



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:33 am BST

PDB ID : 1OUQ
Title : Crystal structure of wild-type Cre recombinase-loxP synapse
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Deposited on : 2003-03-25
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

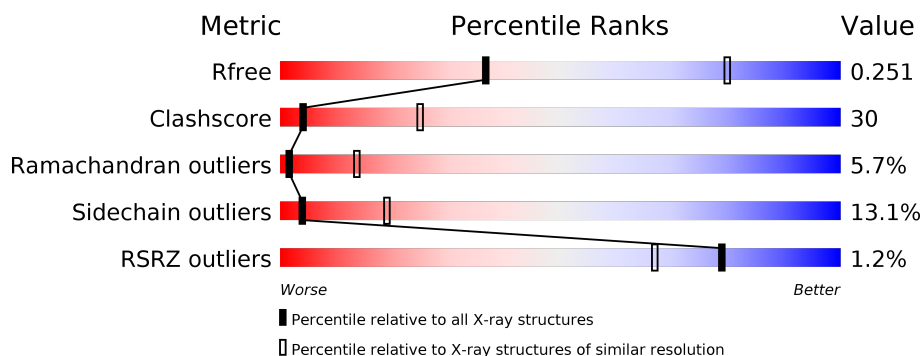
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	16	<div> <div>44%</div> <div>56%</div> </div>
1	G	16	<div> <div>50%</div> <div>38%</div> <div>13%</div> </div>
2	X	21	<div> <div>19%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div>
2	Y	21	<div> <div>14%</div> <div>38%</div> <div>43%</div> <div>19%</div> </div>
3	D	37	<div> <div>22%</div> <div>65%</div> <div>14%</div> </div>
3	H	37	<div> <div>35%</div> <div>62%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	A	343	
4	B	343	
4	E	343	
4	F	343	

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
6	MG	H	307	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13296 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	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			

- 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	H	1	Total Mg 1 1	0	0
6	A	4	Total Mg 4 4	0	0
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is water.

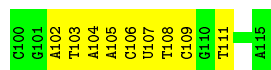
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total O 2 2	0	0
7	F	1	Total O 1 1	0	0

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: 



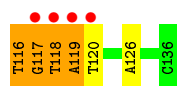
- Molecule 1: loxP DNA

Chain G: 



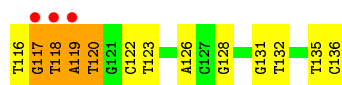
- Molecule 2: loxP DNA

Chain X: 



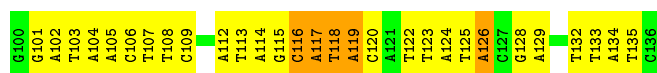
- Molecule 2: loxP DNA

Chain Y: 



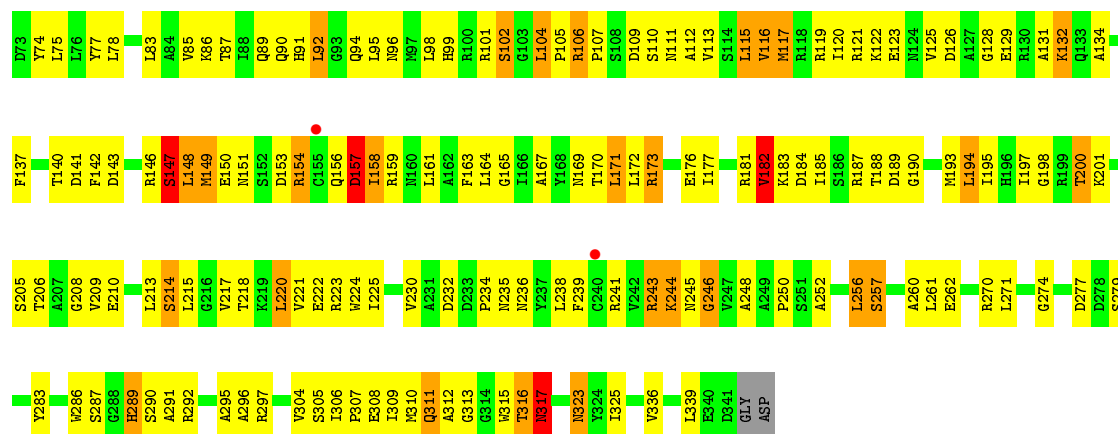
- Molecule 3: loxP DNA

Chain D: 

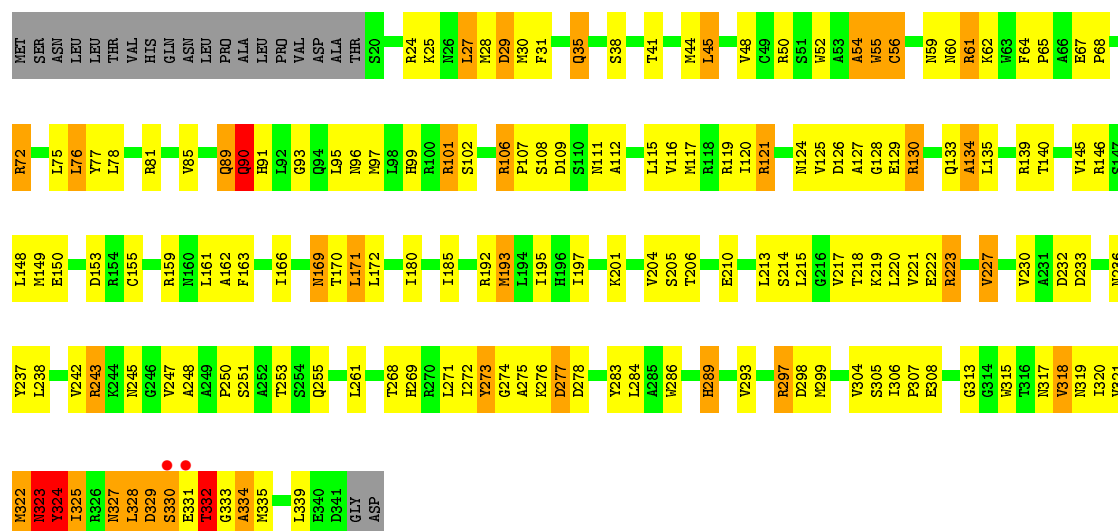


- Molecule 3: loxP DNA

Chain H: 



● Molecule 4: Cre recombinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.50 Å 165.60 Å 193.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 49.29 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (8.00-3.20) 99.1 (49.29-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.19 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.264 0.208 , 0.251	Depositor DCC
R_{free} test set	2949 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13296	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.76	0/316	0.90	0/483
1	G	0.78	0/316	0.97	1/483 (0.2%)
2	X	1.21	2/479 (0.4%)	1.34	7/738 (0.9%)
2	Y	1.17	6/479 (1.3%)	1.42	9/738 (1.2%)
3	D	0.88	0/848	0.95	0/1307
3	H	0.71	0/848	0.87	0/1307
4	A	0.73	1/2663 (0.0%)	0.85	1/3595 (0.0%)
4	B	0.57	0/2591	0.79	0/3493
4	E	0.57	0/2585	0.79	2/3485 (0.1%)
4	F	0.65	0/2591	0.84	2/3493 (0.1%)
All	All	0.72	9/13716 (0.1%)	0.89	22/19122 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
2	X	0	1
3	D	0	5
3	H	0	1
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	120	DT	C5-C7	8.43	1.55	1.50
2	Y	120	DT	C5-C7	8.40	1.55	1.50
2	Y	118	DT	C5-C7	7.68	1.54	1.50
2	Y	119	DA	C5'-C4'	6.60	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	118	DT	C5-C7	6.04	1.53	1.50
2	Y	118	DT	C5'-C4'	5.69	1.57	1.51
2	Y	117	DG	C5'-C4'	5.68	1.57	1.51
4	A	155	CYS	CB-SG	-5.10	1.73	1.81
2	Y	117	DG	P-O5'	5.08	1.64	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	118	DT	O4'-C4'-C3'	-11.85	98.89	106.00
2	Y	117	DG	O4'-C4'-C3'	-10.62	99.63	106.00
4	E	105	PRO	CA-N-CD	-8.19	100.04	111.50
4	F	324	TYR	CB-CG-CD2	7.54	125.53	121.00
2	Y	119	DA	O4'-C4'-C3'	-6.90	101.74	104.50
2	Y	117	DG	O5'-P-OP2	-6.51	99.84	105.70
2	Y	119	DA	OP1-P-OP2	-6.29	110.17	119.60
2	X	119	DA	O4'-C1'-C2'	6.16	110.83	105.90
2	Y	118	DT	C6-C5-C7	-5.99	119.31	122.90
2	X	120	DT	C4'-C3'-C2'	5.92	108.43	103.10
1	G	114	DA	C4'-C3'-C2'	5.89	108.41	103.10
2	X	120	DT	O4'-C4'-C3'	-5.83	102.17	104.50
2	Y	118	DT	C6-N1-C2	5.81	124.20	121.30
2	X	120	DT	C2'-C3'-O3'	-5.61	94.08	112.60
2	Y	119	DA	C3'-C2'-C1'	-5.47	95.93	102.50
2	X	116	DT	C5'-C4'-C3'	5.41	123.84	114.10
2	X	120	DT	O4'-C1'-N1	5.39	111.78	108.00
2	Y	119	DA	C4'-C3'-C2'	5.38	107.94	103.10
2	X	120	DT	N1-C1'-C2'	5.38	122.82	112.60
4	A	107	PRO	CA-N-CD	-5.24	104.17	111.50
4	F	76	LEU	CA-CB-CG	-5.23	103.28	115.30
4	E	317	ASN	N-CA-C	-5.17	97.06	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	116	DC	Sidechain
3	D	117	DA	Sidechain
3	D	118	DT	Sidechain
3	D	119	DA	Sidechain
3	D	126	DA	Sidechain
1	G	105	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	G	106	DC	Sidechain
3	H	105	DA	Sidechain
2	X	117	DG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	326	0	178	12	0
1	G	326	0	178	8	0
2	X	428	0	241	10	0
2	Y	428	0	241	36	0
3	D	756	0	421	34	0
3	H	756	0	421	34	0
4	A	2620	0	2643	163	0
4	B	2550	0	2570	190	0
4	E	2544	0	2566	183	0
4	F	2550	0	2570	161	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	4	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	A	2	0	0	0	0
7	F	1	0	0	0	0
All	All	13296	0	12029	755	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 30.

All (755) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:DA:H2"	1:C:106:DC:H5"	1.20	1.15
4:E:193:MET:HG3	4:E:218:THR:HG23	1.22	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:35:GLN:HA	4:B:35:GLN:HE21	1.04	1.10
3:H:105:DA:H2"	3:H:106:DC:H5"	1.35	1.09
4:A:15:PRO:HB2	4:A:18:ALA:HB3	1.34	1.08
4:A:299:MET:HE1	4:A:309:ILE:HA	1.36	1.06
4:A:72:ARG:HG3	4:A:116:VAL:HG21	1.38	1.00
4:A:181:ARG:HH11	4:A:199:ARG:HH22	1.11	0.97
4:B:134:ALA:HA	4:B:283:TYR:CD2	2.01	0.96
4:B:35:GLN:HA	4:B:35:GLN:NE2	1.83	0.94
4:B:194:LEU:HD13	4:B:212:ALA:HB2	1.48	0.94
4:E:121:ARG:O	4:E:125:VAL:HG12	1.67	0.93
3:D:122:DT:H5"	4:B:97:MET:HE2	1.50	0.93
3:H:134:DA:H2"	3:H:135:DT:C5'	1.99	0.93
4:B:58:LEU:O	4:B:58:LEU:HD12	1.69	0.93
4:E:317:ASN:HD22	4:E:317:ASN:H	1.16	0.92
4:F:245:ASN:OD1	4:F:247:VAL:HG23	1.69	0.91
4:E:200:THR:HG22	4:E:201:LYS:H	1.34	0.90
4:E:146:ARG:O	4:E:150:GLU:HB2	1.73	0.89
2:X:116:DT:H5"	4:B:173:ARG:NH2	1.88	0.89
1:G:105:DA:H2"	1:G:106:DC:H5"	1.53	0.89
4:A:15:PRO:HB2	4:A:18:ALA:CB	2.03	0.88
4:A:15:PRO:CB	4:A:18:ALA:HB3	2.04	0.87
4:F:193:MET:HB3	4:F:213:LEU:HD12	1.56	0.87
1:G:115:A3P:O2P	2:Y:116:DT:H5'	1.75	0.87
4:F:134:ALA:HA	4:F:283:TYR:CD2	2.10	0.86
4:A:188:THR:HG22	4:A:190:GLY:H	1.39	0.85
4:E:243:ARG:HG2	4:E:243:ARG:HH11	1.41	0.85
4:A:181:ARG:NH1	4:A:199:ARG:HH22	1.75	0.84
4:A:305:SER:HB2	4:A:307:PRO:HD2	1.59	0.84
4:E:154:ARG:HB3	4:E:154:ARG:HH11	1.40	0.84
4:E:188:THR:HG22	4:E:190:GLY:H	1.45	0.82
4:F:163:PHE:CE1	4:F:261:LEU:HD13	2.15	0.82
4:B:215:LEU:O	4:B:218:THR:HG22	1.79	0.81
4:A:134:ALA:HA	4:A:283:TYR:CD2	2.15	0.81
2:Y:118:DT:H3	3:H:119:DA:H61	1.28	0.81
3:H:134:DA:H2"	3:H:135:DT:H5'	1.61	0.81
4:F:121:ARG:HG3	4:F:121:ARG:HH11	1.42	0.81
4:E:58:LEU:HD12	4:E:58:LEU:O	1.81	0.80
4:A:325:ILE:HB	4:A:328:LEU:HD12	1.64	0.80
3:H:134:DA:H2"	3:H:135:DT:H5"	1.62	0.80
4:B:113:VAL:O	4:B:116:VAL:HG12	1.81	0.79
4:E:271:LEU:HD23	4:E:271:LEU:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:72:ARG:CG	4:A:116:VAL:HG21	2.13	0.79
4:A:139:ARG:HG3	4:A:139:ARG:O	1.80	0.79
4:B:106:ARG:O	4:B:109:ASP:HB2	1.83	0.79
2:Y:131:DG:H2"	2:Y:132:DT:C5'	2.13	0.78
4:E:117:MET:HE3	4:E:120:ILE:HD12	1.65	0.78
4:A:243:ARG:HH11	4:A:243:ARG:HG2	1.48	0.78
2:Y:118:DT:H72	4:F:319:ASN:ND2	1.98	0.78
4:B:35:GLN:CA	4:B:35:GLN:HE21	1.93	0.78
1:C:105:DA:C2'	1:C:106:DC:H5"	2.10	0.78
4:B:182:VAL:HG23	4:B:236:ASN:O	1.84	0.78
3:D:132:DT:H2"	3:D:133:DT:H5"	1.67	0.77
2:Y:117:DG:H5"	4:F:320:ILE:HD11	1.67	0.76
4:B:258:THR:HA	4:B:261:LEU:HD12	1.66	0.76
4:A:19:THR:HG22	4:A:23:VAL:HG23	1.66	0.76
4:B:185:ILE:HD13	4:B:193:MET:CE	2.15	0.76
3:H:105:DA:C2'	3:H:106:DC:H5"	2.14	0.76
2:X:117:DG:OP2	4:B:320:ILE:HG13	1.86	0.76
2:X:116:DT:C5'	4:B:173:ARG:NH2	2.48	0.76
4:A:299:MET:CE	4:A:309:ILE:HA	2.16	0.75
4:F:317:ASN:ND2	4:F:319:ASN:H	1.84	0.75
4:E:148:LEU:O	4:E:149:MET:HB2	1.84	0.75
4:E:171:LEU:HD23	4:E:171:LEU:N	2.01	0.74
4:E:48:VAL:HG21	4:E:91:HIS:HA	1.68	0.74
4:F:130:ARG:HH11	4:F:130:ARG:HB3	1.51	0.74
4:F:297:ARG:HG2	4:F:297:ARG:HH11	1.51	0.74
4:F:62:LYS:NZ	4:F:62:LYS:HB2	2.02	0.74
4:A:90:GLN:HE21	4:A:90:GLN:HA	1.52	0.73
4:F:317:ASN:HD22	4:F:319:ASN:H	1.35	0.73
4:F:243:ARG:HG2	4:F:243:ARG:HH11	1.53	0.73
4:E:74:TYR:O	4:E:77:TYR:HB3	1.89	0.73
4:A:145:VAL:HG22	4:A:272:ILE:HD11	1.71	0.73
4:A:166:ILE:O	4:A:170:THR:HG23	1.89	0.73
4:E:122:LYS:O	4:E:126:ASP:HB2	1.89	0.73
4:F:52:TRP:O	4:F:56:CYS:HB2	1.89	0.73
2:Y:131:DG:H2"	2:Y:132:DT:H5"	1.70	0.73
4:F:163:PHE:HE1	4:F:261:LEU:HD13	1.51	0.72
4:B:315:TRP:CZ2	4:B:324:TYR:CE2	2.78	0.72
2:Y:135:DT:H2"	2:Y:136:DC:C6	2.25	0.72
4:F:230:VAL:HG12	4:F:250:PRO:HB3	1.71	0.72
4:A:181:ARG:HH11	4:A:199:ARG:NH2	1.86	0.71
4:A:187:ARG:HH11	4:A:187:ARG:HB3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:315:TRP:CZ2	4:B:324:TYR:CD2	2.78	0.71
1:C:102:DA:H2"	1:C:103:DT:H5"	1.73	0.71
2:Y:117:DG:H5"	4:F:320:ILE:CD1	2.20	0.71
4:E:32:ARG:HD2	4:F:72:ARG:HH21	1.55	0.70
4:B:193:MET:HE1	4:B:221:VAL:HG11	1.74	0.70
4:B:233:ASP:O	4:B:236:ASN:HB2	1.90	0.70
4:E:317:ASN:N	4:E:317:ASN:HD22	1.87	0.70
4:A:161:LEU:HD22	4:A:220:LEU:CD1	2.22	0.70
4:F:323:ASN:CG	4:F:324:TYR:N	2.45	0.70
4:B:204:VAL:CG2	4:E:125:VAL:HG11	2.22	0.70
4:A:27:LEU:HD13	4:A:102:SER:CB	2.22	0.70
4:A:217:VAL:O	4:A:221:VAL:HG23	1.92	0.69
4:B:204:VAL:HG22	4:E:125:VAL:HG11	1.74	0.69
4:B:147:SER:O	4:B:148:LEU:HB2	1.91	0.69
4:B:261:LEU:HA	4:B:264:ILE:HD12	1.73	0.69
4:E:159:ARG:HB2	4:E:224:TRP:CE3	2.27	0.69
4:F:329:ASP:HA	4:F:332:THR:HG23	1.75	0.69
4:A:243:ARG:NH1	4:A:243:ARG:HG2	2.08	0.69
4:E:159:ARG:HB2	4:E:224:TRP:CZ3	2.27	0.69
2:Y:128:DG:H1	3:H:109:DC:H42	1.41	0.69
2:X:126:DA:OP1	4:A:288:GLY:N	2.25	0.68
4:B:328:LEU:O	4:B:332:THR:HG23	1.93	0.68
4:A:19:THR:HG22	4:A:23:VAL:CG2	2.24	0.68
4:E:182:VAL:HG23	4:E:234:PRO:O	1.93	0.68
4:B:326:ARG:HH11	4:B:326:ARG:HG3	1.59	0.68
4:E:169:ASN:OD1	4:F:339:LEU:HD12	1.94	0.68
4:A:23:VAL:O	4:A:27:LEU:HB2	1.94	0.68
4:E:117:MET:HA	4:E:117:MET:CE	2.24	0.68
4:A:27:LEU:CD1	4:A:102:SER:HB3	2.24	0.67
4:E:305:SER:OG	4:E:308:GLU:HG3	1.94	0.67
3:D:115:DG:H2"	3:D:116:DC:O4'	1.95	0.67
4:E:209:VAL:O	4:E:210:GLU:HG3	1.94	0.67
2:Y:118:DT:H3	3:H:119:DA:N6	1.92	0.67
4:A:192:ARG:HB3	4:A:215:LEU:HD23	1.77	0.67
4:B:245:ASN:OD1	4:B:247:VAL:HG23	1.94	0.67
4:A:139:ARG:HB2	4:A:168:TYR:OH	1.95	0.67
3:D:120:DC:H3'	4:B:106:ARG:NH2	2.10	0.67
4:E:75:LEU:HD11	4:E:92:LEU:HG	1.78	0.66
4:B:330:SER:C	4:B:332:THR:H	1.98	0.66
4:A:27:LEU:HD13	4:A:102:SER:HB3	1.78	0.66
4:E:181:ARG:HB2	4:E:236:ASN:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:DG:H2''	3:D:102:DA:C8	2.30	0.66
4:E:134:ALA:HA	4:E:283:TYR:CD2	2.30	0.66
4:F:313:GLY:HA3	4:F:315:TRP:CZ3	2.31	0.66
4:E:170:THR:OG1	4:E:172:LEU:HD12	1.95	0.66
1:C:102:DA:H2''	1:C:103:DT:C5'	2.26	0.66
4:F:148:LEU:HD23	4:F:148:LEU:O	1.95	0.66
4:F:215:LEU:O	4:F:218:THR:HG22	1.96	0.66
4:E:183:LYS:HG2	4:E:234:PRO:HB2	1.78	0.66
4:B:206:THR:HB	4:E:131:ALA:HB2	1.78	0.66
4:A:14:LEU:HD12	4:A:19:THR:HG23	1.78	0.65
4:B:172:LEU:HD21	4:B:197:ILE:HG13	1.77	0.65
4:E:107:PRO:O	4:E:113:VAL:HG21	1.96	0.65
4:E:317:ASN:H	4:E:317:ASN:ND2	1.93	0.65
2:Y:117:DG:H3'	4:F:317:ASN:HB2	1.78	0.65
4:B:134:ALA:HA	4:B:283:TYR:HD2	1.57	0.65
1:G:105:DA:C2'	1:G:106:DC:H5''	2.25	0.65
4:E:313:GLY:HA3	4:E:315:TRP:CZ3	2.33	0.64
4:F:172:LEU:HD21	4:F:197:ILE:HG13	1.79	0.64
4:B:257:SER:O	4:B:260:ALA:HB3	1.97	0.64
4:A:161:LEU:HD22	4:A:220:LEU:HD11	1.80	0.64
3:H:106:DC:H2'	3:H:107:DT:H72	1.80	0.64
2:X:116:DT:H5''	4:B:173:ARG:HH22	1.59	0.64
4:B:185:ILE:HD11	4:B:238:LEU:HD22	1.79	0.64
2:Y:131:DG:H2''	2:Y:132:DT:H5'	1.78	0.64
4:A:121:ARG:O	4:A:125:VAL:HG23	1.97	0.64
1:C:103:DT:H2''	1:C:104:DA:C8	2.33	0.64
4:B:295:ALA:O	4:B:299:MET:HG3	1.98	0.64
2:Y:119:DA:H61	3:H:118:DT:H3	1.46	0.64
4:B:330:SER:O	4:B:332:THR:N	2.31	0.63
3:D:108:DT:H2''	3:D:109:DC:H5'	1.79	0.63
4:F:146:ARG:O	4:F:150:GLU:HB2	1.98	0.63
4:B:146:ARG:O	4:B:148:LEU:N	2.31	0.63
4:B:315:TRP:HZ2	4:B:324:TYR:CE2	2.16	0.63
4:A:307:PRO:HG3	4:B:306:ILE:CD1	2.29	0.63
2:Y:117:DG:H3'	4:F:317:ASN:CB	2.29	0.63
3:H:106:DC:H2'	3:H:107:DT:C7	2.29	0.63
4:A:101:ARG:CZ	4:B:115:LEU:HD21	2.29	0.63
4:E:197:ILE:HG22	4:E:209:VAL:C	2.20	0.63
4:E:148:LEU:H	4:E:148:LEU:HD23	1.64	0.62
4:E:217:VAL:O	4:E:221:VAL:HG23	1.99	0.62
4:E:117:MET:HA	4:E:117:MET:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:193:MET:CB	4:F:213:LEU:HD12	2.27	0.62
4:A:11:LEU:HD13	4:A:14:LEU:HD21	1.81	0.62
4:A:15:PRO:CG	4:A:18:ALA:HB3	2.27	0.62
4:B:166:ILE:O	4:B:170:THR:HG23	2.00	0.62
4:E:110:SER:OG	4:E:113:VAL:HG23	1.99	0.62
4:E:317:ASN:N	4:E:317:ASN:ND2	2.48	0.62
4:F:306:ILE:N	4:F:307:PRO:HD2	2.15	0.62
2:Y:122:DC:H2''	2:Y:123:DT:H5'	1.81	0.62
4:F:242:VAL:HG23	4:F:242:VAL:O	1.99	0.62
4:E:143:ASP:O	4:E:146:ARG:HG2	1.99	0.62
4:B:228:SER:OG	4:B:230:VAL:HG13	2.00	0.62
4:F:297:ARG:HG2	4:F:297:ARG:NH1	2.15	0.62
4:A:106:ARG:O	4:A:109:ASP:HB2	2.00	0.62
4:B:89:GLN:HG2	4:B:117:MET:HE2	1.81	0.62
4:B:169:ASN:OD1	4:E:339:LEU:HD12	1.99	0.62
4:A:197:ILE:O	4:A:197:ILE:HG13	1.99	0.62
2:Y:117:DG:C2'	2:Y:118:DT:H71	2.28	0.62
4:A:318:VAL:HG23	4:A:319:ASN:N	2.13	0.62
2:Y:135:DT:H2''	2:Y:136:DC:H6	1.64	0.61
4:B:96:ASN:HD21	4:B:108:SER:HB2	1.64	0.61
4:E:116:VAL:O	4:E:119:ARG:HB3	2.00	0.61
4:E:85:VAL:HG23	4:E:129:GLU:OE2	2.00	0.61
3:H:102:DA:H2''	3:H:103:DT:O5'	2.00	0.61
4:E:74:TYR:CE1	4:E:78:LEU:HD11	2.36	0.61
4:F:272:ILE:C	4:F:273:TYR:HD1	2.04	0.61
4:B:236:ASN:ND2	4:B:250:PRO:HB3	2.16	0.61
1:C:108:DT:H2''	1:C:109:DC:H5'	1.81	0.61
4:F:325:ILE:CG2	4:F:327:ASN:ND2	2.64	0.61
4:E:311:GLN:HG3	4:E:312:ALA:N	2.14	0.61
2:Y:123:DT:H3'	4:E:38:SER:OG	2.01	0.61
4:F:333:GLY:O	4:F:334:ALA:HB3	1.99	0.61
4:B:330:SER:C	4:B:332:THR:N	2.54	0.61
4:F:323:ASN:CG	4:F:324:TYR:H	2.05	0.60
4:A:164:LEU:HD11	4:A:268:THR:HG21	1.84	0.60
4:B:89:GLN:HG2	4:B:117:MET:CE	2.31	0.60
4:B:194:LEU:HD13	4:B:212:ALA:CB	2.27	0.60
4:E:158:ILE:HD13	4:E:223:ARG:HG2	1.83	0.60
4:E:169:ASN:ND2	4:E:213:LEU:HA	2.17	0.60
4:F:214:SER:O	4:F:218:THR:HB	2.02	0.60
4:F:272:ILE:HG22	4:F:273:TYR:CD1	2.37	0.60
4:B:94:GLN:HA	4:B:94:GLN:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:78:LEU:N	4:E:78:LEU:HD12	2.17	0.59
4:F:320:ILE:HD12	4:F:320:ILE:N	2.17	0.59
4:E:200:THR:HG22	4:E:201:LYS:N	2.14	0.59
4:E:154:ARG:NH1	4:E:154:ARG:HB3	2.12	0.59
4:E:72:ARG:HE	4:E:116:VAL:HG13	1.67	0.59
4:A:11:LEU:HD22	4:A:12:PRO:HD3	1.84	0.59
4:A:20:SER:O	4:A:21:ASP:HB2	2.03	0.59
4:E:193:MET:CG	4:E:218:THR:HG23	2.15	0.59
4:B:30:MET:SD	4:B:101:ARG:HG2	2.43	0.59
4:A:169:ASN:HD22	4:A:169:ASN:C	2.03	0.58
4:A:181:ARG:HB2	4:A:236:ASN:O	2.02	0.58
4:E:243:ARG:CG	4:E:243:ARG:HH11	2.13	0.58
4:B:29:ASP:O	4:B:32:ARG:HB3	2.02	0.58
4:F:180:ILE:HD13	4:F:195:ILE:HG21	1.85	0.58
4:F:320:ILE:O	4:F:321:VAL:C	2.41	0.58
4:B:61:ARG:HH11	4:B:61:ARG:HG2	1.67	0.58
3:D:120:DC:H3'	4:B:106:ARG:HH21	1.67	0.58
4:F:62:LYS:HB2	4:F:62:LYS:HZ3	1.68	0.58
4:A:161:LEU:HD13	4:A:220:LEU:HD11	1.85	0.58
4:E:106:ARG:HD3	4:E:109:ASP:OD2	2.03	0.58
4:F:126:ASP:C	4:F:128:GLY:H	2.06	0.58
4:F:242:VAL:HG12	4:F:248:ALA:HA	1.86	0.58
4:F:72:ARG:HH11	4:F:72:ARG:CG	2.16	0.58
4:B:236:ASN:HD21	4:B:250:PRO:HB3	1.69	0.57
4:B:45:LEU:C	4:B:45:LEU:HD23	2.23	0.57
4:E:171:LEU:HD23	4:E:171:LEU:H	1.67	0.57
4:F:121:ARG:NH1	4:F:121:ARG:HG3	2.14	0.57
2:Y:122:DC:H2''	2:Y:123:DT:C5'	2.35	0.57
4:A:193:MET:HE1	4:A:221:VAL:HB	1.86	0.57
4:A:22:GLU:C	4:A:24:ARG:H	2.08	0.57
4:A:299:MET:HE2	4:A:304:VAL:HG11	1.87	0.57
4:E:163:PHE:CE2	4:E:261:LEU:HD22	2.40	0.57
4:F:320:ILE:O	4:F:323:ASN:N	2.38	0.57
4:F:149:MET:HE3	4:F:161:LEU:HB2	1.87	0.57
4:B:22:GLU:O	4:B:25:LYS:N	2.33	0.57
4:B:238:LEU:O	4:B:238:LEU:HD12	2.05	0.57
4:B:116:VAL:O	4:B:120:ILE:HG13	2.05	0.57
4:F:325:ILE:HG22	4:F:327:ASN:ND2	2.19	0.57
1:G:111:DT:OP2	4:F:50:ARG:NH1	2.38	0.56
4:A:106:ARG:O	4:A:109:ASP:CB	2.53	0.56
4:B:74:TYR:O	4:B:77:TYR:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:217:VAL:O	4:F:221:VAL:HG23	2.05	0.56
4:F:323:ASN:O	4:F:325:ILE:N	2.38	0.56
4:F:97:MET:O	4:F:101:ARG:HB2	2.05	0.56
4:B:226:SER:OG	4:B:227:VAL:N	2.39	0.56
4:B:161:LEU:HD23	4:B:220:LEU:HD13	1.88	0.56
3:D:112:DA:OP1	4:A:81:ARG:NH2	2.39	0.56
4:B:306:ILE:N	4:B:307:PRO:HD2	2.20	0.56
4:B:306:ILE:HG21	4:B:318:VAL:HG13	1.86	0.56
4:A:170:THR:OG1	4:A:172:LEU:HG	2.06	0.56
4:A:22:GLU:C	4:A:24:ARG:N	2.55	0.56
2:Y:117:DG:C8	2:Y:118:DT:H73	2.40	0.56
4:E:96:ASN:OD1	4:E:106:ARG:HB2	2.06	0.56
4:A:27:LEU:HD13	4:A:102:SER:HB2	1.86	0.56
4:B:168:TYR:CD2	4:B:168:TYR:C	2.79	0.56
4:B:96:ASN:ND2	4:B:108:SER:HB2	2.21	0.56
4:E:142:PHE:CZ	4:E:165:GLY:HA2	2.40	0.56
4:E:22:GLU:HG3	4:E:23:VAL:N	2.20	0.56
4:A:11:LEU:CD2	4:A:12:PRO:HD3	2.36	0.56
3:D:114:DA:H5''	4:A:132:LYS:O	2.05	0.56
4:A:193:MET:CE	4:A:221:VAL:HB	2.35	0.56
4:A:27:LEU:O	4:A:31:PHE:HD1	1.88	0.56
1:C:102:DA:C2'	1:C:103:DT:H5''	2.35	0.56
2:Y:117:DG:H2''	2:Y:118:DT:H71	1.87	0.56
4:B:209:VAL:HG22	4:B:210:GLU:N	2.21	0.55
4:F:297:ARG:CG	4:F:297:ARG:HH11	2.18	0.55
4:F:243:ARG:HG2	4:F:243:ARG:NH1	2.21	0.55
2:Y:117:DG:H2'	2:Y:118:DT:H71	1.89	0.55
4:B:214:SER:HA	4:E:336:VAL:HG13	1.89	0.55
4:F:323:ASN:ND2	4:F:324:TYR:N	2.55	0.55
4:A:161:LEU:HD22	4:A:220:LEU:HD12	1.88	0.55
4:F:121:ARG:O	4:F:125:VAL:HG23	2.06	0.55
4:F:313:GLY:HA3	4:F:315:TRP:CE3	2.42	0.55
3:D:122:DT:OP2	4:B:101:ARG:NH1	2.39	0.55
4:E:169:ASN:HD22	4:E:213:LEU:HA	1.72	0.55
2:Y:118:DT:H72	4:F:319:ASN:CG	2.27	0.55
3:D:133:DT:H2'	3:D:134:DA:C8	2.41	0.55
3:D:135:DT:H1'	4:B:244:LYS:HD3	1.89	0.55
4:A:192:ARG:HH11	4:B:331:GLU:HA	1.72	0.55
1:C:111:DT:OP2	4:B:50:ARG:NH2	2.35	0.55
3:H:113:DT:C7	4:E:87:THR:HG23	2.37	0.55
4:F:272:ILE:HG22	4:F:273:TYR:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:119:DA:H2''	2:Y:120:DT:O5'	2.06	0.55
4:A:55:TRP:O	4:A:59:ASN:HB2	2.07	0.54
4:E:270:ARG:HA	4:E:274:GLY:O	2.07	0.54
4:E:92:LEU:HD12	4:E:117:MET:SD	2.47	0.54
4:A:72:ARG:CD	4:A:116:VAL:HG21	2.37	0.54
4:B:45:LEU:O	4:B:45:LEU:HD23	2.07	0.54
4:A:168:TYR:HA	4:A:291:ALA:HB1	1.89	0.54
2:X:116:DT:C5'	4:B:173:ARG:HH21	2.20	0.54
4:B:315:TRP:HE1	4:B:324:TYR:HE2	1.56	0.54
4:B:159:ARG:HB2	4:B:224:TRP:CZ3	2.42	0.54
4:F:126:ASP:C	4:F:128:GLY:N	2.61	0.54
4:B:111:ASN:O	4:B:115:LEU:HG	2.08	0.54
4:B:195:ILE:HG22	4:B:196:HIS:N	2.22	0.54
4:F:317:ASN:ND2	4:F:319:ASN:OD1	2.41	0.54
3:H:109:DC:H2''	3:H:110:DG:C8	2.43	0.54
4:A:90:GLN:HE21	4:A:90:GLN:CA	2.17	0.54
4:A:233:ASP:O	4:A:236:ASN:HB2	2.08	0.54
4:A:304:VAL:HG12	4:A:309:ILE:HG13	1.89	0.54
4:F:48:VAL:HG21	4:F:91:HIS:HA	1.89	0.54
4:A:101:ARG:NH1	4:B:115:LEU:HD21	2.22	0.54
4:E:182:VAL:O	4:E:185:ILE:N	2.37	0.54
2:X:116:DT:C5'	4:B:173:ARG:HH22	2.18	0.54
4:A:83:LEU:HD22	4:A:87:THR:HG21	1.90	0.53
4:B:204:VAL:O	4:B:204:VAL:HG13	2.09	0.53
4:A:307:PRO:HG3	4:B:306:ILE:HD13	1.88	0.53
4:B:31:PHE:HD1	4:B:42:TRP:CH2	2.26	0.53
4:B:261:LEU:HA	4:B:264:ILE:CD1	2.36	0.53
4:E:304:VAL:HG12	4:E:309:ILE:HG13	1.88	0.53
4:A:171:LEU:O	4:A:292:ARG:NH1	2.42	0.53
3:D:117:DA:H2''	3:D:118:DT:OP2	2.08	0.53
4:B:248:ALA:O	4:B:249:ALA:HB2	2.08	0.53
4:B:234:PRO:C	4:B:236:ASN:H	2.10	0.53
4:B:315:TRP:NE1	4:B:324:TYR:HE2	2.07	0.53
4:B:31:PHE:HD1	4:B:42:TRP:HH2	1.55	0.53
3:H:116:DC:OP1	4:E:292:ARG:NH2	2.42	0.53
4:F:237:TYR:CE1	4:F:255:GLN:HB3	2.43	0.53
4:F:272:ILE:CG2	4:F:273:TYR:CE1	2.92	0.53
4:A:11:LEU:HD22	4:A:12:PRO:CD	2.39	0.52
4:B:235:ASN:HD22	4:B:235:ASN:N	2.07	0.52
4:E:60:ASN:O	4:E:61:ARG:HD3	2.09	0.52
4:B:299:MET:O	4:B:304:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:234:PRO:O	4:B:236:ASN:N	2.30	0.52
4:E:172:LEU:HD23	4:E:176:GLU:OE2	2.09	0.52
3:H:118:DT:H2''	3:H:119:DA:C8	2.44	0.52
4:B:320:ILE:HA	4:B:323:ASN:HB2	1.92	0.52
3:H:117:DA:H4'	3:H:118:DT:OP1	2.09	0.52
4:A:126:ASP:C	4:A:128:GLY:H	2.13	0.52
4:A:317:ASN:O	4:A:319:ASN:N	2.42	0.52
4:F:268:THR:O	4:F:268:THR:HG22	2.10	0.52
4:A:229:GLY:O	4:A:250:PRO:HG2	2.10	0.52
4:E:287:SER:H	4:E:290:SER:HG	1.58	0.52
4:E:78:LEU:HB3	4:E:83:LEU:HD12	1.92	0.52
4:A:326:ARG:HD3	4:F:210:GLU:HG3	1.91	0.52
4:F:24:ARG:O	4:F:28:MET:HB2	2.10	0.52
4:A:59:ASN:O	4:A:61:ARG:HD3	2.09	0.52
3:D:119:DA:P	4:B:121:ARG:HH22	2.33	0.52
4:F:146:ARG:HA	4:F:161:LEU:HD11	1.92	0.52
4:A:201:LYS:HG3	4:A:202:THR:OG1	2.09	0.51
3:D:112:DA:H1'	3:D:113:DT:H5''	1.92	0.51
4:E:245:ASN:OD1	4:E:246:GLY:N	2.42	0.51
4:B:251:SER:OG	4:B:252:ALA:N	2.42	0.51
3:D:125:DT:H2''	3:D:126:DA:O5'	2.11	0.51
4:B:226:SER:O	4:B:228:SER:N	2.43	0.51
3:H:113:DT:H71	4:E:87:THR:HG23	1.93	0.51
3:H:118:DT:H2''	3:H:119:DA:N7	2.25	0.51
4:F:335:MET:HE3	4:F:335:MET:HA	1.93	0.51
4:B:332:THR:HG22	4:B:333:GLY:H	1.75	0.51
3:D:123:DT:C2	3:D:124:DA:C8	2.98	0.51
3:H:116:DC:H5''	4:E:173:ARG:HH22	1.76	0.51
4:E:137:PHE:CE2	4:E:141:ASP:HB3	2.46	0.51
4:F:45:LEU:O	4:F:45:LEU:HD23	2.10	0.51
4:F:55:TRP:CD1	4:F:56:CYS:N	2.79	0.51
4:A:124:ASN:ND2	4:A:129:GLU:OE2	2.43	0.51
4:A:141:ASP:O	4:A:145:VAL:HG23	2.11	0.51
4:B:185:ILE:HD13	4:B:193:MET:HE3	1.93	0.51
4:E:101:ARG:HA	4:F:111:ASN:HD21	1.76	0.51
3:H:103:DT:H2''	3:H:104:DA:C8	2.46	0.51
4:A:154:ARG:HH11	4:A:154:ARG:HG3	1.76	0.51
4:E:197:ILE:HG12	4:E:197:ILE:O	2.11	0.51
4:F:25:LYS:HD3	4:F:29:ASP:OD1	2.10	0.51
4:F:322:MET:HA	4:F:322:MET:CE	2.40	0.51
2:Y:117:DG:C2'	2:Y:118:DT:C7	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:108:DT:H2"	3:H:109:DC:C5'	2.41	0.51
4:F:170:THR:O	4:F:171:LEU:HB2	2.10	0.50
4:B:90:GLN:HE21	4:B:94:GLN:HG2	1.74	0.50
4:F:331:GLU:O	4:F:332:THR:OG1	2.29	0.50
4:A:192:ARG:HE	4:A:215:LEU:CD2	2.24	0.50
4:B:214:SER:OG	4:B:217:VAL:HG23	2.11	0.50
4:B:80:ALA:C	4:B:82:GLY:H	2.14	0.50
4:E:256:LEU:HD22	4:E:260:ALA:CB	2.41	0.50
4:E:163:PHE:HE2	4:E:261:LEU:HD13	1.76	0.50
4:B:249:ALA:H	4:B:250:PRO:HD3	1.76	0.50
4:B:249:ALA:N	4:B:250:PRO:HD3	2.26	0.50
4:B:110:SER:O	4:B:112:ALA:N	2.44	0.50
4:B:156:GLN:HB3	4:B:242:VAL:HG11	1.92	0.50
4:E:126:ASP:C	4:E:128:GLY:H	2.15	0.50
4:E:156:GLN:C	4:E:158:ILE:H	2.15	0.50
4:B:293:VAL:HG22	4:B:294:GLY:N	2.25	0.50
4:E:195:ILE:HD11	4:E:213:LEU:HD21	1.94	0.50
4:F:116:VAL:HG13	4:F:117:MET:N	2.26	0.50
4:A:34:ARG:C	4:A:36:ALA:H	2.15	0.50
4:E:85:VAL:HG23	4:E:129:GLU:CD	2.32	0.50
4:F:115:LEU:O	4:F:116:VAL:C	2.48	0.50
4:A:30:MET:HA	4:B:115:LEU:HD12	1.93	0.50
4:B:263:GLY:HA2	4:B:266:GLU:HG3	1.94	0.50
4:E:297:ARG:HA	4:E:325:ILE:HG22	1.94	0.50
3:H:101:DG:H2"	3:H:102:DA:OP2	2.11	0.50
4:B:193:MET:HE1	4:B:221:VAL:CG1	2.41	0.50
4:E:163:PHE:CD1	4:E:164:LEU:HD23	2.47	0.49
4:E:68:PRO:HG2	4:E:69:GLU:H	1.77	0.49
4:F:126:ASP:O	4:F:128:GLY:N	2.45	0.49
4:A:34:ARG:O	4:A:36:ALA:N	2.45	0.49
4:E:182:VAL:O	4:E:183:LYS:C	2.48	0.49
4:E:113:VAL:O	4:E:116:VAL:HG23	2.11	0.49
3:H:134:DA:C8	3:H:135:DT:H72	2.48	0.49
4:A:192:ARG:HE	4:A:215:LEU:HD21	1.77	0.49
4:A:158:ILE:HD11	4:A:223:ARG:CZ	2.42	0.49
4:B:28:MET:O	4:B:29:ASP:C	2.50	0.49
4:E:173:ARG:HG2	4:E:173:ARG:HH11	1.77	0.49
4:F:106:ARG:O	4:F:109:ASP:HB2	2.13	0.49
4:A:72:ARG:HD2	4:A:116:VAL:HG21	1.94	0.49
4:A:13:ALA:O	4:A:15:PRO:N	2.46	0.49
4:A:195:ILE:HD12	4:A:213:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:204:VAL:O	4:F:204:VAL:HG13	2.13	0.49
4:B:258:THR:HA	4:B:261:LEU:CD1	2.38	0.49
4:E:197:ILE:CG2	4:E:209:VAL:HA	2.43	0.49
4:F:331:GLU:C	4:F:332:THR:OG1	2.50	0.49
4:A:320:ILE:O	4:A:322:MET:N	2.46	0.49
4:E:156:GLN:O	4:E:158:ILE:N	2.46	0.49
4:E:289:HIS:O	4:E:290:SER:C	2.51	0.49
4:E:90:GLN:HE21	4:E:94:GLN:HG2	1.78	0.49
2:Y:119:DA:N6	3:H:118:DT:H3	2.08	0.49
4:A:107:PRO:O	4:A:108:SER:C	2.49	0.49
4:A:145:VAL:HG22	4:A:272:ILE:CD1	2.42	0.49
4:B:226:SER:O	4:B:229:GLY:N	2.46	0.49
4:B:45:LEU:CD2	4:B:45:LEU:C	2.81	0.49
4:E:154:ARG:HG3	4:E:157:ASP:HB2	1.94	0.49
4:F:218:THR:CG2	4:F:219:LYS:N	2.75	0.49
3:D:122:DT:C5'	4:B:97:MET:HE2	2.34	0.49
4:E:287:SER:N	4:E:290:SER:OG	2.44	0.49
4:E:57:LYS:O	4:E:58:LEU:HB2	2.13	0.49
4:F:227:VAL:O	4:F:227:VAL:CG1	2.61	0.49
4:F:273:TYR:CD1	4:F:273:TYR:N	2.80	0.49
4:A:245:ASN:OD1	4:A:247:VAL:HB	2.13	0.48
4:E:185:ILE:HG21	4:E:193:MET:CE	2.43	0.48
4:E:238:LEU:HD23	4:E:238:LEU:O	2.13	0.48
3:H:134:DA:C2'	3:H:135:DT:H5"	2.38	0.48
4:B:326:ARG:NH1	4:B:326:ARG:HG3	2.28	0.48
4:E:235:ASN:HD22	4:E:235:ASN:N	2.09	0.48
4:E:68:PRO:O	4:E:69:GLU:C	2.52	0.48
4:F:180:ILE:HD13	4:F:195:ILE:HD13	1.95	0.48
4:A:80:ALA:C	4:A:82:GLY:N	2.65	0.48
4:B:221:VAL:O	4:B:225:ILE:HG13	2.13	0.48
4:A:200:THR:HG21	4:A:205:SER:OG	2.13	0.48
3:D:103:DT:O2	4:A:244:LYS:HE3	2.12	0.48
4:B:217:VAL:O	4:B:221:VAL:HG23	2.14	0.48
4:F:169:ASN:HD22	4:F:169:ASN:C	2.14	0.48
3:H:114:DA:H5"	4:E:132:LYS:O	2.13	0.48
4:E:221:VAL:O	4:E:225:ILE:HG13	2.13	0.48
4:E:187:ARG:HH22	4:E:222:GLU:HG2	1.78	0.48
4:F:72:ARG:CG	4:F:72:ARG:NH1	2.77	0.48
4:A:321:VAL:HG23	4:A:321:VAL:O	2.14	0.48
4:B:145:VAL:HG11	4:B:164:LEU:HD12	1.94	0.48
4:E:248:ALA:O	4:E:250:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:78:LEU:HD12	4:E:78:LEU:H	1.77	0.48
4:F:333:GLY:O	4:F:334:ALA:CB	2.61	0.48
4:B:78:LEU:HD22	4:B:83:LEU:HD12	1.96	0.48
2:X:118:DT:H2"	2:X:119:DA:C8	2.49	0.48
4:E:171:LEU:HD22	4:E:295:ALA:CB	2.43	0.48
4:F:146:ARG:O	4:F:150:GLU:N	2.47	0.48
1:G:106:DC:H2"	1:G:107:UMP:O5'	2.14	0.48
4:A:14:LEU:HD12	4:A:19:THR:CG2	2.42	0.48
4:E:163:PHE:CD2	4:E:261:LEU:HD22	2.48	0.48
2:Y:117:DG:H2'	2:Y:118:DT:C7	2.44	0.47
4:E:74:TYR:O	4:E:78:LEU:HD13	2.14	0.47
4:A:134:ALA:HA	4:A:283:TYR:CE2	2.49	0.47
4:B:90:GLN:HE21	4:B:94:GLN:CG	2.27	0.47
4:E:256:LEU:HD22	4:E:260:ALA:HB3	1.96	0.47
3:H:108:DT:H2"	3:H:109:DC:H5"	1.96	0.47
4:A:317:ASN:O	4:A:318:VAL:C	2.52	0.47
4:B:258:THR:CA	4:B:261:LEU:HD12	2.40	0.47
4:E:187:ARG:HH12	4:E:222:GLU:CD	2.18	0.47
4:F:107:PRO:C	4:F:109:ASP:H	2.17	0.47
4:A:256:LEU:HD23	4:A:256:LEU:HA	1.50	0.47
4:A:92:LEU:HD21	4:A:108:SER:HB2	1.96	0.47
4:E:163:PHE:HB2	4:E:239:PHE:CE2	2.50	0.47
4:E:23:VAL:HA	4:E:26:ASN:HD22	1.79	0.47
4:F:329:ASP:O	4:F:330:SER:C	2.53	0.47
4:F:339:LEU:HD23	4:F:339:LEU:HA	1.57	0.47
4:F:121:ARG:NH1	4:F:121:ARG:CG	2.75	0.47
4:A:177:ILE:HG23	4:A:180:ILE:HD12	1.96	0.47
4:E:256:LEU:O	4:E:257:SER:O	2.33	0.47
4:E:26:ASN:CB	4:E:102:SER:HA	2.45	0.47
4:E:49:CYS:SG	4:E:98:LEU:HD22	2.55	0.47
4:F:272:ILE:CG2	4:F:273:TYR:HE1	2.27	0.47
4:E:102:SER:C	4:E:104:LEU:H	2.17	0.47
4:E:243:ARG:NH1	4:E:243:ARG:CG	2.75	0.47
4:F:161:LEU:HG	4:F:161:LEU:O	2.15	0.47
4:A:310:MET:HE3	4:A:318:VAL:N	2.30	0.47
1:C:106:DC:H2"	1:C:107:UMP:H6	1.80	0.47
4:E:154:ARG:CB	4:E:154:ARG:NH1	2.79	0.46
4:E:156:GLN:C	4:E:158:ILE:N	2.68	0.46
4:F:185:ILE:HD11	4:F:238:LEU:HD22	1.95	0.46
4:F:320:ILE:HD12	4:F:320:ILE:H	1.78	0.46
4:F:60:ASN:C	4:F:61:ARG:HD3	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:269:HIS:C	4:F:271:LEU:H	2.19	0.46
4:F:64:PHE:HA	4:F:65:PRO:C	2.34	0.46
3:H:124:DA:H2'	3:H:125:DT:H72	1.97	0.46
4:B:139:ARG:HG2	4:B:139:ARG:NH1	2.30	0.46
4:B:319:ASN:ND2	4:B:319:ASN:O	2.48	0.46
4:E:142:PHE:CE1	4:E:165:GLY:HA2	2.50	0.46
4:E:86:LYS:O	4:E:86:LYS:HD3	2.16	0.46
4:E:195:ILE:CD1	4:E:213:LEU:HD21	2.45	0.46
4:F:236:ASN:OD1	4:F:251:SER:O	2.34	0.46
4:B:148:LEU:HD11	4:B:271:LEU:HD12	1.98	0.46
4:B:57:LYS:O	4:B:59:ASN:N	2.48	0.46
4:F:38:SER:O	4:F:41:THR:N	2.45	0.46
3:D:105:DA:H2''	3:D:106:DC:O5'	2.14	0.46
4:F:230:VAL:C	4:F:232:ASP:H	2.19	0.46
1:G:106:DC:H2''	1:G:107:UMP:H6	1.81	0.46
4:A:204:VAL:HG22	4:A:204:VAL:O	2.16	0.46
3:D:107:DT:H2''	3:D:108:DT:H5'	1.96	0.46
4:F:166:ILE:HG12	4:F:213:LEU:HD21	1.97	0.46
2:Y:116:DT:O5'	4:F:201:LYS:HE3	2.15	0.46
4:F:329:ASP:CA	4:F:332:THR:HG23	2.45	0.46
4:E:173:ARG:O	4:E:177:ILE:HG13	2.15	0.46
4:E:44:MET:HA	4:E:47:SER:HB3	1.98	0.46
4:A:318:VAL:CG2	4:A:319:ASN:N	2.79	0.46
3:D:118:DT:H2''	3:D:119:DA:N7	2.31	0.46
3:D:123:DT:H2''	3:D:124:DA:H5''	1.98	0.45
4:E:165:GLY:O	4:E:169:ASN:HB2	2.16	0.45
4:E:74:TYR:O	4:E:78:LEU:CD1	2.65	0.45
3:H:122:DT:OP2	4:F:101:ARG:NH1	2.49	0.45
4:B:245:ASN:OD1	4:B:247:VAL:CG2	2.63	0.45
4:E:248:ALA:C	4:E:250:PRO:HD3	2.36	0.45
4:F:276:LYS:O	4:F:277:ASP:O	2.35	0.45
4:A:224:TRP:CZ3	4:A:228:SER:HB3	2.51	0.45
4:B:270:ARG:HG2	4:B:274:GLY:O	2.17	0.45
4:B:61:ARG:NH1	4:B:61:ARG:HG2	2.32	0.45
4:E:94:GLN:HA	4:E:94:GLN:NE2	2.31	0.45
2:Y:118:DT:H1'	2:Y:119:DA:C5	2.50	0.45
4:A:181:ARG:O	4:A:184:ASP:HB2	2.15	0.45
3:D:104:DA:H2''	3:D:105:DA:O5'	2.16	0.45
4:E:306:ILE:N	4:E:307:PRO:HD2	2.32	0.45
4:F:25:LYS:O	4:F:25:LYS:HD3	2.17	0.45
4:A:80:ALA:C	4:A:82:GLY:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:DG:O6	4:A:86:LYS:HE2	2.16	0.45
4:A:182:VAL:C	4:A:184:ASP:H	2.19	0.45
4:A:340:GLU:OE2	4:F:192:ARG:NH1	2.50	0.45
4:E:167:ALA:O	4:E:291:ALA:HB1	2.17	0.45
4:F:329:ASP:O	4:F:332:THR:N	2.50	0.45
4:E:209:VAL:HG12	4:E:209:VAL:O	2.16	0.45
4:E:316:THR:HG23	4:E:317:ASN:ND2	2.31	0.45
4:F:238:LEU:O	4:F:238:LEU:HD12	2.17	0.45
4:B:237:TYR:CE1	4:B:255:GLN:HG2	2.52	0.45
4:B:293:VAL:CG2	4:B:294:GLY:N	2.78	0.45
4:F:223:ARG:HH11	4:F:223:ARG:HG2	1.82	0.45
4:F:72:ARG:HH11	4:F:72:ARG:HG3	1.81	0.45
2:X:116:DT:H4'	4:B:202:THR:CG2	2.46	0.45
4:A:15:PRO:CB	4:A:18:ALA:CB	2.81	0.45
4:A:97:MET:O	4:A:98:LEU:C	2.55	0.45
4:B:142:PHE:CZ	4:B:165:GLY:HA2	2.52	0.45
3:D:128:DG:H2''	3:D:129:DA:H5'	1.98	0.45
4:A:64:PHE:HA	4:A:65:PRO:C	2.36	0.45
4:F:67:GLU:HG3	4:F:68:PRO:HD2	1.99	0.45
4:B:319:ASN:ND2	4:B:323:ASN:OD1	2.50	0.44
4:B:327:ASN:OD1	4:B:328:LEU:HD12	2.17	0.44
4:E:23:VAL:CG2	4:E:24:ARG:N	2.80	0.44
4:E:32:ARG:HD2	4:F:72:ARG:NH2	2.28	0.44
4:F:305:SER:OG	4:F:307:PRO:HG2	2.17	0.44
4:F:54:ALA:O	4:F:55:TRP:C	2.55	0.44
4:B:181:ARG:O	4:B:184:ASP:HB2	2.17	0.44
4:A:20:SER:O	4:A:21:ASP:CB	2.65	0.44
2:X:116:DT:O5'	4:B:173:ARG:NH2	2.50	0.44
1:C:108:DT:C2'	1:C:109:DC:H5'	2.47	0.44
4:B:25:LYS:O	4:B:28:MET:N	2.51	0.44
4:B:52:TRP:O	4:B:56:CYS:HB2	2.17	0.44
4:B:42:TRP:O	4:B:43:LYS:C	2.56	0.44
4:E:163:PHE:HD1	4:E:164:LEU:HD23	1.81	0.44
2:Y:135:DT:O2	4:E:244:LYS:HD3	2.18	0.44
4:E:311:GLN:CG	4:E:312:ALA:N	2.80	0.44
4:E:72:ARG:HE	4:E:116:VAL:CG1	2.31	0.44
4:F:219:LYS:HD3	4:F:222:GLU:OE1	2.17	0.44
4:F:245:ASN:CG	4:F:247:VAL:HG23	2.35	0.44
3:D:133:DT:C2'	3:D:134:DA:C8	3.01	0.44
4:E:243:ARG:NH1	4:E:243:ARG:HG2	2.19	0.44
4:A:145:VAL:O	4:A:145:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:13:ALA:O	4:A:15:PRO:CD	2.66	0.44
4:A:72:ARG:HD2	4:A:116:VAL:CG2	2.47	0.44
4:B:319:ASN:HD22	4:B:319:ASN:C	2.21	0.44
4:B:31:PHE:O	4:B:34:ARG:HB3	2.18	0.44
4:E:295:ALA:O	4:E:296:ALA:C	2.55	0.44
2:Y:131:DG:C2'	2:Y:132:DT:H5''	2.45	0.44
4:A:68:PRO:O	4:A:69:GLU:C	2.54	0.44
4:B:158:ILE:HA	4:B:158:ILE:HD13	1.82	0.44
4:E:111:ASN:O	4:E:115:LEU:HB2	2.17	0.44
4:E:177:ILE:O	4:E:177:ILE:HG22	2.18	0.44
4:F:269:HIS:HB2	4:F:286:TRP:CE3	2.53	0.44
4:A:187:ARG:CB	4:A:187:ARG:HH11	2.29	0.43
4:A:320:ILE:C	4:A:322:MET:N	2.71	0.43
4:A:59:ASN:HB3	4:A:61:ARG:HH11	1.83	0.43
4:B:92:LEU:HD23	4:B:117:MET:HG2	1.99	0.43
4:E:310:MET:CE	4:E:317:ASN:O	2.66	0.43
4:F:322:MET:HA	4:F:322:MET:HE3	2.00	0.43
4:F:335:MET:CE	4:F:335:MET:HA	2.47	0.43
4:A:101:ARG:NH2	4:B:115:LEU:HD21	2.33	0.43
4:B:31:PHE:CD1	4:B:42:TRP:CH2	3.05	0.43
3:D:134:DA:C8	3:D:135:DT:H72	2.53	0.43
4:A:126:ASP:C	4:A:128:GLY:N	2.70	0.43
4:A:192:ARG:HH21	4:A:215:LEU:HD21	1.83	0.43
4:A:14:LEU:HG	4:A:27:LEU:CD2	2.48	0.43
4:B:185:ILE:HG21	4:B:193:MET:CE	2.48	0.43
4:E:306:ILE:HG22	4:F:306:ILE:HD11	2.01	0.43
3:H:133:DT:H2''	3:H:134:DA:C8	2.53	0.43
4:A:84:ALA:O	4:A:88:ILE:HG13	2.19	0.43
4:B:171:LEU:O	4:B:292:ARG:HG3	2.18	0.43
4:E:106:ARG:HG3	4:E:106:ARG:HH11	1.83	0.43
4:E:323:ASN:HD22	4:E:323:ASN:HA	1.56	0.43
4:E:339:LEU:HD23	4:E:339:LEU:HA	1.79	0.43
4:F:325:ILE:HG21	4:F:327:ASN:ND2	2.34	0.43
3:D:119:DA:OP1	4:B:121:ARG:NH2	2.37	0.43
4:E:289:HIS:O	4:E:291:ALA:N	2.52	0.43
4:E:78:LEU:CD1	4:E:78:LEU:H	2.31	0.43
4:F:289:HIS:O	4:F:293:VAL:HG12	2.17	0.43
2:Y:118:DT:H2'	2:Y:118:DT:H6	1.55	0.43
4:F:159:ARG:O	4:F:162:ALA:N	2.39	0.43
1:G:115:A3P:O3'	2:Y:116:DT:C5'	2.67	0.43
4:B:170:THR:OG1	4:B:172:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:209:VAL:CG2	4:B:210:GLU:N	2.81	0.43
4:B:309:ILE:HG21	4:B:321:VAL:HG13	2.00	0.43
4:F:124:ASN:O	4:F:129:GLU:HB3	2.19	0.43
4:F:89:GLN:O	4:F:90:GLN:C	2.57	0.43
4:F:99:HIS:O	4:F:102:SER:N	2.52	0.43
4:A:182:VAL:C	4:A:184:ASP:N	2.72	0.43
4:A:95:LEU:HD12	4:A:95:LEU:HA	1.83	0.43
4:B:193:MET:HG3	4:B:218:THR:OG1	2.19	0.43
3:D:126:DA:OP2	4:B:262:GLU:OE1	2.36	0.43
4:E:35:GLN:HB2	4:F:119:ARG:HD2	2.01	0.43
4:F:93:GLY:O	4:F:96:ASN:HB2	2.19	0.43
4:A:169:ASN:C	4:A:169:ASN:ND2	2.70	0.43
4:A:306:ILE:N	4:A:307:PRO:CD	2.82	0.43
4:A:310:MET:SD	4:A:318:VAL:HG12	2.58	0.43
4:A:63:TRP:O	4:A:64:PHE:HB2	2.19	0.43
4:B:163:PHE:CE1	4:B:261:LEU:HD22	2.54	0.43
4:A:260:ALA:O	4:A:264:ILE:HG13	2.19	0.43
4:B:24:ARG:O	4:B:28:MET:HG2	2.19	0.43
4:B:332:THR:HG22	4:B:333:GLY:N	2.33	0.43
4:E:230:VAL:CG1	4:E:236:ASN:HB3	2.49	0.43
4:B:96:ASN:OD1	4:B:107:PRO:HG2	2.19	0.42
4:E:161:LEU:HD23	4:E:220:LEU:HD21	2.01	0.42
4:F:116:VAL:O	4:F:120:ILE:HG13	2.19	0.42
3:H:126:DA:OP1	4:F:289:HIS:N	2.45	0.42
4:B:139:ARG:HD2	4:B:139:ARG:O	2.19	0.42
4:B:68:PRO:O	4:B:69:GLU:C	2.57	0.42
4:F:145:VAL:HG11	4:F:268:THR:HG21	2.01	0.42
1:G:101:DG:H2'	1:G:102:DA:O5'	2.19	0.42
4:A:12:PRO:HG2	4:A:63:TRP:CZ3	2.54	0.42
4:B:221:VAL:C	4:B:223:ARG:N	2.71	0.42
4:E:26:ASN:HB3	4:E:102:SER:HA	2.00	0.42
4:E:41:THR:O	4:E:42:TRP:C	2.57	0.42
4:F:271:LEU:HD13	4:F:271:LEU:C	2.40	0.42
2:Y:126:DA:OP2	4:E:262:GLU:OE1	2.36	0.42
4:A:192:ARG:HB3	4:A:215:LEU:CD2	2.45	0.42
4:E:126:ASP:C	4:E:128:GLY:N	2.72	0.42
4:E:48:VAL:HG11	4:E:94:GLN:HB2	2.01	0.42
4:F:328:LEU:HD12	4:F:328:LEU:H	1.84	0.42
2:Y:117:DG:O6	3:H:120:DC:N3	2.52	0.42
4:B:107:PRO:C	4:B:109:ASP:H	2.23	0.42
4:B:115:LEU:N	4:B:115:LEU:HD23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:185:ILE:HG21	4:B:193:MET:HE3	2.01	0.42
4:B:328:LEU:H	4:B:328:LEU:HD12	1.84	0.42
3:D:118:DT:OP1	4:A:202:THR:HG23	2.18	0.42
4:E:213:LEU:HD22	4:E:213:LEU:H	1.83	0.42
4:F:272:ILE:HG22	4:F:273:TYR:HD1	1.83	0.42
4:E:304:VAL:CG1	4:E:309:ILE:HG13	2.49	0.42
4:F:139:ARG:O	4:F:140:THR:C	2.58	0.42
4:E:194:LEU:HD11	4:F:329:ASP:OD1	2.20	0.42
4:A:215:LEU:O	4:A:218:THR:HB	2.18	0.42
4:B:67:GLU:O	4:B:68:PRO:C	2.58	0.42
4:F:112:ALA:O	4:F:116:VAL:HG12	2.20	0.42
4:F:75:LEU:O	4:F:78:LEU:HB2	2.19	0.42
4:A:164:LEU:CD1	4:A:268:THR:HG21	2.49	0.42
4:A:78:LEU:O	4:A:79:GLN:C	2.55	0.42
4:B:116:VAL:HG13	4:B:117:MET:N	2.34	0.42
4:B:334:ALA:O	4:B:337:ARG:N	2.52	0.42
4:E:236:ASN:OD1	4:E:252:ALA:HB2	2.19	0.42
4:F:304:VAL:HG12	4:F:308:GLU:HB2	2.02	0.42
4:A:158:ILE:HD11	4:A:223:ARG:NH2	2.34	0.42
4:E:57:LYS:O	4:E:58:LEU:CB	2.68	0.42
4:B:159:ARG:HB2	4:B:224:TRP:CE3	2.55	0.42
4:B:226:SER:O	4:B:227:VAL:C	2.56	0.42
1:C:106:DC:H2''	1:C:107:UMP:C6	2.54	0.42
4:E:181:ARG:O	4:E:184:ASP:N	2.53	0.42
4:F:35:GLN:HB2	4:F:35:GLN:HE21	1.64	0.42
4:E:313:GLY:HA3	4:E:315:TRP:CE3	2.56	0.41
4:F:161:LEU:HG	4:F:220:LEU:HD22	2.02	0.41
4:A:177:ILE:HG21	4:A:177:ILE:HD13	1.83	0.41
4:B:76:LEU:HA	4:B:76:LEU:HD23	1.65	0.41
3:D:112:DA:H2''	3:D:113:DT:H5'	2.01	0.41
4:E:106:ARG:NH1	4:E:106:ARG:HG3	2.36	0.41
4:E:112:ALA:O	4:E:116:VAL:HG22	2.20	0.41
4:A:121:ARG:NH1	4:F:204:VAL:HG13	2.35	0.41
4:A:106:ARG:O	4:A:109:ASP:HB3	2.20	0.41
4:A:172:LEU:HA	4:A:172:LEU:HD23	1.88	0.41
4:A:85:VAL:HG23	4:A:129:GLU:OE1	2.21	0.41
4:B:336:VAL:O	4:B:340:GLU:HG3	2.20	0.41
4:E:66:ALA:HB3	4:E:99:HIS:NE2	2.36	0.41
4:F:44:MET:HB3	4:F:90:GLN:OE1	2.20	0.41
4:B:168:TYR:CD2	4:B:168:TYR:O	2.72	0.41
4:E:75:LEU:HD23	4:E:75:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:31:PHE:CD1	4:F:31:PHE:N	2.87	0.41
4:B:223:ARG:O	4:B:226:SER:N	2.53	0.41
4:B:58:LEU:O	4:B:58:LEU:CD1	2.55	0.41
4:F:27:LEU:HD12	4:F:30:MET:CE	2.50	0.41
4:F:89:GLN:O	4:F:91:HIS:N	2.53	0.41
4:A:182:VAL:O	4:A:184:ASP:N	2.53	0.41
4:B:139:ARG:HB2	4:B:168:TYR:OH	2.20	0.41
4:B:193:MET:SD	4:B:221:VAL:HB	2.60	0.41
4:B:75:LEU:HD23	4:B:75:LEU:HA	1.84	0.41
1:C:107:UMP:OP2	4:B:257:SER:HB3	2.20	0.41
2:Y:117:DG:OP2	4:F:320:ILE:HD13	2.20	0.41
4:F:318:VAL:O	4:F:322:MET:HB2	2.20	0.41
4:A:307:PRO:HG3	4:B:306:ILE:HD11	1.99	0.41
4:A:74:TYR:O	4:A:77:TYR:HB3	2.20	0.41
4:B:270:ARG:O	4:B:272:ILE:N	2.54	0.41
4:E:147:SER:OG	4:E:148:LEU:N	2.53	0.41
4:E:230:VAL:HG12	4:E:236:ASN:HB3	2.03	0.41
4:F:62:LYS:HB2	4:F:62:LYS:HZ2	1.82	0.41
4:A:277:ASP:HB3	4:A:284:LEU:HD13	2.03	0.41
4:A:325:ILE:HG13	4:A:325:ILE:O	2.21	0.41
4:A:328:LEU:HA	4:A:328:LEU:HD23	1.87	0.41
4:A:34:ARG:C	4:A:36:ALA:N	2.74	0.41
4:B:195:ILE:CG2	4:B:196:HIS:N	2.84	0.41
4:E:200:THR:HG21	4:E:205:SER:HB2	2.02	0.41
4:A:157:ASP:O	4:A:158:ILE:C	2.55	0.41
3:D:105:DA:C2	3:D:106:DC:C2	3.09	0.41
4:E:214:SER:OG	4:E:215:LEU:N	2.52	0.41
4:A:201:LYS:HB2	4:A:201:LYS:HE3	1.81	0.41
4:A:320:ILE:C	4:A:322:MET:H	2.24	0.41
4:B:71:VAL:O	4:B:74:TYR:HB3	2.21	0.41
3:H:106:DC:H4'	4:E:241:ARG:HG3	2.03	0.41
4:E:64:PHE:C	4:E:64:PHE:CD1	2.94	0.41
4:F:163:PHE:C	4:F:163:PHE:CD2	2.94	0.41
4:B:269:HIS:CG	4:B:285:ALA:HB1	2.56	0.40
4:B:320:ILE:O	4:B:323:ASN:N	2.54	0.40
4:B:83:LEU:HD23	4:B:83:LEU:HA	1.87	0.40
3:D:108:DT:H1'	3:D:109:DC:H5''	2.03	0.40
4:A:164:LEU:HD23	4:A:164:LEU:HA	1.86	0.40
4:B:104:LEU:HB3	4:B:105:PRO:HD2	2.03	0.40
4:B:116:VAL:CG1	4:B:117:MET:N	2.85	0.40
4:F:106:ARG:HD3	4:F:109:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:58:LEU:HG	4:A:58:LEU:O	2.22	0.40
4:B:74:TYR:O	4:B:77:TYR:N	2.55	0.40
4:E:185:ILE:HG21	4:E:193:MET:HE1	2.02	0.40
4:E:78:LEU:CD1	4:E:78:LEU:N	2.83	0.40
4:F:233:ASP:HB3	4:F:236:ASN:ND2	2.37	0.40
4:F:297:ARG:O	4:F:299:MET:N	2.54	0.40
4:A:163:PHE:O	4:A:164:LEU:C	2.60	0.40
4:B:171:LEU:HD13	4:B:312:ALA:O	2.20	0.40
4:B:330:SER:O	4:B:332:THR:OG1	2.37	0.40
4:E:119:ARG:O	4:E:123:GLU:HB2	2.21	0.40
4:E:188:THR:C	4:E:190:GLY:H	2.24	0.40
4:A:11:LEU:HD13	4:A:14:LEU:CD2	2.49	0.40
4:E:171:LEU:HD12	4:E:313:GLY:HA2	2.03	0.40
4:F:85:VAL:HG23	4:F:129:GLU:OE2	2.22	0.40
4:F:48:VAL:HG22	4:F:91:HIS:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	330/343 (96%)	274 (83%)	42 (13%)	14 (4%)	3	20
4	B	320/343 (93%)	232 (72%)	64 (20%)	24 (8%)	1	7
4	E	319/343 (93%)	239 (75%)	63 (20%)	17 (5%)	2	15
4	F	320/343 (93%)	259 (81%)	42 (13%)	19 (6%)	1	12
All	All	1289/1372 (94%)	1004 (78%)	211 (16%)	74 (6%)	1	14

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	21	ASP
4	A	200	THR
4	B	148	LEU
4	B	248	ALA
4	B	327	ASN
4	E	58	LEU
4	E	149	MET
4	E	182	VAL
4	E	232	ASP
4	E	257	SER
4	E	277	ASP
4	F	134	ALA
4	F	275	ALA
4	F	277	ASP
4	F	324	TYR
4	F	327	ASN
4	F	328	LEU
4	F	330	SER
4	A	12	PRO
4	A	35	GLN
4	A	111	ASN
4	A	205	SER
4	A	277	ASP
4	A	318	VAL
4	B	54	ALA
4	B	58	LEU
4	B	111	ASN
4	B	147	SER
4	B	227	VAL
4	B	235	ASN
4	B	249	ALA
4	B	271	LEU
4	B	286	TRP
4	B	331	GLU
4	E	200	THR
4	E	208	GLY
4	E	214	SER
4	F	90	GLN
4	F	227	VAL
4	F	274	GLY
4	F	334	ALA
4	A	182	VAL
4	B	68	PRO

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Mol	Chain	Res	Type
4	B	81	ARG
4	B	250	PRO
4	E	147	SER
4	E	157	ASP
4	E	198	GLY
4	E	286	TRP
4	F	59	ASN
4	F	89	GLN
4	F	332	THR
4	A	183	LYS
4	A	244	LYS
4	A	279	SER
4	B	55	TRP
4	B	160	ASN
4	B	302	ALA
4	B	335	MET
4	E	102	SER
4	E	244	LYS
4	F	108	SER
4	F	127	ALA
4	F	298	ASP
4	A	193	MET
4	B	128	GLY
4	B	328	LEU
4	E	279	SER
4	F	54	ALA
4	F	323	ASN
4	A	25	LYS
4	B	226	SER
4	E	246	GLY
4	B	23	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	277/287 (96%)	240 (87%)	37 (13%)	4	18
4	B	269/287 (94%)	242 (90%)	27 (10%)	7	30
4	E	268/287 (93%)	230 (86%)	38 (14%)	3	15
4	F	269/287 (94%)	229 (85%)	40 (15%)	3	14
All	All	1083/1148 (94%)	941 (87%)	142 (13%)	4	19

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	19	THR
4	A	24	ARG
4	A	34	ARG
4	A	39	GLU
4	A	61	ARG
4	A	63	TRP
4	A	67	GLU
4	A	68	PRO
4	A	69	GLU
4	A	87	THR
4	A	90	GLN
4	A	92	LEU
4	A	95	LEU
4	A	98	LEU
4	A	101	ARG
4	A	108	SER
4	A	140	THR
4	A	144	GLN
4	A	161	LEU
4	A	169	ASN
4	A	170	THR
4	A	187	ARG
4	A	203	LEU
4	A	214	SER
4	A	220	LEU
4	A	225	ILE
4	A	232	ASP
4	A	238	LEU
4	A	242	VAL
4	A	247	VAL

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Mol	Chain	Res	Type
4	A	256	LEU
4	A	258	THR
4	A	278	ASP
4	A	289	HIS
4	A	311	GLN
4	A	316	THR
4	A	317	ASN
4	B	21	ASP
4	B	27	LEU
4	B	30	MET
4	B	35	GLN
4	B	56	CYS
4	B	58	LEU
4	B	60	ASN
4	B	63	TRP
4	B	95	LEU
4	B	101	ARG
4	B	106	ARG
4	B	108	SER
4	B	118	ARG
4	B	133	GLN
4	B	140	THR
4	B	144	GLN
4	B	156	GLN
4	B	171	LEU
4	B	176	GLU
4	B	206	THR
4	B	242	VAL
4	B	261	LEU
4	B	271	LEU
4	B	304	VAL
4	B	311	GLN
4	B	318	VAL
4	B	319	ASN
4	E	27	LEU
4	E	30	MET
4	E	38	SER
4	E	48	VAL
4	E	57	LYS
4	E	58	LEU
4	E	60	ASN
4	E	89	GLN

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Mol	Chain	Res	Type
4	E	92	LEU
4	E	95	LEU
4	E	104	LEU
4	E	106	ARG
4	E	115	LEU
4	E	116	VAL
4	E	117	MET
4	E	132	LYS
4	E	140	THR
4	E	147	SER
4	E	148	LEU
4	E	151	ASN
4	E	153	ASP
4	E	154	ARG
4	E	157	ASP
4	E	158	ILE
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	220	LEU
4	E	243	ARG
4	E	256	LEU
4	E	289	HIS
4	E	311	GLN
4	E	316	THR
4	E	317	ASN
4	E	323	ASN
4	F	27	LEU
4	F	29	ASP
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	76	LEU
4	F	77	TYR
4	F	81	ARG
4	F	90	GLN

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Mol	Chain	Res	Type
4	F	95	LEU
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	153	ASP
4	F	155	CYS
4	F	169	ASN
4	F	171	LEU
4	F	193	MET
4	F	205	SER
4	F	206	THR
4	F	223	ARG
4	F	243	ARG
4	F	253	THR
4	F	273	TYR
4	F	278	ASP
4	F	284	LEU
4	F	289	HIS
4	F	297	ARG
4	F	318	VAL
4	F	322	MET
4	F	323	ASN
4	F	325	ILE
4	F	329	ASP
4	F	332	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	89	GLN
4	A	90	GLN
4	A	133	GLN
4	A	196	HIS
4	A	311	GLN
4	B	35	GLN
4	B	40	HIS
4	B	60	ASN
4	B	90	GLN
4	B	156	GLN

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Mol	Chain	Res	Type
4	B	235	ASN
4	B	236	ASN
4	B	255	GLN
4	B	319	ASN
4	E	26	ASN
4	E	35	GLN
4	E	79	GLN
4	E	89	GLN
4	E	90	GLN
4	E	94	GLN
4	E	144	GLN
4	E	235	ASN
4	E	317	ASN
4	E	323	ASN
4	F	35	GLN
4	F	59	ASN
4	F	94	GLN
4	F	96	ASN
4	F	111	ASN
4	F	133	GLN
4	F	144	GLN
4	F	236	ASN
4	F	281	GLN
4	F	317	ASN
4	F	319	ASN
4	F	327	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	14,20,21	1.19	1 (7%)	14,28,31	1.29	1 (7%)
1	A3P	C	115	1,4	18,26,29	1.99	3 (16%)	17,37,45	1.75	6 (35%)
1	UMP	G	107	1,3	14,20,21	1.11	1 (7%)	14,28,31	1.19	1 (7%)
1	A3P	G	115	1,3,4	18,26,29	1.15	1 (5%)	17,37,45	1.58	1 (5%)

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	-	1/4/21/22	0/2/2/2
1	A3P	C	115	1,4	-	2/5/25/31	0/3/3/3
1	UMP	G	107	1,3	-	0/4/21/22	0/2/2/2
1	A3P	G	115	1,3,4	-	0/5/25/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	A3P	O4'-C4'	-6.70	1.30	1.45
1	C	115	A3P	O3'-C3'	-3.45	1.41	1.45
1	C	107	UMP	C4-N3	3.09	1.38	1.33
1	G	115	A3P	O3'-C3'	-3.08	1.41	1.45
1	G	107	UMP	C4-N3	2.98	1.38	1.33
1	C	115	A3P	O5'-C5'	-2.14	1.39	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	115	A3P	C2'-C1'-N9	4.36	124.33	114.27
1	C	107	UMP	C5-C4-N3	-3.97	114.58	123.31
1	G	107	UMP	C5-C4-N3	-3.94	114.64	123.31
1	C	115	A3P	O4'-C4'-C5'	-3.31	98.47	109.37
1	C	115	A3P	C2'-C1'-N9	2.92	121.00	114.27
1	C	115	A3P	O3'-C3'-C4'	-2.64	100.96	108.66
1	C	115	A3P	C5-C6-N6	2.31	123.86	120.35
1	C	115	A3P	C4'-O4'-C1'	-2.12	104.34	109.45
1	C	115	A3P	C5'-C4'-C3'	2.11	119.34	114.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	115	A3P	O4'-C4'-C5'-O5'
1	C	115	A3P	C3'-C4'-C5'-O5'
1	C	107	UMP	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	107	UMP	3	0
1	G	107	UMP	2	0
1	G	115	A3P	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	14/16 (87%)	-0.33	0 100 100	26, 58, 80, 81	0
1	G	14/16 (87%)	-0.19	0 100 100	31, 58, 109, 136	0
2	X	21/21 (100%)	0.61	4 (19%) 1 1	22, 43, 86, 97	4 (19%)
2	Y	21/21 (100%)	0.62	3 (14%) 2 1	39, 72, 93, 99	3 (14%)
3	D	37/37 (100%)	-0.40	0 100 100	21, 44, 79, 89	0
3	H	37/37 (100%)	-0.23	0 100 100	31, 61, 91, 108	0
4	A	332/343 (96%)	-0.31	1 (0%) 94 92	15, 40, 80, 121	0
4	B	322/343 (93%)	-0.02	4 (1%) 79 67	28, 59, 91, 126	0
4	E	321/343 (93%)	0.07	4 (1%) 79 67	35, 69, 101, 137	0
4	F	322/343 (93%)	-0.25	2 (0%) 89 83	23, 52, 86, 126	0
All	All	1441/1520 (94%)	-0.12	18 (1%) 79 67	15, 56, 93, 137	7 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	117	DG	7.2
2	Y	118	DT	6.9
2	Y	117	DG	6.7
2	Y	119	DA	5.6
2	X	118	DT	5.6
2	X	119	DA	5.6
4	E	155	CYS	3.7
4	F	331	GLU	3.6
4	E	240	CYS	3.6
4	A	19	THR	3.3
4	F	330	SER	3.2
2	X	120	DT	2.9
4	E	49	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
4	B	155	CYS	2.7
4	E	63	TRP	2.3
4	B	330	SER	2.2
4	B	244	LYS	2.0
4	B	49	CYS	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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	A3P	C	115	24/27	0.93	0.22	29,42,50,56	0
1	UMP	C	107	19/20	0.96	0.15	48,56,62,65	0
1	UMP	G	107	19/20	0.96	0.18	51,56,60,63	0
1	A3P	G	115	24/27	0.96	0.18	23,27,36,44	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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	310	1/1	0.64	0.31	46,46,46,46	0
6	MG	H	307	1/1	0.71	0.55	70,70,70,70	1
6	MG	A	344	1/1	0.86	0.34	43,43,43,43	0
6	MG	F	344	1/1	0.86	1.11	25,25,25,25	1
6	MG	A	345	1/1	0.88	0.41	48,48,48,48	0
6	MG	A	347	1/1	0.91	0.29	42,42,42,42	0
6	MG	A	346	1/1	0.96	0.57	36,36,36,36	0
5	IOD	C	1107	1/1	0.97	0.10	53,53,53,53	1
5	IOD	F	2107	1/1	0.97	0.15	54,54,54,54	1

6.5 Other polymers [i](#)

There are no such residues in this entry.