33	0.64
4:F:145:VAL:HG22	4:F:272:ILE:HD11	1.80	0.63
4:A:310:MET:SD	4:A:318:VAL:HG12	2.38	0.63
1:C:108:DT:H2''	1:C:109:DC:H5'	1.80	0.63
4:A:243:ARG:HH11	4:A:243:ARG:HG2	1.64	0.63
4:E:90:GLN:HE21	4:E:94:GLN:HG2	1.63	0.63
4:A:134:ALA:HA	4:A:283:TYR:CD2	2.33	0.63
4:E:230:VAL:CG1	4:E:236:ASN:HB3	2.29	0.63
4:B:30:MET:SD	4:B:101:ARG:HG2	2.39	0.63
4:F:204:VAL:O	4:F:204:VAL:HG13	1.97	0.63
4:F:78:LEU:HD22	4:F:83:LEU:CD1	2.29	0.63
4:E:26:ASN:HB3	4:E:102:SER:HA	1.81	0.63
4:A:187:ARG:NH2	4:A:222:GLU:OE2	2.31	0.62
4:B:330:SER:C	4:B:332:THR:H	2.02	0.62
4:A:245:ASN:OD1	4:A:247:VAL:HB	1.99	0.62
4:E:74:TYR:O	4:E:77:TYR:HB3	2.00	0.62
4:F:325:ILE:CG2	4:F:327:ASN:ND2	2.62	0.62
4:B:204:VAL:O	4:B:204:VAL:HG13	1.99	0.62
3:H:103:DT:H2''	3:H:104:DA:C8	2.34	0.62
4:B:146:ARG:O	4:B:148:LEU:N	2.33	0.62
4:E:228:SER:OG	4:E:230:VAL:HG23	2.00	0.62
4:F:270:ARG:O	4:F:274:GLY:HA2	2.00	0.62
4:B:204:VAL:CG2	4:E:125:VAL:HG11	2.30	0.62
4:B:206:THR:HG22	4:E:130:ARG:CA	2.30	0.62
4:E:27:LEU:CD2	4:E:102:SER:HB3	2.30	0.62
4:A:192:ARG:HB3	4:A:215:LEU:HD23	1.81	0.62
4:E:230:VAL:HG22	4:E:250:PRO:HG3	1.82	0.61
4:E:159:ARG:HB2	4:E:224:TRP:CZ3	2.35	0.61
4:A:72:ARG:HD2	4:A:116:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:230:VAL:HG13	4:E:236:ASN:HB3	1.83	0.61
4:E:78:LEU:H	4:E:78:LEU:HD12	1.64	0.61
4:E:143:ASP:O	4:E:146:ARG:HG2	1.99	0.61
4:E:22:GLU:HG3	4:E:23:VAL:N	2.14	0.61
3:H:105:DA:H2''	3:H:106:DC:C5'	2.24	0.61
4:B:325:ILE:HG22	4:B:326:ARG:N	2.16	0.60
4:A:161:LEU:HD22	4:A:220:LEU:HD11	1.83	0.60
4:F:72:ARG:HD2	4:F:116:VAL:HB	1.82	0.60
4:E:217:VAL:O	4:E:221:VAL:HG23	2.02	0.60
4:E:169:ASN:HD21	4:E:213:LEU:HA	1.64	0.60
4:B:325:ILE:HG22	4:B:327:ASN:H	1.66	0.60
4:E:279:SER:OG	4:E:281:GLN:HG3	2.00	0.60
2:Y:117:DG:H2'	2:Y:118:DT:H72	1.84	0.60
4:E:306:ILE:N	4:E:307:PRO:HD2	2.16	0.60
4:E:318:VAL:O	4:E:322:MET:HG2	2.02	0.60
4:B:317:ASN:ND2	4:B:320:ILE:CG1	2.56	0.60
4:F:126:ASP:C	4:F:128:GLY:H	2.05	0.60
4:A:161:LEU:HD13	4:A:220:LEU:HD11	1.83	0.59
4:E:117:MET:HA	4:E:117:MET:CE	2.32	0.59
4:B:74:TYR:O	4:B:77:TYR:HB3	2.01	0.59
4:A:72:ARG:NH1	4:F:33:ASP:OD2	2.36	0.59
4:A:243:ARG:NH1	4:A:243:ARG:HG2	2.17	0.59
4:B:172:LEU:HD21	4:B:197:ILE:HG13	1.85	0.59
4:E:304:VAL:HG12	4:E:308:GLU:HB2	1.84	0.59
3:H:124:DA:H5'	4:F:201:LYS:HG3	1.85	0.59
1:C:115:A3P:O2P	2:X:116:DT:H5'	2.02	0.59
4:B:159:ARG:HB2	4:B:224:TRP:CZ3	2.37	0.59
4:E:35:GLN:HB2	4:F:119:ARG:HD2	1.84	0.59
4:B:325:ILE:HG21	4:B:327:ASN:HD22	1.67	0.59
3:D:108:DT:H2''	3:D:109:DC:H5'	1.84	0.58
4:B:310:MET:HG2	4:B:321:VAL:HG21	1.84	0.58
4:F:148:LEU:HD23	4:F:148:LEU:O	2.03	0.58
4:F:146:ARG:O	4:F:150:GLU:HB2	2.03	0.58
4:A:306:ILE:HB	4:A:307:PRO:HD3	1.86	0.58
4:F:233:ASP:HB3	4:F:236:ASN:ND2	2.19	0.58
4:B:71:VAL:O	4:B:75:LEU:HG	2.03	0.58
4:E:154:ARG:CB	4:E:154:ARG:HH11	2.12	0.58
1:C:111:DT:OP1	4:B:50:ARG:NH1	2.37	0.58
4:E:200:THR:HG22	4:E:201:LYS:N	2.10	0.58
4:B:72:ARG:HG3	4:B:116:VAL:HG11	1.86	0.58
4:B:171:LEU:O	4:B:292:ARG:NH1	2.37	0.58
1:C:100:DC:H2'	1:C:101:DG:C8	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:78:LEU:HD22	4:F:83:LEU:HD12	1.86	0.57
4:F:25:LYS:O	4:F:25:LYS:HD3	2.04	0.57
1:C:115:A3P:C2'	2:X:116:DT:C5'	2.83	0.57
4:E:173:ARG:HG2	4:E:173:ARG:NH1	2.18	0.57
4:A:116:VAL:O	4:A:120:ILE:HG13	2.04	0.57
4:E:48:VAL:HG11	4:E:94:GLN:HB2	1.85	0.57
4:E:209:VAL:O	4:E:209:VAL:HG12	2.05	0.57
1:C:115:A3P:C2'	2:X:116:DT:H5''	2.34	0.57
3:H:117:DA:H2''	3:H:118:DT:H71	1.86	0.57
4:E:316:THR:HG23	4:E:317:ASN:HD22	1.70	0.57
4:E:111:ASN:O	4:E:115:LEU:HB2	2.03	0.57
4:F:67:GLU:HB3	4:F:70:ASP:OD2	2.05	0.57
1:C:114:DA:H5''	4:B:132:LYS:O	2.04	0.57
4:A:188:THR:HG22	4:A:190:GLY:N	2.09	0.57
4:E:183:LYS:HD3	4:E:235:ASN:ND2	2.19	0.57
4:B:148:LEU:O	4:B:148:LEU:HD13	2.04	0.57
4:E:32:ARG:HD2	4:F:72:ARG:HH21	1.69	0.57
4:F:121:ARG:CG	4:F:121:ARG:NH1	2.67	0.57
1:G:100:DC:H2''	1:G:101:DG:O5'	2.05	0.57
3:H:108:DT:C2'	3:H:109:DC:H5''	2.34	0.57
4:B:258:THR:O	4:B:262:GLU:HG3	2.05	0.56
4:E:96:ASN:ND2	4:E:108:SER:OG	2.36	0.56
4:F:325:ILE:HG21	4:F:327:ASN:ND2	2.20	0.56
4:B:236:ASN:HD21	4:B:250:PRO:HB3	1.70	0.56
4:F:163:PHE:CE1	4:F:261:LEU:HD13	2.39	0.56
4:E:78:LEU:HB3	4:E:83:LEU:HD12	1.87	0.56
2:X:117:DG:OP2	2:X:117:DG:H8	1.88	0.56
4:E:256:LEU:HD22	4:E:260:ALA:HB3	1.87	0.56
1:C:115:A3P:O1P	4:B:292:ARG:NH2	2.38	0.56
1:C:115:A3P:O1P	4:B:292:ARG:CZ	2.53	0.56
4:A:187:ARG:CB	4:A:187:ARG:HH11	2.14	0.56
4:F:60:ASN:C	4:F:61:ARG:HD3	2.26	0.56
3:H:108:DT:H2''	3:H:109:DC:H5''	1.86	0.55
3:D:134:DA:H2''	3:D:135:DT:O5'	2.05	0.55
4:B:330:SER:O	4:B:332:THR:N	2.38	0.55
4:F:242:VAL:HG23	4:F:242:VAL:O	2.06	0.55
4:A:204:VAL:HG23	4:B:326:ARG:NH2	2.21	0.55
4:B:31:PHE:O	4:B:34:ARG:HB3	2.06	0.55
4:B:325:ILE:HG21	4:B:327:ASN:ND2	2.22	0.55
4:A:121:ARG:O	4:A:125:VAL:HG23	2.05	0.55
4:A:169:ASN:OD1	4:A:213:LEU:HA	2.05	0.55
1:C:115:A3P:O1P	4:B:292:ARG:NE	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:317:ASN:N	4:E:317:ASN:ND2	2.55	0.55
4:E:74:TYR:CD1	4:E:78:LEU:HD11	2.41	0.55
4:A:307:PRO:HG3	4:B:306:ILE:HD11	1.89	0.55
4:B:106:ARG:HH12	4:B:108:SER:HB3	1.70	0.55
4:A:161:LEU:HD22	4:A:220:LEU:HD12	1.88	0.55
4:E:197:ILE:HG22	4:E:209:VAL:C	2.27	0.55
4:F:243:ARG:NH1	4:F:243:ARG:HG2	2.19	0.55
4:E:96:ASN:HD21	4:E:108:SER:HG	1.53	0.54
3:D:108:DT:H1'	3:D:109:DC:H5''	1.90	0.54
4:F:277:ASP:OD1	4:F:278:ASP:N	2.40	0.54
3:H:107:DT:H2''	3:H:108:DT:O5'	2.08	0.54
4:B:156:GLN:HB3	4:B:242:VAL:HG11	1.87	0.54
4:F:320:ILE:O	4:F:323:ASN:N	2.40	0.54
4:F:323:ASN:CG	4:F:324:TYR:N	2.60	0.54
3:D:119:DA:OP1	4:B:121:ARG:NH1	2.39	0.54
4:F:320:ILE:H	4:F:320:ILE:CD1	2.19	0.54
4:A:197:ILE:O	4:A:197:ILE:HG13	2.08	0.54
4:A:145:VAL:HG22	4:A:272:ILE:CD1	2.38	0.54
3:D:120:DC:H3'	4:B:106:ARG:NH2	2.23	0.53
4:B:313:GLY:HA3	4:B:315:TRP:CZ3	2.44	0.53
4:A:15:PRO:CG	4:A:18:ALA:HB3	2.38	0.53
4:E:78:LEU:N	4:E:78:LEU:HD12	2.23	0.53
2:X:135:DT:H2''	2:X:136:DC:OP2	2.08	0.53
4:E:215:LEU:HG	4:F:340:GLU:OE1	2.08	0.53
4:A:121:ARG:NH1	4:F:204:VAL:HG13	2.24	0.53
4:F:116:VAL:O	4:F:120:ILE:HG13	2.07	0.53
4:B:237:TYR:CE1	4:B:255:GLN:HG2	2.44	0.53
4:F:271:LEU:HD13	4:F:271:LEU:C	2.29	0.53
4:F:316:THR:HG22	4:F:316:THR:O	2.07	0.53
3:D:118:DT:H2''	3:D:119:DA:N7	2.24	0.53
4:E:72:ARG:HG3	4:E:116:VAL:HG11	1.91	0.53
4:E:117:MET:HE2	4:E:117:MET:HA	1.90	0.53
4:A:145:VAL:HG22	4:A:272:ILE:HD11	1.91	0.53
3:D:101:DG:H2''	3:D:102:DA:C8	2.44	0.53
4:A:161:LEU:HD13	4:A:220:LEU:CD1	2.39	0.53
1:C:107:UMP:OP2	4:B:257:SER:HB3	2.09	0.52
2:Y:131:DG:C2'	2:Y:132:DT:H5''	2.39	0.52
4:B:326:ARG:HG3	4:B:326:ARG:NH1	2.21	0.52
4:B:77:TYR:O	4:B:80:ALA:HB3	2.09	0.52
4:F:306:ILE:N	4:F:307:PRO:HD2	2.24	0.52
4:A:112:ALA:O	4:A:116:VAL:HG23	2.09	0.52
4:E:154:ARG:CB	4:E:154:ARG:NH1	2.71	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:108:DT:H2''	3:H:109:DC:H5'	1.91	0.52
2:Y:117:DG:H5'	4:F:316:THR:HB	1.91	0.52
2:Y:117:DG:C8	2:Y:118:DT:H72	2.44	0.52
4:E:159:ARG:HB2	4:E:224:TRP:CE3	2.44	0.52
4:F:58:LEU:O	4:F:58:LEU:HD23	2.09	0.52
3:D:115:DG:H2''	3:D:116:DC:C6	2.45	0.52
3:D:115:DG:H2''	3:D:116:DC:H6	1.75	0.52
4:A:277:ASP:OD1	4:A:278:ASP:N	2.43	0.52
4:E:163:PHE:CE2	4:E:261:LEU:HD22	2.45	0.52
3:D:103:DT:O2	4:A:244:LYS:HE3	2.09	0.52
3:D:112:DA:OP1	4:A:81:ARG:NH2	2.43	0.52
2:X:117:DG:H3'	4:B:317:ASN:HB3	1.92	0.52
4:B:182:VAL:HG23	4:B:236:ASN:O	2.09	0.52
4:E:79:GLN:NE2	4:E:120:ILE:HG23	2.25	0.52
4:A:192:ARG:NH1	4:B:331:GLU:HG2	2.25	0.52
4:E:154:ARG:C	4:E:156:GLN:H	2.13	0.51
4:B:97:MET:O	4:B:101:ARG:HB2	2.09	0.51
4:A:24:ARG:O	4:A:28:MET:HB2	2.10	0.51
4:E:116:VAL:O	4:E:120:ILE:HG13	2.10	0.51
2:X:135:DT:H2''	2:X:136:DC:C6	2.45	0.51
2:X:117:DG:OP2	2:X:117:DG:C8	2.63	0.51
4:A:187:ARG:NH1	4:A:187:ARG:HB3	2.17	0.51
4:E:258:THR:O	4:E:262:GLU:HG3	2.10	0.51
4:F:154:ARG:HD3	4:F:157:ASP:OD2	2.10	0.51
4:F:159:ARG:HB2	4:F:224:TRP:CZ3	2.46	0.51
4:F:64:PHE:HA	4:F:65:PRO:C	2.31	0.51
1:G:110:DG:H2''	1:G:111:DT:OP2	2.10	0.51
4:F:339:LEU:O	4:F:341:ASP:N	2.44	0.51
4:B:236:ASN:HD22	4:B:250:PRO:HB3	1.73	0.51
2:Y:118:DT:H3	3:H:119:DA:H61	1.57	0.51
4:A:202:THR:HG22	4:A:203:LEU:N	2.25	0.51
1:G:101:DG:H2''	1:G:102:DA:O5'	2.11	0.51
3:H:109:DC:H2''	3:H:110:DG:C8	2.46	0.51
2:X:117:DG:P	4:B:320:ILE:HG13	2.51	0.51
4:F:52:TRP:O	4:F:56:CYS:HB2	2.11	0.51
4:F:187:ARG:NH2	4:F:222:GLU:OE2	2.45	0.50
4:A:12:PRO:O	4:A:13:ALA:HB2	2.11	0.50
4:E:32:ARG:CZ	4:F:72:ARG:HE	2.25	0.50
4:B:45:LEU:C	4:B:45:LEU:HD23	2.31	0.50
1:C:102:DA:H1'	1:C:103:DT:H5''	1.92	0.50
4:A:27:LEU:HD13	4:A:102:SER:HB2	1.93	0.50
1:G:111:DT:OP2	4:F:50:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:108:DT:H2''	1:G:109:DC:C5'	2.41	0.50
4:B:118:ARG:HG3	4:B:118:ARG:HH11	1.75	0.50
1:C:102:DA:H2''	1:C:103:DT:H5'	1.92	0.50
3:D:125:DT:H71	4:B:40:HIS:CD2	2.46	0.50
4:A:119:ARG:O	4:A:123:GLU:HG3	2.11	0.50
4:B:235:ASN:HD22	4:B:235:ASN:N	2.10	0.50
4:A:74:TYR:O	4:A:77:TYR:HB3	2.12	0.50
4:E:197:ILE:HG23	4:E:197:ILE:O	2.11	0.50
4:A:168:TYR:HA	4:A:291:ALA:HB1	1.94	0.50
4:E:185:ILE:HG21	4:E:193:MET:CE	2.42	0.49
1:G:106:DC:H2''	1:G:107:UMP:O5'	2.12	0.49
4:F:320:ILE:HD12	4:F:320:ILE:N	2.22	0.49
4:B:299:MET:O	4:B:304:VAL:HG23	2.12	0.49
2:Y:123:DT:H3'	4:E:38:SER:OG	2.12	0.49
4:A:20:SER:O	4:A:21:ASP:HB2	2.11	0.49
4:B:270:ARG:HG2	4:B:274:GLY:O	2.12	0.49
3:D:117:DA:OP1	4:A:201:LYS:HD3	2.12	0.49
4:F:55:TRP:CD1	4:F:55:TRP:C	2.85	0.49
4:E:64:PHE:CD1	4:E:64:PHE:C	2.85	0.49
4:E:243:ARG:CG	4:E:243:ARG:HH11	2.22	0.49
4:F:30:MET:SD	4:F:101:ARG:HG2	2.51	0.49
3:D:124:DA:H2'	3:D:125:DT:C7	2.41	0.49
4:B:237:TYR:CZ	4:B:255:GLN:HG2	2.48	0.49
4:F:119:ARG:O	4:F:123:GLU:HG3	2.12	0.49
4:F:62:LYS:HB2	4:F:62:LYS:NZ	2.27	0.49
4:E:182:VAL:O	4:E:183:LYS:C	2.49	0.49
4:A:72:ARG:NH1	4:A:116:VAL:HG22	2.28	0.49
3:H:116:DC:OP1	4:E:292:ARG:NH2	2.45	0.49
4:A:107:PRO:O	4:A:108:SER:HB3	2.13	0.49
4:A:14:LEU:HB3	4:A:19:THR:OG1	2.13	0.49
4:E:23:VAL:HG23	4:E:24:ARG:N	2.27	0.49
4:F:147:SER:HA	4:F:150:GLU:OE2	2.13	0.49
4:E:132:LYS:NZ	4:E:132:LYS:HB3	2.28	0.49
4:B:194:LEU:CD1	4:B:212:ALA:HB2	2.42	0.48
4:E:221:VAL:O	4:E:225:ILE:HG13	2.13	0.48
4:E:161:LEU:HD23	4:E:220:LEU:HD21	1.94	0.48
4:A:19:THR:CG2	4:A:23:VAL:HG23	2.42	0.48
4:F:126:ASP:C	4:F:128:GLY:N	2.66	0.48
2:X:124:DA:H2'	2:X:125:DT:C7	2.43	0.48
4:F:146:ARG:O	4:F:150:GLU:N	2.43	0.48
4:F:96:ASN:HD21	4:F:108:SER:HB2	1.78	0.48
4:B:181:ARG:HD3	4:B:183:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:200:THR:OG1	4:B:203:LEU:HD23	2.13	0.48
4:B:216:GLY:O	4:B:219:LYS:HB3	2.13	0.48
4:E:117:MET:CE	4:E:120:ILE:HD12	2.43	0.48
4:B:227:VAL:O	4:B:227:VAL:HG12	2.13	0.48
4:F:134:ALA:HA	4:F:283:TYR:CD2	2.49	0.48
4:B:330:SER:C	4:B:332:THR:N	2.66	0.48
4:B:320:ILE:HA	4:B:323:ASN:HB2	1.96	0.48
4:E:213:LEU:HD22	4:E:213:LEU:N	2.29	0.48
4:F:163:PHE:HE1	4:F:261:LEU:HD13	1.79	0.48
4:F:158:ILE:HG12	4:F:223:ARG:NH1	2.29	0.48
4:F:297:ARG:NH1	4:F:297:ARG:HG2	2.28	0.48
4:B:78:LEU:HD22	4:B:83:LEU:HD12	1.96	0.48
4:A:158:ILE:HD11	4:A:223:ARG:NH2	2.29	0.48
4:A:158:ILE:HD11	4:A:223:ARG:CZ	2.44	0.47
4:F:27:LEU:O	4:F:31:PHE:HD1	1.95	0.47
4:E:304:VAL:CG1	4:E:308:GLU:HB2	2.43	0.47
4:E:261:LEU:HA	4:E:264:ILE:HD12	1.94	0.47
4:E:59:ASN:O	4:E:60:ASN:HB2	2.13	0.47
4:B:320:ILE:C	4:B:323:ASN:HB2	2.34	0.47
4:A:106:ARG:C	4:A:107:PRO:O	2.49	0.47
4:B:306:ILE:N	4:B:307:PRO:HD2	2.29	0.47
4:E:106:ARG:HG2	4:E:109:ASP:OD2	2.15	0.47
4:B:328:LEU:H	4:B:328:LEU:HD12	1.79	0.47
4:B:319:ASN:ND2	4:B:323:ASN:OD1	2.45	0.47
3:D:106:DC:H2"	3:D:107:DT:H5'	1.96	0.47
4:F:96:ASN:HD21	4:F:108:SER:CB	2.27	0.47
1:C:115:A3P:O2P	2:X:116:DT:C5'	2.62	0.47
4:E:26:ASN:CB	4:E:102:SER:HA	2.44	0.47
4:B:25:LYS:O	4:B:28:MET:N	2.48	0.47
4:B:221:VAL:O	4:B:225:ILE:HG13	2.14	0.47
4:E:231:ALA:O	4:E:232:ASP:C	2.53	0.47
4:B:317:ASN:OD1	4:B:319:ASN:HB3	2.15	0.47
1:C:109:DC:H2"	1:C:110:DG:C8	2.50	0.47
4:B:80:ALA:C	4:B:82:GLY:H	2.18	0.47
4:A:71:VAL:O	4:A:75:LEU:HG	2.15	0.47
3:D:107:DT:H2"	3:D:108:DT:H5'	1.96	0.47
4:E:23:VAL:HA	4:E:26:ASN:HD22	1.80	0.47
3:D:100:DG:H2"	3:D:101:DG:O5'	2.14	0.47
2:Y:125:DT:H2"	2:Y:126:DA:H5'	1.96	0.47
4:F:237:TYR:CE1	4:F:255:GLN:HB3	2.50	0.47
4:B:249:ALA:N	4:B:250:PRO:HD3	2.29	0.47
3:H:101:DG:H2"	3:H:102:DA:OP2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:200:IOD:I	4:B:260:ALA:HA	2.85	0.47
3:H:112:DA:H1'	3:H:113:DT:H5''	1.96	0.47
4:A:306:ILE:N	4:A:307:PRO:CD	2.77	0.46
4:A:27:LEU:HD13	4:A:102:SER:CB	2.45	0.46
4:B:192:ARG:NH1	4:E:340:GLU:OE2	2.49	0.46
4:A:307:PRO:HG3	4:B:306:ILE:HD13	1.97	0.46
1:C:110:DG:H2''	1:C:111:DT:OP2	2.15	0.46
4:B:94:GLN:HA	4:B:94:GLN:OE1	2.15	0.46
4:F:135:LEU:HD23	4:F:283:TYR:O	2.15	0.46
4:B:217:VAL:O	4:B:221:VAL:HG23	2.15	0.46
4:F:326:ARG:HH11	4:F:326:ARG:HG2	1.80	0.46
4:B:45:LEU:C	4:B:45:LEU:CD2	2.84	0.46
4:F:269:HIS:HB2	4:F:286:TRP:CE3	2.51	0.46
4:E:74:TYR:O	4:E:78:LEU:HD12	2.15	0.46
4:F:272:ILE:HB	4:F:273:TYR:CD1	2.51	0.46
4:E:92:LEU:HD23	4:E:92:LEU:O	2.16	0.46
4:B:22:GLU:O	4:B:25:LYS:N	2.48	0.46
4:F:20:SER:O	4:F:24:ARG:HG2	2.16	0.46
4:E:171:LEU:CD2	4:E:171:LEU:N	2.75	0.46
4:A:158:ILE:HD13	4:A:223:ARG:HG2	1.96	0.46
4:B:195:ILE:HG22	4:B:196:HIS:N	2.31	0.46
4:B:325:ILE:CG2	4:B:326:ARG:N	2.79	0.46
4:E:243:ARG:NH1	4:E:243:ARG:HG2	2.27	0.46
2:X:124:DA:H2'	2:X:125:DT:C6	2.51	0.46
4:F:168:TYR:HA	4:F:291:ALA:HB1	1.96	0.46
4:B:35:GLN:CA	4:B:35:GLN:HE21	1.98	0.46
4:B:106:ARG:HH11	4:B:106:ARG:HB2	1.80	0.46
4:F:273:TYR:CD1	4:F:273:TYR:N	2.84	0.46
4:F:97:MET:O	4:F:101:ARG:HB2	2.16	0.46
4:F:276:LYS:O	4:F:277:ASP:O	2.34	0.46
2:Y:134:DA:C8	2:Y:135:DT:H72	2.51	0.46
4:B:337:ARG:O	4:B:341:ASP:HB2	2.16	0.46
4:B:169:ASN:C	4:B:169:ASN:HD22	2.19	0.46
4:B:315:TRP:CE2	4:B:324:TYR:CD2	3.04	0.45
2:X:117:DG:C2'	2:X:118:DT:H5'	2.44	0.45
4:E:75:LEU:HA	4:E:78:LEU:HD13	1.97	0.45
2:X:118:DT:H73	4:B:319:ASN:CB	2.42	0.45
4:B:185:ILE:HD13	4:B:193:MET:HE1	1.95	0.45
3:D:105:DA:C2	3:D:106:DC:C2	3.04	0.45
4:B:226:SER:OG	4:B:227:VAL:N	2.49	0.45
4:B:161:LEU:HG	4:B:220:LEU:HD13	1.97	0.45
3:D:104:DA:H2''	3:D:105:DA:O5'	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:155:CYS:SG	4:E:227:VAL:HG12	2.56	0.45
4:E:305:SER:HB2	4:E:307:PRO:HD2	1.98	0.45
3:D:118:DT:H3'	4:B:121:ARG:NH1	2.32	0.45
4:F:169:ASN:HD22	4:F:169:ASN:C	2.20	0.45
4:F:81:ARG:HH11	4:F:81:ARG:HG3	1.81	0.45
3:D:114:DA:N7	4:A:86:LYS:HD2	2.31	0.45
4:B:62:LYS:HE3	4:B:62:LYS:HB2	1.78	0.45
4:E:42:TRP:CE3	4:E:45:LEU:HD23	2.52	0.45
4:B:33:ASP:C	4:B:35:GLN:N	2.70	0.45
2:Y:118:DT:H73	4:F:319:ASN:CG	2.37	0.45
4:E:282:ARG:O	4:E:283:TYR:HB2	2.16	0.45
4:B:270:ARG:HA	4:B:274:GLY:O	2.17	0.45
4:B:209:VAL:HG22	4:B:210:GLU:N	2.31	0.45
4:B:33:ASP:C	4:B:35:GLN:H	2.20	0.45
3:H:108:DT:H1'	3:H:109:DC:H5''	1.99	0.45
1:G:107:UMP:OP2	4:F:256:LEU:HD12	2.17	0.45
2:Y:118:DT:C7	4:F:319:ASN:ND2	2.76	0.45
4:E:154:ARG:H	4:E:154:ARG:HG2	1.48	0.44
3:D:106:DC:H2'	3:D:107:DT:H72	1.99	0.44
3:H:133:DT:H2''	3:H:134:DA:C8	2.53	0.44
4:E:306:ILE:N	4:E:307:PRO:CD	2.80	0.44
4:B:310:MET:HG2	4:B:321:VAL:CG2	2.47	0.44
4:F:60:ASN:O	4:F:61:ARG:HD3	2.17	0.44
4:F:297:ARG:HH11	4:F:297:ARG:HG2	1.81	0.44
4:E:207:ALA:HB2	4:E:314:GLY:HA3	2.00	0.44
4:B:320:ILE:CA	4:B:323:ASN:HB2	2.47	0.44
4:E:213:LEU:HD22	4:E:213:LEU:H	1.83	0.44
1:C:105:DA:H2''	1:C:106:DC:C5'	2.24	0.44
4:E:200:THR:HG21	4:E:205:SER:CB	2.43	0.44
4:E:78:LEU:HD21	4:E:91:HIS:ND1	2.33	0.44
4:A:20:SER:O	4:A:21:ASP:CB	2.65	0.44
4:B:22:GLU:O	4:B:25:LYS:HB3	2.17	0.44
4:A:299:MET:CE	4:B:334:ALA:HB1	2.48	0.44
4:B:218:THR:O	4:B:222:GLU:HG3	2.18	0.44
4:E:171:LEU:HD23	4:E:171:LEU:H	1.77	0.44
4:A:11:LEU:HD13	4:A:14:LEU:HD21	2.00	0.44
4:B:116:VAL:O	4:B:120:ILE:HG13	2.18	0.44
4:F:158:ILE:HG12	4:F:223:ARG:HH12	1.82	0.44
4:F:155:CYS:SG	4:F:227:VAL:HG12	2.57	0.44
2:Y:128:DG:H1	3:H:109:DC:H42	1.65	0.44
4:B:315:TRP:HZ2	4:B:324:TYR:CE2	2.32	0.44
4:A:92:LEU:HD22	4:A:96:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:108:DT:H1'	3:D:109:DC:C5'	2.47	0.44
4:F:215:LEU:C	4:F:218:THR:HG22	2.38	0.44
4:F:55:TRP:O	4:F:59:ASN:HB2	2.18	0.44
4:E:59:ASN:HB3	4:E:61:ARG:NH1	2.32	0.44
4:A:231:ALA:O	4:A:233:ASP:N	2.50	0.44
2:X:117:DG:C5'	4:B:316:THR:OG1	2.63	0.44
4:A:72:ARG:HH11	4:A:116:VAL:CG2	2.30	0.44
3:D:135:DT:H1'	4:B:244:LYS:HD3	1.98	0.44
4:A:14:LEU:HG	4:A:27:LEU:HD23	1.99	0.44
3:D:117:DA:OP1	4:A:201:LYS:CE	2.66	0.44
4:F:172:LEU:HD21	4:F:197:ILE:HG13	2.00	0.44
4:F:310:MET:HG3	4:F:321:VAL:HG21	1.99	0.44
4:A:193:MET:CE	4:A:221:VAL:HB	2.47	0.44
4:B:45:LEU:O	4:B:45:LEU:HD23	2.18	0.44
4:A:64:PHE:HA	4:A:65:PRO:C	2.39	0.44
4:E:188:THR:C	4:E:190:GLY:N	2.72	0.43
4:F:315:TRP:CZ2	4:F:324:TYR:CE1	3.05	0.43
4:E:65:PRO:HB3	4:E:104:LEU:HD21	1.99	0.43
4:E:169:ASN:OD1	4:F:339:LEU:HD12	2.18	0.43
4:A:181:ARG:HB2	4:A:236:ASN:O	2.18	0.43
1:G:105:DA:H4'	4:F:242:VAL:O	2.18	0.43
3:H:126:DA:OP2	4:F:262:GLU:OE2	2.36	0.43
4:A:72:ARG:HH12	4:F:33:ASP:CG	2.21	0.43
2:Y:131:DG:C2'	2:Y:132:DT:C5'	2.86	0.43
4:E:317:ASN:H	4:E:317:ASN:ND2	2.06	0.43
4:A:23:VAL:O	4:A:27:LEU:HB2	2.18	0.43
4:E:306:ILE:HG22	4:F:306:ILE:HD11	2.00	0.43
3:H:122:DT:C6	3:H:123:DT:H72	2.53	0.43
4:A:213:LEU:N	4:A:213:LEU:HD23	2.34	0.43
4:F:297:ARG:CG	4:F:297:ARG:HH11	2.30	0.43
4:B:122:LYS:O	4:B:126:ASP:HB2	2.18	0.43
3:D:124:DA:H2'	3:D:125:DT:H72	1.99	0.43
4:A:171:LEU:O	4:A:292:ARG:NH1	2.52	0.43
4:B:139:ARG:HB2	4:B:168:TYR:OH	2.19	0.43
4:F:171:LEU:O	4:F:292:ARG:HG3	2.18	0.43
4:B:29:ASP:O	4:B:32:ARG:HB3	2.19	0.43
4:B:110:SER:O	4:B:112:ALA:N	2.52	0.43
1:C:115:A3P:C2'	2:X:116:DT:H5'	2.49	0.43
4:F:272:ILE:HB	4:F:273:TYR:HD1	1.82	0.43
4:F:20:SER:HB3	4:F:23:VAL:HG23	2.01	0.43
4:A:72:ARG:HH11	4:A:116:VAL:HG22	1.84	0.43
4:E:200:THR:CG2	4:E:201:LYS:N	2.78	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:115:A3P:O3'	2:Y:116:DT:C5'	2.67	0.43
4:E:185:ILE:HG21	4:E:193:MET:HE1	2.01	0.43
4:E:74:TYR:O	4:E:78:LEU:CD1	2.67	0.43
4:F:126:ASP:O	4:F:128:GLY:N	2.51	0.43
4:B:159:ARG:HB2	4:B:224:TRP:CE3	2.54	0.43
4:A:277:ASP:HB3	4:A:284:LEU:HD13	2.00	0.43
4:F:340:GLU:O	4:F:341:ASP:C	2.57	0.43
4:F:121:ARG:O	4:F:125:VAL:HG23	2.18	0.43
3:D:133:DT:H2''	3:D:134:DA:C8	2.54	0.42
4:F:61:ARG:HG2	4:F:70:ASP:OD1	2.19	0.42
1:G:108:DT:H2''	1:G:109:DC:O5'	2.19	0.42
4:F:326:ARG:O	4:F:326:ARG:HG3	2.18	0.42
3:H:118:DT:H2''	3:H:119:DA:N7	2.33	0.42
4:E:243:ARG:NH1	4:E:243:ARG:CG	2.81	0.42
4:A:121:ARG:HH11	4:F:204:VAL:HG13	1.83	0.42
2:X:126:DA:OP2	4:A:262:GLU:OE1	2.38	0.42
3:H:122:DT:OP2	4:F:101:ARG:NH1	2.51	0.42
4:A:65:PRO:HG3	4:A:104:LEU:HD13	2.00	0.42
3:D:128:DG:H2''	3:D:129:DA:H5'	2.00	0.42
2:X:118:DT:C7	4:B:319:ASN:HB3	2.45	0.42
4:E:200:THR:CG2	4:E:201:LYS:H	2.11	0.42
4:F:329:ASP:O	4:F:330:SER:C	2.57	0.42
4:F:84:ALA:O	4:F:85:VAL:C	2.58	0.42
4:F:61:ARG:NH1	4:F:61:ARG:HG2	2.34	0.42
4:A:299:MET:HE2	4:A:309:ILE:HA	2.02	0.42
4:F:332:THR:HB	4:F:333:GLY:H	1.56	0.42
4:E:215:LEU:O	4:E:218:THR:HB	2.20	0.42
4:A:202:THR:HG22	4:A:204:VAL:H	1.85	0.42
4:E:57:LYS:O	4:E:58:LEU:HB2	2.20	0.42
4:E:119:ARG:O	4:E:123:GLU:HB2	2.20	0.42
4:E:92:LEU:HD21	4:E:108:SER:OG	2.18	0.42
4:E:317:ASN:HB3	4:E:319:ASN:OD1	2.18	0.42
4:B:154:ARG:O	4:B:158:ILE:HG12	2.20	0.42
4:F:270:ARG:HH11	4:F:270:ARG:HG3	1.85	0.42
4:A:141:ASP:O	4:A:145:VAL:HG23	2.20	0.42
4:B:118:ARG:HG3	4:B:118:ARG:NH1	2.35	0.42
3:H:129:DA:C8	3:H:129:DA:H5'	2.55	0.42
4:E:188:THR:C	4:E:190:GLY:H	2.23	0.42
3:H:123:DT:C2	3:H:124:DA:C8	3.08	0.42
4:A:268:THR:HG22	4:A:286:TRP:HZ3	1.84	0.42
4:B:20:SER:O	4:B:24:ARG:HD2	2.20	0.42
4:B:20:SER:OG	4:B:21:ASP:N	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:F:99:HIS:O	4:F:102:SER:HB2	2.19	0.42
4:B:90:GLN:HE21	4:B:94:GLN:HG2	1.85	0.42
4:E:235:ASN:HD22	4:E:235:ASN:N	2.18	0.41
3:D:119:DA:P	4:B:121:ARG:NH1	2.89	0.41
4:F:55:TRP:CD1	4:F:56:CYS:N	2.88	0.41
4:E:84:ALA:O	4:E:88:ILE:HG13	2.20	0.41
4:E:223:ARG:HH11	4:E:223:ARG:HG3	1.85	0.41
4:E:52:TRP:HZ3	4:E:74:TYR:HB2	1.85	0.41
4:E:78:LEU:CD1	4:E:78:LEU:H	2.30	0.41
4:A:215:LEU:HG	4:B:340:GLU:OE1	2.20	0.41
2:X:135:DT:H5'	2:X:135:DT:H6	1.85	0.41
4:F:140:THR:HG22	4:F:141:ASP:N	2.35	0.41
4:B:319:ASN:C	4:B:323:ASN:OD1	2.59	0.41
4:B:63:TRP:O	4:B:64:PHE:HB2	2.19	0.41
2:Y:119:DA:H2''	2:Y:120:DT:O5'	2.20	0.41
2:Y:135:DT:H2''	2:Y:136:DC:C6	2.55	0.41
4:B:111:ASN:O	4:B:115:LEU:HG	2.20	0.41
4:A:106:ARG:O	4:A:109:ASP:CB	2.57	0.41
4:A:318:VAL:HG13	4:B:318:VAL:HG11	2.02	0.41
4:A:22:GLU:C	4:A:24:ARG:N	2.72	0.41
4:B:76:LEU:HA	4:B:76:LEU:HD23	1.73	0.41
4:F:259:ARG:HD2	4:F:259:ARG:HA	1.89	0.41
4:B:305:SER:O	4:B:309:ILE:HG13	2.21	0.41
4:A:325:ILE:HB	4:A:328:LEU:HD12	2.03	0.41
3:H:134:DA:C8	3:H:135:DT:H72	2.56	0.41
4:E:57:LYS:H	4:E:57:LYS:CD	2.33	0.41
4:A:19:THR:HG23	4:A:23:VAL:HG23	2.01	0.41
4:F:145:VAL:O	4:F:145:VAL:HG12	2.20	0.41
4:E:323:ASN:HD22	4:E:323:ASN:HA	1.62	0.41
1:C:105:DA:H4'	4:B:242:VAL:O	2.20	0.41
4:B:185:ILE:HG21	4:B:193:MET:CE	2.51	0.41
4:E:173:ARG:CG	4:E:173:ARG:NH1	2.81	0.41
3:H:113:DT:H2''	3:H:114:DA:H8	1.86	0.41
3:D:123:DT:H3'	4:B:38:SER:HB2	2.03	0.41
4:F:193:MET:HE1	4:F:221:VAL:HG11	2.03	0.41
4:E:49:CYS:SG	4:E:98:LEU:HD22	2.61	0.41
4:B:289:HIS:CD2	4:B:292:ARG:HD3	2.56	0.41
1:C:106:DC:H2''	1:C:107:UMP:H6	1.86	0.41
1:G:106:DC:H2''	1:G:107:UMP:C6	2.56	0.41
4:A:92:LEU:HD21	4:A:108:SER:HB2	2.02	0.41
4:E:173:ARG:O	4:E:176:GLU:HB2	2.21	0.41
4:A:204:VAL:O	4:A:204:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:206:THR:HG21	4:E:129:GLU:HG2	2.03	0.41
4:F:272:ILE:C	4:F:273:TYR:CD1	2.95	0.41
4:E:64:PHE:HA	4:E:65:PRO:C	2.41	0.41
4:B:227:VAL:O	4:B:227:VAL:CG1	2.68	0.41
4:F:333:GLY:O	4:F:334:ALA:HB3	2.21	0.41
4:F:193:MET:HB3	4:F:213:LEU:HD12	2.03	0.41
4:B:327:ASN:OD1	4:B:328:LEU:HD12	2.20	0.41
4:E:222:GLU:O	4:E:223:ARG:C	2.60	0.41
4:B:84:ALA:O	4:B:88:ILE:HG13	2.21	0.41
4:E:154:ARG:C	4:E:156:GLN:N	2.74	0.40
4:F:163:PHE:CZ	4:F:261:LEU:HB3	2.56	0.40
4:B:285:ALA:O	4:B:286:TRP:C	2.59	0.40
4:B:319:ASN:ND2	4:B:319:ASN:O	2.55	0.40
4:A:318:VAL:O	4:A:319:ASN:C	2.59	0.40
4:B:74:TYR:CZ	4:B:78:LEU:HD11	2.56	0.40
3:D:124:DA:H8	3:D:124:DA:H5'	1.87	0.40
4:B:297:ARG:O	4:B:300:ALA:N	2.53	0.40
4:A:95:LEU:HD12	4:A:95:LEU:HA	1.79	0.40
4:E:85:VAL:HG23	4:E:129:GLU:OE2	2.21	0.40
4:A:207:ALA:HA	4:A:314:GLY:HA2	2.03	0.40
1:C:100:DC:C2'	1:C:101:DG:C8	3.05	0.40
4:A:15:PRO:HB2	4:A:18:ALA:H	1.86	0.40
4:A:217:VAL:O	4:A:221:VAL:HG23	2.20	0.40
4:F:27:LEU:HD12	4:F:27:LEU:HA	1.82	0.40
2:Y:117:DG:O6	3:H:120:DC:N3	2.54	0.40
4:B:325:ILE:C	4:B:326:ARG:HG3	2.41	0.40
4:E:197:ILE:HG12	4:E:197:ILE:O	2.21	0.40
4:F:113:VAL:O	4:F:116:VAL:HG12	2.21	0.40
3:H:123:DT:O2	4:F:201:LYS:HE2	2.22	0.40
4:A:186:SER:OG	4:A:196:HIS:HE1	2.05	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	
4	A	330/347 (95%)	297 (90%)	25 (8%)	8 (2%)	9	34
4	B	320/347 (92%)	265 (83%)	39 (12%)	16 (5%)	3	10
4	E	319/347 (92%)	265 (83%)	42 (13%)	12 (4%)	5	18
4	F	320/347 (92%)	278 (87%)	32 (10%)	10 (3%)	7	25
All	All	1289/1388 (93%)	1105 (86%)	138 (11%)	46 (4%)	5	21

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	13	ALA
4	A	182	VAL
4	B	148	LEU
4	B	248	ALA
4	B	327	ASN
4	E	58	LEU
4	E	147	SER
4	E	149	MET
4	E	182	VAL
4	E	232	ASP
4	F	277	ASP
4	F	327	ASN
4	F	328	LEU
4	F	330	SER
4	A	21	ASP
4	A	214	SER
4	A	232	ASP
4	A	279	SER
4	B	81	ARG
4	B	111	ASN
4	B	286	TRP
4	B	328	LEU
4	B	331	GLU
4	E	155	CYS
4	F	59	ASN
4	F	275	ALA
4	F	340	GLU
4	B	128	GLY
4	B	147	SER
4	B	271	LEU
4	B	332	THR
4	B	334	ALA
4	E	286	TRP

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Mol	Chain	Res	Type
4	F	324	TYR
4	A	206	THR
4	E	200	THR
4	E	214	SER
4	E	244	LYS
4	F	127	ALA
4	B	127	ALA
4	B	326	ARG
4	E	189	ASP
4	E	250	PRO
4	F	274	GLY
4	B	68	PRO
4	A	12	PRO

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	
4	A	277/291 (95%)	249 (90%)	28 (10%)	11	32
4	B	269/291 (92%)	243 (90%)	26 (10%)	12	34
4	E	268/291 (92%)	237 (88%)	31 (12%)	8	23
4	F	269/291 (92%)	242 (90%)	27 (10%)	11	32
All	All	1083/1164 (93%)	971 (90%)	112 (10%)	10	30

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	24	ARG
4	A	34	ARG
4	A	61	ARG
4	A	89	GLN
4	A	92	LEU
4	A	95	LEU
4	A	98	LEU
4	A	101	ARG
4	A	106	ARG

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Mol	Chain	Res	Type
4	A	109	ASP
4	A	130	ARG
4	A	140	THR
4	A	155	CYS
4	A	161	LEU
4	A	169	ASN
4	A	186	SER
4	A	187	ARG
4	A	203	LEU
4	A	222	GLU
4	A	238	LEU
4	A	244	LYS
4	A	247	VAL
4	A	277	ASP
4	A	278	ASP
4	A	289	HIS
4	A	311	GLN
4	A	316	THR
4	A	321	VAL
4	B	21	ASP
4	B	27	LEU
4	B	30	MET
4	B	35	GLN
4	B	56	CYS
4	B	60	ASN
4	B	95	LEU
4	B	101	ARG
4	B	106	ARG
4	B	108	SER
4	B	144	GLN
4	B	156	GLN
4	B	157	ASP
4	B	169	ASN
4	B	171	LEU
4	B	203	LEU
4	B	206	THR
4	B	235	ASN
4	B	242	VAL
4	B	270	ARG
4	B	271	LEU
4	B	289	HIS
4	B	293	VAL

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Mol	Chain	Res	Type
4	B	317	ASN
4	B	319	ASN
4	B	332	THR
4	E	30	MET
4	E	48	VAL
4	E	57	LYS
4	E	58	LEU
4	E	95	LEU
4	E	101	ARG
4	E	104	LEU
4	E	106	ARG
4	E	115	LEU
4	E	116	VAL
4	E	132	LYS
4	E	135	LEU
4	E	148	LEU
4	E	151	ASN
4	E	153	ASP
4	E	154	ARG
4	E	157	ASP
4	E	171	LEU
4	E	173	ARG
4	E	182	VAL
4	E	189	ASP
4	E	194	LEU
4	E	206	THR
4	E	238	LEU
4	E	243	ARG
4	E	256	LEU
4	E	311	GLN
4	E	316	THR
4	E	317	ASN
4	E	323	ASN
4	E	338	LEU
4	F	27	LEU
4	F	35	GLN
4	F	45	LEU
4	F	55	TRP
4	F	56	CYS
4	F	61	ARG
4	F	72	ARG
4	F	95	LEU

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Mol	Chain	Res	Type
4	F	101	ARG
4	F	106	ARG
4	F	121	ARG
4	F	130	ARG
4	F	133	GLN
4	F	135	LEU
4	F	155	CYS
4	F	169	ASN
4	F	193	MET
4	F	273	TYR
4	F	289	HIS
4	F	292	ARG
4	F	293	VAL
4	F	297	ARG
4	F	318	VAL
4	F	319	ASN
4	F	323	ASN
4	F	329	ASP
4	F	332	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	40	HIS
4	A	89	GLN
4	A	90	GLN
4	A	96	ASN
4	A	133	GLN
4	A	196	HIS
4	A	255	GLN
4	A	311	GLN
4	B	35	GLN
4	B	40	HIS
4	B	60	ASN
4	B	90	GLN
4	B	133	GLN
4	B	156	GLN
4	B	235	ASN
4	B	236	ASN
4	B	255	GLN
4	E	26	ASN
4	E	35	GLN

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Mol	Chain	Res	Type
4	E	89	GLN
4	E	90	GLN
4	E	94	GLN
4	E	96	ASN
4	E	144	GLN
4	E	169	ASN
4	E	235	ASN
4	E	317	ASN
4	E	323	ASN
4	F	35	GLN
4	F	94	GLN
4	F	96	ASN
4	F	133	GLN
4	F	281	GLN
4	F	319	ASN
4	F	327	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 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	C	107	1,3	18,20,21	0.89	1 (5%)	20,28,31	0.72	0
1	A3P	C	115	1,3,4	21,26,29	1.56	2 (9%)	27,37,45	2.60	3 (11%)
1	UMP	G	107	1,3	18,20,21	0.69	0	20,28,31	0.75	0
1	A3P	G	115	1,3,4	21,26,29	1.11	1 (4%)	27,37,45	2.25	2 (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	C	107	1,3	-	0/5/21/22	0/2/2/2
1	A3P	C	115	1,3,4	-	0/10/25/31	0/1/3/3
1	UMP	G	107	1,3	-	0/5/21/22	0/2/2/2
1	A3P	G	115	1,3,4	-	0/10/25/31	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	A3P	C4'-C3'	-4.42	1.48	1.53
1	C	115	A3P	C2'-C3'	-4.01	1.50	1.52
1	C	107	UMP	P-OP1	2.66	1.49	1.46
1	G	115	A3P	C2'-C3'	-2.47	1.51	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	A3P	C2'-C1'-N9	11.96	126.12	113.39
1	G	115	A3P	C2'-C1'-N9	10.31	124.37	113.39
1	C	115	A3P	O3'-C3'-C4'	-3.55	101.51	112.48
1	C	115	A3P	P1-O3'-C3'	-2.57	110.77	122.32
1	G	115	A3P	P2-O5'-C5'	-2.23	114.48	123.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	16/16 (100%)	-0.08	0 100 100	39, 69, 89, 93	0
1	G	16/16 (100%)	-0.29	0 100 100	43, 61, 114, 131	0
2	X	21/21 (100%)	0.03	0 100 100	35, 56, 95, 99	0
2	Y	21/21 (100%)	0.19	2 (9%) 8 11	49, 77, 115, 120	0
3	D	37/37 (100%)	-0.19	0 100 100	34, 57, 92, 96	0
3	H	37/37 (100%)	-0.25	0 100 100	44, 74, 104, 115	0
4	A	332/347 (95%)	-0.18	6 (1%) 65 75	29, 54, 93, 134	0
4	B	322/347 (92%)	0.12	12 (3%) 39 46	42, 73, 104, 139	0
4	E	321/347 (92%)	0.14	11 (3%) 43 51	48, 82, 114, 150	0
4	F	322/347 (92%)	-0.01	9 (2%) 50 59	36, 65, 99, 139	0
All	All	1445/1536 (94%)	0.00	40 (2%) 50 59	29, 69, 106, 150	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	330	SER	8.8
4	F	331	GLU	6.5
4	B	330	SER	6.2
4	F	329	ASP	4.5
4	B	331	GLU	3.9
4	B	329	ASP	3.8
4	F	319	ASN	3.7
4	E	155	CYS	3.6
4	E	278	ASP	3.4
4	F	326	ARG	3.3
4	E	201	LYS	3.0
4	E	274	GLY	3.0
4	B	277	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	E	208	GLY	2.8
2	Y	117	DG	2.8
4	B	275	ALA	2.8
4	A	201	LYS	2.7
4	E	204	VAL	2.7
4	E	244	LYS	2.7
4	F	275	ALA	2.6
4	E	199	ARG	2.5
4	F	62	LYS	2.4
4	B	244	LYS	2.4
4	A	202	THR	2.4
4	F	281	GLN	2.4
4	F	270	ARG	2.3
4	B	31	PHE	2.3
4	B	130	ARG	2.3
4	A	203	LEU	2.3
4	A	196	HIS	2.2
4	B	279	SER	2.2
4	A	278	ASP	2.2
4	B	284	LEU	2.2
4	E	151	ASN	2.2
4	B	276	LYS	2.2
4	B	281	GLN	2.1
4	E	200	THR	2.1
4	A	19	THR	2.1
4	E	280	GLY	2.1
2	Y	119	DA	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	A3P	C	115	24/27	0.24	0.36	42,55,81,83	0
1	UMP	G	107	19/20	0.17	-0.02	58,62,66,67	0
1	A3P	G	115	24/27	0.18	-0.34	31,40,73,74	0
1	UMP	C	107	19/20	0.15	-1.18	61,69,75,78	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	IOD	C	200	1/1	0.20	324259173170677.00	74,74,74,74	1
6	MG	D	310	1/1	0.53	82.97	47,47,47,47	1
6	MG	A	346	1/1	0.55	37.33	50,50,50,50	0
6	MG	F	345	1/1	0.78	32.20	69,69,69,69	0
6	MG	A	345	1/1	0.21	5.77	47,47,47,47	0
6	MG	A	347	1/1	0.36	4.78	49,49,49,49	0
6	MG	A	344	1/1	0.39	4.07	51,51,51,51	0
6	MG	A	348	1/1	0.18	1.50	44,44,44,44	1
5	IOD	F	344	1/1	0.17	1.00	73,73,73,73	1

6.5 Other polymers ⓘ

There are no such residues in this entry.