



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 22, 2018 – 12:03 PM EST

PDB ID : 6F42
EMDB ID: : EMD-4182
Title : RNA Polymerase III closed complex CC1.
Authors : Vorlaender, M.K.; Khatter, H.; Wetzels, R.; Hagen, W.J.H.; Mueller, C.W.
Deposited on : 2017-11-29
Resolution : 5.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

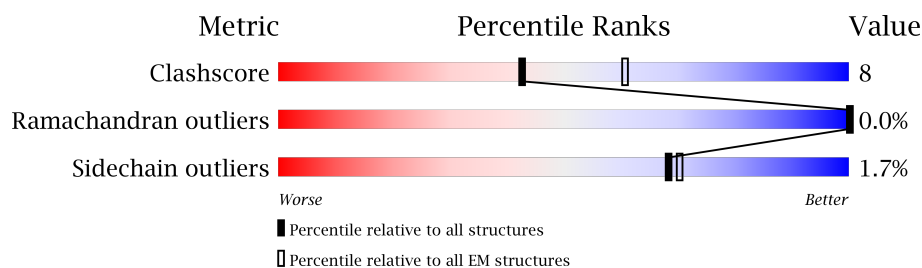
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 ≥ 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	1460	
2	B	1149	
3	C	335	
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	U	240	
19	V	596	
20	W	594	
21	X	81	
22	Y	81	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 45046 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-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10972	6919	1936	2059	58		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	180	Total	C	N	O	S	0	0
			1448	950	231	261	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			255	161	39	49	6		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	159	Total	C	N	O	S	0	0
			1300	835	218	246	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	104	Total	C	N	O	S	0	0
			797	505	143	146	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	534	Total	C	N	O	S	0	0
			4293	2733	736	806	18		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	99	Total	C	N	O	S	0	0
			827	538	127	158	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	35	Total	C	N	O	0	0
			273	181	45	47		

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 19 is a protein called Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	332	Total	C	N	O	S	0	0
			2651	1661	481	495	14		

- Molecule 20 is a protein called Transcription factor TFIIB component B”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	165	Total	C	N	O	S	0	0
			1383	882	245	249	7		

- Molecule 21 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	43	Total	C	N	O	P	0	0
			877	424	146	264	43		

- Molecule 22 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	43	Total	C	N	O	P	0	0
			886	425	166	252	43		

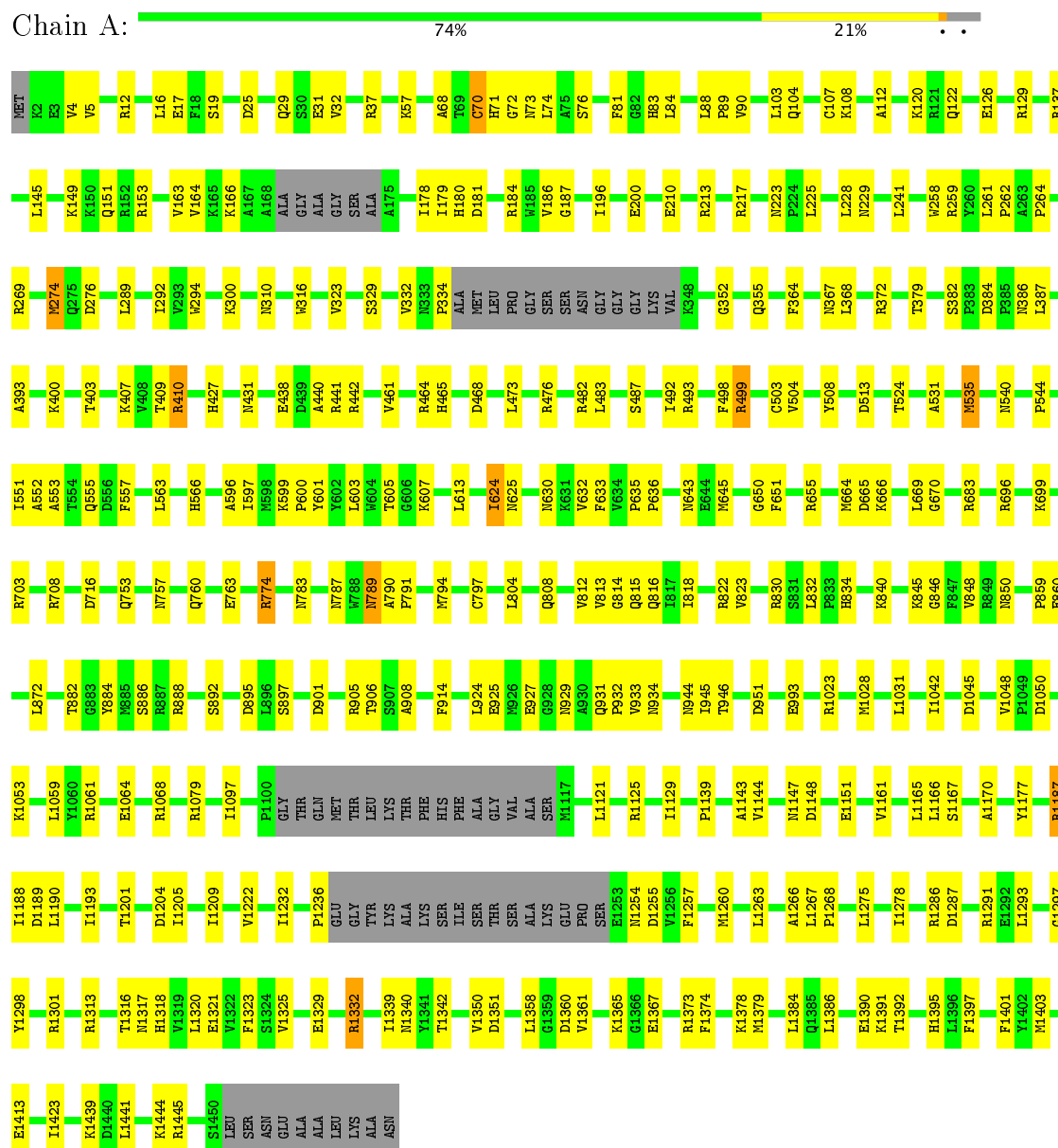
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	J	1	Total	Zn	0
			1	1	
23	B	1	Total	Zn	0
			1	1	
23	I	1	Total	Zn	0
			1	1	
23	V	1	Total	Zn	0
			1	1	
23	A	2	Total	Zn	0
			2	2	
23	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

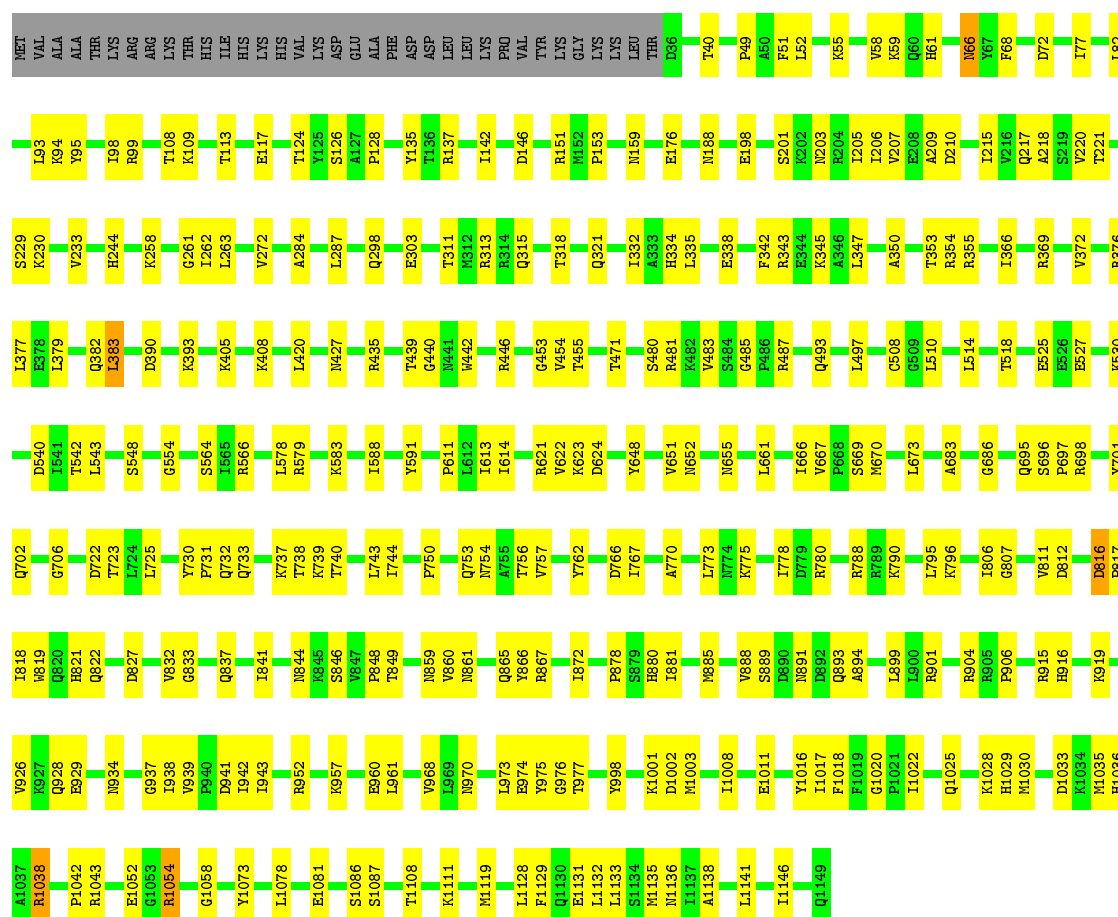
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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-directed RNA polymerase III subunit RPC1

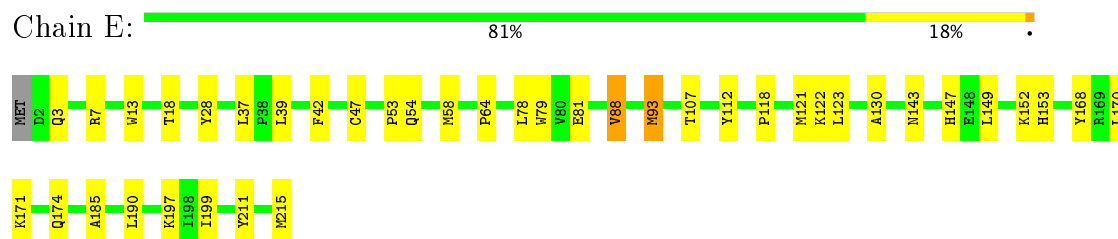


- Molecule 2: DNA-directed RNA polymerase III subunit RPC2

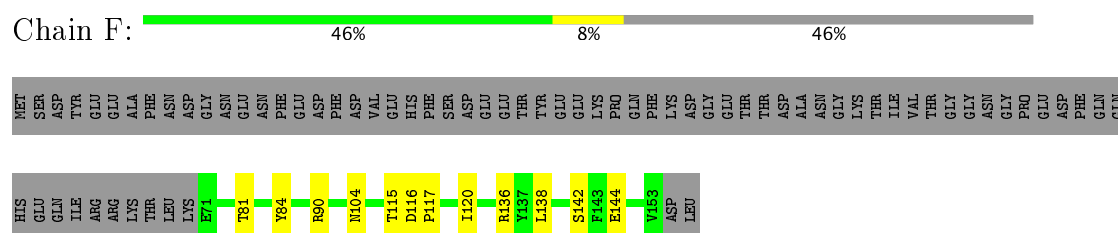
Chain B:  72% 25%



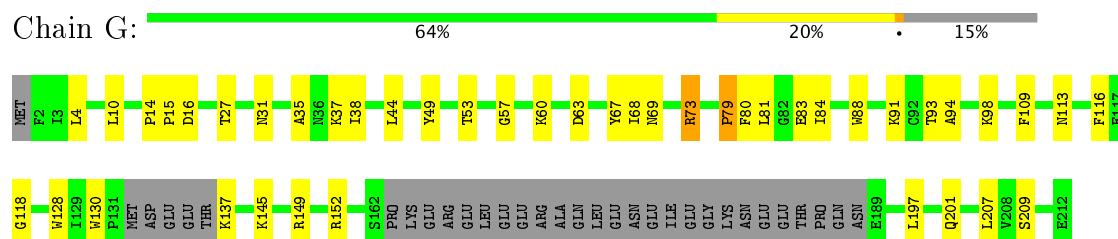
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



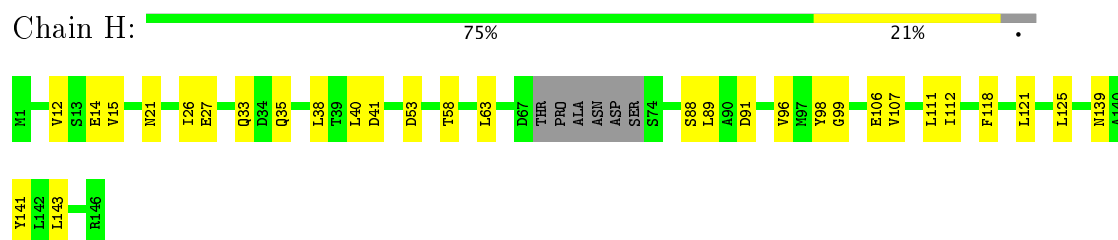
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



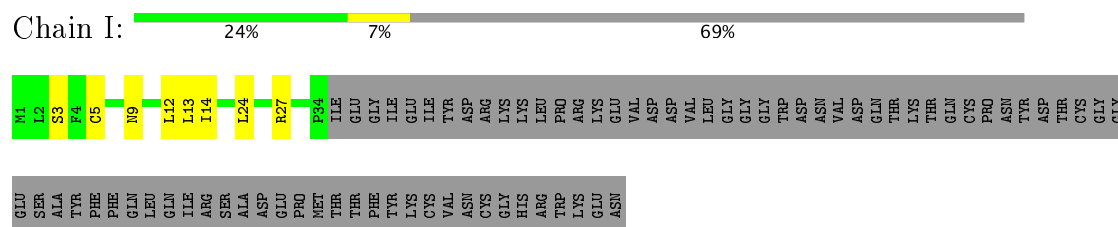
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



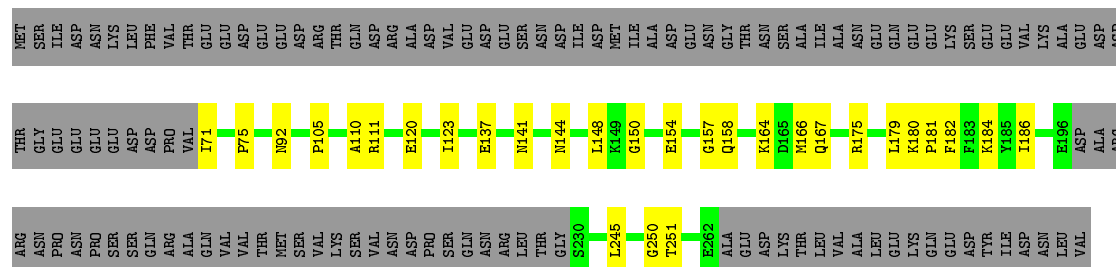
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



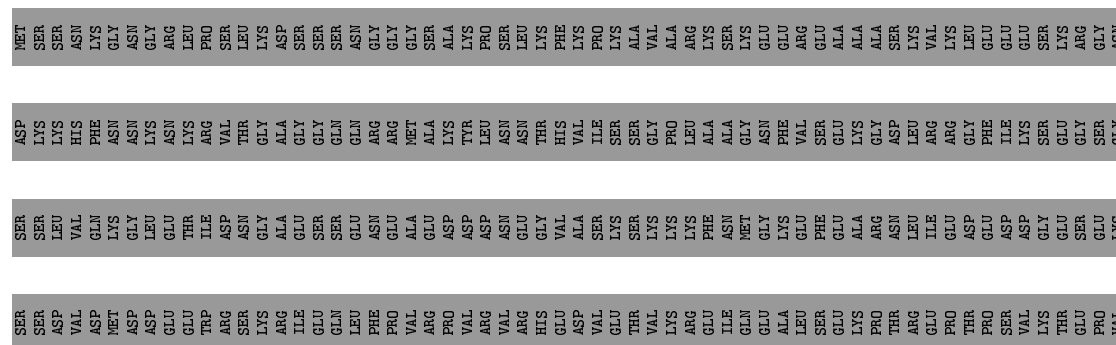
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

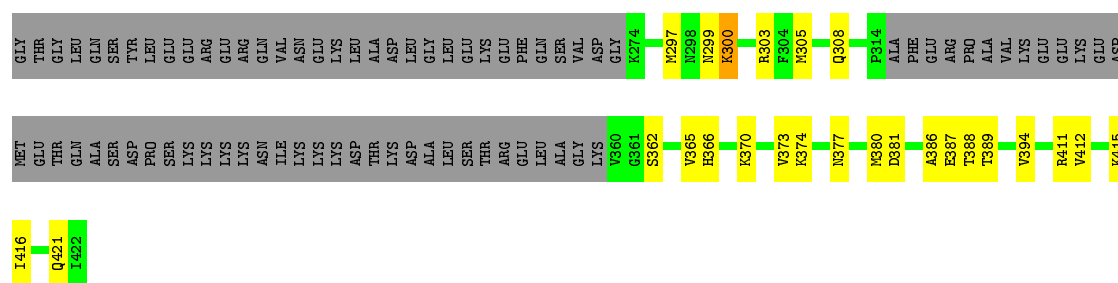


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

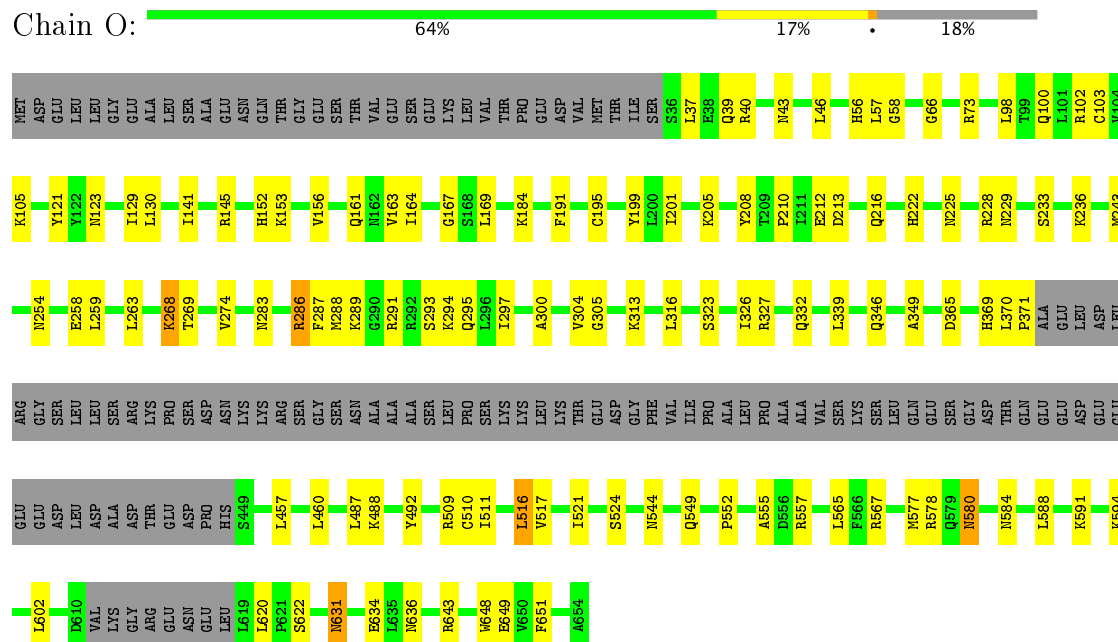


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

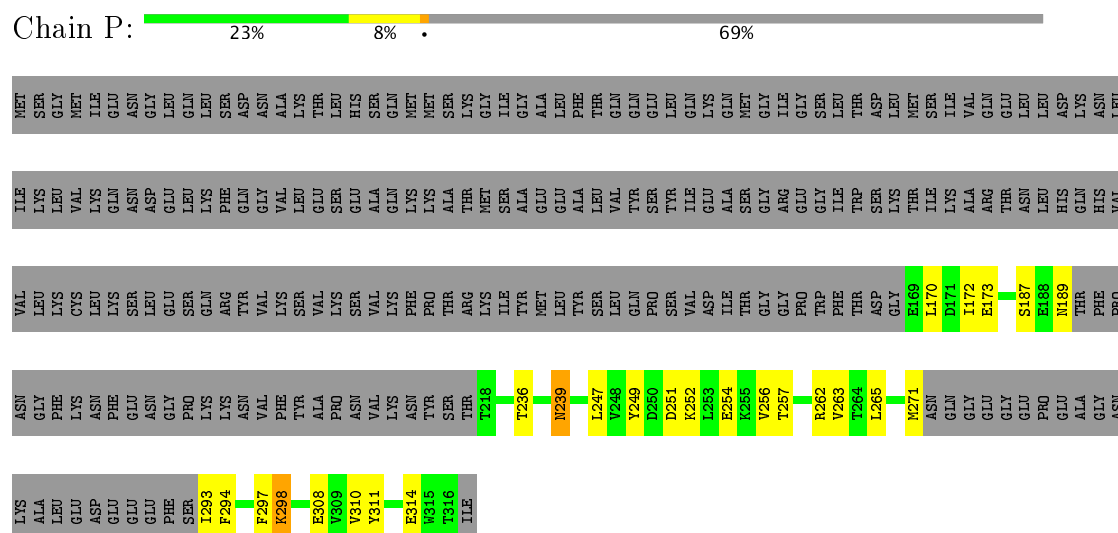




• Molecule 15: DNA-directed RNA polymerase III subunit RPC3



• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

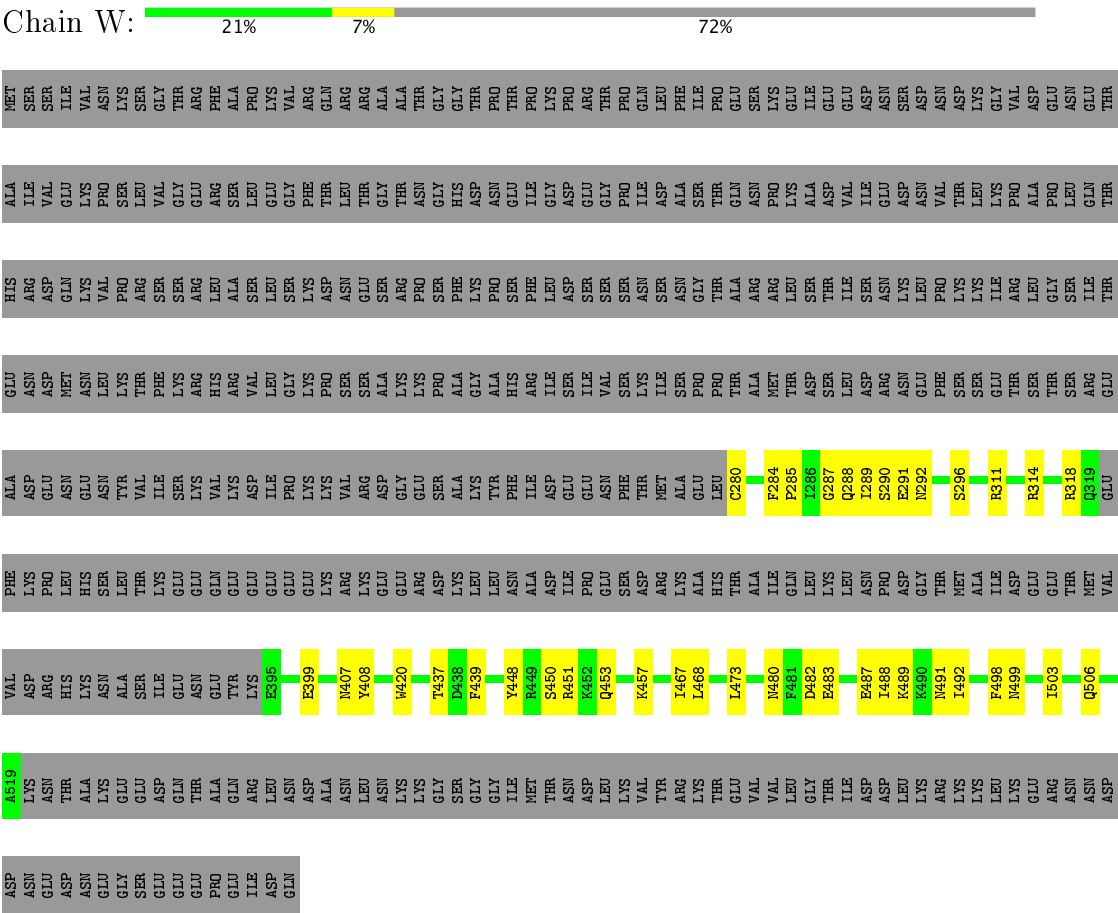


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

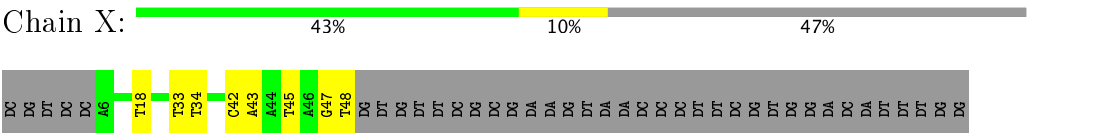
[illegible]

M159	M160	S163	C164	D165	Y185	E186	P187	E188	L189	L193	I194	Y195	R196	M197	P200	K201	I202	V203	L204	Q219	R220	E221	Y224	K239	M240	MET																														
I63	I62	I63	T66	L67	Q68	N69	T73	Y74	T75	T84	L87	H88	A89	R90	E93	Y94	Y94	Y98	Y102	I103	M104	R105	I106	R107	E108	P109	K110	A113	K120	M121	V122	K127	S128	E129	K133	K138	Y139	A140	R141	I142	I143	A149	A150	K151	D154	THR										
ASP	ALA	GLU	GLU	ARG	LEU	LYS	PHE	LYS	GLU	ALA	ASN	LYS	ILE	VAL	PHE	ASP	PRO	ASN	THR	ARG	GLN	VAL	TRP	GLU	ASN	GLN	ASN	ASN	ARG	ASP	GLY	THR	LYS	PRO	ALA	THR	PHE	GLN	SER	GLU	GLU	ASP	ILE	LYS	ARG	ALA	PRO	GLU	SER	GLU	LYS	ASP	THR	SER	ALA	THR

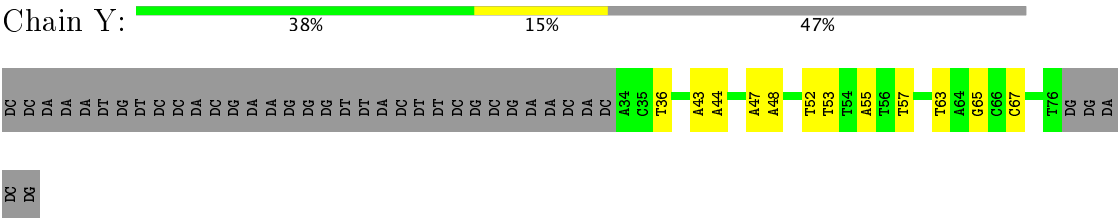
ASP	ASP	ALA	ILE	ILE	LVS	P178	MET
ALA	ASP	ILE	HIS	HIS	GLU	GLU	P2
ILE	PRO	ASP	GLY	GLY	MET	I182	V3
ASP	THR	GLY	THR	THR	PHE	I189	C4
GLY	LVS	SER	GLU	GLU	GLN	D190	K5
LEU	THR	LEU	ASN	ASN	THR	L191	N6
PHE	THR	GLU	ASN	THR	GLU		V30
ARG	ASP	THR	THR	GLU	GLU	S210	
	ALA	ASP	PRO	ARG	ALA	F215	E40
	ALA	THR	LVS	LVS	LEU		VAL
	ALA	C433	ARG	ARG	ASN	R218	THR
	ILE	N441	LEU	LEU	LVS	R219	PHE
	GLY		LEU	ASN	ASN	I223	GLU
	THR	L444	GLU	GLU	PRO	A224	THR
	LEU	L445	VAL	VAL	ILE		ALA
	SER		SER	SER	THR	I228	GLY
	ASP	L452	ILE	ILE	GLN	R233	ALA
	LEU		GLN	GLN	VAL		ALA
	ASP	D458	ASN	ASN	LEU		VAL
	LVS		GLU	GLU	GLY	I237	VAL
	SER	V465	HIS	HIS	GLU	R238	GLN
	GLY		VAL	VAL	GLN	R239	GLY
	LEU	H473	GLU	GLU	GLU		SER
	HIS	L474	GLY	GLY	LEU	T242	PHE
	L475		THR	THR	SER		ILE
	ALA	N476	ASP	ASP	GLU	Q257	GLY
	LEU		LVS	LVS	LVS	R258	ALA
	LVS	A479	GLU	GLU	GLU		GLY
	ALA		THR	THR	VAL	T265	GLN
	ALA	R485	GLU	GLU	VAL	R266	SER
	GLU	T486	GLY	PHE	PHE	A267	HIS
	GLU	N487	THR	THR	THR	A268	ALA
	SER		GLU	LEU	LEU	K269	ALA
	GLY	Q505	GLU	LVS	LVS	V272	PHE
	ASP	GLU	LVS	LVS	GLN	Q273	GLY
	PHE	ALA	VAL	VAL	PHE	Q274	SER
	THR	ASP	LVS	LVS	SER	K274	SER
	THR	ILE	LVS	LVS	GLU	F275	SER
	ALA	ALA	VAL	VAL	ARG		ALA
	ASP	THR	LVS	LVS	ARG	D279	L73
	SER	GLY	THR	THR	ALA		
	VAL	ASN	LVS	LVS	ARG	P287	N115
	LVS	THR	THR	VAL	VAL	P288	
	ASN	SER	SER	VAL	VAL	S289	R135
	MET	VAL	GLU	GLU	GLU	F290	
	GLN	LVS	GLU	ARG	ARG		T139
	LVS	LVS	LVS	LVS	ILE	R294	H140
	ALA	ARG	GLU	GLU	ALA		H141
	SER	THR	ASN	ASN	THR	E297	
	PHE	ARG	GLU	GLU	ASN	ARG	R149
	SER	ARG	SER	SER	GLY	LVS	
	LVS	ARG	GLY	GLY	ILE	ILE	V165
	LVS	ASN	HIS	HIS	ASP	ASP	
	ILE	ASN	PHE	PHE	GLY	SER	I170
	ASN	THR	GLN	GLN	LEU	LEU	P174
	THR	ARG	ASP	ASP	ASN	ASP	



● Molecule 21: Non-template DNA



● Molecule 22: Template DNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.9	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.23	0/11168	0.46	0/15086
10	J	0.23	0/558	0.43	0/750
11	K	0.23	0/803	0.42	0/1083
12	L	0.22	0/360	0.47	0/478
13	M	0.24	0/1331	0.45	0/1800
14	N	0.23	0/805	0.47	0/1081
15	O	0.23	0/4358	0.43	0/5879
16	P	0.24	0/843	0.48	0/1142
17	Q	0.26	0/281	0.45	0/381
18	U	0.25	0/1443	0.46	0/1942
19	V	0.23	0/2693	0.43	0/3628
2	B	0.24	0/8943	0.46	0/12068
20	W	0.24	0/1413	0.42	0/1890
21	X	0.54	0/980	1.09	0/1510
22	Y	0.55	0/996	1.04	0/1535
3	C	0.24	0/2711	0.46	0/3676
4	D	0.24	0/991	0.41	0/1328
5	E	0.23	0/1787	0.44	0/2406
6	F	0.23	0/683	0.41	0/923
7	G	0.24	0/1486	0.43	0/2017
8	H	0.24	0/1138	0.50	0/1540
9	I	0.24	0/261	0.55	0/354
All	All	0.26	0/46032	0.50	0/62497

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	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	CYS	Peptide
2	B	318	THR	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	10972	0	11097	205	0
2	B	8788	0	8904	178	0
3	C	2655	0	2628	50	0
4	D	977	0	983	14	0
5	E	1751	0	1776	23	0
6	F	671	0	692	7	0
7	G	1448	0	1446	31	0
8	H	1120	0	1089	22	0
9	I	255	0	243	5	0
10	J	549	0	559	17	0
11	K	792	0	790	9	0
12	L	358	0	384	15	0
13	M	1300	0	1267	17	0
14	N	797	0	846	16	0
15	O	4293	0	4456	74	0
16	P	827	0	809	18	0
17	Q	273	0	285	4	0
18	U	1416	0	1493	40	0
19	V	2651	0	2673	50	0
20	W	1383	0	1388	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	877	0	493	7	0
22	Y	886	0	487	12	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	V	1	0	0	0	0
All	All	45046	0	44788	727	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 8.

All (727) 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)
15:O:201:ILE:HD13	15:O:283:ASN:HD22	1.46	0.80
2:B:667:VAL:HG12	2:B:669:SER:H	1.47	0.79
15:O:549:GLN:HE21	15:O:567:ARG:HH22	1.31	0.76
3:C:93:GLN:HE21	3:C:96:VAL:HG23	1.52	0.75
2:B:695:GLN:HG2	2:B:697:PRO:HD2	1.67	0.75
3:C:255:VAL:HG21	3:C:273:ASP:HB2	1.70	0.73
3:C:172:GLN:H	3:C:175:GLN:HE21	1.36	0.73
1:A:181:ASP:OD2	1:A:184:ARG:NH2	2.21	0.73
19:V:215:PHE:HB3	19:V:223:ILE:HG21	1.70	0.71
19:V:237:LEU:HB3	20:W:290:SER:HB3	1.71	0.71
1:A:630:ASN:ND2	1:A:650:GLY:O	2.24	0.71
5:E:3:GLN:HE21	5:E:7:ARG:HH22	1.38	0.71
1:A:482:ARG:HD3	1:A:544:PRO:HG3	1.72	0.70
1:A:1441:LEU:HD21	7:G:53:THR:HA	1.73	0.70
1:A:504:VAL:HA	1:A:551:ILE:HD11	1.74	0.69
14:N:366:HIS:HB2	14:N:370:LYS:HB3	1.74	0.69
1:A:151:GLN:NE2	1:A:153:ARG:O	2.24	0.68
16:P:256:VAL:HG22	16:P:257:THR:HG23	1.76	0.68
2:B:818:ILE:H	2:B:821:HIS:HB2	1.59	0.68
2:B:217:GLN:HB2	2:B:233:VAL:HB	1.75	0.68
4:D:129:ALA:H	4:D:157:ILE:HG22	1.59	0.68
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.75	0.67
2:B:888:VAL:HG11	12:L:54:ARG:HH21	1.58	0.67
15:O:591:LYS:HD2	16:P:308:GLU:HG3	1.77	0.67
1:A:757:ASN:HD22	1:A:760:GLN:HE21	1.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:GLN:NE2	2:B:733:GLN:O	2.28	0.66
19:V:257:GLN:OE1	19:V:258:ARG:NH1	2.28	0.66
1:A:599:LYS:HB2	8:H:96:VAL:HG22	1.76	0.66
15:O:293:SER:HB2	15:O:316:LEU:HD11	1.77	0.66
19:V:238:ARG:NH2	20:W:291:GLU:OE2	2.29	0.66
2:B:483:VAL:HG12	2:B:485:GLY:H	1.60	0.66
15:O:39:GLN:O	15:O:43:ASN:ND2	2.28	0.66
13:M:148:LEU:HA	13:M:182:PHE:H	1.61	0.66
18:U:104:MET:HB2	18:U:113:ALA:HB3	1.77	0.66
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.77	0.65
15:O:511:ILE:HG12	15:O:517:VAL:HG11	1.78	0.65
15:O:40:ARG:NH2	16:P:314:GLU:OE1	2.28	0.65
9:I:3:SER:HB2	9:I:12:LEU:HB2	1.79	0.65
2:B:833:GLY:H	2:B:881:ILE:HD11	1.62	0.65
3:C:191:ILE:HG23	10:J:15:GLY:HA3	1.77	0.65
1:A:753:GLN:HB2	1:A:757:ASN:HD21	1.62	0.64
18:U:84:THR:O	18:U:88:HIS:NE2	2.30	0.64
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.30	0.64
2:B:915:ARG:H	2:B:1025:GLN:HE22	1.46	0.64
1:A:19:SER:HA	1:A:1403:MET:HG2	1.80	0.63
1:A:25:ASP:O	1:A:29:GLN:NE2	2.31	0.63
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.80	0.63
1:A:352:GLY:H	1:A:355:GLN:HB2	1.64	0.63
2:B:258:LYS:NZ	2:B:263:LEU:O	2.32	0.63
6:F:115:THR:HG22	6:F:116:ASP:H	1.64	0.62
1:A:153:ARG:HH12	15:O:339:LEU:HB3	1.63	0.62
16:P:187:SER:HA	16:P:263:VAL:HG21	1.81	0.62
13:M:92:ASN:HD21	13:M:181:PRO:HG3	1.64	0.62
19:V:6:ASN:HD22	19:V:30:VAL:HG21	1.64	0.62
2:B:207:VAL:HG12	2:B:217:GLN:HE22	1.64	0.62
13:M:164:LYS:HB3	13:M:167:GLN:HB2	1.81	0.62
15:O:588:LEU:HD21	16:P:310:VAL:HG22	1.81	0.62
1:A:1332:ARG:NH1	1:A:1360:ASP:OD1	2.33	0.62
1:A:929:ASN:O	1:A:931:GLN:NE2	2.33	0.61
2:B:816:ASP:N	2:B:816:ASP:OD1	2.32	0.61
5:E:170:LEU:HB2	5:E:174:GLN:HE21	1.64	0.61
18:U:196:ARG:HG3	18:U:203:VAL:HG12	1.82	0.61
1:A:332:VAL:HG13	1:A:334:PRO:HD3	1.81	0.61
4:D:140:GLU:HG3	4:D:144:ARG:HH12	1.66	0.61
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.82	0.61
18:U:194:ILE:O	18:U:196:ARG:NH1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:730:TYR:OH	3:C:100:ARG:NH1	2.33	0.61
18:U:195:TYR:HD2	18:U:204:LEU:HD21	1.66	0.61
3:C:43:ASN:HB2	3:C:55:ASP:HB2	1.83	0.61
2:B:221:THR:HG21	2:B:334:HIS:H	1.66	0.60
2:B:827:ASP:OD2	12:L:29:TYR:OH	2.20	0.60
14:N:374:LYS:NZ	14:N:377:ASN:O	2.35	0.60
18:U:107:ARG:HB2	20:W:473:LEU:HD22	1.83	0.60
1:A:72:GLY:HA3	1:A:76:SER:HB2	1.84	0.60
1:A:379:THR:HG22	2:B:1035:MET:HA	1.82	0.60
7:G:80:PHE:HB3	7:G:83:GLU:HB2	1.84	0.60
1:A:601:TYR:HD1	3:C:24:SER:HB2	1.67	0.59
15:O:56:HIS:HE1	15:O:130:LEU:HD22	1.67	0.59
1:A:372:ARG:NH1	2:B:1052:GLU:OE1	2.35	0.59
18:U:188:GLU:OE2	19:V:219:ARG:NH2	2.35	0.59
7:G:149:ARG:HH21	7:G:201:GLN:HG2	1.67	0.59
1:A:1263:LEU:HA	1:A:1266:ALA:HB3	1.84	0.59
8:H:106:GLU:HA	8:H:112:ILE:HA	1.85	0.59
1:A:200:GLU:HG2	15:O:516:LEU:HB2	1.84	0.59
3:C:136:LEU:HB3	3:C:167:LEU:HA	1.85	0.58
1:A:493:ARG:HB3	1:A:499:ARG:HH21	1.68	0.58
18:U:93:GLU:OE2	20:W:439:PHE:N	2.33	0.58
20:W:407:ASN:ND2	22:Y:65:DG:OP1	2.33	0.58
1:A:1023:ARG:NH2	1:A:1028:MET:SD	2.76	0.58
18:U:197:MET:HB2	18:U:202:ILE:HG22	1.85	0.58
1:A:409:THR:HG22	1:A:410:ARG:HD2	1.85	0.58
3:C:87:ASN:ND2	12:L:61:THR:O	2.36	0.58
1:A:1048:VAL:O	1:A:1053:LYS:NZ	2.37	0.58
2:B:390:ASP:HA	2:B:393:LYS:HE3	1.85	0.58
8:H:33:GLN:HG3	8:H:35:GLN:H	1.69	0.58
2:B:210:ASP:H	2:B:215:ILE:HG22	1.68	0.58
2:B:683:ALA:HB1	2:B:744:ILE:HD13	1.86	0.58
1:A:815:GLN:NE2	1:A:816:GLN:O	2.37	0.58
2:B:807:GLY:O	2:B:844:ASN:ND2	2.36	0.57
10:J:31:ASP:HB3	10:J:34:THR:HG22	1.84	0.57
16:P:263:VAL:HG12	16:P:265:LEU:H	1.69	0.57
18:U:68:GLN:HE22	18:U:163:SER:H	1.52	0.57
2:B:332:ILE:O	2:B:345:LYS:NZ	2.32	0.57
1:A:1254:ASN:HD21	9:I:13:LEU:HD21	1.69	0.57
1:A:787:ASN:ND2	8:H:21:ASN:OD1	2.38	0.57
2:B:1043:ARG:NH1	2:B:1087:SER:O	2.36	0.57
15:O:199:TYR:HD1	15:O:286:ARG:HD2	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:165:VAL:HG23	19:V:170:ILE:HB	1.87	0.57
1:A:473:LEU:HA	1:A:487:SER:HA	1.85	0.57
11:K:72:LEU:HG	11:K:76:LEU:HD23	1.87	0.57
1:A:945:ILE:HG23	1:A:946:THR:HG23	1.85	0.57
2:B:113:THR:OG1	2:B:117:GLU:OE1	2.21	0.57
2:B:732:GLN:HB3	2:B:753:GLN:HA	1.84	0.56
2:B:1033:ASP:O	2:B:1054:ARG:NH2	2.36	0.56
19:V:476:ASN:HB3	19:V:479:ALA:HB3	1.87	0.56
1:A:1301:ARG:HH21	1:A:1325:VAL:HA	1.69	0.56
1:A:872:LEU:HD21	2:B:701:TYR:HE1	1.70	0.56
3:C:1:MET:HG3	3:C:2:SER:H	1.70	0.56
15:O:233:SER:HB3	15:O:236:LYS:HD3	1.88	0.56
15:O:288:MET:HG3	15:O:326:ILE:HD13	1.86	0.56
18:U:67:LEU:HB3	18:U:160:ILE:HD11	1.88	0.56
1:A:1386:LEU:HB3	1:A:1395:HIS:HD1	1.70	0.56
15:O:100:GLN:HG3	15:O:167:GLY:HA3	1.87	0.56
1:A:12:ARG:HB2	2:B:1146:ILE:HG13	1.87	0.56
1:A:555:GLN:NE2	2:B:767:ILE:O	2.39	0.56
1:A:859:PRO:HD3	2:B:661:LEU:HD11	1.86	0.56
2:B:40:THR:HB	2:B:624:ASP:HB3	1.86	0.56
10:J:22:LEU:O	10:J:26:GLN:NE2	2.39	0.56
19:V:275:PHE:HE2	19:V:279:ASP:HB2	1.71	0.56
15:O:620:LEU:HD23	15:O:622:SER:H	1.70	0.56
18:U:186:GLU:OE1	18:U:189:LEU:N	2.33	0.56
1:A:217:ARG:HH22	15:O:555:ALA:HA	1.70	0.56
1:A:993:GLU:O	5:E:197:LYS:NZ	2.37	0.56
16:P:170:LEU:HD13	16:P:172:ILE:H	1.71	0.56
1:A:951:ASP:O	1:A:1061:ARG:NH2	2.39	0.56
2:B:525:GLU:HG2	2:B:527:GLU:H	1.69	0.56
1:A:179:ILE:HG12	15:O:557:ARG:HH22	1.71	0.56
16:P:236:THR:HG23	16:P:239:ASN:H	1.71	0.56
18:U:94:TYR:HB2	18:U:102:VAL:HG22	1.86	0.56
6:F:138:LEU:HB2	6:F:142:SER:HB3	1.87	0.55
16:P:254:GLU:N	16:P:262:ARG:O	2.29	0.55
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.87	0.55
1:A:1147:ASN:ND2	1:A:1151:GLU:OE2	2.32	0.55
1:A:632:VAL:HG23	1:A:633:PHE:H	1.70	0.55
19:V:165:VAL:HA	19:V:170:ILE:HD13	1.88	0.55
13:M:75:PRO:HA	14:N:362:SER:HA	1.87	0.55
1:A:1445:ARG:NH2	4:D:10:PHE:O	2.40	0.55
2:B:66:ASN:HD21	2:B:159:ASN:HD21	1.53	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:HG23	2:B:651:VAL:HG11	1.88	0.55
18:U:138:LYS:NZ	19:V:465:VAL:O	2.32	0.55
8:H:98:TYR:OH	8:H:139:ASN:ND2	2.40	0.55
16:P:311:TYR:CD2	17:Q:37:PRO:HG2	2.42	0.55
1:A:483:LEU:HD11	1:A:540:ASN:HB3	1.88	0.55
15:O:161:GLN:NE2	17:Q:64:THR:OG1	2.40	0.55
1:A:624:ILE:HG22	1:A:625:ASN:H	1.72	0.55
1:A:683:ARG:NH1	1:A:925:GLU:OE2	2.40	0.55
2:B:795:LEU:HD21	2:B:806:ILE:HD11	1.89	0.55
15:O:129:ILE:HG21	15:O:164:ILE:HD13	1.88	0.55
20:W:467:ILE:HG13	20:W:468:LEU:HD12	1.88	0.55
2:B:723:THR:HA	2:B:790:LYS:HB3	1.88	0.54
19:V:485:ARG:HG3	20:W:498:PHE:HB2	1.88	0.54
21:X:42:DC:H2"	21:X:43:DA:C8	2.42	0.54
2:B:1008:ILE:HD11	11:K:70:HIS:CD2	2.43	0.54
2:B:1108:THR:HA	2:B:1111:LYS:HG2	1.90	0.54
19:V:258:ARG:NH2	22:Y:63:DT:OP2	2.40	0.54
1:A:364:PHE:HA	1:A:368:LEU:HB2	1.88	0.54
2:B:548:SER:OG	14:N:389:THR:O	2.26	0.54
4:D:141:CYS:SG	4:D:144:ARG:NH2	2.80	0.54
15:O:327:ARG:O	15:O:332:GLN:NE2	2.41	0.54
5:E:47:CYS:HB2	5:E:53:PRO:HA	1.90	0.54
15:O:98:LEU:HB2	15:O:103:CYS:HB2	1.89	0.54
7:G:130:TRP:HE3	7:G:137:LYS:HB3	1.73	0.54
20:W:450:SER:H	20:W:453:GLN:NE2	2.06	0.54
1:A:683:ARG:HH12	1:A:925:GLU:HG2	1.73	0.54
1:A:927:GLU:H	1:A:932:PRO:HA	1.73	0.54
4:D:15:GLU:HG3	4:D:18:LYS:HE3	1.89	0.54
3:C:197:ARG:HE	10:J:61:LEU:HD13	1.71	0.54
2:B:206:ILE:HD11	2:B:218:ALA:HB3	1.90	0.54
18:U:224:TYR:HB3	19:V:445:LEU:HD22	1.90	0.54
2:B:788:ARG:HB3	2:B:899:LEU:HD21	1.91	0.53
7:G:93:THR:HG22	7:G:94:ALA:H	1.72	0.53
15:O:457:LEU:HA	15:O:460:LEU:HD13	1.90	0.53
1:A:605:THR:HG23	1:A:607:LYS:H	1.73	0.53
2:B:258:LYS:HG2	2:B:263:LEU:HA	1.90	0.53
1:A:1318:HIS:HD2	1:A:1321:GLU:HB3	1.73	0.53
1:A:553:ALA:HB1	1:A:557:PHE:HB2	1.91	0.53
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.89	0.53
19:V:233:ARG:HE	20:W:285:PRO:HG3	1.72	0.53
1:A:210:GLU:HG3	21:X:48:DT:H5"	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.43	0.53
2:B:667:VAL:HB	2:B:670:MET:HB2	1.90	0.53
7:G:57:GLY:HA2	7:G:68:ILE:HG13	1.89	0.53
3:C:31:TRP:HH2	11:K:127:LEU:HD13	1.74	0.53
18:U:88:HIS:HB2	19:V:475:LEU:HD22	1.91	0.53
1:A:186:VAL:HG13	1:A:187:GLY:H	1.74	0.53
2:B:846:SER:HB3	2:B:866:TYR:HB3	1.91	0.53
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.91	0.53
12:L:29:TYR:HB3	12:L:56:LEU:HD21	1.90	0.53
14:N:305:MET:HA	14:N:412:VAL:HG13	1.91	0.53
1:A:122:GLN:NE2	1:A:126:GLU:OE2	2.42	0.53
1:A:223:ASN:HB2	1:A:316:TRP:HH2	1.74	0.53
1:A:901:ASP:OD2	1:A:905:ARG:NH2	2.42	0.53
3:C:16:THR:O	3:C:295:ARG:NH1	2.42	0.53
18:U:109:PRO:O	18:U:110:LYS:HG3	2.09	0.53
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.92	0.52
3:C:237:GLN:HB2	3:C:288:LYS:HG3	1.91	0.52
5:E:168:TYR:HB2	5:E:170:LEU:HD22	1.91	0.52
2:B:686:GLY:HA3	2:B:740:THR:HG21	1.90	0.52
2:B:369:ARG:NH2	2:B:480:SER:OG	2.42	0.52
2:B:420:LEU:HD12	19:V:149:ARG:HG2	1.92	0.52
1:A:757:ASN:HD22	1:A:760:GLN:NE2	2.08	0.52
2:B:540:ASP:HB3	2:B:543:LEU:HD13	1.92	0.52
1:A:1190:LEU:HD22	1:A:1193:ILE:HD13	1.92	0.52
1:A:812:VAL:HG22	1:A:814:GLY:H	1.74	0.52
8:H:41:ASP:HB2	8:H:121:LEU:HD12	1.91	0.52
2:B:811:VAL:HG12	2:B:816:ASP:HA	1.91	0.52
1:A:1286:ARG:HG2	1:A:1287:ASP:H	1.74	0.52
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.25	0.52
2:B:889:SER:OG	2:B:891:ASN:O	2.28	0.52
1:A:1320:LEU:HD23	1:A:1320:LEU:H	1.75	0.51
1:A:596:ALA:HA	8:H:98:TYR:HB3	1.93	0.51
12:L:38:LEU:HD11	12:L:49:LYS:H	1.75	0.51
1:A:84:LEU:HD12	1:A:261:LEU:HD23	1.92	0.51
2:B:49:PRO:HG3	2:B:743:LEU:HD21	1.92	0.51
1:A:815:GLN:HE21	1:A:846:GLY:HA3	1.75	0.51
15:O:488:LYS:HE2	15:O:651:PHE:HA	1.91	0.51
1:A:1350:VAL:HG23	1:A:1351:ASP:H	1.76	0.51
3:C:59:ILE:HB	3:C:63:ILE:HD11	1.91	0.51
18:U:164:CYS:SG	18:U:165:ASP:N	2.84	0.51
18:U:197:MET:HB3	18:U:200:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:485:ARG:HB2	20:W:499:ASN:HD21	1.76	0.51
13:M:154:GLU:HB3	13:M:175:ARG:HG2	1.93	0.51
1:A:83:HIS:HA	1:A:262:PRO:HA	1.93	0.51
1:A:892:SER:OG	1:A:1379:MET:SD	2.68	0.51
2:B:311:THR:HG23	2:B:313:ARG:HH22	1.76	0.51
2:B:754:ASN:HD21	10:J:48:ARG:HB2	1.74	0.51
11:K:62:SER:HB3	11:K:104:ARG:HH11	1.75	0.51
18:U:185:TYR:HB3	18:U:193:LEU:HG	1.93	0.51
18:U:98:ARG:NH1	22:Y:55:DA:OP1	2.44	0.51
1:A:1079:ARG:HD3	6:F:84:TYR:HE2	1.76	0.51
1:A:1267:LEU:HG	1:A:1268:PRO:HD3	1.93	0.51
2:B:611:PRO:HA	2:B:648:TYR:HA	1.93	0.51
20:W:311:ARG:NH2	22:Y:67:DC:OP1	2.44	0.51
20:W:450:SER:H	20:W:453:GLN:HE22	1.58	0.51
1:A:1050:ASP:HA	1:A:1053:LYS:HE2	1.92	0.51
1:A:1121:LEU:O	1:A:1342:THR:OG1	2.28	0.51
1:A:104:GLN:HB2	1:A:145:LEU:HD11	1.92	0.51
2:B:837:GLN:HG2	2:B:878:PRO:HB3	1.92	0.51
12:L:31:CYS:SG	12:L:32:ALA:N	2.84	0.51
1:A:1187:ARG:NH1	1:A:1189:ASP:OD1	2.43	0.50
1:A:1329:GLU:HG3	5:E:153:HIS:HE1	1.77	0.50
2:B:527:GLU:HA	2:B:530:LYS:HE3	1.93	0.50
2:B:614:ILE:HG23	2:B:621:ARG:HD2	1.91	0.50
14:N:299:ASN:C	14:N:300:LYS:HD2	2.32	0.50
2:B:1081:GLU:OE2	2:B:1086:SER:OG	2.30	0.50
2:B:796:LYS:HA	2:B:893:GLN:HE21	1.76	0.50
8:H:58:THR:HB	8:H:143:LEU:HB2	1.92	0.50
2:B:493:GLN:HE21	2:B:497:LEU:HG	1.74	0.50
2:B:722:ASP:HB2	2:B:725:LEU:HD21	1.94	0.50
2:B:766:ASP:HA	2:B:770:ALA:HB3	1.93	0.50
3:C:245:ARG:NH1	3:C:263:ASP:OD2	2.43	0.50
2:B:272:VAL:O	2:B:354:ARG:NH1	2.44	0.50
2:B:579:ARG:NH1	2:B:588:ILE:O	2.45	0.50
6:F:136:ARG:N	6:F:144:GLU:O	2.45	0.50
19:V:441:ASN:HB2	19:V:444:LEU:HB2	1.93	0.50
2:B:315:GLN:NE2	21:X:45:DT:OP1	2.45	0.50
1:A:261:LEU:HD12	1:A:262:PRO:HD2	1.94	0.50
19:V:233:ARG:HG3	19:V:239:ARG:HH11	1.77	0.50
5:E:171:LYS:H	5:E:174:GLN:NE2	2.09	0.50
1:A:840:LYS:HA	1:A:845:LYS:HE3	1.94	0.50
7:G:207:LEU:HG	7:G:209:SER:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:93:GLU:HG3	18:U:105:ARG:HH12	1.75	0.50
20:W:311:ARG:HH22	20:W:314:ARG:NH2	2.10	0.50
1:A:225:LEU:HD13	1:A:228:LEU:HD21	1.94	0.50
2:B:405:LYS:HA	2:B:408:LYS:HE3	1.94	0.50
8:H:58:THR:O	8:H:143:LEU:N	2.41	0.50
12:L:26:THR:HB	12:L:28:LYS:HG2	1.94	0.49
2:B:819:TRP:HA	2:B:822:GLN:HE22	1.76	0.49
3:C:100:ARG:NH2	10:J:3:VAL:O	2.41	0.49
12:L:53:HIS:HE1	12:L:55:ILE:HB	1.76	0.49
1:A:145:LEU:HG	1:A:149:LYS:HE2	1.94	0.49
2:B:591:TYR:HB2	2:B:652:ASN:HB3	1.93	0.49
2:B:780:ARG:NH2	10:J:10:CYS:O	2.42	0.49
2:B:261:GLY:HA2	2:B:298:GLN:HG3	1.95	0.49
5:E:107:THR:HB	5:E:130:ALA:HB3	1.93	0.49
15:O:199:TYR:HA	15:O:283:ASN:HB3	1.93	0.49
21:X:18:DT:O2	22:Y:65:DG:N2	2.46	0.49
1:A:1161:VAL:HA	1:A:1275:LEU:HD13	1.94	0.49
1:A:274:MET:HG2	1:A:276:ASP:H	1.76	0.49
1:A:914:PHE:HE2	5:E:211:TYR:H	1.60	0.49
8:H:14:GLU:H	8:H:27:GLU:HB2	1.75	0.49
1:A:1205:ILE:O	1:A:1209:ILE:HD12	2.13	0.49
1:A:403:THR:OG1	1:A:464:ARG:O	2.19	0.49
2:B:666:ILE:HD11	2:B:673:LEU:HD12	1.93	0.49
14:N:373:VAL:HG23	14:N:381:ASP:HB2	1.93	0.49
15:O:289:LYS:HD2	15:O:323:SER:HB2	1.94	0.49
1:A:666:LYS:HD2	1:A:670:GLY:HA3	1.94	0.49
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.78	0.49
2:B:1036:HIS:HE1	2:B:1058:GLY:HA3	1.78	0.49
1:A:1236:PRO:HB3	1:A:1255:ASP:HB3	1.93	0.49
1:A:166:LYS:HA	1:A:178:ILE:HG22	1.95	0.49
1:A:4:VAL:HA	7:G:38:ILE:HG22	1.93	0.49
1:A:763:GLU:HG2	1:A:822:ARG:HE	1.77	0.49
1:A:830:ARG:NH2	2:B:655:ASN:O	2.46	0.49
2:B:303:GLU:HB2	2:B:321:GLN:HE21	1.77	0.49
8:H:63:LEU:HG	8:H:89:LEU:HD23	1.95	0.49
18:U:73:THR:HA	18:U:122:VAL:HA	1.95	0.49
19:V:265:THR:HG23	19:V:266:LYS:H	1.77	0.49
1:A:625:ASN:HD22	1:A:655:ARG:HA	1.78	0.49
18:U:142:ILE:HG12	19:V:473:HIS:HD2	1.76	0.49
1:A:19:SER:HB3	2:B:1138:ALA:HB3	1.95	0.49
1:A:703:ARG:NH2	11:K:93:ILE:O	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:129:GLU:HG2	18:U:133:LYS:HE2	1.93	0.49
2:B:904:ARG:NH1	2:B:1030:MET:SD	2.86	0.48
7:G:10:LEU:HA	7:G:69:ASN:HA	1.95	0.48
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.46	0.48
2:B:566:ARG:HD3	14:N:387:GLU:HB3	1.93	0.48
15:O:549:GLN:N	15:O:565:LEU:O	2.42	0.48
1:A:1064:GLU:OE2	1:A:1068:ARG:NE	2.41	0.48
2:B:739:LYS:H	2:B:977:THR:HG22	1.79	0.48
2:B:775:LYS:N	2:B:926:VAL:O	2.44	0.48
5:E:185:ALA:HA	5:E:190:LEU:HD23	1.94	0.48
12:L:29:TYR:CG	12:L:56:LEU:HD11	2.48	0.48
13:M:111:ARG:HD3	13:M:120:GLU:HB2	1.94	0.48
15:O:552:PRO:HB3	15:O:557:ARG:HG3	1.95	0.48
1:A:850:ASN:ND2	1:A:860:GLU:OE2	2.43	0.48
3:C:322:LYS:NZ	3:C:326:GLU:OE1	2.47	0.48
2:B:137:ARG:HH11	2:B:142:ILE:HD13	1.78	0.48
13:M:110:ALA:HB3	13:M:245:LEU:HB2	1.94	0.48
1:A:37:ARG:HG3	1:A:294:TRP:HB2	1.94	0.48
2:B:514:LEU:HD11	2:B:518:THR:HG21	1.96	0.48
2:B:77:ILE:HB	2:B:95:TYR:CE2	2.48	0.48
1:A:427:HIS:CE1	1:A:492:ILE:HG13	2.49	0.48
2:B:849:THR:HG22	2:B:865:GLN:HB2	1.95	0.48
15:O:228:ARG:HG3	15:O:229:ASN:H	1.77	0.48
15:O:327:ARG:HE	15:O:332:GLN:HE22	1.60	0.48
19:V:178:PRO:HB2	19:V:224:ALA:HB2	1.94	0.48
20:W:488:ILE:HA	20:W:491:ASN:HB2	1.95	0.48
18:U:133:LYS:HE3	19:V:452:LEU:HA	1.95	0.48
2:B:128:PRO:HA	2:B:151:ARG:HA	1.96	0.48
8:H:12:VAL:HG22	8:H:53:ASP:H	1.79	0.48
19:V:219:ARG:HH11	22:Y:63:DT:H4'	1.79	0.48
1:A:107:CYS:HB3	1:A:112:ALA:H	1.79	0.47
1:A:544:PRO:HA	1:A:924:LEU:HD13	1.96	0.47
5:E:37:LEU:HD11	5:E:42:PHE:HB2	1.95	0.47
13:M:250:GLY:O	13:M:251:THR:HG22	2.13	0.47
19:V:242:THR:OG1	20:W:296:SER:OG	2.31	0.47
1:A:808:GLN:HG2	1:A:813:VAL:HA	1.96	0.47
2:B:435:ARG:O	2:B:439:THR:OG1	2.32	0.47
15:O:259:LEU:H	15:O:259:LEU:HD23	1.78	0.47
18:U:149:ALA:HB1	18:U:151:LYS:HG2	1.96	0.47
1:A:482:ARG:HH21	2:B:1073:TYR:HA	1.79	0.47
1:A:818:ILE:HD12	1:A:823:VAL:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:SER:OG	2:B:244:HIS:NE2	2.32	0.47
3:C:135:SER:O	3:C:168:LYS:N	2.47	0.47
5:E:47:CYS:HA	5:E:54:GLN:HG3	1.96	0.47
15:O:580:ASN:O	15:O:584:ASN:ND2	2.47	0.47
19:V:189:LEU:HD21	19:V:238:ARG:HG2	1.96	0.47
2:B:126:SER:HA	2:B:153:PRO:HA	1.96	0.47
15:O:287:PHE:O	15:O:291:ARG:N	2.44	0.47
15:O:365:ASP:O	15:O:369:HIS:ND1	2.39	0.47
15:O:57:LEU:HD23	15:O:58:GLY:N	2.30	0.47
2:B:812:ASP:N	2:B:812:ASP:OD1	2.48	0.47
15:O:105:LYS:HE2	15:O:123:ASN:HA	1.96	0.47
15:O:199:TYR:CD1	15:O:286:ARG:HD2	2.48	0.47
14:N:386:ALA:HB2	14:N:416:ILE:HG22	1.96	0.47
2:B:773:LEU:HB3	2:B:942:ILE:HG22	1.97	0.47
19:V:218:ARG:HH22	19:V:288:PRO:HG2	1.79	0.47
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.96	0.47
2:B:284:ALA:HA	2:B:287:LEU:HD13	1.96	0.47
2:B:510:LEU:HD23	2:B:510:LEU:H	1.80	0.47
5:E:78:LEU:HD13	5:E:107:THR:HG23	1.97	0.47
7:G:79:PRO:HB2	7:G:83:GLU:HG2	1.96	0.47
13:M:158:GLN:H	14:N:308:GLN:HA	1.80	0.47
5:E:147:HIS:HE1	5:E:149:LEU:HD23	1.78	0.47
1:A:1373:ARG:HB3	1:A:1391:LYS:HE2	1.97	0.47
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.97	0.47
2:B:756:THR:H	2:B:941:ASP:HB2	1.80	0.47
3:C:100:ARG:HH12	10:J:4:PRO:HA	1.79	0.47
15:O:37:LEU:HA	15:O:40:ARG:HE	1.79	0.47
2:B:841:ILE:HG12	2:B:872:ILE:HG12	1.97	0.47
15:O:254:ASN:O	15:O:258:GLU:N	2.48	0.47
16:P:172:ILE:HG22	16:P:173:GLU:H	1.80	0.47
2:B:929:GLU:HB3	3:C:72:ILE:HD11	1.97	0.46
15:O:121:TYR:HD2	15:O:210:PRO:HG2	1.80	0.46
20:W:318:ARG:NH1	20:W:448:TYR:HB2	2.31	0.46
21:X:34:DT:O4	22:Y:47:DA:N6	2.48	0.46
2:B:420:LEU:O	19:V:149:ARG:NH2	2.44	0.46
8:H:63:LEU:HD21	8:H:143:LEU:HD11	1.98	0.46
15:O:102:ARG:HG3	15:O:208:TYR:HD1	1.79	0.46
18:U:67:LEU:HD12	18:U:160:ILE:HG13	1.97	0.46
20:W:488:ILE:HG22	20:W:492:ILE:HG23	1.97	0.46
2:B:99:ARG:NH2	2:B:146:ASP:OD1	2.48	0.46
13:M:105:PRO:HB2	13:M:123:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1278:ILE:HG22	1:A:1297:GLY:HA3	1.97	0.46
2:B:201:SER:HA	2:B:376:ARG:HG2	1.97	0.46
8:H:107:VAL:N	8:H:111:LEU:O	2.47	0.46
15:O:191:PHE:O	15:O:195:CYS:N	2.47	0.46
1:A:1125:ARG:HH12	1:A:1129:ILE:HD11	1.80	0.46
1:A:1177:TYR:OH	1:A:1260:MET:SD	2.73	0.46
1:A:774:ARG:HH21	1:A:804:LEU:HD11	1.80	0.46
21:X:47:DG:N2	22:Y:36:DT:O2	2.47	0.46
1:A:1170:ALA:HA	1:A:1188:ILE:HA	1.98	0.46
1:A:882:THR:O	1:A:886:SER:N	2.44	0.46
2:B:968:VAL:O	10:J:47:ARG:NE	2.45	0.46
4:D:147:GLU:CD	4:D:148:LYS:H	2.19	0.46
13:M:150:GLY:HA3	13:M:179:LEU:HD23	1.98	0.46
18:U:90:ARG:HB3	19:V:473:HIS:CE1	2.51	0.46
2:B:220:VAL:HA	2:B:230:LYS:HA	1.98	0.46
1:A:107:CYS:SG	1:A:108:LYS:N	2.89	0.46
1:A:1139:PRO:HG3	1:A:1298:TYR:CZ	2.51	0.46
1:A:440:ALA:O	1:A:441:ARG:HG3	2.16	0.46
2:B:915:ARG:N	2:B:1025:GLN:HE22	2.10	0.46
2:B:393:LYS:HE2	2:B:446:ARG:HG2	1.98	0.46
2:B:51:PHE:HD2	2:B:52:LEU:HD12	1.79	0.46
1:A:513:ASP:HB2	2:B:919:LYS:HE2	1.98	0.46
2:B:737:LYS:HE2	2:B:973:LEU:HB3	1.97	0.46
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.97	0.46
16:P:247:LEU:HD12	16:P:252:LYS:HB2	1.98	0.46
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.31	0.46
2:B:737:LYS:N	2:B:974:GLU:O	2.46	0.46
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.97	0.46
1:A:5:VAL:HB	7:G:37:LYS:HB3	1.98	0.46
1:A:89:PRO:HG3	1:A:259:ARG:HG3	1.98	0.46
2:B:696:SER:OG	2:B:697:PRO:HD3	2.16	0.46
15:O:521:ILE:HA	15:O:524:SER:HB3	1.98	0.46
1:A:120:LYS:HB2	1:A:241:LEU:HD21	1.98	0.45
1:A:884:TYR:OH	1:A:888:ARG:NH2	2.49	0.45
2:B:55:LYS:HG2	2:B:59:LYS:HD3	1.99	0.45
3:C:241:GLY:O	3:C:245:ARG:NH1	2.49	0.45
18:U:140:ALA:HA	18:U:143:ILE:HD12	1.98	0.45
21:X:33:DT:O4	22:Y:48:DA:N6	2.49	0.45
1:A:329:SER:HB3	1:A:355:GLN:HG3	1.98	0.45
13:M:182:PHE:HE2	13:M:184:LYS:HD3	1.82	0.45
19:V:458:ASP:OD1	19:V:458:ASP:N	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:O	1:A:181:ASP:N	2.50	0.45
2:B:198:GLU:HB3	2:B:377:LEU:HD12	1.98	0.45
2:B:778:ILE:HD11	2:B:906:PRO:HD2	1.98	0.45
3:C:228:ARG:HB2	3:C:299:ILE:HB	1.98	0.45
7:G:88:TRP:HE1	7:G:145:LYS:HG2	1.82	0.45
8:H:38:LEU:HB3	8:H:125:LEU:HB3	1.97	0.45
15:O:631:ASN:ND2	15:O:634:GLU:OE2	2.50	0.45
20:W:287:GLY:O	20:W:288:GLN:HG3	2.16	0.45
1:A:1045:ASP:O	1:A:1053:LYS:NZ	2.44	0.45
1:A:442:ARG:HG2	19:V:30:VAL:HG22	1.98	0.45
1:A:633:PHE:HE1	1:A:651:PHE:HB2	1.81	0.45
2:B:622:VAL:HG23	2:B:623:LYS:H	1.81	0.45
1:A:84:LEU:N	1:A:261:LEU:O	2.43	0.45
1:A:88:LEU:HB2	1:A:225:LEU:HD21	1.98	0.45
2:B:82:LEU:HD23	2:B:94:LYS:HB3	1.98	0.45
1:A:1444:LYS:O	7:G:49:TYR:OH	2.32	0.45
2:B:860:VAL:HG23	2:B:861:ASN:H	1.82	0.45
10:J:10:CYS:SG	10:J:11:GLY:N	2.89	0.45
1:A:229:ASN:OD1	15:O:544:ASN:ND2	2.49	0.45
15:O:291:ARG:NE	15:O:649:GLU:OE2	2.40	0.45
18:U:68:GLN:NE2	18:U:163:SER:OG	2.49	0.45
1:A:1031:LEU:HD23	1:A:1031:LEU:H	1.81	0.45
1:A:1166:LEU:HD21	1:A:1268:PRO:HA	1.98	0.45
1:A:552:ALA:HB1	1:A:670:GLY:HA2	1.98	0.45
2:B:343:ARG:HD3	2:B:542:THR:HG22	1.99	0.45
4:D:106:LEU:HB2	4:D:156:ILE:HG23	1.98	0.45
15:O:295:GLN:HG3	15:O:487:LEU:HD21	1.98	0.45
19:V:239:ARG:NH2	20:W:284:PHE:H	2.14	0.45
1:A:531:ALA:HA	1:A:535:MET:SD	2.57	0.45
2:B:205:ILE:HD11	2:B:355:ARG:NH2	2.32	0.45
2:B:816:ASP:OD1	2:B:817:PRO:HD3	2.17	0.45
15:O:263:LEU:HA	15:O:274:VAL:HA	1.98	0.45
19:V:274:LYS:HG2	19:V:275:PHE:H	1.81	0.45
2:B:338:GLU:HB2	2:B:342:PHE:HD1	1.81	0.45
2:B:737:LYS:O	2:B:976:GLY:N	2.45	0.45
12:L:53:HIS:CE1	12:L:55:ILE:HB	2.51	0.45
1:A:1148:ASP:O	1:A:1291:ARG:NH1	2.50	0.45
3:C:134:LEU:HB2	3:C:169:PHE:HA	1.99	0.45
15:O:268:LYS:O	15:O:269:THR:HG22	2.17	0.45
18:U:154:ASP:N	18:U:154:ASP:OD1	2.50	0.45
2:B:915:ARG:NH2	2:B:960:GLU:OE2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:SER:HB3	3:C:303:GLU:HG2	1.99	0.44
9:I:5:CYS:O	9:I:9:ASN:N	2.39	0.44
14:N:380:MET:HB3	14:N:421:GLN:HE22	1.82	0.44
15:O:141:ILE:O	15:O:145:ARG:NE	2.48	0.44
1:A:1358:LEU:HA	1:A:1361:VAL:HG22	2.00	0.44
1:A:1386:LEU:HB3	1:A:1395:HIS:ND1	2.32	0.44
4:D:133:HIS:NE2	7:G:84:ILE:HG21	2.33	0.44
7:G:116:PHE:HZ	7:G:128:TRP:HE1	1.65	0.44
3:C:195:LYS:NZ	10:J:58:GLU:OE2	2.43	0.44
15:O:105:LYS:HB3	15:O:210:PRO:HD3	1.99	0.44
2:B:487:ARG:HD2	2:B:508:CYS:HB3	2.00	0.44
3:C:256:ILE:HA	3:C:268:LYS:H	1.82	0.44
7:G:31:ASN:O	7:G:35:ALA:N	2.50	0.44
1:A:664:MET:HE2	1:A:669:LEU:HB2	1.99	0.44
2:B:961:LEU:HB2	2:B:1022:ILE:HD11	1.99	0.44
3:C:139:LYS:HG3	3:C:201:GLU:HB3	2.00	0.44
13:M:157:GLY:HA3	14:N:308:GLN:HG3	2.00	0.44
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.44
5:E:118:PRO:O	5:E:122:LYS:NZ	2.36	0.44
15:O:163:VAL:HA	15:O:169:LEU:HG	2.00	0.44
15:O:294:LYS:HD2	15:O:297:ILE:HD11	1.99	0.44
19:V:135:ARG:HG2	19:V:174:PRO:HD2	1.99	0.44
1:A:563:LEU:HA	1:A:566:HIS:HB2	2.00	0.44
2:B:934:ASN:OD1	2:B:938:ILE:N	2.42	0.44
3:C:93:GLN:NE2	3:C:96:VAL:HG23	2.26	0.44
5:E:147:HIS:CE1	5:E:149:LEU:HD23	2.52	0.44
13:M:71:ILE:N	14:N:365:VAL:O	2.50	0.44
16:P:311:TYR:HA	17:Q:40:PRO:HA	2.00	0.44
1:A:1373:ARG:HH21	1:A:1390:GLU:HB3	1.82	0.44
1:A:386:ASN:O	1:A:699:LYS:NZ	2.50	0.44
1:A:57:LYS:HB3	1:A:68:ALA:HB3	1.98	0.44
2:B:928:GLN:HE21	2:B:939:VAL:HG21	1.81	0.44
1:A:103:LEU:HD12	1:A:164:VAL:HG11	2.00	0.44
1:A:1365:LYS:NZ	1:A:1378:LYS:O	2.27	0.44
4:D:130:ASN:ND2	4:D:132:VAL:HG12	2.33	0.44
18:U:219:GLN:HG3	18:U:221:GLU:H	1.83	0.44
2:B:142:ILE:HD11	20:W:399:GLU:HB2	1.99	0.44
1:A:16:LEU:HD13	1:A:17:GLU:N	2.33	0.44
1:A:164:VAL:HA	1:A:180:HIS:HA	2.00	0.44
1:A:258:TRP:HH2	2:B:1135:MET:HA	1.82	0.44
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:LYS:HA	2:B:1018:PHE:HA	2.00	0.44
15:O:152:HIS:HD2	15:O:156:VAL:HB	1.82	0.44
2:B:176:GLU:O	10:J:63:TYR:OH	2.35	0.43
19:V:182:ILE:HG23	19:V:228:ILE:HD11	2.00	0.43
1:A:364:PHE:HE2	1:A:1392:THR:HG21	1.83	0.43
2:B:203:ASN:HB3	2:B:335:LEU:HD11	1.99	0.43
2:B:379:LEU:H	2:B:382:GLN:NE2	2.16	0.43
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.99	0.43
3:C:86:PHE:HE1	12:L:64:LEU:HD12	1.83	0.43
18:U:87:LEU:HD11	19:V:487:TRP:CE3	2.53	0.43
1:A:73:ASN:OD1	1:A:74:LEU:N	2.47	0.43
8:H:121:LEU:HD23	8:H:121:LEU:H	1.84	0.43
1:A:808:GLN:HB3	1:A:813:VAL:HG12	2.00	0.43
3:C:282:TYR:O	3:C:283:GLU:HG3	2.19	0.43
5:E:79:TRP:NE1	5:E:81:GLU:OE2	2.52	0.43
7:G:91:LYS:HZ2	7:G:98:LYS:HE3	1.84	0.43
1:A:503:CYS:HB3	1:A:551:ILE:HG13	2.00	0.43
3:C:86:PHE:CE1	12:L:64:LEU:HD12	2.54	0.43
5:E:93:MET:HG2	5:E:123:LEU:HD11	2.01	0.43
6:F:117:PRO:HA	6:F:120:ILE:HG22	2.00	0.43
13:M:137:GLU:O	13:M:141:ASN:ND2	2.52	0.43
15:O:210:PRO:HD2	15:O:213:ASP:OD2	2.18	0.43
19:V:237:LEU:HD21	20:W:285:PRO:O	2.18	0.43
19:V:4:CYS:SG	19:V:5:LYS:N	2.91	0.43
1:A:407:LYS:HA	1:A:461:VAL:HA	2.00	0.43
2:B:848:PRO:HG3	2:B:866:TYR:HE1	1.84	0.43
3:C:93:GLN:HE22	3:C:95:GLU:HG2	1.83	0.43
15:O:643:ARG:HH22	17:Q:45:GLY:HA3	1.84	0.43
18:U:75:THR:HA	18:U:120:LYS:HG3	2.01	0.43
19:V:139:THR:HG23	19:V:141:HIS:H	1.83	0.43
1:A:1397:PHE:O	1:A:1401:PHE:N	2.46	0.43
1:A:81:PHE:CZ	2:B:1133:LEU:HD23	2.53	0.43
14:N:394:VAL:HG23	14:N:412:VAL:HB	2.00	0.43
15:O:212:GLU:OE2	15:O:216:GLN:NE2	2.44	0.43
2:B:880:HIS:O	2:B:901:ARG:N	2.49	0.43
3:C:33:VAL:O	3:C:37:LYS:N	2.51	0.43
7:G:152:ARG:H	7:G:197:LEU:HB2	1.83	0.43
7:G:81:LEU:H	7:G:81:LEU:HD23	1.84	0.43
15:O:492:TYR:HB2	15:O:577:MET:HE1	2.00	0.43
15:O:578:ARG:HG3	15:O:648:TRP:HE1	1.83	0.43
18:U:68:GLN:HA	18:U:127:LYS:HD2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:HIS:CD2	1:A:1321:GLU:HB3	2.52	0.43
1:A:468:ASP:OD1	1:A:468:ASP:N	2.52	0.43
2:B:738:THR:HG23	2:B:977:THR:HA	2.01	0.43
7:G:10:LEU:HD23	7:G:10:LEU:H	1.84	0.43
15:O:304:VAL:HG22	15:O:305:GLY:H	1.84	0.43
15:O:510:CYS:HA	16:P:249:TYR:CZ	2.54	0.43
22:Y:52:DT:H2"	22:Y:53:DT:H5"	2.00	0.43
2:B:1078:LEU:HD23	2:B:1078:LEU:H	1.84	0.42
2:B:702:GLN:O	2:B:706:GLY:N	2.37	0.42
2:B:998:TYR:CD1	3:C:281:ARG:HD2	2.54	0.42
3:C:318:VAL:HA	3:C:321:LEU:HD13	2.00	0.42
2:B:1011:GLU:HB3	3:C:61:THR:HG21	2.00	0.42
15:O:370:LEU:HD12	15:O:371:PRO:HD2	2.00	0.42
20:W:503:ILE:O	20:W:506:GLN:HG2	2.19	0.42
3:C:26:ASP:N	3:C:26:ASP:OD1	2.50	0.42
7:G:116:PHE:HD2	7:G:118:GLY:H	1.65	0.42
7:G:84:ILE:HD13	7:G:149:ARG:HB3	2.01	0.42
8:H:26:ILE:HG13	8:H:40:LEU:O	2.19	0.42
15:O:102:ARG:HG3	15:O:208:TYR:CD1	2.54	0.42
16:P:297:PHE:O	16:P:298:LYS:HD3	2.19	0.42
19:V:210:SER:HA	19:V:215:PHE:HZ	1.84	0.42
1:A:1374:PHE:O	1:A:1378:LYS:NZ	2.47	0.42
2:B:1003:MET:HB3	2:B:1016:TYR:CD1	2.55	0.42
11:K:58:GLY:O	11:K:113:ALA:N	2.40	0.42
1:A:1143:ALA:HB3	1:A:1293:LEU:HD11	2.00	0.42
1:A:1144:VAL:HG21	1:A:1313:ARG:HH12	1.84	0.42
3:C:92:ILE:H	3:C:92:ILE:HG13	1.72	0.42
5:E:88:VAL:HG13	5:E:112:TYR:HE1	1.84	0.42
2:B:262:ILE:HA	13:M:180:LYS:NZ	2.34	0.42
14:N:388:THR:HG21	14:N:415:LYS:HB3	2.02	0.42
20:W:483:GLU:O	20:W:487:GLU:N	2.51	0.42
1:A:613:LEU:O	1:A:696:ARG:NH1	2.50	0.42
1:A:70:CYS:SG	1:A:71:HIS:N	2.91	0.42
1:A:895:ASP:OD1	1:A:895:ASP:N	2.53	0.42
2:B:124:THR:HG22	2:B:188:ASN:H	1.83	0.42
15:O:222:HIS:HA	15:O:225:ASN:HD22	1.84	0.42
15:O:300:ALA:O	15:O:304:VAL:N	2.49	0.42
19:V:485:ARG:NH2	20:W:487:GLU:OE2	2.52	0.42
1:A:1384:LEU:HD11	1:A:1413:GLU:HG2	2.01	0.42
1:A:264:PRO:O	1:A:269:ARG:NH1	2.34	0.42
2:B:1038:ARG:NH2	2:B:1042:PRO:O	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:THR:HG22	2:B:109:LYS:H	1.83	0.42
2:B:383:LEU:HD21	2:B:442:TRP:CH2	2.55	0.42
2:B:613:ILE:HD11	2:B:673:LEU:HD22	2.02	0.42
2:B:737:LYS:HE3	2:B:975:TYR:HE1	1.84	0.42
3:C:276:SER:O	3:C:277:ARG:HD2	2.20	0.42
1:A:1222:VAL:HG22	1:A:1232:ILE:HD13	2.02	0.42
1:A:636:PRO:HG2	1:A:643:ASN:HA	2.02	0.42
1:A:753:GLN:N	1:A:757:ASN:OD1	2.52	0.42
1:A:933:VAL:HG23	1:A:934:ASN:H	1.85	0.42
2:B:1129:PHE:HA	2:B:1132:LEU:HG	2.01	0.42
2:B:578:LEU:HD22	2:B:583:LYS:HD3	2.00	0.42
8:H:63:LEU:HD13	8:H:141:TYR:CD2	2.54	0.42
1:A:1097:ILE:H	1:A:1097:ILE:HG13	1.76	0.42
1:A:1201:THR:HG23	1:A:1204:ASP:H	1.85	0.42
1:A:16:LEU:HD23	2:B:1141:LEU:HD23	2.01	0.42
14:N:303:ARG:HH12	14:N:411:ARG:CZ	2.32	0.42
15:O:46:LEU:HD21	15:O:66:GLY:HA2	2.00	0.42
1:A:107:CYS:N	1:A:112:ALA:O	2.44	0.42
1:A:90:VAL:HG21	1:A:323:VAL:HG11	2.02	0.42
1:A:563:LEU:HD11	1:A:708:ARG:HD2	2.01	0.42
2:B:68:PHE:HA	2:B:72:ASP:HB2	2.01	0.42
2:B:832:VAL:HG13	12:L:60:ARG:HA	2.02	0.42
2:B:916:HIS:HD1	2:B:957:LYS:HD3	1.85	0.42
19:V:219:ARG:HD3	20:W:408:TYR:CE2	2.54	0.42
2:B:881:ILE:H	2:B:881:ILE:HG13	1.51	0.41
3:C:85:PHE:HE1	3:C:97:LEU:HD11	1.85	0.41
4:D:64:ASN:OD1	4:D:65:TYR:N	2.53	0.41
16:P:293:ILE:HD12	16:P:294:PHE:N	2.35	0.41
19:V:210:SER:HA	19:V:215:PHE:CZ	2.55	0.41
1:A:897:SER:HB3	1:A:1423:ILE:HG13	2.02	0.41
1:A:31:GLU:HG3	1:A:32:VAL:HG13	2.01	0.41
1:A:524:THR:HG23	2:B:1081:GLU:HG3	2.01	0.41
2:B:1036:HIS:CD2	2:B:1054:ARG:HG2	2.55	0.41
2:B:554:GLY:HA2	2:B:564:SER:HA	2.02	0.41
7:G:60:LYS:HD3	7:G:63:ASP:HB2	2.02	0.41
19:V:268:ALA:O	19:V:272:VAL:HG23	2.20	0.41
7:G:38:ILE:HD12	7:G:44:LEU:HB2	2.03	0.41
11:K:107:THR:OG1	11:K:108:TYR:N	2.54	0.41
13:M:186:ILE:H	13:M:186:ILE:HG13	1.64	0.41
15:O:313:LYS:HB3	15:O:313:LYS:HE2	1.91	0.41
1:A:1263:LEU:O	1:A:1267:LEU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.96	0.41
2:B:757:VAL:N	2:B:1020:GLY:O	2.51	0.41
2:B:93:LEU:HD13	2:B:135:TYR:HB3	2.03	0.41
7:G:14:PRO:HA	7:G:15:PRO:HD3	1.90	0.41
18:U:105:ARG:HB2	20:W:437:THR:HG21	2.01	0.41
15:O:346:GLN:HA	15:O:349:ALA:HB3	2.02	0.41
1:A:1373:ARG:NE	1:A:1390:GLU:OE1	2.53	0.41
1:A:438:GLU:OE2	1:A:441:ARG:N	2.53	0.41
1:A:906:THR:HG23	1:A:908:ALA:H	1.86	0.41
3:C:120:LEU:HD23	3:C:124:GLU:HG2	2.02	0.41
7:G:63:ASP:OD2	7:G:67:TYR:OH	2.24	0.41
15:O:98:LEU:HG	15:O:98:LEU:H	1.70	0.41
20:W:420:TRP:NE1	20:W:457:LYS:HD3	2.35	0.41
1:A:1391:LYS:HE3	1:A:1395:HIS:NE2	2.36	0.41
1:A:384:ASP:HB3	1:A:387:LEU:HD22	2.02	0.41
1:A:716:ASP:HB2	1:A:789:ASN:ND2	2.36	0.41
2:B:1003:MET:HB3	2:B:1016:TYR:HD1	1.86	0.41
2:B:1128:LEU:O	2:B:1131:GLU:HG3	2.20	0.41
4:D:99:SER:OG	4:D:101:GLU:OE1	2.38	0.41
5:E:18:THR:HG23	5:E:143:ASN:HB3	2.02	0.41
6:F:104:ASN:HB3	7:G:16:ASP:HB3	2.02	0.41
1:A:1059:LEU:HD11	8:H:112:ILE:HG21	2.02	0.41
1:A:665:ASP:HB2	1:A:797:CYS:HA	2.02	0.41
2:B:929:GLU:HB2	3:C:69:ARG:HG2	2.03	0.41
2:B:934:ASN:OD1	2:B:937:GLY:N	2.54	0.41
5:E:152:LYS:H	5:E:199:ILE:HD11	1.86	0.41
19:V:287:PRO:HD2	19:V:290:PHE:HE1	1.86	0.41
20:W:480:ASN:O	20:W:482:ASP:N	2.52	0.41
1:A:1042:ILE:H	1:A:1042:ILE:HG13	1.67	0.41
1:A:196:ILE:O	1:A:200:GLU:N	2.47	0.41
2:B:209:ALA:HB2	2:B:366:ILE:HG21	2.01	0.41
3:C:229:LEU:HB2	3:C:293:ARG:HD3	2.02	0.41
10:J:48:ARG:O	10:J:52:THR:OG1	2.39	0.41
16:P:263:VAL:HG12	16:P:265:LEU:N	2.35	0.41
2:B:347:LEU:HD22	2:B:350:ALA:HB3	2.03	0.41
2:B:471:THR:HB	2:B:514:LEU:HB3	2.02	0.41
2:B:762:TYR:HB3	2:B:943:ILE:HD13	2.02	0.41
19:V:474:LEU:HD22	19:V:475:LEU:H	1.85	0.41
20:W:289:ILE:H	20:W:289:ILE:HD12	1.86	0.41
1:A:476:ARG:NH1	1:A:508:TYR:O	2.54	0.41
3:C:103:LEU:HB3	10:J:6:ARG:HE	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:69:ASN:ND2	22:Y:57:DT:H1'	2.36	0.41
2:B:1078:LEU:HA	2:B:1081:GLU:HB3	2.03	0.40
2:B:454:VAL:HG13	2:B:455:THR:HG23	2.03	0.40
5:E:28:TYR:HA	5:E:64:PRO:HA	2.03	0.40
15:O:509:ARG:NH1	16:P:251:ASP:OD1	2.54	0.40
15:O:602:LEU:HD23	15:O:602:LEU:H	1.87	0.40
22:Y:43:DA:H2"	22:Y:44:DA:C8	2.55	0.40
1:A:1165:LEU:HG	1:A:1167:SER:H	1.86	0.40
1:A:1339:ILE:HD12	1:A:1340:ASN:N	2.36	0.40
1:A:382:SER:N	1:A:498:PHE:O	2.54	0.40
1:A:535:MET:SD	1:A:535:MET:N	2.95	0.40
2:B:58:VAL:HG12	2:B:61:HIS:HB2	2.03	0.40
6:F:81:THR:OG1	6:F:144:GLU:OE2	2.29	0.40
15:O:57:LEU:HD23	15:O:58:GLY:H	1.86	0.40
18:U:63:ILE:H	18:U:63:ILE:HG13	1.69	0.40
1:A:223:ASN:HB2	1:A:316:TRP:CH2	2.56	0.40
1:A:300:LYS:HB3	1:A:300:LYS:HE2	1.87	0.40
2:B:77:ILE:HG21	2:B:98:ILE:HD13	2.03	0.40
4:D:130:ASN:HD21	4:D:132:VAL:HG12	1.87	0.40
4:D:13:ASP:HB3	4:D:66:LEU:HD21	2.02	0.40
5:E:13:TRP:CD2	5:E:39:LEU:HD23	2.56	0.40
7:G:27:THR:HG22	7:G:31:ASN:HD21	1.86	0.40
7:G:91:LYS:NZ	7:G:93:THR:OG1	2.55	0.40
8:H:88:SER:N	8:H:91:ASP:OD2	2.54	0.40
2:B:733:GLN:HE21	10:J:52:THR:HA	1.87	0.40
10:J:7:CYS:HB3	10:J:11:GLY:H	1.87	0.40
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.55	0.40
1:A:1323:PHE:CZ	1:A:1367:GLU:HA	2.57	0.40
1:A:599:LYS:HB3	1:A:600:PRO:HD3	2.02	0.40
2:B:1002:ASP:O	2:B:1017:ILE:N	2.42	0.40
2:B:350:ALA:HA	2:B:353:THR:HG22	2.03	0.40
2:B:440:GLY:O	2:B:453:GLY:N	2.54	0.40
7:G:4:LEU:HD13	7:G:73:ARG:HG3	2.04	0.40
12:L:40:LEU:HD13	12:L:41:SER:O	2.22	0.40
15:O:102:ARG:HA	15:O:208:TYR:HE1	1.86	0.40
19:V:233:ARG:NH2	20:W:280:CYS:O	2.54	0.40
1:A:789:ASN:HD22	1:A:790:ALA:N	2.19	0.40
1:A:832:LEU:HD23	1:A:834:HIS:H	1.86	0.40
3:C:51:GLU:N	3:C:310:PRO:HG3	2.37	0.40
7:G:98:LYS:HD3	7:G:109:PHE:HD1	1.87	0.40
9:I:14:ILE:HD13	9:I:24:LEU:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:141:ILE:HD12	15:O:153:LYS:NZ	2.36	0.40
18:U:66:THR:HG23	18:U:68:GLN:NE2	2.36	0.40
19:V:191:LEU:HA	19:V:238:ARG:HH22	1.85	0.40
19:V:273:GLN:HG2	19:V:274:LYS:HB2	2.03	0.40
20:W:489:LYS:HB3	20:W:489:LYS:HE2	1.91	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	1388/1460 (95%)	1263 (91%)	125 (9%)	0	100	100
2	B	1112/1149 (97%)	1011 (91%)	101 (9%)	0	100	100
3	C	333/335 (99%)	303 (91%)	30 (9%)	0	100	100
4	D	113/161 (70%)	101 (89%)	12 (11%)	0	100	100
5	E	212/215 (99%)	198 (93%)	14 (7%)	0	100	100
6	F	81/155 (52%)	72 (89%)	9 (11%)	0	100	100
7	G	174/212 (82%)	157 (90%)	16 (9%)	1 (1%)	28	70
8	H	136/146 (93%)	121 (89%)	15 (11%)	0	100	100
9	I	32/110 (29%)	25 (78%)	7 (22%)	0	100	100
10	J	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
11	K	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
12	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
13	M	155/282 (55%)	143 (92%)	12 (8%)	0	100	100
14	N	100/422 (24%)	89 (89%)	11 (11%)	0	100	100
15	O	528/654 (81%)	497 (94%)	31 (6%)	0	100	100
16	P	93/317 (29%)	84 (90%)	9 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	33/251 (13%)	29 (88%)	4 (12%)	0	100	100
18	U	178/240 (74%)	169 (95%)	9 (5%)	0	100	100
19	V	326/596 (55%)	303 (93%)	23 (7%)	0	100	100
20	W	161/594 (27%)	142 (88%)	19 (12%)	0	100	100
All	All	5362/7581 (71%)	4897 (91%)	464 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	79	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 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	1214/1257 (97%)	1194 (98%)	20 (2%)	68	85
2	B	975/1006 (97%)	962 (99%)	13 (1%)	73	87
3	C	296/296 (100%)	294 (99%)	2 (1%)	87	93
4	D	110/145 (76%)	105 (96%)	5 (4%)	32	63
5	E	196/197 (100%)	191 (97%)	5 (3%)	51	75
6	F	73/137 (53%)	72 (99%)	1 (1%)	71	86
7	G	160/190 (84%)	158 (99%)	2 (1%)	73	87
8	H	123/128 (96%)	123 (100%)	0	100	100
9	I	31/98 (32%)	30 (97%)	1 (3%)	44	71
10	J	62/65 (95%)	61 (98%)	1 (2%)	68	85
11	K	91/130 (70%)	90 (99%)	1 (1%)	78	89
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	138/249 (55%)	136 (99%)	2 (1%)	71	86
14	N	88/360 (24%)	86 (98%)	2 (2%)	56	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	490/593 (83%)	479 (98%)	11 (2%)	57	80
16	P	95/285 (33%)	91 (96%)	4 (4%)	34	65
17	Q	31/212 (15%)	30 (97%)	1 (3%)	44	71
18	U	152/205 (74%)	147 (97%)	5 (3%)	43	70
19	V	292/513 (57%)	288 (99%)	4 (1%)	71	86
20	W	149/534 (28%)	147 (99%)	2 (1%)	73	87
All	All	4806/6657 (72%)	4724 (98%)	82 (2%)	68	84

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
1	A	137	ARG
1	A	213	ARG
1	A	274	MET
1	A	310	ASN
1	A	367	ASN
1	A	410	ARG
1	A	499	ARG
1	A	535	MET
1	A	624	ILE
1	A	645	MET
1	A	774	ARG
1	A	783	ASN
1	A	789	ASN
1	A	794	MET
1	A	848	VAL
1	A	944	ASN
1	A	1187	ARG
1	A	1332	ARG
1	A	1439	LYS
2	B	66	ASN
2	B	383	LEU
2	B	427	ASN
2	B	481	ARG
2	B	816	ASP
2	B	859	ASN
2	B	867	ARG
2	B	885	MET
2	B	970	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1038	ARG
2	B	1054	ARG
2	B	1119	MET
2	B	1136	ASN
3	C	174	ARG
3	C	277	ARG
4	D	71	ASN
4	D	98	MET
4	D	120	LYS
4	D	130	ASN
4	D	153	MET
5	E	58	MET
5	E	88	VAL
5	E	93	MET
5	E	121	MET
5	E	215	MET
6	F	90	ARG
7	G	73	ARG
7	G	113	ASN
9	I	27	ARG
10	J	56	LEU
11	K	74	ASN
13	M	144	ASN
13	M	166	MET
14	N	297	MET
14	N	300	LYS
15	O	73	ARG
15	O	184	LYS
15	O	205	LYS
15	O	243	MET
15	O	268	LYS
15	O	286	ARG
15	O	516	LEU
15	O	580	ASN
15	O	594	LYS
15	O	631	ASN
15	O	636	ASN
16	P	189	ASN
16	P	239	ASN
16	P	271	MET
16	P	298	LYS
17	Q	57	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	U	104	MET
18	U	110	LYS
18	U	141	ARG
18	U	159	ASN
18	U	239	LYS
19	V	115	ASN
19	V	237	LEU
19	V	269	LYS
19	V	294	ARG
20	W	292	ASN
20	W	451	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	367	ASN
1	A	539	ASN
1	A	578	GLN
1	A	692	ASN
1	A	760	GLN
1	A	783	ASN
1	A	815	GLN
1	A	864	HIS
1	A	899	GLN
1	A	1058	GLN
1	A	1254	ASN
1	A	1318	HIS
2	B	66	ASN
2	B	159	ASN
2	B	203	ASN
2	B	217	GLN
2	B	315	GLN
2	B	321	GLN
2	B	427	ASN
2	B	596	GLN
2	B	600	HIS
2	B	733	GLN
2	B	753	GLN
2	B	801	HIS
2	B	859	ASN
2	B	893	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	928	GLN
2	B	1036	HIS
2	B	1136	ASN
3	C	175	GLN
3	C	207	HIS
3	C	234	ASN
3	C	296	ASN
4	D	71	ASN
4	D	130	ASN
5	E	3	GLN
5	E	61	GLN
5	E	153	HIS
5	E	174	GLN
7	G	31	ASN
7	G	113	ASN
8	H	139	ASN
10	J	26	GLN
10	J	53	HIS
11	K	74	ASN
13	M	92	ASN
13	M	128	GLN
13	M	141	ASN
13	M	144	ASN
13	M	190	ASN
15	O	56	HIS
15	O	152	HIS
15	O	161	GLN
15	O	225	ASN
15	O	283	ASN
15	O	332	GLN
15	O	549	GLN
15	O	580	ASN
15	O	584	ASN
15	O	631	ASN
15	O	636	ASN
16	P	189	ASN
16	P	239	ASN
18	U	68	GLN
18	U	91	ASN
18	U	144	GLN
18	U	159	ASN
19	V	6	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	V	21	ASN
19	V	115	ASN
19	V	473	HIS
19	V	505	GLN
20	W	292	ASN
20	W	491	ASN
20	W	499	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 ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.