Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 08:56 PM EDT

PDB ID	:	1Q3U
Title	:	Crystal structure of a wild-type Cre recombinase-loxP synapse: pre-cleavage complex
Authors	:	Ennifar, E.; Meyer, J.E.W.; Buchholz, F.; Stewart, A.F.; Suck, D.
Deposited on	:	2003-08-01
Resolution	:	2.90 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 (i) symbol.

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

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

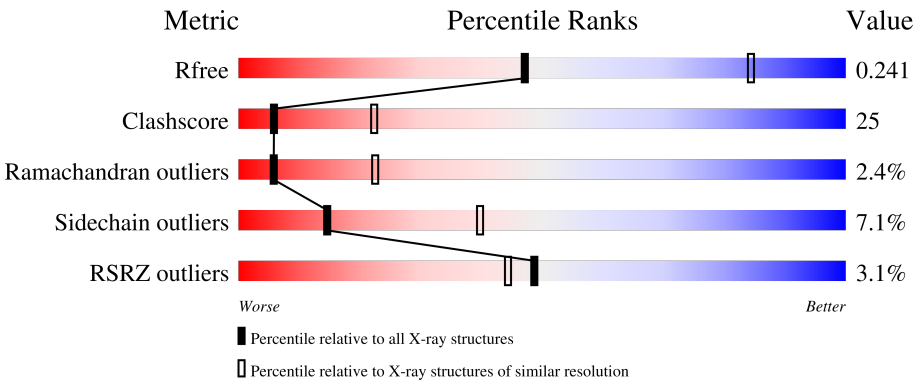
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	37	32% 65% •
1	G	37	3% 41% 54% 5%
2	D	37	3% 32% 68%
2	H	37	3% 35% 62% •
3	A	347	4% 57% 32% 7% •

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Mol	Chain	Length	Quality of chain
3	B	347	2% 51% 36% 5% 7%
3	E	347	5% 50% 38% • 7%
3	F	347	% 57% 31% • 7%

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
5	MG	H	307	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13299 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called loxP DNA.

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

- Molecule 2 is a DNA chain called loxP DNA.

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

- Molecule 3 is a protein called Cre recombinase.

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is IODIDE ION (three-letter code: IOD) (formula: I).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0
5	D	2	Total Mg 2 2	0	0
5	G	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	A	4	Total Mg 4 4	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is water.

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

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

3 Residue-property plots (i)

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

• Molecule 1: loxP DNA

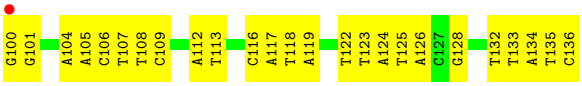
Chain C:

• Molecule 1: loxP DNA

Chain G:

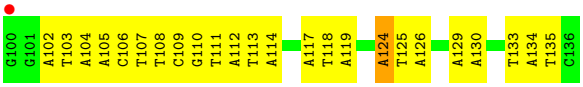
• Molecule 2: loxP DNA

Chain D:



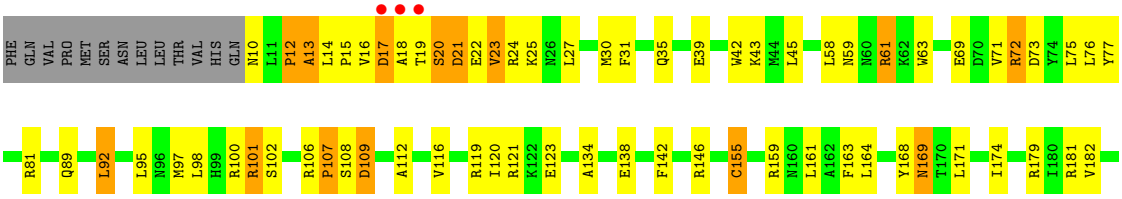
• Molecule 2: loxP DNA

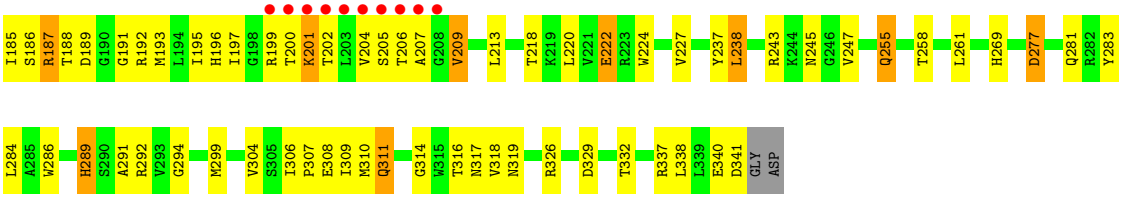
Chain H:



• Molecule 3: Cre recombinase

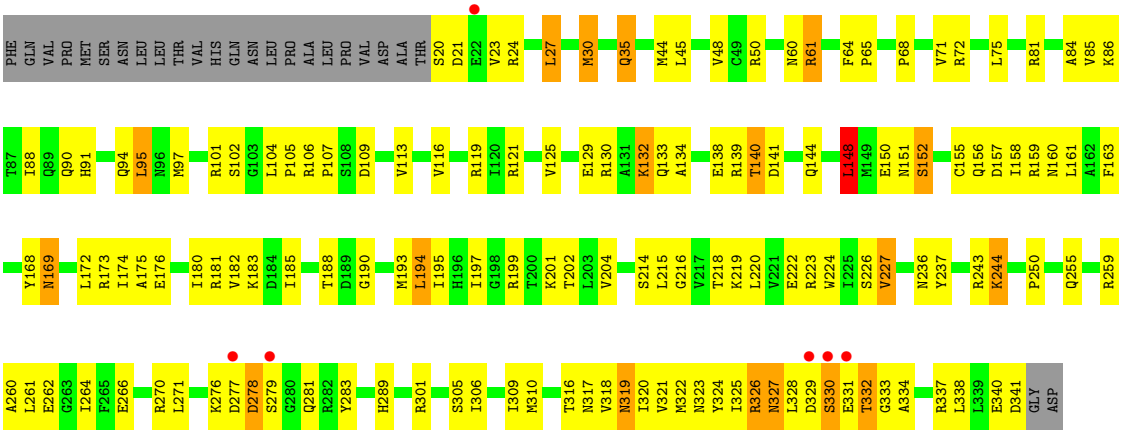
Chain A:





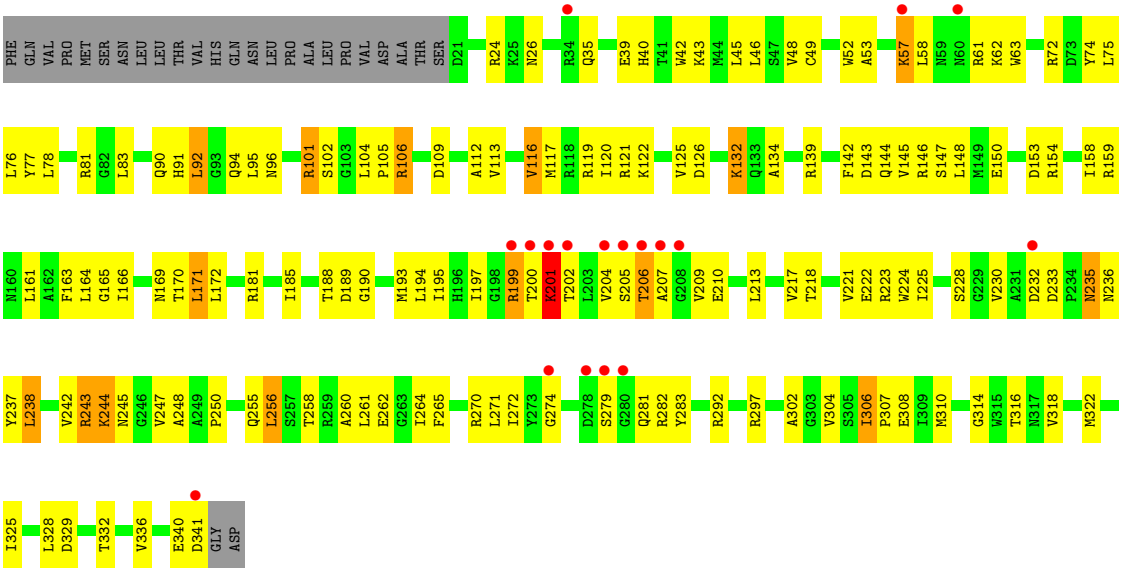
• Molecule 3: Cre recombinase

Chain B:



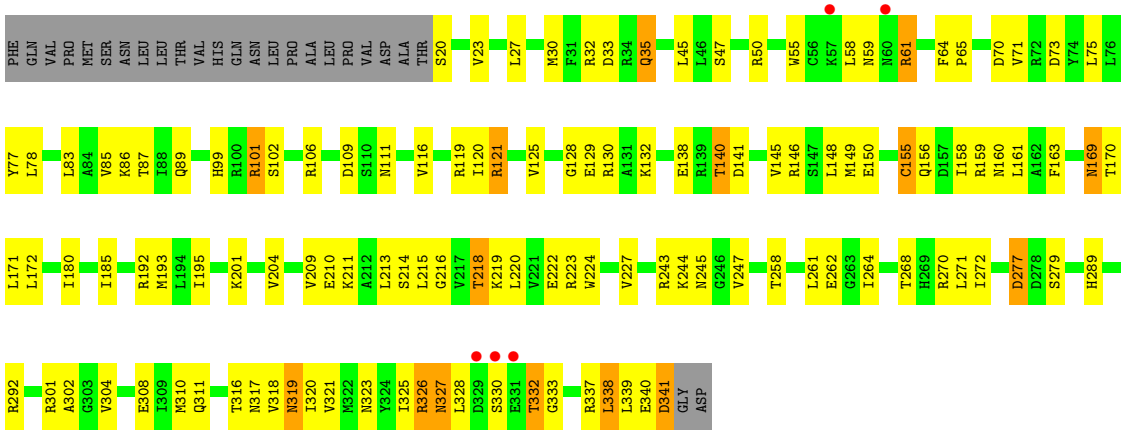
• Molecule 3: Cre recombinase

Chain E:



• Molecule 3: Cre recombinase

Chain F:


PHE GLN VAL PRO MET SER ASN LEU LEU THR VAL HIS GLN ASN LEU PRO ALA LEU PRO VAL ASP ALA THR S20 V23 L27 M30 F31 R32 D33 R34 Q35 L45 L46 S47 R50 W55 C56 K57 L58 N59 N60 R61 F64 P65 D70 V71 R72 D73 Y74 L75 L76
Y77 L78 L83 A84 V85 K86 T87 I88 Q89 H99 R100 R101 S102 R106 D109 S110 N111 V116 R119 I120 R121 V125 G128 E129 R130 A131 K132 E138 R139 T140 D141 V145 R146 S147 L148 M149 E150 C155 Q156 D157 I158 R159 N160 L161 A162 F163 N169 T170
L171 L172 I180 I185 R192 M193 L194 I195 K201 V204 V209 E210 K211 A212 L213 S214 L215 G216 V217 T218 K219 L220 V221 E222 R223 W224 V227 R243 K244 N245 G246 V247 T258 L261 E262 G263 I264 T268 H269 R270 L271 I272 D277 D278 S279 H289
R292 R301 A302 G303 V304 E308 I309 M310 Q311 T316 N317 V318 N319 I320 V321 M322 N323 Y324 I325 R326 N327 L328 D329 S330 E331 T332 G333 R337 L338 L339 E340 D341 GLY ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.99Å 161.06Å 196.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.03 – 2.90 20.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.03-2.90) 99.2 (20.03-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.244 0.215 , 0.241	Depositor DCC
R_{free} test set	3492 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13299	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	C	0.57	0/823	0.85	0/1266
1	G	0.46	0/823	0.80	0/1266
2	D	0.55	0/848	0.82	0/1307
2	H	0.45	0/848	0.78	0/1307
3	A	0.44	0/2663	0.67	0/3595
3	B	0.37	0/2591	0.61	0/3493
3	E	0.34	0/2585	0.58	0/3485
3	F	0.39	0/2591	0.62	0/3493
All	All	0.42	0/13772	0.68	0/19212

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	3
2	D	0	2
2	H	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	108	DT	Sidechain

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Mol	Chain	Res	Type	Group
2	D	104	DA	Sidechain
2	D	126	DA	Sidechain
1	G	115	DA	Sidechain
1	G	117	DG	Sidechain
1	G	124	DA	Sidechain
2	H	124	DA	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	754	0	420	35	0
1	G	754	0	420	20	0
2	D	756	0	421	37	0
2	H	756	0	421	32	0
3	A	2620	0	2643	130	0
3	B	2550	0	2571	143	0
3	E	2544	0	2566	186	0
3	F	2550	0	2571	128	0
4	C	1	0	0	1	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	2	0	0	0	0
6	F	1	0	0	0	0
All	All	13299	0	12033	636	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 25.

All (636) 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)
2:H:105:DA:H2"	2:H:106:DC:H5"	1.24	1.18
2:D:132:DT:H2"	2:D:133:DT:H5"	1.36	1.03
3:A:299:MET:HE1	3:A:309:ILE:HA	1.41	1.01
1:C:105:DA:H2"	1:C:106:DC:H5"	1.42	1.00
3:E:199:ARG:HA	3:F:130:ARG:HH21	1.25	1.00
3:A:10:ASN:HD22	3:A:31:PHE:HE2	1.09	0.97
3:E:199:ARG:HA	3:F:130:ARG:NH2	1.80	0.97
3:F:214:SER:O	3:F:218:THR:HG22	1.65	0.96
3:F:277:ASP:OD2	3:F:279:SER:HB2	1.68	0.94
3:A:72:ARG:HG3	3:A:116:VAL:HG21	1.47	0.93
1:C:112:DA:H62	3:B:44:MET:CE	1.80	0.93
3:F:333:GLY:HA2	3:F:337:ARG:HG3	1.48	0.92
2:H:134:DA:H2"	2:H:135:DT:H5"	1.51	0.92
3:F:35:GLN:H	3:F:35:GLN:HE21	1.19	0.91
3:B:332:THR:HG22	3:B:333:GLY:H	1.32	0.91
2:H:134:DA:H2"	2:H:135:DT:C5'	2.01	0.91
1:G:131:DG:H2"	1:G:132:DT:C5'	2.00	0.91
3:E:169:ASN:ND2	3:E:213:LEU:HA	1.84	0.91
2:D:108:DT:H2"	2:D:109:DC:H5'	1.53	0.90
3:A:15:PRO:HB2	3:A:18:ALA:HB3	1.53	0.90
3:B:319:ASN:HD22	3:B:320:ILE:H	1.15	0.89
1:G:105:DA:H2"	1:G:106:DC:H5"	1.51	0.89
3:E:193:MET:HG3	3:E:218:THR:HG23	1.54	0.89
2:H:105:DA:C2'	2:H:106:DC:H5"	2.02	0.88
1:G:131:DG:H2"	1:G:132:DT:H5"	1.55	0.87
3:F:317:ASN:ND2	3:F:319:ASN:H	1.72	0.87
3:E:154:ARG:HB3	3:E:154:ARG:NH1	1.91	0.86
3:E:243:ARG:HG3	3:E:243:ARG:HH11	1.40	0.86
3:E:48:VAL:HG21	3:E:91:HIS:HA	1.59	0.85
3:A:277:ASP:HB3	3:A:284:LEU:HD13	1.58	0.85
3:E:53:ALA:O	3:E:57:LYS:HD3	1.77	0.84
3:F:121:ARG:HG3	3:F:121:ARG:HH11	1.41	0.84
3:F:35:GLN:H	3:F:35:GLN:NE2	1.75	0.84
3:E:169:ASN:HD22	3:E:213:LEU:HD13	1.43	0.82
3:B:319:ASN:ND2	3:B:320:ILE:H	1.77	0.82
3:A:72:ARG:CG	3:A:116:VAL:HG21	2.10	0.81
1:C:112:DA:H62	3:B:44:MET:HE3	1.46	0.80
2:H:106:DC:H2'	2:H:107:DT:H72	1.63	0.80
3:A:299:MET:CE	3:A:309:ILE:HA	2.12	0.80
2:D:132:DT:C2'	2:D:133:DT:H5"	2.11	0.80
3:E:204:VAL:HG13	3:F:323:ASN:HD21	1.48	0.79
3:A:106:ARG:O	3:A:109:ASP:HB2	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:306:ILE:O	3:B:310:MET:HG2	1.83	0.78
3:E:221:VAL:O	3:E:225:ILE:HG13	1.84	0.78
3:A:10:ASN:ND2	3:A:31:PHE:HE2	1.82	0.78
3:F:180:ILE:HD13	3:F:195:ILE:HG21	1.64	0.78
3:E:169:ASN:HD21	3:E:213:LEU:HA	1.49	0.77
2:H:102:DA:H2"	2:H:103:DT:O5'	1.83	0.77
2:D:122:DT:H5"	3:B:97:MET:HE2	1.67	0.76
3:B:319:ASN:HD22	3:B:320:ILE:N	1.84	0.76
3:E:72:ARG:HG3	3:E:116:VAL:HG11	1.68	0.76
3:E:48:VAL:HG11	3:E:94:GLN:HB2	1.67	0.75
3:E:169:ASN:OD1	3:F:339:LEU:HD12	1.86	0.75
3:F:321:VAL:O	3:F:325:ILE:HG12	1.85	0.75
3:B:332:THR:HG22	3:B:333:GLY:N	2.01	0.75
1:C:108:DT:H2"	1:C:109:DC:H5'	1.68	0.75
3:F:185:ILE:HD13	3:F:193:MET:HE3	1.67	0.75
3:B:71:VAL:O	3:B:75:LEU:HG	1.88	0.74
3:A:192:ARG:HH11	3:B:331:GLU:HG2	1.53	0.74
3:A:72:ARG:HD2	3:A:116:VAL:HG21	1.70	0.74
3:E:217:VAL:O	3:E:221:VAL:HG23	1.89	0.73
3:F:145:VAL:HG13	3:F:149:MET:CE	2.19	0.73
3:F:317:ASN:ND2	3:F:319:ASN:HB2	2.04	0.73
3:A:193:MET:HG3	3:A:218:THR:HG23	1.71	0.73
3:E:154:ARG:HB3	3:E:154:ARG:HH11	1.53	0.72
3:A:317:ASN:HB3	3:A:319:ASN:OD1	1.89	0.72
2:H:108:DT:H2"	2:H:109:DC:H5'	1.71	0.72
3:E:117:MET:HE2	3:E:117:MET:HA	1.70	0.72
3:E:230:VAL:HG12	3:E:236:ASN:HB3	1.71	0.71
2:D:100:DG:H2"	2:D:101:DG:O5'	1.91	0.71
1:G:131:DG:H2"	1:G:132:DT:H5'	1.71	0.71
3:A:200:THR:HG22	3:A:201:LYS:HG2	1.72	0.71
2:D:135:DT:H1'	3:B:244:LYS:HD2	1.73	0.71
3:E:62:LYS:H	3:E:62:LYS:HD2	1.54	0.70
3:F:146:ARG:O	3:F:150:GLU:HB2	1.91	0.70
3:A:72:ARG:CD	3:A:116:VAL:HG21	2.21	0.69
3:E:185:ILE:HG21	3:E:193:MET:CE	2.23	0.69
3:B:180:ILE:HD13	3:B:195:ILE:HG21	1.73	0.69
1:C:105:DA:C2'	1:C:106:DC:H5"	2.22	0.69
2:H:103:DT:H2"	2:H:104:DA:C8	2.27	0.69
2:H:106:DC:H2'	2:H:107:DT:C7	2.22	0.69
3:E:48:VAL:HG11	3:E:94:GLN:CB	2.22	0.69
3:A:161:LEU:HD22	3:A:220:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:235:ASN:N	3:E:235:ASN:HD22	1.90	0.69
3:E:35:GLN:HB2	3:F:119:ARG:HG3	1.74	0.68
3:B:35:GLN:HB3	3:E:119:ARG:HG3	1.75	0.68
3:F:85:VAL:O	3:F:89:GLN:HG3	1.93	0.68
3:F:160:ASN:ND2	3:F:264:ILE:HG23	2.09	0.68
1:C:103:DT:H2"	1:C:104:DA:C8	2.29	0.68
3:A:187:ARG:HH11	3:A:187:ARG:HB3	1.57	0.68
3:B:133:GLN:HE22	3:B:324:TYR:HA	1.57	0.68
3:E:258:THR:O	3:E:262:GLU:HG3	1.94	0.68
2:H:134:DA:C2'	2:H:135:DT:H5"	2.23	0.68
3:E:159:ARG:HB2	3:E:224:TRP:CZ3	2.28	0.68
3:A:20:SER:O	3:A:21:ASP:HB2	1.93	0.67
3:E:185:ILE:HG21	3:E:193:MET:HE2	1.77	0.67
3:E:209:VAL:HB	3:F:326:ARG:NH2	2.09	0.67
3:A:197:ILE:O	3:A:197:ILE:HG13	1.95	0.67
3:B:159:ARG:HB2	3:B:224:TRP:CZ3	2.30	0.67
3:F:218:THR:O	3:F:222:GLU:HG3	1.95	0.67
2:D:133:DT:H2"	2:D:134:DA:C8	2.31	0.66
3:E:121:ARG:O	3:E:125:VAL:HG12	1.95	0.66
3:F:121:ARG:HH11	3:F:121:ARG:CG	2.09	0.66
2:H:134:DA:H2"	2:H:135:DT:H5'	1.76	0.66
3:A:16:VAL:HA	3:A:24:ARG:NH2	2.10	0.66
3:E:230:VAL:HG22	3:E:250:PRO:HG3	1.78	0.66
3:E:228:SER:OG	3:E:230:VAL:HG23	1.95	0.66
3:A:207:ALA:HA	3:A:314:GLY:HA3	1.78	0.66
3:B:30:MET:SD	3:B:101:ARG:HG2	2.37	0.65
3:E:207:ALA:HA	3:E:314:GLY:HA2	1.78	0.65
3:F:243:ARG:HG2	3:F:243:ARG:HH11	1.61	0.65
3:A:59:ASN:O	3:A:61:ARG:HD3	1.97	0.65
3:E:134:ALA:HA	3:E:283:TYR:CD2	2.31	0.65
2:H:104:DA:H1'	3:E:244:LYS:HB3	1.78	0.64
3:A:14:LEU:HG	3:A:27:LEU:CD2	2.27	0.64
3:A:100:ARG:HH21	3:A:101:ARG:CZ	2.09	0.64
3:B:204:VAL:HG23	3:E:125:VAL:HG11	1.79	0.64
3:F:158:ILE:HG12	3:F:223:ARG:NH1	2.12	0.64
3:E:92:LEU:HD22	3:E:96:ASN:HD21	1.63	0.64
3:E:204:VAL:HG12	3:E:206:THR:HG23	1.78	0.64
3:E:210:GLU:CG	3:F:326:ARG:HH21	2.11	0.64
3:A:161:LEU:HD23	3:A:161:LEU:O	1.98	0.64
3:A:107:PRO:C	3:A:109:ASP:H	2.01	0.63
1:C:106:DC:H2"	1:C:107:UMP:O5'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:DA:C2'	1:G:106:DC:H5"	2.26	0.63
3:F:35:GLN:HE21	3:F:35:GLN:N	1.93	0.63
3:E:132:LYS:NZ	3:E:132:LYS:HB3	2.14	0.63
3:E:163:PHE:HE2	3:E:261:LEU:HD13	1.64	0.63
1:C:133:DT:H2"	1:C:134:DA:C8	2.34	0.63
3:B:155:CYS:SG	3:B:227:VAL:HG12	2.39	0.62
2:D:112:DA:OP1	3:A:81:ARG:NH2	2.32	0.62
3:E:204:VAL:HG13	3:F:323:ASN:ND2	2.13	0.62
3:B:214:SER:O	3:B:218:THR:HG22	2.00	0.62
3:A:15:PRO:HB2	3:A:18:ALA:CB	2.26	0.62
3:B:134:ALA:HA	3:B:283:TYR:CD2	2.34	0.62
3:E:101:ARG:HA	3:F:111:ASN:HD21	1.64	0.62
3:A:192:ARG:NH1	3:B:331:GLU:HG2	2.13	0.62
3:A:311:GLN:HG3	3:B:325:ILE:CG2	2.29	0.62
3:E:197:ILE:HG13	3:E:197:ILE:O	1.99	0.62
3:A:205:SER:C	3:B:326:ARG:HH21	2.03	0.62
3:E:318:VAL:O	3:E:322:MET:HG2	2.00	0.62
3:B:163:PHE:CE1	3:B:261:LEU:HD22	2.34	0.62
2:D:119:DA:OP1	3:B:121:ARG:NH1	2.32	0.62
3:A:179:ARG:HG2	3:A:255:GLN:HE22	1.63	0.62
3:F:328:LEU:CB	3:F:332:THR:HA	2.30	0.61
3:A:243:ARG:HG2	3:A:243:ARG:HH11	1.64	0.61
3:E:209:VAL:HB	3:F:326:ARG:HH22	1.63	0.61
3:B:158:ILE:HD12	3:B:223:ARG:HE	1.64	0.61
2:D:112:DA:H2"	2:D:113:DT:C5'	2.31	0.61
3:A:119:ARG:O	3:A:123:GLU:HG3	2.01	0.61
3:B:319:ASN:O	3:B:320:ILE:HB	2.01	0.61
2:D:122:DT:H5"	3:B:97:MET:CE	2.31	0.61
3:E:223:ARG:HG3	3:E:223:ARG:HH11	1.66	0.61
1:C:111:DT:OP2	3:B:50:ARG:NH1	2.34	0.61
3:E:194:LEU:HD11	3:E:210:GLU:HB3	1.83	0.61
3:E:166:ILE:HG12	3:E:213:LEU:HD11	1.81	0.61
1:G:131:DG:C2'	1:G:132:DT:H5"	2.26	0.60
3:A:326:ARG:HD3	3:F:210:GLU:HG3	1.82	0.60
2:D:108:DT:C2'	2:D:109:DC:H5'	2.30	0.60
3:E:188:THR:HG22	3:E:189:ASP:N	2.16	0.60
3:A:23:VAL:O	3:A:27:LEU:HB2	2.01	0.60
3:E:163:PHE:CE2	3:E:261:LEU:HD22	2.37	0.60
1:C:103:DT:H3	2:D:134:DA:H61	1.49	0.60
3:F:272:ILE:HG22	3:F:272:ILE:O	2.02	0.59
3:A:311:GLN:HG3	3:B:325:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:ARG:NH1	3:F:70:ASP:OD1	2.36	0.59
3:B:333:GLY:HA2	3:B:337:ARG:HG3	1.85	0.59
3:A:159:ARG:HB2	3:A:224:TRP:CZ3	2.37	0.59
3:E:210:GLU:CB	3:F:326:ARG:HH21	2.16	0.59
3:B:236:ASN:HD22	3:B:250:PRO:HB3	1.66	0.58
3:A:77:TYR:OH	3:A:81:ARG:HD2	2.02	0.58
1:C:100:DC:H2'	1:C:101:DG:C8	2.38	0.58
3:B:319:ASN:ND2	3:B:320:ILE:N	2.49	0.58
3:F:145:VAL:HG13	3:F:149:MET:HE2	1.85	0.58
3:B:90:GLN:NE2	3:B:94:GLN:HE21	2.02	0.58
3:E:205:SER:O	3:E:207:ALA:N	2.35	0.58
3:F:161:LEU:HG	3:F:220:LEU:HD13	1.85	0.58
3:F:271:LEU:HD13	3:F:271:LEU:O	2.04	0.58
3:A:12:PRO:O	3:A:13:ALA:HB2	2.04	0.58
3:E:271:LEU:HD23	3:E:271:LEU:O	2.04	0.58
3:F:99:HIS:O	3:F:102:SER:HB2	2.02	0.58
1:C:116:DT:H4'	3:B:202:THR:HG21	1.86	0.57
3:E:90:GLN:HE21	3:E:94:GLN:HG2	1.69	0.57
3:B:161:LEU:HG	3:B:220:LEU:HD13	1.86	0.57
3:A:35:GLN:HB2	3:B:119:ARG:HG3	1.86	0.57
3:B:151:ASN:O	3:B:152:SER:C	2.43	0.57
3:A:14:LEU:HG	3:A:27:LEU:HD23	1.85	0.57
3:E:233:ASP:O	3:E:236:ASN:HB2	2.04	0.57
3:E:146:ARG:O	3:E:150:GLU:HB2	2.04	0.57
3:A:14:LEU:HB3	3:A:19:THR:HG21	1.85	0.57
3:B:113:VAL:O	3:B:116:VAL:HG12	2.04	0.57
3:F:332:THR:HG22	3:F:333:GLY:H	1.70	0.57
3:B:218:THR:O	3:B:222:GLU:HG3	2.05	0.57
3:E:74:TYR:CZ	3:E:78:LEU:HD21	2.40	0.57
2:H:114:DA:H5"	3:E:132:LYS:O	2.05	0.56
3:B:90:GLN:HE22	3:B:94:GLN:HE21	1.53	0.56
3:B:262:GLU:O	3:B:266:GLU:HG3	2.04	0.56
3:E:236:ASN:ND2	3:E:250:PRO:HB3	2.20	0.56
3:F:159:ARG:HB2	3:F:224:TRP:CZ3	2.39	0.56
2:D:132:DT:H2"	2:D:133:DT:C5'	2.25	0.56
1:G:100:DC:H2"	1:G:101:DG:O5'	2.06	0.56
3:F:116:VAL:O	3:F:120:ILE:HG13	2.05	0.56
2:D:112:DA:H2"	2:D:113:DT:H5'	1.88	0.56
3:A:161:LEU:CD2	3:A:220:LEU:HD13	2.34	0.56
3:F:30:MET:SD	3:F:101:ARG:HG2	2.46	0.56
3:A:30:MET:HE2	3:A:42:TRP:HH2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:328:LEU:HB2	3:F:332:THR:HA	1.87	0.56
3:B:182:VAL:HG23	3:B:236:ASN:O	2.05	0.56
3:A:310:MET:SD	3:A:318:VAL:HG12	2.45	0.56
3:E:170:THR:OG1	3:E:172:LEU:HD12	2.06	0.56
3:F:185:ILE:HD13	3:F:193:MET:CE	2.35	0.56
3:A:100:ARG:NH2	3:A:101:ARG:CZ	2.69	0.56
3:F:121:ARG:O	3:F:125:VAL:HG23	2.06	0.56
3:A:72:ARG:HD2	3:A:116:VAL:CG2	2.35	0.56
3:A:243:ARG:HG2	3:A:243:ARG:NH1	2.21	0.55
3:E:39:GLU:HG3	3:E:40:HIS:N	2.21	0.55
3:E:193:MET:CG	3:E:218:THR:HG23	2.33	0.55
3:A:12:PRO:HB2	3:A:63:TRP:CZ2	2.41	0.55
3:B:188:THR:HG23	3:B:194:LEU:CD2	2.36	0.55
3:E:279:SER:C	3:E:281:GLN:H	2.10	0.55
1:C:102:DA:H1'	1:C:103:DT:H5"	1.89	0.55
3:E:106:ARG:HG2	3:E:109:ASP:OD2	2.06	0.55
1:C:109:DC:H2"	1:C:110:DG:C8	2.42	0.55
3:B:236:ASN:ND2	3:B:250:PRO:HB3	2.21	0.55
3:F:216:GLY:O	3:F:219:LYS:HB2	2.07	0.55
3:A:106:ARG:C	3:A:107:PRO:O	2.41	0.55
3:E:117:MET:CE	3:E:120:ILE:HD12	2.37	0.55
3:F:78:LEU:HD22	3:F:83:LEU:CD1	2.36	0.55
3:F:148:LEU:HD21	3:F:271:LEU:HD11	1.89	0.55
3:F:317:ASN:HD22	3:F:319:ASN:HB2	1.70	0.55
3:E:271:LEU:HD23	3:E:271:LEU:C	2.27	0.55
3:A:181:ARG:HA	3:A:237:TYR:HA	1.88	0.54
3:F:61:ARG:HH11	3:F:61:ARG:CG	2.20	0.54
2:H:117:DA:H2"	2:H:118:DT:H72	1.88	0.54
3:A:22:GLU:HA	3:A:25:LYS:HB3	1.89	0.54
3:A:76:LEU:HD23	3:A:120:ILE:HD11	1.90	0.54
3:A:209:VAL:HG22	3:B:130:ARG:HH12	1.72	0.54
3:E:206:THR:OG1	3:E:316:THR:HG21	2.07	0.54
3:E:230:VAL:CG1	3:E:236:ASN:HB3	2.38	0.54
3:E:74:TYR:O	3:E:77:TYR:HB3	2.07	0.54
3:F:148:LEU:O	3:F:148:LEU:HD23	2.08	0.54
1:C:112:DA:H62	3:B:44:MET:HE2	1.66	0.54
2:H:111:DT:H73	3:E:43:LYS:HD2	1.89	0.54
3:A:107:PRO:O	3:A:109:ASP:N	2.41	0.54
3:B:158:ILE:HD11	3:B:223:ARG:HH21	1.73	0.54
3:E:206:THR:HG22	3:F:323:ASN:HA	1.89	0.54
3:F:71:VAL:O	3:F:75:LEU:HG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:170:THR:O	3:F:171:LEU:HB2	2.07	0.54
3:F:332:THR:HG22	3:F:333:GLY:N	2.22	0.54
3:A:187:ARG:NH2	3:A:222:GLU:OE2	2.40	0.54
3:E:222:GLU:HA	3:E:225:ILE:HD12	1.90	0.54
3:F:61:ARG:HH11	3:F:61:ARG:HG3	1.73	0.54
2:H:107:DT:H2'	2:H:108:DT:H71	1.90	0.54
3:B:144:GLN:O	3:B:148:LEU:HB2	2.08	0.54
3:B:305:SER:O	3:B:309:ILE:HG13	2.09	0.53
3:E:171:LEU:HD13	3:E:292:ARG:HA	1.89	0.53
3:E:304:VAL:CG1	3:E:308:GLU:HB3	2.38	0.53
3:E:218:THR:O	3:E:222:GLU:HG3	2.07	0.53
3:B:325:ILE:O	3:B:326:ARG:HD2	2.08	0.53
2:D:135:DT:H2"	2:D:136:DC:C6	2.44	0.53
3:E:117:MET:HA	3:E:117:MET:CE	2.38	0.53
3:A:112:ALA:O	3:A:116:VAL:HG23	2.09	0.53
3:A:121:ARG:HG2	3:A:121:ARG:HH11	1.73	0.53
3:B:97:MET:O	3:B:101:ARG:HB2	2.08	0.53
3:E:245:ASN:OD1	3:E:247:VAL:HG23	2.09	0.53
3:F:172:LEU:HD21	3:F:211:LYS:HG3	1.90	0.53
2:H:108:DT:H2"	2:H:109:DC:C5'	2.38	0.52
2:H:112:DA:H2"	2:H:113:DT:C5'	2.39	0.52
3:A:107:PRO:C	3:A:109:ASP:N	2.63	0.52
2:D:133:DT:C2'	2:D:134:DA:C8	2.93	0.52
3:A:14:LEU:HB3	3:A:19:THR:OG1	2.10	0.52
2:D:124:DA:H2'	2:D:125:DT:C7	2.40	0.52
3:E:142:PHE:CZ	3:E:165:GLY:HA2	2.44	0.52
3:F:128:GLY:C	3:F:130:ARG:HH12	2.13	0.52
2:H:112:DA:H2"	2:H:113:DT:H5"	1.92	0.52
3:B:106:ARG:NH1	3:B:109:ASP:OD2	2.39	0.52
3:B:193:MET:HG3	3:B:218:THR:OG1	2.10	0.52
3:E:78:LEU:HD12	3:E:83:LEU:HD12	1.92	0.52
3:E:188:THR:HG22	3:E:190:GLY:H	1.75	0.52
3:E:242:VAL:HG22	3:E:248:ALA:HA	1.91	0.52
2:D:108:DT:H1'	2:D:109:DC:H5"	1.92	0.52
3:A:340:GLU:OE1	3:F:192:ARG:NH1	2.43	0.51
1:C:100:DC:C2'	1:C:101:DG:C8	2.93	0.51
3:A:15:PRO:CB	3:A:18:ALA:HB3	2.32	0.51
3:B:148:LEU:HD12	3:B:271:LEU:HD11	1.91	0.51
3:F:78:LEU:HD22	3:F:83:LEU:HD12	1.92	0.51
2:D:128:DG:O6	3:B:259:ARG:NE	2.38	0.51
3:F:339:LEU:C	3:F:341:ASP:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:158:ILE:HD12	3:B:223:ARG:NE	2.26	0.51
3:F:59:ASN:O	3:F:61:ARG:HD3	2.10	0.51
3:B:180:ILE:CD1	3:B:195:ILE:HG21	2.41	0.51
3:E:213:LEU:HD12	3:E:217:VAL:HG11	1.93	0.51
3:E:248:ALA:C	3:E:250:PRO:HD3	2.30	0.51
1:C:103:DT:H3	2:D:134:DA:N6	2.08	0.51
3:B:84:ALA:O	3:B:88:ILE:HG13	2.11	0.51
3:E:210:GLU:HB2	3:F:326:ARG:HH21	1.74	0.51
3:E:243:ARG:HG3	3:E:243:ARG:NH1	2.16	0.51
3:F:192:ARG:NH1	3:F:215:LEU:HG	2.25	0.51
3:F:289:HIS:CD2	3:F:292:ARG:HD3	2.46	0.51
3:A:10:ASN:ND2	3:A:31:PHE:CE2	2.71	0.51
1:C:102:DA:H2"	1:C:103:DT:H5'	1.92	0.51
3:B:204:VAL:CG2	3:E:125:VAL:HG11	2.41	0.51
3:B:226:SER:OG	3:B:227:VAL:N	2.44	0.51
3:F:132:LYS:NZ	3:F:132:LYS:HB3	2.26	0.51
3:B:140:THR:HG22	3:B:141:ASP:N	2.25	0.51
3:E:159:ARG:HB2	3:E:224:TRP:CE3	2.46	0.51
3:F:328:LEU:HB3	3:F:332:THR:HA	1.92	0.51
3:E:132:LYS:HB3	3:E:132:LYS:HZ3	1.77	0.50
1:C:124:DA:H8	1:C:124:DA:H5"	1.76	0.50
3:F:169:ASN:OD1	3:F:213:LEU:HA	2.11	0.50
2:H:108:DT:H1'	2:H:109:DC:H5"	1.93	0.50
3:B:318:VAL:HG12	3:B:322:MET:HG2	1.94	0.50
3:E:52:TRP:HZ3	3:E:74:TYR:HB2	1.75	0.50
3:E:74:TYR:CE2	3:E:78:LEU:HD21	2.47	0.50
3:E:94:GLN:HA	3:E:94:GLN:NE2	2.26	0.50
3:E:304:VAL:HG12	3:E:308:GLU:HB3	1.93	0.50
3:E:340:GLU:O	3:E:341:ASP:HB2	2.12	0.50
2:D:106:DC:H2"	2:D:107:DT:H5'	1.93	0.50
3:B:185:ILE:HG21	3:B:193:MET:HE2	1.93	0.50
3:F:160:ASN:HD22	3:F:264:ILE:HG23	1.77	0.50
3:B:172:LEU:HD21	3:B:197:ILE:HG13	1.94	0.50
3:F:58:LEU:O	3:F:58:LEU:HD23	2.12	0.50
3:B:321:VAL:O	3:B:325:ILE:HG13	2.12	0.50
3:E:310:MET:SD	3:E:318:VAL:HG12	2.52	0.50
3:A:204:VAL:CG2	3:B:323:ASN:HB2	2.41	0.50
3:E:262:GLU:O	3:E:265:PHE:HB2	2.12	0.50
3:A:188:THR:HG22	3:A:189:ASP:N	2.27	0.49
3:A:329:ASP:HA	3:A:332:THR:HG23	1.94	0.49
3:B:64:PHE:HA	3:B:65:PRO:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:270:ARG:HG3	3:B:270:ARG:HH11	1.76	0.49
3:E:112:ALA:O	3:E:116:VAL:HG22	2.11	0.49
3:F:145:VAL:HG13	3:F:149:MET:HE3	1.91	0.49
3:B:181:ARG:HD3	3:B:183:LYS:HE2	1.94	0.49
3:B:328:LEU:CB	3:B:332:THR:HA	2.42	0.49
3:E:256:LEU:HD22	3:E:260:ALA:HB3	1.94	0.49
2:H:112:DA:OP1	3:E:81:ARG:NH2	2.46	0.49
3:E:210:GLU:HG3	3:F:326:ARG:NH2	2.28	0.49
3:E:325:ILE:HB	3:E:328:LEU:HD12	1.95	0.49
3:F:128:GLY:C	3:F:130:ARG:NH1	2.65	0.49
2:D:108:DT:H1'	2:D:109:DC:C5'	2.42	0.49
3:B:130:ARG:NH2	3:B:326:ARG:CZ	2.76	0.49
3:F:209:VAL:HG22	3:F:210:GLU:N	2.28	0.49
3:B:140:THR:CG2	3:B:141:ASP:N	2.75	0.49
3:E:62:LYS:HD2	3:E:62:LYS:N	2.25	0.49
3:E:209:VAL:HB	3:F:326:ARG:CZ	2.43	0.49
3:A:61:ARG:NH2	3:A:73:ASP:OD1	2.45	0.49
3:B:20:SER:O	3:B:24:ARG:HG3	2.13	0.49
3:E:117:MET:HE2	3:E:120:ILE:HD12	1.94	0.49
2:D:136:DC:H5'	3:B:244:LYS:HD3	1.94	0.49
2:H:133:DT:H2"	2:H:134:DA:C8	2.48	0.49
3:B:90:GLN:HE21	3:B:94:GLN:CG	2.26	0.49
3:E:92:LEU:CD1	3:E:117:MET:HG3	2.43	0.49
1:C:112:DA:OP1	3:B:81:ARG:NH2	2.45	0.49
2:H:118:DT:H2"	2:H:119:DA:N7	2.28	0.49
3:B:216:GLY:O	3:B:219:LYS:HB3	2.12	0.48
3:E:42:TRP:CE3	3:E:45:LEU:HD23	2.48	0.48
3:E:210:GLU:HG3	3:F:326:ARG:HH21	1.77	0.48
3:F:128:GLY:CA	3:F:130:ARG:HH12	2.27	0.48
3:E:144:GLN:OE1	3:E:272:ILE:HD13	2.12	0.48
3:F:138:GLU:OE2	3:F:301:ARG:NH2	2.43	0.48
3:B:90:GLN:HE21	3:B:94:GLN:HG2	1.78	0.48
3:F:310:MET:HE3	3:F:316:THR:HA	1.96	0.48
3:E:260:ALA:O	3:E:264:ILE:HG13	2.13	0.48
3:F:47:SER:O	3:F:50:ARG:HG2	2.13	0.48
1:C:102:DA:H2"	1:C:103:DT:C5'	2.43	0.48
3:A:337:ARG:O	3:A:341:ASP:N	2.47	0.48
3:E:204:VAL:CG1	3:F:323:ASN:ND2	2.76	0.48
3:E:235:ASN:N	3:E:235:ASN:ND2	2.60	0.48
3:E:270:ARG:HA	3:E:274:GLY:O	2.14	0.48
3:E:158:ILE:HG22	3:E:224:TRP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:DA:H2"	1:G:135:DT:O5'	2.13	0.48
1:C:117:DG:H5"	3:B:316:THR:OG1	2.14	0.48
3:A:19:THR:HG22	3:A:24:ARG:CG	2.44	0.48
3:B:328:LEU:O	3:B:332:THR:HG23	2.14	0.47
3:B:259:ARG:HG3	3:B:259:ARG:HH11	1.79	0.47
2:H:124:DA:H2'	2:H:125:DT:H72	1.96	0.47
2:D:116:DC:H2"	2:D:117:DA:C8	2.50	0.47
3:A:138:GLU:HG2	3:A:294:GLY:HA2	1.97	0.47
3:B:148:LEU:CD1	3:B:271:LEU:HD11	2.44	0.47
3:B:259:ARG:HG3	3:B:259:ARG:NH1	2.29	0.47
3:E:256:LEU:HD13	3:E:261:LEU:HD21	1.96	0.47
3:A:72:ARG:HH11	3:A:116:VAL:HG22	1.80	0.47
2:H:105:DA:H5'	3:E:244:LYS:HA	1.95	0.47
2:H:109:DC:H2"	2:H:110:DG:C8	2.49	0.47
2:H:124:DA:H5'	3:F:201:LYS:HG3	1.95	0.47
3:E:72:ARG:HG3	3:E:116:VAL:CG1	2.43	0.47
2:D:125:DT:OP2	3:B:175:ALA:HB2	2.14	0.47
3:A:195:ILE:HD11	3:A:213:LEU:HD11	1.97	0.47
3:B:326:ARG:O	3:B:327:ASN:O	2.33	0.47
3:F:158:ILE:HG12	3:F:223:ARG:HH12	1.79	0.47
3:F:185:ILE:CG2	3:F:193:MET:HE2	2.44	0.47
3:E:201:LYS:N	3:E:201:LYS:HD2	2.30	0.47
3:A:27:LEU:HD13	3:A:102:SER:HB2	1.96	0.47
3:E:329:ASP:O	3:E:332:THR:HG23	2.15	0.47
3:F:148:LEU:HD23	3:F:148:LEU:C	2.34	0.47
3:B:271:LEU:O	3:B:271:LEU:HD22	2.16	0.46
3:B:279:SER:OG	3:B:281:GLN:NE2	2.47	0.46
3:E:48:VAL:CG2	3:E:91:HIS:HA	2.40	0.46
3:E:202:THR:HG22	3:E:204:VAL:N	2.30	0.46
3:E:256:LEU:HD13	3:E:261:LEU:CD2	2.45	0.46
3:B:169:ASN:C	3:B:169:ASN:HD22	2.18	0.46
3:E:48:VAL:HG23	3:E:91:HIS:CG	2.50	0.46
3:E:78:LEU:HD12	3:E:83:LEU:CD1	2.45	0.46
3:E:243:ARG:NH1	3:E:243:ARG:CG	2.76	0.46
1:G:131:DG:C2'	1:G:132:DT:C5'	2.84	0.46
3:A:155:CYS:SG	3:A:227:VAL:HG12	2.55	0.46
3:A:202:THR:HG22	3:A:204:VAL:H	1.80	0.46
3:E:209:VAL:HB	3:F:326:ARG:NH1	2.30	0.46
2:D:112:DA:H2"	2:D:113:DT:H5"	1.97	0.46
3:B:107:PRO:O	3:B:113:VAL:HB	2.15	0.46
3:E:92:LEU:HD22	3:E:96:ASN:ND2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:169:ASN:C	3:F:169:ASN:HD22	2.19	0.46
1:C:116:DT:H4'	3:B:202:THR:CG2	2.45	0.46
2:D:106:DC:H2'	2:D:107:DT:C6	2.50	0.46
3:B:325:ILE:HG22	3:B:326:ARG:N	2.29	0.46
3:E:204:VAL:HG12	3:E:204:VAL:O	2.16	0.46
3:F:163:PHE:CE1	3:F:261:LEU:HD22	2.51	0.46
3:F:317:ASN:HD22	3:F:319:ASN:H	1.58	0.46
1:C:126:DA:H5'	1:C:126:DA:C8	2.51	0.46
3:E:75:LEU:HA	3:E:78:LEU:HD23	1.97	0.46
3:B:20:SER:HB3	3:B:23:VAL:HG23	1.98	0.46
3:E:143:ASP:O	3:E:146:ARG:HG2	2.16	0.46
3:F:243:ARG:HG2	3:F:243:ARG:NH1	2.27	0.46
3:B:130:ARG:HH21	3:B:326:ARG:CZ	2.29	0.46
3:B:325:ILE:O	3:B:326:ARG:CD	2.64	0.46
3:B:106:ARG:O	3:B:109:ASP:HB2	2.16	0.45
1:C:114:DA:H5"	3:B:132:LYS:O	2.15	0.45
3:E:104:LEU:HB3	3:E:105:PRO:HD2	1.96	0.45
3:A:227:VAL:HG12	3:A:227:VAL:O	2.17	0.45
1:C:112:DA:N6	3:B:44:MET:HE3	2.23	0.45
3:B:279:SER:CB	3:B:281:GLN:HE21	2.29	0.45
3:B:340:GLU:O	3:B:341:ASP:HB2	2.15	0.45
3:E:171:LEU:O	3:E:292:ARG:HD2	2.16	0.45
3:F:145:VAL:HG21	3:F:268:THR:CG2	2.46	0.45
1:G:115:DA:H2"	1:G:116:DT:H5'	1.98	0.45
3:A:30:MET:CE	3:A:42:TRP:CH2	3.00	0.45
3:A:338:LEU:HD11	3:F:302:ALA:CB	2.47	0.45
3:B:223:ARG:O	3:B:227:VAL:HG23	2.16	0.45
3:E:147:SER:C	3:E:148:LEU:HD23	2.37	0.45
3:F:170:THR:HB	3:F:172:LEU:HG	1.99	0.45
3:A:245:ASN:CG	3:A:247:VAL:HG23	2.37	0.45
3:E:139:ARG:HG2	3:E:139:ARG:HH11	1.81	0.45
3:E:200:THR:O	3:E:202:THR:N	2.50	0.45
3:E:202:THR:HG22	3:E:204:VAL:C	2.37	0.45
3:E:74:TYR:O	3:E:78:LEU:HD22	2.17	0.45
3:E:199:ARG:CA	3:F:130:ARG:HH21	2.12	0.45
3:F:20:SER:HB3	3:F:23:VAL:HG23	1.99	0.45
3:F:272:ILE:O	3:F:272:ILE:CG2	2.65	0.45
1:G:113:DT:H71	3:F:87:THR:HG23	1.98	0.45
3:A:17:ASP:OD1	3:A:18:ALA:N	2.49	0.45
3:A:163:PHE:CE1	3:A:261:LEU:HD22	2.51	0.45
3:B:185:ILE:HG21	3:B:193:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:310:MET:HE1	3:E:318:VAL:HG13	1.98	0.45
3:E:188:THR:CG2	3:E:189:ASP:N	2.80	0.45
3:A:75:LEU:HD11	3:A:92:LEU:HG	2.00	0.44
3:A:174:ILE:HD12	3:A:258:THR:HB	1.98	0.44
3:B:317:ASN:ND2	3:B:319:ASN:HB2	2.32	0.44
3:E:26:ASN:HB3	3:E:102:SER:HA	1.99	0.44
3:E:144:GLN:CD	3:E:272:ILE:HD13	2.38	0.44
3:E:146:ARG:CG	3:E:147:SER:N	2.80	0.44
3:F:185:ILE:HG23	3:F:193:MET:HE2	1.98	0.44
3:A:45:LEU:HD22	3:A:97:MET:CE	2.47	0.44
3:A:204:VAL:HG13	3:A:204:VAL:O	2.16	0.44
3:F:106:ARG:O	3:F:109:ASP:HB2	2.17	0.44
3:B:121:ARG:O	3:B:125:VAL:HG23	2.17	0.44
3:B:138:GLU:OE2	3:B:301:ARG:NH2	2.35	0.44
3:F:215:LEU:O	3:F:218:THR:HG23	2.17	0.44
1:G:106:DC:H2"	1:G:107:UMP:O5'	2.18	0.44
3:A:72:ARG:NH1	3:F:33:ASP:OD1	2.49	0.44
3:A:188:THR:CG2	3:A:189:ASP:N	2.79	0.44
3:E:92:LEU:HD12	3:E:117:MET:HG3	1.99	0.44
1:C:126:DA:H5'	1:C:126:DA:H8	1.83	0.44
2:H:105:DA:H2"	2:H:106:DC:C5'	2.17	0.44
3:A:14:LEU:HB3	3:A:19:THR:CG2	2.47	0.44
3:A:192:ARG:NH1	3:B:331:GLU:CG	2.78	0.44
3:B:61:ARG:HG2	3:B:61:ARG:HH11	1.83	0.44
3:E:72:ARG:CG	3:E:116:VAL:HG11	2.43	0.44
3:E:202:THR:HB	3:E:205:SER:OG	2.18	0.44
3:F:270:ARG:HG3	3:F:270:ARG:HH11	1.83	0.44
3:A:69:GLU:OE1	3:F:32:ARG:NH1	2.49	0.44
3:A:171:LEU:O	3:A:292:ARG:NH1	2.49	0.44
3:B:85:VAL:HG23	3:B:129:GLU:OE2	2.17	0.44
3:E:90:GLN:NE2	3:E:94:GLN:HG2	2.33	0.44
2:D:107:DT:H1'	2:D:108:DT:H5"	1.99	0.44
2:H:124:DA:H2"	2:H:125:DT:C6	2.52	0.44
3:A:187:ARG:HH11	3:A:187:ARG:CB	2.26	0.44
3:B:173:ARG:O	3:B:176:GLU:HB2	2.17	0.44
3:F:64:PHE:HA	3:F:65:PRO:C	2.37	0.44
3:A:169:ASN:C	3:A:169:ASN:HD22	2.21	0.44
3:B:129:GLU:HG2	3:B:130:ARG:N	2.33	0.44
3:B:243:ARG:HH11	3:B:243:ARG:HG2	1.83	0.44
3:A:71:VAL:O	3:A:75:LEU:HG	2.18	0.44
3:A:329:ASP:O	3:A:332:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:91:HIS:O	3:B:95:LEU:HD22	2.17	0.44
3:E:122:LYS:O	3:E:126:ASP:HB2	2.18	0.44
3:E:145:VAL:HG11	3:E:164:LEU:HD12	1.99	0.43
3:E:195:ILE:CD1	3:E:213:LEU:HD21	2.48	0.43
1:G:115:DA:H2"	3:F:320:ILE:HD11	1.99	0.43
3:A:185:ILE:HD11	3:A:238:LEU:HG	2.00	0.43
3:E:52:TRP:NE1	3:E:63:TRP:O	2.45	0.43
3:A:277:ASP:HB3	3:A:284:LEU:CD1	2.39	0.43
3:B:199:ARG:NH1	3:E:122:LYS:HE3	2.33	0.43
3:E:139:ARG:HG2	3:E:139:ARG:NH1	2.32	0.43
3:F:317:ASN:CG	3:F:318:VAL:H	2.22	0.43
2:D:118:DT:OP2	3:A:202:THR:HG23	2.18	0.43
3:A:14:LEU:HD13	3:A:14:LEU:HA	1.84	0.43
3:E:197:ILE:O	3:E:197:ILE:CG1	2.67	0.43
3:F:61:ARG:NH1	3:F:61:ARG:CG	2.78	0.43
3:F:245:ASN:OD1	3:F:247:VAL:HB	2.18	0.43
3:F:326:ARG:NH1	3:F:326:ARG:HG2	2.33	0.43
3:E:42:TRP:O	3:E:46:LEU:HG	2.19	0.43
1:C:124:DA:H2'	1:C:125:DT:C7	2.49	0.43
2:D:108:DT:H2"	2:D:109:DC:C5'	2.35	0.43
3:A:200:THR:HG22	3:A:201:LYS:N	2.33	0.43
3:B:328:LEU:HB2	3:B:332:THR:HA	2.00	0.43
3:E:142:PHE:CE1	3:E:165:GLY:HA2	2.54	0.43
3:A:299:MET:HE2	3:A:309:ILE:HG12	2.01	0.43
3:A:304:VAL:HG12	3:A:308:GLU:HB3	2.00	0.43
3:E:213:LEU:HD12	3:E:217:VAL:CG1	2.47	0.43
3:F:121:ARG:CG	3:F:121:ARG:NH1	2.72	0.43
3:E:146:ARG:HG2	3:E:147:SER:N	2.34	0.43
3:E:163:PHE:CD2	3:E:261:LEU:HD22	2.54	0.43
1:G:114:DA:C8	3:F:86:LYS:HD3	2.54	0.43
3:E:48:VAL:HG23	3:E:91:HIS:CD2	2.54	0.43
3:E:52:TRP:HZ3	3:E:74:TYR:CB	2.31	0.43
3:E:336:VAL:O	3:E:340:GLU:HG3	2.19	0.43
3:A:187:ARG:HB3	3:A:187:ARG:NH1	2.27	0.43
1:C:124:DA:H8	1:C:124:DA:C5'	2.31	0.42
3:A:187:ARG:HH12	3:A:191:GLY:C	2.23	0.42
3:A:306:ILE:HB	3:A:307:PRO:HD3	2.00	0.42
3:B:138:GLU:CD	3:B:301:ARG:HH22	2.21	0.42
3:B:173:ARG:HD2	3:B:176:GLU:OE2	2.19	0.42
3:B:181:ARG:HA	3:B:237:TYR:HA	2.01	0.42
3:E:297:ARG:HH11	3:E:297:ARG:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:159:ARG:HB2	3:A:224:TRP:CE3	2.54	0.42
3:A:326:ARG:HD3	3:F:210:GLU:CG	2.46	0.42
1:C:131:DG:H2"	1:C:132:DT:H5'	2.01	0.42
3:B:139:ARG:HB2	3:B:168:TYR:OH	2.19	0.42
3:B:160:ASN:ND2	3:B:264:ILE:HG23	2.35	0.42
3:B:327:ASN:HB3	3:B:328:LEU:H	1.48	0.42
1:C:107:UMP:H2'	1:C:108:DT:H71	2.01	0.42
3:A:316:THR:O	3:A:316:THR:HG22	2.19	0.42
3:E:24:ARG:HH11	3:E:24:ARG:HB2	1.84	0.42
3:A:100:ARG:HH21	3:A:101:ARG:NE	2.18	0.42
3:B:215:LEU:C	3:B:218:THR:HG22	2.40	0.42
3:E:48:VAL:CG1	3:E:49:CYS:N	2.82	0.42
3:A:16:VAL:HA	3:A:24:ARG:HH21	1.81	0.42
3:A:142:PHE:O	3:A:146:ARG:HB2	2.18	0.42
3:E:113:VAL:O	3:E:116:VAL:HG23	2.20	0.42
3:F:55:TRP:CZ3	3:F:77:TYR:CG	3.08	0.42
2:D:105:DA:H2"	2:D:106:DC:O5'	2.20	0.42
2:H:112:DA:C2'	2:H:113:DT:H5"	2.50	0.42
3:A:311:GLN:HE21	3:A:311:GLN:HB3	1.68	0.42
3:B:90:GLN:NE2	3:B:94:GLN:HG2	2.34	0.42
3:E:45:LEU:O	3:E:48:VAL:HG12	2.19	0.42
3:F:155:CYS:SG	3:F:227:VAL:HG12	2.59	0.42
3:F:325:ILE:CG2	3:F:327:ASN:ND2	2.83	0.42
3:A:19:THR:HG22	3:A:24:ARG:HG3	2.02	0.42
3:B:20:SER:OG	3:B:21:ASP:N	2.52	0.42
3:E:144:GLN:O	3:E:148:LEU:HG	2.20	0.42
3:E:185:ILE:HG21	3:E:193:MET:HE3	1.98	0.42
3:F:140:THR:HG22	3:F:141:ASP:N	2.34	0.42
4:C:200:IOD:I	3:B:260:ALA:HA	2.90	0.42
1:G:108:DT:H2"	1:G:109:DC:C5'	2.50	0.42
3:B:318:VAL:HG12	3:B:322:MET:CG	2.49	0.42
3:B:331:GLU:O	3:B:332:THR:C	2.58	0.42
3:E:154:ARG:HB3	3:E:154:ARG:CZ	2.47	0.42
3:B:276:LYS:O	3:B:278:ASP:N	2.53	0.41
3:E:169:ASN:HD22	3:E:213:LEU:HA	1.75	0.41
3:B:329:ASP:O	3:B:330:SER:O	2.37	0.41
3:E:76:LEU:HD21	3:E:119:ARG:NH1	2.33	0.41
3:A:72:ARG:HH11	3:A:116:VAL:CG2	2.33	0.41
3:A:134:ALA:HA	3:A:283:TYR:CD2	2.55	0.41
3:A:281:GLN:HB2	3:A:284:LEU:HD21	2.01	0.41
3:B:27:LEU:HD22	3:B:102:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:330:SER:C	3:B:332:THR:H	2.23	0.41
3:F:258:THR:O	3:F:262:GLU:HG3	2.20	0.41
1:C:131:DG:H1'	1:C:132:DT:H5"	2.02	0.41
2:D:123:DT:O2	3:B:201:LYS:NZ	2.53	0.41
3:A:168:TYR:HA	3:A:291:ALA:HB1	2.03	0.41
3:F:328:LEU:HD12	3:F:333:GLY:N	2.35	0.41
3:B:188:THR:HG23	3:B:194:LEU:HD22	2.02	0.41
2:D:106:DC:H2'	2:D:107:DT:H71	2.02	0.41
3:B:104:LEU:HB3	3:B:105:PRO:HD2	2.01	0.41
3:E:106:ARG:HG3	3:E:106:ARG:HH11	1.85	0.41
3:E:237:TYR:O	3:E:238:LEU:C	2.59	0.41
3:F:85:VAL:HG23	3:F:129:GLU:OE2	2.21	0.41
3:F:138:GLU:CD	3:F:301:ARG:HH22	2.23	0.41
2:D:108:DT:C2'	2:D:109:DC:C5'	2.97	0.41
3:B:48:VAL:HG11	3:B:91:HIS:HA	2.02	0.41
3:B:237:TYR:CE1	3:B:255:GLN:HB3	2.55	0.41
3:E:146:ARG:HA	3:E:161:LEU:HD11	2.01	0.41
3:F:155:CYS:SG	3:F:227:VAL:CG1	3.09	0.41
3:A:164:LEU:HD23	3:A:164:LEU:HA	1.82	0.41
3:A:186:SER:OG	3:A:196:HIS:HE1	2.02	0.41
3:E:306:ILE:N	3:E:307:PRO:HD2	2.36	0.41
1:G:101:DG:H2"	1:G:102:DA:O5'	2.21	0.41
1:G:122:DC:H2"	1:G:123:DT:H5'	2.03	0.41
3:A:14:LEU:C	3:A:19:THR:OG1	2.60	0.41
3:A:77:TYR:CZ	3:A:81:ARG:HD2	2.56	0.41
3:A:207:ALA:HA	3:A:314:GLY:CA	2.47	0.41
3:A:289:HIS:CD2	3:A:292:ARG:HD3	2.56	0.41
3:B:188:THR:C	3:B:190:GLY:N	2.70	0.41
3:E:243:ARG:HD2	3:E:243:ARG:N	2.34	0.41
3:E:279:SER:O	3:E:281:GLN:N	2.52	0.41
3:E:306:ILE:O	3:E:310:MET:HG3	2.21	0.41
3:F:317:ASN:CG	3:F:318:VAL:N	2.74	0.41
1:C:126:DA:H2"	1:C:127:DC:O5'	2.21	0.41
1:C:132:DT:H2'	1:C:133:DT:H71	2.03	0.41
2:D:124:DA:H2'	2:D:125:DT:C6	2.56	0.41
2:H:126:DA:OP2	3:F:262:GLU:OE2	2.39	0.41
2:H:129:DA:H2"	2:H:130:DA:C8	2.56	0.41
3:B:174:ILE:HG13	3:B:175:ALA:N	2.36	0.41
3:B:199:ARG:NH1	3:E:122:LYS:CE	2.84	0.41
3:B:333:GLY:CA	3:B:337:ARG:HG3	2.50	0.41
3:B:337:ARG:O	3:B:340:GLU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:62:LYS:H	3:E:62:LYS:CD	2.29	0.41
3:E:256:LEU:HD22	3:E:260:ALA:CB	2.51	0.41
3:E:302:ALA:HB2	3:F:338:LEU:HD21	2.02	0.41
3:F:204:VAL:O	3:F:204:VAL:HG13	2.21	0.41
2:D:117:DA:H3'	3:A:202:THR:HG23	2.02	0.40
1:G:104:DA:O4'	3:F:244:LYS:HE2	2.21	0.40
3:A:23:VAL:CG2	3:A:24:ARG:N	2.84	0.40
3:A:30:MET:CE	3:A:42:TRP:HH2	2.34	0.40
3:B:20:SER:HB3	3:B:23:VAL:CG2	2.51	0.40
3:E:94:GLN:HA	3:E:94:GLN:HE21	1.86	0.40
3:E:248:ALA:O	3:E:250:PRO:HD3	2.21	0.40
1:G:123:DT:H2"	1:G:124:DA:H8	1.85	0.40
1:C:113:DT:H2"	3:B:86:LYS:HB3	2.03	0.40
1:G:109:DC:H2"	1:G:110:DG:C8	2.56	0.40
3:A:269:HIS:HB2	3:A:286:TRP:CE3	2.57	0.40
3:E:57:LYS:N	3:E:57:LYS:CD	2.84	0.40
3:A:204:VAL:O	3:A:204:VAL:HG22	2.21	0.40
3:A:39:GLU:O	3:A:43:LYS:HG2	2.21	0.40
3:E:237:TYR:CD1	3:E:255:GLN:HB3	2.55	0.40
3:F:304:VAL:HG12	3:F:308:GLU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	330/347 (95%)	306 (93%)	15 (4%)	9 (3%)	5 19
3	B	320/347 (92%)	279 (87%)	30 (9%)	11 (3%)	3 15
3	E	319/347 (92%)	277 (87%)	37 (12%)	5 (2%)	9 32
3	F	320/347 (92%)	295 (92%)	19 (6%)	6 (2%)	8 28
All	All	1289/1388 (93%)	1157 (90%)	101 (8%)	31 (2%)	6 22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	13	ALA
3	A	21	ASP
3	B	277	ASP
3	B	327	ASN
3	B	330	SER
3	B	332	THR
3	E	58	LEU
3	E	201	LYS
3	F	327	ASN
3	F	330	SER
3	A	199	ARG
3	A	201	LYS
3	A	277	ASP
3	B	152	SER
3	B	326	ARG
3	E	206	THR
3	E	244	LYS
3	F	326	ARG
3	B	148	LEU
3	B	278	ASP
3	A	108	SER
3	B	244	LYS
3	B	334	ALA
3	F	277	ASP
3	F	340	GLU
3	E	199	ARG
3	F	332	THR
3	B	227	VAL
3	A	182	VAL
3	A	12	PRO
3	A	107	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	277/291 (95%)	255 (92%)	22 (8%)	12	34
3	B	269/291 (92%)	249 (93%)	20 (7%)	13	38
3	E	268/291 (92%)	249 (93%)	19 (7%)	14	40
3	F	269/291 (92%)	253 (94%)	16 (6%)	19	49
All	All	1083/1164 (93%)	1006 (93%)	77 (7%)	14	40

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	17	ASP
3	A	20	SER
3	A	23	VAL
3	A	58	LEU
3	A	61	ARG
3	A	72	ARG
3	A	89	GLN
3	A	92	LEU
3	A	95	LEU
3	A	98	LEU
3	A	101	ARG
3	A	109	ASP
3	A	155	CYS
3	A	169	ASN
3	A	187	ARG
3	A	206	THR
3	A	209	VAL
3	A	222	GLU
3	A	238	LEU
3	A	255	GLN
3	A	289	HIS
3	A	311	GLN
3	B	27	LEU
3	B	30	MET
3	B	35	GLN
3	B	45	LEU
3	B	60	ASN
3	B	61	ARG
3	B	68	PRO
3	B	72	ARG
3	B	95	LEU
3	B	132	LYS
3	B	140	THR

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Mol	Chain	Res	Type
3	B	148	LEU
3	B	150	GLU
3	B	156	GLN
3	B	157	ASP
3	B	169	ASN
3	B	194	LEU
3	B	289	HIS
3	B	319	ASN
3	B	338	LEU
3	E	57	LYS
3	E	61	ARG
3	E	92	LEU
3	E	95	LEU
3	E	101	ARG
3	E	106	ARG
3	E	116	VAL
3	E	132	LYS
3	E	153	ASP
3	E	171	LEU
3	E	181	ARG
3	E	201	LYS
3	E	232	ASP
3	E	235	ASN
3	E	238	LEU
3	E	243	ARG
3	E	256	LEU
3	E	282	ARG
3	E	306	ILE
3	F	27	LEU
3	F	35	GLN
3	F	45	LEU
3	F	61	ARG
3	F	73	ASP
3	F	101	ARG
3	F	121	ARG
3	F	140	THR
3	F	155	CYS
3	F	156	GLN
3	F	169	ASN
3	F	218	THR
3	F	311	GLN
3	F	319	ASN

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Mol	Chain	Res	Type
3	F	338	LEU
3	F	341	ASP

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

Mol	Chain	Res	Type
3	A	59	ASN
3	A	79	GLN
3	A	89	GLN
3	A	90	GLN
3	A	94	GLN
3	A	133	GLN
3	A	196	HIS
3	A	255	GLN
3	A	289	HIS
3	A	311	GLN
3	B	35	GLN
3	B	60	ASN
3	B	90	GLN
3	B	133	GLN
3	B	156	GLN
3	B	236	ASN
3	B	281	GLN
3	B	317	ASN
3	B	319	ASN
3	B	327	ASN
3	E	35	GLN
3	E	90	GLN
3	E	94	GLN
3	E	169	ASN
3	E	235	ASN
3	E	236	ASN
3	E	323	ASN
3	F	35	GLN
3	F	94	GLN
3	F	111	ASN
3	F	133	GLN
3	F	156	GLN
3	F	281	GLN
3	F	317	ASN
3	F	323	ASN
3	F	327	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	UMP	C	107	2,1	17,20,21	0.54	0	24,28,31	0.52	0
1	UMP	G	107	2,1	17,20,21	0.41	0	24,28,31	0.45	0

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	2,1	-	0/7/21/22	0/2/2/2
1	UMP	G	107	2,1	-	1/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	107	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	36/37 (97%)	-0.45	0	100	100	27, 48, 81, 90	0
1	G	36/37 (97%)	-0.15	1 (2%)	53	49	34, 62, 89, 140	0
2	D	37/37 (100%)	-0.45	1 (2%)	54	50	28, 44, 79, 88	0
2	H	37/37 (100%)	-0.27	1 (2%)	54	50	33, 66, 91, 109	0
3	A	332/347 (95%)	-0.21	13 (3%)	39	35	12, 43, 88, 143	0
3	B	322/347 (92%)	-0.23	6 (1%)	66	65	22, 57, 92, 137	0
3	E	321/347 (92%)	-0.00	18 (5%)	24	20	32, 66, 103, 150	0
3	F	322/347 (92%)	-0.27	5 (1%)	72	71	25, 52, 90, 133	0
All	All	1443/1536 (93%)	-0.19	45 (3%)	49	44	12, 55, 93, 150	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	202	THR	6.8
3	B	330	SER	6.3
3	E	208	GLY	6.1
3	E	204	VAL	6.0
3	B	331	GLU	5.1
3	E	201	LYS	4.9
3	A	208	GLY	4.8
3	F	331	GLU	4.7
3	A	205	SER	4.7
3	A	204	VAL	4.6
3	E	206	THR	4.5
3	F	330	SER	4.3
3	E	200	THR	4.2
3	E	202	THR	4.1
3	A	19	THR	3.9
3	E	205	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	100	DC	3.5
3	F	329	ASP	3.3
3	A	201	LYS	3.3
3	A	203	LEU	3.2
3	E	199	ARG	3.1
3	B	329	ASP	3.1
3	A	200	THR	3.0
3	A	207	ALA	2.9
3	A	206	THR	2.9
3	E	57	LYS	2.9
3	E	279	SER	2.6
3	A	17	ASP	2.6
3	E	278	ASP	2.6
3	B	22	GLU	2.6
3	B	277	ASP	2.6
3	E	60	ASN	2.5
3	A	199	ARG	2.4
2	H	100	DG	2.4
3	E	341	ASP	2.3
2	D	100	DG	2.3
3	A	18	ALA	2.3
3	E	274	GLY	2.3
3	E	207	ALA	2.2
3	F	57	LYS	2.2
3	F	60	ASN	2.2
3	E	34	ARG	2.1
3	E	280	GLY	2.1
3	B	279	SER	2.1
3	E	232	ASP	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	UMP	C	107	19/20	0.95	0.14	37,51,66,68	0
1	UMP	G	107	19/20	0.97	0.15	49,53,58,59	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	MG	H	307	1/1	0.77	0.97	53,53,53,53	1
5	MG	C	308	1/1	0.85	0.17	44,44,44,44	0
5	MG	A	347	1/1	0.86	0.59	63,63,63,63	0
5	MG	D	301	1/1	0.88	0.26	60,60,60,60	0
5	MG	A	346	1/1	0.89	0.42	56,56,56,56	0
5	MG	G	306	1/1	0.90	0.26	55,55,55,55	0
5	MG	F	345	1/1	0.91	0.39	32,32,32,32	1
4	IOD	C	200	1/1	0.94	0.16	52,52,52,52	1
5	MG	A	344	1/1	0.96	0.13	41,41,41,41	0
5	MG	A	345	1/1	0.97	0.35	39,39,39,39	0
5	MG	D	310	1/1	0.98	0.20	58,58,58,58	0
4	IOD	F	344	1/1	0.98	0.16	46,46,46,46	1

6.5 Other polymers (i)

There are no such residues in this entry.