



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:46 PM GMT

PDB ID : 1C9B
Title : CRYSTAL STRUCTURE OF A HUMAN TBP CORE DOMAIN-HUMAN
TFIIB CORE DOMAIN COMPLEX BOUND TO AN EXTENDED, MODI-
FIED ADENOVIRAL MAJOR LATE PROMOTER (ADMLP)
Authors : Tsai, F.T.F.; Sigler, P.B.
Deposited on : 1999-08-01
Resolution : 2.65 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

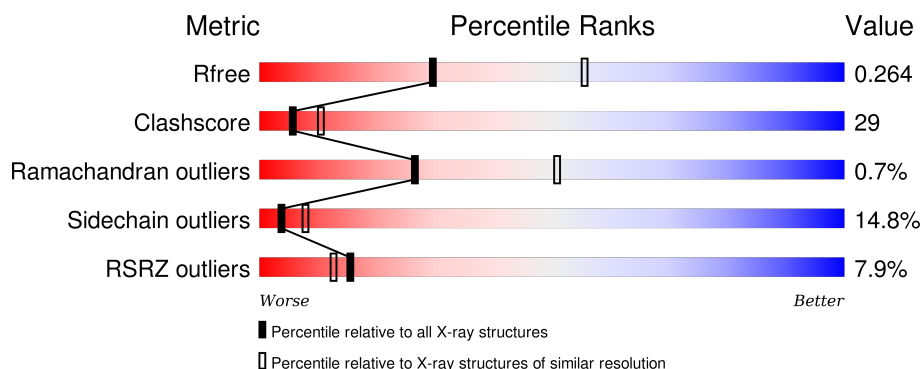
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.





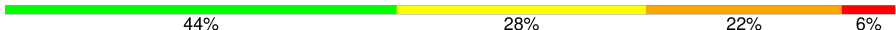
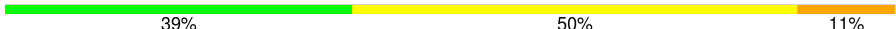
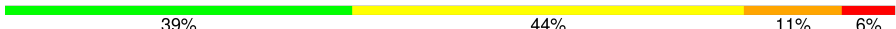






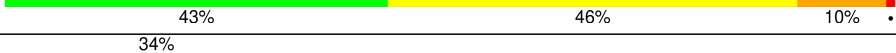

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	18	<div> <div>44%</div> <div>33%</div> <div>22%</div> </div>
1	G	18	<div> <div>39%</div> <div>44%</div> <div>17%</div> </div>
1	K	18	<div> <div>44%</div> <div>39%</div> <div>17%</div> </div>
1	O	18	<div> <div>33%</div> <div>61%</div> <div>6%</div> </div>
1	S	18	<div> <div>44%</div> <div>44%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	18	
2	H	18	
2	L	18	
2	P	18	
2	T	18	
3	A	207	
3	E	207	
3	I	207	
3	M	207	
3	Q	207	
4	B	180	
4	F	180	
4	J	180	
4	N	180	
4	R	180	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19199 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 ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	G	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	K	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	O	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	S	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			

- Molecule 2 is a DNA chain called ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	H	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	L	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	P	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	T	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			

- Molecule 3 is a protein called GENERAL TRANSCRIPTION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	I	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	M	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	Q	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			

- Molecule 4 is a protein called TATA BOX BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	F	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	J	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	N	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	R	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	158	GLY	SER	CONFLICT	UNP P20226
F	158	GLY	SER	CONFLICT	UNP P20226
J	158	GLY	SER	CONFLICT	UNP P20226
N	158	GLY	SER	CONFLICT	UNP P20226
R	158	GLY	SER	CONFLICT	UNP P20226

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total	O	0	0
			28	28		
5	B	44	Total	O	0	0
			44	44		
5	C	15	Total	O	0	0
			15	15		

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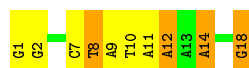
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	15	Total 15	O 15	0	0
5	E	56	Total 56	O 56	0	0
5	F	29	Total 29	O 29	0	0
5	G	7	Total 7	O 7	0	0
5	H	14	Total 14	O 14	0	0
5	I	12	Total 12	O 12	0	0
5	J	22	Total 22	O 22	0	0
5	K	7	Total 7	O 7	0	0
5	L	8	Total 8	O 8	0	0
5	M	15	Total 15	O 15	0	0
5	N	14	Total 14	O 14	0	0
5	O	7	Total 7	O 7	0	0
5	P	9	Total 9	O 9	0	0
5	Q	10	Total 10	O 10	0	0
5	R	9	Total 9	O 9	0	0
5	S	4	Total 4	O 4	0	0
5	T	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

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

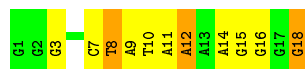
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain C: 



- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain G: 



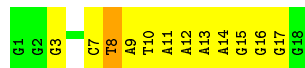
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain K: 



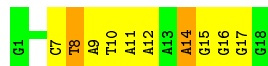
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain O: 



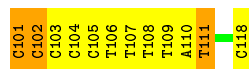
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain S: 



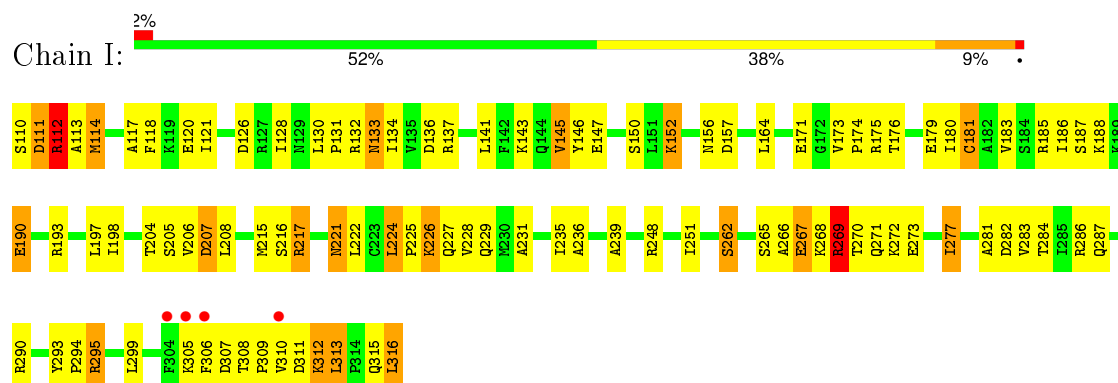
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain D: 

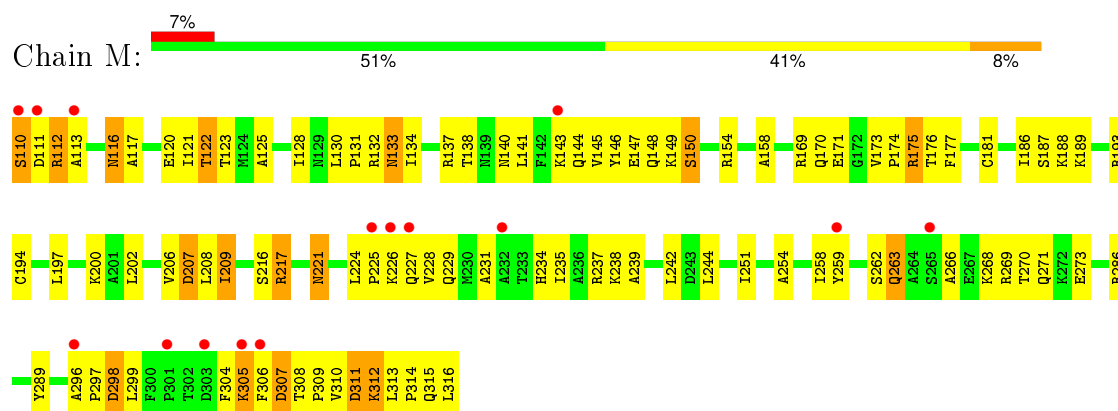


P225	K226	Q227	V228	K237	K238	L251	S262	S265	K268	R269	T270	Q271	K272	E273	D276	I277	A278	D282	V283	Q287	S288	Y289	Y293	R293	R294	R295	A296	T297	D298	L299	T302	K305	F306	V310	D311	K312	L313	Q314	Q315	L316	P310	D111	A113	M114	K119	E120	T121	T122	T123	P131	R132	M133	R137	T138	M139	S150	L151	R154	D157	R169	Q170	P174	T176	F177	K178	E179	R185	L186	S187	K188	K189	E190	R193	K196	L197	L202	E203	T204	S205	V206	S216	R217	F218	L220
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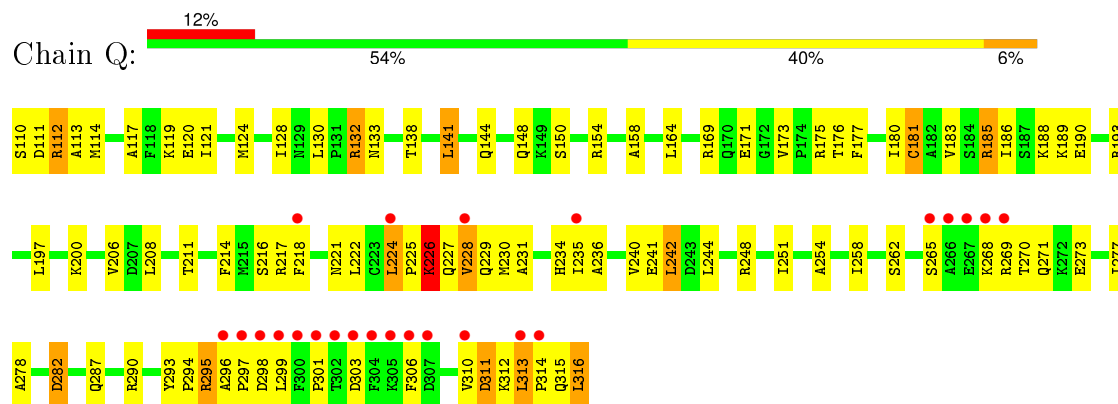
- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



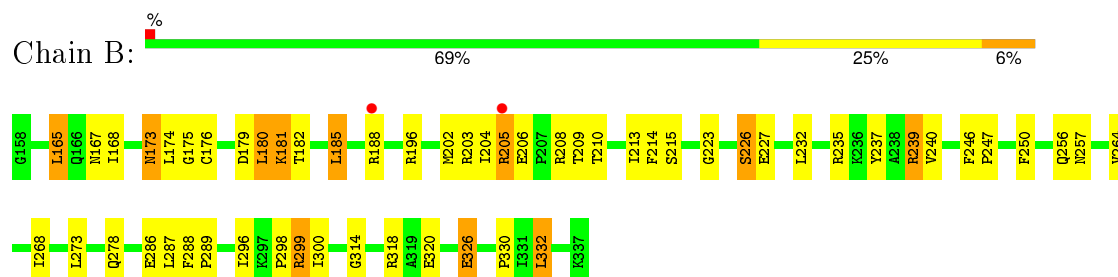
- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



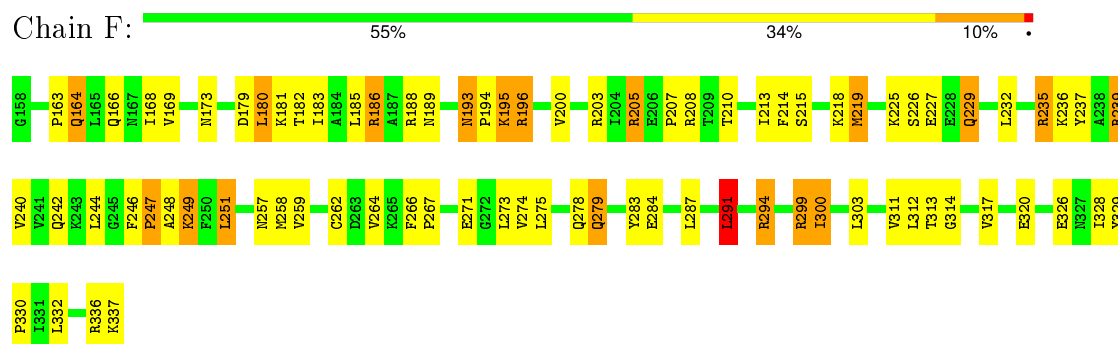
- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



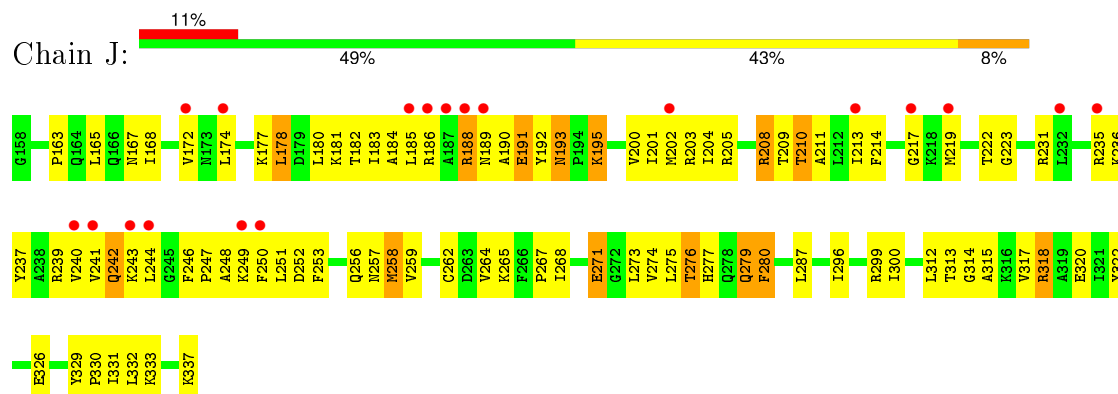
- Molecule 4: TATA BOX BINDING PROTEIN



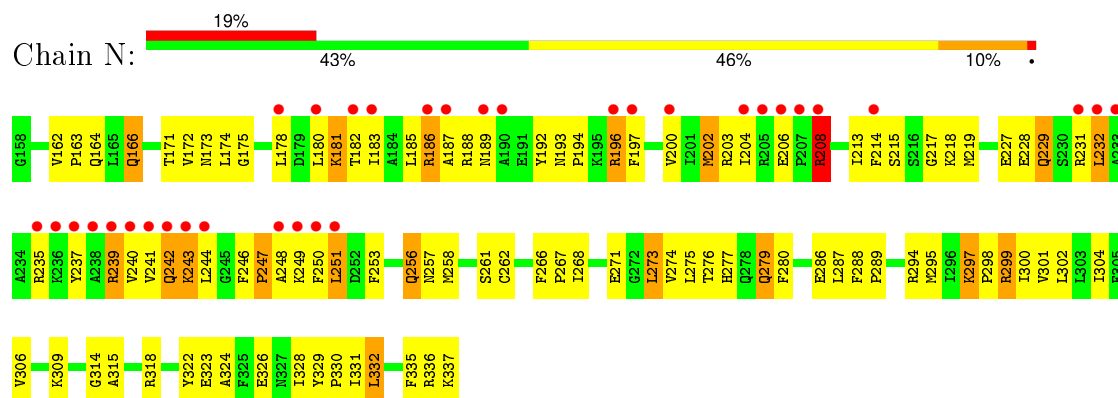
• Molecule 4: TATA BOX BINDING PROTEIN



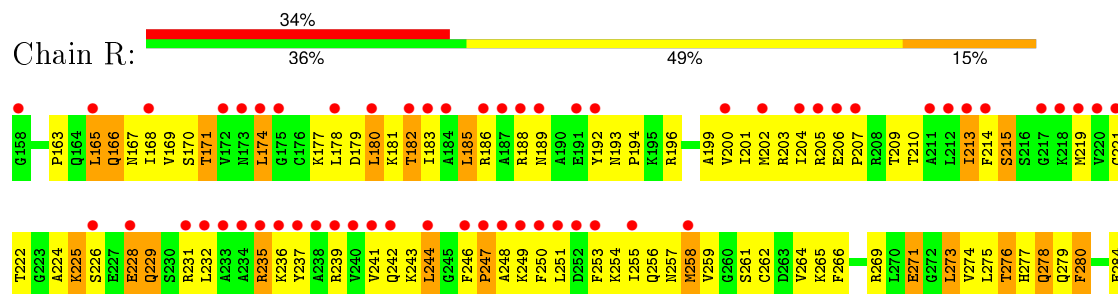
• Molecule 4: TATA BOX BINDING PROTEIN

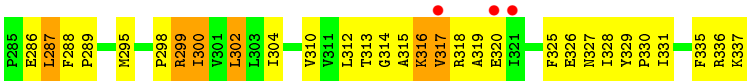


• Molecule 4: TATA BOX BINDING PROTEIN



• Molecule 4: TATA BOX BINDING PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.45Å 122.30Å 140.22Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 46.74 – 2.66	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.65) 94.7 (46.74-2.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.65Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.229 , 0.260 0.234 , 0.264	Depositor DCC
R_{free} test set	5030 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 99505 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19199	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.10	0/423	1.07	0/653
1	G	1.03	0/423	1.06	0/653
1	K	0.96	0/423	1.05	0/653
1	O	0.94	0/423	1.07	0/653
1	S	0.88	0/423	1.04	0/653
2	D	1.01	0/397	1.08	0/609
2	H	1.09	0/397	1.14	1/609 (0.2%)
2	L	0.85	0/397	1.08	1/609 (0.2%)
2	P	0.88	0/397	1.09	0/609
2	T	0.86	0/397	1.07	1/609 (0.2%)
3	A	0.67	1/1639 (0.1%)	0.78	1/2209 (0.0%)
3	E	0.68	0/1639	0.73	2/2209 (0.1%)
3	I	0.64	0/1639	0.73	1/2209 (0.0%)
3	M	0.62	1/1639 (0.1%)	0.72	0/2209
3	Q	0.68	1/1639 (0.1%)	0.79	2/2209 (0.1%)
4	B	0.77	0/1453	0.84	0/1953
4	F	0.68	0/1453	0.85	2/1953 (0.1%)
4	J	0.65	0/1453	0.80	0/1953
4	N	0.69	0/1453	0.82	2/1953 (0.1%)
4	R	0.73	0/1453	0.76	0/1953
All	All	0.75	3/19560 (0.0%)	0.86	13/27120 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
1	G	0	3
1	K	0	4
1	O	0	2
1	S	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	3
2	H	0	1
2	L	0	5
2	P	0	2
2	T	0	3
3	I	0	1
4	N	0	1
All	All	0	31

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	181	CYS	CB-SG	-7.45	1.69	1.82
3	Q	181	CYS	CB-SG	-5.49	1.72	1.81
3	M	181	CYS	CB-SG	-5.07	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	169	ARG	NE-CZ-NH1	11.56	126.08	120.30
4	N	235	ARG	NE-CZ-NH1	7.09	123.85	120.30
4	F	291	LEU	CA-CB-CG	6.97	131.34	115.30
4	N	235	ARG	CG-CD-NE	-6.24	98.70	111.80
3	I	269	ARG	CG-CD-NE	-5.89	99.44	111.80
2	L	101	DC	N1-C1'-C2'	-5.79	101.59	112.60
3	E	197	LEU	CA-CB-CG	5.41	127.73	115.30
4	F	196	ARG	CG-CD-NE	5.35	123.03	111.80
3	Q	132	ARG	NE-CZ-NH2	-5.33	117.63	120.30
2	T	101	DC	N1-C1'-C2'	-5.27	102.58	112.60
2	H	101	DC	N1-C1'-C2'	-5.24	102.64	112.60
3	E	169	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	Q	132	ARG	CA-CB-CG	5.06	124.53	113.40

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	12	DA	Sidechain
1	C	14	DA	Sidechain
1	C	18	DG	Sidechain
1	C	8	DT	Sidechain

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Mol	Chain	Res	Type	Group
2	D	101	DC	Sidechain
2	D	102	DC	Sidechain
2	D	111	DT	Sidechain
1	G	12	DA	Sidechain
1	G	18	DG	Sidechain
1	G	8	DT	Sidechain
2	H	101	DC	Sidechain
3	I	269	ARG	Sidechain
1	K	13	DA	Sidechain
1	K	14	DA	Sidechain
1	K	18	DG	Sidechain
1	K	8	DT	Sidechain
2	L	101	DC	Sidechain
2	L	102	DC	Sidechain
2	L	103	DC	Sidechain
2	L	110	DA	Sidechain
2	L	111	DT	Sidechain
4	N	299	ARG	Sidechain
1	O	13	DA	Sidechain
1	O	8	DT	Sidechain
2	P	101	DC	Sidechain
2	P	102	DC	Sidechain
1	S	14	DA	Sidechain
1	S	8	DT	Sidechain
2	T	101	DC	Sidechain
2	T	102	DC	Sidechain
2	T	110	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	375	0	202	17	0
1	G	375	0	202	20	0
1	K	375	0	202	9	0
1	O	375	0	202	14	0
1	S	375	0	202	13	0
2	D	357	0	205	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	357	0	205	13	0
2	L	357	0	205	14	0
2	P	357	0	205	19	0
2	T	357	0	205	24	0
3	A	1615	0	1670	90	0
3	E	1615	0	1670	65	0
3	I	1615	0	1670	117	0
3	M	1615	0	1670	115	0
3	Q	1615	0	1670	91	0
4	B	1427	0	1517	46	0
4	F	1427	0	1517	103	0
4	J	1427	0	1517	93	0
4	N	1427	0	1517	111	0
4	R	1427	0	1517	137	0
5	A	28	0	0	4	0
5	B	44	0	0	2	0
5	C	15	0	0	2	0
5	D	15	0	0	0	0
5	E	56	0	0	2	0
5	F	29	0	0	1	0
5	G	7	0	0	1	0
5	H	14	0	0	0	0
5	I	12	0	0	2	0
5	J	22	0	0	0	0
5	K	7	0	0	1	0
5	L	8	0	0	0	0
5	M	15	0	0	1	0
5	N	14	0	0	2	0
5	O	7	0	0	1	0
5	P	9	0	0	0	0
5	Q	10	0	0	0	0
5	R	9	0	0	1	0
5	S	4	0	0	0	0
5	T	4	0	0	0	0
All	All	19199	0	17970	1074	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 29.

All (1074) 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)
4:N:193:ASN:HB3	4:N:196:ARG:NE	1.37	1.35
4:N:193:ASN:CB	4:N:196:ARG:HE	1.47	1.26
3:Q:224:LEU:CD2	3:Q:228:VAL:HG21	1.67	1.23
4:N:188:ARG:HG3	4:N:189:ASN:H	1.04	1.20
1:G:11:DA:H2''	1:G:12:DA:H5'	1.22	1.16
1:O:11:DA:H2''	1:O:12:DA:H5'	1.23	1.16
3:Q:295:ARG:HG2	3:Q:295:ARG:HH11	1.11	1.16
4:R:259:VAL:HG22	4:R:313:THR:HG22	1.20	1.13
3:I:309:PRO:HG2	3:I:312:LYS:HG2	1.22	1.12
3:A:270:THR:HG22	3:A:273:GLU:H	1.05	1.11
4:B:181:LYS:H	4:B:181:LYS:HD2	1.02	1.11
1:S:11:DA:H2''	1:S:12:DA:H5'	1.30	1.10
4:N:229:GLN:HA	4:N:229:GLN:HE21	1.17	1.09
4:N:229:GLN:NE2	4:N:229:GLN:HA	1.66	1.09
1:K:11:DA:H2''	1:K:12:DA:H5'	1.17	1.08
4:F:181:LYS:H	4:F:181:LYS:HD2	0.96	1.08
4:F:193:ASN:ND2	4:F:195:LYS:HD2	1.68	1.08
4:R:269:ARG:HG2	4:R:337:LYS:HG2	1.35	1.06
4:N:180:LEU:HD21	4:N:215:SER:HB3	1.37	1.05
3:Q:224:LEU:HD22	3:Q:228:VAL:HG21	1.09	1.04
4:R:242:GLN:HG2	4:R:248:ALA:HB3	1.07	1.04
4:N:188:ARG:HG3	4:N:189:ASN:N	1.68	1.03
4:F:180:LEU:HD21	4:F:215:SER:HB3	1.36	1.02
3:I:133:ASN:HD22	3:I:133:ASN:H	1.07	1.02
4:F:188:ARG:HG3	4:F:189:ASN:H	1.23	1.02
3:Q:128:ILE:CG2	3:Q:183:VAL:HG11	1.89	1.02
4:J:188:ARG:HG2	4:J:189:ASN:N	1.75	1.01
4:R:213:ILE:HD13	4:R:219:MET:HB3	1.40	1.01
4:F:193:ASN:HD21	4:F:195:LYS:HD2	1.15	1.00
3:M:125:ALA:HA	3:M:130:LEU:HD12	1.39	1.00
4:N:295:MET:HE1	4:N:324:ALA:HA	1.39	1.00
3:M:209:ILE:HD12	3:M:209:ILE:H	1.24	1.00
4:F:229:GLN:HE21	4:F:229:GLN:HA	1.26	1.00
3:M:305:LYS:CD	3:M:305:LYS:H	1.71	0.99
4:F:180:LEU:HD22	4:F:180:LEU:H	1.26	0.99
4:R:207:PRO:HB3	4:R:229:GLN:OE1	1.64	0.98
4:R:286:GLU:HG3	5:R:338:HOH:O	1.62	0.97
3:M:175:ARG:HG2	3:M:175:ARG:HH11	1.27	0.97
3:I:312:LYS:HD3	3:I:312:LYS:N	1.79	0.97
3:I:270:THR:HG23	3:I:273:GLU:H	1.29	0.97
4:N:243:LYS:O	4:N:243:LYS:HD3	1.64	0.97
4:R:259:VAL:HG22	4:R:313:THR:CG2	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:181:LYS:HD2	4:F:181:LYS:N	1.82	0.95
3:Q:224:LEU:HD23	3:Q:228:VAL:HG11	1.47	0.95
4:F:205:ARG:H	4:F:205:ARG:HD2	1.31	0.95
4:J:279:GLN:HG3	4:J:280:PHE:CE2	2.02	0.95
4:R:181:LYS:O	4:R:185:LEU:HD13	1.67	0.94
4:F:205:ARG:H	4:F:205:ARG:CD	1.77	0.94
3:Q:242:LEU:HB3	3:Q:244:LEU:HD13	1.46	0.94
4:N:193:ASN:O	4:N:196:ARG:HG3	1.66	0.94
2:D:108:DT:H2''	2:D:109:DT:H5'	1.50	0.94
2:T:110:DA:H2''	2:T:111:DT:H5'	1.49	0.94
2:P:110:DA:H5'	4:N:166:GLN:HG2	1.48	0.94
2:T:110:DA:H5'	4:R:166:GLN:HG2	1.48	0.94
3:Q:128:ILE:HG23	3:Q:183:VAL:HG11	1.50	0.94
3:I:295:ARG:HH11	3:I:295:ARG:HG3	1.32	0.93
1:C:11:DA:H2''	1:C:12:DA:H5'	1.50	0.93
4:R:242:GLN:HG2	4:R:248:ALA:CB	1.99	0.93
2:H:108:DT:H2''	2:H:109:DT:H5'	1.49	0.93
4:R:213:ILE:CD1	4:R:219:MET:HB3	1.98	0.93
3:I:204:THR:HG22	3:I:205:SER:H	1.35	0.92
4:N:229:GLN:CA	4:N:229:GLN:HE21	1.82	0.92
4:R:188:ARG:NH2	4:R:189:ASN:HD21	1.68	0.91
4:J:193:ASN:ND2	4:J:195:LYS:HG3	1.85	0.91
3:I:312:LYS:HD3	3:I:312:LYS:H	1.32	0.91
4:N:229:GLN:HE22	4:N:232:LEU:HD12	1.34	0.90
1:G:3:DG:N3	5:G:147:HOH:O	2.03	0.90
3:M:289:TYR:CE2	3:M:316:LEU:HD12	2.07	0.90
4:J:279:GLN:HG3	4:J:280:PHE:HE2	1.37	0.89
3:Q:189:LYS:HE2	3:Q:193:ARG:HH21	1.35	0.89
3:Q:189:LYS:HE2	3:Q:193:ARG:NH2	1.87	0.89
3:M:224:LEU:HB3	3:M:228:VAL:HG21	1.52	0.89
4:R:165:LEU:O	4:R:225:LYS:HD3	1.72	0.89
4:R:271:GLU:CD	4:R:271:GLU:H	1.76	0.89
3:A:189:LYS:HE2	3:A:193:ARG:NH2	1.86	0.89
3:I:133:ASN:ND2	3:I:133:ASN:H	1.68	0.89
3:Q:224:LEU:HD22	3:Q:228:VAL:CG2	2.01	0.88
3:I:185:ARG:HG2	5:I:318:HOH:O	1.71	0.88
4:F:259:VAL:HG22	4:F:313:THR:HG22	1.52	0.88
4:B:181:LYS:H	4:B:181:LYS:CD	1.87	0.88
2:P:110:DA:H2''	2:P:111:DT:H5'	1.54	0.88
4:R:288:PHE:CD2	4:R:289:PRO:HD2	2.08	0.87
1:G:9:DA:H2''	1:G:10:DT:H5'	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:181:LYS:HD2	4:B:181:LYS:N	1.87	0.87
3:A:267:GLU:HA	3:A:267:GLU:OE2	1.69	0.87
4:J:167:ASN:HD21	4:J:223:GLY:H	1.22	0.87
3:M:209:ILE:HD12	3:M:209:ILE:N	1.89	0.87
3:E:133:ASN:H	3:E:133:ASN:HD22	1.17	0.87
3:A:270:THR:HG22	3:A:273:GLU:N	1.89	0.86
4:F:235:ARG:HH21	4:F:235:ARG:HG3	1.38	0.86
4:R:242:GLN:CG	4:R:248:ALA:HB3	2.01	0.86
4:J:193:ASN:HD21	4:J:195:LYS:HG3	1.38	0.85
4:R:179:ASP:OD1	4:R:182:THR:HG22	1.76	0.85
3:I:270:THR:HG22	3:I:273:GLU:CG	2.05	0.85
3:I:221:ASN:N	3:I:221:ASN:HD22	1.73	0.85
3:I:270:THR:HG22	3:I:273:GLU:HG3	1.57	0.85
4:N:256:GLN:HE21	4:N:256:GLN:HA	1.42	0.85
4:N:193:ASN:CG	4:N:196:ARG:HG2	1.98	0.84
3:Q:121:ILE:HD13	3:Q:138:THR:HG22	1.58	0.84
3:M:224:LEU:HD21	3:M:269:ARG:HE	1.43	0.84
3:M:305:LYS:HD2	3:M:305:LYS:H	1.41	0.84
4:N:178:LEU:HD11	4:N:217:GLY:HA2	1.58	0.84
3:A:133:ASN:HD22	3:A:133:ASN:H	1.26	0.83
3:Q:225:PRO:O	3:Q:228:VAL:HG13	1.78	0.83
3:M:189:LYS:HE2	3:M:193:ARG:NH1	1.93	0.83
3:A:133:ASN:HD22	3:A:133:ASN:N	1.77	0.82
2:P:108:DT:H2''	2:P:109:DT:H5'	1.61	0.82
4:R:224:ALA:HA	4:R:229:GLN:HE22	1.42	0.82
1:O:8:DT:H2''	1:O:9:DA:H5'	1.61	0.82
3:A:226:LYS:HG2	3:A:230:MET:HE2	1.61	0.82
4:F:229:GLN:HE21	4:F:229:GLN:CA	1.93	0.82
4:N:231:ARG:HA	4:N:253:PHE:CE2	2.15	0.81
3:M:140:ASN:O	3:M:144:GLN:HG3	1.79	0.81
4:N:257:ASN:HD21	4:N:314:GLY:H	1.28	0.81
1:G:11:DA:H2''	1:G:12:DA:C5'	2.08	0.81
4:F:188:ARG:HG3	4:F:189:ASN:N	1.94	0.81
2:L:110:DA:H2''	2:L:111:DT:H5'	1.62	0.81
1:C:8:DT:H2''	1:C:9:DA:H5'	1.63	0.81
3:I:306:PHE:CE1	3:I:310:VAL:HG22	2.16	0.81
4:F:299:ARG:O	4:F:300:ILE:HD13	1.81	0.80
3:Q:231:ALA:O	3:Q:235:ILE:HG13	1.80	0.80
1:K:9:DA:H2''	1:K:10:DT:H5'	1.64	0.80
3:M:263:GLN:HG2	3:M:314:PRO:HG2	1.64	0.80
2:T:107:DT:OP1	4:R:196:ARG:NH2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:305:LYS:N	3:M:305:LYS:CD	2.42	0.80
4:J:205:ARG:O	4:J:205:ARG:HD3	1.81	0.80
1:G:18:DG:O3'	3:M:316:LEU:HD23	1.81	0.79
3:I:295:ARG:HH11	3:I:295:ARG:CG	1.94	0.79
4:B:179:ASP:OD1	4:B:182:THR:HG23	1.82	0.79
4:J:186:ARG:NH1	4:J:244:LEU:HD22	1.96	0.79
4:B:257:ASN:HD21	4:B:314:GLY:H	1.31	0.79
4:N:295:MET:CE	4:N:324:ALA:HA	2.12	0.79
3:I:270:THR:CG2	3:I:273:GLU:H	1.95	0.79
1:K:11:DA:H2''	1:K:12:DA:C5'	2.07	0.79
4:N:239:ARG:HG2	4:N:242:GLN:HE22	1.48	0.79
2:T:108:DT:H1'	4:R:167:ASN:HD21	1.47	0.79
2:T:108:DT:H2''	2:T:109:DT:H5'	1.64	0.79
3:M:141:LEU:O	3:M:145:VAL:HG23	1.83	0.79
4:N:180:LEU:CD2	4:N:215:SER:HB3	2.13	0.78
4:R:207:PRO:HB3	4:R:229:GLN:CD	2.04	0.78
4:N:328:ILE:HG23	4:N:332:LEU:HD22	1.66	0.78
4:J:276:THR:OG1	4:J:277:HIS:HD2	1.65	0.78
4:F:181:LYS:H	4:F:181:LYS:CD	1.83	0.78
4:R:213:ILE:HD13	4:R:219:MET:CB	2.14	0.78
3:Q:295:ARG:NH1	3:Q:295:ARG:HG2	1.85	0.78
4:N:178:LEU:CD1	4:N:217:GLY:HA2	2.13	0.77
4:F:179:ASP:O	4:F:182:THR:HG22	1.83	0.77
2:T:109:DT:H5''	4:R:167:ASN:HD22	1.49	0.77
3:I:267:GLU:HB2	3:I:269:ARG:HH11	1.49	0.77
3:I:248:ARG:HH22	3:I:287:GLN:NE2	1.83	0.77
3:I:190:GLU:OE2	3:I:193:ARG:NH1	2.17	0.77
2:T:109:DT:H5''	4:R:167:ASN:ND2	1.99	0.77
4:N:318:ARG:HG2	4:N:322:TYR:CE2	2.20	0.77
4:N:193:ASN:O	4:N:196:ARG:CG	2.32	0.77
3:I:157:ASP:HB2	3:I:185:ARG:NH2	1.99	0.76
4:F:259:VAL:HG22	4:F:313:THR:CG2	2.16	0.76
1:G:15:DG:H2''	1:G:16:DG:H5''	1.66	0.76
3:Q:295:ARG:CG	3:Q:295:ARG:HH11	1.95	0.76
3:I:309:PRO:HG2	3:I:312:LYS:CG	2.11	0.76
4:F:193:ASN:HD21	4:F:195:LYS:CD	1.97	0.76
4:J:186:ARG:HH11	4:J:244:LEU:HD22	1.50	0.76
4:R:186:ARG:CZ	4:R:244:LEU:HG	2.15	0.76
3:M:270:THR:HG23	3:M:273:GLU:H	1.51	0.76
4:J:259:VAL:HG22	4:J:313:THR:HG22	1.67	0.76
4:R:186:ARG:NH1	4:R:244:LEU:O	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:173:VAL:O	3:M:173:VAL:HG23	1.84	0.76
3:M:131:PRO:HG2	3:M:134:ILE:HG12	1.67	0.76
4:R:257:ASN:HD21	4:R:314:GLY:H	1.31	0.75
1:G:11:DA:C2'	1:G:12:DA:H5'	2.12	0.75
1:S:14:DA:H1'	4:R:214:PHE:CZ	2.22	0.75
3:I:131:PRO:HB2	3:I:133:ASN:HD21	1.49	0.75
4:J:204:ILE:HD12	4:J:236:LYS:HD2	1.68	0.75
4:J:188:ARG:HG2	4:J:189:ASN:H	1.46	0.75
3:A:221:ASN:HD22	3:A:221:ASN:N	1.84	0.74
4:F:266:PHE:CD1	4:F:336:ARG:HG3	2.21	0.74
3:I:286:ARG:O	3:I:290:ARG:HG3	1.86	0.74
3:Q:226:LYS:H	3:Q:226:LYS:HD3	1.53	0.74
3:I:267:GLU:OE2	3:I:267:GLU:N	2.20	0.74
3:I:176:THR:OG1	3:I:179:GLU:HG3	1.87	0.74
1:S:7:DC:H2''	1:S:8:DT:H5'	1.68	0.74
4:J:181:LYS:O	4:J:185:LEU:HG	1.87	0.74
3:Q:224:LEU:CD2	3:Q:228:VAL:CG2	2.58	0.74
4:F:226:SER:OG	4:F:229:GLN:HB2	1.86	0.74
2:L:108:DT:H2''	2:L:109:DT:H5'	1.70	0.74
4:N:188:ARG:CG	4:N:189:ASN:H	1.94	0.73
3:M:112:ARG:O	3:M:112:ARG:HG3	1.88	0.73
4:F:188:ARG:CG	4:F:189:ASN:H	2.00	0.73
4:N:247:PRO:O	4:N:249:LYS:HE2	1.89	0.73
3:M:125:ALA:CA	3:M:130:LEU:HD12	2.18	0.73
2:T:110:DA:C5'	4:R:166:GLN:HG2	2.19	0.73
3:I:176:THR:HG22	3:I:251:ILE:HD13	1.70	0.73
3:M:137:ARG:HE	3:M:170:GLN:NE2	1.86	0.73
3:Q:235:ILE:HG23	3:Q:299:LEU:HB3	1.71	0.73
3:E:133:ASN:ND2	3:E:133:ASN:H	1.87	0.73
4:N:240:VAL:O	4:N:244:LEU:HG	1.89	0.73
2:H:110:DA:H2''	2:H:111:DT:H5'	1.71	0.73
4:R:209:THR:HG23	4:R:222:THR:O	1.88	0.72
4:F:229:GLN:NE2	4:F:229:GLN:HA	2.01	0.72
3:Q:173:VAL:CG1	3:Q:175:ARG:NH2	2.53	0.72
3:E:270:THR:HG23	3:E:273:GLU:OE1	1.89	0.72
4:N:186:ARG:HG2	4:N:244:LEU:HD22	1.71	0.72
3:I:114:MET:HG2	3:I:118:PHE:CZ	2.24	0.72
2:L:101:DC:H4'	3:I:152:LYS:HD3	1.71	0.72
3:I:112:ARG:HG2	3:I:112:ARG:O	1.90	0.72
2:P:111:DT:H5''	4:N:309:LYS:HD2	1.72	0.71
3:I:268:LYS:NZ	3:I:308:THR:OG1	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:205:ARG:NH1	4:B:208:ARG:HE	1.88	0.71
4:R:174:LEU:CD1	4:R:241:VAL:HG11	2.20	0.71
2:L:108:DT:OP1	4:J:210:THR:HG21	1.90	0.71
3:Q:290:ARG:NH2	3:Q:316:LEU:O	2.22	0.71
4:F:180:LEU:CD2	4:F:180:LEU:H	2.01	0.71
3:M:137:ARG:HE	3:M:170:GLN:HE22	1.38	0.71
4:J:318:ARG:HG2	4:J:322:TYR:CE2	2.26	0.71
3:Q:224:LEU:HD23	3:Q:228:VAL:CG1	2.20	0.71
3:M:305:LYS:N	3:M:305:LYS:HD3	2.03	0.71
3:A:128:ILE:HG12	3:A:183:VAL:HG11	1.73	0.71
4:R:166:GLN:NE2	4:R:261:SER:HB3	2.06	0.71
3:M:306:PHE:HD1	3:M:308:THR:O	1.75	0.70
3:A:248:ARG:CG	3:A:248:ARG:HH21	2.03	0.70
1:G:8:DT:H2"	1:G:9:DA:H5'	1.72	0.70
4:R:186:ARG:NE	4:R:244:LEU:HG	2.05	0.70
4:R:235:ARG:HA	4:R:250:PHE:CE1	2.26	0.70
3:M:143:LYS:HE2	3:M:147:GLU:OE2	1.92	0.70
3:I:222:LEU:HD23	3:I:277:ILE:HD13	1.72	0.70
4:F:205:ARG:HD2	4:F:205:ARG:N	2.02	0.70
2:D:110:DA:H2"	2:D:111:DT:H5'	1.73	0.70
4:N:237:TYR:O	4:N:241:VAL:HG23	1.90	0.70
4:N:304:ILE:HD13	4:N:332:LEU:HD11	1.72	0.70
3:I:309:PRO:CG	3:I:312:LYS:HG2	2.13	0.69
3:M:225:PRO:O	3:M:228:VAL:HG22	1.92	0.69
1:S:9:DA:H2"	1:S:10:DT:H5'	1.73	0.69
4:B:196:ARG:NH2	5:B:381:HOH:O	2.23	0.69
4:B:298:PRO:HB2	4:B:300:ILE:HD13	1.73	0.69
3:M:304:PHE:CZ	3:M:305:LYS:HE3	2.28	0.69
3:M:112:ARG:HH21	3:M:112:ARG:HG3	1.56	0.69
3:I:270:THR:CG2	3:I:273:GLU:HG3	2.22	0.69
2:P:110:DA:H2"	2:P:111:DT:C5'	2.22	0.69
4:N:256:GLN:NE2	4:N:256:GLN:HA	2.07	0.69
4:R:235:ARG:HA	4:R:250:PHE:HE1	1.57	0.69
4:B:300:ILE:HD11	4:B:320:GLU:HB3	1.73	0.69
4:N:279:GLN:NE2	4:N:280:PHE:CE2	2.59	0.69
4:F:180:LEU:HD23	4:F:181:LYS:NZ	2.07	0.69
4:F:194:PRO:HG2	4:F:195:LYS:HE3	1.74	0.69
3:I:111:ASP:C	3:I:113:ALA:H	1.95	0.69
4:N:202:MET:HE3	4:N:213:ILE:HD11	1.73	0.69
4:F:257:ASN:HD21	4:F:314:GLY:H	1.39	0.69
3:M:231:ALA:O	3:M:235:ILE:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:179:ASP:HB3	4:R:182:THR:CG2	2.23	0.69
1:K:8:DT:H2''	1:K:9:DA:H5'	1.74	0.69
3:Q:236:ALA:O	3:Q:240:VAL:HG23	1.92	0.69
4:F:203:ARG:HG2	4:F:210:THR:HG23	1.76	0.68
3:E:224:LEU:HD21	3:E:269:ARG:HD3	1.75	0.68
1:C:7:DC:H2'	1:C:8:DT:C6	2.29	0.68
1:C:9:DA:H2''	1:C:10:DT:H5'	1.73	0.68
3:I:204:THR:HG22	3:I:205:SER:N	2.08	0.68
4:J:276:THR:OG1	4:J:277:HIS:CD2	2.47	0.68
3:E:137:ARG:HE	3:E:170:GLN:NE2	1.91	0.68
2:D:105:DC:H2''	2:D:106:DT:H5'	1.75	0.68
4:R:271:GLU:N	4:R:271:GLU:OE2	2.26	0.68
3:I:143:LYS:O	3:I:147:GLU:HG3	1.94	0.68
3:Q:224:LEU:HD23	3:Q:228:VAL:HG21	1.71	0.67
4:J:279:GLN:HG2	4:J:280:PHE:HD2	1.58	0.67
1:G:7:DC:H2''	1:G:8:DT:H5'	1.76	0.67
1:S:11:DA:H2''	1:S:12:DA:C5'	2.17	0.67
3:I:225:PRO:HG2	3:I:228:VAL:HG23	1.76	0.67
3:M:112:ARG:HH21	3:M:112:ARG:CG	2.06	0.67
4:R:165:LEU:O	4:R:225:LYS:CD	2.41	0.67
4:R:188:ARG:CZ	4:R:189:ASN:HD21	2.07	0.67
2:L:105:DC:H2''	2:L:106:DT:H5'	1.76	0.67
4:J:279:GLN:CG	4:J:280:PHE:CD2	2.77	0.67
2:T:110:DA:H2''	2:T:111:DT:C5'	2.24	0.67
3:M:134:ILE:HD13	3:M:171:GLU:HG3	1.77	0.67
3:Q:173:VAL:HG12	3:Q:173:VAL:O	1.94	0.67
1:O:11:DA:H2''	1:O:12:DA:C5'	2.14	0.66
1:O:9:DA:H2''	1:O:10:DT:H5'	1.78	0.66
4:J:209:THR:HG22	4:J:210:THR:N	2.09	0.66
1:K:11:DA:C2'	1:K:12:DA:H5'	2.11	0.66
3:M:175:ARG:CG	3:M:175:ARG:HH11	2.06	0.66
3:I:221:ASN:ND2	3:I:221:ASN:N	2.44	0.66
3:M:311:ASP:N	3:M:311:ASP:OD2	2.28	0.66
3:I:271:GLN:NE2	3:I:316:LEU:HD21	2.11	0.66
4:F:173:ASN:HB2	4:F:218:LYS:HE2	1.76	0.66
4:N:267:PRO:HG2	4:N:337:LYS:HB2	1.77	0.66
4:R:204:ILE:HG23	4:R:237:TYR:CE1	2.30	0.66
3:A:134:ILE:HD12	3:A:171:GLU:HG3	1.78	0.66
3:Q:128:ILE:HG13	3:Q:130:LEU:HG	1.78	0.66
4:N:276:THR:HG21	4:N:335:PHE:HZ	1.60	0.66
3:Q:270:THR:OG1	3:Q:273:GLU:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:190:GLU:OE2	3:Q:193:ARG:NH1	2.30	0.66
2:T:109:DT:C5'	4:R:167:ASN:HD22	2.08	0.65
4:N:297:LYS:HE3	4:N:298:PRO:HA	1.77	0.65
3:M:111:ASP:C	3:M:113:ALA:H	2.00	0.65
4:B:268:ILE:HD13	4:B:332:LEU:HG	1.77	0.65
3:A:271:GLN:NE2	3:A:316:LEU:HD21	2.11	0.65
4:R:259:VAL:CG2	4:R:313:THR:HG22	2.10	0.65
4:N:202:MET:HE3	4:N:213:ILE:CD1	2.26	0.65
3:Q:226:LYS:CD	3:Q:226:LYS:H	2.07	0.65
2:H:107:DT:OP1	4:F:196:ARG:NH1	2.26	0.65
4:N:180:LEU:HD22	4:N:180:LEU:H	1.62	0.65
3:I:225:PRO:CD	3:I:267:GLU:HG3	2.25	0.65
4:R:255:ILE:O	4:R:316:LYS:HD2	1.96	0.65
3:Q:217:ARG:O	3:Q:221:ASN:OD1	2.13	0.65
3:A:111:ASP:C	3:A:113:ALA:H	2.00	0.65
3:E:157:ASP:HB2	3:E:185:ARG:NH2	2.12	0.65
3:M:224:LEU:HD21	3:M:269:ARG:NE	2.12	0.65
4:N:288:PHE:CD1	4:N:289:PRO:HD2	2.32	0.65
4:F:168:ILE:HD13	4:F:258:MET:HB3	1.78	0.65
4:B:296:ILE:HG23	4:B:299:ARG:NH1	2.12	0.64
4:F:213:ILE:HG12	4:F:219:MET:CE	2.27	0.64
4:J:268:ILE:HD13	4:J:332:LEU:HG	1.79	0.64
3:A:270:THR:HG23	3:A:272:LYS:H	1.62	0.64
3:M:227:GLN:OE1	3:M:305:LYS:HE2	1.97	0.64
3:M:209:ILE:CD1	3:M:209:ILE:H	1.90	0.64
3:Q:228:VAL:HG22	3:Q:229:GLN:N	2.13	0.64
3:E:310:VAL:HG13	3:E:311:ASP:OD1	1.98	0.64
4:N:204:ILE:HG23	4:N:237:TYR:CE1	2.33	0.64
4:J:267:PRO:HG2	4:J:337:LYS:HB2	1.79	0.64
2:H:108:DT:OP1	4:F:203:ARG:NH2	2.31	0.64
3:Q:226:LYS:HD3	3:Q:226:LYS:N	2.13	0.64
3:Q:111:ASP:C	3:Q:113:ALA:H	2.00	0.64
3:Q:306:PHE:CZ	3:Q:310:VAL:HG23	2.33	0.64
3:M:225:PRO:HG2	3:M:228:VAL:HG13	1.78	0.63
3:Q:173:VAL:CG1	3:Q:173:VAL:O	2.46	0.63
4:J:205:ARG:CD	4:J:205:ARG:O	2.45	0.63
4:R:329:TYR:HB3	4:R:330:PRO:HD3	1.80	0.63
4:R:254:LYS:HD3	4:R:256:GLN:HE22	1.62	0.63
4:R:269:ARG:HG3	4:R:335:PHE:O	1.97	0.63
4:N:329:TYR:HB3	4:N:330:PRO:HD3	1.79	0.63
4:J:279:GLN:HG3	4:J:280:PHE:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:196:ARG:HH22	4:R:201:ILE:CD1	2.12	0.63
4:J:209:THR:CG2	4:J:210:THR:N	2.62	0.62
4:R:299:ARG:O	4:R:300:ILE:HD12	1.99	0.62
4:N:229:GLN:NE2	4:N:232:LEU:HD12	2.10	0.62
3:A:193:ARG:NH1	5:A:334:HOH:O	2.33	0.62
4:J:296:ILE:HG23	4:J:299:ARG:NH2	2.14	0.62
4:J:178:LEU:CD2	4:J:183:ILE:HD11	2.30	0.62
3:Q:128:ILE:HG21	3:Q:183:VAL:HG11	1.78	0.62
3:M:312:LYS:HG2	3:M:312:LYS:O	1.98	0.62
3:M:133:ASN:ND2	3:M:133:ASN:H	1.97	0.62
4:B:173:ASN:ND2	4:B:175:GLY:H	1.96	0.62
4:N:171:THR:HG23	4:N:256:GLN:HG3	1.81	0.62
3:A:112:ARG:HD3	3:A:112:ARG:N	2.09	0.62
4:R:209:THR:HG22	4:R:210:THR:N	2.13	0.62
4:N:193:ASN:CB	4:N:196:ARG:HG2	2.29	0.62
3:A:174:PRO:O	3:A:217:ARG:NH2	2.33	0.62
3:E:305:LYS:HD3	3:E:305:LYS:O	2.00	0.62
2:L:101:DC:H4'	3:I:152:LYS:CD	2.30	0.62
3:E:111:ASP:C	3:E:113:ALA:H	2.04	0.61
4:R:163:PRO:HA	4:R:262:CYS:HB3	1.82	0.61
4:R:179:ASP:O	4:R:182:THR:HG23	2.00	0.61
4:J:296:ILE:HG23	4:J:299:ARG:HH22	1.64	0.61
4:R:171:THR:CG2	4:R:256:GLN:HG2	2.30	0.61
3:I:133:ASN:N	3:I:133:ASN:ND2	2.44	0.61
2:P:110:DA:C5'	4:N:166:GLN:HG2	2.27	0.61
4:N:257:ASN:HD21	4:N:314:GLY:N	1.95	0.61
3:I:225:PRO:HD2	3:I:267:GLU:HG3	1.82	0.61
3:M:254:ALA:O	3:M:258:ILE:HG13	2.00	0.61
4:J:257:ASN:HD21	4:J:314:GLY:H	1.47	0.61
2:H:102:DC:H2''	2:H:103:DC:O5'	2.01	0.61
4:N:300:ILE:HD11	4:N:315:ALA:HB2	1.81	0.61
4:R:174:LEU:HD12	4:R:241:VAL:HG11	1.83	0.61
2:H:106:DT:H2''	2:H:107:DT:H5'	1.81	0.61
3:M:117:ALA:O	3:M:121:ILE:HG13	2.00	0.61
3:A:269:ARG:CG	3:A:269:ARG:HH11	2.14	0.61
3:I:295:ARG:NH1	3:I:295:ARG:HG3	2.12	0.61
4:N:173:ASN:ND2	4:N:175:GLY:H	1.98	0.61
3:Q:112:ARG:N	3:Q:112:ARG:HD2	2.15	0.61
1:C:2:DG:OP2	5:C:172:HOH:O	2.16	0.61
3:M:224:LEU:HB3	3:M:228:VAL:CG2	2.28	0.61
4:F:196:ARG:NH2	5:F:361:HOH:O	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:DA:H1'	4:J:214:PHE:CZ	2.36	0.61
3:M:262:SER:OG	3:M:269:ARG:N	2.34	0.60
2:T:106:DT:H2''	2:T:107:DT:H5'	1.81	0.60
3:M:270:THR:HG22	3:M:273:GLU:CD	2.21	0.60
4:R:174:LEU:HD11	4:R:241:VAL:HG21	1.82	0.60
4:R:278:GLN:OE1	4:R:278:GLN:HA	2.00	0.60
2:D:108:DT:OP1	4:B:203:ARG:NH2	2.32	0.60
1:O:8:DT:H2''	1:O:9:DA:C5'	2.31	0.60
3:Q:173:VAL:CG1	3:Q:175:ARG:HH22	2.12	0.60
4:N:256:GLN:HE21	4:N:256:GLN:CA	2.10	0.60
2:T:105:DC:H2''	2:T:106:DT:H5'	1.82	0.60
2:D:101:DC:H2''	2:D:102:DC:H5'	1.83	0.60
3:I:231:ALA:O	3:I:235:ILE:HG13	2.02	0.60
3:I:216:SER:HA	3:I:229:GLN:NE2	2.17	0.60
4:J:172:VAL:HG21	4:J:250:PHE:CE1	2.37	0.60
2:T:108:DT:H1'	4:R:167:ASN:ND2	2.17	0.60
4:J:211:ALA:HB1	4:J:219:MET:CE	2.32	0.60
3:M:289:TYR:CD2	3:M:316:LEU:HD12	2.36	0.60
4:N:237:TYR:O	4:N:240:VAL:HG22	2.02	0.60
3:A:221:ASN:HD22	3:A:221:ASN:H	1.48	0.60
3:M:268:LYS:NZ	3:M:308:THR:OG1	2.34	0.59
4:F:271:GLU:H	4:F:271:GLU:CD	2.06	0.59
4:J:279:GLN:HG2	4:J:280:PHE:CD2	2.37	0.59
3:M:263:GLN:HG2	3:M:314:PRO:CG	2.30	0.59
4:N:249:LYS:HB3	4:N:251:LEU:CD1	2.32	0.59
4:N:268:ILE:HD13	4:N:332:LEU:HG	1.84	0.59
3:I:282:ASP:O	3:I:286:ARG:HG3	2.02	0.59
4:R:171:THR:CG2	4:R:256:GLN:CG	2.80	0.59
4:J:191:GLU:HG3	4:J:201:ILE:O	2.02	0.59
3:M:298:ASP:N	3:M:298:ASP:OD2	2.35	0.59
3:M:207:ASP:OD2	3:M:207:ASP:N	2.27	0.59
3:I:112:ARG:O	3:I:112:ARG:CG	2.51	0.59
1:G:18:DG:O3'	3:M:316:LEU:CD2	2.50	0.59
3:M:169:ARG:NH2	3:M:206:VAL:HG23	2.18	0.59
2:L:110:DA:H2''	2:L:111:DT:C5'	2.31	0.59
3:Q:173:VAL:HG13	3:Q:175:ARG:NH2	2.18	0.59
3:A:158:ALA:HA	3:A:186:ILE:HG13	1.85	0.59
4:F:235:ARG:HH21	4:F:235:ARG:CG	2.12	0.59
3:M:131:PRO:HG2	3:M:134:ILE:CG1	2.32	0.59
4:F:239:ARG:HH21	4:F:242:GLN:HE22	1.50	0.59
3:A:248:ARG:HH21	3:A:248:ARG:HG3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:204:THR:HG22	3:E:205:SER:N	2.18	0.59
1:C:14:DA:H1'	4:B:214:PHE:CE1	2.38	0.59
4:R:199:ALA:HB1	4:R:213:ILE:O	2.03	0.58
4:R:171:THR:HG23	4:R:256:GLN:HG2	1.84	0.58
4:F:203:ARG:CG	4:F:210:THR:HG23	2.33	0.58
3:M:125:ALA:HA	3:M:130:LEU:CD1	2.23	0.58
3:M:110:SER:O	3:M:113:ALA:HB2	2.03	0.58
3:M:238:LYS:HB3	3:M:299:LEU:HD22	1.84	0.58
4:R:179:ASP:CG	4:R:182:THR:HG22	2.23	0.58
4:N:239:ARG:HG2	4:N:242:GLN:NE2	2.17	0.58
4:R:279:GLN:HB3	4:R:280:PHE:CE2	2.38	0.58
4:N:306:VAL:HG22	5:N:340:HOH:O	2.02	0.58
3:A:133:ASN:ND2	3:A:133:ASN:N	2.50	0.58
2:P:105:DC:H2''	2:P:106:DT:H5'	1.85	0.58
1:S:7:DC:H2''	1:S:8:DT:C5'	2.34	0.58
4:R:317:VAL:HG23	4:R:319:ALA:H	1.67	0.58
4:J:209:THR:HG23	4:J:222:THR:O	2.04	0.58
4:J:205:ARG:HD3	4:J:208:ARG:HG3	1.86	0.58
3:I:225:PRO:CG	3:I:267:GLU:HG3	2.34	0.58
4:R:205:ARG:O	4:R:205:ARG:HG3	2.03	0.58
3:Q:176:THR:HG22	3:Q:251:ILE:CD1	2.34	0.58
2:P:106:DT:H2''	2:P:107:DT:H5'	1.86	0.58
1:G:11:DA:OP1	4:F:294:ARG:NH2	2.35	0.57
4:F:180:LEU:N	4:F:180:LEU:HD22	2.10	0.57
2:D:104:DC:H2''	2:D:105:DC:H5'	1.85	0.57
4:F:229:GLN:NE2	4:F:229:GLN:CA	2.65	0.57
3:A:122:THR:HG22	3:A:123:THR:N	2.17	0.57
4:R:178:LEU:HD22	4:R:246:PHE:CD2	2.39	0.57
3:I:226:LYS:H	3:I:226:LYS:HE2	1.70	0.57
3:I:130:LEU:HD22	3:I:134:ILE:HD12	1.87	0.57
1:O:14:DA:H1'	4:N:214:PHE:CZ	2.39	0.57
4:N:295:MET:HE2	4:N:324:ALA:CB	2.35	0.57
3:Q:111:ASP:O	3:Q:114:MET:HG3	2.04	0.57
4:N:196:ARG:HG3	4:N:197:PHE:H	1.69	0.57
4:R:224:ALA:HA	4:R:229:GLN:NE2	2.16	0.57
4:N:202:MET:CE	4:N:213:ILE:CD1	2.83	0.57
4:R:325:PHE:O	4:R:328:ILE:HG22	2.04	0.57
2:P:111:DT:H5''	4:N:309:LYS:CD	2.34	0.57
1:C:7:DC:H2''	1:C:8:DT:H5'	1.85	0.57
3:A:286:ARG:HG2	3:A:316:LEU:HD23	1.86	0.57
4:J:279:GLN:CG	4:J:280:PHE:HD2	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:179:ASP:OD1	4:F:182:THR:HG22	2.05	0.57
2:T:102:DC:H2"	2:T:103:DC:O5'	2.04	0.57
3:M:173:VAL:O	3:M:173:VAL:CG2	2.53	0.57
3:A:224:LEU:CD2	3:A:269:ARG:NH1	2.67	0.57
4:F:283:TYR:HB2	4:F:291:LEU:HD22	1.87	0.57
3:E:150:SER:C	3:E:151:LEU:HD12	2.25	0.57
3:M:175:ARG:NH1	3:M:175:ARG:HG2	2.07	0.56
3:I:222:LEU:HB2	3:I:224:LEU:HD12	1.85	0.56
3:A:157:ASP:HB2	3:A:185:ARG:NH2	2.20	0.56
3:I:173:VAL:O	3:I:173:VAL:HG23	2.04	0.56
4:R:269:ARG:CG	4:R:337:LYS:HG2	2.22	0.56
4:R:271:GLU:N	4:R:271:GLU:CD	2.55	0.56
3:M:270:THR:HG22	3:M:273:GLU:CG	2.36	0.56
3:I:137:ARG:HD2	3:I:171:GLU:HG2	1.87	0.56
1:G:15:DG:C2'	1:G:16:DG:H5"	2.34	0.56
4:R:209:THR:HG21	4:R:221:CYS:SG	2.45	0.56
3:Q:164:LEU:HD23	3:Q:180:ILE:HD12	1.86	0.56
3:Q:262:SER:OG	3:Q:269:ARG:N	2.38	0.56
3:I:132:ARG:NH1	3:I:136:ASP:OD1	2.39	0.56
3:I:207:ASP:OD1	3:I:207:ASP:N	2.29	0.56
3:A:133:ASN:ND2	3:A:133:ASN:H	2.01	0.56
3:I:131:PRO:HB2	3:I:133:ASN:ND2	2.19	0.56
3:I:225:PRO:HG3	3:I:267:GLU:OE1	2.06	0.56
3:A:117:ALA:O	3:A:121:ILE:HG13	2.06	0.56
3:Q:117:ALA:O	3:Q:121:ILE:HG13	2.06	0.56
4:B:205:ARG:HH12	4:B:208:ARG:HE	1.54	0.56
4:F:213:ILE:HG12	4:F:219:MET:HE3	1.88	0.56
3:A:309:PRO:HG3	3:A:312:LYS:HE3	1.88	0.56
3:I:157:ASP:CB	3:I:185:ARG:NH2	2.69	0.56
4:F:163:PRO:HA	4:F:262:CYS:HB3	1.88	0.56
3:M:308:THR:HG23	3:M:312:LYS:HD2	1.87	0.56
3:E:133:ASN:N	3:E:133:ASN:ND2	2.54	0.56
3:M:121:ILE:HD13	3:M:138:THR:HG22	1.88	0.56
3:Q:176:THR:HG22	3:Q:251:ILE:HD13	1.88	0.56
1:O:7:DC:H2'	1:O:8:DT:C6	2.41	0.56
4:R:280:PHE:N	4:R:280:PHE:CD2	2.74	0.56
4:N:286:GLU:HG3	5:N:338:HOH:O	2.05	0.56
3:I:221:ASN:H	3:I:221:ASN:HD22	1.50	0.55
3:A:204:THR:HG22	3:A:205:SER:H	1.70	0.55
3:M:186:ILE:HG22	3:M:187:SER:N	2.21	0.55
3:I:295:ARG:NH1	3:I:295:ARG:CG	2.62	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:148:GLN:NE2	3:A:150:SER:OG	2.35	0.55
3:Q:262:SER:OG	3:Q:268:LYS:HA	2.07	0.55
4:J:279:GLN:H	4:J:279:GLN:HE21	1.53	0.55
3:Q:154:ARG:NH2	3:Q:190:GLU:OE1	2.37	0.55
4:N:294:ARG:HG2	4:N:301:VAL:HG22	1.87	0.55
2:P:101:DC:H2''	2:P:102:DC:O5'	2.07	0.55
4:J:317:VAL:HG23	4:J:320:GLU:HG3	1.87	0.55
3:I:270:THR:HG22	3:I:273:GLU:CB	2.36	0.55
3:I:221:ASN:ND2	3:I:221:ASN:H	2.04	0.55
4:R:278:GLN:CA	4:R:278:GLN:OE1	2.55	0.55
3:E:196:LYS:HE2	5:E:371:HOH:O	2.06	0.55
3:E:131:PRO:HB2	3:E:133:ASN:HD21	1.72	0.55
4:J:174:LEU:HD12	4:J:248:ALA:HB1	1.89	0.55
4:B:204:ILE:HG23	4:B:237:TYR:CE1	2.42	0.55
3:M:209:ILE:CD1	3:M:209:ILE:N	2.58	0.54
4:J:239:ARG:NH1	4:J:242:GLN:HE22	2.05	0.54
4:J:329:TYR:HB3	4:J:330:PRO:HD3	1.90	0.54
3:I:309:PRO:CG	3:I:312:LYS:HE2	2.37	0.54
4:F:259:VAL:HG13	4:F:313:THR:CG2	2.36	0.54
2:L:101:DC:H2''	2:L:102:DC:H5'	1.89	0.54
3:A:289:TYR:CD2	3:A:316:LEU:HD22	2.41	0.54
3:A:186:ILE:HG22	3:A:187:SER:N	2.22	0.54
4:F:179:ASP:O	4:F:182:THR:CG2	2.54	0.54
4:R:231:ARG:HB3	4:R:231:ARG:NH1	2.22	0.54
4:N:295:MET:HE2	4:N:324:ALA:HB1	1.90	0.54
3:Q:193:ARG:O	3:Q:197:LEU:HD22	2.08	0.54
3:Q:193:ARG:O	3:Q:197:LEU:CD2	2.55	0.54
4:R:196:ARG:HH22	4:R:201:ILE:HD11	1.72	0.54
3:M:307:ASP:C	3:M:307:ASP:OD1	2.46	0.54
4:F:264:VAL:HG11	4:F:332:LEU:HD23	1.88	0.54
3:E:110:SER:O	3:E:113:ALA:HB2	2.08	0.54
3:A:189:LYS:CE	3:A:193:ARG:NH2	2.66	0.54
4:R:209:THR:CG2	4:R:210:THR:N	2.70	0.54
4:F:180:LEU:HD23	4:F:181:LYS:HZ1	1.73	0.54
4:J:237:TYR:O	4:J:240:VAL:HG22	2.08	0.54
3:Q:128:ILE:CG2	3:Q:183:VAL:CG1	2.77	0.54
3:E:296:ALA:N	3:E:297:PRO:HD2	2.24	0.54
4:N:273:LEU:O	4:N:273:LEU:HD23	2.07	0.54
1:O:11:DA:C2'	1:O:12:DA:H5'	2.15	0.53
3:I:293:TYR:HB3	3:I:294:PRO:HD3	1.91	0.53
3:I:141:LEU:O	3:I:145:VAL:CG2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:259:VAL:HG13	4:J:313:THR:CG2	2.39	0.53
4:F:205:ARG:CD	4:F:205:ARG:N	2.56	0.53
3:M:228:VAL:HG23	3:M:229:GLN:N	2.24	0.53
3:A:296:ALA:N	3:A:297:PRO:HD2	2.23	0.53
1:S:7:DC:H2'	1:S:8:DT:C6	2.43	0.53
3:Q:128:ILE:HD11	3:Q:130:LEU:HD11	1.89	0.53
1:C:7:DC:H2''	1:C:8:DT:C5'	2.37	0.53
4:B:168:ILE:HD12	4:B:226:SER:C	2.29	0.53
4:R:170:SER:OG	4:R:221:CYS:HB3	2.08	0.53
2:D:101:DC:H2''	2:D:102:DC:C5'	2.39	0.53
4:R:213:ILE:HD11	4:R:219:MET:HB3	1.87	0.53
3:A:134:ILE:HG22	3:A:135:VAL:N	2.24	0.53
4:N:173:ASN:HB2	4:N:218:LYS:HD3	1.91	0.53
4:J:251:LEU:N	4:J:251:LEU:HD23	2.23	0.53
3:E:154:ARG:NH1	3:E:190:GLU:OE1	2.42	0.53
4:F:259:VAL:CG2	4:F:313:THR:HG22	2.32	0.52
4:J:277:HIS:CE1	4:J:331:ILE:HD13	2.44	0.52
3:Q:234:HIS:CG	3:Q:301:PRO:HG3	2.44	0.52
4:F:207:PRO:HD3	4:F:236:LYS:HE3	1.91	0.52
3:A:310:VAL:O	3:A:313:LEU:HB2	2.10	0.52
3:I:133:ASN:N	3:I:133:ASN:HD22	1.91	0.52
4:J:178:LEU:HD23	4:J:183:ILE:HD11	1.90	0.52
3:I:141:LEU:O	3:I:145:VAL:HG23	2.09	0.52
4:J:243:LYS:HB3	4:J:243:LYS:HZ2	1.75	0.52
4:F:180:LEU:CD2	4:F:215:SER:HB3	2.25	0.52
4:N:163:PRO:HA	4:N:262:CYS:HB3	1.89	0.52
3:A:215:MET:HG3	3:A:233:THR:OG1	2.09	0.52
3:A:270:THR:HG23	3:A:272:LYS:N	2.25	0.52
3:E:137:ARG:HE	3:E:170:GLN:HE22	1.54	0.52
4:B:288:PHE:CD1	4:B:289:PRO:HD2	2.44	0.52
1:O:3:DG:N3	5:O:225:HOH:O	2.33	0.52
3:I:312:LYS:CD	3:I:312:LYS:N	2.56	0.52
4:N:229:GLN:HE22	4:N:232:LEU:CD1	2.15	0.52
4:J:203:ARG:HG2	4:J:210:THR:HB	1.90	0.52
2:L:106:DT:H2''	2:L:107:DT:H5'	1.91	0.52
3:A:176:THR:OG1	3:A:179:GLU:HG3	2.09	0.52
3:M:112:ARG:CG	3:M:112:ARG:NH2	2.70	0.52
3:E:224:LEU:HD21	3:E:269:ARG:CD	2.40	0.52
3:A:310:VAL:HA	3:A:313:LEU:HD22	1.91	0.52
3:Q:254:ALA:O	3:Q:258:ILE:HG13	2.09	0.52
3:I:181:CYS:SG	3:I:188:LYS:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:228:GLU:OE2	4:N:228:GLU:HA	2.08	0.52
3:I:310:VAL:O	3:I:313:LEU:HB2	2.09	0.52
3:A:221:ASN:N	3:A:221:ASN:ND2	2.56	0.52
3:A:259:TYR:CE2	3:A:271:GLN:HG3	2.44	0.52
1:O:14:DA:H1'	4:N:214:PHE:CE1	2.45	0.52
2:P:102:DC:H2''	2:P:103:DC:O5'	2.09	0.52
4:F:185:LEU:HD23	4:F:185:LEU:C	2.29	0.52
2:H:108:DT:H2''	2:H:109:DT:C5'	2.31	0.52
4:N:288:PHE:CG	4:N:289:PRO:HD2	2.45	0.52
1:C:18:DG:H3'	3:E:271:GLN:NE2	2.24	0.52
4:F:180:LEU:HB3	4:F:200:VAL:CG2	2.40	0.51
4:J:174:LEU:HD23	4:J:217:GLY:O	2.09	0.51
1:G:7:DC:H2'	1:G:8:DT:C6	2.45	0.51
3:Q:169:ARG:NH1	4:R:284:GLU:OE1	2.31	0.51
4:J:231:ARG:HA	4:J:253:PHE:CE2	2.45	0.51
4:N:162:VAL:HG13	4:N:162:VAL:O	2.11	0.51
4:N:193:ASN:ND2	4:N:196:ARG:HG2	2.25	0.51
3:A:131:PRO:HB2	3:A:133:ASN:ND2	2.25	0.51
4:F:179:ASP:HB3	4:F:182:THR:CG2	2.41	0.51
4:F:182:THR:HG23	4:F:183:ILE:N	2.25	0.51
3:A:157:ASP:HB2	3:A:185:ARG:HH21	1.74	0.51
3:M:174:PRO:O	3:M:217:ARG:NH1	2.32	0.51
4:R:207:PRO:CB	4:R:229:GLN:OE1	2.50	0.51
1:C:18:DG:O3'	3:E:316:LEU:CD1	2.59	0.51
4:J:246:PHE:O	4:J:248:ALA:N	2.36	0.51
4:R:317:VAL:HG22	4:R:320:GLU:HG3	1.91	0.51
3:M:148:GLN:HB3	3:M:150:SER:OG	2.11	0.51
4:R:249:LYS:HB2	4:R:251:LEU:CD1	2.40	0.51
4:F:180:LEU:HB3	4:F:200:VAL:HG23	1.92	0.51
4:N:219:MET:HE1	4:N:237:TYR:HB3	1.93	0.51
4:J:259:VAL:HG13	4:J:313:THR:HG22	1.93	0.51
3:A:248:ARG:CG	3:A:248:ARG:NH2	2.71	0.51
4:J:243:LYS:HB3	4:J:243:LYS:NZ	2.25	0.51
3:M:231:ALA:HB2	3:M:304:PHE:CE2	2.46	0.51
3:Q:176:THR:CG2	3:Q:251:ILE:HD13	2.40	0.51
4:R:327:ASN:O	4:R:331:ILE:HD12	2.11	0.51
1:S:8:DT:H2''	1:S:9:DA:H5'	1.93	0.50
3:A:248:ARG:HG3	3:A:248:ARG:NH2	2.25	0.50
4:B:173:ASN:HD22	4:B:174:LEU:N	2.08	0.50
4:R:251:LEU:H	4:R:251:LEU:HD12	1.76	0.50
3:M:154:ARG:HD3	3:M:194:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:GLU:OE2	3:A:217:ARG:NH1	2.44	0.50
2:D:102:DC:H2''	2:D:103:DC:O5'	2.10	0.50
3:E:224:LEU:HD23	3:E:269:ARG:HH11	1.77	0.50
4:R:192:TYR:CD1	4:R:194:PRO:HD3	2.46	0.50
4:F:249:LYS:HB2	4:F:251:LEU:HD22	1.94	0.50
3:M:224:LEU:CD2	3:M:269:ARG:HE	2.19	0.50
3:A:224:LEU:HD21	3:A:269:ARG:HH11	1.74	0.50
4:N:246:PHE:C	4:N:248:ALA:H	2.14	0.50
2:T:104:DC:OP1	3:Q:193:ARG:NH2	2.44	0.50
4:J:178:LEU:HD22	4:J:183:ILE:HD11	1.92	0.50
4:J:246:PHE:C	4:J:248:ALA:H	2.15	0.50
3:E:204:THR:CG2	3:E:205:SER:N	2.75	0.50
3:Q:169:ARG:NH2	3:Q:206:VAL:HG23	2.26	0.50
3:I:311:ASP:C	3:I:313:LEU:H	2.15	0.50
4:N:202:MET:CE	4:N:213:ILE:HD11	2.42	0.50
4:B:257:ASN:HD21	4:B:314:GLY:N	2.03	0.50
4:J:204:ILE:HG23	4:J:237:TYR:CE1	2.46	0.50
3:I:111:ASP:C	3:I:113:ALA:N	2.64	0.50
4:J:180:LEU:HB3	4:J:200:VAL:HG23	1.94	0.50
4:J:167:ASN:HD21	4:J:223:GLY:N	2.00	0.50
4:J:167:ASN:ND2	4:J:168:ILE:H	2.09	0.50
4:F:257:ASN:HD21	4:F:314:GLY:N	2.07	0.50
3:M:116:ASN:OD1	3:M:116:ASN:N	2.44	0.50
4:R:236:LYS:O	4:R:239:ARG:HB2	2.12	0.50
4:F:274:VAL:O	4:F:278:GLN:HG2	2.11	0.50
3:M:304:PHE:CE2	3:M:305:LYS:HE3	2.45	0.49
3:A:131:PRO:HB2	3:A:133:ASN:HD21	1.77	0.49
3:A:137:ARG:HD2	3:A:171:GLU:OE1	2.11	0.49
1:S:15:DG:H2''	1:S:16:DG:H5''	1.93	0.49
2:T:104:DC:P	3:Q:193:ARG:NH2	2.86	0.49
3:I:267:GLU:H	3:I:267:GLU:CD	2.16	0.49
2:H:105:DC:H2''	2:H:106:DT:H5'	1.95	0.49
3:E:289:TYR:CE2	3:E:316:LEU:HD23	2.47	0.49
4:R:266:PHE:HB2	4:R:336:ARG:HD2	1.94	0.49
3:A:245:VAL:HG21	3:A:253:VAL:HG21	1.93	0.49
3:A:270:THR:CG2	3:A:272:LYS:HB3	2.42	0.49
2:H:109:DT:OP1	4:F:208:ARG:NH2	2.45	0.49
4:F:179:ASP:HB3	4:F:182:THR:HG22	1.93	0.49
3:I:193:ARG:O	3:I:197:LEU:HD23	2.12	0.49
4:B:227:GLU:OE1	4:B:318:ARG:NH1	2.37	0.49
4:R:171:THR:HG23	4:R:256:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:128:ILE:CD1	3:Q:130:LEU:HD11	2.42	0.49
4:J:280:PHE:CD2	4:J:280:PHE:N	2.80	0.49
3:I:204:THR:CG2	3:I:205:SER:H	2.16	0.49
4:F:317:VAL:HG22	4:F:320:GLU:OE2	2.11	0.49
3:M:306:PHE:CD1	3:M:308:THR:O	2.60	0.49
3:Q:293:TYR:CE2	3:Q:314:PRO:O	2.66	0.49
4:N:203:ARG:HD3	4:N:208:ARG:HH21	1.77	0.49
3:Q:185:ARG:O	3:Q:185:ARG:HG3	2.13	0.49
4:F:299:ARG:C	4:F:300:ILE:HD13	2.32	0.49
3:E:311:ASP:C	3:E:313:LEU:H	2.16	0.49
3:M:259:TYR:CE2	3:M:271:GLN:HG3	2.48	0.49
3:A:286:ARG:HD2	5:A:324:HOH:O	2.12	0.49
4:R:205:ARG:HB3	4:R:206:GLU:OE1	2.12	0.49
4:B:202:MET:HE3	4:B:213:ILE:CD1	2.43	0.49
4:N:295:MET:CE	4:N:324:ALA:CA	2.89	0.49
3:Q:177:PHE:CE2	4:R:287:LEU:HD13	2.48	0.49
3:E:311:ASP:N	3:E:311:ASP:OD1	2.46	0.49
4:F:273:LEU:HD12	4:F:273:LEU:O	2.13	0.49
4:B:205:ARG:HD2	4:B:205:ARG:HA	1.60	0.48
4:R:278:GLN:O	4:R:278:GLN:OE1	2.30	0.48
3:A:120:GLU:HA	3:A:120:GLU:OE2	2.13	0.48
3:Q:177:PHE:HB3	3:Q:188:LYS:HG3	1.95	0.48
3:I:235:ILE:HG23	3:I:299:LEU:HB3	1.94	0.48
4:B:326:GLU:O	4:B:330:PRO:HD3	2.12	0.48
3:M:221:ASN:HD22	3:M:221:ASN:N	2.10	0.48
3:E:176:THR:HG22	3:E:251:ILE:CD1	2.43	0.48
3:E:177:PHE:HB3	3:E:188:LYS:HG3	1.95	0.48
3:I:179:GLU:OE1	3:I:217:ARG:NH2	2.46	0.48
4:B:205:ARG:NH2	4:B:208:ARG:HD2	2.28	0.48
3:A:113:ALA:HA	3:A:116:ASN:ND2	2.27	0.48
3:I:266:ALA:HB2	3:I:307:ASP:OD2	2.13	0.48
2:L:101:DC:H2''	2:L:102:DC:C5'	2.42	0.48
4:N:202:MET:CE	4:N:213:ILE:HD12	2.43	0.48
3:Q:306:PHE:CZ	3:Q:310:VAL:CG2	2.96	0.48
4:N:229:GLN:N	4:N:229:GLN:HE21	2.10	0.48
3:Q:214:PHE:HB3	3:Q:218:PHE:CE1	2.49	0.48
3:M:237:ARG:HG3	3:M:237:ARG:HH21	1.79	0.48
4:R:225:LYS:H	4:R:229:GLN:NE2	2.11	0.48
3:Q:248:ARG:HH22	3:Q:287:GLN:NE2	2.11	0.48
4:N:277:HIS:NE2	4:N:331:ILE:HD13	2.28	0.48
4:R:246:PHE:C	4:R:248:ALA:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:205:ARG:CG	4:F:205:ARG:HH11	2.26	0.48
3:I:114:MET:HE1	3:I:146:TYR:CD1	2.48	0.48
3:I:226:LYS:CE	3:I:226:LYS:H	2.26	0.48
3:A:311:ASP:C	3:A:313:LEU:H	2.17	0.48
1:C:18:DG:H3'	3:E:271:GLN:HE22	1.78	0.48
4:N:196:ARG:HG3	4:N:197:PHE:N	2.29	0.48
3:M:128:ILE:HG13	3:M:130:LEU:HG	1.96	0.48
3:A:113:ALA:HA	3:A:116:ASN:HD22	1.78	0.48
3:E:313:LEU:HD12	3:E:314:PRO:CD	2.43	0.48
4:N:266:PHE:CD1	4:N:336:ARG:HB2	2.49	0.48
4:R:188:ARG:NH2	4:R:189:ASN:ND2	2.49	0.48
4:J:168:ILE:HD13	4:J:258:MET:HB3	1.95	0.48
3:E:151:LEU:HD12	3:E:151:LEU:N	2.28	0.48
3:E:176:THR:HG22	3:E:251:ILE:HD11	1.95	0.48
3:E:193:ARG:O	3:E:197:LEU:HD22	2.14	0.48
4:N:231:ARG:HA	4:N:253:PHE:HE2	1.74	0.48
4:R:315:ALA:HA	4:R:320:GLU:OE1	2.14	0.48
4:J:178:LEU:HD12	4:J:217:GLY:HA2	1.96	0.47
3:I:157:ASP:CB	3:I:185:ARG:HH21	2.27	0.47
3:Q:133:ASN:ND2	3:Q:171:GLU:CD	2.67	0.47
3:M:259:TYR:CE2	3:M:271:GLN:CG	2.97	0.47
2:T:101:DC:H2''	2:T:102:DC:C5'	2.45	0.47
3:I:222:LEU:CB	3:I:224:LEU:HD12	2.45	0.47
4:J:317:VAL:CG2	4:J:320:GLU:HG3	2.44	0.47
3:I:174:PRO:O	3:I:217:ARG:NH1	2.48	0.47
3:I:293:TYR:OH	3:I:315:GLN:HG2	2.14	0.47
4:F:267:PRO:HG2	4:F:337:LYS:HB2	1.97	0.47
4:J:259:VAL:HG22	4:J:313:THR:CG2	2.39	0.47
4:N:279:GLN:NE2	4:N:280:PHE:HE2	2.10	0.47
1:C:1:DG:H2''	5:C:172:HOH:O	2.14	0.47
4:J:235:ARG:CG	4:J:250:PHE:CZ	2.98	0.47
2:T:101:DC:H2''	2:T:102:DC:H5'	1.97	0.47
3:A:226:LYS:CG	3:A:230:MET:HE2	2.39	0.47
3:I:110:SER:O	3:I:113:ALA:HB2	2.15	0.47
4:R:295:MET:SD	4:R:298:PRO:HD2	2.55	0.47
3:M:208:LEU:HD12	3:M:208:LEU:HA	1.68	0.47
3:M:296:ALA:N	3:M:297:PRO:HD2	2.30	0.47
1:K:13:DA:C4'	4:J:256:GLN:HG3	2.45	0.47
4:B:209:THR:CG2	4:B:210:THR:N	2.78	0.47
3:M:311:ASP:C	3:M:313:LEU:H	2.17	0.47
3:I:128:ILE:HG23	3:I:183:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:209:THR:CG2	4:R:210:THR:H	2.28	0.47
4:N:267:PRO:HB2	4:N:337:LYS:HD2	1.96	0.47
3:A:224:LEU:HD23	3:A:269:ARG:NH1	2.30	0.47
3:I:281:ALA:O	3:I:284:THR:HB	2.15	0.47
4:J:163:PRO:HA	4:J:262:CYS:HB3	1.97	0.47
3:M:308:THR:HG23	3:M:309:PRO:HD2	1.96	0.47
4:N:243:LYS:C	4:N:243:LYS:HD3	2.32	0.47
3:M:271:GLN:HE22	3:M:316:LEU:CD2	2.28	0.47
4:R:228:GLU:OE2	4:R:231:ARG:NH1	2.32	0.47
4:F:235:ARG:CG	4:F:235:ARG:NH2	2.73	0.46
4:B:205:ARG:CZ	4:B:208:ARG:HG3	2.45	0.46
4:J:172:VAL:HG21	4:J:250:PHE:CD1	2.50	0.46
3:E:154:ARG:NH1	3:E:190:GLU:OE2	2.48	0.46
4:B:167:ASN:HD21	4:B:223:GLY:H	1.63	0.46
4:R:276:THR:HG1	4:R:277:HIS:HD1	1.63	0.46
1:O:7:DC:H2''	1:O:8:DT:H5'	1.96	0.46
2:D:106:DT:H2''	2:D:107:DT:H5'	1.97	0.46
3:E:310:VAL:O	3:E:313:LEU:HB2	2.14	0.46
3:A:157:ASP:CG	3:A:185:ARG:HH21	2.18	0.46
4:J:188:ARG:CG	4:J:189:ASN:N	2.60	0.46
4:R:224:ALA:CA	4:R:229:GLN:HE22	2.22	0.46
4:N:166:GLN:NE2	4:N:261:SER:OG	2.49	0.46
2:L:109:DT:H6	2:L:109:DT:H2'	1.43	0.46
3:I:145:VAL:HG11	3:I:198:ILE:HG12	1.97	0.46
4:R:249:LYS:CB	4:R:251:LEU:HD11	2.46	0.46
3:M:176:THR:HG22	3:M:251:ILE:HD13	1.97	0.46
3:M:120:GLU:OE2	3:M:120:GLU:HA	2.15	0.46
1:G:12:DA:C2	4:F:169:VAL:HG21	2.50	0.46
2:H:109:DT:H2''	2:H:110:DA:C8	2.51	0.46
3:I:186:ILE:HG22	3:I:187:SER:N	2.31	0.46
3:A:200:LYS:HD3	3:A:200:LYS:HA	1.88	0.46
3:Q:224:LEU:HD23	3:Q:228:VAL:CG2	2.37	0.46
4:R:213:ILE:HG22	4:R:213:ILE:O	2.16	0.46
1:G:18:DG:HO3'	3:M:316:LEU:HD23	1.79	0.46
3:Q:111:ASP:C	3:Q:113:ALA:N	2.68	0.46
4:N:300:ILE:CD1	4:N:315:ALA:HB2	2.46	0.46
4:N:298:PRO:HG3	4:N:323:GLU:HB3	1.98	0.46
4:F:219:MET:HE1	4:F:237:TYR:HB3	1.98	0.46
4:R:325:PHE:HA	4:R:328:ILE:HG22	1.97	0.46
3:E:189:LYS:O	3:E:193:ARG:HG3	2.16	0.46
4:R:168:ILE:HD12	4:R:226:SER:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:271:GLN:HB3	3:Q:282:ASP:HB3	1.97	0.46
4:R:186:ARG:NH1	4:R:244:LEU:HG	2.31	0.46
4:N:279:GLN:NE2	4:N:280:PHE:CD2	2.84	0.46
3:A:110:SER:O	3:A:113:ALA:HB2	2.15	0.46
4:N:172:VAL:HG21	4:N:250:PHE:CD1	2.51	0.46
4:J:167:ASN:ND2	4:J:168:ILE:N	2.64	0.46
3:Q:265:SER:O	3:Q:268:LYS:NZ	2.38	0.46
1:G:14:DA:H1'	4:F:214:PHE:CZ	2.51	0.46
4:R:177:LYS:HE3	4:R:177:LYS:HB3	1.79	0.46
4:B:176:CYS:SG	4:B:247:PRO:HD2	2.56	0.46
4:B:165:LEU:HA	4:B:165:LEU:HD12	1.75	0.46
3:I:311:ASP:HB2	3:I:312:LYS:NZ	2.31	0.45
4:R:178:LEU:HD13	4:R:183:ILE:HD11	1.96	0.45
3:E:310:VAL:HA	3:E:313:LEU:HD22	1.97	0.45
4:N:246:PHE:O	4:N:248:ALA:N	2.37	0.45
3:M:289:TYR:CD2	3:M:316:LEU:CD1	2.99	0.45
4:F:182:THR:HG23	4:F:183:ILE:H	1.82	0.45
3:I:262:SER:O	3:I:268:LYS:HA	2.16	0.45
3:I:114:MET:CE	3:I:146:TYR:CD1	3.00	0.45
4:F:239:ARG:NH2	4:F:242:GLN:HE22	2.12	0.45
2:P:101:DC:H2''	2:P:102:DC:C5'	2.46	0.45
3:M:154:ARG:HH21	3:M:154:ARG:HG3	1.82	0.45
4:R:192:TYR:CE1	4:R:194:PRO:HD3	2.51	0.45
1:O:15:DG:H2''	1:O:16:DG:H5''	1.98	0.45
3:A:307:ASP:OD1	3:A:307:ASP:C	2.55	0.45
3:E:176:THR:OG1	3:E:179:GLU:HG3	2.16	0.45
3:A:267:GLU:CA	3:A:267:GLU:OE2	2.51	0.45
4:N:256:GLN:NE2	4:N:256:GLN:CA	2.76	0.45
1:C:1:DG:H5''	5:K:176:HOH:O	2.16	0.45
4:J:235:ARG:HG3	4:J:250:PHE:CZ	2.51	0.45
4:J:167:ASN:ND2	4:J:223:GLY:H	2.03	0.45
3:I:193:ARG:O	3:I:197:LEU:CD2	2.65	0.45
4:B:173:ASN:HD22	4:B:173:ASN:C	2.20	0.45
3:A:179:GLU:CD	3:A:217:ARG:HH12	2.20	0.45
1:C:14:DA:H1'	4:B:214:PHE:CZ	2.52	0.45
3:E:237:ARG:HA	3:E:237:ARG:HD2	1.72	0.45
3:M:111:ASP:C	3:M:113:ALA:N	2.68	0.45
4:B:173:ASN:C	4:B:173:ASN:ND2	2.70	0.45
3:E:111:ASP:O	3:E:114:MET:HG3	2.16	0.45
3:E:131:PRO:HB2	3:E:133:ASN:ND2	2.32	0.45
3:Q:306:PHE:CE2	3:Q:310:VAL:HG23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:103:DC:OP1	3:Q:154:ARG:NH1	2.49	0.45
1:C:7:DC:H2'	1:C:8:DT:H71	1.99	0.45
2:D:104:DC:H2''	2:D:105:DC:C5'	2.47	0.45
3:A:234:HIS:CD2	3:A:237:ARG:HH22	2.35	0.45
4:N:188:ARG:HD2	4:N:189:ASN:OD1	2.17	0.44
4:F:189:ASN:ND2	4:F:205:ARG:HH21	2.15	0.44
3:Q:188:LYS:NZ	4:R:286:GLU:O	2.45	0.44
2:H:103:DC:H2''	2:H:104:DC:O5'	2.17	0.44
3:I:117:ALA:O	3:I:121:ILE:HG13	2.16	0.44
3:I:164:LEU:HD23	3:I:180:ILE:HD12	1.98	0.44
2:T:101:DC:H2''	2:T:102:DC:O5'	2.18	0.44
1:G:9:DA:H2''	1:G:10:DT:C5'	2.39	0.44
4:J:214:PHE:N	4:J:214:PHE:CD1	2.85	0.44
3:A:309:PRO:HG3	3:A:312:LYS:CE	2.47	0.44
4:R:273:LEU:O	4:R:273:LEU:HD23	2.17	0.44
1:G:12:DA:H8	1:G:12:DA:H2'	1.67	0.44
4:F:180:LEU:HD23	4:F:181:LYS:HZ2	1.78	0.44
3:M:122:THR:HG22	3:M:123:THR:N	2.32	0.44
1:G:8:DT:H2''	1:G:9:DA:C5'	2.43	0.44
3:I:217:ARG:O	3:I:221:ASN:ND2	2.50	0.44
3:M:137:ARG:HH22	3:M:144:GLN:HE22	1.65	0.44
4:N:318:ARG:CG	4:N:322:TYR:CE2	2.96	0.44
4:R:249:LYS:HB2	4:R:251:LEU:HD12	1.99	0.44
4:N:181:LYS:O	4:N:185:LEU:HD23	2.18	0.44
3:M:266:ALA:HA	3:M:307:ASP:OD2	2.17	0.44
4:R:259:VAL:HG13	4:R:313:THR:HG23	2.00	0.44
2:T:109:DT:H2'	2:T:109:DT:H6	1.55	0.44
4:J:209:THR:CG2	4:J:210:THR:H	2.29	0.44
2:L:102:DC:H2''	2:L:103:DC:O5'	2.17	0.44
4:B:296:ILE:HG23	4:B:299:ARG:HH12	1.82	0.44
3:A:165:TYR:O	5:A:319:HOH:O	2.21	0.44
4:R:229:GLN:HB3	4:R:229:GLN:HE21	1.43	0.44
4:J:280:PHE:HD2	4:J:280:PHE:N	2.16	0.44
3:I:267:GLU:HB2	3:I:269:ARG:NH1	2.26	0.44
4:B:264:VAL:HG11	4:B:332:LEU:HD23	2.00	0.44
3:A:224:LEU:CD2	3:A:269:ARG:HH11	2.30	0.44
4:R:276:THR:HG21	4:R:335:PHE:HZ	1.82	0.44
2:H:110:DA:H2''	2:H:111:DT:C5'	2.43	0.44
3:Q:181:CYS:SG	3:Q:188:LYS:HA	2.57	0.44
3:A:157:ASP:CB	3:A:185:ARG:HH21	2.30	0.44
4:B:235:ARG:HG2	4:B:250:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:238:LYS:HB3	3:E:299:LEU:CD2	2.48	0.44
3:A:173:VAL:O	3:A:173:VAL:HG23	2.18	0.44
3:Q:141:LEU:HD12	3:Q:141:LEU:HA	1.83	0.44
4:F:329:TYR:HB3	4:F:330:PRO:HD3	2.00	0.44
3:I:157:ASP:OD2	3:I:185:ARG:NH2	2.50	0.44
3:M:145:VAL:HG22	3:M:202:LEU:HD11	1.99	0.44
2:D:110:DA:H2''	2:D:111:DT:C5'	2.46	0.44
2:L:107:DT:H2'	2:L:107:DT:H6	1.70	0.44
3:A:196:LYS:HE2	5:A:335:HOH:O	2.18	0.44
3:Q:224:LEU:HA	3:Q:225:PRO:HD2	1.93	0.43
3:I:295:ARG:O	3:I:299:LEU:HG	2.18	0.43
4:R:203:ARG:HG2	4:R:210:THR:OG1	2.18	0.43
3:A:148:GLN:HB3	3:A:150:SER:OG	2.17	0.43
1:C:18:DG:O3'	3:E:316:LEU:HD11	2.18	0.43
4:F:189:ASN:OD1	4:F:189:ASN:N	2.50	0.43
4:F:235:ARG:NH2	4:F:235:ARG:HG3	2.17	0.43
3:I:266:ALA:HB3	3:I:267:GLU:OE2	2.18	0.43
4:R:231:ARG:HA	4:R:253:PHE:CE1	2.53	0.43
4:J:249:LYS:HB3	4:J:251:LEU:HD21	2.00	0.43
4:F:166:GLN:NE2	4:F:225:LYS:NZ	2.66	0.43
4:J:189:ASN:N	4:J:189:ASN:OD1	2.51	0.43
3:I:173:VAL:HG23	3:I:175:ARG:NH2	2.33	0.43
4:F:205:ARG:NH1	4:F:205:ARG:CG	2.81	0.43
3:M:238:LYS:HB3	3:M:299:LEU:CD2	2.48	0.43
4:R:179:ASP:O	4:R:182:THR:CG2	2.67	0.43
4:R:193:ASN:HB3	4:R:196:ARG:HB3	2.01	0.43
3:Q:311:ASP:C	3:Q:313:LEU:H	2.22	0.43
3:M:169:ARG:HG2	3:M:174:PRO:HG3	2.00	0.43
4:R:246:PHE:O	4:R:248:ALA:N	2.42	0.43
3:M:262:SER:O	3:M:268:LYS:HA	2.18	0.43
3:M:309:PRO:HG2	3:M:312:LYS:HB3	2.00	0.43
3:A:111:ASP:C	3:A:113:ALA:N	2.70	0.43
3:Q:310:VAL:O	3:Q:313:LEU:HB2	2.18	0.43
4:F:271:GLU:O	4:F:274:VAL:HG12	2.19	0.43
3:I:164:LEU:CD2	3:I:180:ILE:HD12	2.48	0.43
4:R:304:ILE:HG12	4:R:310:VAL:HG22	2.00	0.43
3:A:139:ASN:HD22	3:A:139:ASN:N	2.16	0.43
3:E:174:PRO:O	5:E:359:HOH:O	2.22	0.43
1:K:15:DG:H2''	1:K:16:DG:H5''	2.01	0.43
4:N:258:MET:HG2	4:N:315:ALA:O	2.18	0.43
3:A:215:MET:CG	3:A:233:THR:OG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:259:VAL:HG13	4:F:313:THR:HG23	2.00	0.43
4:J:235:ARG:HG2	4:J:250:PHE:CE1	2.54	0.43
4:F:326:GLU:O	4:F:330:PRO:HD3	2.19	0.43
1:O:12:DA:H8	1:O:12:DA:H2'	1.70	0.43
4:F:188:ARG:CG	4:F:189:ASN:N	2.66	0.43
1:K:8:DT:H2''	1:K:9:DA:C5'	2.46	0.43
4:R:264:VAL:O	4:R:265:LYS:HB2	2.18	0.43
2:H:101:DC:H5'	2:P:118:DC:H2''	2.01	0.43
4:N:193:ASN:HA	4:N:194:PRO:HD2	1.76	0.43
2:P:110:DA:N7	2:P:111:DT:C4	2.87	0.43
3:I:248:ARG:NH2	3:I:287:GLN:NE2	2.62	0.43
3:I:152:LYS:HG3	3:I:152:LYS:H	1.45	0.43
3:I:265:SER:O	3:I:268:LYS:HG3	2.19	0.43
3:A:295:ARG:C	3:A:297:PRO:HD2	2.39	0.43
3:E:282:ASP:OD1	3:E:283:VAL:N	2.52	0.43
3:Q:303:ASP:CG	3:Q:303:ASP:O	2.57	0.43
4:J:253:PHE:C	4:J:253:PHE:CD1	2.92	0.42
4:N:204:ILE:HG12	4:N:237:TYR:OH	2.19	0.42
4:J:178:LEU:HD22	4:J:183:ILE:CD1	2.49	0.42
3:A:269:ARG:CG	3:A:269:ARG:NH1	2.80	0.42
3:I:310:VAL:HA	3:I:313:LEU:HD22	2.01	0.42
1:S:12:DA:H2	4:R:169:VAL:HG21	1.84	0.42
4:B:204:ILE:HG23	4:B:237:TYR:CZ	2.54	0.42
3:Q:293:TYR:N	3:Q:294:PRO:CD	2.82	0.42
4:R:302:LEU:HD23	4:R:312:LEU:HG	2.01	0.42
4:J:177:LYS:HE3	4:J:177:LYS:HB3	1.71	0.42
4:N:239:ARG:O	4:N:240:VAL:C	2.56	0.42
3:Q:110:SER:O	3:Q:113:ALA:HB2	2.20	0.42
3:E:293:TYR:HB3	3:E:294:PRO:HD3	2.01	0.42
1:S:12:DA:C2	4:R:169:VAL:HG21	2.55	0.42
1:G:7:DC:H2''	1:G:8:DT:C5'	2.47	0.42
4:N:257:ASN:ND2	4:N:314:GLY:CA	2.82	0.42
3:A:221:ASN:H	3:A:221:ASN:ND2	2.16	0.42
3:I:271:GLN:HE22	3:I:316:LEU:HD21	1.84	0.42
4:J:182:THR:HG22	4:J:183:ILE:N	2.34	0.42
3:A:224:LEU:HD23	3:A:269:ARG:HH12	1.83	0.42
3:E:151:LEU:CD1	3:E:151:LEU:N	2.82	0.42
3:A:245:VAL:HG21	3:A:253:VAL:CG2	2.50	0.42
3:I:156:ASN:ND2	5:I:325:HOH:O	2.51	0.42
4:F:240:VAL:O	4:F:244:LEU:HG	2.20	0.42
4:J:193:ASN:C	4:J:193:ASN:HD22	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:186:ILE:CG2	3:Q:190:GLU:HB3	2.49	0.42
3:M:313:LEU:HD22	3:M:314:PRO:HD2	2.02	0.42
4:N:326:GLU:O	4:N:330:PRO:HD3	2.19	0.42
3:M:121:ILE:CG2	3:M:138:THR:HG21	2.49	0.42
4:R:231:ARG:HB3	4:R:231:ARG:HH11	1.83	0.42
3:E:186:ILE:HG22	3:E:187:SER:N	2.34	0.42
4:B:286:GLU:HG3	5:B:338:HOH:O	2.19	0.42
4:N:193:ASN:O	4:N:196:ARG:HG2	2.18	0.42
3:I:270:THR:HG23	3:I:273:GLU:N	2.12	0.42
3:I:143:LYS:HE2	3:I:147:GLU:OE1	2.18	0.42
4:F:213:ILE:HG12	4:F:219:MET:HE2	2.00	0.42
1:O:16:DG:H2''	1:O:17:DG:O5'	2.20	0.42
3:A:114:MET:CE	3:A:143:LYS:HG3	2.49	0.42
4:J:264:VAL:O	4:J:265:LYS:HB2	2.20	0.42
4:F:164:GLN:HB2	4:F:164:GLN:HE21	1.65	0.42
4:R:246:PHE:HA	4:R:247:PRO:HD3	1.77	0.42
3:I:131:PRO:HG2	3:I:134:ILE:HG13	2.02	0.42
4:R:244:LEU:HA	4:R:244:LEU:HD12	1.74	0.42
3:E:157:ASP:HB2	3:E:185:ARG:HH21	1.84	0.42
3:E:112:ARG:HH22	3:E:114:MET:HE2	1.84	0.42
4:R:249:LYS:CB	4:R:251:LEU:CD1	2.98	0.42
3:A:141:LEU:HA	3:A:141:LEU:HD23	1.86	0.42
4:R:178:LEU:HD13	4:R:183:ILE:CD1	2.50	0.42
2:P:108:DT:H6	2:P:108:DT:H2'	1.67	0.42
4:J:213:ILE:HG12	4:J:219:MET:HE3	2.02	0.42
4:R:317:VAL:HG23	4:R:319:ALA:N	2.34	0.42
1:S:16:DG:H2''	1:S:17:DG:O5'	2.20	0.42
4:N:183:ILE:O	4:N:187:ALA:HB3	2.18	0.42
4:J:271:GLU:O	4:J:274:VAL:HG12	2.20	0.42
3:E:169:ARG:HH22	4:F:284:GLU:CD	2.23	0.42
3:E:265:SER:O	3:E:268:LYS:NZ	2.52	0.42
4:F:180:LEU:CD2	4:F:180:LEU:N	2.78	0.42
2:T:110:DA:H5'	4:R:166:GLN:CG	2.35	0.42
4:R:186:ARG:NH1	4:R:244:LEU:HB3	2.34	0.42
1:S:15:DG:C2'	1:S:16:DG:H5''	2.50	0.42
3:E:169:ARG:HB3	3:E:206:VAL:HG11	2.01	0.42
3:E:225:PRO:HG2	3:E:228:VAL:HG23	2.02	0.42
4:B:256:GLN:HA	4:B:256:GLN:HE21	1.84	0.42
3:M:228:VAL:O	3:M:231:ALA:HB3	2.20	0.41
3:M:235:ILE:HG23	3:M:299:LEU:HB3	2.02	0.41
4:F:328:ILE:HG13	4:F:332:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:167:ASN:ND2	4:B:223:GLY:H	2.18	0.41
3:I:236:ALA:O	3:I:239:ALA:HB3	2.20	0.41
4:J:202:MET:SD	4:J:240:VAL:HG21	2.60	0.41
4:J:184:ALA:HB2	4:J:192:TYR:HB2	2.02	0.41
1:C:12:DA:H2'	1:C:12:DA:H8	1.70	0.41
3:A:189:LYS:CE	3:A:193:ARG:HH21	2.32	0.41
3:M:186:ILE:CG2	3:M:187:SER:N	2.83	0.41
4:F:185:LEU:HD23	4:F:186:ARG:N	2.35	0.41
4:F:279:GLN:H	4:F:279:GLN:HG3	1.11	0.41
4:R:179:ASP:CB	4:R:182:THR:HG22	2.50	0.41
3:E:112:ARG:HA	3:E:112:ARG:HD3	1.85	0.41
3:E:293:TYR:CZ	3:E:315:GLN:HG3	2.55	0.41
4:R:180:LEU:HD22	4:R:215:SER:OG	2.21	0.41
3:M:216:SER:HA	3:M:229:GLN:NE2	2.34	0.41
3:M:234:HIS:HD2	3:M:299:LEU:O	2.04	0.41
2:T:102:DC:O3'	3:Q:154:ARG:NH1	2.53	0.41
4:N:253:PHE:CD1	4:N:253:PHE:C	2.93	0.41
2:P:107:DT:H2'	2:P:107:DT:H6	1.76	0.41
4:F:303:LEU:HB2	4:F:311:VAL:HB	2.02	0.41
4:B:180:LEU:HD22	4:B:215:SER:HB3	2.02	0.41
3:Q:222:LEU:HB3	3:Q:224:LEU:HD12	2.02	0.41
3:Q:158:ALA:HA	3:Q:186:ILE:HG13	2.02	0.41
4:J:190:ALA:O	4:J:191:GLU:HG2	2.21	0.41
3:Q:176:THR:HG22	3:Q:251:ILE:HD11	2.02	0.41
3:E:218:PHE:CZ	3:E:278:ALA:HA	2.56	0.41
3:A:262:SER:O	3:A:268:LYS:HA	2.21	0.41
4:F:294:ARG:HG2	4:F:299:ARG:HH12	1.85	0.41
4:R:177:LYS:O	4:R:178:LEU:HD23	2.20	0.41
4:R:271:GLU:O	4:R:274:VAL:HG12	2.21	0.41
3:M:189:LYS:CE	3:M:193:ARG:NH1	2.76	0.41
3:I:225:PRO:HG2	3:I:228:VAL:CG2	2.47	0.41
3:E:313:LEU:HA	3:E:313:LEU:HD12	1.90	0.41
4:J:178:LEU:HD21	4:J:241:VAL:HG13	2.02	0.41
4:F:251:LEU:N	4:F:251:LEU:HD13	2.35	0.41
3:A:293:TYR:N	3:A:294:PRO:CD	2.82	0.41
2:D:118:DC:H2''	2:L:101:DC:H5'	2.02	0.41
3:E:137:ARG:NE	3:E:170:GLN:HE22	2.19	0.41
3:E:265:SER:O	3:E:268:LYS:HG2	2.21	0.41
3:M:286:ARG:HD2	5:M:322:HOH:O	2.19	0.41
4:N:193:ASN:HB3	4:N:196:ARG:CZ	2.31	0.41
4:N:192:TYR:CE1	4:N:194:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:306:PHE:CZ	3:I:310:VAL:HG22	2.56	0.41
3:A:270:THR:HG21	3:A:272:LYS:HB3	2.03	0.41
3:M:262:SER:OG	3:M:268:LYS:HA	2.20	0.41
2:T:111:DT:H2'	2:T:111:DT:H6	1.62	0.41
4:N:240:VAL:HG23	4:N:241:VAL:N	2.36	0.41
4:N:302:LEU:HD12	4:N:302:LEU:N	2.35	0.41
3:M:111:ASP:OD2	3:M:146:TYR:HE1	2.03	0.41
3:A:295:ARG:NH1	3:A:298:ASP:OD1	2.54	0.41
4:B:180:LEU:CD2	4:B:215:SER:HB3	2.50	0.41
3:M:239:ALA:HA	3:M:244:LEU:HD12	2.02	0.41
4:J:300:ILE:HD13	4:J:312:LEU:HB3	2.03	0.41
3:Q:120:GLU:O	3:Q:124:MET:HG3	2.21	0.41
4:F:246:PHE:HA	4:F:247:PRO:HD3	1.82	0.41
4:F:246:PHE:C	4:F:248:ALA:H	2.20	0.41
4:R:258:MET:HE1	4:R:318:ARG:HG3	2.02	0.41
3:Q:277:ILE:HG22	3:Q:278:ALA:N	2.36	0.41
4:B:205:ARG:NH1	4:B:208:ARG:NE	2.64	0.41
3:E:121:ILE:HG21	3:E:139:ASN:ND2	2.36	0.41
4:F:189:ASN:ND2	4:F:203:ARG:O	2.54	0.40
4:F:205:ARG:H	4:F:205:ARG:NE	2.16	0.40
3:M:111:ASP:OD2	3:M:146:TYR:CE1	2.74	0.40
3:E:227:GLN:HG2	3:E:305:LYS:HE3	2.03	0.40
3:E:262:SER:O	3:E:268:LYS:HA	2.22	0.40
3:Q:296:ALA:N	3:Q:297:PRO:HD2	2.36	0.40
4:B:239:ARG:HH11	4:B:239:ARG:HD3	1.77	0.40
4:B:185:LEU:HD12	4:B:185:LEU:HA	1.79	0.40
2:P:111:DT:H2'	2:P:111:DT:H6	1.57	0.40
4:J:258:MET:HG2	4:J:315:ALA:O	2.21	0.40
2:P:109:DT:H2'	2:P:109:DT:H6	1.56	0.40
4:N:302:LEU:HD22	4:N:328:ILE:HG12	2.04	0.40
3:E:112:ARG:HH22	3:E:114:MET:CE	2.34	0.40
3:M:177:PHE:HB3	3:M:188:LYS:HG3	2.04	0.40
3:Q:181:CYS:SG	3:Q:188:LYS:CA	3.10	0.40
3:I:120:GLU:HG2	3:I:157:ASP:OD1	2.21	0.40
3:M:311:ASP:O	3:M:313:LEU:N	2.54	0.40
3:E:111:ASP:C	3:E:113:ALA:N	2.73	0.40
3:M:158:ALA:HA	3:M:186:ILE:HG13	2.02	0.40
3:M:271:GLN:NE2	3:M:316:LEU:HD21	2.37	0.40
3:I:176:THR:HG22	3:I:251:ILE:CD1	2.46	0.40
4:R:326:GLU:O	4:R:330:PRO:HD3	2.22	0.40
2:P:101:DC:H2''	2:P:102:DC:H5'	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:329:TYR:N	4:F:330:PRO:CD	2.85	0.40
4:F:166:GLN:NE2	4:F:225:LYS:HZ2	2.18	0.40
4:R:180:LEU:HD21	4:R:215:SER:HB2	2.03	0.40
3:I:176:THR:CG2	3:I:251:ILE:HD13	2.47	0.40
3:A:269:ARG:HH11	3:A:269:ARG:HG2	1.84	0.40
4:B:246:PHE:HA	4:B:247:PRO:HD3	1.89	0.40
3:Q:144:GLN:O	3:Q:148:GLN:HB2	2.22	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	205/207 (99%)	195 (95%)	8 (4%)	2 (1%)	19	41
3	E	205/207 (99%)	192 (94%)	11 (5%)	2 (1%)	19	41
3	I	205/207 (99%)	194 (95%)	9 (4%)	2 (1%)	19	41
3	M	205/207 (99%)	191 (93%)	13 (6%)	1 (0%)	34	59
3	Q	205/207 (99%)	191 (93%)	12 (6%)	2 (1%)	19	41
4	B	178/180 (99%)	167 (94%)	11 (6%)	0	100	100
4	F	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	30	54
4	J	178/180 (99%)	163 (92%)	14 (8%)	1 (1%)	30	54
4	N	178/180 (99%)	159 (89%)	17 (10%)	2 (1%)	17	38
4	R	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	30	54
All	All	1915/1935 (99%)	1776 (93%)	125 (6%)	14 (1%)	26	51

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	312	LYS
3	M	312	LYS
3	E	312	LYS
3	I	112	ARG
3	Q	312	LYS
3	E	226	LYS
3	I	312	LYS
3	A	226	LYS
3	Q	226	LYS
4	N	208	ARG
4	R	247	PRO
4	F	247	PRO
4	N	247	PRO
4	J	247	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	176/176 (100%)	155 (88%)	21 (12%)	6	13
3	E	176/176 (100%)	149 (85%)	27 (15%)	3	7
3	I	176/176 (100%)	148 (84%)	28 (16%)	3	6
3	M	176/176 (100%)	152 (86%)	24 (14%)	5	9
3	Q	176/176 (100%)	152 (86%)	24 (14%)	5	9
4	B	154/154 (100%)	136 (88%)	18 (12%)	7	13
4	F	154/154 (100%)	132 (86%)	22 (14%)	4	8
4	J	154/154 (100%)	133 (86%)	21 (14%)	5	9
4	N	154/154 (100%)	126 (82%)	28 (18%)	2	4
4	R	154/154 (100%)	123 (80%)	31 (20%)	1	3
All	All	1650/1650 (100%)	1406 (85%)	244 (15%)	4	8

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	110	SER
3	A	122	THR
3	A	128	ILE
3	A	133	ASN
3	A	136	ASP
3	A	164	LEU
3	A	185	ARG
3	A	197	LEU
3	A	202	LEU
3	A	204	THR
3	A	215	MET
3	A	221	ASN
3	A	248	ARG
3	A	267	GLU
3	A	269	ARG
3	A	270	THR
3	A	280	VAL
3	A	305	LYS
3	A	310	VAL
3	A	313	LEU
3	A	315	GLN
4	B	165	LEU
4	B	173	ASN
4	B	180	LEU
4	B	181	LYS
4	B	185	LEU
4	B	188	ARG
4	B	205	ARG
4	B	206	GLU
4	B	226	SER
4	B	232	LEU
4	B	239	ARG
4	B	240	VAL
4	B	273	LEU
4	B	278	GLN
4	B	287	LEU
4	B	299	ARG
4	B	326	GLU
4	B	332	LEU
3	E	111	ASP
3	E	112	ARG
3	E	119	LYS
3	E	123	THR

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Mol	Chain	Res	Type
3	E	132	ARG
3	E	133	ASN
3	E	150	SER
3	E	169	ARG
3	E	175	ARG
3	E	185	ARG
3	E	197	LEU
3	E	202	LEU
3	E	205	SER
3	E	216	SER
3	E	237	ARG
3	E	238	LYS
3	E	262	SER
3	E	269	ARG
3	E	270	THR
3	E	276	ASP
3	E	283	VAL
3	E	287	GLN
3	E	302	THR
3	E	305	LYS
3	E	311	ASP
3	E	312	LYS
3	E	313	LEU
4	F	164	GLN
4	F	180	LEU
4	F	186	ARG
4	F	193	ASN
4	F	195	LYS
4	F	205	ARG
4	F	219	MET
4	F	227	GLU
4	F	229	GLN
4	F	232	LEU
4	F	235	ARG
4	F	239	ARG
4	F	249	LYS
4	F	251	LEU
4	F	275	LEU
4	F	279	GLN
4	F	287	LEU
4	F	291	LEU
4	F	294	ARG

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Mol	Chain	Res	Type
4	F	299	ARG
4	F	300	ILE
4	F	312	LEU
3	I	111	ASP
3	I	112	ARG
3	I	114	MET
3	I	126	ASP
3	I	133	ASN
3	I	145	VAL
3	I	150	SER
3	I	152	LYS
3	I	181	CYS
3	I	190	GLU
3	I	206	VAL
3	I	207	ASP
3	I	208	LEU
3	I	215	MET
3	I	217	ARG
3	I	221	ASN
3	I	224	LEU
3	I	226	LYS
3	I	227	GLN
3	I	262	SER
3	I	267	GLU
3	I	272	LYS
3	I	277	ILE
3	I	283	VAL
3	I	295	ARG
3	I	305	LYS
3	I	313	LEU
3	I	316	LEU
4	J	165	LEU
4	J	178	LEU
4	J	188	ARG
4	J	191	GLU
4	J	193	ASN
4	J	195	LYS
4	J	208	ARG
4	J	210	THR
4	J	242	GLN
4	J	252	ASP
4	J	258	MET

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Mol	Chain	Res	Type
4	J	271	GLU
4	J	273	LEU
4	J	275	LEU
4	J	276	THR
4	J	279	GLN
4	J	280	PHE
4	J	287	LEU
4	J	318	ARG
4	J	326	GLU
4	J	333	LYS
3	M	110	SER
3	M	112	ARG
3	M	116	ASN
3	M	122	THR
3	M	132	ARG
3	M	133	ASN
3	M	149	LYS
3	M	150	SER
3	M	175	ARG
3	M	197	LEU
3	M	200	LYS
3	M	207	ASP
3	M	209	ILE
3	M	217	ARG
3	M	221	ASN
3	M	226	LYS
3	M	242	LEU
3	M	263	GLN
3	M	298	ASP
3	M	305	LYS
3	M	307	ASP
3	M	310	VAL
3	M	311	ASP
3	M	315	GLN
4	N	164	GLN
4	N	166	GLN
4	N	174	LEU
4	N	181	LYS
4	N	182	THR
4	N	186	ARG
4	N	196	ARG
4	N	200	VAL

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Mol	Chain	Res	Type
4	N	202	MET
4	N	206	GLU
4	N	208	ARG
4	N	227	GLU
4	N	229	GLN
4	N	232	LEU
4	N	239	ARG
4	N	242	GLN
4	N	243	LYS
4	N	251	LEU
4	N	256	GLN
4	N	271	GLU
4	N	273	LEU
4	N	274	VAL
4	N	275	LEU
4	N	279	GLN
4	N	287	LEU
4	N	297	LYS
4	N	299	ARG
4	N	332	LEU
3	Q	112	ARG
3	Q	119	LYS
3	Q	132	ARG
3	Q	141	LEU
3	Q	150	SER
3	Q	185	ARG
3	Q	200	LYS
3	Q	208	LEU
3	Q	211	THR
3	Q	216	SER
3	Q	224	LEU
3	Q	226	LYS
3	Q	227	GLN
3	Q	228	VAL
3	Q	230	MET
3	Q	241	GLU
3	Q	242	LEU
3	Q	282	ASP
3	Q	295	ARG
3	Q	298	ASP
3	Q	311	ASP
3	Q	313	LEU

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Mol	Chain	Res	Type
3	Q	315	GLN
3	Q	316	LEU
4	R	165	LEU
4	R	166	GLN
4	R	171	THR
4	R	174	LEU
4	R	180	LEU
4	R	182	THR
4	R	185	LEU
4	R	200	VAL
4	R	202	MET
4	R	213	ILE
4	R	215	SER
4	R	225	LYS
4	R	228	GLU
4	R	229	GLN
4	R	232	LEU
4	R	235	ARG
4	R	243	LYS
4	R	244	LEU
4	R	258	MET
4	R	271	GLU
4	R	273	LEU
4	R	275	LEU
4	R	276	THR
4	R	278	GLN
4	R	280	PHE
4	R	287	LEU
4	R	299	ARG
4	R	300	ILE
4	R	302	LEU
4	R	316	LYS
4	R	317	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	116	ASN
3	A	133	ASN
3	A	139	ASN
3	A	144	GLN
3	A	148	GLN

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Mol	Chain	Res	Type
3	A	170	GLN
3	A	221	ASN
3	A	234	HIS
3	A	263	GLN
4	B	166	GLN
4	B	167	ASN
4	B	173	ASN
4	B	256	GLN
4	B	257	ASN
4	B	278	GLN
4	B	327	ASN
3	E	133	ASN
3	E	139	ASN
3	E	148	GLN
3	E	170	GLN
3	E	227	GLN
3	E	263	GLN
4	F	164	GLN
4	F	166	GLN
4	F	167	ASN
4	F	193	ASN
4	F	229	GLN
4	F	256	GLN
4	F	257	ASN
4	F	279	GLN
4	F	327	ASN
3	I	116	ASN
3	I	133	ASN
3	I	139	ASN
3	I	156	ASN
3	I	221	ASN
3	I	229	GLN
3	I	263	GLN
3	I	287	GLN
4	J	166	GLN
4	J	167	ASN
4	J	193	ASN
4	J	242	GLN
4	J	257	ASN
4	J	277	HIS
4	J	279	GLN
4	J	327	ASN

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Mol	Chain	Res	Type
3	M	133	ASN
3	M	144	GLN
3	M	170	GLN
3	M	221	ASN
3	M	234	HIS
4	N	164	GLN
4	N	166	GLN
4	N	173	ASN
4	N	229	GLN
4	N	242	GLN
4	N	256	GLN
4	N	257	ASN
4	N	279	GLN
4	N	327	ASN
3	Q	116	ASN
3	Q	148	GLN
3	Q	156	ASN
3	Q	227	GLN
3	Q	263	GLN
3	Q	287	GLN
3	Q	315	GLN
4	R	166	GLN
4	R	167	ASN
4	R	189	ASN
4	R	229	GLN
4	R	256	GLN
4	R	257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	C	18/18 (100%)	0.16	0	100	100	27, 41, 52, 58	0
1	G	18/18 (100%)	-0.02	0	100	100	25, 43, 50, 57	0
1	K	18/18 (100%)	-0.13	0	100	100	32, 45, 52, 59	0
1	O	18/18 (100%)	-0.12	0	100	100	29, 44, 58, 65	0
1	S	18/18 (100%)	-0.27	0	100	100	33, 49, 58, 62	0
2	D	18/18 (100%)	0.12	0	100	100	25, 37, 52, 53	0
2	H	18/18 (100%)	0.03	0	100	100	26, 40, 50, 50	0
2	L	18/18 (100%)	-0.20	0	100	100	31, 42, 54, 55	0
2	P	18/18 (100%)	-0.27	0	100	100	31, 45, 51, 53	0
2	T	18/18 (100%)	-0.41	0	100	100	36, 47, 54, 55	0
3	A	207/207 (100%)	0.18	4 (1%)	70	69	31, 49, 66, 75	0
3	E	207/207 (100%)	0.37	4 (1%)	70	69	25, 45, 65, 71	0
3	I	207/207 (100%)	0.23	4 (1%)	70	69	33, 52, 68, 72	0
3	M	207/207 (100%)	0.49	15 (7%)	18	16	34, 54, 69, 75	0
3	Q	207/207 (100%)	0.64	24 (11%)	6	4	34, 53, 69, 75	0
4	B	180/180 (100%)	0.42	2 (1%)	82	82	23, 42, 62, 72	0
4	F	180/180 (100%)	0.18	0	100	100	25, 46, 65, 73	0
4	J	180/180 (100%)	0.48	19 (10%)	8	6	30, 49, 66, 73	0
4	N	180/180 (100%)	0.72	34 (18%)	2	1	32, 53, 69, 74	0
4	R	180/180 (100%)	1.56	61 (33%)	0	0	35, 56, 70, 75	0
All	All	2115/2115 (100%)	0.46	167 (7%)	15	13	23, 49, 68, 75	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	110	SER	9.7
4	R	237	TYR	7.6
3	M	110	SER	6.9
4	R	241	VAL	6.2
4	R	238	ALA	6.0
3	Q	301	PRO	5.8
4	R	217	GLY	5.8
4	R	204	ILE	5.6
4	R	174	LEU	5.4
4	R	202	MET	5.4
4	R	219	MET	5.2
4	R	249	LYS	5.1
4	R	180	LEU	5.0
3	Q	299	LEU	4.9
4	R	244	LEU	4.9
4	R	186	ARG	4.9
4	R	172	VAL	4.6
3	Q	306	PHE	4.6
4	R	253	PHE	4.5
3	Q	267	GLU	4.4
4	R	240	VAL	4.3
4	R	250	PHE	4.1
4	R	187	ALA	4.1
4	R	188	ARG	4.1
4	R	189	ASN	4.0
4	N	249	LYS	4.0
3	Q	302	THR	3.9
3	Q	304	PHE	3.9
4	R	239	ARG	3.9
3	Q	266	ALA	3.8
4	R	236	LYS	3.8
4	R	247	PRO	3.8
4	R	183	ILE	3.8
4	N	205	ARG	3.7
3	M	111	ASP	3.7
4	J	188	ARG	3.7
3	Q	314	PRO	3.6
4	N	180	LEU	3.6
4	R	213	ILE	3.6
4	R	232	LEU	3.6
3	Q	297	PRO	3.5
4	N	206	GLU	3.5
4	R	233	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	Q	313	LEU	3.4
3	E	306	PHE	3.4
4	R	251	LEU	3.4
4	R	178	LEU	3.3
4	R	246	PHE	3.3
4	R	184	ALA	3.3
3	M	303	ASP	3.3
4	J	189	ASN	3.3
4	R	248	ALA	3.2
4	R	255	ILE	3.2
4	R	173	ASN	3.2
4	R	228	GLU	3.2
3	Q	310	VAL	3.2
4	R	218	LYS	3.2
3	Q	307	ASP	3.2
4	R	207	PRO	3.2
4	J	174	LEU	3.1
4	R	212	LEU	3.1
4	R	205	ARG	3.1
3	Q	300	PHE	3.1
4	N	214	PHE	3.1
4	R	192	TYR	3.1
4	N	242	GLN	3.1
4	N	237	TYR	3.1
4	N	183	ILE	3.0
4	R	242	GLN	3.0
4	R	321	ILE	3.0
3	I	310	VAL	3.0
4	J	185	LEU	3.0
3	I	306	PHE	3.0
4	N	241	VAL	3.0
4	N	238	ALA	3.0
4	J	240	VAL	3.0
4	R	214	PHE	2.9
3	M	296	ALA	2.9
3	I	304	PHE	2.9
4	J	186	ARG	2.9
4	N	244	LEU	2.9
4	N	189	ASN	2.9
4	R	258	MET	2.8
4	R	211	ALA	2.8
3	I	305	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
4	N	204	ILE	2.8
4	R	206	GLU	2.8
4	N	243	LYS	2.7
4	N	248	ALA	2.7
4	R	220	VAL	2.7
3	Q	296	ALA	2.7
4	R	158	GLY	2.7
4	R	200	VAL	2.7
4	J	232	LEU	2.7
4	J	213	ILE	2.7
4	J	202	MET	2.7
4	J	241	VAL	2.7
3	M	225	PRO	2.7
4	N	207	PRO	2.7
4	N	232	LEU	2.7
3	E	111	ASP	2.6
4	N	190	ALA	2.6
3	Q	228	VAL	2.6
4	R	168	ILE	2.6
4	R	191	GLU	2.6
4	N	231	ARG	2.6
4	J	243	LYS	2.6
4	J	235	ARG	2.5
4	N	208	ARG	2.5
3	M	306	PHE	2.5
3	Q	305	LYS	2.5
3	Q	218	PHE	2.5
4	N	239	ARG	2.5
3	M	305	LYS	2.5
3	Q	269	ARG	2.5
4	R	234	ALA	2.5
4	N	186	ARG	2.5
4	N	196	ARG	2.5
4	R	235	ARG	2.5
3	M	227	GLN	2.5
3	Q	235	ILE	2.4
4	B	205	ARG	2.4
4	J	244	LEU	2.4
3	E	312	LYS	2.4
3	Q	303	ASP	2.4
4	J	250	PHE	2.4
3	Q	268	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	N	233	ALA	2.4
4	N	250	PHE	2.4
4	R	317	VAL	2.4
4	N	197	PHE	2.4
4	J	187	ALA	2.4
4	J	219	MET	2.3
3	A	111	ASP	2.3
4	N	235	ARG	2.3
3	M	143	LYS	2.3
3	Q	224	LEU	2.3
4	J	172	VAL	2.3
4	R	182	THR	2.3
3	Q	265	SER	2.2
4	N	187	ALA	2.2
4	N	182	THR	2.2
4	N	178	LEU	2.2
3	A	134	ILE	2.2
4	R	231	ARG	2.2
3	M	265	SER	2.2
4	R	320	GLU	2.2
3	Q	298	ASP	2.2
4	R	165	LEU	2.2
4	N	200	VAL	2.1
4	B	188	ARG	2.1
4	R	175	GLY	2.1
4	R	252	ASP	2.1
3	M	113	ALA	2.1
3	M	232	ALA	2.1
3	M	301	PRO	2.1
3	A	312	LYS	2.1
4	R	226	SER	2.1
4	J	249	LYS	2.1
4	N	251	LEU	2.1
4	J	217	GLY	2.1
4	R	221	CYS	2.1
3	M	259	TYR	2.0
3	M	226	LYS	2.0
4	N	240	VAL	2.0
3	E	305	LYS	2.0
4	N	236	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.