



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 1Q3U / pdb_00001q3u
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

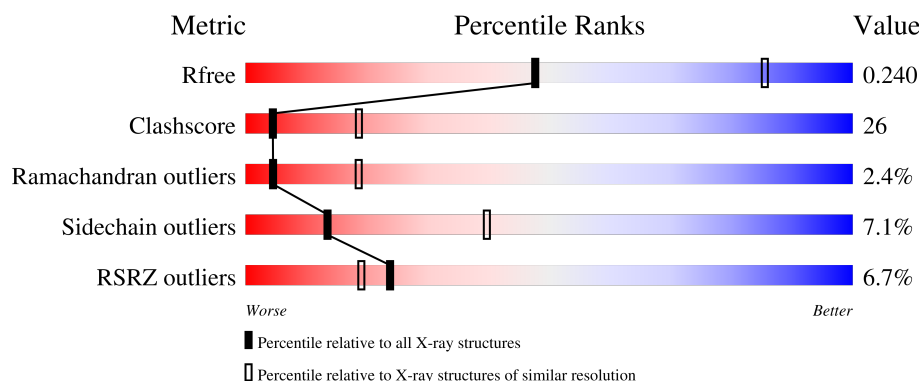
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	37	8% 32% 62% 5%
1	G	37	5% 41% 54% 5%
2	D	37	5% 32% 68%
2	H	37	16% 35% 62% .
3	A	347	7% 56% 33% 7% .

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Mol	Chain	Length	Quality of chain
3	B	347	4% 49% 38% 5% 7%
3	E	347	8% 46% 42% 5% 7%
3	F	347	5% 54% 33% 5% 7%

2 Entry composition

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

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

- Molecule 1 is a DNA chain called loxP DNA.

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

- Molecule 2 is a DNA chain called loxP DNA.

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

- Molecule 3 is a protein called Cre recombinase.

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

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 (CCD ID: 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 (CCD ID: 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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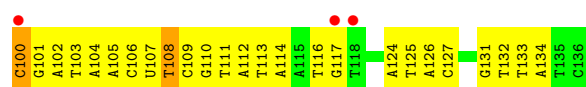
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	O	0	0
			1	1		

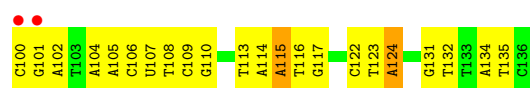
3 Residue-property plots [i](#)

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



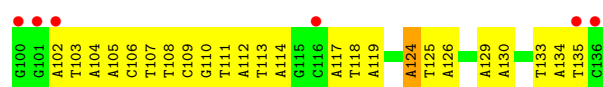
- Molecule 1: loxP DNA



- Molecule 2: loxP DNA

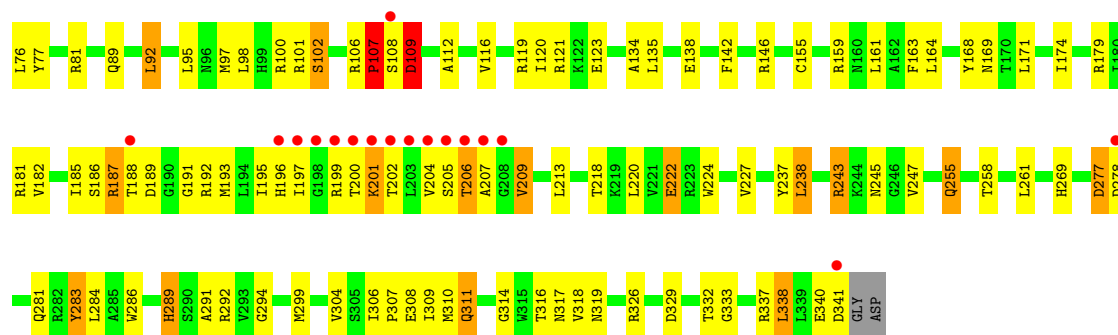


- Molecule 2: loxP DNA

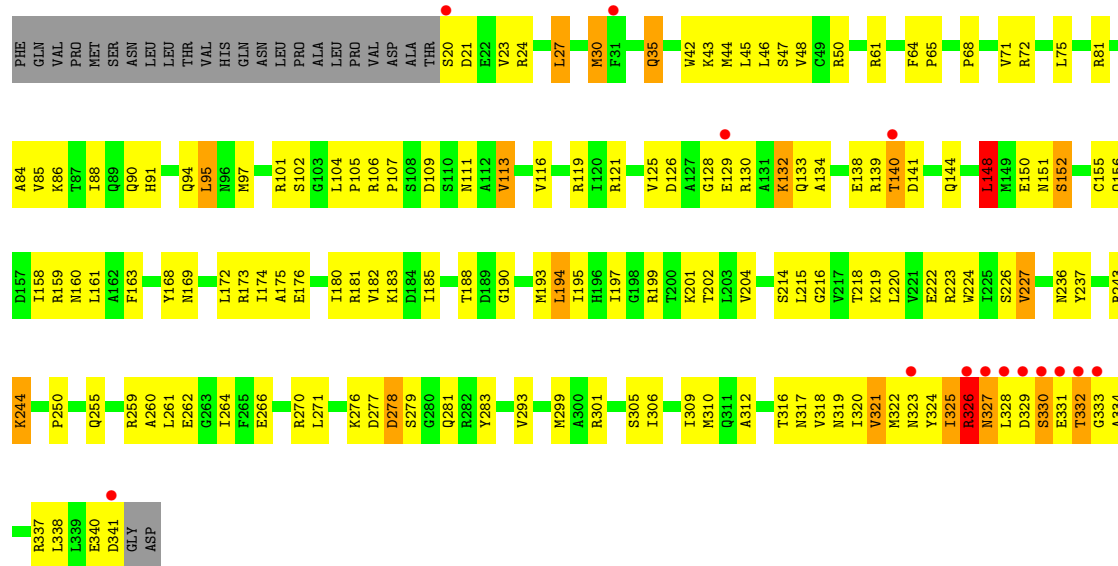


- Molecule 3: Cre recombinase

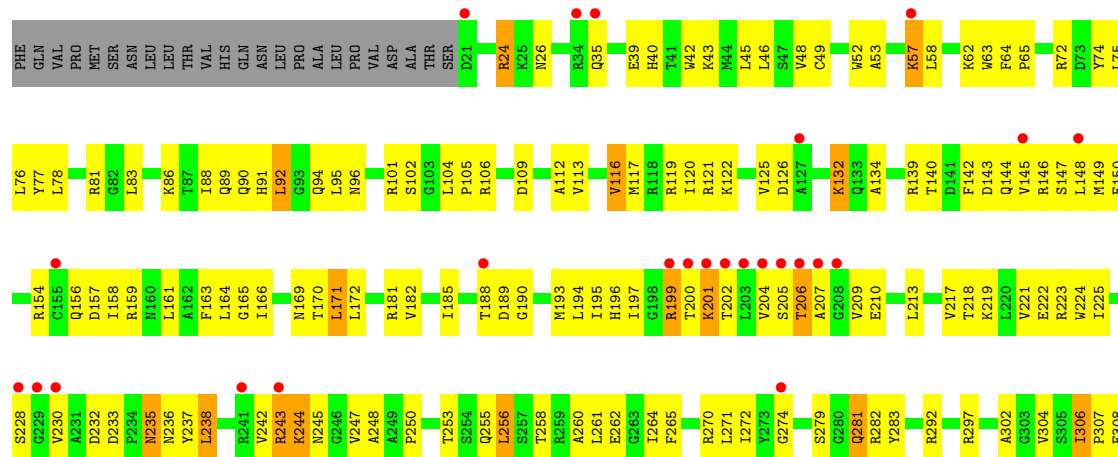


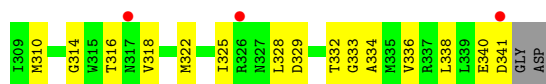


• Molecule 3: Cre recombinase

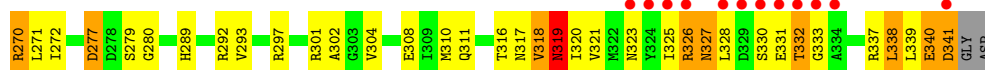
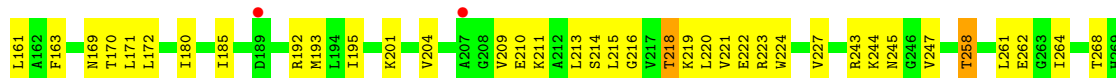


• Molecule 3: Cre recombinase





● Molecule 3: Cre recombinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, 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) 99.0 (20.03-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.244 0.215 , 0.240	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 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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

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	0.38	0/823	0.83	1/1266 (0.1%)
1	G	0.35	0/823	0.81	0/1266
2	D	0.37	0/848	0.83	0/1307
2	H	0.33	0/848	0.77	0/1307
3	A	0.57	0/2663	0.99	8/3595 (0.2%)
3	B	0.49	0/2591	0.93	3/3493 (0.1%)
3	E	0.45	0/2585	0.89	5/3485 (0.1%)
3	F	0.50	0/2591	0.96	6/3493 (0.2%)
All	All	0.47	0/13772	0.91	23/19212 (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	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.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	333	GLY	N-CA-C	8.88	122.51	111.85
3	A	109	ASP	N-CA-C	-8.79	102.29	113.72
3	B	321	VAL	N-CA-C	-7.36	103.11	110.62
3	E	333	GLY	N-CA-C	6.45	120.13	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	331	GLU	N-CA-C	-6.41	104.33	111.71
3	F	319	ASN	N-CA-C	6.38	121.90	111.37
3	B	325	ILE	N-CA-C	6.26	117.50	108.48
3	A	24	ARG	N-CA-C	-6.08	104.77	111.82
3	E	149	MET	N-CA-C	-5.89	107.33	114.75
3	A	107	PRO	N-CA-C	-5.88	100.35	112.47
3	A	243	ARG	N-CA-C	5.88	118.46	110.35
3	A	135	LEU	N-CA-C	-5.84	101.20	109.96
3	E	253	THR	N-CA-C	-5.74	106.91	114.31
3	E	334	ALA	N-CA-C	5.60	117.39	111.28
1	C	100	DC	O5'-C5'-C4'	-5.57	102.44	110.80
3	F	36	ALA	N-CA-C	-5.52	106.55	113.28
3	A	283	TYR	N-CA-C	5.43	119.20	111.92
3	F	280	GLY	N-CA-C	-5.30	108.31	115.36
3	F	258	THR	N-CA-C	-5.15	106.25	112.54
3	F	103	GLY	N-CA-C	-5.10	108.20	115.64
3	A	102	SER	N-CA-C	-5.06	105.81	112.94
3	B	326	ARG	N-CA-C	-5.05	100.04	110.80
3	E	24	ARG	N-CA-C	-5.04	105.68	111.07

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	108	DT	Sidechain
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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	135	0
3	B	2550	0	2571	151	0
3	E	2544	0	2566	192	0
3	F	2550	0	2571	138	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	665	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 26.

All (665) 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
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
1:C:112:DA:H62	3:B:44:MET:HE3	1.30	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:185:ILE:HG21	3:B:193:MET:HE2	1.51	0.90
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:117:MET:HE2	3:E:117:MET:HA	1.58	0.86
3:F:185:ILE:HG21	3:F:193:MET:HE3	1.58	0.85
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:A:30:MET:HE3	3:A:42:TRP:CH2	2.13	0.83
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:DT:H2''	1:C:109:DC:H5'	1.68	0.75
3:B:71:VAL:O	3:B:75:LEU:HG	1.88	0.74
2:D:122:DT:H5''	3:B:97:MET:HE2	1.69	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:A:299:MET:HE1	3:A:309:ILE:HA	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:185:ILE:HG21	3:E:193:MET:HE2	1.72	0.71
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:185:ILE:CG2	3:F:193:MET:HE3	2.21	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
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:107:PRO:C	3:A:109:ASP:H	2.01	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:F:145:VAL:HG13	3:F:149:MET:HE3	1.75	0.68
1:C:112:DA:N6	3:B:44:MET:HE3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:205:SER:C	3:B:326:ARG:HH21	2.03	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:A:299:MET:HE2	3:A:309:ILE:HA	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:30:MET:HE3	3:A:42:TRP:HH2	1.61	0.63
1:C:106:DC:H2''	1:C:107:UMP:O5'	1.98	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:151:ASN:O	3:B:152:SER:C	2.43	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
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:B:299:MET:HE1	3:B:312:ALA:HB2	1.83	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
3:E:279:SER:C	3:E:281:GLN:H	2.10	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:299:MET:HE2	3:A:309:ILE:HG12	1.85	0.59
3:A:311:GLN:HG3	3:B:325:ILE:HG21	1.84	0.59
3:E:271:LEU:HD23	3:E:271:LEU:C	2.27	0.59
3:A:106:ARG:C	3:A:107:PRO:O	2.41	0.59
3:F:61:ARG:NH1	3:F:70:ASP:OD1	2.36	0.59
3:B:319:ASN:O	3:B:320:ILE:HB	2.01	0.59
3:B:333:GLY:HA2	3:B:337:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:185:ILE:HD13	3:F:193:MET:CE	2.35	0.57
3:F:332:THR:HG22	3:F:333:GLY:H	1.70	0.57
3:F:193:MET:HE1	3:F:221:VAL:HG11	1.86	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:F:339:LEU:C	3:F:341:ASP:H	2.14	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:248:ALA:C	3:E:250:PRO:HD3	2.30	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:F:310:MET:HE3	3:F:316:THR:HA	1.87	0.56
3:A:243:ARG:HG2	3:A:243:ARG:NH1	2.21	0.55
3:E:193:MET:CG	3:E:218:THR:HG23	2.33	0.55
3:F:128:GLY:C	3:F:130:ARG:HH12	2.13	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
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: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: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:B:64:PHE:HA	3:B:65:PRO:C	2.32	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:128:GLY:C	3:F:130:ARG:NH1	2.65	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
3:E:39:GLU:HG3	3:E:40:HIS:N	2.21	0.53
2:D:135:DT:H2''	2:D:136:DC:C6	2.44	0.53
3:F:170:THR:O	3:F:171:LEU:HB2	2.07	0.53
3:F:185:ILE:HD13	3:F:193:MET:HE3	1.89	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
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
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
3:F:148:LEU:HD23	3:F:148:LEU:C	2.34	0.52
2:D:108:DT:H1'	2:D:109:DC:H5''	1.92	0.52
3:A:107:PRO:C	3:A:109:ASP:N	2.63	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:B:158:ILE:HD12	3:B:223:ARG:NE	2.26	0.51
3:B:169:ASN:C	3:B:169:ASN:HD22	2.18	0.51
3:F:59:ASN:O	3:F:61:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:169:ASN:C	3:F:169:ASN:HD22	2.19	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:140:THR:HG22	3:B:141:ASP:N	2.25	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: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:A:245:ASN:CG	3:A:247:VAL:HG23	2.37	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:202:THR:HG22	3:E:204:VAL:C	2.37	0.50
3:E:262:GLU:O	3:E:265:PHE:HB2	2.12	0.50
3:A:329:ASP:HA	3:A:332:THR:HG23	1.94	0.49
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:E:147:SER:C	3:E:148:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:64:PHE:HA	3:F:65:PRO:C	2.37	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:144:GLN:CD	3:E:272:ILE:HD13	2.38	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
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:E:117:MET:HA	3:E:117:MET:CE	2.38	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
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:A:188:THR:HG22	3:A:189:ASP:N	2.27	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:317:ASN:CG	3:F:318:VAL:H	2.22	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:270:ARG:HA	3:E:274:GLY:O	2.14	0.48
3:F:209:VAL:HG22	3:F:210:GLU:N	2.28	0.48
3:E:158:ILE:HG22	3:E:224:TRP:HB2	1.95	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:GLU:CD	3:B:301:ARG:HH22	2.21	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:187:ARG:HH12	3:A:191:GLY:C	2.23	0.47
3:A:195:ILE:HD11	3:A:213:LEU:HD11	1.97	0.47
3:B:215:LEU:C	3:B:218:THR:HG22	2.40	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:A:169:ASN:C	3:A:169:ASN:HD22	2.21	0.47
3:B:330:SER:C	3:B:332:THR:H	2.23	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: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:B:331:GLU:O	3:B:332:THR:C	2.58	0.46
3:E:48:VAL:CG2	3:E:91:HIS:HA	2.40	0.46
3:E:88:ILE:HG21	3:E:117:MET:HE1	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:107:PRO:O	3:B:113:VAL:HB	2.15	0.46
3:B:188:THR:C	3:B:190:GLY:N	2.70	0.46
3:E:92:LEU:HD22	3:E:96:ASN:ND2	2.29	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:E:237:TYR:O	3:E:238:LEU:C	2.59	0.46
3:F:138:GLU:CD	3:F:301:ARG:HH22	2.23	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:A:14:LEU:C	3:A:19:THR:OG1	2.60	0.45
3:E:104:LEU:HB3	3:E:105:PRO:HD2	1.96	0.45
3:F:317:ASN:CG	3:F:318:VAL:N	2.74	0.45
3:A:227:VAL:HG12	3:A:227:VAL:O	2.17	0.45
3:A:64:PHE:HA	3:A:65:PRO:C	2.42	0.45
3:B:279:SER:CB	3:B:281:GLN:HE21	2.29	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: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:F:170:THR:HB	3:F:172:LEU:HG	1.99	0.45
3:B:340:GLU:O	3:B:341:ASP:HB2	2.15	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:74:TYR:O	3:E:78:LEU:HD22	2.17	0.45
1:C:112:DA:N7	3:B:44:MET:HE1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:146:ARG:CG	3:E:147:SER:N	2.80	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:129:GLU:C	3:F:130:ARG:HH11	2.26	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:B:126:ASP:C	3:B:128:GLY:H	2.26	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:E:139:ARG:O	3:E:140:THR:C	2.61	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:F:80:ALA:C	3:F:82:GLY:H	2.25	0.44
3:A:71:VAL:O	3:A:75:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:329:ASP:O	3:A:332:THR:HG23	2.18	0.44
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:202:THR:CG2	3:E:204:VAL:C	2.91	0.44
3:B:126:ASP:C	3:B:128:GLY:N	2.76	0.43
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:310:MET:HE3	3:F:316:THR:CA	2.47	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:169:ASN:C	3:F:169:ASN:ND2	2.76	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: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:45:LEU:HD22	3:A:97:MET:HE2	2.00	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:E:243:ARG:C	3:E:245:ASN:H	2.27	0.43
3:F:121:ARG:CG	3:F:121:ARG:NH1	2.72	0.43
3:F:340:GLU:O	3:F:341:ASP:C	2.60	0.43
3:A:200:THR:HG22	3:A:201:LYS:N	2.33	0.43
3:A:277:ASP:CG	3:A:278:ASP:N	2.76	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:156:GLN:O	3:E:157:ASP:C	2.62	0.43
3:E:336:VAL:O	3:E:340:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:187:ARG:HB3	3:A:187:ARG:NH1	2.27	0.43
3:A:206:THR:O	3:A:207:ALA:C	2.62	0.43
3:E:310:MET:HE1	3:E:318:VAL:HG13	2.01	0.43
1:C:124:DA:H8	1:C:124:DA:C5'	2.31	0.42
3:A:306:ILE:HB	3:A:307:PRO:HD3	2.00	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:B:185:ILE:CG2	3:B:193:MET:HE2	2.36	0.42
3:E:64:PHE:HA	3:E:65:PRO:C	2.43	0.42
3:E:297:ARG:HH11	3:E:297:ARG:HG2	1.84	0.42
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: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:B:42:TRP:O	3:B:43:LYS:C	2.62	0.42
3:E:144:GLN:O	3:E:148:LEU:HG	2.20	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:226:SER:O	3:B:227:VAL:C	2.62	0.42
3:B:318:VAL:HG12	3:B:322:MET:CG	2.49	0.42
3:E:154:ARG:HB3	3:E:154:ARG:CZ	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:80:ALA:C	3:F:82:GLY:N	2.77	0.41
3:B:133:GLN:O	3:B:134:ALA:C	2.62	0.41
3:B:188:THR:C	3:B:190:GLY:H	2.28	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
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:126:ASP:C	3:F:128:GLY:N	2.79	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:F:85:VAL:HG23	3:F:129:GLU:OE2	2.21	0.41
3:F:140:THR:HG22	3:F:141:ASP:N	2.34	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:A:317:ASN:O	3:A:318:VAL:C	2.62	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: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:E:146:ARG:C	3:E:148:LEU:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:LEU:O	3:B:47:SER:C	2.63	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
3:E:62:LYS:H	3:E:62:LYS:CD	2.29	0.41
3:E:117:MET:HE2	3:E:120:ILE:HD12	2.02	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: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
1:G:123:DT:H2''	1:G:124:DA:H8	1.85	0.40
3:F:126:ASP:C	3:F:128:GLY:H	2.29	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:F:34:ARG:C	3:F:36:ALA:H	2.29	0.40
3:A:204:VAL:O	3:A:204:VAL:HG22	2.21	0.40
3:E:146:ARG:C	3:E:148:LEU:N	2.79	0.40
3:E:248:ALA:O	3:E:250:PRO:HD3	2.21	0.40
3:F:310:MET:HE3	3:F:316:THR:C	2.46	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	330/347 (95%)	306 (93%)	15 (4%)	9 (3%)	4	16
3	B	320/347 (92%)	279 (87%)	30 (9%)	11 (3%)	3	12
3	E	319/347 (92%)	277 (87%)	37 (12%)	5 (2%)	7	27
3	F	320/347 (92%)	295 (92%)	19 (6%)	6 (2%)	6	23
All	All	1289/1388 (93%)	1157 (90%)	101 (8%)	31 (2%)	4	18

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	258 (93%)	19 (7%)	14	41
3	B	269/291 (92%)	252 (94%)	17 (6%)	16	45
3	E	268/291 (92%)	247 (92%)	21 (8%)	11	35
3	F	269/291 (92%)	249 (93%)	20 (7%)	13	38
All	All	1083/1164 (93%)	1006 (93%)	77 (7%)	13	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	72	ARG
3	A	89	GLN
3	A	92	LEU
3	A	95	LEU
3	A	98	LEU
3	A	109	ASP
3	A	187	ARG
3	A	206	THR

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Mol	Chain	Res	Type
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	A	338	LEU
3	B	27	LEU
3	B	30	MET
3	B	35	GLN
3	B	45	LEU
3	B	68	PRO
3	B	72	ARG
3	B	95	LEU
3	B	111	ASN
3	B	113	VAL
3	B	132	LYS
3	B	140	THR
3	B	148	LEU
3	B	150	GLU
3	B	156	GLN
3	B	194	LEU
3	B	293	VAL
3	B	338	LEU
3	E	57	LYS
3	E	86	LYS
3	E	89	GLN
3	E	92	LEU
3	E	95	LEU
3	E	116	VAL
3	E	132	LYS
3	E	171	LEU
3	E	181	ARG
3	E	182	VAL
3	E	196	HIS
3	E	219	LYS
3	E	232	ASP
3	E	235	ASN
3	E	238	LEU
3	E	243	ARG
3	E	256	LEU
3	E	281	GLN

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Mol	Chain	Res	Type
3	E	282	ARG
3	E	306	ILE
3	E	338	LEU
3	F	27	LEU
3	F	35	GLN
3	F	45	LEU
3	F	61	ARG
3	F	62	LYS
3	F	121	ARG
3	F	132	LYS
3	F	140	THR
3	F	145	VAL
3	F	155	CYS
3	F	156	GLN
3	F	218	THR
3	F	270	ARG
3	F	293	VAL
3	F	297	ARG
3	F	311	GLN
3	F	318	VAL
3	F	319	ASN
3	F	338	LEU
3	F	341	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	10	ASN
3	A	59	ASN
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	A	317	ASN
3	A	323	ASN
3	B	35	GLN
3	B	60	ASN
3	B	89	GLN

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Mol	Chain	Res	Type
3	B	90	GLN
3	B	133	GLN
3	B	144	GLN
3	B	156	GLN
3	B	236	ASN
3	B	281	GLN
3	B	289	HIS
3	B	317	ASN
3	B	319	ASN
3	B	327	ASN
3	E	35	GLN
3	E	79	GLN
3	E	90	GLN
3	E	94	GLN
3	E	156	GLN
3	E	169	ASN
3	E	235	ASN
3	E	323	ASN
3	F	35	GLN
3	F	89	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 ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UMP	C	107	1,2	17,20,21	0.46	0	23,28,31	0.53	0
1	UMP	G	107	1,2	17,20,21	0.37	0	23,28,31	0.46	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	1,2	-	0/7/21/22	0/2/2/2
1	UMP	G	107	1,2	-	2/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	G	107	UMP	O4'-C4'-C5'-O5'
1	G	107	UMP	C3'-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
1	G	107	UMP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.18	3 (8%) 17 14	27, 48, 81, 90	0
1	G	36/37 (97%)	0.66	2 (5%) 30 23	34, 62, 89, 140	0
2	D	37/37 (100%)	0.20	2 (5%) 31 24	28, 44, 79, 88	0
2	H	37/37 (100%)	0.86	6 (16%) 4 4	33, 66, 91, 109	0
3	A	332/347 (95%)	0.22	26 (7%) 19 16	12, 43, 88, 143	0
3	B	322/347 (92%)	0.35	14 (4%) 40 31	22, 57, 92, 137	0
3	E	321/347 (92%)	0.58	28 (8%) 16 13	32, 66, 103, 150	0
3	F	322/347 (92%)	0.29	16 (4%) 34 27	25, 52, 90, 133	0
All	All	1443/1536 (93%)	0.37	97 (6%) 24 19	12, 55, 93, 150	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	202	THR	7.7
1	G	100	DC	7.7
3	B	328	LEU	7.3
3	E	204	VAL	7.1
3	A	207	ALA	6.8
3	E	206	THR	6.7
3	A	19	THR	6.6
2	H	100	DG	6.4
3	A	201	LYS	6.0
3	A	204	VAL	6.0
3	B	331	GLU	5.9
3	E	208	GLY	5.5
3	B	330	SER	5.2
3	A	203	LEU	5.1
3	A	208	GLY	5.0
3	F	329	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
3	E	203	LEU	4.8
3	F	328	LEU	4.7
3	A	206	THR	4.4
3	E	341	ASP	4.3
3	E	200	THR	4.2
3	F	331	GLU	4.2
3	A	200	THR	4.2
2	D	100	DG	4.2
3	E	201	LYS	4.1
3	E	207	ALA	3.9
1	G	101	DG	3.9
3	F	330	SER	3.8
3	A	17	ASP	3.8
3	F	326	ARG	3.7
3	E	21	ASP	3.6
3	B	327	ASN	3.5
3	A	196	HIS	3.5
3	B	332	THR	3.4
3	E	202	THR	3.4
3	F	325	ILE	3.4
3	E	57	LYS	3.3
3	E	205	SER	3.3
1	C	100	DC	3.3
3	B	326	ARG	3.3
3	A	18	ALA	3.2
3	A	21	ASP	3.2
3	E	274	GLY	3.1
3	F	332	THR	3.1
3	A	24	ARG	3.1
3	E	199	ARG	3.1
3	B	329	ASP	3.1
3	A	12	PRO	3.0
2	H	136	DC	3.0
2	H	101	DG	2.9
3	B	140	THR	2.9
3	E	326	ARG	2.9
3	A	205	SER	2.9
3	A	197	ILE	2.9
3	F	323	ASN	2.8
3	F	324	TYR	2.8
3	A	14	LEU	2.7
3	E	155	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	341	ASP	2.7
3	E	35	GLN	2.6
3	A	108	SER	2.6
3	E	230	VAL	2.6
3	B	341	ASP	2.6
3	A	22	GLU	2.5
3	F	153	ASP	2.5
3	E	148	LEU	2.5
3	A	188	THR	2.5
3	B	323	ASN	2.4
3	A	199	ARG	2.4
3	B	20	SER	2.4
3	A	198	GLY	2.4
3	F	189	ASP	2.4
3	E	243	ARG	2.4
3	E	241	ARG	2.4
3	B	129	GLU	2.3
3	F	341	ASP	2.3
3	E	34	ARG	2.3
3	E	127	ALA	2.2
3	E	145	VAL	2.2
2	H	116	DC	2.2
3	E	229	GLY	2.2
3	F	333	GLY	2.2
3	B	333	GLY	2.2
3	E	228	SER	2.2
3	E	188	THR	2.1
1	C	118	DT	2.1
3	F	334	ALA	2.1
3	A	16	VAL	2.1
3	A	278	ASP	2.1
3	E	317	ASN	2.1
1	C	117	DG	2.1
3	B	31	PHE	2.1
2	H	135	DT	2.1
2	H	102	DA	2.1
2	D	135	DT	2.0
3	F	140	THR	2.0
3	F	207	ALA	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	0.92	0.12	37,51,66,68	0
1	UMP	G	107	19/20	0.94	0.10	49,53,58,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	0.81	0.67	53,53,53,53	1
5	MG	A	347	1/1	0.82	0.29	63,63,63,63	0
5	MG	D	301	1/1	0.89	0.21	60,60,60,60	0
5	MG	D	310	1/1	0.90	0.26	58,58,58,58	0
5	MG	F	345	1/1	0.91	0.29	32,32,32,32	1
5	MG	A	346	1/1	0.92	0.30	56,56,56,56	0
4	IOD	C	200	1/1	0.93	0.10	52,52,52,52	1
5	MG	C	308	1/1	0.93	0.16	44,44,44,44	0
5	MG	A	345	1/1	0.94	0.33	39,39,39,39	0
5	MG	A	344	1/1	0.95	0.17	41,41,41,41	0
5	MG	G	306	1/1	0.96	0.27	55,55,55,55	0
4	IOD	F	344	1/1	0.98	0.12	46,46,46,46	1

6.5 Other polymers [i](#)

There are no such residues in this entry.