



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Dec 13, 2016 – 07:55 PM EST

PDB ID : 5FKV  
EMDB ID: : EMD-3198  
Title : cryo-EM structure of the E. coli replicative DNA polymerase complex bound to DNA (DNA polymerase III alpha, beta, epsilon, tau complex)  
Authors : Fernandez-Leiro, R.; Conrad, J.; Scheres, S.H.W.; Lamers, M.H.  
Deposited on : 2015-10-20  
Resolution : 8.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

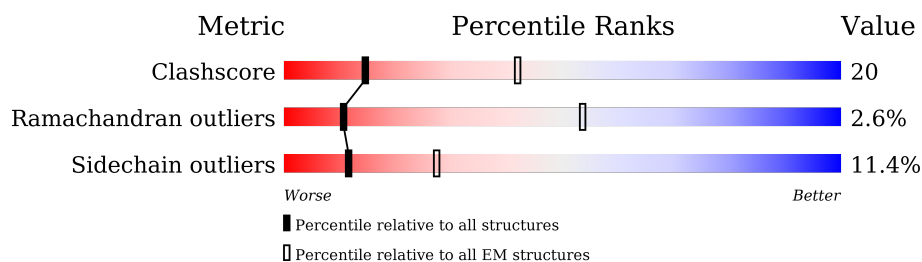
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1160	
2	B	366	
2	C	366	
3	D	243	
4	E	144	
5	P	25	
6	T	29	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18386 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called DNA POLYMERASE III SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1145	Total	C	N	O	S	0	0
			9020	5721	1562	1690	47		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	921	LEU	ALA	ENGINEERED MUTATION	UNP P10443
A	923	LEU	MET	ENGINEERED MUTATION	UNP P10443

- Molecule 2 is a protein called DNA POLYMERASE III BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		
2	C	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		

- Molecule 3 is a protein called DNA POLYMERASE III EPSILON.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	219	Total	C	N	O	S	0	0
			1717	1090	299	319	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	LEU	THR	ENGINEERED MUTATION	UNP P03007
D	185	LEU	MET	ENGINEERED MUTATION	UNP P03007
D	186	PRO	ALA	ENGINEERED MUTATION	UNP P03007
D	187	LEU	PHE	ENGINEERED MUTATION	UNP P03007

- Molecule 4 is a protein called DNA POLYMERASE III TAU.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	117	Total	C	N	O	S	0	0
			914	567	165	180	2		

- Molecule 5 is a DNA chain called PRIMER-TEMPLATE DUPLEX DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	25	Total	C	N	O	P	0	0
			522	246	105	146	25		

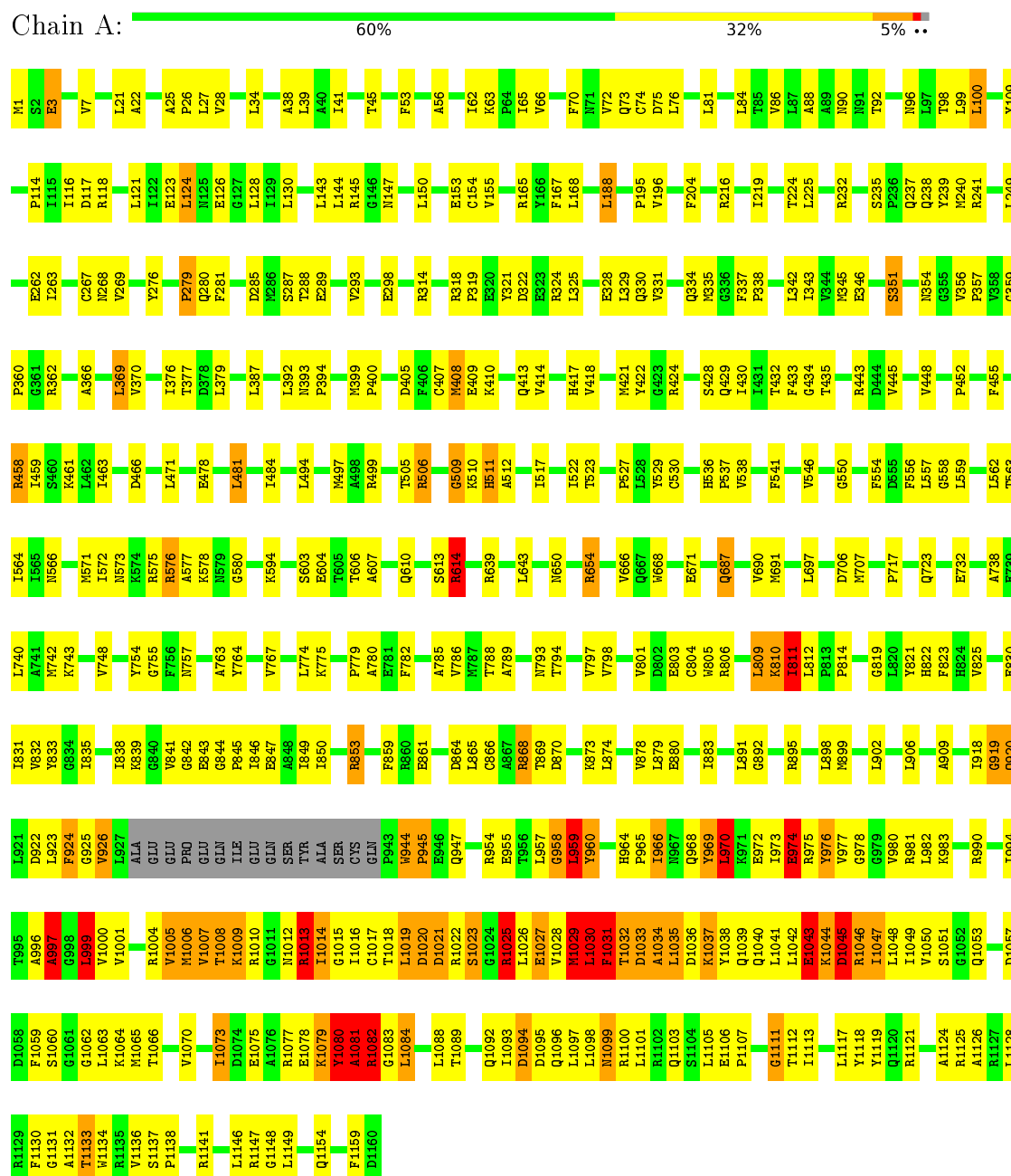
- Molecule 6 is a DNA chain called PRIMER-TEMPLATE DUPLEX DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	26	Total	C	N	O	P	0	0
			525	251	88	160	26		

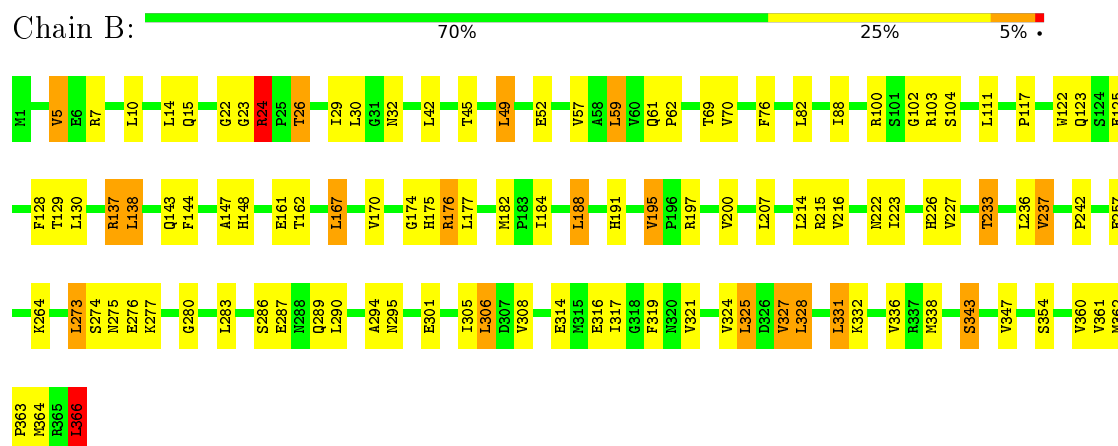
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

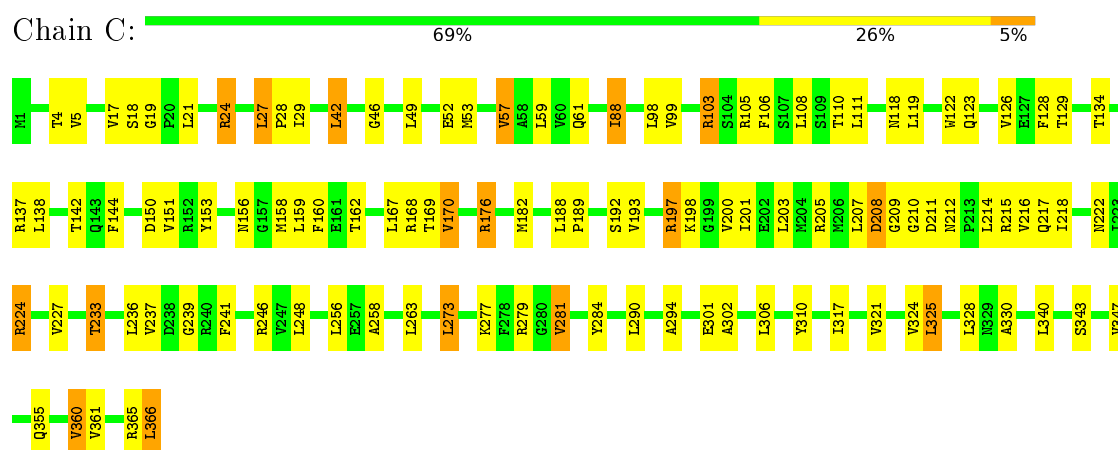
#### • Molecule 1: DNA POLYMERASE III SUBUNIT ALPHA



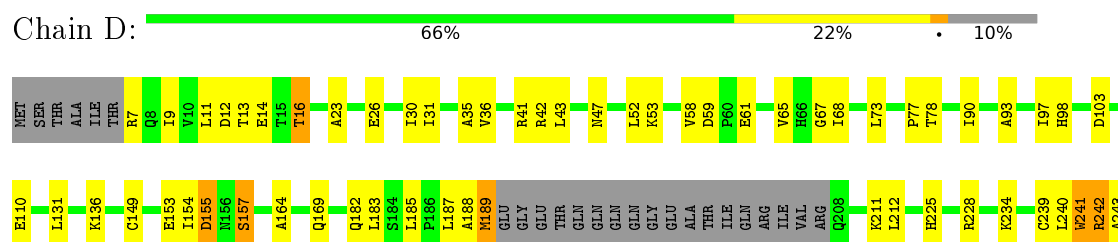
- Molecule 2: DNA POLYMERASE III BETA



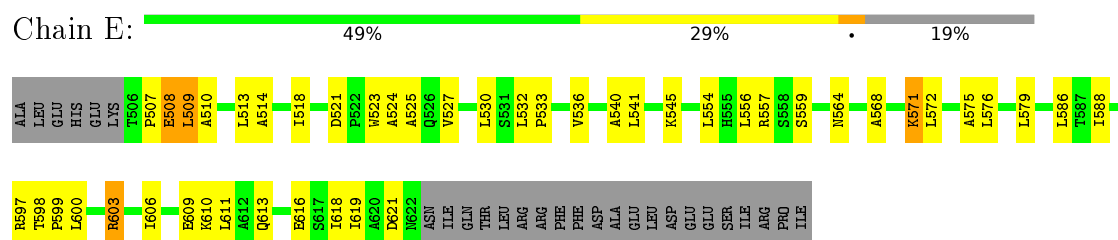
- Molecule 2: DNA POLYMERASE III BETA



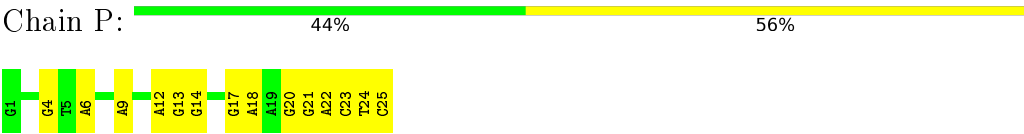
- Molecule 3: DNA POLYMERASE III EPSILON



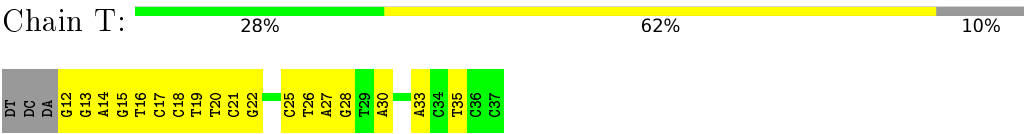
- Molecule 4: DNA POLYMERASE III TAU



● Molecule 5: PRIMER-TEMPLATE DUPLEX DNA



● Molecule 6: PRIMER-TEMPLATE DUPLEX DNA



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	5663	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	28409	Depositor
Image detector	GATAN K2 SUMMIT	Depositor



## 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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.59	8/9199 (0.1%)	0.88	20/12427 (0.2%)
2	B	0.51	0/2893	0.92	3/3915 (0.1%)
2	C	0.52	0/2893	0.92	4/3915 (0.1%)
3	D	0.57	1/1747 (0.1%)	0.75	4/2358 (0.2%)
4	E	0.65	0/927	0.82	0/1259
5	P	0.39	0/588	0.81	0/907
6	T	0.44	0/585	0.94	0/899
All	All	0.56	9/18832 (0.0%)	0.88	31/25680 (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	A	0	8
2	B	0	1
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	242	ARG	N-CA	-12.04	1.22	1.46
1	A	687	GLN	CG-CD	10.32	1.74	1.51
1	A	1045	ASP	C-N	-8.38	1.14	1.34
1	A	687	GLN	CD-OE1	6.76	1.38	1.24
1	A	1080	TYR	CB-CG	-6.71	1.41	1.51
1	A	687	GLN	CB-CG	6.59	1.70	1.52
1	A	1080	TYR	CA-CB	-6.21	1.40	1.53
1	A	960	TYR	CE1-CZ	-6.10	1.30	1.38
1	A	1079	LYS	N-CA	-5.55	1.35	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1045	ASP	O-C-N	-12.69	102.40	122.70
1	A	1081	ALA	N-CA-C	-10.74	82.01	111.00
1	A	687	GLN	CB-CG-CD	8.18	132.87	111.60
1	A	1082	ARG	CA-CB-CG	7.99	130.99	113.40
1	A	614	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	1081	ALA	CB-CA-C	6.92	120.48	110.10
1	A	1025	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	232	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	B	366	LEU	CA-CB-CG	6.26	129.69	115.30
1	A	424	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	1029	MET	N-CA-CB	5.97	121.35	110.60
2	B	24	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	1080	TYR	C-N-CA	-5.91	106.92	121.70
3	D	155	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	1082	ARG	CG-CD-NE	5.77	123.92	111.80
3	D	242	ARG	N-CA-CB	-5.72	100.31	110.60
2	C	224	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	999	LEU	CB-CG-CD1	5.52	120.38	111.00
2	C	366	LEU	CA-CB-CG	5.49	127.92	115.30
2	C	27	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	165	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	997	ALA	N-CA-CB	-5.34	102.62	110.10
1	A	506	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	D	241	TRP	CA-C-N	-5.24	105.67	117.20
1	A	1082	ARG	N-CA-C	-5.18	97.03	111.00
1	A	1082	ARG	N-CA-CB	5.17	119.91	110.60
2	B	137	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	1125	ARG	NE-CZ-NH1	5.14	122.87	120.30
3	D	241	TRP	N-CA-C	-5.13	97.16	111.00
1	A	853	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	C	168	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1027	GLU	Peptide
1	A	1033	ASP	Peptide
1	A	1045	ASP	Mainchain
1	A	1080	TYR	Peptide
1	A	1084	LEU	Peptide
1	A	509	GLY	Peptide
1	A	511	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	996	ALA	Peptide
2	B	237	VAL	Peptide

## 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	A	9020	0	8985	497	0
2	B	2844	0	2861	67	0
2	C	2844	0	2861	46	0
3	D	1717	0	1715	58	0
4	E	914	0	915	30	0
5	P	522	0	280	39	0
6	T	525	0	295	31	0
All	All	18386	0	17912	725	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 20.

All (725) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:CD	1:A:687:GLN:CG	1.74	1.55
1:A:1040:GLN:O	1:A:1043:GLU:HG3	1.29	1.32
1:A:1079:LYS:NZ	1:A:1083:GLY:O	1.66	1.29
1:A:1040:GLN:O	1:A:1043:GLU:CG	1.81	1.26
1:A:977:VAL:HB	1:A:981:ARG:HB2	1.20	1.18
1:A:1080:TYR:O	1:A:1082:ARG:HG3	1.43	1.18
1:A:1079:LYS:CE	1:A:1083:GLY:O	1.90	1.17
3:D:188:ALA:HA	3:D:189:MET:CB	1.72	1.15
1:A:775:LYS:O	1:A:779:PRO:HB3	1.41	1.15
1:A:977:VAL:CB	1:A:981:ARG:HB2	1.81	1.10
1:A:1080:TYR:O	1:A:1082:ARG:CG	2.00	1.09
1:A:1013:ARG:CG	1:A:1014:ILE:HG22	1.82	1.08
1:A:1080:TYR:CD2	1:A:1081:ALA:N	2.22	1.08
3:D:188:ALA:HA	3:D:189:MET:HB2	1.07	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:VAL:HG23	1:A:1029:MET:HB2	1.29	1.05
1:A:809:LEU:HD22	1:A:811:ILE:CD1	1.87	1.05
3:D:188:ALA:CA	3:D:189:MET:HB2	1.87	1.05
1:A:1045:ASP:O	1:A:1047:ILE:N	1.89	1.05
1:A:1079:LYS:HE2	1:A:1083:GLY:O	1.55	1.04
1:A:977:VAL:HB	1:A:981:ARG:CB	1.90	1.01
1:A:1013:ARG:HG2	1:A:1014:ILE:HG22	1.39	1.01
1:A:1080:TYR:C	1:A:1082:ARG:HD3	1.81	1.00
3:D:239:CYS:SG	3:D:242:ARG:HD2	2.00	0.99
1:A:1080:TYR:HB3	1:A:1082:ARG:NH1	1.77	0.99
1:A:1080:TYR:CA	1:A:1082:ARG:HD3	1.92	0.98
4:E:507:PRO:O	4:E:509:LEU:N	1.97	0.97
5:P:25:DC:N3	6:T:13:DG:O6	1.96	0.97
1:A:775:LYS:O	1:A:779:PRO:CB	2.12	0.97
1:A:432:THR:O	1:A:509:GLY:HA3	1.65	0.97
1:A:809:LEU:HD22	1:A:811:ILE:HD13	1.42	0.96
1:A:1028:VAL:HA	1:A:1029:MET:CB	1.96	0.95
6:T:17:DC:H2'	6:T:18:DC:C6	2.03	0.93
4:E:513:LEU:HD11	4:E:606:ILE:HB	1.51	0.93
5:P:22:DA:H2''	5:P:23:DC:C5	2.04	0.92
1:A:1028:VAL:CG2	1:A:1029:MET:HB2	1.98	0.92
1:A:1045:ASP:O	1:A:1046:ARG:C	2.01	0.91
1:A:1029:MET:O	1:A:1030:LEU:HB2	1.68	0.91
3:D:240:LEU:C	3:D:242:ARG:H	1.58	0.91
1:A:1040:GLN:O	1:A:1043:GLU:HG2	1.70	0.90
1:A:1079:LYS:CG	1:A:1082:ARG:HB3	2.02	0.90
2:B:242:PRO:HB2	3:D:187:LEU:HD22	1.54	0.89
1:A:1079:LYS:HG3	1:A:1082:ARG:HB3	1.54	0.88
1:A:1080:TYR:HB3	1:A:1082:ARG:HH11	1.35	0.88
1:A:918:ILE:HG23	1:A:920:GLN:HB3	1.55	0.88
1:A:564:ILE:HD11	1:A:789:ALA:HB2	1.56	0.87
1:A:510:LYS:HB3	6:T:17:DC:H2''	1.53	0.87
1:A:918:ILE:HG23	1:A:920:GLN:CB	2.05	0.87
1:A:1080:TYR:N	1:A:1082:ARG:NE	2.23	0.86
1:A:1020:ASP:HA	1:A:1021:ASP:O	1.75	0.86
1:A:954:ARG:O	1:A:959:LEU:N	2.07	0.86
1:A:977:VAL:CG1	1:A:981:ARG:HB2	2.05	0.85
1:A:1034:ALA:HB2	1:A:1038:TYR:CD1	2.11	0.85
2:B:30:LEU:HD11	2:B:49:LEU:HD13	1.58	0.85
1:A:1080:TYR:N	1:A:1082:ARG:CD	2.40	0.85
3:D:240:LEU:C	3:D:242:ARG:N	2.20	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:ILE:O	1:A:920:GLN:N	2.09	0.84
1:A:780:ALA:HB1	1:A:831:ILE:HD11	1.60	0.83
4:E:524:ALA:HB2	4:E:599:PRO:HB3	1.60	0.83
1:A:966:ILE:HG23	1:A:970:LEU:HA	1.60	0.83
1:A:969:TYR:O	1:A:970:LEU:O	1.96	0.82
3:D:241:TRP:HB3	3:D:242:ARG:HG3	1.61	0.82
1:A:1080:TYR:CA	1:A:1082:ARG:CD	2.58	0.82
1:A:1080:TYR:HB3	1:A:1082:ARG:HD3	1.60	0.81
1:A:960:TYR:HE1	1:A:964:HIS:CE1	2.00	0.80
1:A:1080:TYR:CB	1:A:1082:ARG:NH1	2.43	0.80
2:C:317:ILE:HD12	2:C:343:SER:HA	1.64	0.80
1:A:1080:TYR:CG	1:A:1081:ALA:N	2.41	0.80
1:A:1080:TYR:CB	1:A:1082:ARG:HD3	2.10	0.80
1:A:1008:THR:O	1:A:1009:LYS:HG2	1.82	0.80
1:A:1094:ASP:HA	1:A:1097:LEU:HD13	1.64	0.80
1:A:1040:GLN:HG3	1:A:1043:GLU:CD	2.01	0.80
2:B:24:ARG:N	2:B:24:ARG:HD2	1.97	0.79
1:A:977:VAL:HG12	1:A:980:VAL:HG13	1.65	0.79
1:A:1028:VAL:HA	1:A:1029:MET:HB2	1.64	0.79
2:C:158:MET:HG3	2:C:170:VAL:O	1.83	0.79
1:A:810:LYS:HA	1:A:811:ILE:CG1	2.12	0.79
1:A:1013:ARG:HG3	1:A:1014:ILE:HG22	1.64	0.78
1:A:408:MET:SD	6:T:16:DT:H3'	2.24	0.78
1:A:1103:GLN:O	1:A:1107:PRO:HD2	1.83	0.78
1:A:1080:TYR:O	1:A:1082:ARG:HD3	1.83	0.78
1:A:1028:VAL:HA	1:A:1029:MET:CG	2.14	0.78
1:A:1080:TYR:O	1:A:1082:ARG:CD	2.31	0.77
1:A:1027:GLU:HB2	1:A:1029:MET:SD	2.24	0.77
5:P:20:DG:H2''	5:P:21:DG:C8	2.19	0.77
1:A:1080:TYR:H	1:A:1082:ARG:NE	1.84	0.76
5:P:9:DA:C2	6:T:30:DA:C2	2.74	0.76
1:A:76:LEU:HD22	1:A:150:LEU:HD12	1.65	0.75
1:A:1028:VAL:HG23	1:A:1029:MET:CB	2.11	0.75
1:A:775:LYS:O	1:A:779:PRO:HG3	1.86	0.75
1:A:1042:LEU:O	1:A:1043:GLU:O	2.04	0.75
5:P:12:DA:C2	6:T:27:DA:C2	2.75	0.75
3:D:9:ILE:HG21	3:D:90:ILE:HG22	1.67	0.74
1:A:809:LEU:HD22	1:A:811:ILE:HD11	1.67	0.74
1:A:775:LYS:O	1:A:779:PRO:CG	2.35	0.74
1:A:1080:TYR:CG	1:A:1081:ALA:CA	2.70	0.73
2:B:128:PHE:HB3	2:B:188:LEU:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:LYS:HA	1:A:811:ILE:CB	2.17	0.73
3:D:240:LEU:HA	3:D:243:ALA:HB2	1.70	0.73
1:A:1048:LEU:HD11	1:A:1050:VAL:HG13	1.71	0.73
1:A:1040:GLN:HA	1:A:1043:GLU:HG2	1.71	0.72
4:E:616:GLU:O	4:E:619:ILE:HG22	1.89	0.72
1:A:1080:TYR:CB	1:A:1082:ARG:CZ	2.68	0.72
3:D:240:LEU:HA	3:D:243:ALA:CB	2.20	0.72
1:A:809:LEU:N	1:A:810:LYS:HE3	2.04	0.72
5:P:22:DA:H2"	5:P:23:DC:C6	2.25	0.72
1:A:964:HIS:N	1:A:970:LEU:HD21	2.05	0.71
1:A:429:GLN:HB2	1:A:538:VAL:HG12	1.72	0.71
1:A:1078:GLU:HB3	1:A:1082:ARG:HH21	1.54	0.71
2:B:7:ARG:NH2	2:B:82:LEU:O	2.24	0.71
1:A:109:TYR:OH	1:A:530:CYS:O	2.09	0.71
4:E:536:VAL:HG22	4:E:568:ALA:HA	1.73	0.71
2:C:256:LEU:HD12	2:C:310:TYR:CD1	2.26	0.70
1:A:564:ILE:HG23	1:A:785:ALA:CB	2.21	0.70
1:A:1075:GLU:O	1:A:1082:ARG:NH2	2.25	0.70
1:A:1093:ILE:HG12	1:A:1096:GLN:HG2	1.74	0.70
1:A:614:ARG:HG2	1:A:614:ARG:HH11	1.57	0.70
1:A:1040:GLN:CG	1:A:1043:GLU:CD	2.61	0.69
1:A:167:PHE:HA	1:A:195:PRO:O	1.91	0.69
1:A:958:GLY:O	1:A:959:LEU:O	2.11	0.69
1:A:1048:LEU:HD21	1:A:1050:VAL:HG13	1.73	0.69
1:A:1079:LYS:HG2	1:A:1083:GLY:H	1.58	0.69
1:A:974:GLU:O	1:A:975:ARG:HG3	1.92	0.69
1:A:168:LEU:HB2	1:A:196:VAL:HG12	1.73	0.69
1:A:1030:LEU:O	1:A:1031:PHE:HB2	1.93	0.69
1:A:564:ILE:HG23	1:A:785:ALA:HB1	1.74	0.68
1:A:1038:TYR:O	1:A:1042:LEU:HG	1.92	0.68
1:A:1007:VAL:HG11	2:B:276:GLU:HB3	1.75	0.68
5:P:6:DA:C2	6:T:33:DA:C2	2.81	0.68
1:A:1028:VAL:CA	1:A:1029:MET:HB2	2.23	0.68
1:A:357:PRO:HB3	1:A:562:LEU:HD12	1.76	0.68
1:A:919:GLY:O	1:A:920:GLN:O	2.12	0.68
1:A:965:PRO:HB3	1:A:1077:ARG:HA	1.76	0.67
1:A:1012:ASN:O	1:A:1013:ARG:NE	2.28	0.67
3:D:240:LEU:C	3:D:243:ALA:H	1.97	0.67
4:E:523:TRP:CE2	4:E:554:LEU:HD21	2.29	0.67
1:A:879:LEU:HD12	1:A:906:LEU:HD21	1.76	0.67
2:C:176:ARG:HB2	2:C:361:VAL:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:GLN:C	1:A:1043:GLU:HG2	2.16	0.66
1:A:960:TYR:CE1	1:A:964:HIS:CE1	2.81	0.66
1:A:573:ASN:O	1:A:576:ARG:HB3	1.95	0.66
1:A:1078:GLU:O	1:A:1082:ARG:O	2.13	0.66
1:A:463:ILE:CD1	1:A:481:LEU:HD21	2.25	0.66
2:B:5:VAL:HG13	2:B:59:LEU:HD12	1.78	0.66
1:A:1030:LEU:HD21	3:D:153:GLU:HA	1.78	0.66
1:A:1136:VAL:HG12	1:A:1137:SER:O	1.96	0.66
1:A:1027:GLU:CB	1:A:1029:MET:SD	2.84	0.65
1:A:1080:TYR:HB3	1:A:1082:ARG:CZ	2.26	0.65
1:A:1077:ARG:NE	1:A:1138:PRO:O	2.28	0.65
3:D:240:LEU:O	3:D:242:ARG:N	2.28	0.65
1:A:830:GLU:O	1:A:831:ILE:HD13	1.97	0.65
2:B:176:ARG:HB3	2:B:361:VAL:HG12	1.78	0.65
1:A:822:HIS:CD2	1:A:823:PHE:H	2.14	0.65
3:D:14:GLU:HG2	3:D:164:ALA:HB2	1.79	0.65
1:A:1028:VAL:CB	1:A:1029:MET:HB2	2.27	0.65
1:A:432:THR:O	1:A:509:GLY:CA	2.44	0.65
1:A:968:GLN:HB2	1:A:969:TYR:CD1	2.32	0.65
4:E:530:LEU:HD13	4:E:575:ALA:HB1	1.79	0.65
1:A:810:LYS:HA	1:A:811:ILE:HB	1.77	0.64
1:A:810:LYS:HA	1:A:811:ILE:HG12	1.77	0.64
2:B:147:ALA:O	2:B:197:ARG:NH1	2.29	0.64
1:A:975:ARG:HB3	1:A:981:ARG:NE	2.12	0.64
4:E:524:ALA:HB2	4:E:599:PRO:CB	2.27	0.64
1:A:1034:ALA:HB3	1:A:1038:TYR:HB2	1.77	0.64
1:A:357:PRO:CB	1:A:562:LEU:HD12	2.28	0.64
3:D:16:THR:HG22	3:D:58:VAL:HA	1.78	0.64
2:B:214:LEU:HD13	2:B:227:VAL:HG22	1.80	0.64
1:A:1100:ARG:HA	1:A:1103:GLN:HG2	1.80	0.64
1:A:1079:LYS:HB3	1:A:1083:GLY:N	2.13	0.64
1:A:86:VAL:HG13	1:A:130:LEU:CD2	2.27	0.64
1:A:825:VAL:HG12	1:A:830:GLU:O	1.98	0.64
5:P:20:DG:C5	5:P:21:DG:O6	2.51	0.63
1:A:812:LEU:HB2	1:A:832:VAL:HG12	1.80	0.63
1:A:975:ARG:HB3	1:A:981:ARG:CD	2.29	0.63
1:A:356:VAL:HG22	1:A:410:LYS:HB3	1.79	0.63
1:A:918:ILE:HG23	1:A:920:GLN:HB2	1.78	0.63
1:A:944:TRP:CE2	1:A:947:GLN:CD	2.72	0.63
1:A:1040:GLN:CA	1:A:1043:GLU:HG2	2.28	0.63
1:A:45:THR:HG23	1:A:70:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:240:LEU:O	3:D:243:ALA:N	2.24	0.63
3:D:241:TRP:HB3	3:D:242:ARG:CG	2.29	0.63
1:A:1105:LEU:HD22	1:A:1136:VAL:CG2	2.29	0.63
1:A:788:THR:CG2	1:A:822:HIS:CD2	2.81	0.63
1:A:1080:TYR:HB2	1:A:1082:ARG:CZ	2.29	0.62
1:A:393:ASN:ND2	1:A:706:ASP:OD2	2.31	0.62
1:A:430:ILE:O	1:A:512:ALA:HA	1.98	0.62
5:P:20:DG:C4	5:P:21:DG:C6	2.87	0.62
1:A:167:PHE:CD2	1:A:263:ILE:HD11	2.35	0.62
3:D:239:CYS:SG	3:D:242:ARG:CD	2.84	0.62
4:E:527:VAL:HG13	4:E:532:LEU:HD22	1.81	0.62
1:A:1080:TYR:CD2	1:A:1081:ALA:CA	2.82	0.62
1:A:969:TYR:HB2	1:A:973:ILE:HG13	1.80	0.62
1:A:1031:PHE:CZ	3:D:155:ASP:HB2	2.35	0.62
1:A:167:PHE:CE2	1:A:263:ILE:HD11	2.34	0.62
1:A:902:LEU:O	1:A:906:LEU:HG	2.00	0.62
4:E:518:ILE:HG23	4:E:525:ALA:HA	1.81	0.62
1:A:924:PHE:HD1	1:A:925:GLY:H	1.47	0.61
1:A:1053:GLN:HE22	3:D:157:SER:CB	2.13	0.61
1:A:1040:GLN:HG3	1:A:1043:GLU:OE1	1.99	0.61
1:A:990:ARG:HB3	1:A:1053:GLN:HB3	1.83	0.61
2:B:24:ARG:HD2	2:B:24:ARG:H	1.66	0.61
1:A:1094:ASP:CA	1:A:1097:LEU:HD13	2.30	0.61
1:A:1028:VAL:CA	1:A:1029:MET:CB	2.75	0.61
1:A:433:PHE:O	5:P:23:DC:H5"	2.00	0.61
1:A:687:GLN:NE2	1:A:687:GLN:CG	2.61	0.61
1:A:1025:ARG:O	1:A:1026:LEU:HD23	2.00	0.61
2:C:17:VAL:HG22	2:C:53:MET:HG3	1.82	0.61
1:A:1029:MET:O	1:A:1030:LEU:CB	2.46	0.61
1:A:1050:VAL:HG12	1:A:1070:VAL:HG13	1.81	0.61
1:A:975:ARG:O	1:A:976:TYR:CD1	2.54	0.61
1:A:314:ARG:O	1:A:318:ARG:HB2	2.00	0.61
1:A:944:TRP:CZ3	1:A:947:GLN:HG3	2.36	0.61
2:B:195:VAL:HG22	2:B:200:VAL:HG12	1.83	0.61
2:B:5:VAL:HG11	2:B:57:VAL:HG21	1.82	0.60
1:A:360:PRO:HG3	1:A:767:VAL:HG21	1.82	0.60
2:C:150:ASP:H	2:C:156:ASN:HD21	1.49	0.60
5:P:20:DG:H2"	5:P:21:DG:N7	2.16	0.60
1:A:1012:ASN:O	1:A:1013:ARG:HB3	2.00	0.60
1:A:960:TYR:CE1	1:A:964:HIS:ND1	2.69	0.60
1:A:964:HIS:CE1	1:A:965:PRO:HD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:536:VAL:HG21	4:E:571:LYS:HB3	1.83	0.60
1:A:964:HIS:ND1	1:A:965:PRO:HD2	2.17	0.60
3:D:241:TRP:CB	3:D:242:ARG:HG3	2.32	0.60
1:A:1007:VAL:O	1:A:1008:THR:HG22	2.02	0.60
1:A:1079:LYS:CG	1:A:1082:ARG:CB	2.75	0.60
1:A:944:TRP:CD2	1:A:945:PRO:HD2	2.36	0.60
1:A:775:LYS:C	1:A:779:PRO:HB3	2.20	0.60
3:D:239:CYS:SG	3:D:242:ARG:HB2	2.41	0.59
1:A:362:ARG:HG3	1:A:377:THR:HG22	1.85	0.59
1:A:798:VAL:O	1:A:801:VAL:HG22	2.01	0.59
1:A:510:LYS:CB	6:T:17:DC:H2"	2.29	0.59
5:P:20:DG:C4	5:P:21:DG:C5	2.90	0.59
2:C:258:ALA:HB3	2:C:263:LEU:HD22	1.85	0.59
1:A:1032:THR:HG21	1:A:1039:GLN:HG2	1.83	0.59
1:A:455:PHE:HA	1:A:1060:SER:OG	2.03	0.59
1:A:331:VAL:HG23	1:A:394:PRO:HB3	1.84	0.59
1:A:804:CYS:HB3	1:A:809:LEU:HB3	1.83	0.59
1:A:1040:GLN:CG	1:A:1043:GLU:OE2	2.51	0.59
1:A:1001:VAL:O	1:A:1016:ILE:HB	2.03	0.59
5:P:20:DG:C2	5:P:21:DG:C6	2.91	0.59
1:A:1080:TYR:HB3	1:A:1082:ARG:CD	2.32	0.58
1:A:821:TYR:HA	1:A:835:ILE:HG22	1.84	0.58
1:A:557:LEU:HD21	1:A:559:LEU:HD12	1.84	0.58
2:C:279:ARG:HB3	2:C:321:VAL:HG12	1.86	0.58
1:A:944:TRP:CZ3	1:A:945:PRO:HG2	2.38	0.58
1:A:235:SER:H	1:A:238:GLN:HE21	1.51	0.58
1:A:346:GLU:OE1	1:A:417:HIS:CE1	2.57	0.58
1:A:650:ASN:O	1:A:654:ARG:CG	2.52	0.58
5:P:17:DG:C2	6:T:22:DG:C2	2.91	0.58
1:A:1079:LYS:HG2	1:A:1083:GLY:N	2.18	0.58
1:A:977:VAL:HG11	1:A:981:ARG:HB2	1.85	0.58
1:A:801:VAL:O	1:A:805:TRP:HD1	1.87	0.57
1:A:955:GLU:HA	1:A:959:LEU:HB2	1.85	0.57
2:B:7:ARG:CZ	2:B:82:LEU:O	2.53	0.57
2:C:281:VAL:HG23	2:C:294:ALA:HB2	1.85	0.57
4:E:507:PRO:HB2	4:E:510:ALA:HB3	1.86	0.57
1:A:576:ARG:HG3	1:A:577:ALA:N	2.18	0.57
1:A:843:GLU:O	1:A:846:ILE:HG12	2.05	0.57
1:A:279:PRO:CD	1:A:343:ILE:HD11	2.34	0.57
1:A:557:LEU:HD21	1:A:559:LEU:CG	2.35	0.57
4:E:523:TRP:CZ2	4:E:554:LEU:HD21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:20:DG:N3	5:P:21:DG:C5	2.72	0.57
1:A:957:LEU:HD13	1:A:1022:ARG:HG2	1.86	0.57
1:A:1105:LEU:HD22	1:A:1136:VAL:HG21	1.87	0.57
1:A:835:ILE:O	1:A:838:ILE:HG22	2.04	0.57
2:C:208:ASP:O	2:C:210:GLY:N	2.36	0.57
5:P:17:DG:N2	6:T:22:DG:C2	2.72	0.57
1:A:41:ILE:HD12	1:A:53:PHE:CD1	2.40	0.56
1:A:866:CYS:HB3	1:A:909:ALA:HB2	1.87	0.56
1:A:1009:LYS:NZ	2:B:274:SER:OG	2.25	0.56
1:A:1043:GLU:O	1:A:1044:LYS:HB2	2.06	0.56
1:A:794:THR:O	1:A:798:VAL:HG23	2.05	0.56
3:D:43:LEU:HD11	3:D:169:GLN:HE22	1.70	0.56
1:A:1019:LEU:HD13	1:A:1026:LEU:HD12	1.87	0.56
1:A:650:ASN:O	1:A:654:ARG:HG2	2.06	0.56
1:A:1119:TYR:CD1	4:E:618:ILE:CD1	2.89	0.56
1:A:864:ASP:O	1:A:868:ARG:HD3	2.05	0.56
1:A:610:GLN:NE2	1:A:764:TYR:HB3	2.20	0.56
1:A:98:THR:HG21	1:A:523:THR:O	2.06	0.56
2:B:32:ASN:HB3	2:B:69:THR:HG22	1.87	0.56
1:A:803:GLU:O	1:A:806:ARG:HG2	2.06	0.56
1:A:969:TYR:HD2	1:A:973:ILE:HD12	1.71	0.56
2:C:134:THR:HG23	2:C:182:MET:CE	2.36	0.56
3:D:11:LEU:HD12	3:D:35:ALA:HB2	1.88	0.56
2:B:275:ASN:HD21	2:B:277:LYS:HE2	1.71	0.56
3:D:16:THR:HG23	3:D:31:ILE:CG2	2.36	0.56
4:E:507:PRO:O	4:E:510:ALA:N	2.39	0.56
1:A:983:LYS:NZ	1:A:1063:LEU:HD11	2.21	0.55
1:A:321:TYR:CD2	1:A:369:LEU:HD11	2.41	0.55
1:A:1080:TYR:C	1:A:1082:ARG:CD	2.61	0.55
1:A:944:TRP:CZ2	1:A:947:GLN:OE1	2.59	0.55
6:T:20:DT:C4	6:T:21:DC:N4	2.75	0.55
1:A:219:ILE:HG13	1:A:448:VAL:HG21	1.87	0.55
1:A:428:SER:HB2	1:A:522:ILE:HG21	1.88	0.55
1:A:814:PRO:HA	1:A:833:TYR:HB2	1.89	0.55
2:B:24:ARG:N	2:B:24:ARG:CD	2.69	0.55
1:A:268:ASN:OD1	3:D:225:HIS:HA	2.06	0.55
1:A:966:ILE:HD11	1:A:969:TYR:CE2	2.41	0.55
2:B:29:ILE:HD11	2:B:69:THR:HG21	1.88	0.55
1:A:1029:MET:HB3	1:A:1065:MET:O	2.05	0.55
2:B:331:LEU:HD23	2:B:336:VAL:HG22	1.89	0.55
2:C:273:LEU:HB2	2:C:302:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:240:LEU:HD23	3:D:243:ALA:HB2	1.89	0.55
1:A:880:GLU:O	1:A:883:ILE:HG22	2.07	0.55
1:A:1121:ARG:HB3	1:A:1124:ALA:O	2.07	0.55
2:B:128:PHE:CD1	2:B:184:ILE:HD11	2.42	0.55
1:A:1045:ASP:C	1:A:1047:ILE:N	2.56	0.54
1:A:606:THR:HG21	1:A:803:GLU:OE2	2.07	0.54
2:B:5:VAL:HG11	2:B:57:VAL:CG2	2.37	0.54
1:A:1146:LEU:HD13	1:A:1147:ARG:HG2	1.89	0.54
1:A:1050:VAL:HG12	1:A:1070:VAL:CG1	2.37	0.54
1:A:28:VAL:HG21	1:A:56:ALA:CB	2.38	0.54
1:A:969:TYR:CD2	1:A:973:ILE:HD12	2.42	0.54
1:A:1088:LEU:HD23	1:A:1089:THR:N	2.23	0.54
1:A:788:THR:HG21	1:A:822:HIS:CD2	2.42	0.54
1:A:919:GLY:HA3	2:C:365:ARG:O	2.07	0.54
3:D:239:CYS:O	3:D:242:ARG:C	2.46	0.54
3:D:52:LEU:HA	3:D:77:PRO:O	2.07	0.54
1:A:805:TRP:CZ3	1:A:810:LYS:HG2	2.42	0.54
1:A:845:PRO:HB3	1:A:874:LEU:HD23	1.90	0.54
1:A:918:ILE:O	1:A:918:ILE:HG12	2.08	0.54
1:A:1080:TYR:CD1	1:A:1081:ALA:HA	2.43	0.54
5:P:20:DG:H1'	5:P:21:DG:C8	2.42	0.54
1:A:1080:TYR:CB	1:A:1082:ARG:CD	2.84	0.54
1:A:1148:GLY:C	1:A:1149:LEU:HD12	2.28	0.54
1:A:478:GLU:HB3	1:A:481:LEU:HD22	1.90	0.54
1:A:445:VAL:HG12	1:A:494:LEU:HG	1.89	0.54
1:A:1008:THR:O	1:A:1009:LYS:CG	2.54	0.54
1:A:1033:ASP:O	1:A:1038:TYR:CG	2.61	0.54
1:A:964:HIS:HB3	1:A:966:ILE:HG22	1.89	0.54
1:A:968:GLN:HB2	1:A:969:TYR:CE1	2.43	0.54
1:A:853:ARG:HB2	1:A:859:PHE:CE2	2.43	0.54
2:C:347:VAL:O	2:C:360:VAL:HB	2.07	0.54
1:A:966:ILE:HD11	1:A:969:TYR:CD2	2.43	0.53
1:A:690:VAL:HG22	1:A:748:VAL:HG13	1.91	0.53
2:B:280:GLY:HA2	2:B:366:LEU:HD21	1.90	0.53
2:B:29:ILE:CG1	2:B:69:THR:HG21	2.37	0.53
5:P:20:DG:C2	5:P:21:DG:N1	2.76	0.53
1:A:357:PRO:HB2	1:A:562:LEU:HB3	1.90	0.53
1:A:883:ILE:HD11	1:A:895:ARG:HG2	1.89	0.53
4:E:523:TRP:HB2	4:E:545:LYS:HB2	1.88	0.53
1:A:429:GLN:HB3	1:A:512:ALA:HB2	1.90	0.53
1:A:1008:THR:HG23	1:A:1008:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:ASP:C	1:A:1047:ILE:H	2.12	0.53
1:A:1063:LEU:HD12	1:A:1063:LEU:N	2.23	0.53
1:A:1078:GLU:HB3	1:A:1082:ARG:NH2	2.22	0.53
1:A:610:GLN:HE22	1:A:764:TYR:HB3	1.73	0.53
5:P:20:DG:C6	5:P:21:DG:O6	2.61	0.53
1:A:445:VAL:CG1	1:A:494:LEU:HG	2.39	0.53
1:A:379:LEU:HD11	1:A:763:ALA:HA	1.89	0.53
1:A:1040:GLN:HG2	1:A:1043:GLU:OE2	2.09	0.53
1:A:76:LEU:HD21	1:A:153:GLU:HB3	1.90	0.53
3:D:149:CYS:HA	3:D:154:ILE:HD12	1.90	0.53
1:A:1030:LEU:O	1:A:1031:PHE:CB	2.57	0.53
1:A:1093:ILE:CG1	1:A:1096:GLN:H	2.22	0.53
1:A:167:PHE:CE2	1:A:195:PRO:HB2	2.44	0.53
1:A:841:VAL:HG22	1:A:878:VAL:HG13	1.90	0.53
3:D:98:HIS:CE1	3:D:131:LEU:HD13	2.44	0.53
2:C:21:LEU:HD21	2:C:46:GLY:HA3	1.90	0.52
5:P:23:DC:H2"	5:P:24:DT:H72	1.90	0.52
1:A:65:ILE:HG23	1:A:267:CYS:HB3	1.91	0.52
2:C:52:GLU:HB2	2:C:119:LEU:HD22	1.91	0.52
4:E:507:PRO:O	4:E:508:GLU:C	2.48	0.52
1:A:1034:ALA:CB	1:A:1038:TYR:CD1	2.89	0.52
1:A:879:LEU:CD1	1:A:906:LEU:HD21	2.38	0.52
1:A:964:HIS:CG	1:A:965:PRO:HD2	2.44	0.52
3:D:241:TRP:C	3:D:242:ARG:HG3	2.30	0.52
1:A:1020:ASP:CB	1:A:1021:ASP:HA	2.39	0.52
2:B:129:THR:HG22	2:B:215:ARG:HB2	1.90	0.52
2:B:15:GLN:HA	2:B:76:PHE:CZ	2.43	0.52
2:C:159:LEU:HD11	2:C:192:SER:HB3	1.91	0.52
5:P:21:DG:C2	5:P:22:DA:C5	2.97	0.52
1:A:838:ILE:HG23	1:A:841:VAL:HB	1.92	0.52
1:A:892:GLY:HA3	1:A:898:LEU:HD21	1.92	0.52
1:A:434:GLY:HA2	5:P:23:DC:H5"	1.91	0.52
1:A:100:LEU:HD11	1:A:121:LEU:HD23	1.92	0.52
5:P:23:DC:H2"	5:P:24:DT:OP2	2.09	0.52
1:A:1013:ARG:HG3	1:A:1014:ILE:CG2	2.38	0.52
1:A:957:LEU:HD13	1:A:1022:ARG:CG	2.40	0.52
1:A:1106:GLU:HB3	1:A:1107:PRO:HD3	1.91	0.52
1:A:809:LEU:O	1:A:810:LYS:HG3	2.09	0.52
1:A:1126:ALA:HB3	4:E:618:ILE:HG13	1.93	0.51
1:A:923:LEU:O	1:A:924:PHE:C	2.48	0.51
1:A:1093:ILE:CD1	1:A:1095:ASP:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:GLU:O	1:A:775:LYS:NZ	2.43	0.51
1:A:861:GLU:HA	1:A:891:LEU:HD13	1.91	0.51
2:B:184:ILE:HG21	2:B:188:LEU:HD22	1.91	0.51
3:D:36:VAL:HG12	3:D:47:ASN:CG	2.31	0.51
1:A:387:LEU:HD23	1:A:691:MET:HE2	1.92	0.51
1:A:1053:GLN:HE21	1:A:1066:THR:CG2	2.23	0.51
1:A:74:CYS:HB3	1:A:118:ARG:HB2	1.92	0.51
5:P:20:DG:C2'	5:P:21:DG:C8	2.91	0.51
1:A:1111:GLY:O	1:A:1113:ILE:HG13	2.10	0.51
1:A:944:TRP:CE3	1:A:947:GLN:HG3	2.46	0.51
1:A:925:GLY:HA3	1:A:926:VAL:HB	1.93	0.51
1:A:969:TYR:N	1:A:969:TYR:CD1	2.79	0.51
2:B:321:VAL:HG22	2:B:325:LEU:HD22	1.93	0.51
2:C:281:VAL:CG2	2:C:294:ALA:HB2	2.40	0.51
6:T:16:DT:H1'	6:T:17:DC:H5'	1.92	0.51
1:A:1048:LEU:HD21	1:A:1050:VAL:CG1	2.39	0.51
4:E:530:LEU:HD21	4:E:579:LEU:HB2	1.92	0.51
1:A:1093:ILE:HG13	1:A:1095:ASP:N	2.25	0.51
1:A:143:LEU:HD21	1:A:188:LEU:HD12	1.93	0.51
1:A:606:THR:O	1:A:607:ALA:HB3	2.11	0.50
2:B:161:GLU:O	2:B:167:LEU:HA	2.11	0.50
3:D:11:LEU:CD1	3:D:35:ALA:HB2	2.40	0.50
1:A:849:ILE:HG12	1:A:874:LEU:HD11	1.93	0.50
1:A:997:ALA:CB	1:A:1048:LEU:HD12	2.40	0.50
4:E:554:LEU:HD12	4:E:586:LEU:HD11	1.93	0.50
1:A:471:LEU:HD13	1:A:499:ARG:HG3	1.93	0.50
2:C:217:GLN:HE21	2:C:224:ARG:HH11	1.58	0.50
1:A:505:THR:HG22	1:A:506:ARG:N	2.26	0.50
3:D:239:CYS:HG	3:D:242:ARG:HD2	1.73	0.50
1:A:1033:ASP:O	1:A:1038:TYR:CD2	2.65	0.50
1:A:1133:THR:HB	1:A:1134:TRP:CE3	2.47	0.50
2:B:273:LEU:HD23	2:B:301:GLU:N	2.27	0.50
1:A:793:ASN:O	1:A:797:VAL:HG23	2.12	0.50
1:A:870:ASP:OD1	1:A:873:LYS:HD3	2.11	0.50
1:A:994:ILE:HA	1:A:1051:SER:HA	1.93	0.50
1:A:1079:LYS:CB	1:A:1083:GLY:N	2.75	0.49
1:A:997:ALA:HA	1:A:1018:THR:O	2.13	0.49
1:A:1048:LEU:HD11	1:A:1050:VAL:CG1	2.42	0.49
1:A:1080:TYR:CG	1:A:1081:ALA:HA	2.47	0.49
1:A:22:ALA:HB3	1:A:27:LEU:HD21	1.94	0.49
1:A:28:VAL:HG21	1:A:56:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ILE:HG13	1:A:874:LEU:HD21	1.95	0.49
1:A:975:ARG:HD2	1:A:981:ARG:NH1	2.28	0.49
1:A:1117:LEU:HD13	1:A:1118:TYR:N	2.27	0.49
1:A:1040:GLN:C	1:A:1043:GLU:CG	2.68	0.49
1:A:732:GLU:OE2	1:A:738:ALA:HB2	2.12	0.49
1:A:918:ILE:CG2	1:A:920:GLN:CB	2.87	0.49
3:D:188:ALA:N	3:D:189:MET:HB2	2.28	0.49
6:T:13:DG:H2"	6:T:14:DA:C8	2.46	0.49
1:A:1093:ILE:CG1	1:A:1096:GLN:HG2	2.42	0.49
1:A:511:HIS:CD2	6:T:18:DC:P	3.05	0.49
1:A:98:THR:CG2	1:A:523:THR:O	2.61	0.49
6:T:12:DG:C4	6:T:13:DG:N7	2.81	0.49
6:T:17:DC:C4	6:T:18:DC:N4	2.80	0.49
1:A:405:ASP:HB2	1:A:557:LEU:HB2	1.94	0.49
2:B:176:ARG:CB	2:B:361:VAL:HG12	2.41	0.49
5:P:22:DA:C2	6:T:17:DC:O2	2.66	0.49
1:A:1080:TYR:C	1:A:1082:ARG:CG	2.76	0.49
1:A:1105:LEU:HD22	1:A:1136:VAL:HG22	1.94	0.49
1:A:38:ALA:HA	1:A:62:ILE:HG23	1.93	0.49
1:A:819:GLY:O	1:A:853:ARG:NH2	2.46	0.49
2:B:283:LEU:O	2:B:316:GLU:HA	2.13	0.49
1:A:944:TRP:CE3	1:A:945:PRO:CD	2.96	0.49
1:A:977:VAL:HG12	1:A:980:VAL:CG1	2.41	0.49
4:E:541:LEU:HA	4:E:599:PRO:HG2	1.95	0.48
1:A:1048:LEU:CD1	1:A:1050:VAL:HG13	2.42	0.48
1:A:964:HIS:H	1:A:970:LEU:HD21	1.77	0.48
2:C:134:THR:HG23	2:C:182:MET:HE2	1.95	0.48
1:A:1018:THR:HA	1:A:1025:ARG:HA	1.94	0.48
1:A:351:SER:HB2	1:A:356:VAL:HB	1.95	0.48
1:A:564:ILE:HG23	1:A:785:ALA:HB3	1.95	0.48
1:A:804:CYS:HB3	1:A:809:LEU:HD13	1.94	0.48
1:A:25:ALA:HB3	1:A:26:PRO:HD3	1.95	0.48
1:A:944:TRP:CE2	1:A:947:GLN:OE1	2.67	0.48
1:A:959:LEU:O	1:A:960:TYR:CD1	2.67	0.48
1:A:510:LYS:HB2	6:T:17:DC:H4'	1.96	0.48
1:A:1040:GLN:HG3	1:A:1043:GLU:OE2	2.14	0.48
1:A:86:VAL:HG13	1:A:130:LEU:HD23	1.94	0.48
1:A:966:ILE:HG23	1:A:970:LEU:CA	2.37	0.48
2:C:321:VAL:HG22	2:C:325:LEU:HD22	1.96	0.48
5:P:21:DG:C2	5:P:22:DA:C4	3.01	0.48
1:A:1020:ASP:HB2	1:A:1021:ASP:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLY:C	1:A:1063:LEU:HD12	2.34	0.48
1:A:1080:TYR:O	1:A:1082:ARG:CB	2.59	0.48
2:C:24:ARG:O	2:C:24:ARG:HG2	2.14	0.48
4:E:521:ASP:OD2	4:E:599:PRO:HB3	2.14	0.48
1:A:1021:ASP:O	1:A:1023:SER:N	2.46	0.48
3:D:9:ILE:HG12	3:D:93:ALA:HB1	1.96	0.48
4:E:527:VAL:HG21	4:E:540:ALA:HB1	1.96	0.48
1:A:954:ARG:O	1:A:958:GLY:N	2.45	0.48
3:D:16:THR:HG23	3:D:31:ILE:HG21	1.95	0.48
5:P:17:DG:C2	6:T:22:DG:N2	2.82	0.48
1:A:1015:GLY:O	1:A:1027:GLU:OE1	2.32	0.48
1:A:1019:LEU:HD13	1:A:1026:LEU:CD1	2.44	0.48
1:A:1044:LYS:O	1:A:1047:ILE:O	2.32	0.47
1:A:289:GLU:O	1:A:293:VAL:HG23	2.13	0.47
2:C:284:TYR:O	2:C:290:LEU:HD12	2.14	0.47
6:T:18:DC:H2"	6:T:19:DT:C6	2.49	0.47
2:B:286:SER:HA	2:B:314:GLU:HG2	1.96	0.47
2:C:144:PHE:CE1	2:C:330:ALA:CB	2.97	0.47
3:D:61:GLU:O	3:D:65:VAL:HG23	2.14	0.47
4:E:514:ALA:HB2	4:E:603:ARG:NH2	2.29	0.47
1:A:1048:LEU:HD13	1:A:1049:ILE:N	2.29	0.47
2:C:273:LEU:HD23	2:C:301:GLU:O	2.14	0.47
1:A:1028:VAL:HA	1:A:1029:MET:HG2	1.94	0.47
1:A:1093:ILE:CD1	1:A:1096:GLN:HG2	2.44	0.47
1:A:650:ASN:O	1:A:654:ARG:HG3	2.14	0.47
1:A:1130:PHE:CE2	1:A:1132:ALA:HB3	2.49	0.47
1:A:429:GLN:HE22	1:A:536:HIS:HA	1.80	0.47
1:A:557:LEU:HD21	1:A:559:LEU:CD1	2.44	0.47
1:A:557:LEU:HD23	1:A:557:LEU:C	2.35	0.47
5:P:20:DG:C1'	5:P:21:DG:N7	2.78	0.47
1:A:100:LEU:HG	1:A:124:LEU:HD23	1.96	0.47
2:C:128:PHE:HE1	2:C:218:ILE:HD11	1.79	0.47
1:A:668:TRP:HA	1:A:740:LEU:HD12	1.96	0.47
2:B:347:VAL:O	2:B:360:VAL:HA	2.15	0.47
5:P:20:DG:C5	5:P:21:DG:C6	3.03	0.47
1:A:1084:LEU:C	1:A:1154:GLN:HE22	2.17	0.47
1:A:639:ARG:NH2	1:A:754:TYR:O	2.36	0.47
1:A:835:ILE:CG2	1:A:846:ILE:HB	2.45	0.47
1:A:1047:ILE:O	1:A:1048:LEU:HB2	2.14	0.47
1:A:835:ILE:HG12	1:A:846:ILE:HG22	1.97	0.47
1:A:1006:MET:SD	2:C:24:ARG:HD3	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:PRO:HG2	1:A:1059:PHE:CZ	2.50	0.46
2:C:4:THR:HB	2:C:61:GLN:HB2	1.97	0.46
1:A:838:ILE:CG2	1:A:841:VAL:HB	2.45	0.46
1:A:966:ILE:CG1	1:A:969:TYR:CD2	2.98	0.46
2:B:366:LEU:C	3:D:41:ARG:HE	2.18	0.46
3:D:31:ILE:HD12	3:D:68:ILE:HG21	1.98	0.46
6:T:12:DG:C6	6:T:13:DG:O6	2.68	0.46
1:A:1034:ALA:O	1:A:1035:LEU:HD12	2.16	0.46
1:A:1078:GLU:HA	1:A:1113:ILE:HD11	1.98	0.46
1:A:557:LEU:HD21	1:A:559:LEU:HG	1.96	0.46
2:B:295:ASN:HD21	3:D:42:ARG:HH22	1.61	0.46
1:A:1048:LEU:HD13	1:A:1048:LEU:C	2.36	0.46
2:B:61:GLN:HB3	2:B:62:PRO:CD	2.45	0.46
1:A:1036:ASP:CG	2:C:28:PRO:HB2	2.36	0.46
5:P:20:DG:C2'	5:P:21:DG:N7	2.78	0.46
1:A:288:THR:HG22	1:A:338:PRO:HB2	1.97	0.46
1:A:409:GLU:OE1	1:A:563:THR:HG23	2.16	0.46
1:A:558:GLY:O	1:A:559:LEU:HG	2.16	0.46
2:B:129:THR:HG22	2:B:215:ARG:CB	2.46	0.46
2:C:159:LEU:HB2	2:C:241:PHE:CD1	2.51	0.46
2:C:52:GLU:N	2:C:233:THR:O	2.47	0.46
4:E:564:ASN:ND2	4:E:588:ILE:HB	2.30	0.46
1:A:1119:TYR:CD1	4:E:618:ILE:HD11	2.50	0.46
1:A:407:CYS:SG	1:A:562:LEU:HB2	2.56	0.46
1:A:841:VAL:HG12	1:A:842:GLY:O	2.15	0.46
1:A:919:GLY:O	1:A:920:GLN:C	2.55	0.46
2:B:317:ILE:HD12	2:B:343:SER:HA	1.98	0.46
1:A:34:LEU:HD12	1:A:240:MET:HE1	1.97	0.45
2:B:317:ILE:HD11	2:B:363:PRO:HB3	1.97	0.45
6:T:20:DT:C5	6:T:21:DC:N4	2.84	0.45
1:A:455:PHE:CA	1:A:1060:SER:OG	2.63	0.45
1:A:458:ARG:HA	1:A:461:LYS:HE3	1.98	0.45
1:A:918:ILE:CG2	1:A:920:GLN:HB2	2.46	0.45
1:A:954:ARG:C	1:A:959:LEU:H	2.11	0.45
2:C:159:LEU:HD22	2:C:241:PHE:CG	2.51	0.45
1:A:782:PHE:O	1:A:786:VAL:HG23	2.17	0.45
1:A:825:VAL:HG23	1:A:825:VAL:O	2.16	0.45
2:B:10:LEU:O	2:B:14:LEU:HB2	2.15	0.45
1:A:1095:ASP:O	1:A:1099:ASN:HB3	2.17	0.45
1:A:966:ILE:O	1:A:970:LEU:N	2.50	0.45
1:A:354:ASN:HB2	1:A:413:GLN:HE22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:THR:HG23	1:A:839:LYS:HD3	1.98	0.45
2:B:214:LEU:HD13	2:B:227:VAL:CG2	2.45	0.45
2:B:45:THR:HG23	2:B:52:GLU:HG3	1.99	0.45
4:E:600:LEU:C	4:E:600:LEU:HD23	2.37	0.45
5:P:14:DG:N2	6:T:25:DC:O2	2.49	0.45
1:A:324:ARG:HD2	1:A:328:GLU:OE2	2.17	0.45
3:D:240:LEU:C	3:D:243:ALA:N	2.69	0.45
1:A:983:LYS:HZ3	1:A:1063:LEU:HD11	1.82	0.45
1:A:969:TYR:OH	1:A:1082:ARG:HD2	2.17	0.45
3:D:7:ARG:NH1	3:D:93:ALA:HB2	2.31	0.45
1:A:1016:ILE:HD13	1:A:1027:GLU:OE1	2.16	0.45
1:A:1048:LEU:HD11	1:A:1050:VAL:HG22	1.98	0.45
1:A:1081:ALA:HB3	1:A:1159:PHE:HB2	1.98	0.45
6:T:16:DT:C6	6:T:17:DC:C5	3.04	0.45
6:T:17:DC:H2'	6:T:18:DC:C5	2.49	0.45
1:A:1048:LEU:HD13	1:A:1049:ILE:CA	2.47	0.44
1:A:527:PRO:HD3	1:A:541:PHE:CZ	2.51	0.44
1:A:797:VAL:O	1:A:801:VAL:HG13	2.16	0.44
2:B:174:GLY:HA2	3:D:185:LEU:HD12	2.00	0.44
2:C:197:ARG:O	2:C:201:ILE:HG12	2.16	0.44
1:A:944:TRP:CE3	1:A:945:PRO:HD2	2.52	0.44
1:A:366:ALA:HB1	1:A:379:LEU:HD12	2.00	0.44
5:P:18:DA:OP2	5:P:18:DA:H8	2.00	0.44
1:A:1040:GLN:HG2	1:A:1043:GLU:CD	2.37	0.44
1:A:1098:LEU:O	1:A:1099:ASN:HB2	2.17	0.44
1:A:96:ASN:HD21	1:A:126:GLU:HB2	1.81	0.44
1:A:999:LEU:HD12	1:A:1018:THR:HG23	1.98	0.44
1:A:999:LEU:HD13	1:A:1000:VAL:N	2.33	0.44
2:C:42:LEU:HB3	2:C:57:VAL:HG13	1.99	0.44
5:P:20:DG:N3	5:P:21:DG:C6	2.85	0.44
1:A:76:LEU:HD21	1:A:153:GLU:CB	2.47	0.44
1:A:318:ARG:NH1	1:A:322:ASP:OD2	2.50	0.44
1:A:822:HIS:CD2	1:A:823:PHE:CD1	3.06	0.44
1:A:960:TYR:CE2	1:A:976:TYR:HD2	2.35	0.44
4:E:507:PRO:O	4:E:509:LEU:CA	2.63	0.44
1:A:1053:GLN:HE22	3:D:157:SER:HB2	1.83	0.44
1:A:429:GLN:O	1:A:538:VAL:HA	2.18	0.44
3:D:23:ALA:HB3	3:D:26:GLU:HB2	2.00	0.44
1:A:1080:TYR:CB	1:A:1082:ARG:NE	2.80	0.44
1:A:801:VAL:O	1:A:805:TRP:CD1	2.70	0.44
2:B:175:HIS:HA	2:B:362:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LEU:HD13	2:B:182:MET:HG3	2.00	0.44
1:A:1057:ASP:HB2	1:A:1064:LYS:HG2	2.00	0.43
1:A:76:LEU:HD13	1:A:154:CYS:SG	2.57	0.43
3:D:12:ASP:O	3:D:164:ALA:HB1	2.18	0.43
3:D:16:THR:HG23	3:D:31:ILE:HG23	2.00	0.43
2:C:122:TRP:CD2	2:C:222:ASN:HB2	2.53	0.43
1:A:63:LYS:HG3	3:D:228:ARG:HG3	2.00	0.43
5:P:20:DG:N2	5:P:21:DG:C2	2.86	0.43
1:A:1111:GLY:O	1:A:1113:ILE:N	2.52	0.43
1:A:429:GLN:CB	1:A:538:VAL:HG12	2.44	0.43
1:A:918:ILE:C	1:A:920:GLN:N	2.69	0.43
2:C:160:PHE:O	2:C:192:SER:HA	2.18	0.43
1:A:1080:TYR:HB2	1:A:1082:ARG:NH1	2.29	0.43
1:A:100:LEU:HD22	1:A:116:ILE:HG21	1.98	0.43
5:P:20:DG:C1'	5:P:21:DG:C8	3.01	0.43
1:A:1048:LEU:CD2	1:A:1050:VAL:HG13	2.46	0.43
1:A:72:VAL:O	1:A:81:LEU:HA	2.19	0.43
2:B:264:LYS:HG3	2:B:328:LEU:HB3	2.00	0.43
2:C:214:LEU:HD13	2:C:227:VAL:CG2	2.48	0.43
1:A:343:ILE:HG12	1:A:422:TYR:OH	2.19	0.43
1:A:335:MET:SD	1:A:392:LEU:HD11	2.58	0.43
1:A:564:ILE:HD11	1:A:789:ALA:CB	2.40	0.43
1:A:576:ARG:O	1:A:580:GLY:N	2.51	0.43
2:B:29:ILE:CD1	2:B:69:THR:HG21	2.48	0.43
1:A:558:GLY:C	6:T:15:DG:H4'	2.39	0.43
1:A:944:TRP:CD1	1:A:947:GLN:NE2	2.87	0.43
2:B:130:LEU:N	2:B:130:LEU:HD23	2.34	0.43
2:B:290:LEU:HB3	2:B:306:LEU:HG	2.01	0.43
2:B:305:ILE:HB	2:C:103:ARG:HB2	2.00	0.43
2:C:160:PHE:CE2	2:C:169:THR:HG22	2.53	0.43
2:C:88:ILE:HD12	2:C:99:VAL:CG1	2.49	0.43
2:B:364:MET:HE3	3:D:182:GLN:HB2	2.01	0.43
1:A:1009:LYS:HZ3	2:B:274:SER:HG	1.55	0.43
1:A:237:GLN:HE21	1:A:241:ARG:HH22	1.66	0.43
1:A:318:ARG:N	1:A:319:PRO:HD2	2.34	0.43
1:A:517:ILE:HD12	1:A:554:PHE:CE2	2.53	0.43
2:B:294:ALA:O	2:B:301:GLU:HA	2.19	0.43
6:T:16:DT:C5	6:T:17:DC:C4	3.07	0.43
1:A:966:ILE:O	1:A:966:ILE:HG23	2.19	0.43
1:A:1032:THR:HG21	1:A:1039:GLN:CG	2.48	0.42
1:A:1088:LEU:HD13	1:A:1092:GLN:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TYR:O	1:A:537:PRO:HA	2.19	0.42
1:A:844:GLY:O	1:A:847:GLU:HG2	2.18	0.42
2:C:17:VAL:HG22	2:C:53:MET:CG	2.49	0.42
1:A:999:LEU:HB3	1:A:1018:THR:CG2	2.48	0.42
2:B:223:ILE:O	2:B:233:THR:HA	2.20	0.42
1:A:1077:ARG:HD2	1:A:1141:ARG:HB2	2.01	0.42
1:A:325:LEU:HD12	1:A:370:VAL:HG22	2.01	0.42
2:B:363:PRO:HD2	3:D:183:LEU:HD12	2.01	0.42
2:B:24:ARG:NH2	6:T:28:DG:OP2	2.52	0.42
3:D:30:ILE:HG22	3:D:52:LEU:HD12	2.02	0.42
1:A:838:ILE:HG21	1:A:841:VAL:CG2	2.49	0.42
1:A:924:PHE:HD1	1:A:925:GLY:N	2.14	0.42
1:A:455:PHE:N	1:A:1060:SER:CB	2.82	0.42
1:A:73:GLN:O	1:A:117:ASP:HA	2.20	0.42
1:A:977:VAL:HB	1:A:981:ARG:HB3	1.91	0.42
1:A:1007:VAL:CG1	2:B:276:GLU:HB3	2.46	0.42
1:A:997:ALA:CB	1:A:1048:LEU:HB3	2.50	0.42
2:B:162:THR:HG22	2:B:167:LEU:HG	2.02	0.42
1:A:351:SER:CB	1:A:356:VAL:HB	2.49	0.42
1:A:359:GLY:HA3	1:A:557:LEU:HD13	2.02	0.42
1:A:668:TRP:HA	1:A:740:LEU:CD1	2.50	0.42
1:A:835:ILE:HD11	1:A:849:ILE:HD12	2.01	0.42
2:B:49:LEU:HD11	2:B:117:PRO:HG2	2.01	0.42
1:A:1027:GLU:O	1:A:1029:MET:HG2	2.20	0.42
1:A:109:TYR:HB3	1:A:114:PRO:HA	2.01	0.42
1:A:204:PHE:O	1:A:239:TYR:HA	2.20	0.42
1:A:362:ARG:NE	1:A:376:ILE:O	2.38	0.42
1:A:668:TRP:CE2	1:A:743:LYS:HG2	2.55	0.42
3:D:97:ILE:HG21	3:D:103:ASP:HB2	2.01	0.42
1:A:88:ALA:HA	1:A:128:LEU:HD23	2.02	0.42
1:A:512:ALA:HB1	1:A:556:PHE:CE1	2.55	0.42
3:D:240:LEU:HD23	3:D:243:ALA:CB	2.49	0.42
1:A:1078:GLU:OE1	1:A:1082:ARG:NH2	2.53	0.41
1:A:557:LEU:HD23	1:A:558:GLY:N	2.35	0.41
1:A:572:ILE:O	1:A:575:ARG:HB2	2.19	0.41
1:A:66:VAL:HG21	1:A:269:VAL:HG11	2.00	0.41
1:A:960:TYR:CD1	1:A:964:HIS:ND1	2.88	0.41
2:C:129:THR:HG22	2:C:215:ARG:HA	2.01	0.41
5:P:21:DG:N1	5:P:22:DA:C6	2.88	0.41
1:A:1064:LYS:HA	1:A:1064:LYS:HD3	1.82	0.41
2:B:122:TRP:CE2	2:B:222:ASN:CB	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:4:DG:N2	6:T:35:DT:O2	2.53	0.41
1:A:1073:ILE:HD13	1:A:1073:ILE:O	2.19	0.41
1:A:330:GLN:O	1:A:334:GLN:HG3	2.20	0.41
1:A:459:ILE:HG23	1:A:484:ILE:HD11	2.01	0.41
1:A:958:GLY:O	1:A:959:LEU:C	2.58	0.41
2:B:331:LEU:HD23	2:B:336:VAL:CG2	2.51	0.41
1:A:1077:ARG:HD2	1:A:1141:ARG:CB	2.50	0.41
1:A:276:TYR:HA	1:A:550:GLY:O	2.21	0.41
1:A:346:GLU:OE1	1:A:417:HIS:HE1	2.04	0.41
1:A:944:TRP:CE3	1:A:945:PRO:HG2	2.56	0.41
2:B:144:PHE:CE2	2:B:327:VAL:HG12	2.55	0.41
5:P:13:DG:N2	6:T:26:DT:O2	2.53	0.41
1:A:1005:VAL:HG12	1:A:1006:MET:H	1.85	0.41
1:A:1093:ILE:HG13	1:A:1095:ASP:H	1.85	0.41
1:A:76:LEU:HD22	1:A:150:LEU:CD1	2.43	0.41
1:A:814:PRO:HG3	1:A:833:TYR:CD2	2.55	0.41
1:A:458:ARG:CD	1:A:983:LYS:HE3	2.51	0.41
1:A:997:ALA:HB3	1:A:1048:LEU:HD12	2.02	0.41
1:A:944:TRP:CD2	1:A:947:GLN:CD	2.94	0.41
2:B:184:ILE:HD13	2:B:188:LEU:HD21	2.02	0.41
6:T:16:DT:N1	6:T:17:DC:C5	2.89	0.41
1:A:1037:LYS:O	1:A:1041:LEU:HG	2.21	0.41
1:A:742:MET:HA	1:A:742:MET:CE	2.51	0.41
2:B:24:ARG:O	2:B:26:THR:N	2.54	0.41
1:A:1078:GLU:N	1:A:1138:PRO:HB3	2.35	0.41
1:A:1079:LYS:HG2	1:A:1082:ARG:HB3	1.97	0.41
1:A:1093:ILE:O	1:A:1094:ASP:CB	2.69	0.41
1:A:1117:LEU:HD13	1:A:1118:TYR:C	2.42	0.41
1:A:811:ILE:HG22	1:A:811:ILE:O	2.20	0.41
2:B:324:VAL:O	2:B:328:LEU:HD22	2.21	0.41
2:C:17:VAL:HG13	2:C:53:MET:HB3	2.03	0.41
4:E:598:THR:HB	4:E:599:PRO:HD2	2.02	0.41
1:A:865:LEU:O	1:A:869:THR:HG22	2.21	0.41
1:A:977:VAL:CG2	1:A:981:ARG:HD3	2.50	0.41
1:A:1027:GLU:HB2	1:A:1029:MET:CE	2.52	0.40
1:A:614:ARG:HG2	1:A:614:ARG:NH1	2.31	0.40
1:A:847:GLU:HA	1:A:850:ILE:HG12	2.04	0.40
1:A:924:PHE:CD1	1:A:925:GLY:N	2.89	0.40
2:C:18:SER:HA	2:C:21:LEU:HD22	2.03	0.40
1:A:92:THR:HG21	1:A:126:GLU:HB3	2.03	0.40
1:A:357:PRO:HG2	1:A:566:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:LEU:HD22	2:C:241:PHE:CD2	2.56	0.40
2:C:98:LEU:HA	2:C:106:PHE:O	2.22	0.40
1:A:1078:GLU:O	1:A:1079:LYS:C	2.59	0.40
1:A:1101:LEU:HD13	1:A:1101:LEU:C	2.41	0.40
1:A:969:TYR:C	1:A:970:LEU:O	2.56	0.40
1:A:978:GLY:O	1:A:982:LEU:HG	2.21	0.40
1:A:976:TYR:HD1	1:A:976:TYR:O	2.04	0.40
3:D:52:LEU:O	3:D:73:LEU:HB3	2.22	0.40
5:P:22:DA:C2'	5:P:23:DC:C5	2.91	0.40
1:A:1093:ILE:HD12	1:A:1095:ASP:HB2	2.04	0.40
1:A:687:GLN:NE2	1:A:755:GLY:O	2.46	0.40
2:B:138:LEU:HD13	2:B:182:MET:CG	2.52	0.40
3:D:30:ILE:HD12	3:D:110:GLU:HG3	2.04	0.40
4:E:556:LEU:HD22	4:E:564:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	A	1141/1160 (98%)	1028 (90%)	70 (6%)	43 (4%)	4	37
2	B	364/366 (100%)	338 (93%)	21 (6%)	5 (1%)	14	58
2	C	364/366 (100%)	339 (93%)	19 (5%)	6 (2%)	12	56
3	D	215/243 (88%)	199 (93%)	14 (6%)	2 (1%)	21	67
4	E	115/144 (80%)	108 (94%)	5 (4%)	2 (2%)	11	55
All	All	2199/2279 (96%)	2012 (92%)	129 (6%)	58 (3%)	11	45

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	279	PRO
1	A	280	GLN
1	A	466	ASP
1	A	576	ARG
1	A	811	ILE
1	A	919	GLY
1	A	920	GLN
1	A	945	PRO
1	A	959	LEU
1	A	970	LEU
1	A	974	GLU
1	A	997	ALA
1	A	1013	ARG
1	A	1021	ASP
1	A	1029	MET
1	A	1030	LEU
1	A	1031	PHE
1	A	1032	THR
1	A	1034	ALA
1	A	1035	LEU
1	A	1043	GLU
1	A	1046	ARG
1	A	1080	TYR
1	A	1094	ASP
1	A	1099	ASN
1	A	1112	THR
2	C	239	GLY
4	E	508	GLU
1	A	281	PHE
1	A	924	PHE
1	A	1131	GLY
2	B	23	GLY
2	C	19	GLY
2	C	153	TYR
2	C	208	ASP
2	C	209	GLY
4	E	533	PRO
1	A	1007	VAL
1	A	1009	LYS
1	A	1045	ASP
1	A	1081	ALA
1	A	1133	THR

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Mol	Chain	Res	Type
2	B	102	GLY
2	B	287	GLU
3	D	212	LEU
1	A	400	PRO
1	A	966	ILE
3	D	67	GLY
2	B	343	SER
1	A	717	PRO
2	C	189	PRO
1	A	958	GLY
1	A	1111	GLY
1	A	1047	ILE
1	A	926	VAL
2	B	22	GLY
1	A	337	PHE

### 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 PDB entries followed by that with respect to all EM entries.

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	
1	A	952/965 (99%)	860 (90%)	92 (10%)	10	40
2	B	313/313 (100%)	268 (86%)	45 (14%)	4	25
2	C	313/313 (100%)	261 (83%)	52 (17%)	3	19
3	D	180/200 (90%)	170 (94%)	10 (6%)	26	62
4	E	97/122 (80%)	84 (87%)	13 (13%)	5	27
All	All	1855/1913 (97%)	1643 (89%)	212 (11%)	11	33

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	7	VAL
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	39	LEU
1	A	75	ASP
1	A	84	LEU
1	A	90	ASN
1	A	99	LEU
1	A	100	LEU
1	A	123	GLU
1	A	124	LEU
1	A	144	LEU
1	A	145	ARG
1	A	147	ASN
1	A	155	VAL
1	A	188	LEU
1	A	216	ARG
1	A	224	THR
1	A	225	LEU
1	A	249	LEU
1	A	262	GLU
1	A	285	ASP
1	A	287	SER
1	A	298	GLU
1	A	329	LEU
1	A	342	LEU
1	A	345	MET
1	A	351	SER
1	A	369	LEU
1	A	399	MET
1	A	408	MET
1	A	414	VAL
1	A	418	VAL
1	A	421	MET
1	A	435	THR
1	A	443	ARG
1	A	458	ARG
1	A	481	LEU
1	A	497	MET
1	A	546	VAL
1	A	571	MET
1	A	578	LYS
1	A	594	LYS
1	A	603	SER
1	A	613	SER

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Mol	Chain	Res	Type
1	A	614	ARG
1	A	643	LEU
1	A	654	ARG
1	A	666	VAL
1	A	671	GLU
1	A	697	LEU
1	A	707	MET
1	A	723	GLN
1	A	757	ASN
1	A	774	LEU
1	A	809	LEU
1	A	810	LYS
1	A	811	ILE
1	A	868	ARG
1	A	899	MET
1	A	922	ASP
1	A	944	TRP
1	A	959	LEU
1	A	969	TYR
1	A	970	LEU
1	A	972	GLU
1	A	974	GLU
1	A	976	TYR
1	A	999	LEU
1	A	1004	ARG
1	A	1005	VAL
1	A	1006	MET
1	A	1008	THR
1	A	1010	ARG
1	A	1013	ARG
1	A	1014	ILE
1	A	1017	CYS
1	A	1019	LEU
1	A	1020	ASP
1	A	1023	SER
1	A	1025	ARG
1	A	1029	MET
1	A	1030	LEU
1	A	1031	PHE
1	A	1037	LYS
1	A	1043	GLU
1	A	1044	LYS

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Mol	Chain	Res	Type
1	A	1045	ASP
1	A	1073	ILE
1	A	1082	ARG
1	A	1128	LEU
2	B	5	VAL
2	B	24	ARG
2	B	26	THR
2	B	42	LEU
2	B	49	LEU
2	B	59	LEU
2	B	70	VAL
2	B	88	ILE
2	B	100	ARG
2	B	103	ARG
2	B	104	SER
2	B	111	LEU
2	B	123	GLN
2	B	125	GLU
2	B	137	ARG
2	B	138	LEU
2	B	143	GLN
2	B	148	HIS
2	B	167	LEU
2	B	170	VAL
2	B	176	ARG
2	B	177	LEU
2	B	188	LEU
2	B	191	HIS
2	B	195	VAL
2	B	207	LEU
2	B	216	VAL
2	B	226	HIS
2	B	233	THR
2	B	236	LEU
2	B	237	VAL
2	B	257	GLU
2	B	273	LEU
2	B	289	GLN
2	B	306	LEU
2	B	308	VAL
2	B	319	PHE
2	B	325	LEU

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Mol	Chain	Res	Type
2	B	327	VAL
2	B	328	LEU
2	B	331	LEU
2	B	332	LYS
2	B	338	MET
2	B	354	SER
2	B	366	LEU
2	C	5	VAL
2	C	24	ARG
2	C	27	LEU
2	C	29	ILE
2	C	42	LEU
2	C	49	LEU
2	C	57	VAL
2	C	59	LEU
2	C	88	ILE
2	C	103	ARG
2	C	105	ARG
2	C	108	LEU
2	C	110	THR
2	C	111	LEU
2	C	118	ASN
2	C	123	GLN
2	C	126	VAL
2	C	137	ARG
2	C	138	LEU
2	C	142	THR
2	C	151	VAL
2	C	162	THR
2	C	167	LEU
2	C	170	VAL
2	C	176	ARG
2	C	188	LEU
2	C	193	VAL
2	C	197	ARG
2	C	198	LYS
2	C	200	VAL
2	C	203	LEU
2	C	205	ARG
2	C	207	LEU
2	C	211	ASP
2	C	212	ASN

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Mol	Chain	Res	Type
2	C	216	VAL
2	C	233	THR
2	C	236	LEU
2	C	237	VAL
2	C	246	ARG
2	C	248	LEU
2	C	273	LEU
2	C	277	LYS
2	C	281	VAL
2	C	306	LEU
2	C	324	VAL
2	C	325	LEU
2	C	328	LEU
2	C	340	LEU
2	C	355	GLN
2	C	360	VAL
2	C	366	LEU
3	D	13	THR
3	D	16	THR
3	D	53	LYS
3	D	59	ASP
3	D	78	THR
3	D	136	LYS
3	D	157	SER
3	D	189	MET
3	D	211	LYS
3	D	234	LYS
4	E	509	LEU
4	E	557	ARG
4	E	559	SER
4	E	571	LYS
4	E	572	LEU
4	E	576	LEU
4	E	597	ARG
4	E	603	ARG
4	E	609	GLU
4	E	610	LYS
4	E	611	LEU
4	E	613	GLN
4	E	621	ASP

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

Mol	Chain	Res	Type
1	A	90	ASN
1	A	125	ASN
1	A	147	ASN
1	A	220	HIS
1	A	237	GLN
1	A	238	GLN
1	A	413	GLN
1	A	417	HIS
1	A	429	GLN
1	A	511	HIS
1	A	610	GLN
1	A	650	ASN
1	A	692	GLN
1	A	723	GLN
1	A	822	HIS
1	A	824	HIS
1	A	920	GLN
1	A	947	GLN
1	A	1039	GLN
1	A	1053	GLN
2	B	143	GLN
2	B	149	GLN
2	B	156	ASN
2	B	186	GLN
2	B	212	ASN
2	B	275	ASN
2	B	288	ASN
2	B	295	ASN
2	B	348	GLN
2	C	156	ASN
2	C	217	GLN
2	C	355	GLN
3	D	8	GLN
3	D	98	HIS
3	D	169	GLN
3	D	208	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1045:ASP	C	1046:ARG	N	1.14