Full wwPDB EM Validation Report ⓘ

Apr 24, 2023 – 12:23 PM JST

PDB ID	:	8HSR
EMDB ID	:	EMD-35004
Title	:	Thermus thermophilus Rho-engaged RNAP elongation complex
Authors	:	Murayama, Y.; Ehara, H.; Sekine, S.
Deposited on	:	2022-12-20
Resolution	:	4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

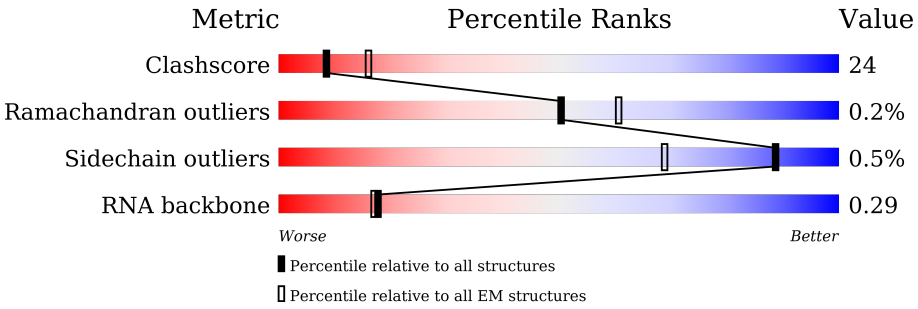
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 4.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	428	6% 36% 48% 16%
1	B	428	10% 39% 45% 16%
1	C	428	9% 39% 46% 14%
1	D	428	9% 42% 42% 16%
1	E	428	6% 38% 45% 16%
1	F	428	7% 39% 44% 16%
2	G	315	49% 23% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	315	47% 26% 27%
3	I	1119	5% 64% 36%
4	J	1532	8% 58% 27% 15%
5	K	99	20% 53% 37% 8%
6	T	184	16% 79%
7	R	125	7% 7% 12% 77%
8	N	180	7% 8% 84%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	BEF	B	502	-	-	X	-
11	BEF	C	1004	-	-	X	-
11	BEF	D	1002	-	-	X	-
11	BEF	F	1002	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 42577 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
1	B	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
1	C	367	Total	C	N	O	S	0	0
			2882	1814	526	535	7		
1	D	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
1	E	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		
1	F	361	Total	C	N	O	S	0	0
			2842	1790	517	528	7		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q5SJE9
A	0	PRO	-	expression tag	UNP Q5SJE9
B	-1	GLY	-	expression tag	UNP Q5SJE9
B	0	PRO	-	expression tag	UNP Q5SJE9
C	-1	GLY	-	expression tag	UNP Q5SJE9
C	0	PRO	-	expression tag	UNP Q5SJE9
D	-1	GLY	-	expression tag	UNP Q5SJE9
D	0	PRO	-	expression tag	UNP Q5SJE9
E	-1	GLY	-	expression tag	UNP Q5SJE9
E	0	PRO	-	expression tag	UNP Q5SJE9
F	-1	GLY	-	expression tag	UNP Q5SJE9
F	0	PRO	-	expression tag	UNP Q5SJE9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		
2	H	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	1119	Total	C	N	O	S	0	0
			8829	5581	1577	1647	24		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	1303	Total	C	N	O	S	0	0
			10280	6508	1821	1919	32		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1525	ASP	-	expression tag	UNP Q8RQE8
J	1526	TYR	-	expression tag	UNP Q8RQE8
J	1527	LYS	-	expression tag	UNP Q8RQE8
J	1528	ASP	-	expression tag	UNP Q8RQE8
J	1529	ASP	-	expression tag	UNP Q8RQE8
J	1530	ASP	-	expression tag	UNP Q8RQE8
J	1531	ASP	-	expression tag	UNP Q8RQE8
J	1532	LYS	-	expression tag	UNP Q8RQE8

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	91	Total	C	N	O	S	0	0
			735	467	129	135	4		

- Molecule 6 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	38	Total	C	N	O	P	0	0
			786	371	154	223	38		

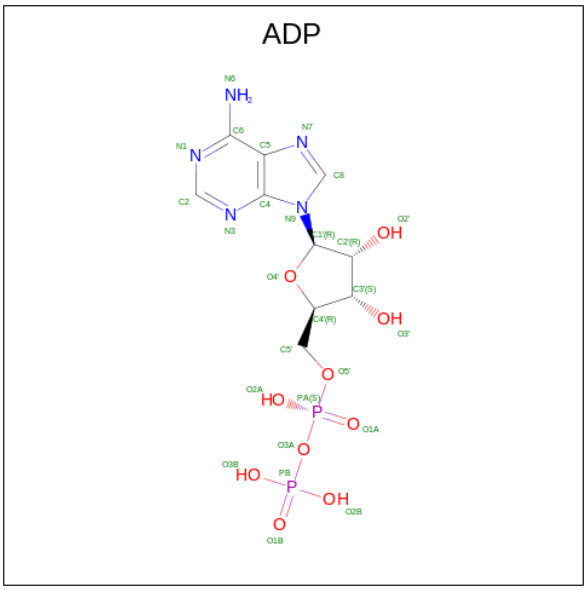
- Molecule 7 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	29	Total	C	N	O	P	0	0
			474	208	47	190	29		

- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	28	Total	C	N	O	P	0	0
			574	273	99	174	28		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

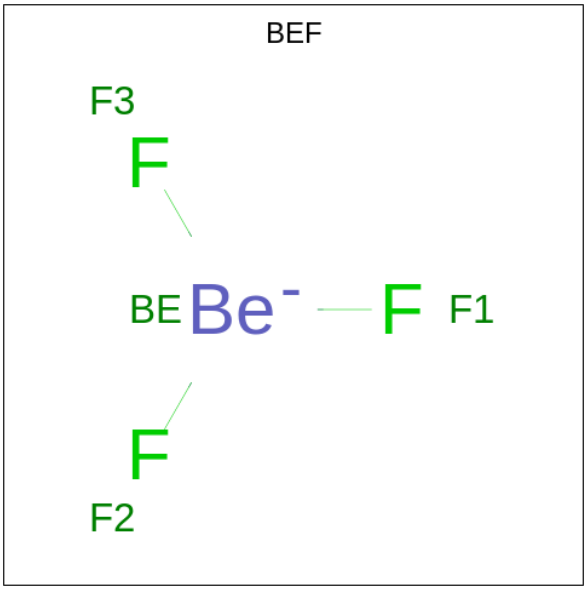


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Mg 1 1	0
10	C	2	Total Mg 2 2	0
10	D	1	Total Mg 1 1	0
10	E	1	Total Mg 1 1	0
10	F	1	Total Mg 1 1	0
10	J	1	Total Mg 1 1	0

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total Be F 4 1 3	0
11	B	1	Total Be F 4 1 3	0
11	C	1	Total Be F 4 1 3	0
11	D	1	Total Be F 4 1 3	0
11	E	1	Total Be F 4 1 3	0
11	F	1	Total Be F 4 1 3	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

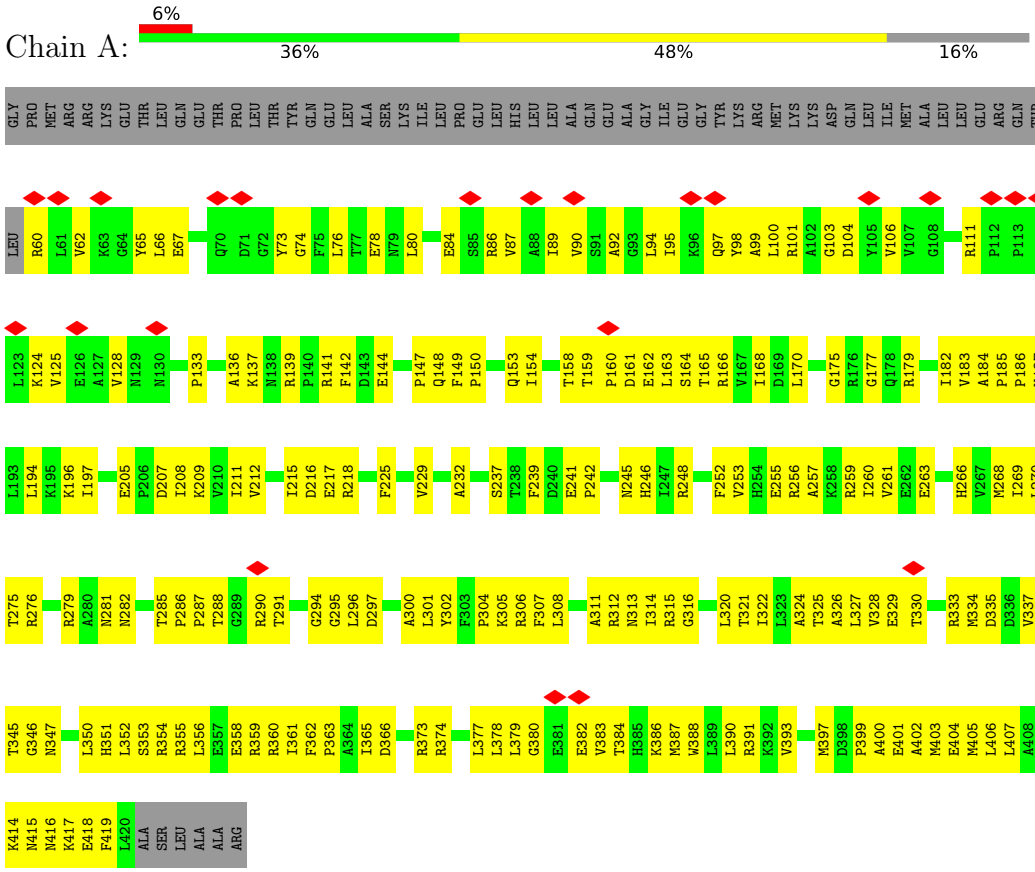
Mol	Chain	Residues	Atoms	AltConf
12	J	2	Total Zn 2 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

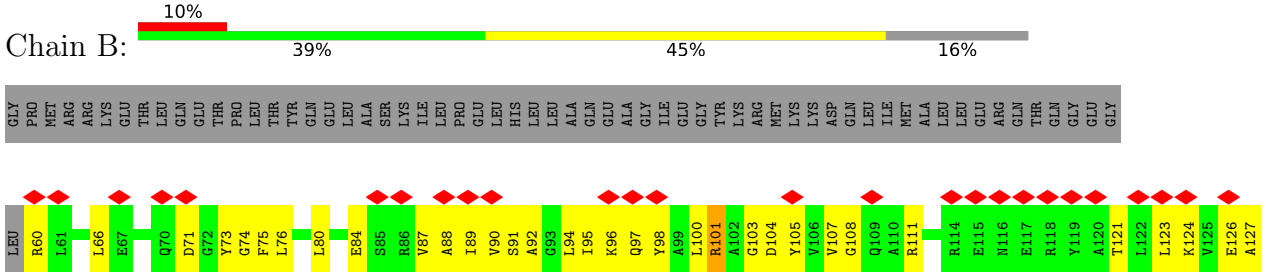
• Molecule 1: Transcription termination factor Rho

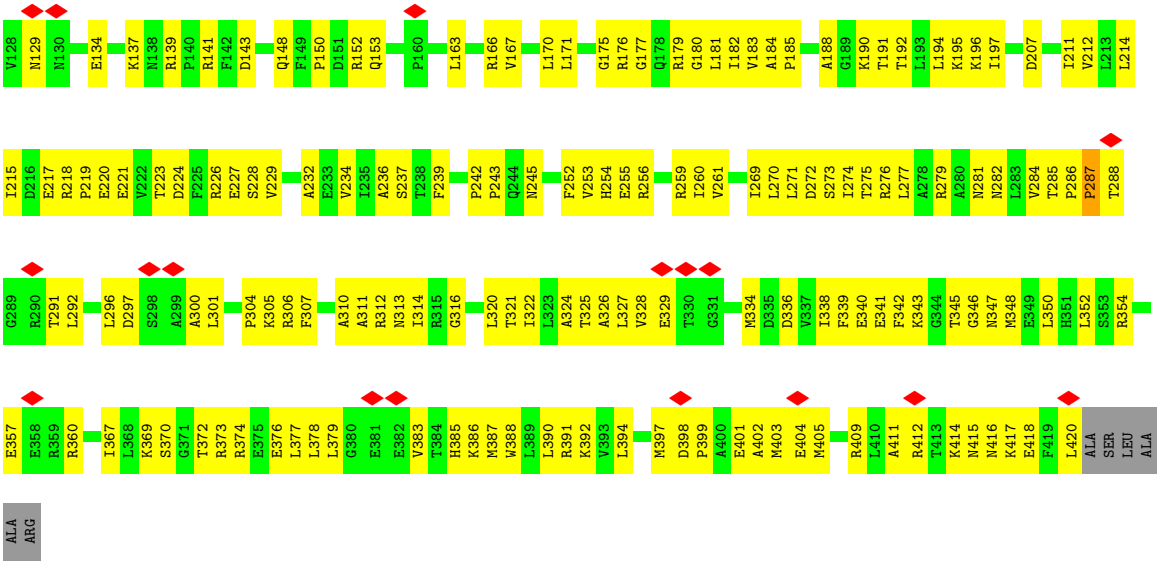
Chain A:



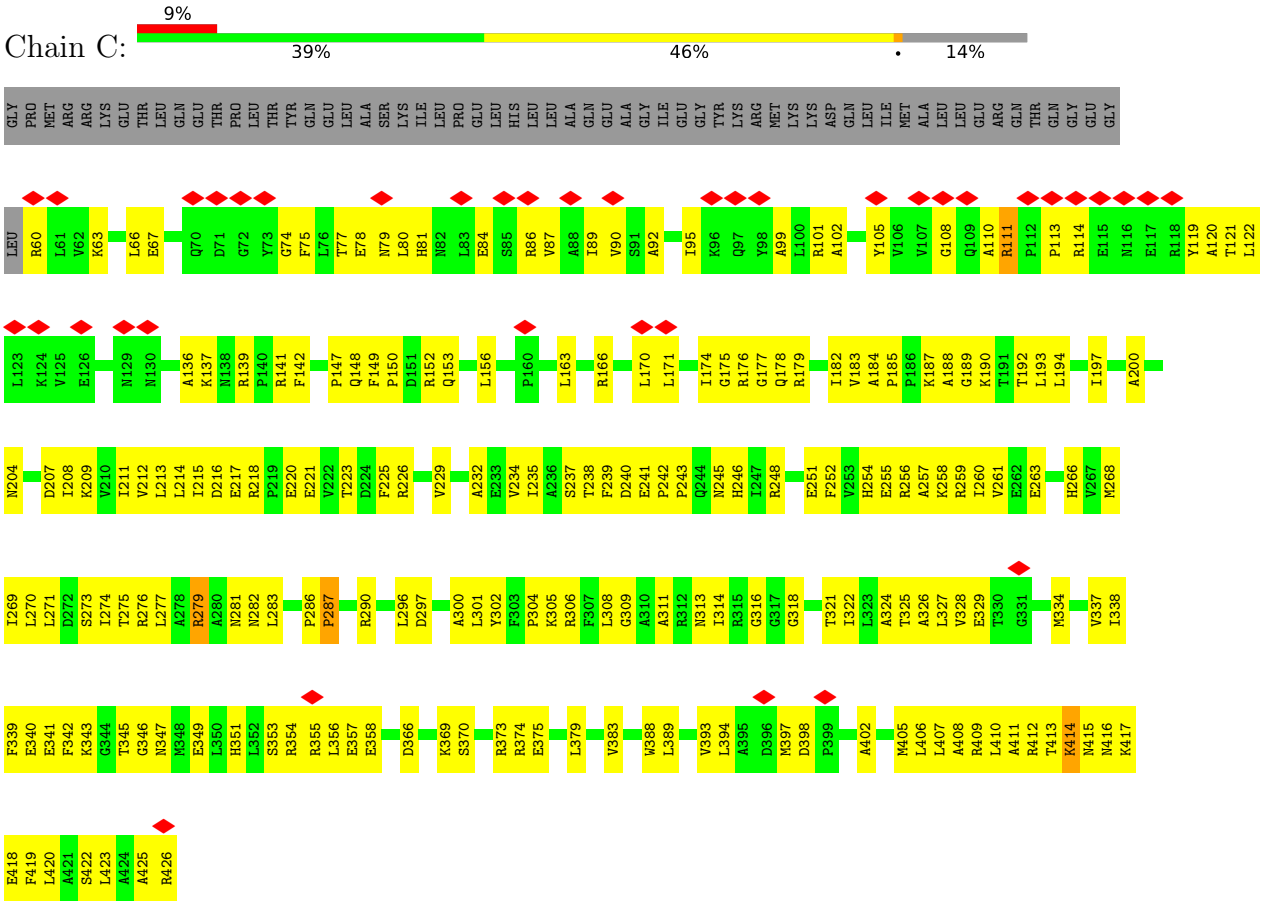
• Molecule 1: Transcription termination factor Rho

Chain B:

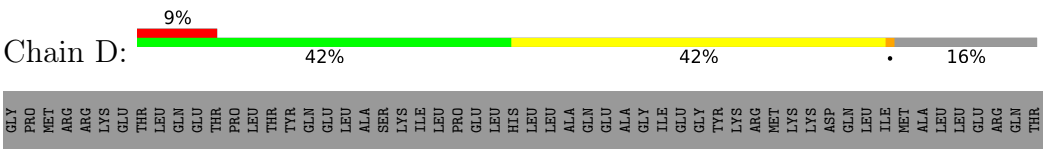


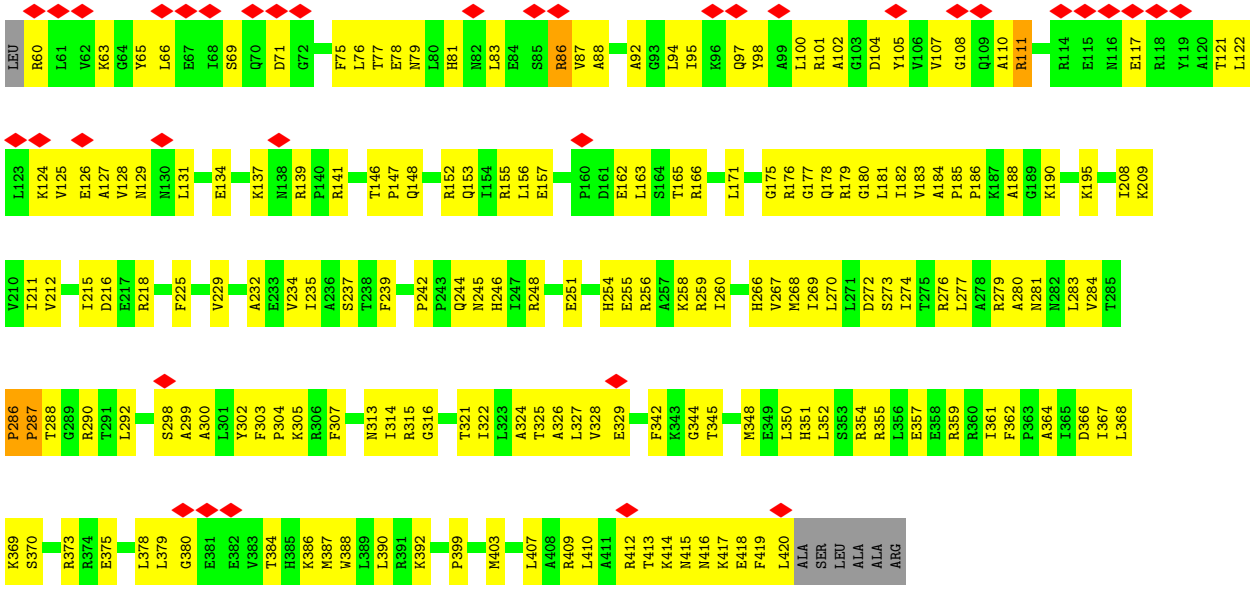


• Molecule 1: Transcription termination factor Rho

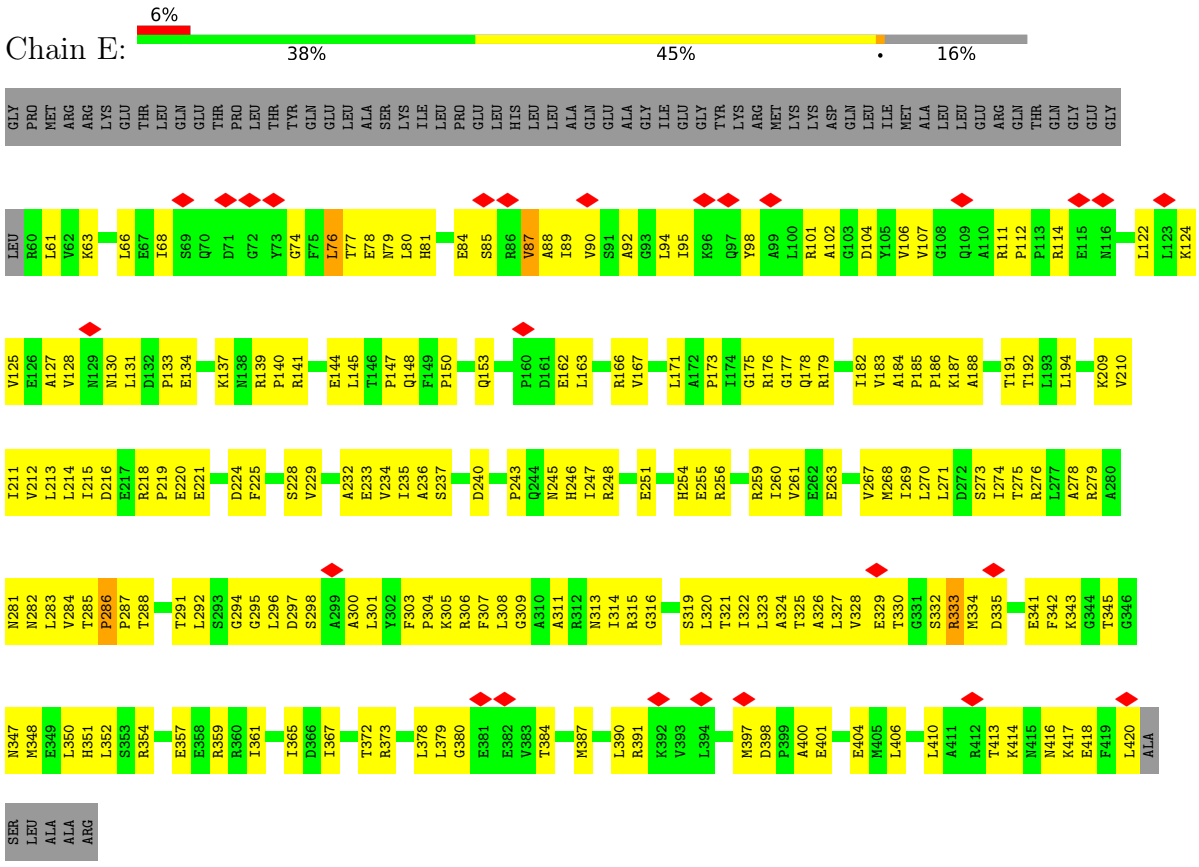


• Molecule 1: Transcription termination factor Rho

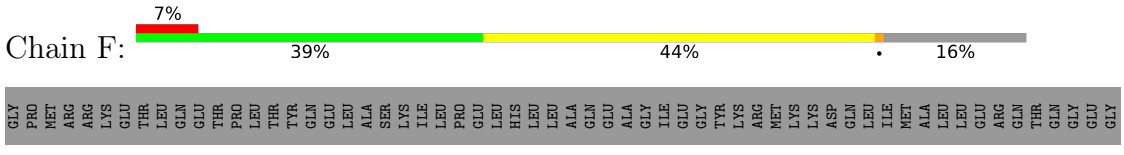


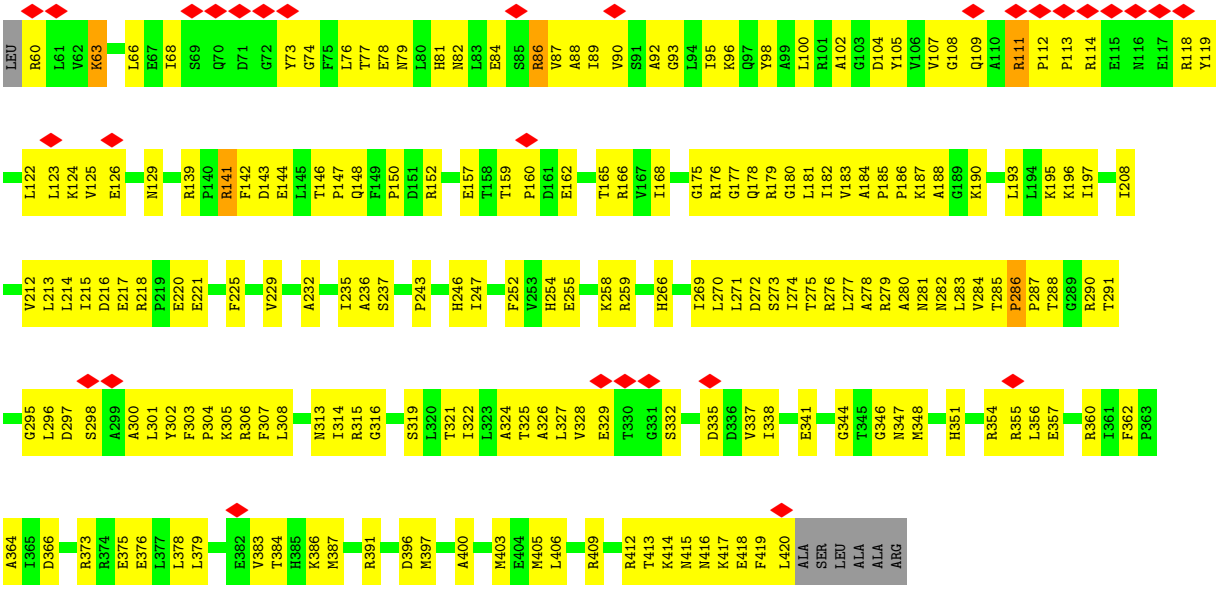


• Molecule 1: Transcription termination factor Rho



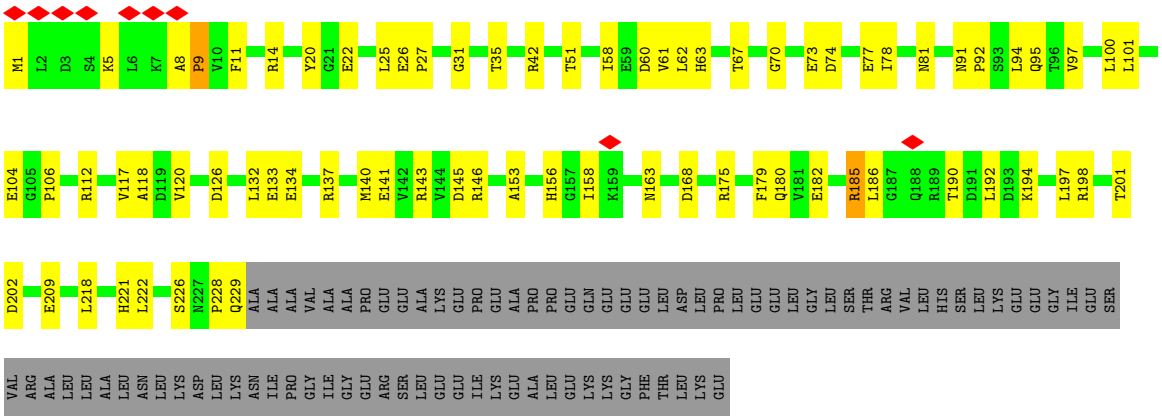
• Molecule 1: Transcription termination factor Rho





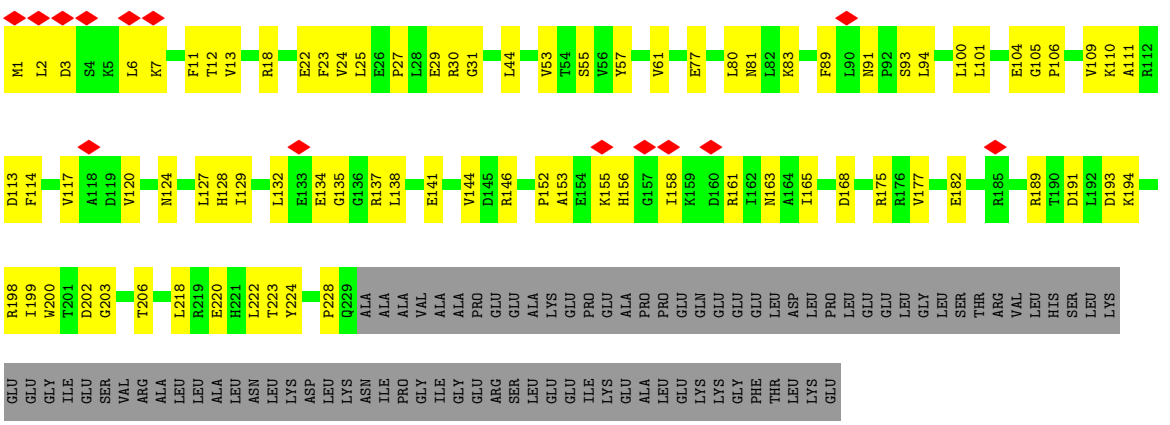
• Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain G:



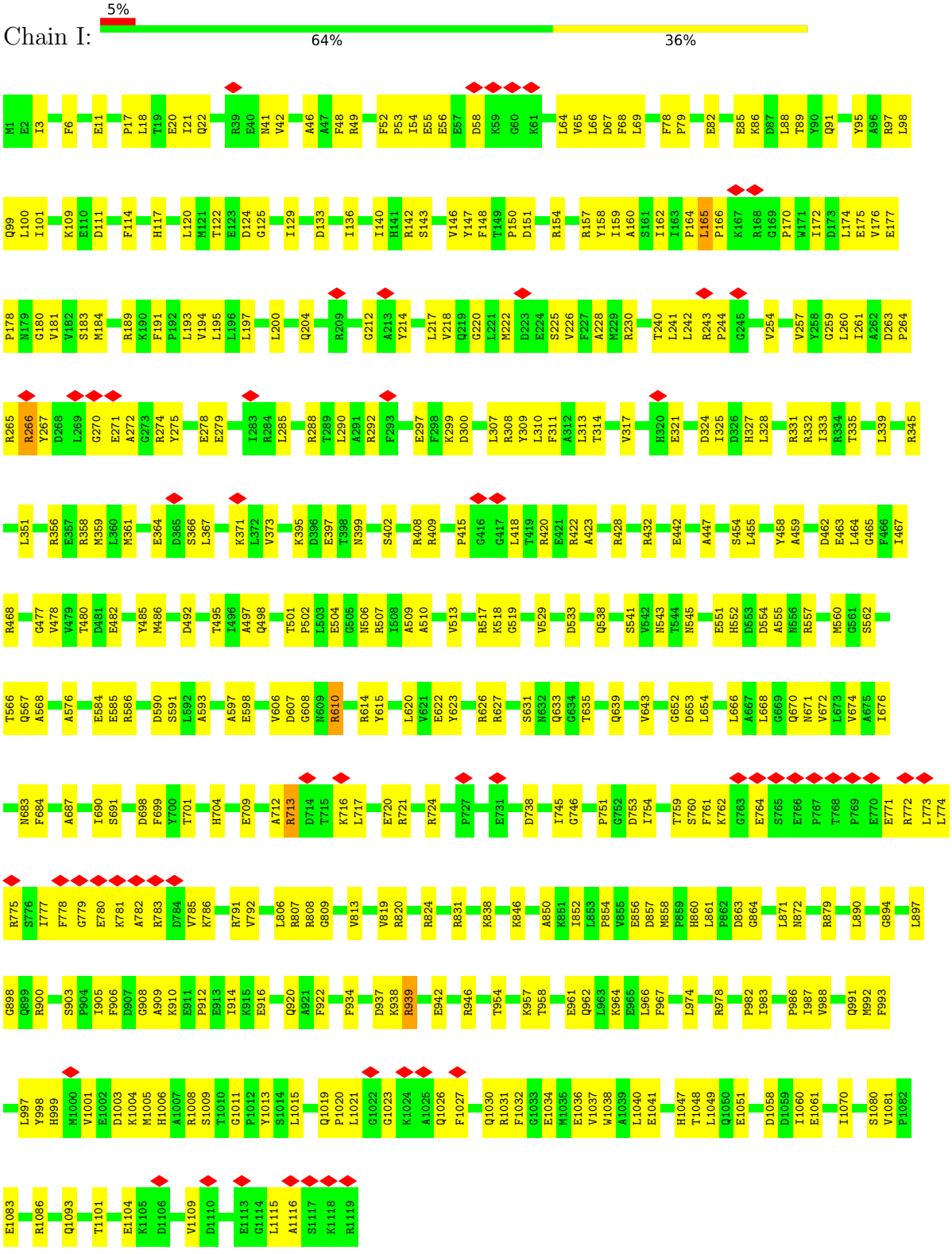
• Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain H:



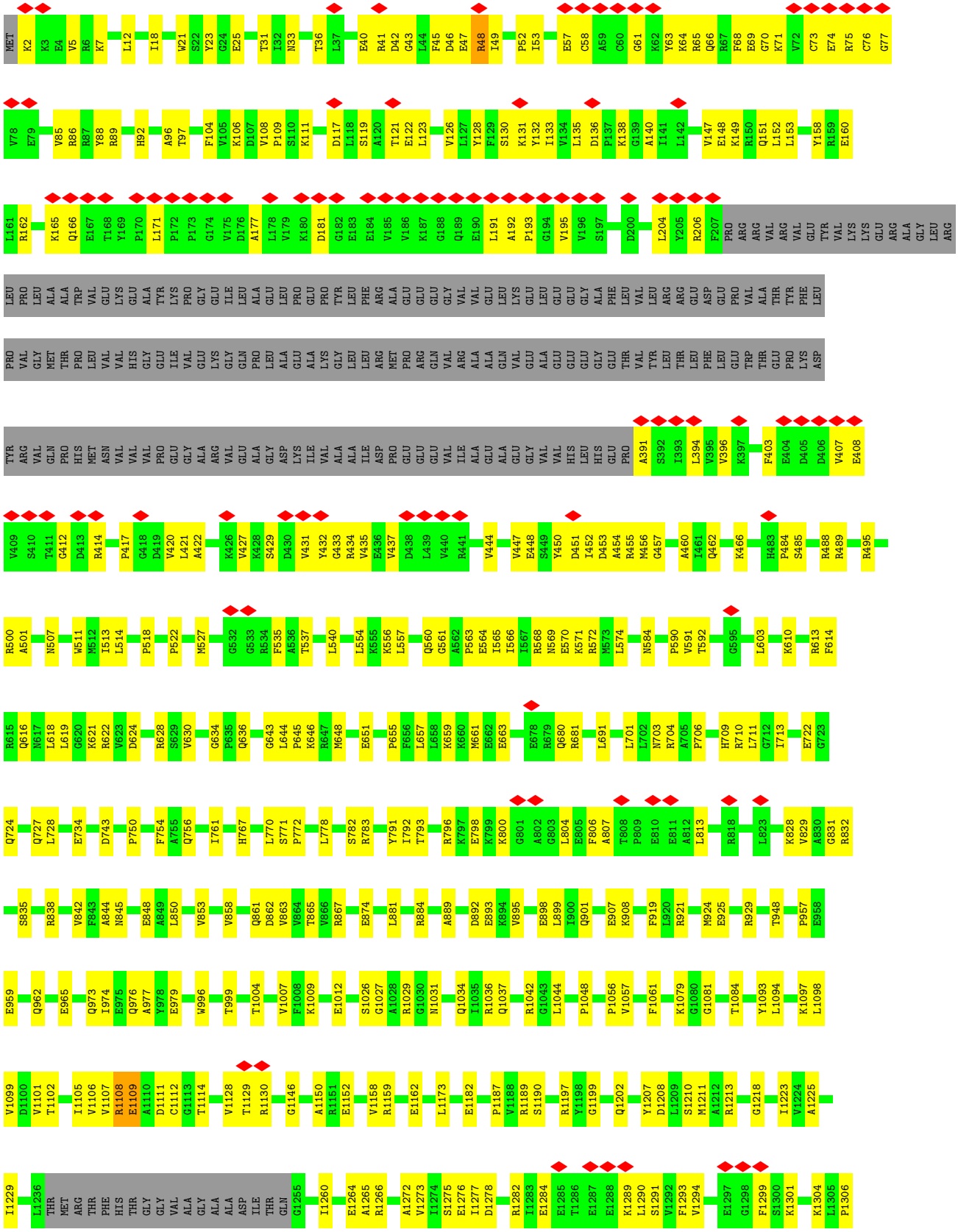
• Molecule 3: DNA-directed RNA polymerase subunit beta

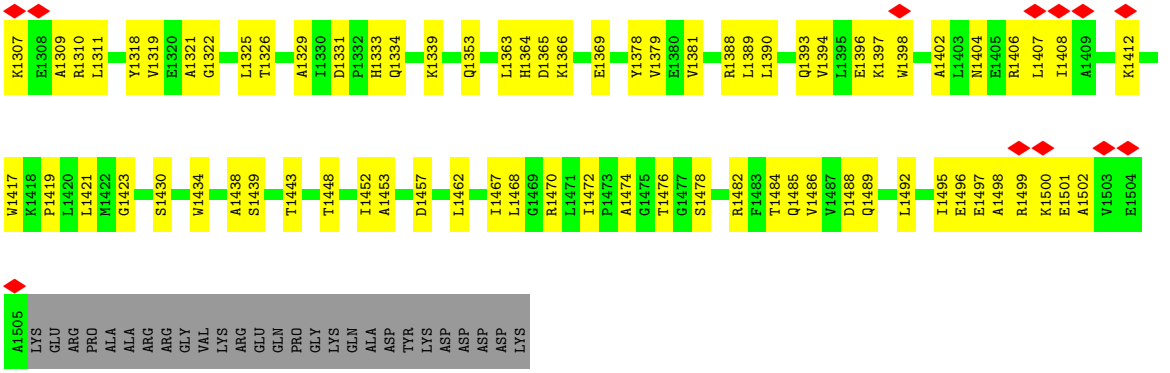
Chain I:



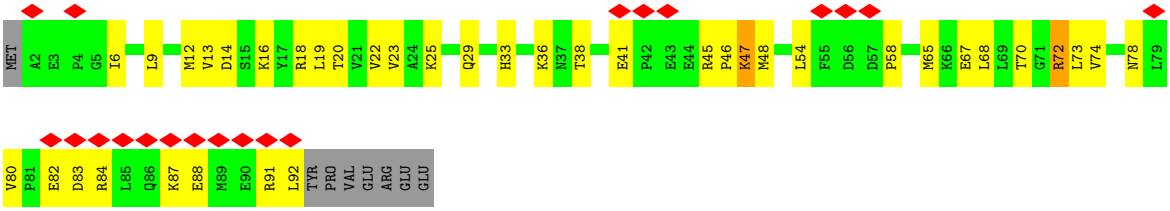
• Molecule 4: DNA-directed RNA polymerase subunit beta'

Chain J:

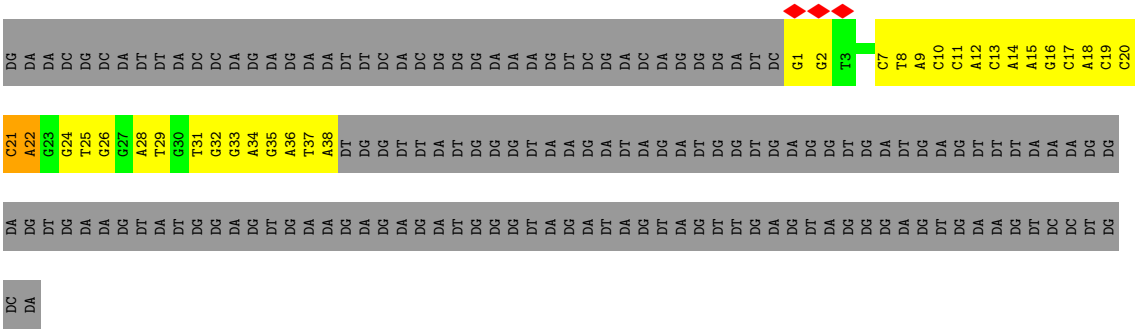

MET K2 K3 E4 V5 R6 K7 L12 I18 W21 S22 Y23 G24 E25 T31 I32 N33 T36 L37 E40 R41 D42 G43 L44 F45 D46 E47 R48 I49 P52 I53 E57 C58 A59 C60 G61 K62 Y63 K64 R65 Q66 R67 F68 E69 G70 K71 V72 C73 E74 R75 C76 G77
V78 E79 V85 R86 R87 Y88 R89 H92 A96 T97 F104 V105 K106 D107 V108 P109 S110 K111 D117 L118 S119 A120 T121 E122 L123 V126 L127 Y128 F129 S130 K131 Y132 I133 V134 L135 D136 P137 K138 G139 A140 I141 L142 V147 E148 K149 R150 Q151 L152 L153 Y158 R159 E160
L161 R162 K165 Q166 E167 T168 Y169 P170 L171 P172 P173 G174 V175 D176 A177 L178 V179 K180 D181 G182 E183 E184 V185 V186 K187 G188 Q189 E190 L191 A192 P193 G194 V195 V196 S197 D200 L204 Y205 R206 F207 PRO ARG ARG VAL ARG VAL GLU TYR VAL LYS LYS GLU ARG ALA GLY LEU ARG
LEU PRO LEU ALA ALA TRP VAL GLU LYS GLU ALA TYR LYS PRO GLY GLU ILE LEU ALA GLU LEU PRO GLU PRO TYR LEU PHE ARG ALA GLU GLU GLU GLY VAL VAL GLU LEU LYS GLU LEU GLU GLU GLY ALA PHE LEU VAL LEU ARG ARG GLU ASP GLU PRO VAL ALA THR TYR PHE LEU
PRO VAL GLY MET THR PRO LEU VAL VAL VAL HIS GLY GLY GLU ILE VAL GLU LYS GLY GLN PRO LEU ALA GLU ALA LYS GLY LEU LEU ARG MET PRO ARG GLN VAL ARG ALA ALA GLN VAL GLU ALA GLU GLU GLU GLY GLU THR VAL TYR LEU THR LEU PHE LEU GLU TRP THR GLU PRO LYS ASP
TYR ARG VAL GLN PRO HIS MET ASN VAL VAL VAL PRO GLU GLY ALA ARG VAL GLU ALA GLY ASP LYS ILE VAL ALA ALA ILE ASP PRO GLU GLU GLU VAL ILE ALA GLU ALA GLU GLY VAL VAL HIS LEU HIS GLU PRO A391 S392 I393 L394 V395 V396 K397 F403 E404 D405 D406 V407 E408
V409 S410 T411 G412 D413 R414 P417 G418 D419 V420 L421 A422 K426 V427 K428 S429 D430 V431 Y432 G433 R434 V435 E436 V437 D438 L439 V440 R441 V444 V447 E448 S449 Y450 D451 I452 D453 A454 R455 M456 G457 A460 I461 Q462 K466 H483 P484 S485 R488 R489 R495
R500 A501 N507 W511 M512 I513 L514 P518 P522 M527 G532 G533 R534 F535 A536 T537 L540 L554 K555 K556 L557 Q560 G561 A562 P563 E564 I565 I566 I567 R568 N569 E570 K571 R572 M573 L574 N584 P590 V591 T592 G596 L603 K610 R613 F614
R615 Q616 N617 L618 L619 G620 K621 R622 V623 D624 R628 S629 V630 G634 P635 Q636 G643 L644 P645 K646 R647 M648 E651 P655 F656 L657 L658 K659 K660 M661 E662 E663 E678 R679 Q680 R681 L691 L701 L702 N703 R704 A705 P706 H709 R710 L711 G712 I713 E722 G723
Q724 Q727 L728 E734 D743 P750 F754 A755 Q756 I761 H767 L770 S771 P772 L778 S782 R783 Y791 I792 T793 R796 K797 E798 K799 K800 G801 A802 G803 L804 E805 F806 A807 T808 P809 E810 E811 A812 L813 R818 L823 K828 V829 A830 G831 R832
S835 R838 V842 F843 A844 N845 E848 A849 L850 V853 V858 Q861 D862 V863 V864 T865 V866 R867 E874 L881 R884 A889 D892 E893 K894 V895 E898 L899 I900 Q901 E907 K908 F919 L920 R921 M924 E925 R929 T948 P957 E958
E959 Q962 E965 Q973 I974 E975 Q976 A977 Y978 E979 W996 T999 T1004 V1007 F1008 K1009 E1012 S1026 G1027 A1028 R1029 G1030 N1031 Q1034 I1035 R1036 Q1037 R1042 G1043 L1044 P1048 P1056 V1057 F1061 K1079 G1080 G1081 T1084 Y1093 L1094 K1097 L1098
V1099 D1100 V1101 T1102 I1105 V1106 V1107 R1108 E1109 A1110 D1111 C1112 G1113 T1114 V1128 T1129 R1130 G1146 A1150 R1151 E1152 V1158 R1159 E1162 L1173 E1182 P1187 Y1188 R1189 S1190 R1197 Y1198 G1199 Q1202 Y1207 D1208 L1209 S1210 M1211 A1212 R1213 G1218 I1223 V1224 A1225
I1229 L1236 THR MET ARG THR PHE HIS THR GLY GLY VAL ALA GLY ALA ALA ASP ILE THR GLN G1255 I1260 E1264 A1265 R1266 A1272 V1273 I1274 S1275 E1276 I1277 D1278 R1282 I1283 E1284 E1285 T1286 E1287 E1288 K1289 L1290 S1291 V1292 F1293 V1294 E1297 G1298 F1299 S1300 K1301 K1304 L1305 P1306



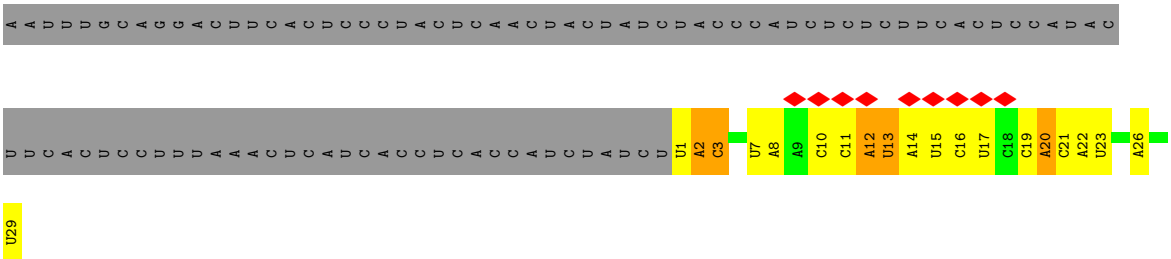
• Molecule 5: DNA-directed RNA polymerase subunit omega



• Molecule 6: DNA (41-MER)

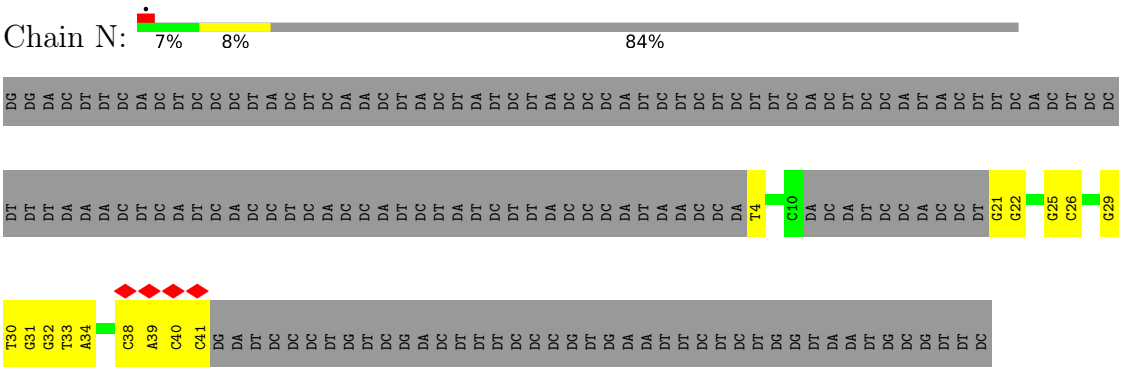


• Molecule 7: RNA (29-MER)



• Molecule 8: DNA (31-MER)

Chain N:


7%
8%
84%
T4
C10
G21
G22
G25
C26
G29
T30
G31
G32
T33
A34
C38
A39
C40
C41

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	17.972	Depositor
Minimum map value	-6.489	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.925	Depositor
Recommended contour level	4.4	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/2886	0.59	0/3900
1	B	0.31	0/2886	0.59	0/3900
1	C	0.30	0/2926	0.61	0/3954
1	D	0.29	0/2886	0.58	0/3900
1	E	0.30	0/2886	0.61	2/3900 (0.1%)
1	F	0.28	0/2886	0.58	0/3900
2	G	0.31	0/1838	0.54	0/2498
2	H	0.29	0/1838	0.54	0/2498
3	I	0.32	0/8997	0.56	1/12164 (0.0%)
4	J	0.31	0/10452	0.54	0/14116
5	K	0.30	0/747	0.60	0/1005
6	T	0.74	0/884	1.03	4/1363 (0.3%)
7	R	0.35	0/520	0.85	0/801
8	N	0.60	0/640	1.00	0/984
All	All	0.33	0/43272	0.60	7/58883 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
4	J	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	32	DG	O5'-P-OP1	-8.37	98.17	105.70
6	T	31	DT	OP1-P-O3'	7.46	121.61	105.20
1	E	76	LEU	CA-CB-CG	6.44	130.11	115.30
6	T	21	DC	P-O3'-C3'	6.26	127.21	119.70
3	I	165	LEU	CA-CB-CG	5.43	127.79	115.30
6	T	22	DA	O4'-C4'-C3'	-5.34	102.37	104.50
1	E	87	VAL	CG1-CB-CG2	-5.30	102.42	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	9	PRO	Peptide
4	J	1109	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2842	0	2924	204	0
1	B	2842	0	2924	198	0
1	C	2882	0	2968	239	0
1	D	2842	0	2924	196	0
1	E	2842	0	2924	209	0
1	F	2842	0	2925	211	0
2	G	1806	0	1861	58	0
2	H	1806	0	1861	68	0
3	I	8829	0	8933	342	0
4	J	10280	0	10509	357	0
5	K	735	0	752	75	0
6	T	786	0	422	78	0
7	R	474	0	246	14	0
8	N	574	0	317	50	0
9	A	27	0	12	8	0
9	B	27	0	12	8	0
9	C	27	0	12	8	0
9	D	27	0	12	5	0
9	E	27	0	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	27	0	10	3	0
10	A	1	0	0	0	0
10	C	2	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	J	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	4	0
11	C	4	0	0	5	0
11	D	4	0	0	2	0
11	E	4	0	0	1	0
11	F	4	0	0	2	0
12	J	2	0	0	0	0
All	All	42577	0	42559	2039	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 24.

All (2039) 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)
6:T:10:DC:N3	8:N:32:DG:N1	1.62	1.46
6:T:10:DC:N4	8:N:32:DG:O6	1.58	1.35
6:T:10:DC:O2	8:N:32:DG:N2	1.57	1.35
1:C:413:THR:OG1	5:K:84:ARG:NH2	1.61	1.34
1:C:412:ARG:HD2	5:K:83:ASP:OD2	1.23	1.31
1:B:297:ASP:OD2	1:C:290:ARG:NH1	1.68	1.26
4:J:1492:LEU:HD22	5:K:74:VAL:HG21	1.20	1.18
1:E:218:ARG:NH2	1:F:344:GLY:O	1.77	1.17
1:C:240:ASP:O	1:D:302:TYR:OH	1.64	1.12
6:T:9:DA:N1	8:N:33:DT:N3	1.97	1.11
1:C:218:ARG:NH2	1:D:344:GLY:O	1.82	1.10
3:I:1031:ARG:HD3	6:T:25:DT:OP2	1.53	1.07
1:E:240:ASP:O	1:F:302:TYR:OH	1.71	1.07
1:E:291:THR:HG23	1:F:290:ARG:HH21	1.12	1.06
1:C:297:ASP:OD1	1:D:290:ARG:NH2	1.91	1.03
1:C:408:ALA:CB	5:K:87:LYS:HE3	1.92	1.00
6:T:10:DC:C2	8:N:32:DG:N2	2.30	0.99
1:C:218:ARG:NH2	1:D:344:GLY:C	2.17	0.97
1:C:192:THR:OG1	9:C:1002:ADP:N7	1.94	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:SER:HB3	1:B:276:ARG:HB3	1.47	0.96
6:T:9:DA:C6	8:N:32:DG:C6	2.53	0.96
4:J:1485:GLN:NE2	5:K:82:GLU:HB3	1.82	0.95
6:T:10:DC:N4	8:N:32:DG:C6	2.35	0.95
1:C:283:LEU:CD2	1:D:298:SER:HB3	1.95	0.95
6:T:9:DA:C6	8:N:32:DG:O6	2.21	0.94
6:T:38:DA:N1	8:N:4:DT:N3	2.16	0.93
1:C:273:SER:HB3	1:C:276:ARG:HB2	1.50	0.93
1:C:412:ARG:CD	5:K:83:ASP:OD2	2.15	0.91
1:C:223:THR:HG21	1:D:147:PRO:HD2	1.54	0.90
1:C:425:ALA:HB1	5:K:88:GLU:OE2	1.71	0.90
6:T:38:DA:C2	8:N:4:DT:N3	2.38	0.90
1:C:217:GLU:OE2	11:C:1004:BEF:F3	1.81	0.88
3:I:240:THR:O	3:I:243:ARG:NH2	2.07	0.88
1:E:273:SER:HB3	1:E:276:ARG:HB2	1.54	0.87
1:C:283:LEU:HD22	1:D:298:SER:HB3	1.55	0.87
1:E:295:GLY:C	1:F:290:ARG:NH2	2.28	0.87
1:C:166:ARG:NH1	1:C:413:THR:O	2.08	0.86
1:C:408:ALA:HB3	5:K:87:LYS:HE3	1.54	0.86
6:T:10:DC:C4	8:N:32:DG:N1	2.43	0.86
1:F:215:ILE:O	1:F:276:ARG:NH2	2.08	0.86
1:C:286:PRO:HG2	1:C:287:PRO:HD3	1.55	0.86
4:J:1485:GLN:HE21	5:K:82:GLU:CB	1.89	0.85
3:I:1031:ARG:HB3	6:T:24:DG:H5”	1.58	0.85
6:T:10:DC:N3	8:N:32:DG:C2	2.44	0.85
1:E:185:PRO:HG3	1:E:354:ARG:HB2	1.59	0.85
1:C:297:ASP:CG	1:D:290:ARG:NH2	2.31	0.84
3:I:324:ASP:HB3	3:I:327:HIS:HB2	1.59	0.84
6:T:38:DA:N1	8:N:4:DT:C4	2.44	0.84
1:E:332:SER:OG	1:E:334:MET:SD	2.35	0.84
4:J:63:TYR:HB2	4:J:73:CYS:HA	1.60	0.83
4:J:1485:GLN:NE2	5:K:82:GLU:CB	2.40	0.83
1:D:186:PRO:O	1:D:354:ARG:NH2	2.12	0.83
4:J:65:ARG:NH2	7:R:13:U:OP1	2.11	0.82
1:B:275:THR:OG1	1:B:327:LEU:N	2.12	0.82
1:C:413:THR:CB	5:K:84:ARG:NH2	2.42	0.82
1:C:413:THR:OG1	5:K:84:ARG:CZ	2.27	0.82
4:J:162:ARG:HH22	4:J:451:ASP:HA	1.43	0.82
1:A:391:ARG:HD3	1:F:360:ARG:HH21	1.45	0.82
1:C:282:ASN:OD1	1:D:290:ARG:NH1	2.12	0.82
1:C:220:GLU:OE2	1:D:179:ARG:NH2	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:VAL:HG22	5:K:92:LEU:HD12	1.61	0.81
1:C:408:ALA:HB1	5:K:87:LYS:HE3	1.60	0.81
1:F:297:ASP:HB2	1:F:300:ALA:HB2	1.61	0.81
1:A:279:ARG:NH1	1:A:335:ASP:OD1	2.14	0.80
6:T:9:DA:N1	8:N:32:DG:C6	2.50	0.80
1:E:288:THR:OG1	1:E:297:ASP:OD1	1.99	0.80
1:A:187:LYS:HE3	1:B:373:ARG:NH1	1.96	0.80
1:D:412:ARG:HG2	1:D:413:THR:HG23	1.64	0.80
1:E:305:LYS:O	1:E:309:GLY:N	2.15	0.80
5:K:6:ILE:HA	5:K:9:LEU:HD12	1.64	0.79
6:T:10:DC:C2	8:N:32:DG:N1	2.49	0.79
1:F:214:LEU:HB2	1:F:236:ALA:HA	1.65	0.79
4:J:206:ARG:O	4:J:391:ALA:HA	1.82	0.79
1:B:184:ALA:HB2	1:B:352:LEU:HB2	1.65	0.79
1:C:101:ARG:HH21	1:C:141:ARG:HD3	1.46	0.78
1:C:217:GLU:OE1	11:C:1004:BEF:F1	1.92	0.78
1:F:182:ILE:HD11	1:F:325:THR:HG22	1.65	0.78
1:F:217:GLU:HG2	1:F:276:ARG:HH22	1.46	0.78
1:F:273:SER:O	1:F:277:LEU:N	2.17	0.78
1:A:275:THR:HB	1:A:279:ARG:HH12	1.47	0.78
1:C:139:ARG:NH1	1:C:263:GLU:OE2	2.16	0.78
1:E:125:VAL:HB	1:E:133:PRO:HG3	1.66	0.78
6:T:10:DC:N3	8:N:32:DG:C6	2.51	0.78
4:J:1485:GLN:NE2	5:K:82:GLU:CA	2.47	0.78
1:D:409:ARG:NH1	1:D:418:GLU:OE2	2.16	0.78
1:C:218:ARG:HH21	1:D:344:GLY:C	1.88	0.78
1:B:217:GLU:OE1	1:B:276:ARG:NH1	2.16	0.77
1:C:414:LYS:O	1:C:418:GLU:N	2.17	0.77
1:C:63:LYS:O	1:C:86:ARG:NH1	2.17	0.77
1:A:379:LEU:HD13	1:A:387:MET:HG3	1.67	0.77
1:F:273:SER:HB3	1:F:276:ARG:HB3	1.66	0.77
1:E:291:THR:HG23	1:F:290:ARG:NH2	1.96	0.77
1:D:180:GLY:HA2	1:D:348:MET:HB3	1.65	0.77
1:B:282:ASN:ND2	1:B:334:MET:SD	2.58	0.77
3:I:274:ARG:NH1	3:I:285:LEU:O	2.18	0.77
4:J:1485:GLN:NE2	5:K:82:GLU:HA	2.00	0.76
4:J:1486:VAL:O	5:K:29:GLN:NE2	2.15	0.76
1:A:74:GLY:H	1:A:90:VAL:H	1.33	0.76
1:A:189:GLY:N	9:A:1000:ADP:O5'	2.06	0.76
1:A:373:ARG:CZ	1:F:218:ARG:HH22	1.99	0.76
1:A:401:GLU:O	1:A:405:MET:HG3	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASP:CA	1:D:290:ARG:HH22	1.99	0.76
2:H:80:LEU:HD21	4:J:867:ARG:HB2	1.67	0.76
1:A:393:VAL:HG13	3:I:773:LEU:HD22	1.68	0.76
4:J:807:ALA:H	4:J:832:ARG:HE	1.34	0.75
1:C:297:ASP:HA	1:D:290:ARG:HH22	1.50	0.75
2:H:53:VAL:HA	2:H:144:VAL:HG22	1.69	0.75
3:I:97:ARG:HG3	3:I:111:ASP:HA	1.66	0.75
1:B:215:ILE:O	1:B:276:ARG:NH2	2.17	0.75
1:A:414:LYS:HE2	1:A:417:LYS:HG3	1.69	0.75
3:I:1049:LEU:HD23	4:J:1472:ILE:HD11	1.68	0.75
1:E:283:LEU:HD12	1:F:298:SER:HB3	1.69	0.74
1:F:328:VAL:HG13	1:F:329:GLU:HG3	1.69	0.74
6:T:10:DC:C2	8:N:32:DG:C2	2.74	0.74
1:E:150:PRO:HB2	1:E:378:LEU:HD21	1.68	0.74
1:B:180:GLY:HA2	1:B:348:MET:HB3	1.69	0.74
4:J:835:SER:H	4:J:838:ARG:HH21	1.34	0.74
1:A:186:PRO:O	1:A:354:ARG:NH2	2.21	0.74
1:A:379:LEU:O	1:A:384:THR:OG1	2.05	0.74
3:I:1023:GLY:N	3:I:1026:GLN:O	2.20	0.74
1:D:102:ALA:O	1:D:259:ARG:NE	2.20	0.74
1:A:216:ASP:O	1:A:276:ARG:NH2	2.19	0.73
1:A:184:ALA:HB3	1:A:190:LYS:HD3	1.69	0.73
1:F:282:ASN:HA	1:F:285:THR:HB	1.70	0.73
3:I:1006:HIS:NE2	6:T:26:DG:H5"	2.02	0.73
1:A:166:ARG:NH2	1:A:410:LEU:O	2.22	0.73
1:C:245:ASN:OD1	1:C:248:ARG:NH2	2.22	0.73
6:T:9:DA:N6	8:N:32:DG:O6	2.22	0.73
6:T:10:DC:C4	8:N:32:DG:C6	2.76	0.73
1:A:245:ASN:OD1	1:A:248:ARG:NH2	2.22	0.73
1:C:179:ARG:NH1	1:C:311:ALA:O	2.21	0.73
3:I:1008:ARG:HH21	3:I:1011:GLY:H	1.34	0.73
1:A:347:ASN:HA	1:A:373:ARG:HD2	1.71	0.73
2:H:182:GLU:HG2	2:H:194:LYS:HB3	1.71	0.73
1:E:295:GLY:C	1:F:290:ARG:HH22	1.92	0.72
3:I:1015:LEU:HG	7:R:19:C:H41	1.53	0.72
1:E:219:PRO:HB2	1:F:147:PRO:HG2	1.70	0.72
1:A:185:PRO:HG2	1:A:354:ARG:HB2	1.72	0.72
1:B:98:TYR:OH	1:B:124:LYS:NZ	2.21	0.72
3:I:189:ARG:NH2	3:I:241:LEU:O	2.23	0.72
1:D:414:LYS:O	1:D:418:GLU:N	2.22	0.72
1:E:304:PRO:HA	1:E:307:PHE:HB2	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:670:GLN:NE2	3:I:699:PHE:O	2.23	0.72
1:E:387:MET:O	1:E:391:ARG:HG3	1.89	0.72
1:A:373:ARG:CZ	1:F:218:ARG:NH2	2.53	0.72
4:J:501:ALA:HB1	4:J:1453:ALA:HB2	1.72	0.72
1:C:398:ASP:O	1:C:402:ALA:N	2.21	0.72
1:C:413:THR:CG2	5:K:84:ARG:NH2	2.53	0.71
1:D:274:ILE:HG21	1:D:324:ALA:HB1	1.71	0.71
4:J:1333:HIS:NE2	4:J:1421:LEU:O	2.23	0.71
1:B:177:GLY:N	1:B:321:THR:OG1	2.23	0.71
1:E:187:LYS:HG3	1:F:373:ARG:NH2	2.05	0.71
3:I:164:PRO:HG2	3:I:170:PRO:HB2	1.72	0.71
1:E:186:PRO:HD3	1:E:330:THR:HG22	1.71	0.71
3:I:367:LEU:HB2	3:I:371:LYS:HB2	1.71	0.71
3:I:626:ARG:HE	3:I:639:GLN:HE22	1.36	0.71
6:T:9:DA:N1	8:N:32:DG:N1	2.38	0.71
2:G:185:ARG:NH1	2:G:186:LEU:O	2.23	0.71
1:E:92:ALA:HA	1:E:95:ILE:HD12	1.73	0.71
1:A:191:THR:N	9:A:1000:ADP:O3B	2.19	0.71
1:A:352:LEU:HD23	1:A:365:ILE:HA	1.73	0.71
1:E:328:VAL:HG13	1:E:329:GLU:HG3	1.72	0.71
4:J:710:ARG:NH2	4:J:1210:SER:OG	2.24	0.71
1:B:105:TYR:HB3	1:B:129:ASN:HA	1.71	0.71
3:I:857:ASP:HB2	3:I:978:ARG:HG2	1.71	0.71
1:A:186:PRO:HG3	1:A:327:LEU:HD23	1.73	0.70
1:F:269:ILE:HB	1:F:322:ILE:HG12	1.72	0.70
3:I:52:PHE:HD2	3:I:68:PHE:HB2	1.55	0.70
1:E:283:LEU:CD1	1:F:298:SER:HB3	2.21	0.70
1:F:284:VAL:O	1:F:286:PRO:HD3	1.91	0.70
3:I:568:ALA:HB3	3:I:668:LEU:HD12	1.73	0.70
1:B:183:VAL:HG12	1:B:326:ALA:HB3	1.72	0.70
4:J:1037:GLN:HG2	4:J:1042:ARG:HB3	1.73	0.70
1:B:103:GLY:HA3	1:B:259:ARG:HH21	1.56	0.70
2:G:112:ARG:NH2	2:G:126:ASP:OD1	2.24	0.70
1:C:302:TYR:HA	1:C:305:LYS:HB2	1.73	0.70
1:A:302:TYR:HA	1:A:305:LYS:HB2	1.73	0.70
3:I:22:GLN:NE2	3:I:136:ILE:O	2.25	0.70
3:I:987:ILE:HA	4:J:948:THR:HG21	1.74	0.70
1:F:216:ASP:N	1:F:237:SER:O	2.22	0.70
4:J:1112:CYS:SG	4:J:1114:THR:OG1	2.48	0.70
1:C:393:VAL:CG2	5:K:92:LEU:HD12	2.22	0.69
1:D:157:GLU:OE2	1:D:166:ARG:NH2	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ARG:HD3	1:F:143:ASP:H	1.56	0.69
1:B:181:LEU:HD11	1:B:274:ILE:HG21	1.74	0.69
1:C:314:ILE:HG22	1:C:316:GLY:H	1.57	0.69
1:B:192:THR:OG1	9:B:501:ADP:C5	2.45	0.69
1:C:218:ARG:CZ	1:D:344:GLY:O	2.40	0.69
1:E:294:GLY:HA2	1:E:333:ARG:HE	1.57	0.69
1:C:328:VAL:HG13	1:C:329:GLU:OE1	1.91	0.69
1:F:301:LEU:O	1:F:305:LYS:N	2.22	0.69
3:I:52:PHE:CD2	3:I:68:PHE:HB2	2.28	0.69
1:A:187:LYS:HG3	1:B:373:ARG:NH2	2.08	0.69
1:B:190:LYS:HD3	1:B:325:THR:HB	1.73	0.69
1:A:158:THR:OG1	1:A:165:THR:OG1	2.10	0.69
1:B:390:LEU:HG	1:B:394:LEU:HD23	1.74	0.69
1:C:190:LYS:HD2	1:C:325:THR:HB	1.74	0.69
1:D:216:ASP:O	1:D:276:ARG:NH1	2.24	0.69
3:I:86:LYS:HD2	3:I:813:VAL:HB	1.73	0.69
4:J:135:LEU:HB2	4:J:453:ASP:HB3	1.72	0.69
4:J:1105:ILE:HG23	4:J:1199:GLY:HA2	1.75	0.69
1:C:422:SER:O	1:C:426:ARG:N	2.26	0.69
1:B:221:GLU:HG3	1:C:149:PHE:CZ	2.28	0.69
1:C:75:PHE:HA	1:C:87:VAL:HB	1.75	0.69
1:E:279:ARG:NH2	1:E:335:ASP:OD2	2.23	0.69
3:I:333:ILE:H	3:I:465:GLY:HA3	1.58	0.69
1:C:101:ARG:HH22	1:C:142:PHE:H	1.41	0.68
1:C:277:LEU:O	1:C:281:ASN:ND2	2.26	0.68
1:F:186:PRO:O	1:F:354:ARG:NH2	2.26	0.68
1:C:166:ARG:NH1	1:C:418:GLU:OE1	2.26	0.68
1:D:166:ARG:HD3	1:D:415:ASN:HB2	1.75	0.68
1:F:108:GLY:HA3	1:F:122:LEU:HD21	1.75	0.68
1:F:247:ILE:HG13	1:F:284:VAL:HG11	1.75	0.68
5:K:9:LEU:HB3	5:K:19:LEU:HD11	1.75	0.68
3:I:66:LEU:HD11	3:I:98:LEU:HD13	1.75	0.68
3:I:158:TYR:HE1	3:I:310:LEU:HG	1.57	0.68
3:I:226:VAL:O	3:I:230:ARG:NH1	2.26	0.68
3:I:1031:ARG:HD2	4:J:622:ARG:HH21	1.59	0.68
1:F:76:LEU:H	1:F:88:ALA:H	1.40	0.68
4:J:1484:THR:O	5:K:25:LYS:HD2	1.94	0.68
1:C:218:ARG:HE	1:D:345:THR:C	1.97	0.68
1:E:76:LEU:HD23	1:E:89:ILE:HB	1.75	0.68
1:E:274:ILE:N	1:E:325:THR:O	2.22	0.68
4:J:584:ASN:ND2	4:J:590:PRO:O	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:PRO:O	2:G:146:ARG:NH1	2.26	0.68
3:I:468:ARG:HB3	3:I:485:TYR:HB3	1.76	0.68
1:B:184:ALA:O	1:B:327:LEU:HA	1.94	0.68
1:F:212:VAL:HG11	1:F:225:PHE:HE2	1.57	0.68
1:B:269:ILE:HB	1:B:322:ILE:HG12	1.76	0.67
1:B:182:ILE:HD12	1:B:350:LEU:HD23	1.75	0.67
1:C:153:GLN:HA	1:C:175:GLY:HA2	1.77	0.67
1:E:218:ARG:NH1	1:E:221:GLU:OE2	2.27	0.67
1:A:409:ARG:NH2	3:I:777:ILE:HB	2.08	0.67
1:C:226:ARG:NH2	1:C:234:VAL:O	2.26	0.67
3:I:724:ARG:NH1	3:I:738:ASP:O	2.27	0.67
4:J:414:ARG:HA	4:J:434:ARG:HA	1.77	0.67
1:B:60:ARG:HE	1:B:111:ARG:HA	1.60	0.67
1:D:111:ARG:NH2	1:D:121:THR:OG1	2.28	0.67
1:F:186:PRO:HG3	1:F:327:LEU:HD23	1.76	0.67
6:T:10:DC:C4	8:N:32:DG:O6	2.46	0.67
1:A:294:GLY:HA3	1:A:334:MET:SD	2.34	0.67
1:D:166:ARG:NH1	1:D:410:LEU:O	2.27	0.67
3:I:82:GLU:HA	3:I:85:GLU:HB3	1.76	0.67
3:I:463:GLU:HG2	3:I:464:LEU:HG	1.75	0.67
3:I:1031:ARG:HB2	6:T:24:DG:O3'	1.94	0.67
4:J:1107:VAL:HG23	4:J:1218:GLY:H	1.59	0.67
1:C:301:LEU:O	1:C:305:LYS:N	2.27	0.67
1:E:282:ASN:HA	1:E:297:ASP:OD2	1.94	0.67
1:A:177:GLY:N	1:A:321:THR:OG1	2.26	0.67
1:E:177:GLY:N	1:E:321:THR:OG1	2.27	0.67
4:J:109:PRO:O	4:J:111:LYS:NZ	2.28	0.67
6:T:9:DA:N6	8:N:32:DG:C6	2.62	0.67
1:A:187:LYS:O	1:A:354:ARG:NH1	2.27	0.67
1:E:186:PRO:O	1:E:354:ARG:NH2	2.19	0.67
3:I:146:VAL:HG22	3:I:162:ILE:HG12	1.75	0.67
3:I:204:GLN:NE2	3:I:228:ALA:O	2.28	0.67
1:C:296:LEU:HD11	1:C:334:MET:HA	1.77	0.67
1:D:186:PRO:HA	9:D:1000:ADP:O2B	1.95	0.67
1:D:412:ARG:HH22	1:D:418:GLU:HA	1.60	0.67
6:T:38:DA:N1	8:N:4:DT:O4	2.28	0.67
1:A:380:GLY:O	1:A:384:THR:N	2.22	0.66
1:C:166:ARG:HH22	1:C:411:ALA:HA	1.60	0.66
1:D:375:GLU:OE1	1:D:375:GLU:N	2.27	0.66
1:F:357:GLU:HG2	1:F:362:PHE:HE1	1.60	0.66
1:E:295:GLY:HA2	1:F:290:ARG:NH2	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:HB3	1:F:360:ARG:HE	1.60	0.66
1:E:153:GLN:HA	1:E:175:GLY:HA2	1.76	0.66
1:C:216:ASP:O	1:C:276:ARG:NH1	2.28	0.66
1:C:389:LEU:HD11	5:K:92:LEU:HD11	1.76	0.66
1:F:185:PRO:HG3	1:F:354:ARG:HG2	1.77	0.66
3:I:432:ARG:HD2	3:I:519:GLY:HA3	1.76	0.66
3:I:775:ARG:HG3	3:I:783:ARG:HB3	1.77	0.66
1:B:275:THR:HG1	1:B:327:LEU:H	1.42	0.66
1:D:63:LYS:O	1:D:86:ARG:NH2	2.28	0.66
3:I:18:LEU:O	3:I:408:ARG:NH1	2.29	0.66
6:T:2:DG:O6	8:N:40:DC:N3	2.29	0.66
1:E:66:LEU:HD22	1:E:104:ASP:HB2	1.78	0.66
1:D:229:VAL:HG22	1:D:232:ALA:HB3	1.77	0.66
1:A:397:MET:HB2	3:I:773:LEU:HD12	1.77	0.66
3:I:158:TYR:OH	3:I:310:LEU:O	2.12	0.66
3:I:1030:GLN:OE1	4:J:628:ARG:NH1	2.28	0.66
4:J:432:TYR:HB3	4:J:450:TYR:HB2	1.77	0.66
4:J:1404:ASN:HA	4:J:1408:ILE:HB	1.77	0.66
1:A:98:TYR:OH	1:A:124:LYS:NZ	2.29	0.66
1:C:156:LEU:O	1:C:415:ASN:ND2	2.29	0.66
1:F:291:THR:HG21	7:R:2:A:H5'	1.78	0.66
1:D:242:PRO:HD2	1:D:245:ASN:HD22	1.60	0.65
1:E:288:THR:HG23	1:E:298:SER:H	1.60	0.65
1:F:105:TYR:O	1:F:129:ASN:N	2.29	0.65
1:F:273:SER:H	1:F:325:THR:HG1	1.41	0.65
4:J:1197:ARG:NH1	4:J:1396:GLU:OE1	2.28	0.65
1:D:148:GLN:HG3	1:D:315:ARG:HG2	1.77	0.65
1:E:216:ASP:N	1:E:237:SER:O	2.28	0.65
1:A:269:ILE:HB	1:A:322:ILE:HG22	1.79	0.65
1:D:209:LYS:HG2	1:D:211:ILE:HD11	1.78	0.65
1:C:286:PRO:CG	1:C:287:PRO:HD3	2.26	0.65
4:J:462:GLN:HB2	4:J:513:ILE:HD11	1.78	0.65
4:J:842:VAL:HG12	4:J:865:THR:HB	1.78	0.65
1:A:391:ARG:HD3	1:F:360:ARG:NH2	2.10	0.65
1:C:351:HIS:O	1:C:366:ASP:N	2.28	0.65
1:D:95:ILE:HA	1:D:100:LEU:HG	1.77	0.65
1:F:279:ARG:HH21	1:F:335:ASP:H	1.45	0.65
3:I:939:ARG:HG2	3:I:982:PRO:HD3	1.77	0.65
1:B:391:ARG:HA	1:B:394:LEU:HG	1.79	0.65
1:C:200:ALA:O	1:C:204:ASN:ND2	2.28	0.65
1:F:190:LYS:HD2	1:F:325:THR:HB	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:LEU:HD13	1:F:196:LYS:HD2	1.78	0.65
3:I:170:PRO:HG3	3:I:263:ASP:HB3	1.77	0.65
1:A:162:GLU:O	1:A:166:ARG:CB	2.44	0.65
1:D:185:PRO:HB2	1:D:354:ARG:NH2	2.12	0.65
1:E:215:ILE:HD11	1:E:246:HIS:HB3	1.78	0.65
1:A:271:LEU:HB3	1:A:324:ALA:HB2	1.79	0.65
1:C:190:LYS:N	9:C:1002:ADP:O2A	2.29	0.65
4:J:1485:GLN:HE21	5:K:82:GLU:CA	2.09	0.65
1:A:216:ASP:N	1:A:237:SER:O	2.24	0.65
3:I:598:GLU:OE1	3:I:615:TYR:OH	2.14	0.65
1:B:98:TYR:HB3	1:B:100:LEU:HG	1.79	0.64
1:B:191:THR:HG23	9:B:501:ADP:O2A	1.97	0.64
3:I:85:GLU:O	3:I:824:ARG:NH2	2.30	0.64
4:J:1394:VAL:HB	4:J:1397:LYS:HG2	1.80	0.64
1:B:221:GLU:HG3	1:C:149:PHE:HZ	1.62	0.64
1:B:254:HIS:CE1	1:B:307:PHE:HA	2.33	0.64
1:C:409:ARG:HG3	5:K:87:LYS:HE2	1.80	0.64
1:E:229:VAL:HG22	1:E:232:ALA:HB3	1.80	0.64
2:H:91:ASN:ND2	2:H:93:SER:OG	2.30	0.64
4:J:569:ASN:OD1	4:J:572:ARG:NH2	2.25	0.64
1:E:269:ILE:HB	1:E:322:ILE:HG12	1.78	0.64
1:E:398:ASP:HB2	1:E:401:GLU:HB2	1.79	0.64
3:I:292:ARG:HD2	3:I:299:LYS:HB3	1.80	0.64
3:I:910:LYS:HB3	3:I:912:PRO:HD2	1.80	0.64
4:J:140:ALA:HA	4:J:147:VAL:HG12	1.78	0.64
1:A:282:ASN:ND2	1:A:295:GLY:O	2.30	0.64
1:E:107:VAL:HB	1:E:127:ALA:HB3	1.79	0.64
2:H:22:GLU:HG2	2:H:198:ARG:HG2	1.80	0.64
1:F:78:GLU:HG2	1:F:86:ARG:HE	1.62	0.64
3:I:1001:VAL:HA	3:I:1004:LYS:HG2	1.79	0.64
1:A:78:GLU:HG3	1:A:80:LEU:H	1.63	0.64
1:C:375:GLU:O	1:C:379:LEU:N	2.29	0.64
2:G:97:VAL:HG11	2:G:120:VAL:HG21	1.80	0.64
3:I:172:ILE:HD11	3:I:184:MET:SD	2.38	0.64
3:I:497:ALA:HB2	3:I:529:VAL:HG11	1.80	0.64
4:J:622:ARG:NH2	6:T:25:DT:OP1	2.31	0.64
4:J:925:GLU:OE2	5:K:6:ILE:HB	1.98	0.64
1:C:394:LEU:HD11	1:C:406:LEU:HD11	1.80	0.64
1:E:295:GLY:CA	1:F:290:ARG:NH2	2.61	0.64
1:B:104:ASP:OD1	1:B:129:ASN:ND2	2.31	0.63
3:I:584:GLU:HB3	3:I:666:LEU:H	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PRO:HB2	1:A:354:ARG:HH21	1.63	0.63
1:D:229:VAL:HG21	1:D:234:VAL:HG23	1.80	0.63
1:F:313:ASN:OD1	1:F:315:ARG:NH2	2.25	0.63
3:I:41:ASN:HD22	3:I:49:ARG:HH12	1.46	0.63
3:I:1031:ARG:CB	6:T:24:DG:H5"	2.26	0.63
4:J:610:LYS:NZ	6:T:22:DA:O5'	2.31	0.63
4:J:1211:MET:CE	5:K:16:LYS:NZ	2.61	0.63
9:F:1000:ADP:O1B	11:F:1002:BEF:F2	2.06	0.63
2:H:106:PRO:HG3	2:H:134:GLU:HA	1.80	0.63
2:H:175:ARG:HH11	2:H:202:ASP:HB3	1.63	0.63
6:T:9:DA:C2	8:N:32:DG:N1	2.66	0.63
1:A:100:LEU:HD11	1:A:128:VAL:HG21	1.80	0.63
1:B:185:PRO:HD2	1:B:354:ARG:HH11	1.62	0.63
2:G:67:THR:HG21	3:I:627:ARG:HD3	1.81	0.63
1:A:150:PRO:HG2	1:A:378:LEU:HD21	1.80	0.63
1:C:166:ARG:NH1	1:C:410:LEU:O	2.31	0.63
3:I:69:LEU:HD12	3:I:97:ARG:HG2	1.81	0.63
5:K:46:PRO:HB2	5:K:54:LEU:HB3	1.80	0.63
1:D:69:SER:OG	1:D:71:ASP:OD1	2.17	0.63
1:E:179:ARG:NE	1:E:345:THR:O	2.30	0.63
4:J:204:LEU:HD12	4:J:394:LEU:HD23	1.80	0.63
1:A:215:ILE:HD11	1:A:246:HIS:HB3	1.79	0.63
1:B:414:LYS:O	1:B:418:GLU:N	2.28	0.63
1:E:94:LEU:HD13	1:E:122:LEU:HD23	1.81	0.63
3:I:774:LEU:HD12	3:I:778:PHE:HE2	1.63	0.63
6:T:7:DC:C4	8:N:34:DA:N6	2.67	0.63
1:A:296:LEU:HD22	1:A:301:LEU:HD11	1.79	0.62
3:I:214:TYR:OH	3:I:308:ARG:O	2.17	0.62
1:B:73:TYR:HB2	1:B:89:ILE:HG23	1.81	0.62
1:F:274:ILE:N	1:F:325:THR:O	2.27	0.62
4:J:138:LYS:HG2	4:J:450:TYR:HD2	1.64	0.62
1:B:292:LEU:N	1:B:296:LEU:O	2.29	0.62
1:D:410:LEU:HD23	1:D:418:GLU:HG3	1.81	0.62
3:I:683:ASN:O	3:I:872:ASN:ND2	2.32	0.62
3:I:1021:LEU:HD13	4:J:622:ARG:HH11	1.65	0.62
4:J:557:LEU:HD23	4:J:570:GLU:HG2	1.81	0.62
1:B:346:GLY:O	1:B:373:ARG:NH1	2.32	0.62
1:D:156:LEU:HB3	1:D:165:THR:HB	1.80	0.62
1:F:184:ALA:HB3	1:F:190:LYS:HD3	1.81	0.62
5:K:70:THR:HG21	5:K:72:ARG:HH21	1.65	0.62
1:A:153:GLN:HA	1:A:175:GLY:HA2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ALA:HA	1:D:95:ILE:HD12	1.80	0.62
1:A:189:GLY:HA3	9:A:1000:ADP:C8	2.34	0.62
1:C:212:VAL:HG11	1:C:225:PHE:HE2	1.63	0.62
1:E:141:ARG:NH2	1:E:144:GLU:OE2	2.28	0.62
1:A:358:GLU:OE2	1:B:369:LYS:HA	1.99	0.62
1:C:101:ARG:HH11	1:C:259:ARG:HH21	1.46	0.62
1:E:380:GLY:O	1:E:384:THR:N	2.20	0.62
3:I:762:LYS:HA	3:I:786:LYS:HB2	1.82	0.62
6:T:10:DC:O2	8:N:32:DG:C2	2.48	0.62
3:I:495:THR:OG1	3:I:517:ARG:NH1	2.33	0.62
4:J:1364:HIS:CD2	4:J:1366:LYS:HG3	2.35	0.62
1:F:185:PRO:O	1:F:190:LYS:NZ	2.33	0.62
2:G:58:ILE:HB	2:G:61:VAL:HG22	1.82	0.62
2:G:9:PRO:HB3	2:G:26:GLU:N	2.15	0.61
3:I:1104:GLU:O	4:J:7:LYS:NZ	2.32	0.61
4:J:618:LEU:HD12	4:J:1467:ILE:HD11	1.82	0.61
1:B:111:ARG:HD3	1:B:123:LEU:HD13	1.81	0.61
1:C:413:THR:HG23	5:K:84:ARG:NH2	2.15	0.61
1:D:79:ASN:O	1:D:81:HIS:ND1	2.33	0.61
1:E:175:GLY:O	1:E:178:GLN:HG2	2.00	0.61
1:D:182:ILE:HD11	1:D:352:LEU:HD21	1.81	0.61
3:I:164:PRO:HB3	3:I:265:ARG:HB2	1.83	0.61
4:J:117:ASP:OD1	4:J:495:ARG:NH1	2.31	0.61
4:J:1472:ILE:HG22	4:J:1474:ALA:H	1.66	0.61
1:A:281:ASN:O	1:A:285:THR:N	2.27	0.61
1:F:243:PRO:HB2	1:F:284:VAL:HG22	1.80	0.61
4:J:889:ALA:O	4:J:929:ARG:NH1	2.34	0.61
1:A:271:LEU:HD23	1:A:274:ILE:HG22	1.81	0.61
1:B:179:ARG:NH1	1:B:311:ALA:O	2.33	0.61
1:C:297:ASP:CG	1:D:290:ARG:CZ	2.69	0.61
1:C:418:GLU:O	1:C:422:SER:OG	2.13	0.61
6:T:7:DC:N4	8:N:34:DA:N6	2.48	0.61
9:B:501:ADP:O3'	1:C:373:ARG:NE	2.32	0.61
1:D:105:TYR:O	1:D:129:ASN:N	2.31	0.61
4:J:128:TYR:HA	4:J:457:GLY:HA2	1.83	0.61
1:E:178:GLN:HB2	1:E:321:THR:HG23	1.81	0.61
1:F:346:GLY:O	1:F:373:ARG:NH1	2.34	0.61
3:I:65:VAL:HB	3:I:101:ILE:HB	1.82	0.61
4:J:1265:ALA:H	4:J:1423:GLY:HA2	1.66	0.61
1:E:78:GLU:HG3	1:E:80:LEU:H	1.66	0.61
1:E:183:VAL:HG12	1:E:326:ALA:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1008:ARG:HH21	3:I:1011:GLY:N	1.99	0.61
2:G:180:GLN:NE2	2:G:182:GLU:OE2	2.34	0.61
4:J:206:ARG:O	4:J:391:ALA:CA	2.49	0.61
4:J:527:MET:HG3	4:J:537:THR:HB	1.82	0.61
4:J:838:ARG:NH1	4:J:874:GLU:OE1	2.34	0.61
1:A:104:ASP:OD2	1:A:139:ARG:NH2	2.24	0.60
1:E:254:HIS:HB2	1:E:307:PHE:CE1	2.36	0.60
1:E:153:GLN:HB3	1:E:378:LEU:HD22	1.84	0.60
3:I:140:ILE:HD11	3:I:331:ARG:HB3	1.82	0.60
3:I:351:LEU:HD11	3:I:373:VAL:HG13	1.83	0.60
1:A:358:GLU:OE2	1:B:369:LYS:HD3	2.02	0.60
1:D:162:GLU:O	1:D:166:ARG:HG3	2.01	0.60
1:E:127:ALA:HB1	1:E:130:ASN:HA	1.83	0.60
1:E:387:MET:HG3	1:E:390:LEU:HD22	1.83	0.60
3:I:56:GLU:HB3	3:I:64:LEU:HB3	1.82	0.60
1:A:183:VAL:HG13	1:A:326:ALA:HB3	1.84	0.60
1:C:417:LYS:HE2	4:J:1502:ALA:HB1	1.82	0.60
1:D:122:LEU:HD21	1:D:125:VAL:HG22	1.84	0.60
1:E:111:ARG:HH11	1:E:114:ARG:HD2	1.66	0.60
1:F:291:THR:HB	7:R:1:U:O3’	2.01	0.60
3:I:1005:MET:N	3:I:1005:MET:SD	2.74	0.60
4:J:121:THR:OG1	4:J:122:GLU:OE1	2.17	0.60
4:J:754:PHE:HZ	4:J:1476:THR:HG21	1.67	0.60
1:C:78:GLU:HA	1:C:86:ARG:HH21	1.67	0.60
1:C:238:THR:OG1	1:C:241:GLU:OE2	2.19	0.60
2:G:77:GLU:O	2:G:81:ASN:ND2	2.33	0.60
2:H:2:LEU:HA	2:H:6:LEU:HB3	1.83	0.60
6:T:9:DA:C2	8:N:33:DT:N3	2.61	0.60
1:A:66:LEU:HB2	1:A:103:GLY:H	1.67	0.60
1:A:98:TYR:OH	1:A:125:VAL:O	2.19	0.60
1:D:416:ASN:HA	1:D:419:PHE:CE2	2.37	0.60
1:F:122:LEU:HD23	1:F:125:VAL:HG22	1.83	0.60
1:F:188:ALA:HA	1:F:357:GLU:HG3	1.83	0.60
4:J:133:ILE:HG23	4:J:455:ARG:H	1.65	0.60
4:J:565:ILE:O	4:J:569:ASN:ND2	2.33	0.60
4:J:1307:LYS:O	4:J:1310:ARG:NH2	2.34	0.60
9:A:1000:ADP:H5’2	1:B:373:ARG:HE	1.65	0.60
1:E:171:LEU:HD21	1:E:367:ILE:HG23	1.82	0.60
1:A:311:ALA:HB2	1:A:322:ILE:HG12	1.84	0.60
1:A:379:LEU:HB3	1:A:383:VAL:HG12	1.84	0.60
1:B:107:VAL:HB	1:B:127:ALA:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:PRO:HG3	1:B:329:GLU:HB3	1.84	0.60
1:E:387:MET:HA	1:E:390:LEU:HB2	1.84	0.60
1:F:148:GLN:OE1	1:F:315:ARG:HG2	2.02	0.60
3:I:265:ARG:HG3	3:I:267:TYR:H	1.67	0.60
3:I:1008:ARG:NH2	4:J:624:ASP:OD1	2.33	0.60
1:A:78:GLU:HG2	1:A:84:GLU:HG3	1.84	0.59
1:E:187:LYS:CG	1:F:373:ARG:NH2	2.65	0.59
1:E:348:MET:SD	1:E:372:THR:HG22	2.42	0.59
1:F:111:ARG:HB2	1:F:112:PRO:HD2	1.84	0.59
3:I:504:GLU:HG3	3:I:509:ALA:HB2	1.83	0.59
4:J:18:ILE:HD12	4:J:518:PRO:HG3	1.84	0.59
4:J:433:GLY:HA3	4:J:447:VAL:O	2.02	0.59
4:J:807:ALA:H	4:J:832:ARG:NE	2.00	0.59
4:J:1152:GLU:OE2	4:J:1159:ARG:NH1	2.35	0.59
1:B:287:PRO:O	1:B:288:THR:HG22	2.03	0.59
4:J:792:ILE:HG23	4:J:793:THR:HG23	1.82	0.59
1:A:192:THR:HG21	9:A:1000:ADP:H2'	1.85	0.59
1:B:296:LEU:HG	1:B:334:MET:HG3	1.83	0.59
1:D:83:LEU:HD12	1:D:87:VAL:HG11	1.84	0.59
1:D:379:LEU:HB2	1:D:387:MET:HE1	1.84	0.59
4:J:643:GLY:HA3	4:J:727:GLN:HB2	1.84	0.59
1:A:275:THR:HB	1:A:279:ARG:NH1	2.17	0.59
1:B:221:GLU:CG	1:C:149:PHE:HZ	2.16	0.59
1:D:328:VAL:HG13	1:D:329:GLU:OE1	2.02	0.59
2:G:229:GLN:NE2	2:H:11:PHE:O	2.36	0.59
2:H:81:ASN:ND2	2:H:129:ILE:O	2.36	0.59
1:A:360:ARG:NH1	1:B:391:ARG:HE	2.00	0.59
1:D:225:PHE:O	1:D:229:VAL:N	2.35	0.59
4:J:1146:GLY:HA2	4:J:1207:TYR:HB3	1.84	0.59
1:A:179:ARG:NH2	1:A:345:THR:O	2.36	0.59
1:C:189:GLY:HA2	9:C:1002:ADP:C8	2.37	0.59
4:J:892:ASP:OD1	4:J:893:GLU:N	2.36	0.59
1:C:229:VAL:HG22	1:C:232:ALA:HB3	1.85	0.59
1:C:405:MET:SD	4:J:2:LYS:NZ	2.76	0.59
1:F:165:THR:HA	1:F:168:ILE:HG12	1.84	0.59
1:F:414:LYS:NZ	1:F:416:ASN:HB3	2.17	0.59
3:I:1047:HIS:O	3:I:1051:GLU:HG2	2.03	0.59
5:K:33:HIS:O	5:K:36:LYS:NZ	2.35	0.59
1:A:301:LEU:O	1:A:305:LYS:N	2.30	0.59
1:C:66:LEU:HG	1:C:102:ALA:HA	1.84	0.59
1:D:314:ILE:HG22	1:D:316:GLY:H	1.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:LYS:NZ	1:E:233:GLU:OE1	2.35	0.59
3:I:266:ARG:HD3	3:I:266:ARG:H	1.66	0.59
1:B:101:ARG:HH21	1:B:139:ARG:CZ	2.16	0.59
1:B:229:VAL:HG22	1:B:232:ALA:HB3	1.85	0.59
1:B:311:ALA:HB2	1:B:322:ILE:HD12	1.83	0.59
1:D:183:VAL:HG12	1:D:328:VAL:HG11	1.83	0.59
3:I:598:GLU:OE1	3:I:623:TYR:OH	2.15	0.59
3:I:721:ARG:HG2	3:I:820:ARG:HH12	1.68	0.59
4:J:1158:VAL:HG21	4:J:1173:LEU:HD21	1.84	0.59
1:B:66:LEU:O	1:B:103:GLY:N	2.27	0.59
1:D:274:ILE:HD13	1:D:324:ALA:HB1	1.84	0.59
2:H:100:LEU:HG	2:H:141:GLU:HB3	1.84	0.59
4:J:119:SER:HB2	4:J:123:LEU:HD13	1.85	0.59
4:J:828:LYS:NZ	4:J:863:VAL:O	2.35	0.59
9:B:501:ADP:O1A	11:B:502:BEF:F1	2.11	0.58
1:D:255:GLU:O	1:D:259:ARG:HD2	2.03	0.58
2:H:110:LYS:N	2:H:113:ASP:OD2	2.33	0.58
4:J:484:PRO:O	4:J:489:ARG:NH2	2.36	0.58
1:A:162:GLU:O	1:A:166:ARG:HB2	2.02	0.58
1:C:77:THR:O	1:C:86:ARG:NH2	2.37	0.58
1:C:305:LYS:HG3	1:C:342:PHE:HE1	1.67	0.58
1:F:229:VAL:HG22	1:F:232:ALA:HB3	1.84	0.58
1:A:360:ARG:CZ	1:B:391:ARG:HE	2.15	0.58
1:C:148:GLN:N	1:C:313:ASN:O	2.34	0.58
1:C:274:ILE:HB	1:C:324:ALA:HB1	1.85	0.58
1:D:152:ARG:HD2	1:D:176:ARG:HD2	1.85	0.58
3:I:399:ASN:O	3:I:402:SER:OG	2.20	0.58
3:I:409:ARG:NH1	7:R:26:A:OP1	2.36	0.58
4:J:138:LYS:HE2	4:J:140:ALA:HB3	1.84	0.58
1:A:388:TRP:CH2	1:F:360:ARG:HB3	2.38	0.58
1:D:66:LEU:HD21	1:D:100:LEU:HD13	1.85	0.58
1:F:162:GLU:O	1:F:166:ARG:HG3	2.03	0.58
1:D:185:PRO:HB2	1:D:354:ARG:HH21	1.68	0.58
3:I:157:ARG:NE	3:I:314:THR:OG1	2.36	0.58
3:I:364:GLU:OE1	3:I:366:SER:N	2.37	0.58
1:B:152:ARG:HD2	1:B:176:ARG:HD2	1.85	0.58
1:C:99:ALA:HB3	1:C:137:LYS:HA	1.85	0.58
1:D:218:ARG:NH2	1:E:343:LYS:O	2.36	0.58
3:I:177:GLU:HB3	3:I:181:VAL:HB	1.84	0.58
1:A:190:LYS:HD2	1:A:325:THR:OG1	2.03	0.58
1:D:255:GLU:OE1	1:D:259:ARG:NH2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLN:N	1:E:313:ASN:O	2.36	0.58
1:E:414:LYS:O	1:E:418:GLU:N	2.24	0.58
3:I:415:PRO:HD2	3:I:418:LEU:HD13	1.86	0.58
4:J:659:LYS:NZ	4:J:663:GLU:OE2	2.24	0.58
4:J:835:SER:N	4:J:838:ARG:HH21	2.01	0.58
1:A:106:VAL:HG22	1:A:128:VAL:HG23	1.85	0.58
3:I:154:ARG:HH21	3:I:178:PRO:HG3	1.69	0.58
1:A:351:HIS:HB2	1:A:366:ASP:HB3	1.86	0.58
1:C:413:THR:HG23	5:K:84:ARG:HH21	1.69	0.58
1:F:176:ARG:HH21	1:F:208:ILE:HG12	1.69	0.58
4:J:1486:VAL:HG21	5:K:25:LYS:HB2	1.85	0.58
1:B:281:ASN:HA	1:B:284:VAL:HB	1.84	0.58
1:E:218:ARG:HD3	1:F:179:ARG:NH2	2.19	0.58
1:F:109:GLN:HE21	1:F:124:LYS:HB3	1.69	0.58
1:F:184:ALA:O	1:F:328:VAL:N	2.34	0.58
4:J:485:SER:H	4:J:488:ARG:HH21	1.49	0.58
3:I:271:GLU:HA	3:I:275:TYR:HB2	1.84	0.57
1:A:182:ILE:O	1:A:325:THR:HA	2.03	0.57
1:B:76:LEU:H	1:B:87:VAL:HA	1.67	0.57
1:C:415:ASN:O	1:C:419:PHE:HB2	2.05	0.57
1:F:95:ILE:HA	1:F:100:LEU:HB2	1.85	0.57
4:J:895:VAL:HG23	4:J:921:ARG:HH12	1.69	0.57
1:A:163:LEU:HD13	1:A:407:LEU:HG	1.87	0.57
1:B:217:GLU:OE2	1:B:218:ARG:NH1	2.37	0.57
1:C:89:ILE:HD11	1:C:119:TYR:HD2	1.68	0.57
1:C:187:LYS:HG3	1:D:373:ARG:HH21	1.70	0.57
3:I:274:ARG:O	3:I:278:GLU:N	2.25	0.57
4:J:1379:VAL:HG12	4:J:1419:PRO:HA	1.85	0.57
1:A:300:ALA:O	1:A:304:PRO:HD2	2.04	0.57
1:B:255:GLU:HB2	1:B:259:ARG:HH12	1.68	0.57
1:D:178:GLN:N	1:D:321:THR:OG1	2.37	0.57
3:I:148:PHE:HE2	3:I:309:TYR:CD2	2.22	0.57
3:I:1031:ARG:HD2	4:J:622:ARG:NH2	2.18	0.57
1:A:314:ILE:HG22	1:A:316:GLY:H	1.70	0.57
1:B:94:LEU:HA	1:B:97:GLN:HE21	1.70	0.57
1:B:218:ARG:NH2	1:C:373:ARG:NH1	2.52	0.57
1:A:161:ASP:O	1:A:165:THR:OG1	2.22	0.57
3:I:709:GLU:HG3	3:I:824:ARG:HG2	1.86	0.57
3:I:974:LEU:HD13	3:I:987:ILE:HB	1.85	0.57
1:A:177:GLY:H	1:A:321:THR:HG1	1.50	0.57
3:I:1001:VAL:HG13	3:I:1004:LYS:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:704:ARG:HG3	4:J:706:PRO:HD2	1.87	0.57
1:A:187:LYS:HE3	1:B:373:ARG:CZ	2.35	0.57
1:B:171:LEU:HD22	1:B:367:ILE:HG23	1.85	0.57
1:C:182:ILE:HG23	1:C:325:THR:HA	1.86	0.57
1:E:214:LEU:N	1:E:235:ILE:O	2.37	0.57
1:F:86:ARG:H	1:F:86:ARG:HD3	1.68	0.57
1:F:93:GLY:HA2	1:F:96:LYS:HE2	1.86	0.57
3:I:82:GLU:HB2	3:I:86:LYS:HE2	1.87	0.57
4:J:132:TYR:HB3	4:J:152:LEU:HD11	1.87	0.57
1:A:76:LEU:H	1:A:87:VAL:HA	1.70	0.57
4:J:1378:TYR:OH	4:J:1430:SER:O	2.14	0.57
4:J:1468:LEU:HD22	4:J:1470:ARG:HD2	1.86	0.57
1:A:164:SER:HA	1:A:363:PRO:HD3	1.85	0.57
1:A:415:ASN:OD1	1:A:416:ASN:N	2.38	0.57
1:B:414:LYS:HE2	1:B:417:LYS:HG3	1.87	0.57
1:F:212:VAL:HG22	1:F:270:LEU:HB2	1.87	0.57
2:H:153:ALA:N	2:H:168:ASP:OD1	2.30	0.57
3:I:271:GLU:HA	3:I:275:TYR:CB	2.35	0.57
1:A:373:ARG:NH2	1:F:218:ARG:HH22	2.02	0.56
1:B:301:LEU:O	1:B:305:LYS:N	2.34	0.56
1:F:157:GLU:OE1	1:F:414:LYS:HD3	2.05	0.56
3:I:154:ARG:NH2	3:I:157:ARG:HG3	2.20	0.56
1:D:95:ILE:HG12	1:D:100:LEU:HD11	1.86	0.56
1:D:153:GLN:HA	1:D:175:GLY:HA2	1.85	0.56
1:D:155:ARG:HD2	1:D:414:LYS:NZ	2.20	0.56
6:T:9:DA:N1	8:N:33:DT:C4	2.71	0.56
1:B:281:ASN:O	1:B:285:THR:N	2.35	0.56
1:B:352:LEU:O	1:B:354:ARG:NH1	2.35	0.56
1:D:134:GLU:HA	1:D:137:LYS:HE2	1.87	0.56
1:D:166:ARG:HD2	1:D:410:LEU:HD22	1.87	0.56
1:D:277:LEU:O	1:D:281:ASN:ND2	2.34	0.56
1:E:379:LEU:O	1:E:384:THR:OG1	2.23	0.56
3:I:631:SER:OG	3:I:635:THR:N	2.36	0.56
4:J:162:ARG:NH1	4:J:452:ILE:O	2.38	0.56
4:J:750:PRO:HG2	4:J:756:GLN:NE2	2.20	0.56
4:J:1211:MET:HG2	4:J:1213:ARG:HE	1.68	0.56
4:J:1321:ALA:O	4:J:1339:LYS:NZ	2.27	0.56
1:C:358:GLU:OE2	1:D:369:LYS:HA	2.04	0.56
1:C:397:MET:HG3	5:K:91:ARG:CZ	2.36	0.56
1:F:79:ASN:C	1:F:81:HIS:HD1	2.09	0.56
3:I:966:LEU:HD21	3:I:986:PRO:HG3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:HB	1:C:322:ILE:HG12	1.87	0.56
9:C:1002:ADP:O2'	1:D:373:ARG:HG2	2.04	0.56
1:D:101:ARG:NH1	1:D:141:ARG:HD2	2.21	0.56
1:D:354:ARG:O	1:D:357:GLU:HG3	2.05	0.56
2:G:185:ARG:HG2	2:G:190:THR:HA	1.88	0.56
2:H:80:LEU:HD11	4:J:844:ALA:HA	1.87	0.56
2:H:105:GLY:H	2:H:135:GLY:HA2	1.70	0.56
1:C:413:THR:OG1	5:K:84:ARG:NH1	2.37	0.56
1:E:76:LEU:CB	1:E:87:VAL:HG23	2.35	0.56
3:I:311:PHE:HA	3:I:314:THR:HG22	1.88	0.56
3:I:988:VAL:HG12	4:J:948:THR:HB	1.86	0.56
4:J:191:LEU:HD12	4:J:195:VAL:HG12	1.88	0.56
9:D:1000:ADP:O2A	11:D:1002:BEF:F1	2.13	0.56
1:F:146:THR:HB	1:F:148:GLN:HE22	1.71	0.56
3:I:442:GLU:HG2	3:I:454:SER:HB2	1.88	0.56
1:B:276:ARG:HB2	1:B:327:LEU:HD12	1.88	0.56
1:C:170:LEU:HD22	1:C:426:ARG:HH12	1.70	0.56
1:C:422:SER:O	1:C:426:ARG:HG2	2.05	0.56
1:E:304:PRO:O	1:E:308:LEU:N	2.35	0.56
3:I:478:VAL:HG23	3:I:506:ASN:HB2	1.88	0.56
4:J:63:TYR:HA	4:J:68:PHE:CE1	2.40	0.56
4:J:1289:LYS:HE3	4:J:1306:PRO:HG3	1.88	0.56
1:C:218:ARG:NE	1:D:345:THR:O	2.35	0.56
1:D:166:ARG:NH1	1:D:413:THR:O	2.39	0.56
1:E:122:LEU:HD21	1:E:125:VAL:HG22	1.87	0.56
2:G:42:ARG:NH2	2:H:31:GLY:O	2.32	0.56
4:J:791:TYR:O	4:J:861:GLN:NE2	2.35	0.56
9:B:501:ADP:O1A	11:B:502:BEF:F3	2.13	0.56
1:D:274:ILE:HG12	1:D:325:THR:O	2.06	0.56
1:D:380:GLY:O	1:D:384:THR:N	2.37	0.56
1:C:268:MET:SD	1:C:321:THR:HB	2.46	0.55
9:C:1002:ADP:O3'	1:D:373:ARG:HD3	2.06	0.55
1:D:155:ARG:HD2	1:D:414:LYS:HZ3	1.72	0.55
3:I:194:VAL:HA	3:I:197:LEU:HD12	1.88	0.55
3:I:557:ARG:HE	3:I:879:ARG:HG2	1.71	0.55
7:R:21:C:H2'	7:R:22:A:C8	2.41	0.55
1:B:416:ASN:O	1:B:420:LEU:N	2.32	0.55
1:C:192:THR:OG1	9:C:1002:ADP:C8	2.59	0.55
1:C:415:ASN:O	1:C:419:PHE:CB	2.55	0.55
1:D:313:ASN:OD1	1:D:315:ARG:NH2	2.28	0.55
9:F:1000:ADP:O1B	11:F:1002:BEF:F1	2.15	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:VAL:HG12	2:H:23:PHE:HD1	1.71	0.55
4:J:710:ARG:HH21	4:J:772:PRO:HG3	1.71	0.55
4:J:973:GLN:O	4:J:976:GLN:HG3	2.07	0.55
4:J:1434:TRP:NE1	4:J:1457:ASP:HB2	2.21	0.55
1:A:288:THR:HG23	1:A:296:LEU:O	2.07	0.55
1:C:86:ARG:HD2	1:C:86:ARG:O	2.06	0.55
4:J:527:MET:HG2	4:J:535:PHE:HB3	1.87	0.55
4:J:1484:THR:H	5:K:25:LYS:NZ	2.05	0.55
1:B:255:GLU:HB2	1:B:259:ARG:NH1	2.22	0.55
1:B:279:ARG:NH1	1:B:327:LEU:HB2	2.22	0.55
1:D:268:MET:SD	1:D:321:THR:HB	2.47	0.55
3:I:653:ASP:OD1	3:I:654:LEU:N	2.37	0.55
3:I:687:ALA:HB1	3:I:850:ALA:HB2	1.88	0.55
4:J:1031:ASN:OD1	4:J:1034:GLN:NE2	2.40	0.55
6:T:8:DT:C4	8:N:33:DT:O4	2.60	0.55
1:D:258:LYS:HE3	1:D:259:ARG:HH12	1.72	0.55
4:J:1389:LEU:HG	4:J:1390:LEU:HG	1.87	0.55
1:A:98:TYR:CZ	1:A:125:VAL:HB	2.42	0.55
1:A:355:ARG:HH12	1:A:400:ALA:HB2	1.70	0.55
1:C:185:PRO:HG3	1:C:329:GLU:OE2	2.07	0.55
1:C:353:SER:HB3	1:C:356:LEU:HD13	1.86	0.55
1:F:296:LEU:HD21	1:F:301:LEU:HG	1.89	0.55
3:I:704:HIS:CE1	3:I:831:ARG:HH21	2.25	0.55
4:J:1276:GLU:OE1	4:J:1276:GLU:N	2.40	0.55
4:J:1485:GLN:HE21	5:K:82:GLU:HA	1.65	0.55
1:F:416:ASN:HA	1:F:419:PHE:CD2	2.42	0.55
2:H:110:LYS:HG2	2:H:128:HIS:HA	1.88	0.55
1:E:251:GLU:O	1:E:255:GLU:HG2	2.07	0.55
1:E:303:PHE:HD1	1:E:306:ARG:HE	1.54	0.55
3:I:162:ILE:HB	3:I:172:ILE:HG22	1.89	0.55
3:I:175:GLU:HG3	3:I:183:SER:HB3	1.89	0.55
1:A:73:TYR:HB2	1:A:89:ILE:HG23	1.89	0.55
1:B:214:LEU:HB2	1:B:236:ALA:HA	1.89	0.55
1:C:213:LEU:HD13	1:C:235:ILE:HG23	1.88	0.55
2:G:8:ALA:HB1	2:H:224:TYR:HE2	1.71	0.55
2:H:7:LYS:HB2	2:H:27:PRO:HG2	1.88	0.55
3:I:142:ARG:HE	3:I:325:ILE:HD11	1.72	0.55
1:D:148:GLN:N	1:D:313:ASN:O	2.31	0.54
1:F:82:ASN:O	1:F:86:ARG:NH2	2.40	0.54
1:E:139:ARG:NH1	1:E:263:GLU:OE2	2.36	0.54
1:F:274:ILE:HB	1:F:324:ALA:HB1	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:LYS:HA	2:G:8:ALA:HB3	1.89	0.54
3:I:838:LYS:HD3	3:I:846:LYS:HE3	1.89	0.54
4:J:456:MET:SD	4:J:568:ARG:HD2	2.47	0.54
6:T:22:DA:H8	6:T:22:DA:OP1	1.90	0.54
1:A:92:ALA:HA	1:A:95:ILE:HD12	1.90	0.54
3:I:292:ARG:HB2	3:I:299:LYS:HG2	1.90	0.54
3:I:1083:GLU:OE2	3:I:1086:ARG:NH1	2.39	0.54
4:J:1306:PRO:HD2	4:J:1309:ALA:HB2	1.87	0.54
1:B:60:ARG:HH21	1:B:111:ARG:HG2	1.73	0.54
1:E:416:ASN:O	1:E:420:LEU:N	2.39	0.54
4:J:657:LEU:HD11	4:J:691:LEU:HD13	1.90	0.54
1:A:101:ARG:HH21	1:A:141:ARG:HD3	1.72	0.54
1:A:218:ARG:HH21	1:B:345:THR:C	2.10	0.54
1:B:91:SER:H	1:B:94:LEU:HD12	1.72	0.54
1:C:113:PRO:HD3	1:C:120:ALA:HB2	1.89	0.54
1:C:179:ARG:O	1:C:347:ASN:N	2.35	0.54
1:F:214:LEU:N	1:F:235:ILE:O	2.41	0.54
2:H:202:ASP:OD1	2:H:203:GLY:N	2.41	0.54
4:J:761:ILE:O	4:J:767:HIS:ND1	2.32	0.54
1:C:256:ARG:O	1:C:260:ILE:HG12	2.08	0.54
1:F:179:ARG:HD2	1:F:308:LEU:HG	1.88	0.54
3:I:468:ARG:HA	3:I:486:MET:O	2.08	0.54
3:I:720:GLU:HG2	3:I:760:SER:HA	1.89	0.54
1:A:162:GLU:O	1:A:166:ARG:HB3	2.08	0.54
1:C:239:PHE:O	1:D:302:TYR:HE1	1.90	0.54
2:H:57:TYR:HE1	2:H:163:ASN:HB3	1.71	0.54
3:I:165:LEU:HG	3:I:166:PRO:HA	1.90	0.54
4:J:46:ASP:HB3	4:J:49:ILE:HG22	1.89	0.54
1:A:165:THR:HA	1:A:168:ILE:HD12	1.90	0.54
1:C:163:LEU:HD13	1:C:407:LEU:HD22	1.90	0.54
1:D:101:ARG:HH12	1:D:141:ARG:HD2	1.71	0.54
1:F:376:GLU:OE1	1:F:376:GLU:N	2.38	0.54
1:F:383:VAL:O	1:F:387:MET:HE2	2.08	0.54
1:D:104:ASP:OD2	1:D:139:ARG:NH2	2.39	0.54
1:F:183:VAL:HA	1:F:326:ALA:HB3	1.90	0.54
1:F:255:GLU:O	1:F:259:ARG:NH1	2.41	0.54
1:F:288:THR:N	1:F:297:ASP:OD1	2.36	0.54
2:G:63:HIS:HB3	3:I:746:GLY:HA2	1.90	0.54
2:G:221:HIS:NE2	2:H:29:GLU:OE2	2.37	0.54
3:I:751:PRO:HD2	4:J:680:GLN:HE22	1.73	0.54
3:I:1031:ARG:HA	4:J:621:LYS:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:42:ASP:OD1	4:J:48:ARG:NH2	2.40	0.54
4:J:421:LEU:HD21	4:J:429:SER:HB2	1.90	0.54
4:J:613:ARG:HD3	4:J:616:GLN:HE21	1.73	0.54
1:A:139:ARG:NH1	1:A:263:GLU:OE2	2.41	0.54
1:E:296:LEU:N	1:F:290:ARG:HH22	2.05	0.54
2:G:106:PRO:HA	2:G:132:LEU:O	2.07	0.54
2:H:175:ARG:NH1	2:H:202:ASP:HB3	2.22	0.54
1:A:154:ILE:HG23	1:A:205:GLU:HG3	1.90	0.53
1:A:182:ILE:HG22	1:A:350:LEU:HB3	1.89	0.53
1:B:185:PRO:HD2	1:B:354:ARG:NH1	2.22	0.53
1:B:243:PRO:HB2	1:B:284:VAL:HG22	1.90	0.53
1:C:207:ASP:N	1:C:207:ASP:OD1	2.41	0.53
1:C:304:PRO:HB2	1:C:342:PHE:HZ	1.74	0.53
3:I:218:VAL:HG22	3:I:222:MET:HG2	1.89	0.53
6:T:38:DA:C6	8:N:4:DT:O4	2.61	0.53
1:C:408:ALA:HB3	5:K:87:LYS:CE	2.34	0.53
1:E:220:GLU:OE1	1:E:220:GLU:N	2.39	0.53
3:I:174:LEU:HD22	3:I:193:LEU:HD22	1.89	0.53
1:B:212:VAL:HG22	1:B:270:LEU:HB2	1.90	0.53
1:B:274:ILE:N	1:B:325:THR:O	2.41	0.53
4:J:554:LEU:HD13	4:J:574:LEU:HD22	1.90	0.53
1:E:68:ILE:HA	1:E:90:VAL:HG11	1.91	0.53
1:F:266:HIS:ND1	1:F:319:SER:OG	2.27	0.53
1:F:351:HIS:HB2	1:F:366:ASP:HB3	1.90	0.53
3:I:399:ASN:ND2	3:I:566:THR:O	2.39	0.53
4:J:122:GLU:HG2	4:J:123:LEU:HD12	1.89	0.53
1:B:338:ILE:HA	1:B:341:GLU:HG2	1.91	0.53
1:C:214:LEU:O	1:C:237:SER:N	2.40	0.53
1:F:104:ASP:OD2	1:F:139:ARG:NH2	2.41	0.53
2:H:104:GLU:HG2	2:H:137:ARG:HE	1.72	0.53
1:E:297:ASP:O	1:E:301:LEU:HG	2.09	0.53
1:F:384:THR:HA	1:F:387:MET:HE3	1.90	0.53
3:I:91:GLN:OE1	3:I:117:HIS:HB3	2.09	0.53
3:I:676:ILE:HB	3:I:988:VAL:HG13	1.91	0.53
3:I:890:LEU:HG	3:I:914:ILE:HD12	1.91	0.53
1:C:184:ALA:O	1:C:327:LEU:HA	2.09	0.53
1:C:226:ARG:NH1	1:C:226:ARG:HB2	2.23	0.53
1:D:163:LEU:HD22	1:D:407:LEU:HA	1.91	0.53
1:E:184:ALA:HB2	1:E:352:LEU:HD12	1.91	0.53
3:I:54:ILE:HG12	3:I:66:LEU:HB3	1.91	0.53
3:I:266:ARG:HE	3:I:345:ARG:NH1	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:942:GLU:OE1	3:I:946:ARG:NH2	2.42	0.53
1:A:409:ARG:O	1:A:412:ARG:HG3	2.09	0.53
1:B:218:ARG:NH1	11:B:502:BEF:F1	2.32	0.53
1:C:101:ARG:NH2	1:C:141:ARG:HD3	2.22	0.53
1:C:209:LYS:HE2	1:C:211:ILE:HD11	1.90	0.53
1:E:295:GLY:HA2	1:F:290:ARG:HH21	1.72	0.53
1:F:166:ARG:HA	1:F:415:ASN:HD21	1.72	0.53
2:G:58:ILE:HG22	2:G:60:ASP:H	1.74	0.53
2:H:152:PRO:HD2	2:H:155:LYS:NZ	2.23	0.53
3:I:200:LEU:HD22	3:I:300:ASP:HB3	1.91	0.53
4:J:122:GLU:OE1	4:J:122:GLU:N	2.41	0.53
1:A:148:GLN:N	1:A:313:ASN:O	2.31	0.53
1:B:74:GLY:H	1:B:90:VAL:H	1.56	0.53
1:C:420:LEU:HD23	1:C:423:LEU:HD12	1.91	0.53
1:D:273:SER:H	1:D:325:THR:HG1	1.56	0.53
4:J:33:ASN:ND2	4:J:40:GLU:OE1	2.41	0.53
4:J:563:PRO:HG2	4:J:566:ILE:HB	1.91	0.53
4:J:1211:MET:CE	5:K:16:LYS:HZ1	2.22	0.53
6:T:9:DA:H2	8:N:33:DT:O2	1.92	0.53
1:B:111:ARG:NH2	1:B:121:THR:OG1	2.42	0.52
1:D:184:ALA:HB2	1:D:352:LEU:HD12	1.90	0.52
1:E:314:ILE:HG22	1:E:316:GLY:H	1.74	0.52
3:I:79:PRO:HD2	3:I:82:GLU:OE2	2.08	0.52
3:I:863:ASP:OD1	3:I:864:GLY:N	2.41	0.52
4:J:162:ARG:HH12	4:J:452:ILE:H	1.56	0.52
4:J:403:PHE:CE1	4:J:444:VAL:HG23	2.44	0.52
4:J:892:ASP:HB3	4:J:895:VAL:HG12	1.91	0.52
4:J:959:GLU:O	4:J:962:GLN:HG2	2.09	0.52
1:A:208:ILE:HG23	1:A:266:HIS:HB3	1.90	0.52
1:D:176:ARG:HD3	1:D:266:HIS:CE1	2.44	0.52
3:I:254:VAL:O	3:I:257:VAL:HG12	2.08	0.52
4:J:800:LYS:HZ3	4:J:831:GLY:HA2	1.73	0.52
1:B:217:GLU:HB2	1:B:276:ARG:NH2	2.24	0.52
1:C:101:ARG:HH11	1:C:259:ARG:NH2	2.07	0.52
1:F:275:THR:OG1	1:F:327:LEU:N	2.37	0.52
5:K:70:THR:HB	5:K:72:ARG:HE	1.74	0.52
1:B:183:VAL:HG11	1:B:339:PHE:HE1	1.73	0.52
1:B:219:PRO:HB2	1:C:147:PRO:HG2	1.89	0.52
1:B:242:PRO:HD2	1:B:245:ASN:HD22	1.73	0.52
4:J:31:THR:HG23	4:J:45:PHE:CD1	2.44	0.52
1:D:379:LEU:HB2	1:D:387:MET:CE	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:PRO:HB2	1:E:354:ARG:NH2	2.25	0.52
1:E:268:MET:SD	1:E:321:THR:HB	2.49	0.52
1:F:177:GLY:N	1:F:321:THR:OG1	2.35	0.52
3:I:1040:LEU:HD21	3:I:1048:THR:HG22	1.92	0.52
1:A:388:TRP:CZ2	1:F:360:ARG:HB3	2.45	0.52
1:B:92:ALA:HA	1:B:95:ILE:HD12	1.92	0.52
1:E:284:VAL:O	1:E:286:PRO:HD3	2.10	0.52
1:F:355:ARG:HH12	1:F:400:ALA:HB2	1.75	0.52
2:H:1:MET:O	2:H:6:LEU:N	2.42	0.52
2:H:104:GLU:HG2	2:H:137:ARG:HH21	1.74	0.52
3:I:165:LEU:H	3:I:265:ARG:HD3	1.74	0.52
7:R:21:C:H2'	7:R:22:A:H8	1.73	0.52
1:A:184:ALA:HB2	1:A:352:LEU:HD12	1.91	0.52
1:B:274:ILE:HB	1:B:324:ALA:HB1	1.92	0.52
1:D:186:PRO:HG3	1:D:327:LEU:HD21	1.90	0.52
1:D:354:ARG:O	1:D:357:GLU:N	2.43	0.52
3:I:48:PHE:O	3:I:53:PRO:HD3	2.10	0.52
3:I:184:MET:HG3	3:I:193:LEU:HD13	1.92	0.52
4:J:63:TYR:HA	4:J:68:PHE:HE1	1.74	0.52
6:T:2:DG:N1	8:N:40:DC:O2	2.37	0.52
3:I:272:ALA:HB2	3:I:464:LEU:HD13	1.91	0.52
3:I:999:HIS:CE1	3:I:1003:ASP:HB3	2.45	0.52
4:J:806:PHE:HZ	4:J:813:LEU:HA	1.75	0.52
4:J:1276:GLU:HG2	4:J:1277:ILE:HG12	1.91	0.52
5:K:83:ASP:HB2	5:K:87:LYS:NZ	2.25	0.52
1:A:402:ALA:O	1:A:406:LEU:HB2	2.10	0.52
1:C:212:VAL:HG11	1:C:225:PHE:CE2	2.43	0.52
1:C:300:ALA:O	1:C:304:PRO:HD2	2.10	0.52
1:D:244:GLN:HB3	1:D:248:ARG:HH12	1.75	0.52
1:E:80:LEU:HB3	1:E:84:GLU:HG2	1.92	0.52
1:E:397:MET:SD	1:E:398:ASP:N	2.82	0.52
3:I:1080:SER:OG	3:I:1081:VAL:N	2.42	0.52
4:J:57:GLU:HA	4:J:64:LYS:HD2	1.92	0.52
4:J:800:LYS:HD3	4:J:829:VAL:CG2	2.40	0.52
4:J:925:GLU:OE2	5:K:6:ILE:N	2.41	0.52
1:E:182:ILE:O	1:E:326:ALA:N	2.30	0.52
4:J:838:ARG:HH11	4:J:874:GLU:HB3	1.74	0.52
4:J:1225:ALA:O	4:J:1229:ILE:HG12	2.09	0.52
1:A:242:PRO:HD2	1:A:245:ASN:HD22	1.74	0.51
1:D:218:ARG:HH22	1:E:373:ARG:NH2	2.08	0.51
1:F:281:ASN:O	1:F:285:THR:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:153:ALA:N	2:G:168:ASP:OD1	2.43	0.51
3:I:367:LEU:HB2	3:I:371:LYS:HD3	1.92	0.51
4:J:636:GLN:NE2	4:J:727:GLN:OE1	2.43	0.51
4:J:1081:GLY:O	4:J:1084:THR:OG1	2.26	0.51
1:B:185:PRO:O	1:B:190:LYS:NZ	2.43	0.51
1:B:417:LYS:HA	1:B:420:LEU:HB2	1.91	0.51
1:C:297:ASP:HA	1:D:290:ARG:NH2	2.23	0.51
1:D:108:GLY:HA2	1:D:126:GLU:HB2	1.93	0.51
1:D:212:VAL:HG22	1:D:270:LEU:HD12	1.91	0.51
3:I:957:LYS:HD3	3:I:961:GLU:HG3	1.91	0.51
1:A:229:VAL:HG22	1:A:232:ALA:HB3	1.93	0.51
1:B:360:ARG:HD3	1:C:388:TRP:CD1	2.45	0.51
1:C:110:ALA:HB2	1:C:122:LEU:HA	1.93	0.51
3:I:204:GLN:CD	3:I:228:ALA:HB1	2.30	0.51
4:J:64:LYS:HE3	4:J:65:ARG:HH11	1.75	0.51
1:B:223:THR:O	1:B:227:GLU:OE1	2.28	0.51
1:B:314:ILE:HG22	1:B:316:GLY:H	1.74	0.51
1:F:166:ARG:NH1	1:F:414:LYS:HA	2.26	0.51
3:I:332:ARG:HE	3:I:464:LEU:HB3	1.75	0.51
3:I:999:HIS:NE2	3:I:1003:ASP:OD2	2.43	0.51
4:J:1211:MET:HE1	5:K:16:LYS:NZ	2.24	0.51
1:A:353:SER:HB3	1:A:356:LEU:HD13	1.93	0.51
1:B:239:PHE:CZ	1:C:345:THR:HG23	2.44	0.51
2:G:11:PHE:HD2	2:H:228:PRO:HA	1.76	0.51
2:H:23:PHE:HE2	2:H:199:ILE:HD12	1.75	0.51
4:J:893:GLU:N	4:J:893:GLU:OE1	2.44	0.51
4:J:1094:LEU:HD13	4:J:1260:ILE:HD13	1.91	0.51
4:J:1406:ARG:O	4:J:1412:LYS:NZ	2.34	0.51
5:K:23:VAL:HG21	5:K:65:MET:HG3	1.93	0.51
6:T:1:DG:H2"	6:T:2:DG:C8	2.46	0.51
6:T:37:DT:H2"	6:T:38:DA:H8	1.75	0.51
1:B:409:ARG:HG2	1:B:412:ARG:NH1	2.26	0.51
1:D:251:GLU:O	1:D:255:GLU:HG2	2.10	0.51
1:E:212:VAL:HG22	1:E:270:LEU:HD12	1.92	0.51
1:F:63:LYS:HB2	1:F:107:VAL:HG22	1.93	0.51
4:J:962:GLN:HA	4:J:965:GLU:HG2	1.91	0.51
1:C:275:THR:C	1:C:279:ARG:HE	2.14	0.51
1:E:185:PRO:HB2	1:E:354:ARG:HH21	1.75	0.51
3:I:158:TYR:OH	3:I:314:THR:N	2.44	0.51
4:J:1106:VAL:HG13	4:J:1108:ARG:HD2	1.91	0.51
5:K:48:MET:SD	5:K:54:LEU:HG	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:THR:HG23	9:B:501:ADP:PA	2.50	0.51
1:E:76:LEU:HB3	1:E:87:VAL:HG23	1.93	0.51
1:E:77:THR:N	1:E:87:VAL:HB	2.25	0.51
1:E:78:GLU:HB3	1:E:87:VAL:HG12	1.92	0.51
3:I:586:ARG:NH2	3:I:590:ASP:OD2	2.31	0.51
4:J:1331:ASP:HB3	4:J:1334:GLN:HG2	1.93	0.51
1:B:179:ARG:NE	1:B:345:THR:O	2.43	0.51
1:C:218:ARG:HA	1:C:239:PHE:HE1	1.75	0.51
1:C:297:ASP:N	1:D:290:ARG:HH22	2.09	0.51
1:E:78:GLU:HG2	1:E:84:GLU:OE1	2.11	0.51
1:E:102:ALA:O	1:E:259:ARG:NE	2.44	0.51
1:E:261:VAL:HG21	1:E:320:LEU:HB2	1.92	0.51
9:E:1000:ADP:O2B	11:E:1002:BEF:F2	2.18	0.51
1:F:187:LYS:HA	9:F:1000:ADP:O3A	2.11	0.51
1:F:288:THR:HA	1:F:297:ASP:HA	1.93	0.51
4:J:412:GLY:HA2	4:J:434:ARG:NH2	2.26	0.51
5:K:38:THR:OG1	5:K:67:GLU:OE2	2.19	0.51
1:B:218:ARG:NH1	1:C:373:ARG:CZ	2.74	0.51
1:D:362:PHE:HB3	9:D:1000:ADP:N6	2.26	0.51
1:D:414:LYS:HZ2	1:D:416:ASN:H	1.59	0.51
3:I:292:ARG:NH2	3:I:297:GLU:OE2	2.44	0.51
3:I:1013:TYR:HA	3:I:1020:PRO:HA	1.93	0.51
4:J:153:LEU:HD11	4:J:158:TYR:HD1	1.76	0.51
4:J:895:VAL:HG23	4:J:921:ARG:NH1	2.26	0.51
1:B:188:ALA:HA	1:B:357:GLU:OE1	2.11	0.50
1:B:350:LEU:HD12	1:B:370:SER:OG	2.11	0.50
1:D:273:SER:N	1:D:325:THR:OG1	2.34	0.50
9:D:1000:ADP:O2B	11:D:1002:BEF:F3	2.20	0.50
1:F:213:LEU:HG	1:F:215:ILE:HD11	1.93	0.50
2:H:175:ARG:N	2:H:200:TRP:O	2.44	0.50
3:I:78:PHE:HB3	3:I:82:GLU:OE2	2.11	0.50
3:I:541:SER:O	3:I:545:ASN:ND2	2.44	0.50
3:I:808:ARG:HD3	3:I:820:ARG:HA	1.92	0.50
3:I:1031:ARG:HD3	6:T:25:DT:P	2.49	0.50
1:B:218:ARG:HH12	1:C:373:ARG:CZ	2.24	0.50
1:B:271:LEU:HD22	1:B:307:PHE:HE2	1.77	0.50
1:C:274:ILE:HG22	1:C:325:THR:O	2.10	0.50
9:C:1002:ADP:O2B	11:C:1004:BEF:F2	2.19	0.50
3:I:158:TYR:CE1	3:I:310:LEU:HG	2.43	0.50
3:I:567:GLN:HG3	3:I:997:LEU:HD22	1.93	0.50
4:J:131:LYS:HZ2	4:J:568:ARG:HG3	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ALA:HA	1:C:95:ILE:HD12	1.93	0.50
1:F:288:THR:HG21	1:F:295:GLY:HA2	1.93	0.50
2:G:218:LEU:HG	2:H:222:LEU:HD11	1.92	0.50
6:T:9:DA:C2	8:N:33:DT:C2	2.99	0.50
1:C:297:ASP:N	1:D:290:ARG:HH12	2.10	0.50
1:E:166:ARG:NE	1:E:410:LEU:HB3	2.26	0.50
1:E:183:VAL:HG23	1:E:351:HIS:HA	1.94	0.50
1:F:78:GLU:HG2	1:F:86:ARG:NE	2.26	0.50
2:H:55:SER:OG	2:H:165:ILE:O	2.27	0.50
3:I:55:GLU:O	3:I:356:ARG:NH2	2.45	0.50
3:I:584:GLU:OE1	3:I:584:GLU:N	2.38	0.50
3:I:1093:GLN:HG3	4:J:21:TRP:CZ3	2.47	0.50
4:J:845:ASN:HB2	4:J:848:GLU:OE1	2.12	0.50
1:A:166:ARG:HG3	1:A:415:ASN:HB3	1.93	0.50
1:D:176:ARG:HE	1:D:208:ILE:HD11	1.77	0.50
1:E:145:LEU:O	1:E:147:PRO:HD3	2.11	0.50
1:E:328:VAL:HG22	1:E:329:GLU:H	1.76	0.50
1:F:217:GLU:CG	1:F:276:ARG:HH22	2.21	0.50
4:J:828:LYS:HD2	4:J:863:VAL:HG22	1.94	0.50
4:J:1093:TYR:CZ	4:J:1097:LYS:HE3	2.46	0.50
1:B:221:GLU:HA	1:C:149:PHE:CE1	2.46	0.50
1:B:288:THR:HG21	1:B:300:ALA:HB2	1.92	0.50
1:F:328:VAL:HG22	1:F:329:GLU:H	1.75	0.50
5:K:14:ASP:OD2	5:K:18:ARG:NH1	2.45	0.50
1:A:383:VAL:HA	1:A:386:LYS:HG2	1.94	0.50
1:B:89:ILE:HD12	1:B:121:THR:HG22	1.93	0.50
1:F:387:MET:O	1:F:391:ARG:HG3	2.12	0.50
3:I:166:PRO:HD3	3:I:266:ARG:HH12	1.77	0.50
3:I:753:ASP:OD1	4:J:681:ARG:NH2	2.45	0.50
4:J:1364:HIS:HD2	4:J:1366:LYS:HG3	1.74	0.50
4:J:1448:THR:O	4:J:1452:ILE:HG12	2.12	0.50
4:J:1462:LEU:HD22	4:J:1472:ILE:HG23	1.94	0.50
4:J:130:SER:OG	4:J:131:LYS:N	2.44	0.50
4:J:996:TRP:CE2	4:J:1056:PRO:HG3	2.47	0.50
1:B:192:THR:O	1:B:196:LYS:HG3	2.12	0.50
1:B:214:LEU:O	1:B:237:SER:N	2.45	0.50
1:E:63:LYS:HA	1:E:106:VAL:O	2.12	0.50
1:E:182:ILE:HA	1:E:350:LEU:HB3	1.92	0.50
1:F:400:ALA:O	1:F:403:MET:HB3	2.11	0.50
4:J:64:LYS:HE3	4:J:65:ARG:NH1	2.27	0.50
1:A:184:ALA:HB2	1:A:352:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:ILE:HG12	1:E:284:VAL:HG21	1.94	0.49
1:E:406:LEU:HG	1:E:410:LEU:HD12	1.94	0.49
1:F:114:ARG:HA	1:F:114:ARG:CZ	2.42	0.49
3:I:420:ARG:HH12	3:I:423:ALA:HB3	1.77	0.49
4:J:66:GLN:NE2	7:R:12:A:H3'	2.27	0.49
4:J:591:VAL:HG22	4:J:592:THR:H	1.77	0.49
6:T:11:DC:H2"	6:T:12:DA:C8	2.47	0.49
1:B:254:HIS:HE1	1:B:306:ARG:HD2	1.76	0.49
1:D:171:LEU:HD21	1:D:370:SER:HB2	1.93	0.49
1:E:225:PHE:O	1:E:229:VAL:N	2.41	0.49
1:F:214:LEU:HD23	1:F:272:ASP:HB2	1.95	0.49
2:H:220:GLU:O	2:H:223:THR:OG1	2.26	0.49
6:T:8:DT:O4	8:N:33:DT:O4	2.30	0.49
1:A:194:LEU:HD11	1:A:270:LEU:HB3	1.94	0.49
1:B:192:THR:OG1	9:B:501:ADP:N7	2.44	0.49
1:B:218:ARG:HD3	1:C:179:ARG:HH21	1.78	0.49
1:B:254:HIS:HB2	1:B:307:PHE:CE1	2.48	0.49
3:I:58:ASP:N	3:I:58:ASP:OD1	2.45	0.49
3:I:502:PRO:HB2	3:I:509:ALA:HB3	1.95	0.49
5:K:9:LEU:HD23	5:K:68:LEU:HD22	1.93	0.49
8:N:38:DC:H2"	8:N:39:DA:C8	2.46	0.49
1:B:286:PRO:HB2	1:B:287:PRO:HD3	1.94	0.49
1:D:178:GLN:O	1:D:321:THR:HA	2.12	0.49
3:I:17:PRO:HB2	3:I:20:GLU:HB3	1.95	0.49
3:I:176:VAL:HG11	3:I:217:LEU:HD21	1.95	0.49
4:J:69:GLU:HG2	4:J:70:GLY:N	2.28	0.49
4:J:455:ARG:HB3	4:J:460:ALA:HB2	1.94	0.49
4:J:907:GLU:HG2	4:J:1026:SER:HA	1.94	0.49
1:A:148:GLN:HE22	1:A:315:ARG:HH21	1.59	0.49
1:B:374:ARG:HB3	1:B:377:LEU:HG	1.94	0.49
1:B:401:GLU:O	1:B:405:MET:HG3	2.13	0.49
1:C:328:VAL:HG22	1:C:329:GLU:H	1.78	0.49
1:D:177:GLY:N	1:D:321:THR:OG1	2.45	0.49
1:F:286:PRO:HD2	1:F:287:PRO:HD3	1.94	0.49
1:F:375:GLU:O	1:F:379:LEU:N	2.45	0.49
3:I:557:ARG:NE	3:I:879:ARG:HG2	2.26	0.49
3:I:806:LEU:HD13	3:I:813:VAL:HG21	1.94	0.49
4:J:138:LYS:HG2	4:J:450:TYR:CD2	2.46	0.49
1:A:330:THR:OG1	1:A:335:ASP:OD2	2.20	0.49
1:F:337:VAL:O	1:F:341:GLU:HG3	2.12	0.49
4:J:160:GLU:OE2	4:J:165:LYS:HD3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLU:HB2	1:B:276:ARG:HH22	1.78	0.49
1:C:67:GLU:O	1:C:74:GLY:HA2	2.12	0.49
1:C:255:GLU:O	1:C:259:ARG:HG2	2.13	0.49
1:C:275:THR:O	1:C:279:ARG:NE	2.36	0.49
1:E:166:ARG:HD2	1:E:410:LEU:HD13	1.94	0.49
1:E:342:PHE:HA	1:E:345:THR:HB	1.95	0.49
1:C:75:PHE:HD2	1:C:87:VAL:HG11	1.78	0.49
1:C:349:GLU:OE2	1:C:369:LYS:NZ	2.45	0.49
1:E:92:ALA:O	1:E:95:ILE:HB	2.12	0.49
3:I:551:GLU:OE2	3:I:552:HIS:NE2	2.46	0.49
4:J:976:GLN:HA	4:J:979:GLU:HG2	1.95	0.49
1:A:391:ARG:CB	1:F:360:ARG:HE	2.25	0.49
1:B:224:ASP:OD2	1:C:374:ARG:NH2	2.46	0.49
1:C:183:VAL:HA	1:C:326:ALA:HB3	1.94	0.49
1:C:279:ARG:O	1:C:283:LEU:HG	2.13	0.49
1:D:101:ARG:HG2	1:D:259:ARG:NH2	2.27	0.49
1:E:255:GLU:O	1:E:259:ARG:HG2	2.13	0.49
1:F:141:ARG:HB3	1:F:144:GLU:OE1	2.12	0.49
5:K:12:MET:SD	5:K:13:VAL:HG13	2.52	0.49
7:R:22:A:H2'	7:R:23:U:C6	2.48	0.49
1:B:171:LEU:HD21	1:B:370:SER:HB2	1.94	0.49
1:D:388:TRP:O	1:D:392:LYS:HD3	2.13	0.49
1:F:280:ALA:O	1:F:284:VAL:HG23	2.12	0.49
2:G:73:GLU:HB3	2:G:77:GLU:HB2	1.93	0.49
4:J:957:PRO:HG2	4:J:1007:VAL:HG22	1.94	0.49
1:A:252:PHE:O	1:A:255:GLU:HG2	2.12	0.48
1:C:297:ASP:CA	1:D:290:ARG:NH2	2.74	0.48
1:D:75:PHE:HB3	1:D:87:VAL:HB	1.95	0.48
1:D:269:ILE:HB	1:D:322:ILE:HG12	1.93	0.48
2:G:104:GLU:OE2	2:G:137:ARG:NE	2.46	0.48
2:G:133:GLU:HG3	2:G:134:GLU:N	2.28	0.48
3:I:333:ILE:HD11	3:I:467:ILE:HD11	1.94	0.48
3:I:1070:ILE:HD13	4:J:655:PRO:HB2	1.95	0.48
6:T:35:DG:C2	6:T:36:DA:C4	3.01	0.48
1:B:388:TRP:O	1:B:392:LYS:HD3	2.13	0.48
1:C:218:ARG:NH1	11:C:1004:BEF:F1	2.36	0.48
4:J:500:ARG:NH1	4:J:1388:ARG:HH22	2.10	0.48
4:J:634:GLY:N	4:J:728:LEU:O	2.46	0.48
1:A:179:ARG:HE	1:A:346:GLY:HA2	1.77	0.48
1:D:104:ASP:OD1	1:D:139:ARG:NH1	2.33	0.48
1:D:128:VAL:N	1:D:131:LEU:O	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:SER:OG	1:D:276:ARG:NH2	2.46	0.48
1:D:302:TYR:HA	1:D:305:LYS:HD2	1.95	0.48
1:E:192:THR:HG21	9:E:1000:ADP:H2'	1.94	0.48
3:I:64:LEU:HD22	3:I:359:MET:HG3	1.95	0.48
3:I:1038:TRP:CH2	4:J:1099:VAL:HG11	2.48	0.48
4:J:1042:ARG:HH11	4:J:1061:PHE:HZ	1.61	0.48
4:J:1150:ALA:HB3	4:J:1187:PRO:HB2	1.94	0.48
1:A:94:LEU:HD13	1:A:122:LEU:HD22	1.94	0.48
1:B:336:ASP:O	1:B:339:PHE:HB3	2.13	0.48
1:E:285:THR:HB	1:E:297:ASP:OD2	2.13	0.48
1:F:82:ASN:H	1:F:86:ARG:NH2	2.11	0.48
1:F:243:PRO:HA	1:F:246:HIS:CG	2.48	0.48
4:J:761:ILE:HG21	5:K:20:THR:HG22	1.94	0.48
4:J:1294:VAL:HB	4:J:1301:LYS:HE3	1.94	0.48
1:B:163:LEU:HD21	1:B:411:ALA:HA	1.96	0.48
1:B:383:VAL:HG12	1:B:387:MET:CE	2.43	0.48
1:B:398:ASP:N	1:B:401:GLU:OE2	2.44	0.48
1:C:218:ARG:NE	1:D:345:THR:HA	2.28	0.48
1:D:76:LEU:HD12	1:D:88:ALA:HB3	1.96	0.48
1:E:84:GLU:HB2	1:E:87:VAL:CG1	2.44	0.48
1:F:279:ARG:HH21	1:F:335:ASP:N	2.10	0.48
2:H:3:ASP:HA	2:H:189:ARG:HH22	1.78	0.48
3:I:162:ILE:HB	3:I:172:ILE:CG2	2.42	0.48
4:J:421:LEU:HB2	4:J:427:VAL:HG12	1.96	0.48
4:J:1048:PRO:HA	4:J:1079:LYS:HE3	1.96	0.48
4:J:1289:LYS:HD3	4:J:1304:LYS:HB3	1.94	0.48
6:T:15:DA:H2"	6:T:16:DG:C8	2.48	0.48
6:T:37:DT:H2"	6:T:38:DA:C8	2.49	0.48
1:B:194:LEU:HD12	1:B:197:ILE:HD11	1.96	0.48
1:C:334:MET:O	1:C:338:ILE:HG12	2.13	0.48
1:E:66:LEU:HB2	1:E:104:ASP:O	2.14	0.48
3:I:191:PHE:CZ	3:I:195:LEU:HB3	2.48	0.48
4:J:1402:ALA:O	4:J:1406:ARG:HG2	2.14	0.48
6:T:15:DA:H2"	6:T:16:DG:H8	1.77	0.48
1:B:301:LEU:HD13	1:B:305:LYS:HE2	1.95	0.48
1:E:352:LEU:HD23	1:E:365:ILE:HA	1.95	0.48
1:F:73:TYR:HB2	1:F:89:ILE:HG12	1.95	0.48
3:I:3:ILE:HG22	3:I:900:ARG:HB2	1.94	0.48
3:I:807:ARG:HG3	3:I:809:GLY:H	1.79	0.48
3:I:894:GLY:O	3:I:898:GLY:N	2.46	0.48
4:J:46:ASP:HB3	4:J:49:ILE:CG2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:417:PRO:HD3	4:J:432:TYR:CD1	2.49	0.48
4:J:908:LYS:HD3	4:J:1027:GLY:HA3	1.95	0.48
4:J:1438:ALA:O	4:J:1443:THR:HG22	2.14	0.48
5:K:48:MET:HG2	5:K:54:LEU:N	2.28	0.48
1:E:74:GLY:O	1:E:89:ILE:HG13	2.14	0.48
3:I:64:LEU:HD12	3:I:100:LEU:HD11	1.94	0.48
3:I:122:THR:OG1	3:I:124:ASP:OD1	2.25	0.48
4:J:806:PHE:H	4:J:832:ARG:HE	1.62	0.48
6:T:34:DA:H2"	6:T:35:DG:C8	2.48	0.48
7:R:16:C:H2'	7:R:17:U:C6	2.49	0.48
1:D:218:ARG:HA	1:D:239:PHE:HE1	1.78	0.48
1:E:224:ASP:O	1:E:228:SER:OG	2.24	0.48
1:F:347:ASN:HA	1:F:373:ARG:HD2	1.96	0.48
1:F:351:HIS:O	1:F:366:ASP:N	2.39	0.48
2:H:18:ARG:NH2	2:H:203:GLY:O	2.26	0.48
3:I:420:ARG:HD2	3:I:422:ARG:HB2	1.95	0.48
3:I:576:ALA:O	3:I:671:ASN:ND2	2.45	0.48
4:J:40:GLU:HG3	4:J:41:ARG:HG2	1.95	0.48
4:J:507:ASN:HB2	4:J:511:TRP:HE1	1.79	0.48
4:J:1496:GLU:O	4:J:1500:LYS:HG2	2.14	0.48
4:J:1498:ALA:HA	4:J:1501:GLU:OE2	2.14	0.48
6:T:34:DA:H2"	6:T:35:DG:H8	1.78	0.48
8:N:39:DA:H2"	8:N:40:DC:C5	2.49	0.48
1:D:279:ARG:O	1:D:283:LEU:HG	2.14	0.48
1:F:414:LYS:O	1:F:418:GLU:N	2.37	0.48
1:C:212:VAL:HG23	1:C:270:LEU:HB2	1.96	0.47
1:D:273:SER:O	1:D:277:LEU:N	2.41	0.47
1:F:78:GLU:HB3	1:F:86:ARG:HG3	1.95	0.47
3:I:275:TYR:O	3:I:279:GLU:HB3	2.14	0.47
3:I:717:LEU:HD23	3:I:761:PHE:HB2	1.96	0.47
3:I:958:THR:N	3:I:961:GLU:OE2	2.43	0.47
4:J:659:LYS:O	4:J:663:GLU:HG2	2.14	0.47
6:T:17:DC:H2"	6:T:18:DA:C8	2.49	0.47
2:G:175:ARG:NH1	2:G:202:ASP:OD1	2.36	0.47
2:H:141:GLU:OE2	2:H:161:ARG:NH1	2.48	0.47
1:C:257:ALA:O	1:C:261:VAL:HG23	2.15	0.47
2:H:80:LEU:HD21	4:J:867:ARG:CB	2.41	0.47
3:I:42:VAL:HA	3:I:46:ALA:HB2	1.95	0.47
3:I:150:PRO:HA	3:I:158:TYR:HB3	1.95	0.47
4:J:23:TYR:HE2	4:J:89:ARG:HG2	1.78	0.47
6:T:13:DC:H2"	6:T:14:DA:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HA	1:A:322:ILE:HD11	1.95	0.47
1:B:291:THR:OG1	7:R:3:C:O2'	2.28	0.47
1:B:399:PRO:O	1:B:403:MET:HG2	2.14	0.47
1:D:288:THR:HG21	1:D:298:SER:N	2.29	0.47
1:E:77:THR:H	1:E:88:ALA:H	1.63	0.47
2:G:229:GLN:HE22	2:H:11:PHE:HB3	1.79	0.47
4:J:108:VAL:HB	4:J:109:PRO:HD3	1.97	0.47
1:A:261:VAL:HG21	1:A:320:LEU:HD22	1.96	0.47
1:A:382:GLU:OE2	1:A:383:VAL:HG23	2.14	0.47
1:A:383:VAL:HG13	1:A:386:LYS:HE3	1.95	0.47
1:C:351:HIS:HB2	1:C:366:ASP:HB3	1.97	0.47
1:F:77:THR:HB	1:F:86:ARG:NH2	2.29	0.47
1:F:181:LEU:HD11	1:F:274:ILE:HD13	1.97	0.47
3:I:180:GLY:HA2	3:I:220:GLY:HA2	1.96	0.47
1:A:225:PHE:O	1:A:229:VAL:N	2.46	0.47
1:A:312:ARG:NE	1:A:314:ILE:HD11	2.30	0.47
1:C:243:PRO:HA	1:C:246:HIS:CG	2.50	0.47
1:D:216:ASP:N	1:D:237:SER:O	2.35	0.47
1:D:412:ARG:NH1	1:D:413:THR:OG1	2.48	0.47
2:G:61:VAL:O	2:G:163:ASN:ND2	2.32	0.47
3:I:257:VAL:O	3:I:263:ASP:HB2	2.15	0.47
3:I:774:LEU:CD1	3:I:778:PHE:HE2	2.26	0.47
4:J:564:GLU:O	4:J:568:ARG:HG2	2.14	0.47
4:J:614:PHE:HD2	4:J:1439:SER:HA	1.80	0.47
4:J:1128:VAL:HG12	4:J:1129:THR:H	1.80	0.47
1:B:141:ARG:NH1	1:B:143:ASP:HB2	2.30	0.47
1:B:255:GLU:HB2	1:B:259:ARG:HH22	1.80	0.47
1:D:274:ILE:HD11	1:D:326:ALA:HB2	1.96	0.47
3:I:395:LYS:HG2	3:I:397:GLU:HG3	1.95	0.47
3:I:1032:PHE:O	3:I:1036:GLU:HB2	2.15	0.47
4:J:1042:ARG:O	4:J:1057:VAL:HB	2.15	0.47
1:A:256:ARG:O	1:A:260:ILE:HG12	2.15	0.47
1:B:148:GLN:N	1:B:313:ASN:O	2.40	0.47
1:B:310:ALA:HA	1:B:312:ARG:HH21	1.80	0.47
1:D:107:VAL:HB	1:D:127:ALA:HB3	1.96	0.47
1:F:146:THR:CB	1:F:148:GLN:HE22	2.28	0.47
1:F:296:LEU:HD23	1:F:297:ASP:O	2.14	0.47
3:I:124:ASP:OD1	3:I:125:GLY:N	2.48	0.47
3:I:922:PHE:HB2	3:I:967:PHE:CD1	2.49	0.47
3:I:1004:LYS:HD3	4:J:724:GLN:NE2	2.30	0.47
1:E:179:ARG:HD2	1:E:308:LEU:HG	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:PHE:HB2	1:E:304:PRO:HD3	1.97	0.47
1:F:255:GLU:O	1:F:259:ARG:HG2	2.14	0.47
3:I:905:ILE:HG13	3:I:906:PHE:HD1	1.80	0.47
4:J:148:GLU:HA	4:J:151:GLN:NE2	2.30	0.47
1:A:101:ARG:HH11	1:A:259:ARG:NH2	2.13	0.47
1:A:211:ILE:HB	1:A:269:ILE:HD13	1.97	0.47
1:B:183:VAL:HG11	1:B:339:PHE:CE1	2.50	0.47
1:B:376:GLU:OE1	1:B:376:GLU:N	2.36	0.47
1:D:184:ALA:O	1:D:327:LEU:HA	2.15	0.47
3:I:11:GLU:OE1	3:I:458:TYR:OH	2.33	0.47
3:I:462:ASP:HB3	3:I:468:ARG:HD2	1.97	0.47
4:J:540:LEU:HD11	4:J:603:LEU:HD22	1.96	0.47
4:J:657:LEU:O	4:J:661:MET:HG3	2.15	0.47
1:A:161:ASP:OD2	1:A:196:LYS:NZ	2.31	0.46
1:B:182:ILE:HD11	1:B:352:LEU:HD11	1.96	0.46
1:B:401:GLU:HA	1:B:404:GLU:OE2	2.15	0.46
1:D:157:GLU:HG3	1:D:166:ARG:HE	1.79	0.46
1:D:163:LEU:HD13	1:D:407:LEU:HG	1.98	0.46
1:D:256:ARG:O	1:D:260:ILE:HG12	2.15	0.46
1:E:68:ILE:HG23	1:E:95:ILE:HD11	1.98	0.46
1:E:254:HIS:HB2	1:E:307:PHE:HE1	1.78	0.46
2:G:222:LEU:HD11	2:H:218:LEU:HG	1.97	0.46
3:I:358:ARG:HA	3:I:361:MET:SD	2.54	0.46
3:I:1009:SER:N	4:J:651:GLU:OE2	2.48	0.46
4:J:65:ARG:HE	7:R:12:A:P	2.38	0.46
4:J:1311:LEU:HA	4:J:1326:THR:HA	1.96	0.46
6:T:7:DC:H2"	6:T:8:DT:C6	2.49	0.46
1:A:101:ARG:HH12	1:A:142:PHE:HB3	1.79	0.46
1:B:166:ARG:CZ	1:B:414:LYS:HA	2.45	0.46
1:C:108:GLY:HA3	1:C:122:LEU:HD11	1.96	0.46
1:C:111:ARG:NH1	1:C:121:THR:H	2.13	0.46
1:C:282:ASN:CG	1:D:290:ARG:NH1	2.69	0.46
1:E:179:ARG:NH1	1:E:311:ALA:O	2.49	0.46
1:F:314:ILE:HG22	1:F:316:GLY:H	1.79	0.46
1:F:338:ILE:HD13	1:F:341:GLU:OE2	2.15	0.46
1:F:386:LYS:HE2	1:F:386:LYS:HB2	1.76	0.46
2:G:209:GLU:OE1	2:G:209:GLU:N	2.48	0.46
3:I:327:HIS:NE2	3:I:492:ASP:OD2	2.46	0.46
3:I:997:LEU:HD23	3:I:997:LEU:HA	1.77	0.46
4:J:65:ARG:O	4:J:69:GLU:N	2.48	0.46
4:J:448:GLU:OE1	4:J:448:GLU:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:O	1:A:301:LEU:HG	2.16	0.46
1:B:211:ILE:HB	1:B:269:ILE:HD13	1.97	0.46
1:C:355:ARG:HG3	1:C:356:LEU:HD12	1.98	0.46
1:E:243:PRO:HA	1:E:246:HIS:CD2	2.51	0.46
1:E:251:GLU:OE2	1:E:306:ARG:NH2	2.48	0.46
1:E:400:ALA:O	1:E:404:GLU:OE1	2.33	0.46
2:H:153:ALA:HA	2:H:156:HIS:HE2	1.80	0.46
3:I:189:ARG:HH12	3:I:243:ARG:N	2.13	0.46
3:I:1031:ARG:HB2	6:T:24:DG:C3'	2.45	0.46
4:J:1101:VAL:HG13	4:J:1102:THR:HG23	1.97	0.46
4:J:1197:ARG:HH11	4:J:1397:LYS:NZ	2.13	0.46
1:E:81:HIS:NE2	1:E:235:ILE:HD12	2.30	0.46
1:E:184:ALA:N	1:E:328:VAL:HG12	2.30	0.46
1:E:218:ARG:HH21	1:F:344:GLY:C	2.15	0.46
1:E:294:GLY:CA	1:E:333:ARG:HE	2.26	0.46
2:H:152:PRO:HD2	2:H:155:LYS:HZ2	1.80	0.46
3:I:1021:LEU:HD13	4:J:622:ARG:NH1	2.29	0.46
4:J:771:SER:HB2	4:J:778:LEU:CD2	2.46	0.46
4:J:1211:MET:HE1	5:K:16:LYS:HZ2	1.80	0.46
1:A:297:ASP:HB3	1:A:300:ALA:HB3	1.98	0.46
1:B:255:GLU:HB2	1:B:259:ARG:NH2	2.30	0.46
1:B:256:ARG:O	1:B:260:ILE:HG12	2.15	0.46
1:B:401:GLU:HA	1:B:404:GLU:CD	2.35	0.46
1:C:163:LEU:HD22	1:C:407:LEU:HD23	1.97	0.46
1:D:215:ILE:HG23	1:D:246:HIS:HD2	1.81	0.46
1:F:141:ARG:NH1	1:F:142:PHE:HB3	2.31	0.46
2:G:70:GLY:H	3:I:607:ASP:CG	2.19	0.46
2:G:91:ASN:OD1	2:G:94:LEU:N	2.47	0.46
3:I:937:ASP:OD1	3:I:938:LYS:N	2.48	0.46
3:I:939:ARG:HB3	3:I:982:PRO:HG3	1.96	0.46
1:A:379:LEU:HB3	1:A:383:VAL:CG1	2.45	0.46
1:B:153:GLN:HA	1:B:175:GLY:HA2	1.98	0.46
1:F:258:LYS:HB2	1:F:259:ARG:NH1	2.31	0.46
1:F:279:ARG:HH22	1:F:332:SER:HB3	1.80	0.46
2:G:1:MET:O	2:G:5:LYS:HB3	2.15	0.46
3:I:292:ARG:HB3	3:I:299:LYS:H	1.80	0.46
3:I:674:VAL:HG11	3:I:992:MET:HG3	1.97	0.46
3:I:1116:ALA:O	4:J:23:TYR:OH	2.33	0.46
4:J:1094:LEU:O	4:J:1098:LEU:HD23	2.15	0.46
1:A:285:THR:HG21	1:A:300:ALA:HB2	1.98	0.46
1:B:218:ARG:NH2	1:C:346:GLY:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:PRO:O	1:D:403:MET:HG3	2.16	0.46
1:E:128:VAL:N	1:E:131:LEU:O	2.47	0.46
1:E:247:ILE:HG13	1:E:284:VAL:HG11	1.98	0.46
2:G:101:LEU:HB3	2:G:140:MET:HG2	1.97	0.46
3:I:52:PHE:O	3:I:54:ILE:N	2.49	0.46
3:I:759:THR:HB	3:I:785:VAL:HG13	1.98	0.46
4:J:996:TRP:CD2	4:J:1056:PRO:HG3	2.50	0.46
4:J:1146:GLY:CA	4:J:1207:TYR:HB3	2.45	0.46
5:K:67:GLU:HB3	5:K:73:LEU:HD11	1.97	0.46
6:T:9:DA:C2	8:N:33:DT:O2	2.68	0.46
1:C:218:ARG:HA	1:C:239:PHE:CE1	2.50	0.46
1:C:422:SER:O	1:C:425:ALA:N	2.49	0.46
1:F:92:ALA:O	1:F:95:ILE:HB	2.15	0.46
2:H:83:LYS:HE2	2:H:168:ASP:HB2	1.96	0.46
3:I:148:PHE:HE2	3:I:309:TYR:HD2	1.64	0.46
4:J:800:LYS:HG2	4:J:804:LEU:HB3	1.97	0.46
4:J:1282:ARG:HB2	4:J:1293:PHE:HB2	1.96	0.46
4:J:1406:ARG:HB2	4:J:1407:LEU:HD12	1.97	0.46
1:B:220:GLU:HG2	1:B:221:GLU:N	2.31	0.46
9:B:501:ADP:HO3'	1:C:373:ARG:HE	1.63	0.46
1:C:170:LEU:HD22	1:C:426:ARG:NH1	2.31	0.46
1:C:252:PHE:HA	1:C:255:GLU:OE2	2.16	0.46
1:C:408:ALA:CB	5:K:87:LYS:CE	2.81	0.46
1:D:303:PHE:HB2	1:D:304:PRO:HD3	1.98	0.46
1:D:361:ILE:O	1:D:364:ALA:HB2	2.16	0.46
1:E:275:THR:OG1	1:E:327:LEU:HB2	2.16	0.46
4:J:976:GLN:O	4:J:979:GLU:HG2	2.15	0.46
4:J:996:TRP:HB3	4:J:1044:LEU:HD21	1.97	0.46
6:T:10:DC:N4	8:N:31:DG:O6	2.49	0.46
1:C:90:VAL:HG12	1:C:95:ILE:HG13	1.98	0.46
1:C:283:LEU:HD21	1:D:298:SER:HB3	1.90	0.46
1:D:304:PRO:HB2	1:D:342:PHE:HZ	1.81	0.46
1:D:378:LEU:O	1:D:379:LEU:HD23	2.16	0.46
3:I:133:ASP:OD1	3:I:133:ASP:N	2.47	0.46
3:I:270:GLY:O	3:I:275:TYR:N	2.49	0.46
3:I:691:SER:HA	3:I:858:MET:HE1	1.97	0.46
4:J:66:GLN:H	4:J:66:GLN:CD	2.18	0.46
4:J:181:ASP:O	4:J:204:LEU:HD23	2.15	0.46
4:J:901:GLN:N	4:J:901:GLN:OE1	2.49	0.46
4:J:1211:MET:HE3	5:K:16:LYS:CE	2.45	0.46
1:A:186:PRO:HD3	1:A:330:THR:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:OD2	1:A:300:ALA:N	2.46	0.45
1:A:412:ARG:NH2	1:A:418:GLU:HG2	2.32	0.45
1:D:182:ILE:HD13	1:D:350:LEU:HD23	1.98	0.45
1:E:63:LYS:HB3	1:E:107:VAL:HG13	1.98	0.45
1:E:347:ASN:O	1:E:348:MET:HE2	2.16	0.45
1:E:401:GLU:HA	1:E:404:GLU:OE2	2.16	0.45
1:F:247:ILE:CG1	1:F:284:VAL:HG21	2.46	0.45
1:F:271:LEU:HB3	1:F:324:ALA:HB2	1.97	0.45
2:H:156:HIS:ND1	2:H:158:ILE:HG13	2.32	0.45
3:I:89:THR:HG23	3:I:129:ILE:HA	1.98	0.45
3:I:597:ALA:O	3:I:652:GLY:N	2.35	0.45
3:I:1031:ARG:N	4:J:622:ARG:HH21	2.14	0.45
8:N:21:DG:H2"	8:N:22:DG:H8	1.82	0.45
1:A:60:ARG:NH2	1:A:86:ARG:HD2	2.31	0.45
1:A:128:VAL:HG11	1:A:136:ALA:HB2	1.97	0.45
1:B:276:ARG:NH1	11:B:502:BEF:F2	2.40	0.45
1:E:148:GLN:O	1:E:313:ASN:HB3	2.16	0.45
2:G:133:GLU:HG3	2:G:134:GLU:H	1.80	0.45
3:I:242:LEU:C	3:I:244:PRO:HD3	2.37	0.45
4:J:158:TYR:OH	4:J:454:ALA:HB2	2.16	0.45
1:B:272:ASP:OD2	1:B:276:ARG:NH2	2.48	0.45
1:C:226:ARG:O	1:C:229:VAL:HG12	2.16	0.45
1:F:215:ILE:HG22	1:F:216:ASP:HB2	1.97	0.45
1:F:379:LEU:O	1:F:384:THR:OG1	2.34	0.45
2:H:101:LEU:HB2	2:H:114:PHE:CE1	2.51	0.45
4:J:76:CYS:SG	4:J:77:GLY:N	2.89	0.45
1:A:159:THR:N	1:A:160:PRO:HD2	2.30	0.45
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.82	0.45
1:A:288:THR:HG21	1:A:291:THR:HA	1.99	0.45
1:B:274:ILE:O	1:B:277:LEU:HB3	2.16	0.45
1:B:383:VAL:O	1:B:386:LYS:HG2	2.16	0.45
1:C:66:LEU:HD23	1:C:101:ARG:O	2.16	0.45
1:E:76:LEU:HB2	1:E:87:VAL:HG23	1.98	0.45
1:E:270:LEU:HA	1:E:323:LEU:O	2.16	0.45
1:F:76:LEU:HB2	1:F:88:ALA:HB3	1.99	0.45
1:F:102:ALA:O	1:F:259:ARG:NE	2.50	0.45
3:I:779:GLY:O	3:I:781:LYS:N	2.49	0.45
3:I:1101:THR:OG1	3:I:1109:VAL:O	2.33	0.45
4:J:1496:GLU:HG3	4:J:1500:LYS:HZ3	1.81	0.45
1:A:268:MET:SD	1:A:321:THR:HB	2.56	0.45
1:A:387:MET:HE2	1:A:390:LEU:HD12	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ARG:NH2	1:C:373:ARG:HH12	2.15	0.45
1:C:266:HIS:CD2	1:C:318:GLY:HA2	2.52	0.45
1:D:211:ILE:HD13	1:D:267:VAL:HG13	1.99	0.45
1:F:356:LEU:HB3	1:F:364:ALA:HB1	1.98	0.45
3:I:420:ARG:NH1	3:I:423:ALA:H	2.14	0.45
5:K:13:VAL:HG21	5:K:19:LEU:HB2	1.98	0.45
1:A:111:ARG:NH2	1:A:121:THR:OG1	2.50	0.45
1:A:147:PRO:HG3	1:A:312:ARG:HH11	1.82	0.45
1:B:226:ARG:NH2	1:B:234:VAL:O	2.50	0.45
1:E:79:ASN:O	1:E:81:HIS:N	2.50	0.45
1:F:95:ILE:HG23	1:F:100:LEU:O	2.17	0.45
2:G:20:TYR:OH	2:G:198:ARG:HD2	2.17	0.45
2:H:189:ARG:HB2	2:H:191:ASP:OD1	2.16	0.45
4:J:12:LEU:HD21	4:J:104:PHE:CZ	2.51	0.45
4:J:47:GLU:HG3	4:J:52:PRO:HA	1.98	0.45
4:J:1485:GLN:HE22	5:K:82:GLU:HB3	1.76	0.45
1:A:286:PRO:HD2	1:A:287:PRO:HD3	1.98	0.45
1:A:346:GLY:O	1:A:373:ARG:NH1	2.49	0.45
1:E:85:SER:C	1:E:87:VAL:HG22	2.36	0.45
2:G:58:ILE:HD11	2:G:140:MET:HE3	1.98	0.45
2:G:94:LEU:HD12	2:G:95:GLN:N	2.32	0.45
2:H:117:VAL:HB	2:H:120:VAL:HG22	1.98	0.45
3:I:533:ASP:HB3	3:I:538:GLN:NE2	2.32	0.45
4:J:895:VAL:HG22	4:J:899:LEU:HD23	1.98	0.45
4:J:1111:ASP:OD1	4:J:1189:ARG:NH2	2.43	0.45
4:J:1472:ILE:HG22	4:J:1474:ALA:N	2.32	0.45
1:A:362:PHE:HB3	9:A:1000:ADP:N6	2.32	0.45
1:C:185:PRO:HB2	1:C:354:ARG:CZ	2.47	0.45
1:E:182:ILE:HD11	1:E:323:LEU:HD12	1.98	0.45
2:H:132:LEU:HD21	2:H:138:LEU:HD22	1.97	0.45
3:I:265:ARG:HG3	3:I:267:TYR:N	2.31	0.45
4:J:131:LYS:NZ	4:J:568:ARG:HG3	2.31	0.45
6:T:28:DA:H2'	6:T:29:DT:C6	2.52	0.45
1:A:149:PHE:CE1	1:F:220:GLU:HG3	2.52	0.45
1:A:175:GLY:HA3	1:A:378:LEU:HD11	1.99	0.45
1:A:296:LEU:HD21	1:A:338:ILE:HD11	1.97	0.45
1:B:221:GLU:HA	1:C:149:PHE:HE1	1.82	0.45
1:C:188:ALA:HA	1:C:357:GLU:HG3	1.99	0.45
1:E:124:LYS:NZ	1:E:133:PRO:HG2	2.32	0.45
1:E:183:VAL:HA	1:E:326:ALA:O	2.17	0.45
1:E:209:LYS:HZ2	1:E:211:ILE:HD11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ARG:HH11	1:F:113:PRO:HB3	1.81	0.45
3:I:317:VAL:O	3:I:317:VAL:HG13	2.16	0.45
3:I:1031:ARG:HG3	4:J:621:LYS:HE3	1.98	0.45
3:I:1038:TRP:CZ2	4:J:1099:VAL:HG11	2.52	0.45
4:J:68:PHE:HB2	4:J:71:LYS:HD2	1.99	0.45
4:J:408:GLU:HG2	4:J:420:VAL:HG12	1.98	0.45
4:J:462:GLN:HG2	4:J:466:LYS:HE2	1.98	0.45
4:J:792:ILE:HD11	4:J:881:LEU:HD23	1.98	0.45
6:T:12:DA:N6	8:N:29:DG:C6	2.85	0.45
1:C:251:GLU:O	1:C:254:HIS:HB3	2.17	0.45
1:D:182:ILE:CD1	1:D:350:LEU:HD23	2.46	0.45
1:E:148:GLN:HE21	1:E:315:ARG:HE	1.65	0.45
1:E:379:LEU:HB2	1:E:384:THR:OG1	2.17	0.45
5:K:47:LYS:O	5:K:54:LEU:HD12	2.17	0.45
6:T:1:DG:H2"	6:T:2:DG:H8	1.82	0.45
1:A:188:ALA:HB2	1:A:354:ARG:NH2	2.32	0.44
1:C:220:GLU:HG2	1:C:221:GLU:N	2.33	0.44
1:C:225:PHE:O	1:C:229:VAL:N	2.50	0.44
1:D:94:LEU:HA	1:D:97:GLN:HG2	1.99	0.44
1:E:140:PRO:HB2	1:E:145:LEU:HD21	1.99	0.44
2:H:177:VAL:HG12	2:H:199:ILE:HG12	1.99	0.44
3:I:903:SER:HB2	3:I:908:GLY:HA2	1.98	0.44
3:I:1019:GLN:HB3	4:J:622:ARG:HB2	1.99	0.44
3:I:1034:GLU:HB3	4:J:619:LEU:CD2	2.47	0.44
4:J:41:ARG:C	4:J:43:GLY:H	2.20	0.44
4:J:166:GLN:OE1	4:J:396:VAL:HG22	2.17	0.44
4:J:556:LYS:O	4:J:560:GLN:HG2	2.18	0.44
5:K:41:GLU:HA	5:K:45:ARG:NE	2.33	0.44
6:T:38:DA:H2	8:N:4:DT:N3	2.08	0.44
1:A:191:THR:H	9:A:1000:ADP:PB	2.40	0.44
1:A:215:ILE:HD12	1:A:237:SER:HB3	2.00	0.44
1:B:336:ASP:O	1:B:340:GLU:OE1	2.35	0.44
1:B:385:HIS:O	1:B:388:TRP:HB3	2.17	0.44
1:C:184:ALA:HB3	1:C:190:LYS:HG3	1.99	0.44
1:F:98:TYR:HB2	1:F:100:LEU:HG	1.99	0.44
2:G:62:LEU:HD11	3:I:745:ILE:HB	1.98	0.44
2:H:124:ASN:OD1	2:H:124:ASN:N	2.51	0.44
3:I:1006:HIS:ND1	3:I:1027:PHE:HB3	2.32	0.44
4:J:1284:GLU:HB2	4:J:1291:SER:OG	2.18	0.44
5:K:18:ARG:O	5:K:22:VAL:HG23	2.17	0.44
1:A:253:VAL:HA	1:A:256:ARG:HH11	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:VAL:HA	1:B:256:ARG:HG2	1.99	0.44
1:C:218:ARG:HH21	1:D:345:THR:N	2.14	0.44
1:D:215:ILE:HG23	1:D:246:HIS:CD2	2.52	0.44
1:F:180:GLY:HA3	1:F:348:MET:HB3	1.99	0.44
4:J:58:CYS:SG	4:J:61:GLY:N	2.89	0.44
4:J:1152:GLU:N	4:J:1162:GLU:HB2	2.32	0.44
1:A:259:ARG:NE	1:A:259:ARG:HA	2.31	0.44
1:A:386:LYS:HD2	1:A:419:PHE:CZ	2.52	0.44
1:D:367:ILE:HG13	1:D:368:LEU:N	2.33	0.44
1:E:259:ARG:HA	1:E:259:ARG:HD3	1.74	0.44
1:F:74:GLY:O	1:F:89:ILE:HA	2.18	0.44
1:F:247:ILE:HG12	1:F:284:VAL:HG21	1.99	0.44
1:F:288:THR:HG22	1:F:291:THR:HA	2.00	0.44
1:F:405:MET:SD	1:F:406:LEU:N	2.91	0.44
1:F:416:ASN:O	1:F:420:LEU:N	2.42	0.44
2:H:31:GLY:N	2:H:193:ASP:OD2	2.50	0.44
3:I:480:THR:HG22	3:I:482:GLU:H	1.81	0.44
3:I:713:ARG:HA	3:I:819:VAL:HA	2.00	0.44
3:I:1041:GLU:HG3	4:J:1223:ILE:HD12	1.98	0.44
3:I:1058:ASP:OD1	3:I:1083:GLU:HB2	2.17	0.44
4:J:65:ARG:HB3	7:R:12:A:OP2	2.17	0.44
1:B:223:THR:O	1:B:226:ARG:HB2	2.17	0.44
1:B:261:VAL:HG21	1:B:320:LEU:HB2	2.00	0.44
1:C:409:ARG:HG2	5:K:87:LYS:HB2	2.00	0.44
1:E:173:PRO:HD2	1:E:372:THR:HG21	2.00	0.44
1:E:184:ALA:O	1:E:327:LEU:HA	2.17	0.44
1:E:414:LYS:N	1:E:417:LYS:HB2	2.32	0.44
1:F:303:PHE:HB2	1:F:304:PRO:HD3	2.00	0.44
3:I:95:TYR:HE1	3:I:114:PHE:HB3	1.82	0.44
3:I:704:HIS:CG	3:I:831:ARG:HE	2.35	0.44
3:I:1101:THR:HB	4:J:5:VAL:HG13	1.99	0.44
4:J:485:SER:HA	4:J:489:ARG:HH21	1.82	0.44
4:J:591:VAL:HG13	4:J:592:THR:O	2.16	0.44
4:J:1353:GLN:NE2	4:J:1363:LEU:O	2.49	0.44
1:B:111:ARG:HH11	1:B:111:ARG:HG3	1.83	0.44
1:B:398:ASP:O	1:B:401:GLU:HG3	2.18	0.44
1:C:79:ASN:O	1:C:81:HIS:ND1	2.50	0.44
1:D:413:THR:HB	1:D:417:LYS:HB2	2.00	0.44
1:F:82:ASN:H	1:F:86:ARG:HH22	1.64	0.44
1:F:414:LYS:HB3	1:F:417:LYS:HD2	1.99	0.44
2:G:42:ARG:HH12	3:I:857:ASP:HB3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:VAL:O	2:H:163:ASN:ND2	2.50	0.44
3:I:160:ALA:HB2	3:I:310:LEU:HD12	1.99	0.44
4:J:1129:THR:O	4:J:1130:ARG:NE	2.48	0.44
5:K:83:ASP:OD1	5:K:83:ASP:N	2.50	0.44
1:C:174:ILE:HD12	1:C:178:GLN:HG2	2.00	0.44
1:D:98:TYR:OH	1:D:124:LYS:HD2	2.18	0.44
1:D:288:THR:HG21	1:D:299:ALA:H	1.83	0.44
1:E:184:ALA:HB2	1:E:352:LEU:HB2	2.00	0.44
1:E:245:ASN:ND2	1:E:248:ARG:HH21	2.16	0.44
2:G:14:ARG:NH2	2:G:22:GLU:OE1	2.50	0.44
2:H:77:GLU:OE2	4:J:867:ARG:NH1	2.51	0.44
3:I:717:LEU:HD21	3:I:764:GLU:HA	1.99	0.44
3:I:957:LYS:HB2	3:I:962:GLN:HG3	1.99	0.44
3:I:1003:ASP:CG	4:J:724:GLN:HE22	2.21	0.44
4:J:485:SER:HB2	4:J:488:ARG:HH22	1.82	0.44
4:J:500:ARG:HG3	4:J:1388:ARG:NH1	2.33	0.44
4:J:734:GLU:OE2	4:J:783:ARG:NH1	2.47	0.44
4:J:1272:ALA:N	4:J:1329:ALA:O	2.42	0.44
6:T:36:DA:C8	6:T:37:DT:H72	2.53	0.44
1:A:187:LYS:CE	1:B:373:ARG:NH1	2.76	0.44
1:A:257:ALA:O	1:A:261:VAL:HG23	2.18	0.44
1:B:134:GLU:HA	1:B:137:LYS:HE2	1.99	0.44
1:D:111:ARG:HD3	1:D:111:ARG:H	1.82	0.44
1:D:190:LYS:HD2	1:D:325:THR:HB	1.99	0.44
1:D:216:ASP:OD2	1:D:276:ARG:HD2	2.18	0.44
1:E:210:VAL:HA	1:E:268:MET:HB2	2.00	0.44
1:F:254:HIS:HE1	1:F:306:ARG:HE	1.63	0.44
2:G:11:PHE:HD1	2:G:25:LEU:HD13	1.83	0.44
2:G:175:ARG:H	2:G:201:THR:HA	1.83	0.44
3:I:140:ILE:HD13	3:I:333:ILE:HG12	2.00	0.44
3:I:259:GLY:O	3:I:264:PRO:HG2	2.18	0.44
3:I:504:GLU:HB2	3:I:507:ARG:HB3	1.99	0.44
3:I:846:LYS:HE3	3:I:997:LEU:HD12	2.00	0.44
4:J:514:LEU:HD23	4:J:514:LEU:H	1.82	0.44
4:J:1277:ILE:HG21	4:J:1299:PHE:CZ	2.52	0.44
5:K:45:ARG:HG3	5:K:46:PRO:HD2	2.00	0.44
1:A:290:ARG:NE	1:F:287:PRO:O	2.51	0.44
1:A:334:MET:SD	1:A:334:MET:N	2.91	0.44
1:A:399:PRO:O	1:A:402:ALA:HB3	2.16	0.44
1:B:397:MET:HG2	1:B:402:ALA:CB	2.48	0.44
1:C:147:PRO:HA	1:C:314:ILE:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LEU:HG	1:C:166:ARG:HH21	1.82	0.44
1:C:218:ARG:HE	1:D:345:THR:CA	2.30	0.44
9:C:1002:ADP:O2B	11:C:1004:BEF:F1	2.26	0.44
1:E:150:PRO:HB3	1:E:178:GLN:OE1	2.18	0.44
4:J:53:ILE:HA	4:J:86:ARG:HD2	1.98	0.44
5:K:14:ASP:OD1	5:K:14:ASP:N	2.50	0.44
1:A:271:LEU:HD22	1:A:307:PHE:HE2	1.82	0.43
1:D:81:HIS:CG	1:D:235:ILE:HD12	2.53	0.43
1:F:254:HIS:CG	1:F:307:PHE:HD1	2.36	0.43
3:I:557:ARG:HD3	3:I:557:ARG:HA	1.79	0.43
3:I:674:VAL:HG11	3:I:992:MET:SD	2.58	0.43
4:J:1277:ILE:HG21	4:J:1299:PHE:CE2	2.53	0.43
1:A:339:PHE:HZ	1:A:351:HIS:HE1	1.67	0.43
1:B:80:LEU:HB3	1:B:84:GLU:OE2	2.18	0.43
1:B:207:ASP:OD1	1:B:207:ASP:N	2.51	0.43
1:C:171:LEU:HD21	1:C:370:SER:HB2	1.99	0.43
1:D:65:TYR:HB2	1:D:77:THR:OG1	2.17	0.43
1:E:134:GLU:HA	1:E:137:LYS:HE2	2.00	0.43
3:I:212:GLY:HA3	3:I:218:VAL:HG21	2.00	0.43
3:I:455:LEU:HD23	3:I:455:LEU:H	1.83	0.43
4:J:46:ASP:OD1	4:J:47:GLU:N	2.52	0.43
4:J:1211:MET:N	4:J:1211:MET:SD	2.91	0.43
4:J:1489:GLN:HB2	5:K:72:ARG:O	2.17	0.43
8:N:31:DG:H2"	8:N:32:DG:H8	1.83	0.43
1:A:99:ALA:HB3	1:A:137:LYS:HA	2.00	0.43
1:A:150:PRO:HA	1:A:313:ASN:ND2	2.33	0.43
1:A:241:GLU:HB2	1:A:246:HIS:HE2	1.83	0.43
1:C:271:LEU:HD21	1:C:277:LEU:HD22	2.00	0.43
1:E:63:LYS:HB2	1:E:107:VAL:HG22	2.01	0.43
1:E:111:ARG:HG2	1:E:114:ARG:NH1	2.33	0.43
1:E:218:ARG:HD3	1:F:179:ARG:HH22	1.83	0.43
1:E:247:ILE:HD11	1:E:281:ASN:OD1	2.18	0.43
1:E:333:ARG:H	1:E:333:ARG:HD3	1.83	0.43
1:F:109:GLN:HE22	1:F:123:LEU:HB3	1.83	0.43
3:I:67:ASP:HB3	3:I:99:GLN:HE21	1.83	0.43
3:I:151:ASP:OD1	3:I:159:ILE:HG23	2.18	0.43
4:J:1273:VAL:O	4:J:1325:LEU:N	2.49	0.43
4:J:1319:VAL:HG21	4:J:1325:LEU:HD21	1.99	0.43
6:T:19:DC:H2"	6:T:20:DC:C5	2.54	0.43
1:A:60:ARG:NE	1:A:62:VAL:HG12	2.34	0.43
1:A:355:ARG:HH22	1:A:400:ALA:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:HE2	1:A:409:ARG:HD2	2.00	0.43
1:B:71:ASP:HB2	1:B:73:TYR:CE1	2.54	0.43
1:B:92:ALA:O	1:B:96:LYS:HG3	2.18	0.43
1:C:208:ILE:HG21	1:C:268:MET:HG2	2.00	0.43
1:E:359:ARG:HB2	1:E:361:ILE:HG12	2.00	0.43
2:H:30:ARG:HH21	3:I:854:PRO:HD3	1.83	0.43
3:I:698:ASP:HB3	3:I:701:THR:HG21	2.00	0.43
1:A:78:GLU:HA	1:A:86:ARG:NH2	2.34	0.43
1:B:300:ALA:O	1:B:304:PRO:HD2	2.19	0.43
1:D:97:GLN:HG3	1:D:98:TYR:CD2	2.54	0.43
1:D:351:HIS:CB	1:D:366:ASP:HB3	2.48	0.43
1:E:77:THR:O	1:E:88:ALA:N	2.51	0.43
1:E:179:ARG:O	1:E:347:ASN:N	2.43	0.43
1:E:328:VAL:HG22	1:E:329:GLU:N	2.34	0.43
1:F:66:LEU:HD13	1:F:90:VAL:HB	2.01	0.43
1:F:214:LEU:O	1:F:237:SER:N	2.52	0.43
3:I:21:ILE:HG23	3:I:22:GLN:H	1.84	0.43
3:I:290:LEU:HD12	3:I:290:LEU:O	2.18	0.43
3:I:557:ARG:HA	3:I:560:MET:HG2	2.01	0.43
3:I:1013:TYR:CE1	3:I:1020:PRO:HG3	2.53	0.43
4:J:1275:SER:O	4:J:1322:GLY:N	2.43	0.43
1:A:391:ARG:HB3	1:F:360:ARG:NE	2.30	0.43
1:B:214:LEU:HD13	1:B:272:ASP:HB2	2.00	0.43
1:B:296:LEU:HD11	1:B:338:ILE:HG13	2.01	0.43
1:E:214:LEU:HB2	1:E:236:ALA:HA	2.01	0.43
1:E:401:GLU:HA	1:E:404:GLU:CD	2.39	0.43
1:F:215:ILE:HA	1:F:237:SER:HB3	2.00	0.43
2:G:156:HIS:ND1	2:G:158:ILE:HG12	2.34	0.43
3:I:140:ILE:HD12	3:I:332:ARG:O	2.17	0.43
3:I:501:THR:HG21	3:I:513:VAL:HG23	2.00	0.43
3:I:716:LYS:HE2	3:I:716:LYS:HB3	1.67	0.43
3:I:1115:LEU:HD23	4:J:85:VAL:HA	1.99	0.43
4:J:1182:GLU:OE1	4:J:1182:GLU:N	2.51	0.43
1:A:98:TYR:CE2	1:A:133:PRO:HB3	2.54	0.43
1:A:170:LEU:HD21	1:A:415:ASN:HB2	2.00	0.43
1:B:76:LEU:HD12	1:B:88:ALA:HB3	2.00	0.43
1:B:338:ILE:HA	1:B:341:GLU:OE2	2.19	0.43
1:C:63:LYS:HE2	1:C:105:TYR:CE1	2.53	0.43
1:C:189:GLY:O	1:C:193:LEU:HD23	2.18	0.43
1:C:229:VAL:HG21	1:C:234:VAL:HB	2.01	0.43
1:C:273:SER:N	1:C:325:THR:OG1	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:VAL:HG21	1:E:234:VAL:HG23	2.01	0.43
1:E:274:ILE:HB	1:E:326:ALA:HA	2.01	0.43
1:F:66:LEU:HD21	1:F:95:ILE:HD11	2.01	0.43
1:F:383:VAL:HG12	1:F:387:MET:CE	2.48	0.43
2:G:51:THR:HG22	2:G:146:ARG:HB2	2.01	0.43
3:I:191:PHE:HZ	3:I:195:LEU:HB3	1.83	0.43
3:I:856:GLU:HG2	3:I:857:ASP:N	2.34	0.43
3:I:922:PHE:CD2	3:I:964:LYS:HG3	2.53	0.43
3:I:1060:ILE:HG13	3:I:1061:GLU:H	1.83	0.43
4:J:25:GLU:HG2	4:J:92:HIS:O	2.18	0.43
4:J:73:CYS:HB3	4:J:76:CYS:C	2.39	0.43
4:J:162:ARG:NH2	4:J:451:ASP:HA	2.24	0.43
4:J:645:PRO:HB2	4:J:648:MET:HG2	2.01	0.43
6:T:20:DC:H2'	6:T:21:DC:C6	2.54	0.43
6:T:25:DT:H2'	6:T:26:DG:H8	1.83	0.43
1:A:189:GLY:O	1:A:192:THR:OG1	2.15	0.43
1:B:276:ARG:HB2	1:B:327:LEU:CD1	2.48	0.43
1:D:146:THR:O	1:D:314:ILE:HA	2.18	0.43
1:D:166:ARG:CZ	1:D:414:LYS:HA	2.49	0.43
1:F:82:ASN:OD1	1:F:84:GLU:HG3	2.19	0.43
3:I:957:LYS:O	3:I:962:GLN:NE2	2.52	0.43
4:J:646:LYS:HE3	4:J:722:GLU:HG2	2.01	0.43
4:J:743:ASP:N	4:J:743:ASP:OD1	2.51	0.43
1:B:271:LEU:O	1:B:324:ALA:HA	2.19	0.43
1:B:397:MET:HG2	1:B:402:ALA:HB2	2.00	0.43
2:H:111:ALA:HB2	2:H:127:LEU:HB3	2.01	0.43
4:J:86:ARG:HB3	4:J:522:PRO:HG2	2.01	0.43
4:J:192:ALA:HB1	4:J:193:PRO:HD2	2.00	0.43
4:J:771:SER:HB2	4:J:778:LEU:HD23	2.00	0.43
4:J:974:ILE:O	4:J:977:ALA:HB3	2.19	0.43
6:T:25:DT:H2'	6:T:26:DG:C8	2.53	0.43
1:A:405:MET:HE1	1:A:409:ARG:NH1	2.34	0.43
1:C:379:LEU:HB3	1:C:383:VAL:HB	2.00	0.43
1:D:273:SER:HB3	1:D:276:ARG:HB2	2.00	0.43
1:D:300:ALA:O	1:D:304:PRO:HD2	2.19	0.43
1:E:101:ARG:HH11	1:E:139:ARG:NH2	2.17	0.43
1:E:305:LYS:HE2	1:E:341:GLU:OE2	2.19	0.43
1:F:152:ARG:O	1:F:175:GLY:HA2	2.19	0.43
1:F:280:ALA:O	1:F:283:LEU:HB3	2.18	0.43
3:I:292:ARG:HB3	3:I:299:LYS:N	2.34	0.43
3:I:954:THR:OG1	3:I:957:LYS:HE3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:701:LEU:HD12	4:J:750:PRO:HD3	2.01	0.43
4:J:828:LYS:HE3	4:J:862:ASP:HA	2.01	0.43
5:K:47:LYS:C	5:K:54:LEU:HD12	2.39	0.43
1:A:218:ARG:HA	1:A:239:PHE:HE1	1.83	0.42
1:B:239:PHE:HE1	1:C:309:GLY:HA3	1.84	0.42
1:C:422:SER:C	1:C:426:ARG:HG2	2.39	0.42
1:D:166:ARG:HD3	1:D:415:ASN:CB	2.48	0.42
1:E:148:GLN:HE21	1:E:315:ARG:NE	2.18	0.42
1:E:256:ARG:O	1:E:260:ILE:HG12	2.19	0.42
1:E:271:LEU:HB2	1:E:324:ALA:HB2	2.01	0.42
1:F:220:GLU:HG2	1:F:221:GLU:N	2.34	0.42
1:F:414:LYS:HZ2	1:F:416:ASN:HB3	1.82	0.42
2:G:74:ASP:O	2:G:78:ILE:HG12	2.19	0.42
2:H:91:ASN:OD1	2:H:94:LEU:HG	2.19	0.42
3:I:21:ILE:HG23	3:I:22:GLN:N	2.34	0.42
3:I:270:GLY:H	3:I:274:ARG:HD3	1.84	0.42
3:I:554:ASP:OD1	3:I:555:ALA:N	2.52	0.42
3:I:1001:VAL:O	3:I:1004:LYS:N	2.52	0.42
3:I:1047:HIS:HB2	4:J:754:PHE:CD2	2.54	0.42
4:J:703:ASN:HB2	4:J:713:ILE:HD13	2.01	0.42
4:J:1289:LYS:CD	4:J:1304:LYS:HB3	2.49	0.42
8:N:30:DT:H2"	8:N:31:DG:C8	2.54	0.42
1:B:188:ALA:HB1	1:B:354:ARG:CZ	2.49	0.42
1:B:271:LEU:HB3	1:B:324:ALA:HB2	2.01	0.42
1:B:274:ILE:HG22	1:B:325:THR:O	2.19	0.42
1:C:150:PRO:HA	1:C:313:ASN:HD22	1.82	0.42
1:C:394:LEU:HA	1:C:397:MET:HB3	1.99	0.42
1:E:212:VAL:O	1:E:235:ILE:N	2.35	0.42
1:F:122:LEU:HD12	1:F:122:LEU:HA	1.83	0.42
1:F:409:ARG:HG2	1:F:412:ARG:HH12	1.85	0.42
1:F:414:LYS:HE3	1:F:417:LYS:HG3	2.01	0.42
2:H:44:LEU:HD13	2:H:177:VAL:HG11	2.00	0.42
3:I:498:GLN:HA	3:I:533:ASP:OD2	2.20	0.42
3:I:1003:ASP:HA	4:J:630:VAL:HG23	2.00	0.42
4:J:1109:GLU:CD	4:J:1202:GLN:H	2.23	0.42
6:T:33:DG:C2	6:T:34:DA:C4	3.08	0.42
1:C:215:ILE:HD13	1:C:237:SER:HB3	2.01	0.42
1:C:282:ASN:ND2	1:D:290:ARG:HH11	2.17	0.42
1:C:338:ILE:HA	1:C:341:GLU:OE1	2.19	0.42
9:D:1000:ADP:H2'	9:D:1000:ADP:N3	2.34	0.42
1:E:417:LYS:HA	1:E:420:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ILE:HG22	1:F:325:THR:O	2.19	0.42
1:F:417:LYS:HA	1:F:420:LEU:HB2	2.01	0.42
3:I:260:LEU:HG	3:I:261:ILE:HG12	2.01	0.42
3:I:455:LEU:HD12	3:I:459:ALA:HB3	2.01	0.42
4:J:709:HIS:NE2	4:J:711:LEU:HB2	2.34	0.42
1:B:166:ARG:O	1:B:170:LEU:HD23	2.20	0.42
1:C:194:LEU:HD12	1:C:197:ILE:HD11	2.00	0.42
1:C:258:LYS:NZ	1:C:306:ARG:HH21	2.18	0.42
1:C:389:LEU:O	1:C:393:VAL:HG23	2.19	0.42
1:D:286:PRO:HG2	1:D:287:PRO:HD3	2.01	0.42
1:E:413:THR:HB	1:E:417:LYS:HB3	2.00	0.42
1:F:68:ILE:HG13	1:F:102:ALA:HB2	2.01	0.42
1:F:108:GLY:C	1:F:122:LEU:HD11	2.40	0.42
2:H:109:VAL:HG11	2:H:138:LEU:HD23	2.01	0.42
3:I:120:LEU:HD23	3:I:120:LEU:HA	1.85	0.42
3:I:328:LEU:HD12	3:I:328:LEU:HA	1.80	0.42
4:J:171:LEU:HD11	4:J:177:ALA:HB2	2.02	0.42
4:J:408:GLU:H	4:J:422:ALA:HA	1.85	0.42
4:J:644:LEU:HD12	4:J:644:LEU:HA	1.92	0.42
4:J:754:PHE:CZ	4:J:1476:THR:HG21	2.50	0.42
1:B:150:PRO:HB2	1:B:378:LEU:HD13	2.01	0.42
1:C:102:ALA:C	1:C:255:GLU:HG3	2.40	0.42
1:C:397:MET:HA	5:K:91:ARG:NH1	2.35	0.42
1:D:134:GLU:OE1	1:D:134:GLU:N	2.37	0.42
1:D:386:LYS:HZ3	1:D:390:LEU:HD11	1.85	0.42
1:E:147:PRO:HA	1:E:314:ILE:HD13	2.01	0.42
1:F:396:ASP:OD1	1:F:397:MET:N	2.52	0.42
2:G:226:SER:O	2:G:228:PRO:HD3	2.20	0.42
2:H:12:THR:OG1	2:H:24:VAL:HB	2.19	0.42
2:H:25:LEU:HD12	2:H:25:LEU:HA	1.88	0.42
3:I:313:LEU:HD13	3:I:321:GLU:HG2	2.02	0.42
3:I:428:ARG:NH1	3:I:447:ALA:O	2.45	0.42
3:I:684:PHE:HZ	4:J:782:SER:HB2	1.83	0.42
4:J:1208:ASP:HB3	4:J:1366:LYS:HZ1	1.84	0.42
1:E:163:LEU:O	1:E:167:VAL:HG23	2.19	0.42
3:I:502:PRO:HD2	3:I:510:ALA:HB2	2.02	0.42
4:J:1009:LYS:HA	4:J:1012:GLU:OE2	2.20	0.42
8:N:25:DG:H1'	8:N:26:DC:H5'	2.01	0.42
1:A:65:TYR:HB3	1:A:103:GLY:HA2	2.02	0.42
1:A:212:VAL:HG22	1:A:270:LEU:HB2	2.00	0.42
1:B:348:MET:SD	1:B:372:THR:HG22	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:HB3	1:C:111:ARG:HA	2.02	0.42
1:C:182:ILE:CG2	1:C:325:THR:HA	2.49	0.42
1:C:282:ASN:CG	1:D:290:ARG:HH11	2.23	0.42
1:E:77:THR:N	1:E:88:ALA:H	2.17	0.42
1:E:216:ASP:O	1:E:276:ARG:NH2	2.52	0.42
1:F:84:GLU:HB2	1:F:86:ARG:CZ	2.50	0.42
1:F:84:GLU:O	1:F:87:VAL:HG13	2.18	0.42
1:F:168:ILE:HD12	1:F:197:ILE:HD13	2.01	0.42
1:F:178:GLN:HB3	1:F:321:THR:HG23	2.01	0.42
2:H:2:LEU:CA	2:H:6:LEU:HB3	2.50	0.42
3:I:151:ASP:HB2	3:I:154:ARG:O	2.19	0.42
3:I:462:ASP:N	3:I:462:ASP:OD1	2.51	0.42
3:I:633:GLN:O	3:I:998:TYR:OH	2.32	0.42
3:I:676:ILE:HD13	3:I:871:LEU:HB2	2.00	0.42
4:J:106:LYS:HD3	4:J:106:LYS:HA	1.89	0.42
4:J:412:GLY:HA2	4:J:434:ARG:HH21	1.83	0.42
4:J:895:VAL:HA	4:J:898:GLU:HG2	2.02	0.42
4:J:1485:GLN:OE1	5:K:80:VAL:HG12	2.19	0.42
1:C:218:ARG:HE	1:D:345:THR:HA	1.85	0.42
1:D:195:LYS:HB2	1:D:225:PHE:CE1	2.54	0.42
1:F:118:ARG:NH2	1:F:119:TYR:OH	2.53	0.42
1:F:252:PHE:O	1:F:255:GLU:HG2	2.20	0.42
2:G:145:ASP:OD1	2:G:146:ARG:N	2.52	0.42
2:H:80:LEU:CD1	4:J:844:ALA:HA	2.50	0.42
3:I:148:PHE:HE2	3:I:309:TYR:CE2	2.37	0.42
3:I:148:PHE:CE2	3:I:309:TYR:HD2	2.38	0.42
3:I:754:ILE:HD13	3:I:791:ARG:HG2	2.01	0.42
1:A:359:ARG:NH2	1:A:404:GLU:OE2	2.40	0.42
1:A:361:ILE:HG21	1:A:403:MET:HB3	2.01	0.42
1:B:108:GLY:HA2	1:B:126:GLU:OE1	2.19	0.42
1:C:301:LEU:HD21	1:C:338:ILE:HD12	2.01	0.42
1:D:292:LEU:HD11	1:D:298:SER:HA	2.02	0.42
1:D:417:LYS:HA	1:D:420:LEU:HD12	2.01	0.42
1:E:111:ARG:NH1	1:E:114:ARG:HD2	2.33	0.42
1:F:108:GLY:HA2	1:F:126:GLU:H	1.84	0.42
1:F:176:ARG:HD3	1:F:266:HIS:CE1	2.55	0.42
3:I:52:PHE:HZ	3:I:98:LEU:HD22	1.85	0.42
3:I:606:VAL:HG21	3:I:643:VAL:HG23	2.01	0.42
4:J:591:VAL:HG22	4:J:592:THR:N	2.34	0.42
4:J:1107:VAL:HG23	4:J:1107:VAL:O	2.20	0.42
6:T:1:DG:N2	8:N:41:DC:H1'	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:SER:H	1:C:325:THR:HG1	1.61	0.42
1:D:181:LEU:HD11	1:D:326:ALA:HB2	2.02	0.42
1:D:272:ASP:OD1	1:D:273:SER:N	2.53	0.42
1:D:286:PRO:CG	1:D:287:PRO:HD3	2.49	0.42
1:E:81:HIS:CE1	1:E:235:ILE:HD12	2.55	0.42
1:F:150:PRO:O	1:F:378:LEU:HD12	2.19	0.42
2:G:192:LEU:HD23	2:G:192:LEU:HA	1.85	0.42
3:I:1006:HIS:HB3	3:I:1027:PHE:HB3	2.01	0.42
3:I:1040:LEU:HD23	3:I:1049:LEU:HD13	2.01	0.42
1:A:141:ARG:HB2	1:A:144:GLU:CD	2.39	0.41
1:A:209:LYS:HE2	1:A:211:ILE:HD11	2.01	0.41
1:A:241:GLU:O	1:A:246:HIS:NE2	2.53	0.41
1:C:183:VAL:HG21	1:C:339:PHE:HE1	1.84	0.41
1:D:280:ALA:O	1:D:284:VAL:HG23	2.20	0.41
1:E:278:ALA:HA	1:E:281:ASN:HD22	1.84	0.41
3:I:751:PRO:HA	3:I:792:VAL:HB	2.02	0.41
4:J:97:THR:OG1	4:J:571:LYS:HE2	2.20	0.41
1:A:149:PHE:CZ	1:F:220:GLU:HG2	2.55	0.41
1:B:163:LEU:O	1:B:167:VAL:HG23	2.20	0.41
1:B:292:LEU:HB2	1:B:296:LEU:HB2	2.02	0.41
1:B:328:VAL:HG22	1:B:329:GLU:N	2.36	0.41
1:C:242:PRO:HD2	1:C:245:ASN:ND2	2.36	0.41
1:C:349:GLU:CD	1:C:351:HIS:HE2	2.23	0.41
1:C:420:LEU:HD23	1:C:420:LEU:HA	1.87	0.41
1:D:188:ALA:HB2	1:D:354:ARG:HE	1.84	0.41
2:G:143:ARG:NH1	2:G:158:ILE:HG21	2.35	0.41
3:I:626:ARG:N	3:I:639:GLN:OE1	2.53	0.41
1:A:207:ASP:N	1:A:207:ASP:OD1	2.49	0.41
1:D:182:ILE:HG22	1:D:324:ALA:O	2.19	0.41
2:H:89:PHE:HD2	2:H:146:ARG:NH2	2.18	0.41
3:I:712:ALA:HB1	3:I:720:GLU:O	2.20	0.41
3:I:1020:PRO:O	4:J:622:ARG:HD3	2.19	0.41
4:J:1484:THR:H	5:K:25:LYS:HZ1	1.67	0.41
4:J:1485:GLN:HE22	5:K:82:GLU:CA	2.31	0.41
4:J:1488:ASP:N	4:J:1488:ASP:OD1	2.43	0.41
6:T:8:DT:H3	8:N:34:DA:N6	2.19	0.41
7:R:20:A:P	7:R:20:A:H8	2.43	0.41
1:A:217:GLU:HG3	1:A:272:ASP:OD2	2.20	0.41
1:B:340:GLU:O	1:B:343:LYS:HB3	2.19	0.41
1:E:303:PHE:HA	1:E:306:ARG:HG2	2.01	0.41
1:F:375:GLU:HB3	1:F:379:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:94:LEU:HD12	2:G:95:GLN:H	1.84	0.41
3:I:266:ARG:O	3:I:288:ARG:NH1	2.53	0.41
3:I:518:LYS:HE3	3:I:518:LYS:HB2	1.77	0.41
3:I:1019:GLN:NE2	4:J:616:GLN:OE1	2.53	0.41
4:J:435:VAL:HG13	4:J:444:VAL:HG13	2.00	0.41
4:J:919:PHE:HE1	4:J:924:MET:SD	2.43	0.41
4:J:1393:GLN:CD	4:J:1398:TRP:HE1	2.23	0.41
1:A:67:GLU:O	1:A:74:GLY:HA2	2.20	0.41
1:A:302:TYR:O	1:A:306:ARG:N	2.34	0.41
1:A:373:ARG:NE	1:F:218:ARG:NH1	2.67	0.41
1:A:409:ARG:HH21	3:I:777:ILE:HB	1.83	0.41
1:A:414:LYS:HE3	1:A:416:ASN:HB3	2.03	0.41
1:B:181:LEU:O	1:B:350:LEU:N	2.54	0.41
1:B:379:LEU:HD13	1:B:387:MET:HE1	2.01	0.41
1:C:252:PHE:HA	1:C:255:GLU:CD	2.40	0.41
1:C:340:GLU:OE1	1:C:340:GLU:HA	2.20	0.41
1:D:254:HIS:HB2	1:D:307:PHE:CE2	2.55	0.41
1:E:292:LEU:HD12	1:E:296:LEU:HB2	2.00	0.41
1:E:416:ASN:O	1:E:420:LEU:HG	2.21	0.41
3:I:6:PHE:CD2	3:I:909:ALA:HB2	2.55	0.41
3:I:109:LYS:HE3	3:I:109:LYS:HB3	1.92	0.41
3:I:897:LEU:HD23	3:I:897:LEU:HA	1.86	0.41
3:I:939:ARG:O	3:I:942:GLU:HG3	2.21	0.41
5:K:54:LEU:HD23	5:K:58:PRO:CG	2.51	0.41
1:B:273:SER:O	1:B:277:LEU:N	2.39	0.41
1:D:163:LEU:HD23	1:D:410:LEU:HB2	2.02	0.41
1:D:218:ARG:NH2	1:E:373:ARG:NH2	2.68	0.41
1:E:243:PRO:HB2	1:E:284:VAL:HG23	2.02	0.41
2:G:31:GLY:O	2:G:35:THR:OG1	2.37	0.41
2:G:100:LEU:HD22	2:G:141:GLU:HG2	2.02	0.41
2:G:117:VAL:HG12	2:G:118:ALA:H	1.86	0.41
2:G:179:PHE:HA	2:G:197:LEU:HA	2.03	0.41
3:I:270:GLY:H	3:I:274:ARG:NE	2.19	0.41
3:I:477:GLY:O	3:I:507:ARG:HA	2.20	0.41
3:I:871:LEU:HD23	3:I:871:LEU:HA	1.84	0.41
4:J:507:ASN:N	4:J:507:ASN:OD1	2.53	0.41
4:J:614:PHE:CD2	4:J:1439:SER:HA	2.55	0.41
4:J:850:LEU:HD12	4:J:884:ARG:NH1	2.35	0.41
6:T:35:DG:H2"	6:T:36:DA:H8	1.86	0.41
6:T:38:DA:H2	8:N:4:DT:C2	2.38	0.41
1:A:187:LYS:CG	1:B:373:ARG:NH2	2.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.73	0.41
1:C:174:ILE:HG23	1:C:178:GLN:HG2	2.03	0.41
1:C:179:ARG:HD2	1:C:308:LEU:HG	2.02	0.41
1:C:339:PHE:CZ	1:C:343:LYS:HD2	2.56	0.41
1:C:418:GLU:O	1:C:422:SER:CB	2.69	0.41
1:D:414:LYS:HD2	1:D:415:ASN:H	1.86	0.41
1:E:101:ARG:HG3	1:E:259:ARG:HD2	2.02	0.41
1:E:229:VAL:CG2	1:E:232:ALA:HB3	2.50	0.41
2:G:198:ARG:HD3	3:I:934:PHE:CZ	2.55	0.41
2:H:222:LEU:HD23	2:H:222:LEU:HA	1.90	0.41
3:I:916:GLU:OE2	3:I:920:GLN:NE2	2.53	0.41
4:J:23:TYR:O	4:J:49:ILE:HG13	2.20	0.41
6:T:38:DA:C2	8:N:4:DT:C2	3.07	0.41
1:A:305:LYS:HE2	1:A:341:GLU:OE2	2.21	0.41
1:A:355:ARG:HH12	1:A:400:ALA:CB	2.33	0.41
1:B:383:VAL:HG12	1:B:387:MET:HE3	2.02	0.41
1:C:80:LEU:HD23	1:C:84:GLU:OE2	2.19	0.41
1:C:389:LEU:CD1	5:K:92:LEU:HD11	2.46	0.41
1:E:61:LEU:HD21	1:E:107:VAL:HG13	2.03	0.41
1:E:78:GLU:CB	1:E:87:VAL:HG12	2.51	0.41
1:E:122:LEU:HD21	1:E:125:VAL:CG2	2.49	0.41
1:E:162:GLU:H	1:E:162:GLU:CD	2.22	0.41
1:E:191:THR:HB	1:E:225:PHE:HZ	1.86	0.41
3:I:270:GLY:H	3:I:274:ARG:CD	2.33	0.41
3:I:771:GLU:O	3:I:774:LEU:HB3	2.20	0.41
3:I:983:ILE:HG21	3:I:987:ILE:HD11	2.02	0.41
3:I:1001:VAL:CG1	3:I:1004:LYS:HB2	2.51	0.41
4:J:74:GLU:HB3	4:J:75:ARG:NH2	2.36	0.41
4:J:96:ALA:HB3	4:J:554:LEU:HD22	2.02	0.41
4:J:770:LEU:HB2	4:J:1210:SER:O	2.21	0.41
4:J:853:VAL:HG22	4:J:858:VAL:HG23	2.02	0.41
1:A:78:GLU:HA	1:A:86:ARG:NE	2.36	0.41
1:A:194:LEU:HD12	1:A:197:ILE:HD11	2.03	0.41
1:A:328:VAL:HG22	1:A:329:GLU:HG3	2.03	0.41
1:A:374:ARG:HG3	1:A:377:LEU:HD12	2.03	0.41
1:B:347:ASN:HA	1:B:373:ARG:HH11	1.85	0.41
1:B:354:ARG:HA	1:B:354:ARG:NE	2.36	0.41
1:C:337:VAL:O	1:C:341:GLU:OE1	2.39	0.41
1:C:413:THR:O	1:C:418:GLU:HB2	2.21	0.41
1:C:414:LYS:N	1:C:417:LYS:HB2	2.36	0.41
1:C:414:LYS:HD2	1:C:416:ASN:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ARG:HH22	1:E:373:ARG:HH22	1.69	0.41
1:E:98:TYR:HE1	1:E:137:LYS:HZ2	1.68	0.41
1:E:124:LYS:HZ2	1:E:133:PRO:HG2	1.84	0.41
1:E:166:ARG:CZ	1:E:410:LEU:HB3	2.51	0.41
1:F:60:ARG:NH2	1:F:119:TYR:HA	2.36	0.41
1:F:76:LEU:O	1:F:87:VAL:HA	2.20	0.41
1:F:195:LYS:HG3	1:F:225:PHE:CE1	2.56	0.41
1:F:300:ALA:O	1:F:304:PRO:HD2	2.20	0.41
1:F:379:LEU:HD13	1:F:387:MET:CE	2.50	0.41
2:H:7:LYS:O	2:H:7:LYS:HG3	2.21	0.41
2:H:153:ALA:HA	2:H:156:HIS:NE2	2.36	0.41
3:I:274:ARG:HG2	3:I:285:LEU:HB3	2.03	0.41
3:I:704:HIS:CB	3:I:831:ARG:HE	2.34	0.41
3:I:772:ARG:HG3	3:I:782:ALA:HB1	2.02	0.41
3:I:860:HIS:ND1	3:I:861:LEU:O	2.47	0.41
3:I:1006:HIS:HE2	6:T:26:DG:H5”	1.82	0.41
4:J:33:ASN:HB2	4:J:36:THR:OG1	2.21	0.41
4:J:204:LEU:HB3	4:J:206:ARG:NH1	2.36	0.41
4:J:407:VAL:HG11	4:J:437:VAL:HG11	2.03	0.41
4:J:560:GLN:HG3	4:J:561:GLY:H	1.85	0.41
4:J:996:TRP:HA	4:J:999:THR:HG22	2.01	0.41
4:J:1381:VAL:HA	4:J:1417:TRP:HA	2.03	0.41
4:J:1497:GLU:HA	4:J:1500:LYS:HE2	2.03	0.41
5:K:54:LEU:HD23	5:K:58:PRO:HG2	2.03	0.41
1:A:353:SER:CB	1:A:356:LEU:HD13	2.51	0.41
1:B:350:LEU:HA	1:B:370:SER:OG	2.21	0.41
1:C:111:ARG:NH2	1:C:114:ARG:HG2	2.36	0.41
1:C:282:ASN:HD21	1:D:290:ARG:HH11	1.69	0.41
1:C:414:LYS:HG2	1:C:415:ASN:H	1.86	0.41
1:D:111:ARG:NH2	1:D:117:GLU:OE2	2.54	0.41
1:D:148:GLN:HG3	1:D:315:ARG:HE	1.85	0.41
1:E:176:ARG:HB3	1:E:319:SER:CB	2.50	0.41
2:G:26:GLU:HA	2:G:27:PRO:HA	1.88	0.41
3:I:86:LYS:HB3	3:I:813:VAL:HG23	2.03	0.41
3:I:222:MET:O	3:I:225:SER:OG	2.38	0.41
3:I:307:LEU:HD23	3:I:307:LEU:HA	1.95	0.41
3:I:610:ARG:HB2	3:I:622:GLU:OE2	2.21	0.41
3:I:670:GLN:O	3:I:993:PHE:HA	2.21	0.41
4:J:417:PRO:HG3	4:J:431:VAL:HA	2.02	0.41
4:J:1190:SER:OG	4:J:1369:GLU:OE1	2.26	0.41
4:J:1495:ILE:O	4:J:1499:ARG:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:48:MET:HG2	5:K:54:LEU:H	1.86	0.41
1:B:304:PRO:HB2	1:B:342:PHE:HZ	1.86	0.40
1:C:271:LEU:O	1:C:325:THR:HG23	2.21	0.40
1:C:414:LYS:HB3	1:C:417:LYS:HD2	2.02	0.40
1:D:78:GLU:HG3	1:D:79:ASN:H	1.86	0.40
1:E:76:LEU:C	1:E:87:VAL:HB	2.41	0.40
1:E:153:GLN:H	1:E:153:GLN:CD	2.25	0.40
1:E:247:ILE:HD13	1:E:247:ILE:HA	1.85	0.40
1:F:278:ALA:HA	1:F:281:ASN:HD22	1.86	0.40
2:G:62:LEU:HA	2:G:163:ASN:OD1	2.21	0.40
3:I:143:SER:O	3:I:147:TYR:OH	2.30	0.40
3:I:335:THR:O	3:I:339:LEU:HG	2.21	0.40
3:I:1037:VAL:HG12	3:I:1041:GLU:OE2	2.21	0.40
4:J:796:ARG:HD3	4:J:862:ASP:OD1	2.21	0.40
4:J:1211:MET:CE	5:K:16:LYS:CE	2.98	0.40
4:J:1278:ASP:HB3	4:J:1318:TYR:OH	2.21	0.40
1:A:184:ALA:O	1:A:327:LEU:HA	2.21	0.40
1:A:190:LYS:HB2	9:A:1000:ADP:PB	2.62	0.40
1:A:271:LEU:HD22	1:A:307:PHE:CE2	2.56	0.40
1:A:400:ALA:O	1:A:404:GLU:OE1	2.39	0.40
1:B:252:PHE:HA	1:B:255:GLU:HG2	2.03	0.40
1:C:136:ALA:O	1:C:139:ARG:NE	2.52	0.40
1:C:177:GLY:N	1:C:321:THR:OG1	2.32	0.40
1:D:355:ARG:HH11	1:D:359:ARG:HD3	1.85	0.40
1:E:220:GLU:HA	1:F:147:PRO:O	2.21	0.40
1:E:267:VAL:HG12	1:E:269:ILE:HG12	2.03	0.40
1:F:243:PRO:HB2	1:F:284:VAL:CG2	2.49	0.40
1:F:413:THR:HB	1:F:417:LYS:HB3	2.02	0.40
2:G:26:GLU:HB2	2:G:194:LYS:HG3	2.03	0.40
2:H:18:ARG:HG2	2:H:206:THR:HG22	2.02	0.40
3:I:585:GLU:HG2	3:I:586:ARG:N	2.35	0.40
3:I:614:ARG:HA	3:I:620:LEU:HA	2.04	0.40
3:I:672:VAL:O	3:I:991:GLN:HA	2.21	0.40
3:I:1115:LEU:HD22	4:J:88:TYR:HD2	1.85	0.40
4:J:12:LEU:HB2	4:J:507:ASN:HD22	1.86	0.40
4:J:1004:THR:OG1	4:J:1036:ARG:HD3	2.21	0.40
4:J:1478:SER:O	4:J:1482:ARG:N	2.54	0.40
1:A:97:GLN:O	1:A:137:LYS:HE3	2.21	0.40
1:A:355:ARG:NH1	1:A:400:ALA:HB2	2.36	0.40
1:B:182:ILE:O	1:B:326:ALA:N	2.40	0.40
1:C:152:ARG:HB2	1:C:176:ARG:HD2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ARG:O	1:D:110:ALA:N	2.43	0.40
1:E:112:PRO:O	1:E:114:ARG:NH1	2.54	0.40
1:E:188:ALA:HA	1:E:357:GLU:HG3	2.02	0.40
1:E:194:LEU:HD12	1:E:270:LEU:HD13	2.04	0.40
1:E:300:ALA:O	1:E:304:PRO:HD2	2.22	0.40
1:F:273:SER:N	1:F:325:THR:OG1	2.36	0.40
3:I:86:LYS:O	3:I:88:LEU:N	2.53	0.40
3:I:89:THR:O	3:I:91:GLN:HG3	2.21	0.40
3:I:151:ASP:OD2	3:I:154:ARG:NH1	2.54	0.40
3:I:957:LYS:HB3	3:I:961:GLU:CG	2.51	0.40
4:J:485:SER:HB2	4:J:488:ARG:NH2	2.36	0.40
4:J:798:GLU:N	4:J:798:GLU:OE1	2.54	0.40
4:J:1353:GLN:NE2	4:J:1365:ASP:OD1	2.54	0.40
1:A:333:ARG:O	1:A:337:VAL:HG23	2.22	0.40
1:B:242:PRO:HD2	1:B:245:ASN:ND2	2.36	0.40
1:B:414:LYS:HG2	1:B:415:ASN:N	2.37	0.40
1:C:241:GLU:HB2	1:C:246:HIS:NE2	2.37	0.40
1:D:244:GLN:HB3	1:D:248:ARG:NH1	2.37	0.40
1:D:287:PRO:HD2	1:D:288:THR:H	1.86	0.40
1:D:403:MET:O	1:D:407:LEU:HB2	2.21	0.40
1:D:412:ARG:NH2	1:D:418:GLU:HA	2.31	0.40
1:F:178:GLN:O	1:F:321:THR:HG23	2.20	0.40
1:F:383:VAL:HG12	1:F:387:MET:HE1	2.04	0.40
2:H:1:MET:C	2:H:6:LEU:H	2.23	0.40
3:I:543:ASN:ND2	3:I:562:SER:O	2.55	0.40
4:J:122:GLU:O	4:J:126:VAL:HG12	2.21	0.40
4:J:136:ASP:HA	4:J:149:LYS:O	2.21	0.40
4:J:701:LEU:CD1	4:J:750:PRO:HD3	2.51	0.40
4:J:800:LYS:HD3	4:J:829:VAL:HG22	2.03	0.40
6:T:18:DA:C4	6:T:19:DC:C5	3.09	0.40
6:T:19:DC:H2"	6:T:20:DC:H5	1.87	0.40
1:A:149:PHE:CZ	1:F:220:GLU:CG	3.05	0.40
1:A:328:VAL:HG22	1:A:329:GLU:N	2.36	0.40
1:B:73:TYR:HE2	1:B:75:PHE:CE1	2.40	0.40
1:B:195:LYS:HE3	1:B:228:SER:HB2	2.04	0.40
1:B:274:ILE:HG23	1:B:275:THR:HG23	2.02	0.40
1:D:63:LYS:H	1:D:86:ARG:NH2	2.20	0.40
1:D:75:PHE:CG	1:D:87:VAL:HB	2.56	0.40
1:D:355:ARG:O	1:D:359:ARG:HG3	2.21	0.40
1:E:213:LEU:HB3	1:E:271:LEU:HD23	2.03	0.40
1:F:159:THR:N	1:F:160:PRO:HD2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ALA:O	1:F:328:VAL:HG12	2.21	0.40
1:F:217:GLU:HG2	1:F:276:ARG:NH2	2.26	0.40
1:F:272:ASP:OD1	1:F:273:SER:OG	2.28	0.40
3:I:591:SER:O	3:I:593:ALA:N	2.54	0.40
3:I:607:ASP:OD1	3:I:608:GLY:N	2.48	0.40
3:I:690:ILE:HD11	3:I:852:ILE:HG12	2.02	0.40
4:J:12:LEU:HA	4:J:12:LEU:HD23	1.78	0.40
4:J:783:ARG:HE	4:J:1029:ARG:NH1	2.19	0.40
4:J:1264:GLU:HG2	4:J:1266:ARG:HE	1.86	0.40
4:J:1290:LEU:HD12	4:J:1290:LEU:H	1.87	0.40
4:J:1291:SER:HB2	4:J:1293:PHE:HE1	1.85	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	359/428 (84%)	339 (94%)	20 (6%)	0	100	100
1	B	359/428 (84%)	337 (94%)	21 (6%)	1 (0%)	41	75
1	C	365/428 (85%)	345 (94%)	19 (5%)	1 (0%)	41	75
1	D	359/428 (84%)	341 (95%)	16 (4%)	2 (1%)	25	63
1	E	359/428 (84%)	335 (93%)	22 (6%)	2 (1%)	25	63
1	F	359/428 (84%)	339 (94%)	19 (5%)	1 (0%)	41	75
2	G	227/315 (72%)	218 (96%)	9 (4%)	0	100	100
2	H	227/315 (72%)	213 (94%)	14 (6%)	0	100	100
3	I	1117/1119 (100%)	1017 (91%)	99 (9%)	1 (0%)	51	84
4	J	1297/1532 (85%)	1204 (93%)	93 (7%)	0	100	100
5	K	89/99 (90%)	78 (88%)	11 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5117/5948 (86%)	4766 (93%)	343 (7%)	8 (0%)	50 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	PRO
1	C	287	PRO
1	D	287	PRO
1	D	286	PRO
3	I	780	GLU
1	E	287	PRO
1	E	286	PRO
1	F	286	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	304/359 (85%)	304 (100%)	0	100 100
1	B	304/359 (85%)	303 (100%)	1 (0%)	92 95
1	C	307/359 (86%)	304 (99%)	3 (1%)	76 86
1	D	304/359 (85%)	302 (99%)	2 (1%)	84 90
1	E	304/359 (85%)	303 (100%)	1 (0%)	92 95
1	F	304/359 (85%)	300 (99%)	4 (1%)	69 82
2	G	202/273 (74%)	201 (100%)	1 (0%)	88 93
2	H	202/273 (74%)	202 (100%)	0	100 100
3	I	941/941 (100%)	937 (100%)	4 (0%)	91 94
4	J	1100/1287 (86%)	1098 (100%)	2 (0%)	93 96
5	K	80/88 (91%)	77 (96%)	3 (4%)	33 59
All	All	4352/5016 (87%)	4331 (100%)	21 (0%)	89 93

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	101	ARG
1	C	111	ARG
1	C	279	ARG
1	C	414	LYS
1	D	86	ARG
1	D	111	ARG
1	E	333	ARG
1	F	63	LYS
1	F	86	ARG
1	F	111	ARG
1	F	141	ARG
2	G	185	ARG
3	I	266	ARG
3	I	610	ARG
3	I	713	ARG
3	I	939	ARG
4	J	48	ARG
4	J	1108	ARG
5	K	47	LYS
5	K	72	ARG
5	K	78	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	GLN
1	B	254	HIS
1	C	415	ASN
1	E	281	ASN
1	F	109	GLN
1	F	148	GLN
1	F	254	HIS
2	G	180	GLN
2	G	229	GLN
2	H	91	ASN
2	H	163	ASN
3	I	1019	GLN
4	J	616	GLN
4	J	1364	HIS
4	J	1485	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	28/125 (22%)	12 (42%)	0

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	2	A
7	R	3	C
7	R	7	U
7	R	8	A
7	R	10	C
7	R	11	C
7	R	12	A
7	R	13	U
7	R	14	A
7	R	15	U
7	R	20	A
7	R	29	U

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BEF	B	502	1	0,3,3	-	-	-		
9	ADP	E	1000	1,10	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
9	ADP	F	1000	1,10	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
11	BEF	D	1002	-	0,3,3	-	-	-		
9	ADP	D	1000	1,10	24,29,29	0.98	1 (4%)	29,45,45	1.58	4 (13%)
11	BEF	A	1002	-	0,3,3	-	-	-		
9	ADP	B	501	1,10	24,29,29	0.94	1 (4%)	29,45,45	1.36	3 (10%)
11	BEF	E	1002	-	0,3,3	-	-	-		
11	BEF	C	1004	-	0,3,3	-	-	-		
9	ADP	A	1000	1,10	24,29,29	0.95	1 (4%)	29,45,45	1.35	3 (10%)
9	ADP	C	1002	10	24,29,29	1.04	1 (4%)	29,45,45	1.58	5 (17%)
11	BEF	F	1002	-	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	E	1000	1,10	-	3/12/32/32	0/3/3/3
9	ADP	F	1000	1,10	-	1/12/32/32	0/3/3/3
9	ADP	D	1000	1,10	-	3/12/32/32	0/3/3/3
9	ADP	B	501	1,10	-	7/12/32/32	0/3/3/3
9	ADP	A	1000	1,10	-	10/12/32/32	0/3/3/3
9	ADP	C	1002	10	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1002	ADP	C5-C4	2.61	1.47	1.40
9	E	1000	ADP	C5-C4	2.55	1.47	1.40
9	D	1000	ADP	C5-C4	2.55	1.47	1.40
9	F	1000	ADP	C5-C4	2.52	1.47	1.40
9	A	1000	ADP	C5-C4	2.43	1.47	1.40
9	B	501	ADP	C5-C4	2.42	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1002	ADP	PA-O3A-PB	-5.24	114.86	132.83
9	D	1000	ADP	PA-O3A-PB	-4.02	119.03	132.83
9	D	1000	ADP	C3'-C2'-C1'	3.85	106.77	100.98
9	E	1000	ADP	C3'-C2'-C1'	3.72	106.57	100.98
9	A	1000	ADP	C3'-C2'-C1'	3.60	106.39	100.98
9	A	1000	ADP	N3-C2-N1	-3.26	123.58	128.68
9	E	1000	ADP	N3-C2-N1	-3.26	123.58	128.68
9	B	501	ADP	C3'-C2'-C1'	3.10	105.64	100.98
9	F	1000	ADP	C3'-C2'-C1'	3.10	105.64	100.98
9	D	1000	ADP	N3-C2-N1	-3.09	123.84	128.68
9	F	1000	ADP	C4-C5-N7	-3.04	106.23	109.40
9	F	1000	ADP	N3-C2-N1	-2.96	124.05	128.68
9	B	501	ADP	N3-C2-N1	-2.95	124.06	128.68
9	C	1002	ADP	C4-C5-N7	-2.87	106.41	109.40
9	E	1000	ADP	PA-O3A-PB	-2.79	123.24	132.83
9	C	1002	ADP	N3-C2-N1	-2.77	124.36	128.68
9	B	501	ADP	C4-C5-N7	-2.67	106.62	109.40
9	A	1000	ADP	C4-C5-N7	-2.58	106.71	109.40
9	E	1000	ADP	C4-C5-N7	-2.54	106.75	109.40
9	F	1000	ADP	PA-O3A-PB	-2.38	124.66	132.83
9	D	1000	ADP	C4-C5-N7	-2.38	106.92	109.40
9	C	1002	ADP	C3'-C2'-C1'	2.15	104.21	100.98
9	C	1002	ADP	O3B-PB-O2B	2.02	115.34	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1000	ADP	PA-O3A-PB-O3B
9	A	1000	ADP	C5'-O5'-PA-O1A
9	B	501	ADP	PA-O3A-PB-O2B
9	B	501	ADP	PA-O3A-PB-O3B
9	B	501	ADP	C5'-O5'-PA-O3A
9	B	501	ADP	O4'-C4'-C5'-O5'
9	E	1000	ADP	PA-O3A-PB-O2B
9	E	1000	ADP	PA-O3A-PB-O3B
9	D	1000	ADP	C3'-C4'-C5'-O5'
9	B	501	ADP	C3'-C4'-C5'-O5'
9	A	1000	ADP	O4'-C4'-C5'-O5'
9	D	1000	ADP	O4'-C4'-C5'-O5'
9	A	1000	ADP	C4'-C5'-O5'-PA
9	D	1000	ADP	PA-O3A-PB-O2B
9	A	1000	ADP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

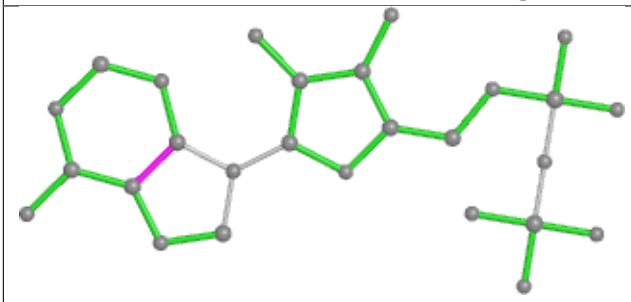
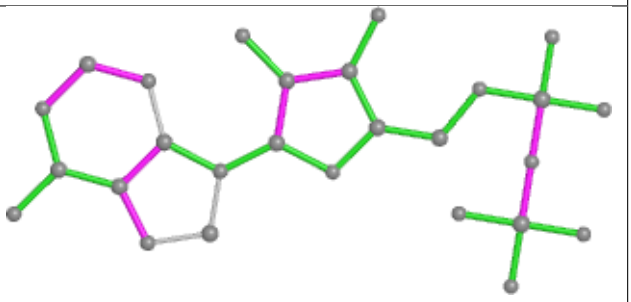
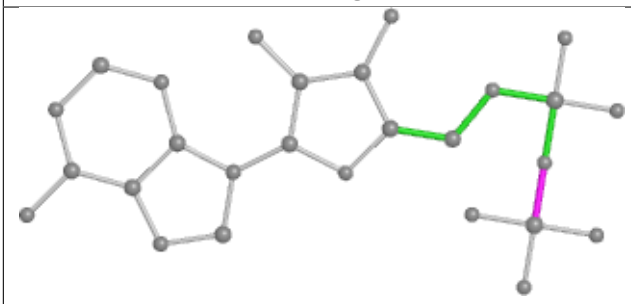
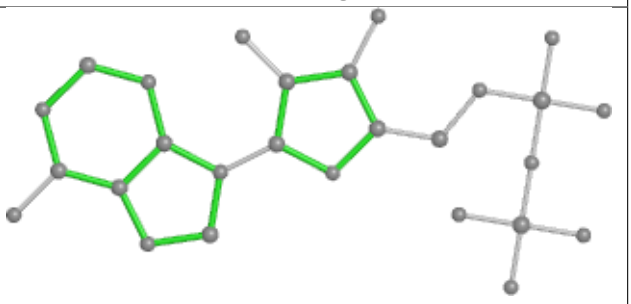
Mol	Chain	Res	Type	Atoms
9	C	1002	ADP	C5'-O5'-PA-O3A
9	A	1000	ADP	PB-O3A-PA-O2A
9	A	1000	ADP	C5'-O5'-PA-O2A
9	B	501	ADP	C5'-O5'-PA-O1A
9	B	501	ADP	C5'-O5'-PA-O2A
9	C	1002	ADP	C5'-O5'-PA-O2A
9	A	1000	ADP	C3'-C4'-C5'-O5'
9	E	1000	ADP	PA-O3A-PB-O1B
9	A	1000	ADP	PA-O3A-PB-O2B
9	C	1002	ADP	PA-O3A-PB-O3B
9	F	1000	ADP	PA-O3A-PB-O2B
9	A	1000	ADP	PB-O3A-PA-O1A

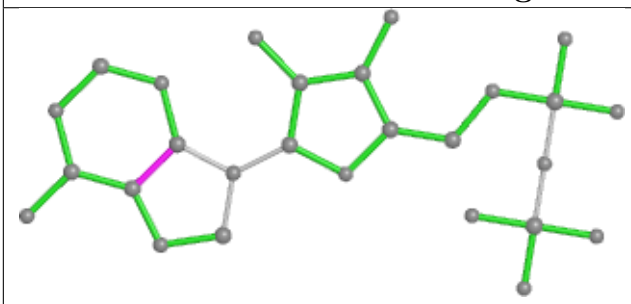
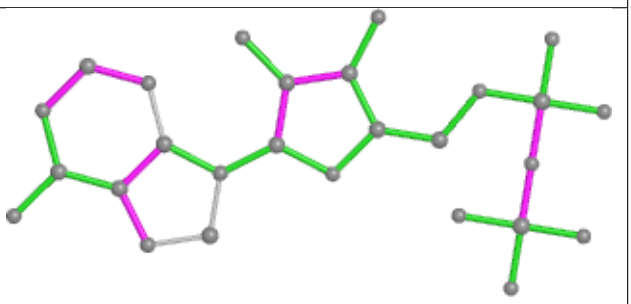
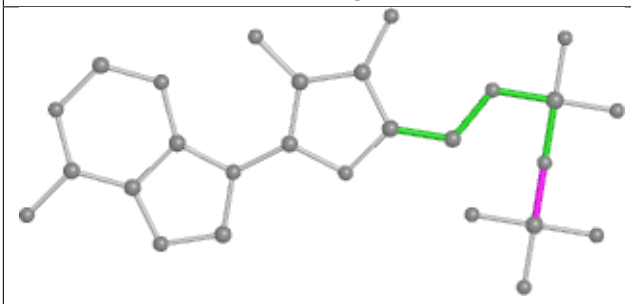
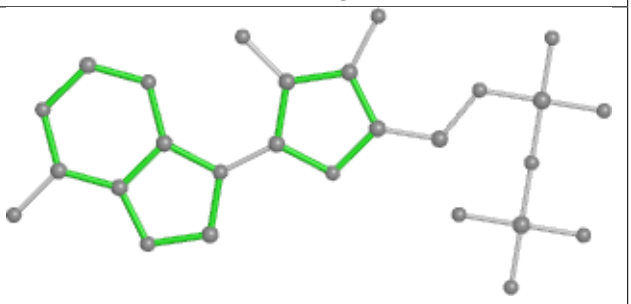
There are no ring outliers.

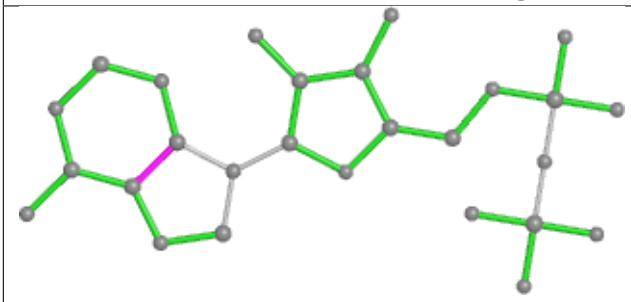
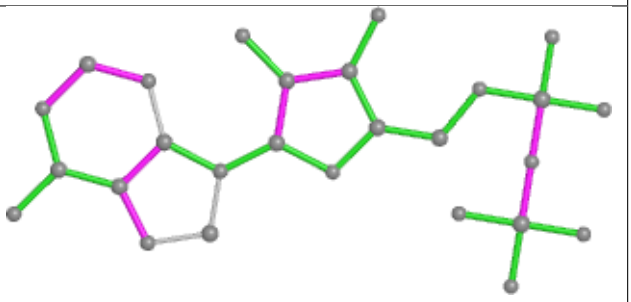
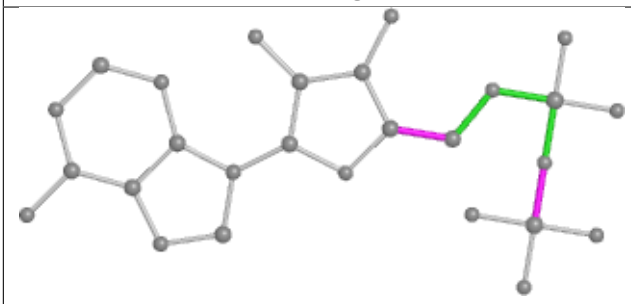
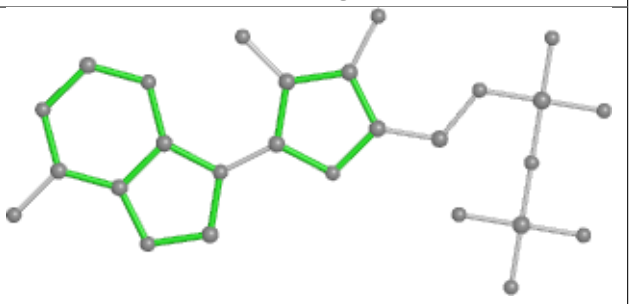
11 monomers are involved in 39 short contacts:

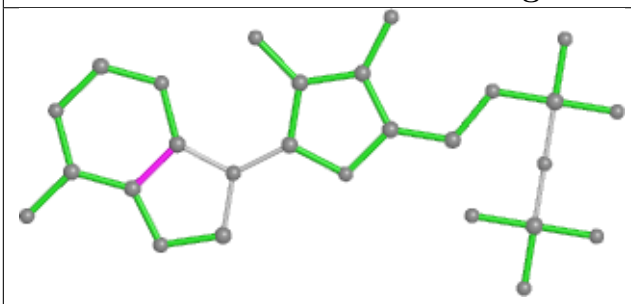
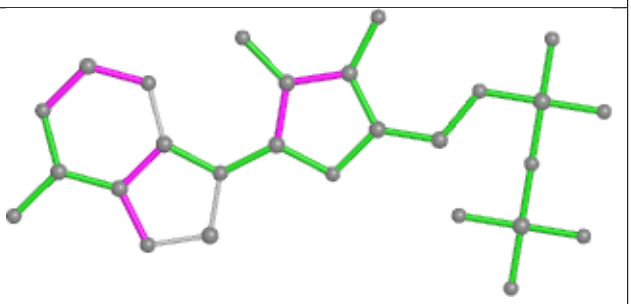
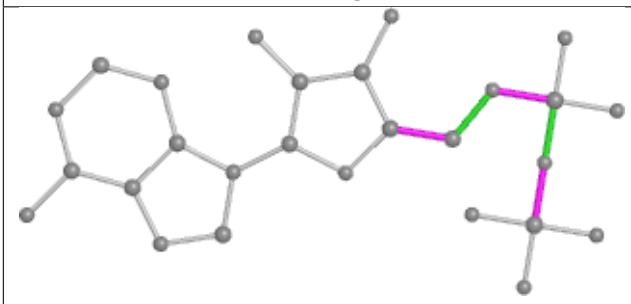
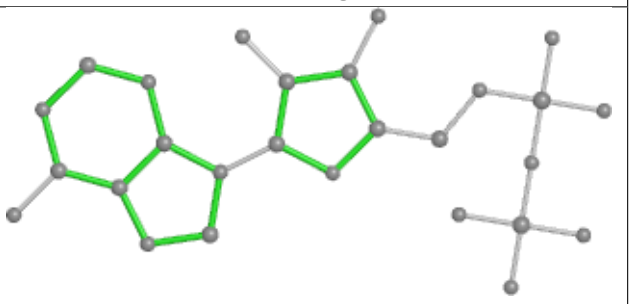
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	502	BEF	4	0
9	E	1000	ADP	2	0
9	F	1000	ADP	3	0
11	D	1002	BEF	2	0
9	D	1000	ADP	5	0
9	B	501	ADP	8	0
11	E	1002	BEF	1	0
11	C	1004	BEF	5	0
9	A	1000	ADP	8	0
9	C	1002	ADP	8	0
11	F	1002	BEF	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

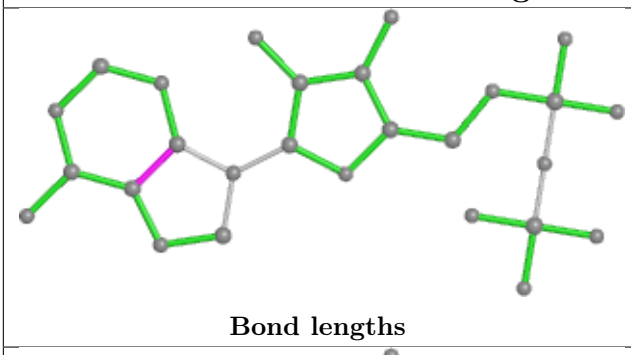
Ligand ADP E 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

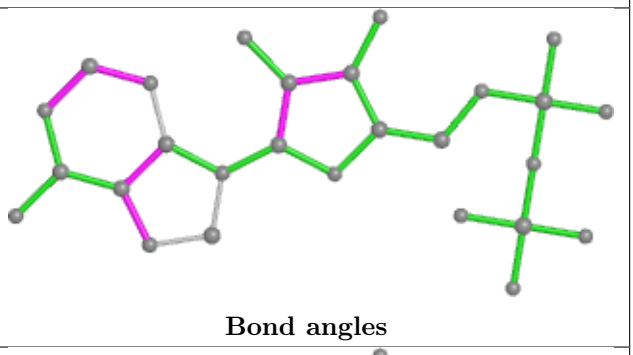
Ligand ADP D 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

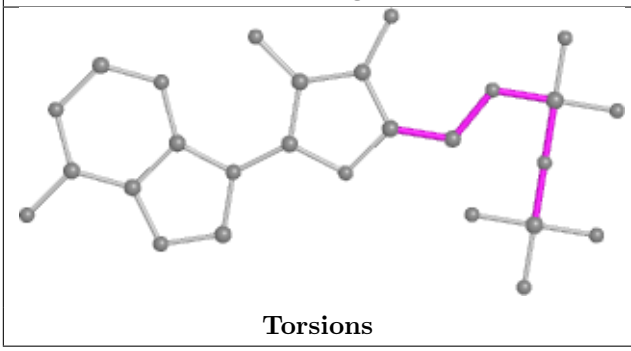
Ligand ADP A 1000



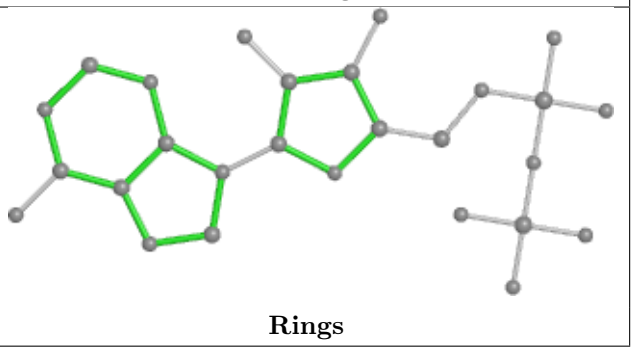
Bond lengths



Bond angles

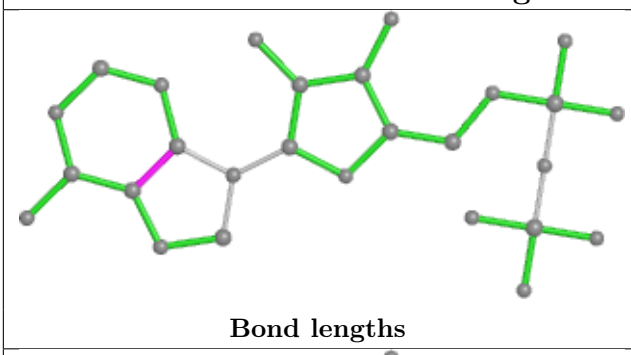


Torsions

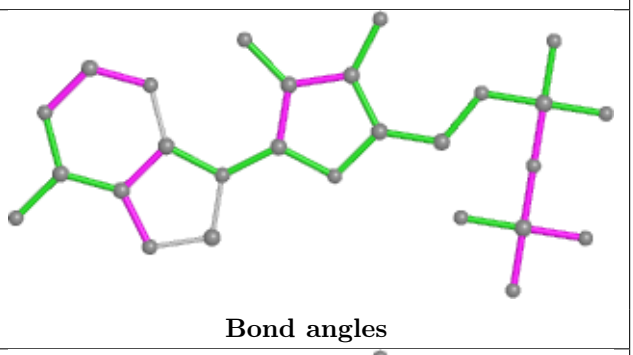


Rings

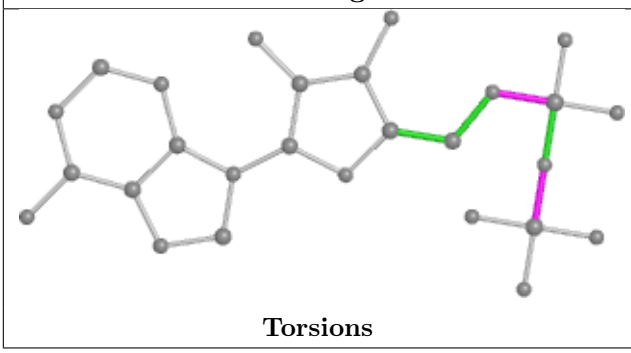
Ligand ADP C 1002



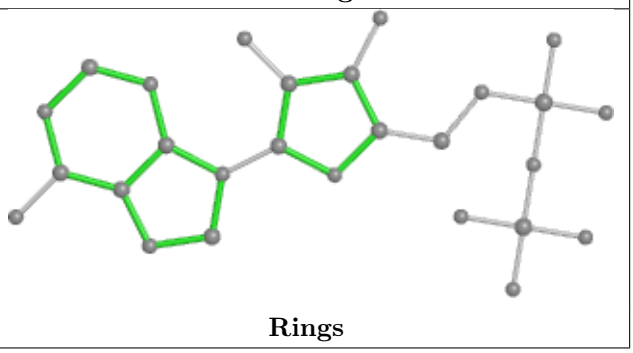
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

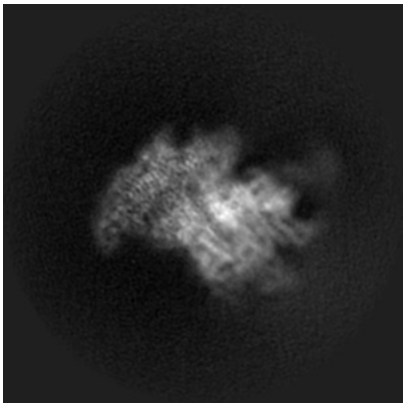
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35004. These allow visual inspection of the internal detail of the map and identification of artifacts.

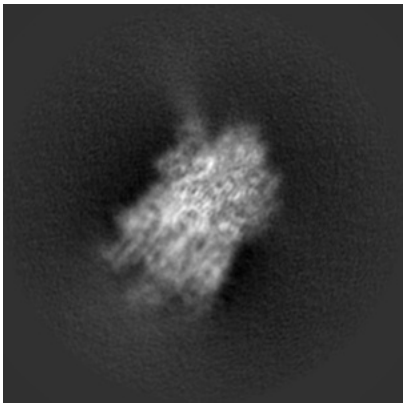
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

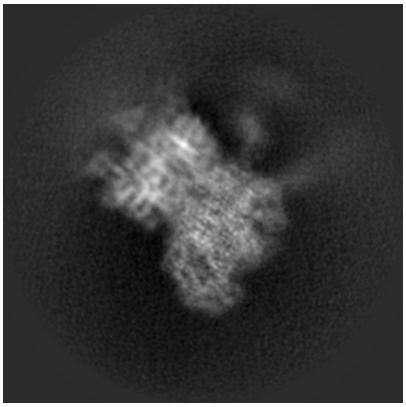
6.1.1 Primary map



X



Y

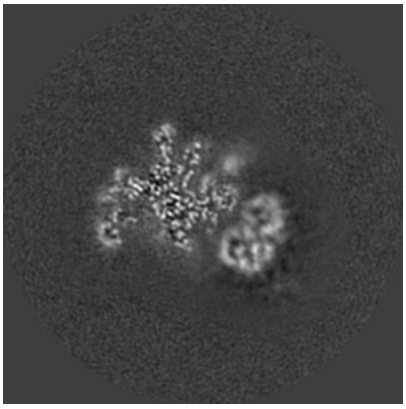


Z

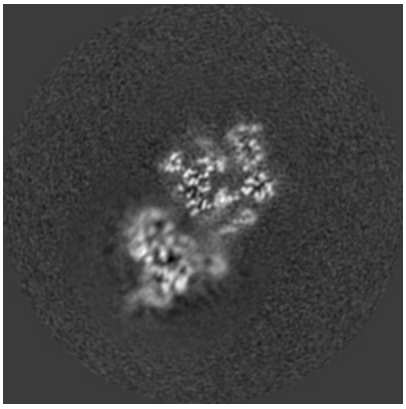
The images above show the map projected in three orthogonal directions.

6.2 Central slices

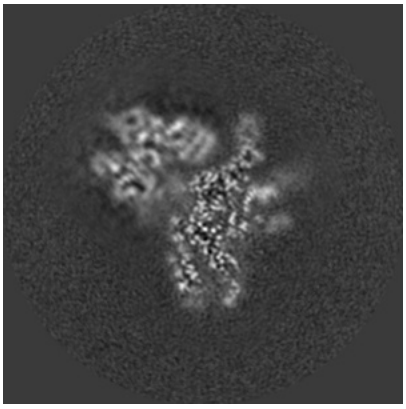
6.2.1 Primary map



X Index: 160



Y Index: 160

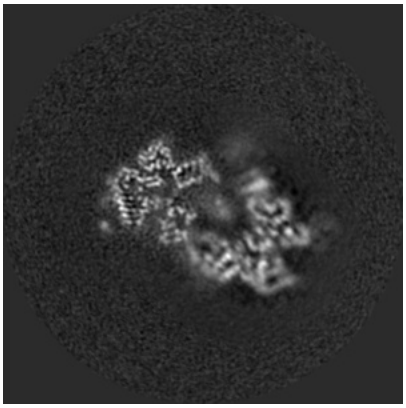


Z Index: 160

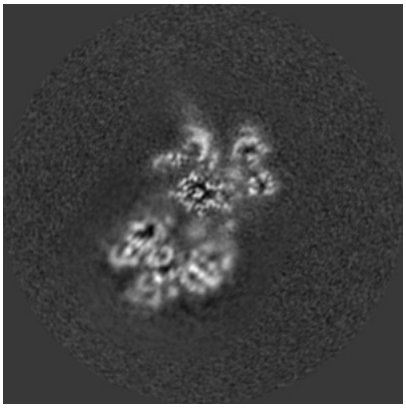
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

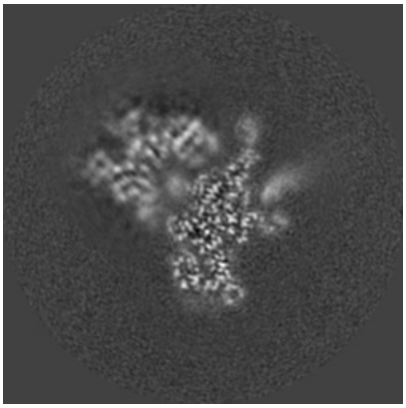
6.3.1 Primary map



X Index: 144



Y Index: 169

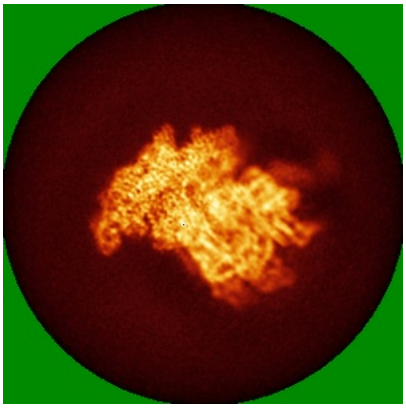


Z Index: 156

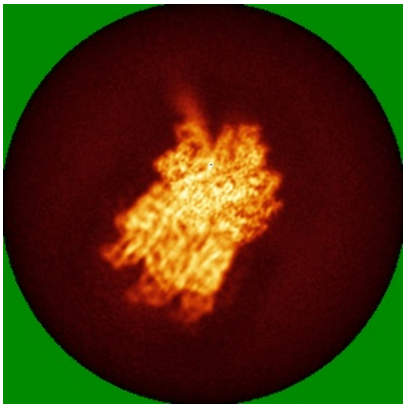
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

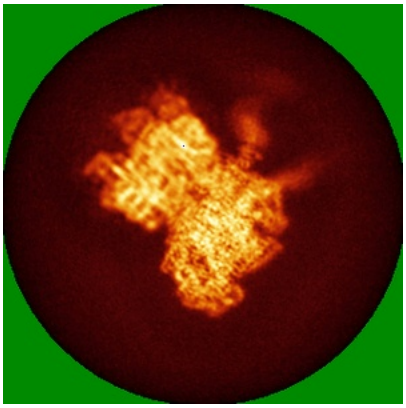
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

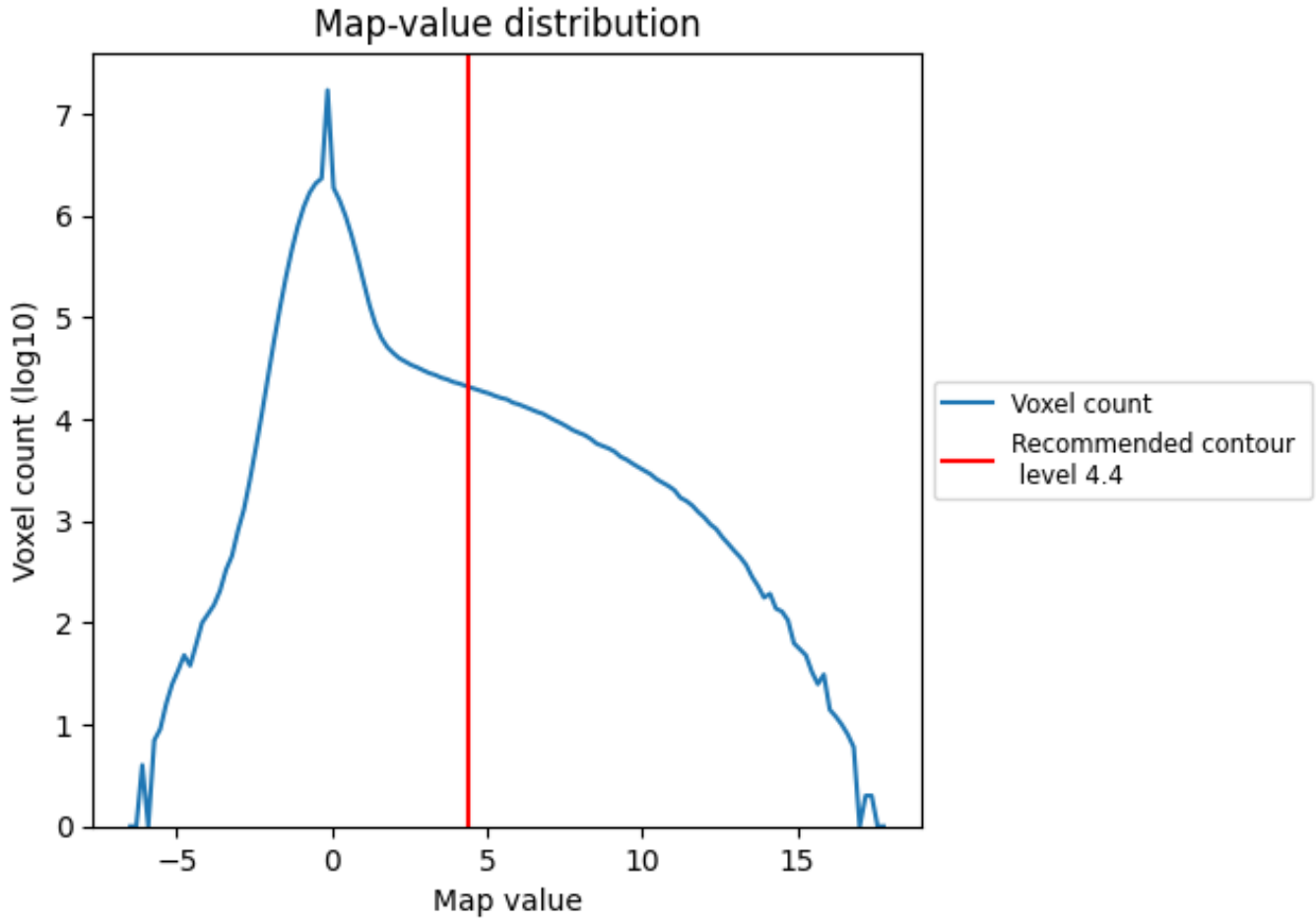
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

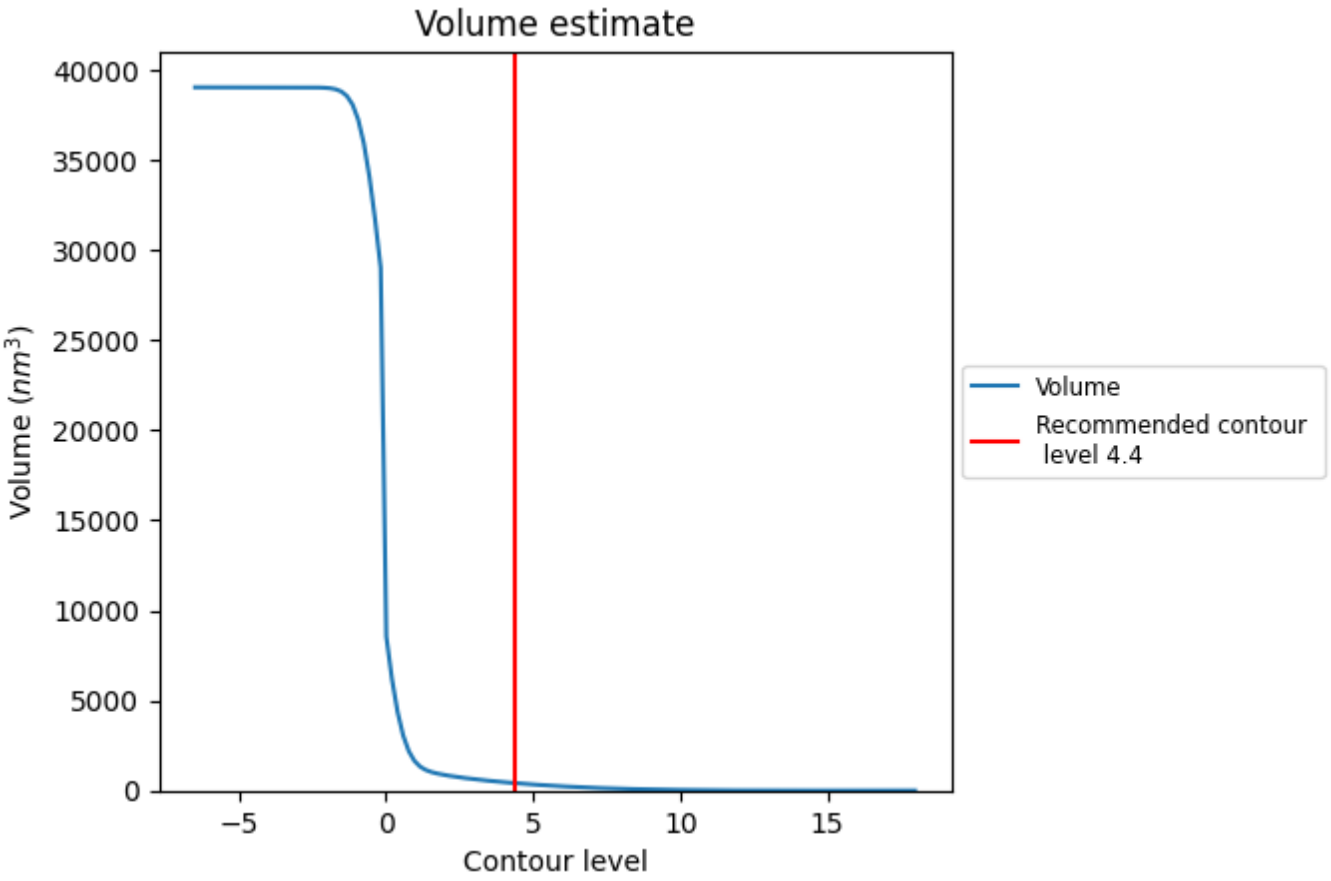
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

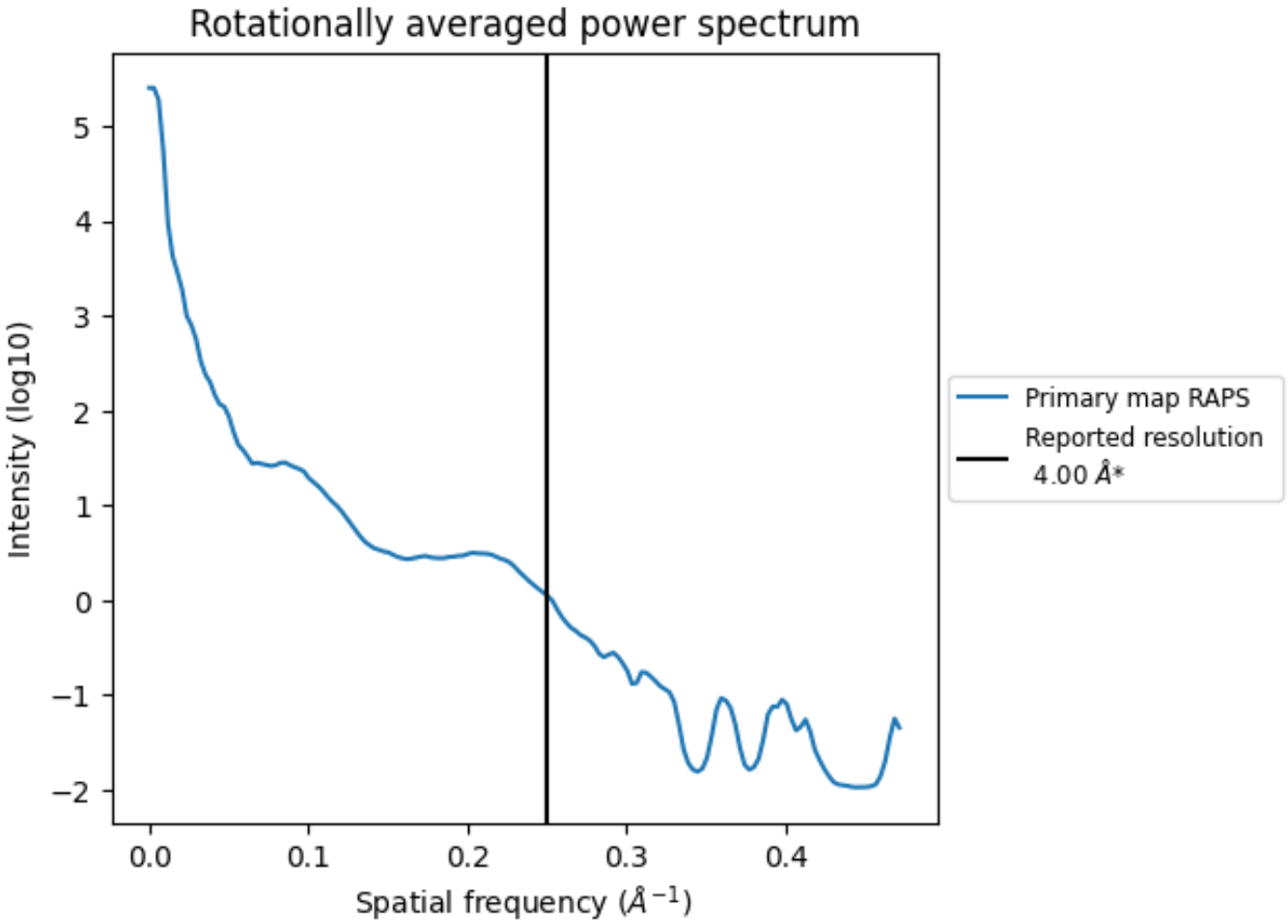
7.2 Volume estimate



The volume at the recommended contour level is 410 nm^3; this corresponds to an approximate mass of 370 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

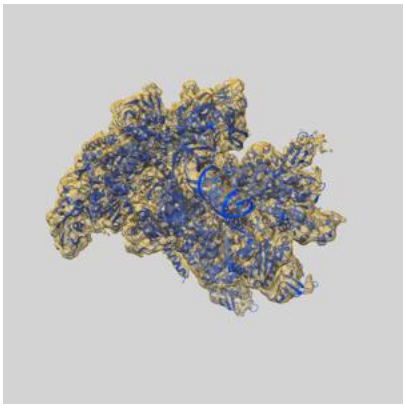
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

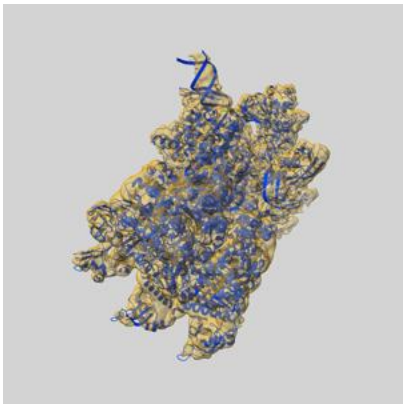
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35004 and PDB model 8HSR. Per-residue inclusion information can be found in section 3 on page 9.

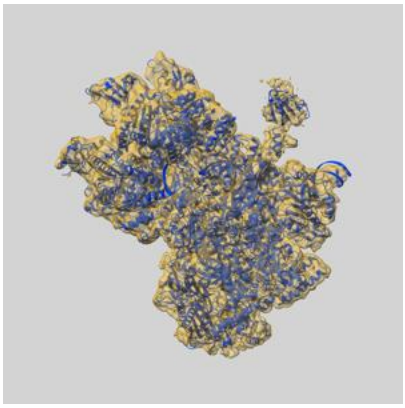
9.1 Map-model overlay



X



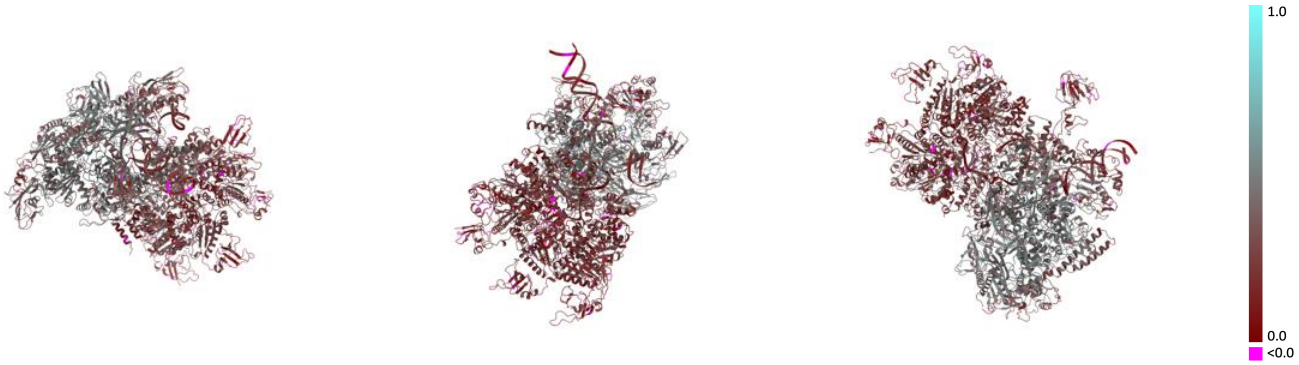
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

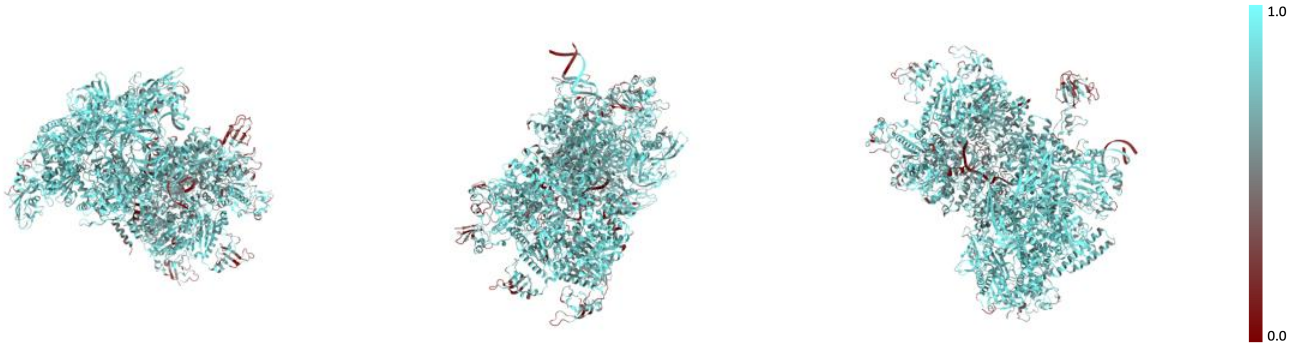
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

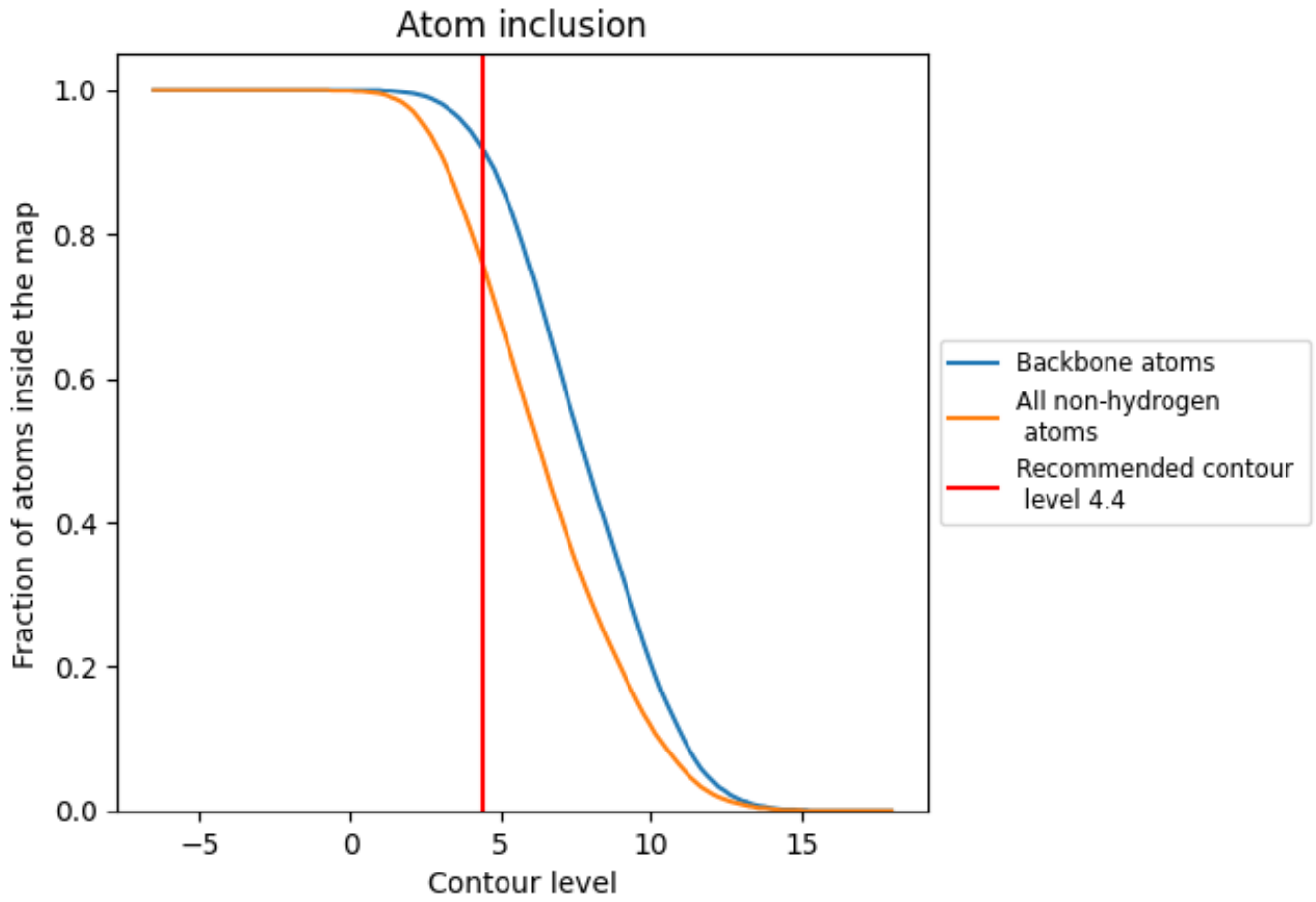
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.4).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.3170
A	0.7530	0.2180
B	0.7350	0.2180
C	0.7230	0.2190
D	0.7390	0.2160
E	0.7570	0.2060
F	0.7710	0.2150
G	0.8000	0.4340
H	0.7640	0.3940
I	0.7960	0.4130
J	0.7530	0.3880
K	0.6250	0.2810
N	0.6810	0.1600
R	0.6650	0.2630
T	0.8300	0.2970