Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID	:	5IYB / pdb_00005iyb
EMDB ID	:	EMD-8136
Title	:	Human core-PIC in the open state
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	3.90 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:

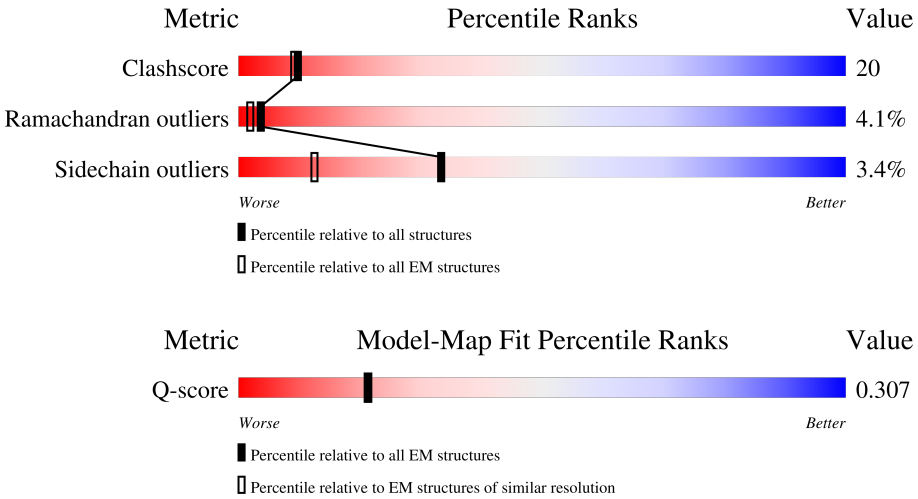
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



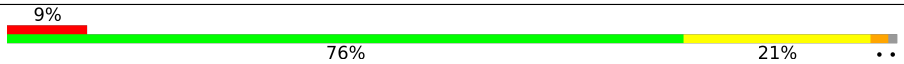
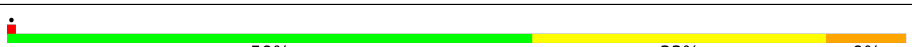
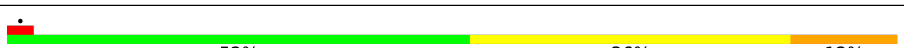
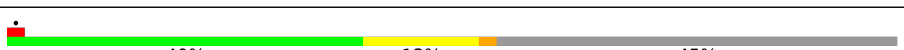
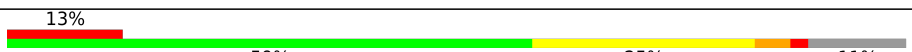
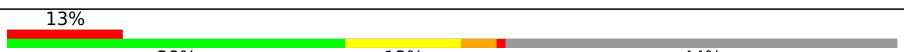
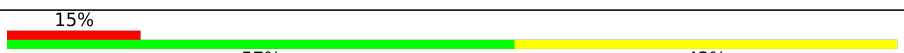
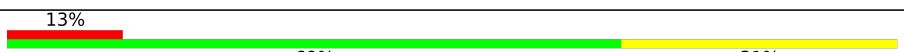
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	1970	47% 22% 26%
2	B	1174	59% 35% 5%
3	C	275	71% 23% 6%
4	D	142	80% 11% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	75	
23	Y	75	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 47728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1454	11515	7234	2058	2150	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1165	9317	5878	1637	1738	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	275	2213	1386	380	440	7	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	129	1062	665	179	214	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1723	1088	301	325	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	86	689	437	120	127	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	310	Total	C	N	O	S	0	0
			2391	1490	426	457	18		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	75	Total	C	N	O	P	0	0
			1553	735	297	447	74		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	75	Total	C	N	O	P	0	0
			1517	721	269	453	74		

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	
24	U	1	Total	Mg	0
			1	1	

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	M	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
25	U	1	1	1	0

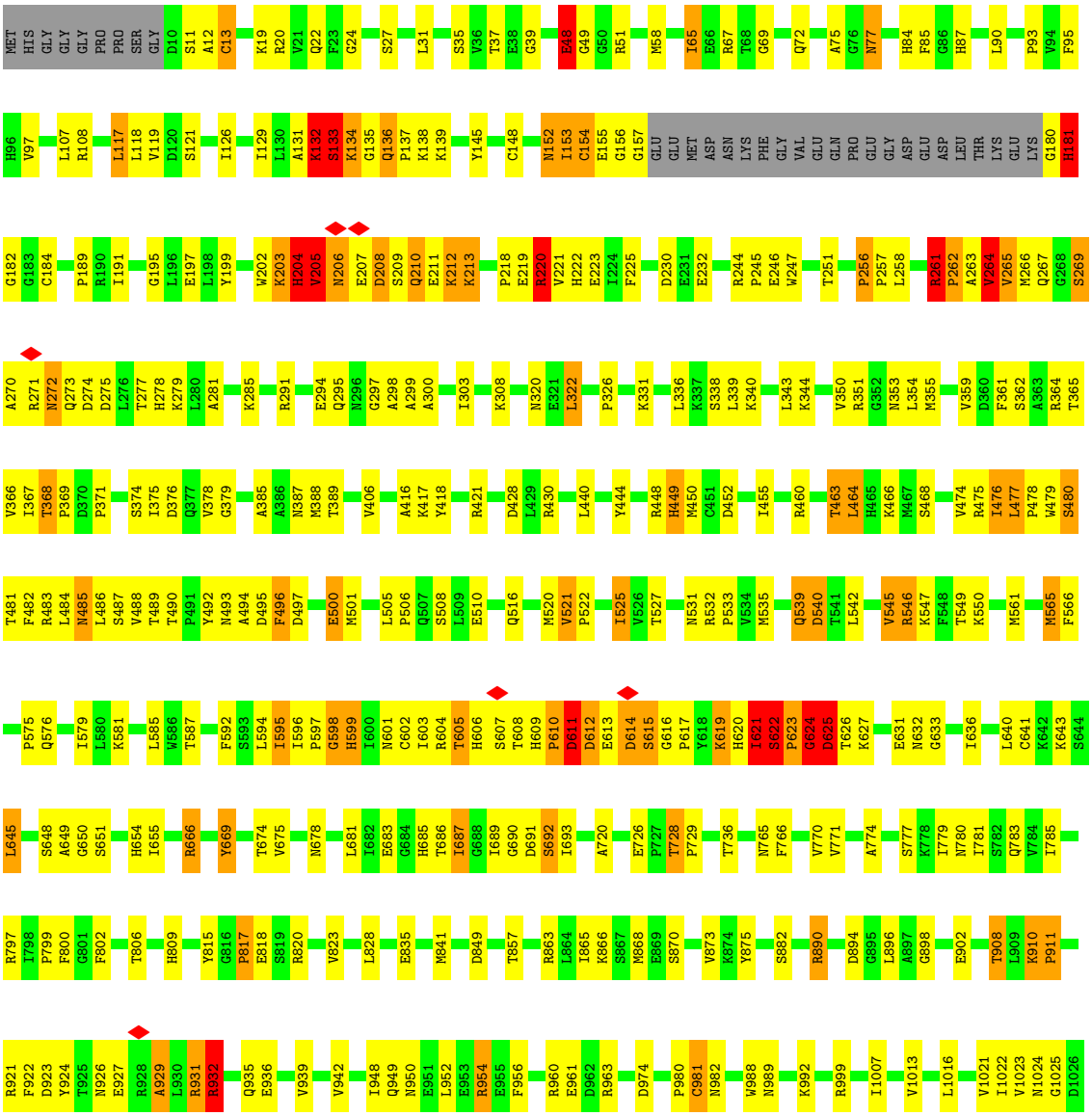
3 Residue-property plots (i)

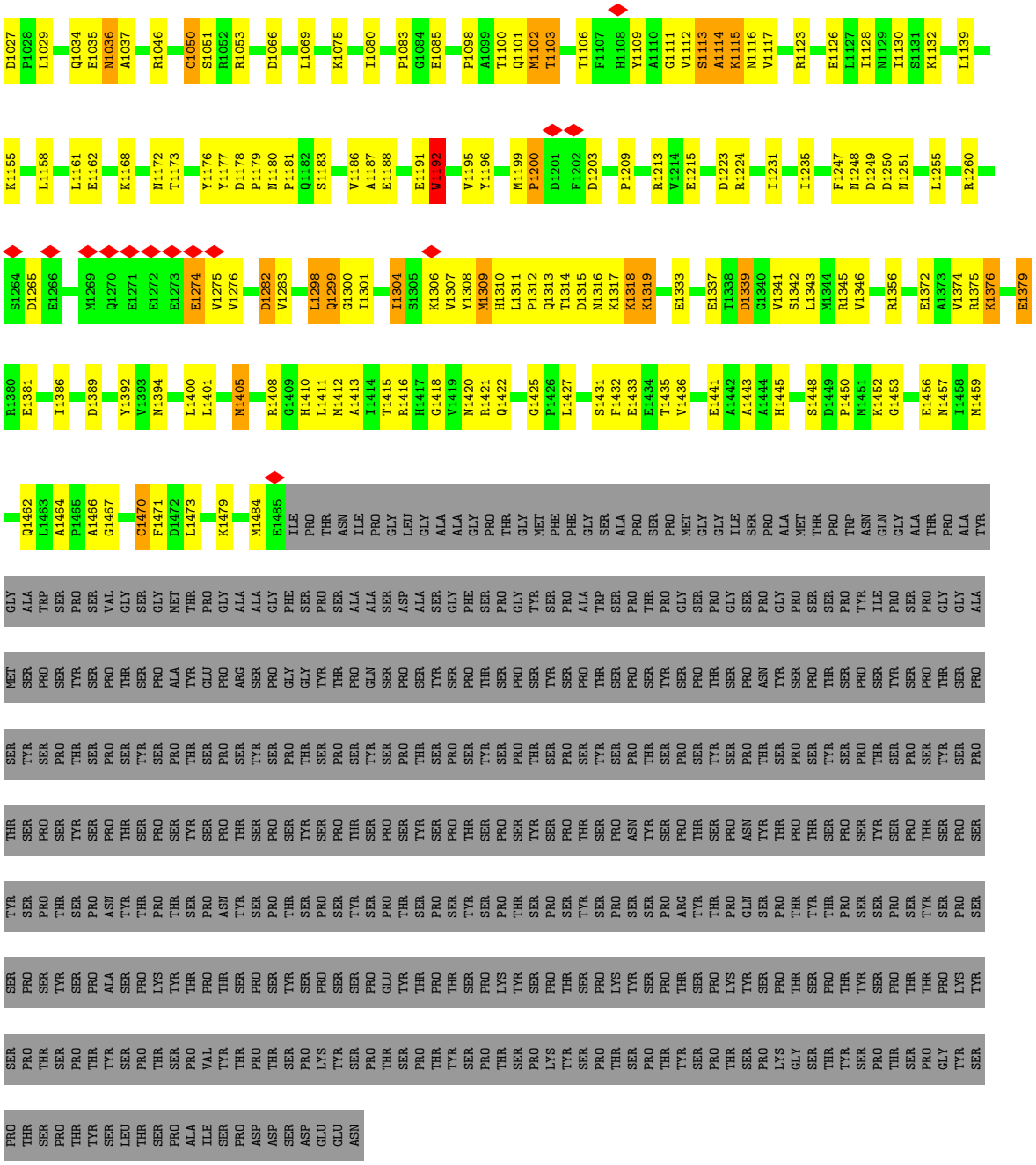
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase II subunit RPB1

Chain A:

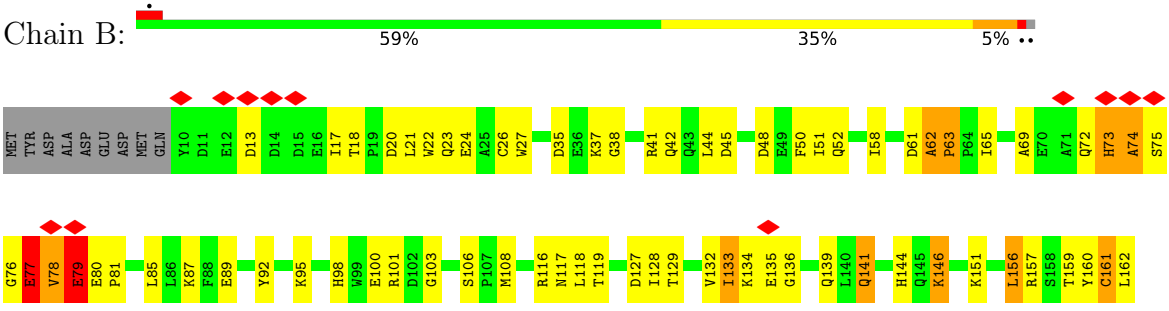


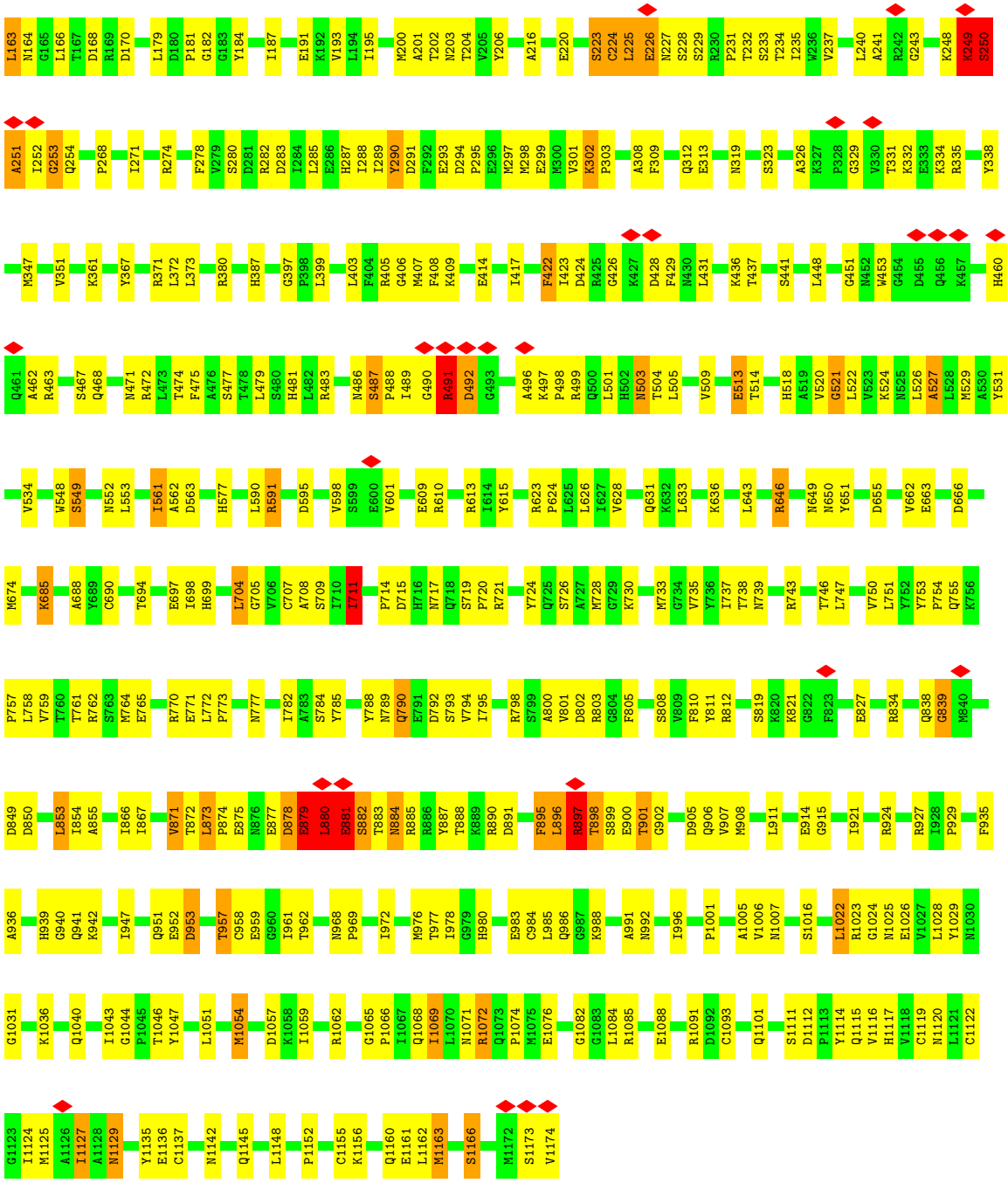




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

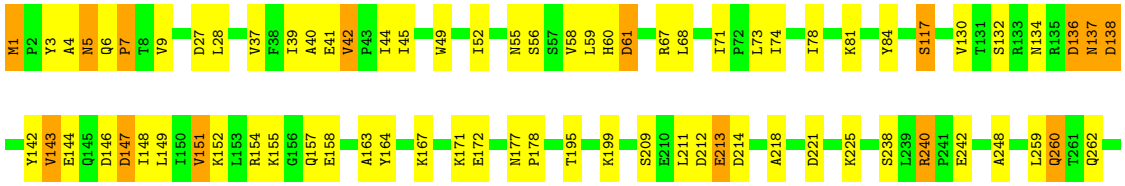


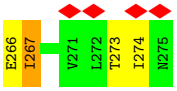


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



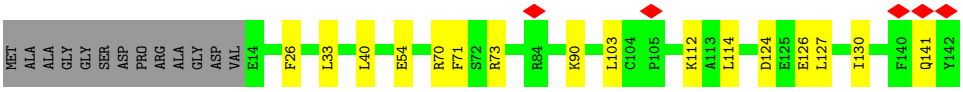




• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:

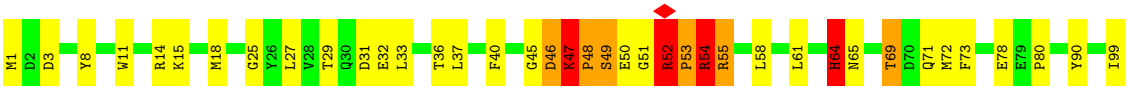




• Molecule 5: DNA-directed RNA polymerase II subunit RPB5

Chain E:



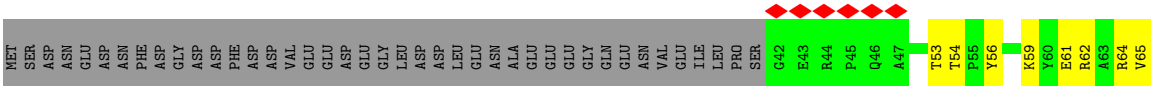


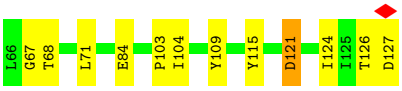


• Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F:



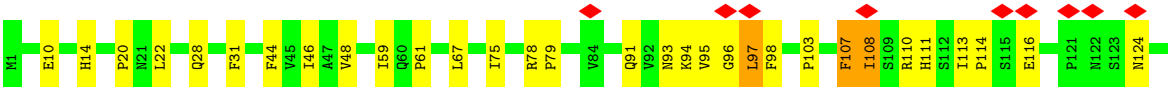


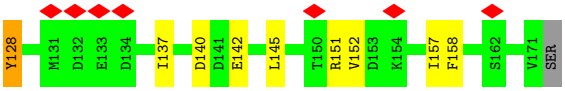


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



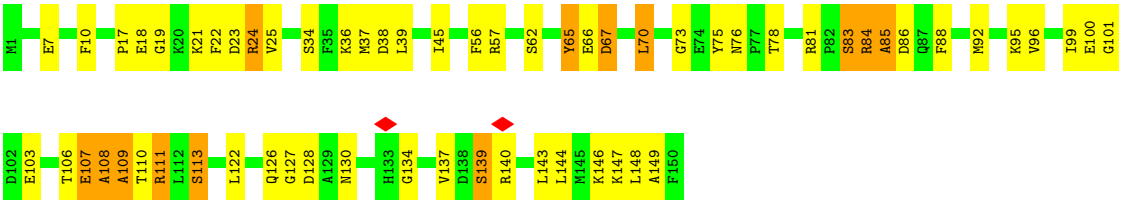




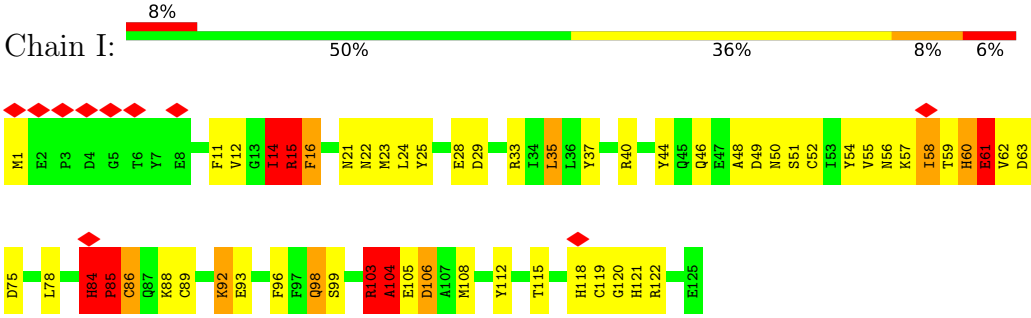
• Molecule 8: DNA-directed RNA polymerase II subunit RPB8

Chain H:

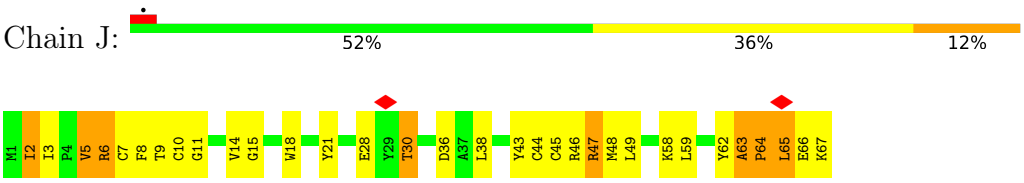




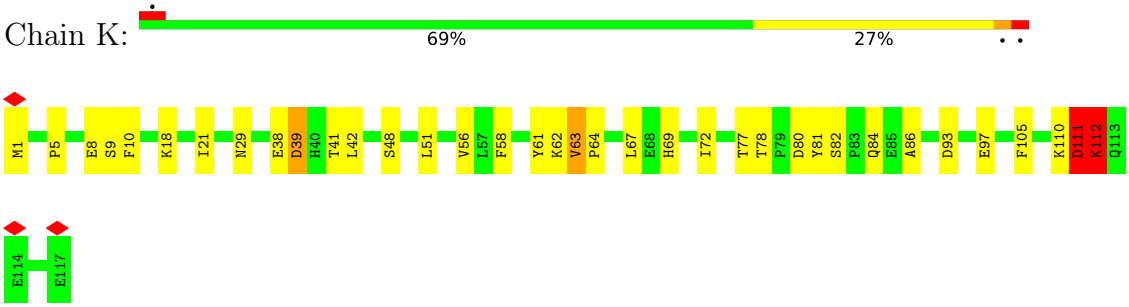
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



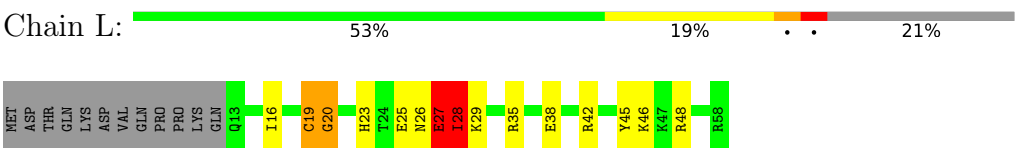
• Molecule 10: DNA-directed RNA polymerase II subunit RPB10



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

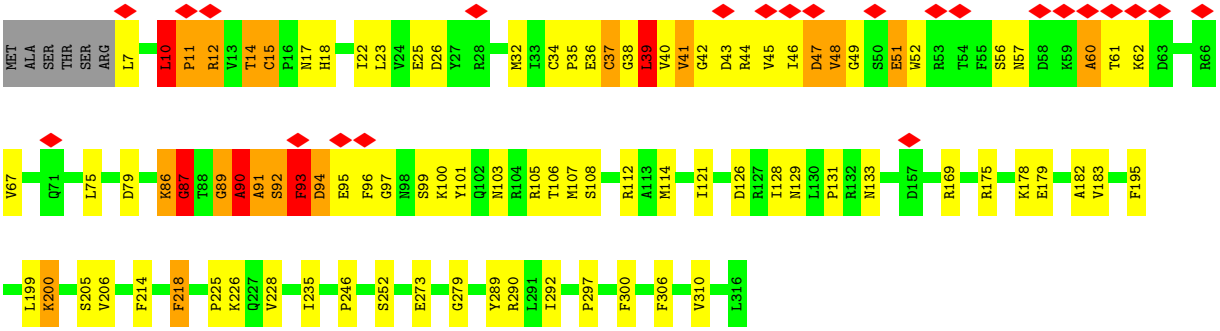


• Molecule 12: DNA-directed RNA polymerase II subunit RPB12



• Molecule 13: Transcription initiation factor IIB

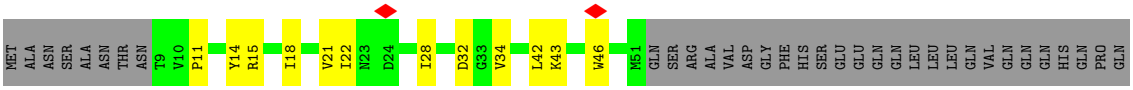




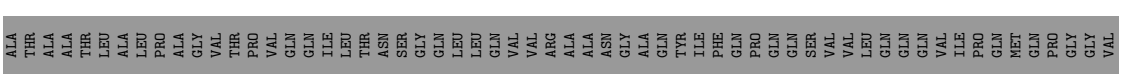
• Molecule 14: Transcription initiation factor IIA subunit 1

Chain N:

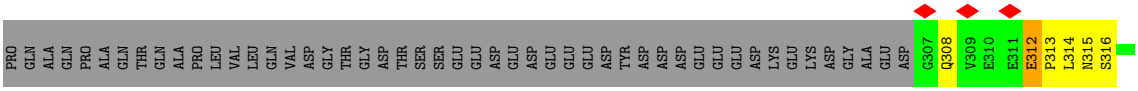


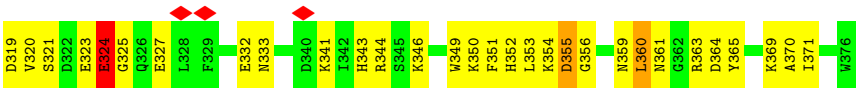








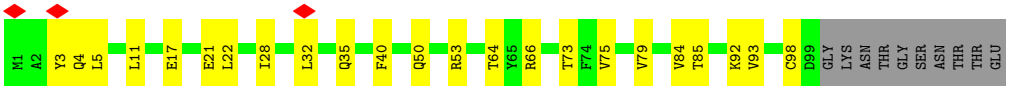




• Molecule 15: Transcription initiation factor IIA subunit 2

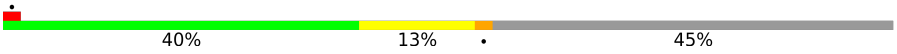
Chain O:

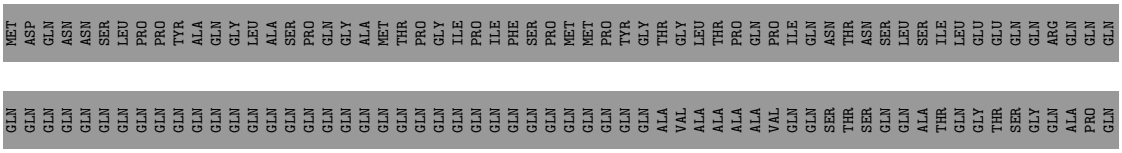


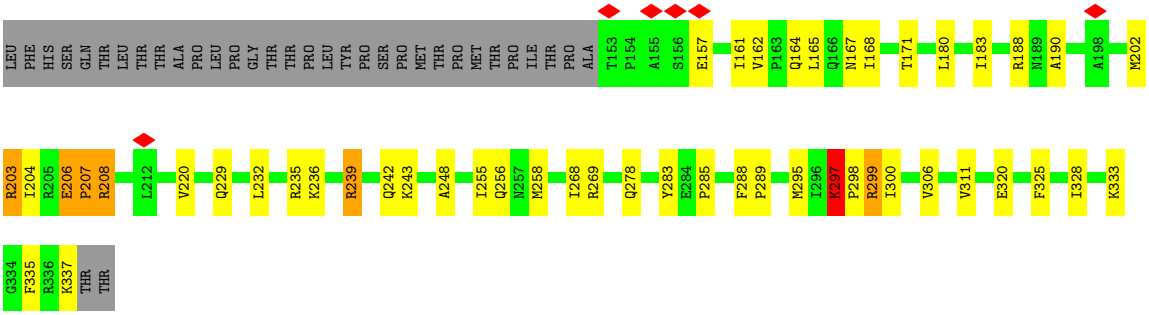


• Molecule 16: TATA-box-binding protein

Chain P:



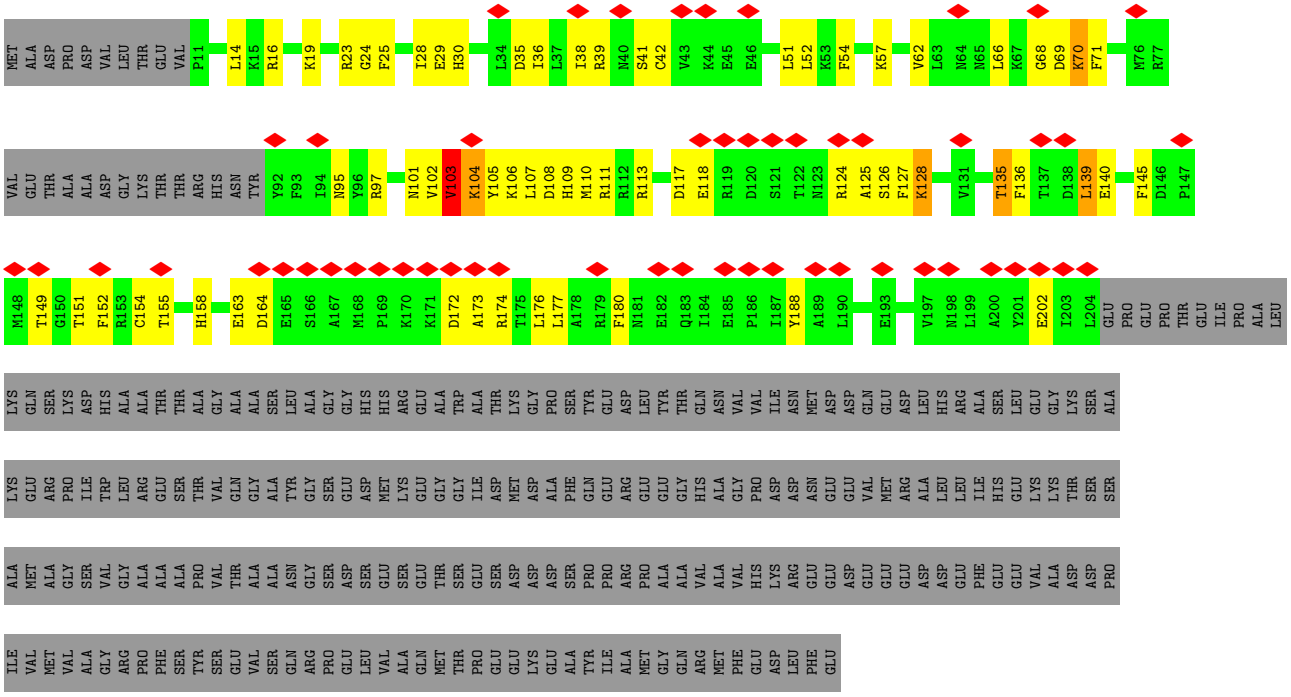




• Molecule 17: General transcription factor IIE subunit 1

Chain Q:

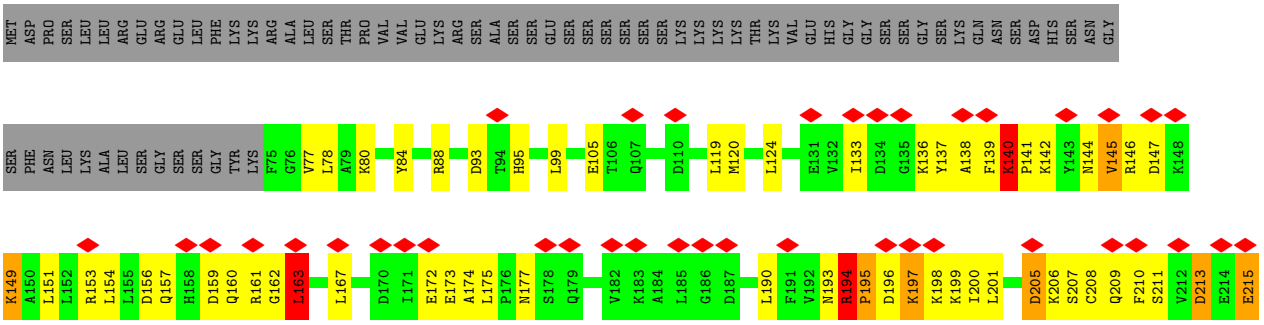


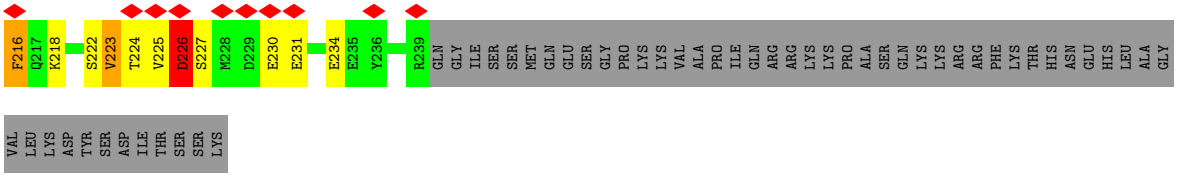


• Molecule 18: Transcription initiation factor IIE subunit beta

Chain R:



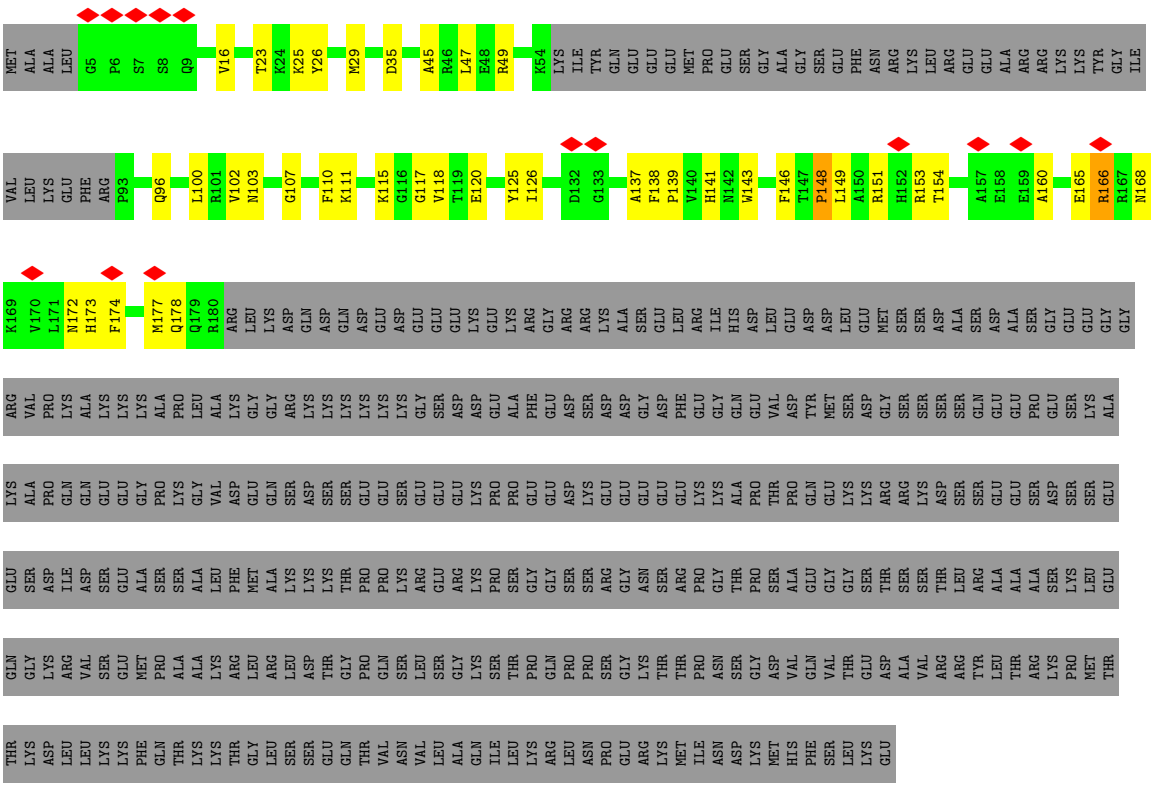




• Molecule 19: General transcription factor IIF subunit 1

Chain S:

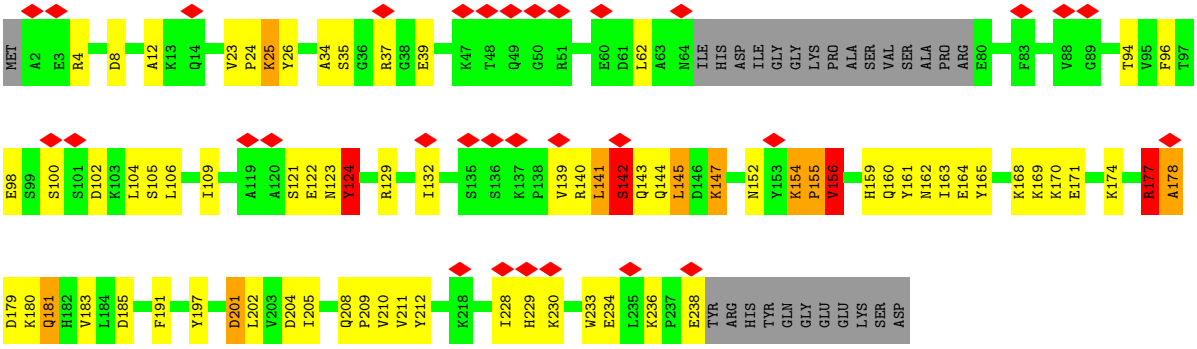




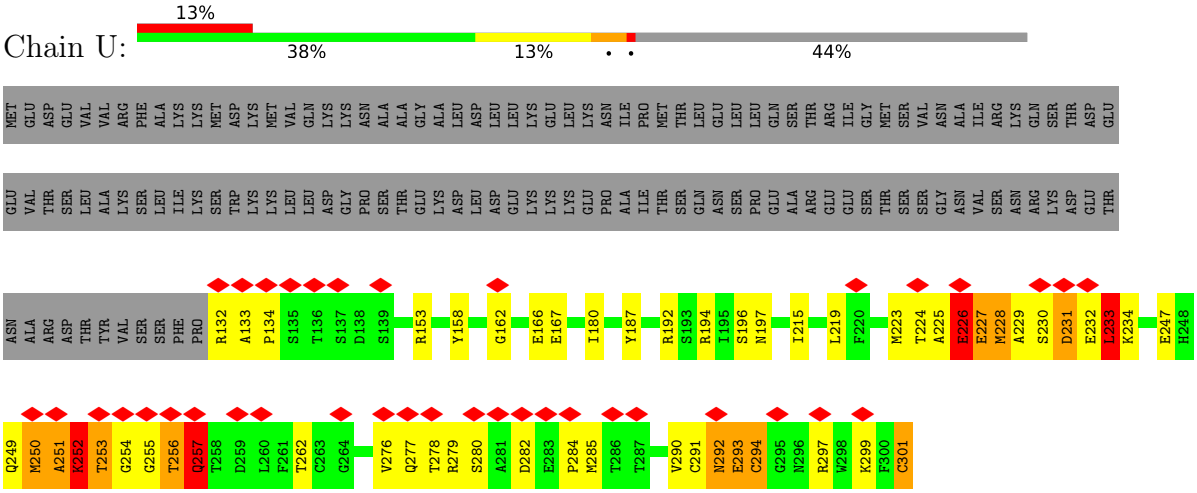
• Molecule 20: General transcription factor IIF subunit 2

Chain T:

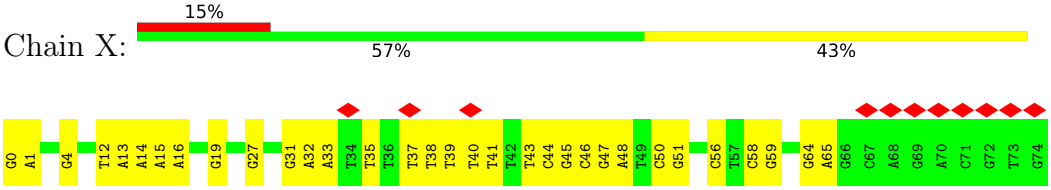




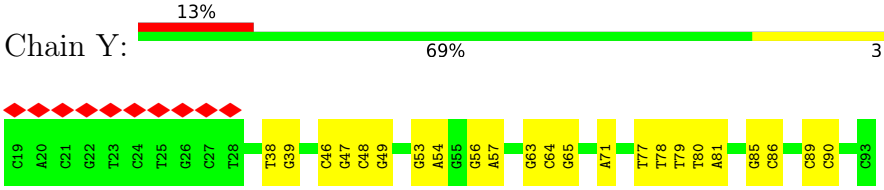
• Molecule 21: Transcription elongation factor A protein 1



• Molecule 22: SCP-X



• Molecule 23: SCP-Y



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	1/11727 (0.0%)	1.17	74/15833 (0.5%)
2	B	0.72	5/9503 (0.1%)	1.19	74/12831 (0.6%)
3	C	0.64	0/2259	1.15	19/3073 (0.6%)
4	D	0.34	0/1077	0.88	1/1446 (0.1%)
5	E	0.52	0/1753	1.12	9/2368 (0.4%)
6	F	0.57	0/700	1.02	4/946 (0.4%)
7	G	0.35	0/1382	0.95	9/1874 (0.5%)
8	H	0.44	0/1227	0.94	4/1654 (0.2%)
9	I	0.44	0/1038	1.28	15/1407 (1.1%)
10	J	0.69	0/542	1.27	3/730 (0.4%)
11	K	0.52	0/956	1.06	8/1294 (0.6%)
12	L	0.49	0/394	0.90	0/524
13	M	0.47	0/2429	1.15	20/3281 (0.6%)
14	N	0.34	0/945	0.94	5/1274 (0.4%)
15	O	0.32	0/816	0.81	0/1105
16	P	0.36	0/1489	0.98	1/2005 (0.0%)
17	Q	0.38	0/1507	1.01	3/2023 (0.1%)
18	R	0.50	0/1380	1.15	7/1854 (0.4%)
19	S	0.33	0/1167	0.80	0/1576
20	T	0.43	0/1817	1.09	14/2445 (0.6%)
21	U	0.45	0/1358	1.06	4/1820 (0.2%)
22	X	0.26	0/1746	0.45	0/2698
23	Y	0.25	0/1696	0.46	0/2612
All	All	0.56	6/48908 (0.0%)	1.08	274/66673 (0.4%)

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	B	0	1
5	E	0	1
8	H	0	1
14	N	0	4
18	R	0	2
19	S	0	1
20	T	0	1
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	947	ILE	CA-CB	-6.48	1.50	1.55
2	B	794	VAL	CA-CB	5.92	1.63	1.54
2	B	801	VAL	CA-CB	5.86	1.61	1.54
1	A	474	VAL	C-O	-5.74	1.15	1.23
2	B	811	TYR	CA-C	-5.05	1.46	1.52
2	B	1046	THR	CA-CB	5.04	1.62	1.53

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1115	LYS	N-CA-C	-20.67	81.74	111.30
13	M	91	ALA	N-CA-C	-16.01	90.67	112.12
9	I	84	HIS	C-N-CD	-14.71	64.71	125.00
9	I	61	GLU	N-CA-C	-13.73	89.02	109.62
16	P	206	GLU	C-N-CD	-13.18	70.96	125.00
1	A	205	VAL	N-CA-C	12.88	127.43	107.98
9	I	103	ARG	N-CA-C	-12.83	83.47	110.80
1	A	261	ARG	C-N-CD	-12.36	74.32	125.00
18	R	194	ARG	C-N-CD	-12.32	74.47	125.00
1	A	545	VAL	N-CA-C	12.22	123.08	110.62
21	U	251	ALA	N-CA-C	-11.39	98.95	111.36
3	C	137	ASN	N-CA-C	-11.38	98.88	111.28
5	E	64	HIS	CA-C-N	-11.13	102.07	120.87
5	E	64	HIS	C-N-CA	-11.13	102.07	120.87
13	M	39	LEU	N-CA-C	10.84	133.88	110.80
13	M	94	ASP	N-CA-C	-10.67	94.93	109.54
1	A	203	LYS	N-CA-C	10.23	126.10	107.99
2	B	249	LYS	N-CA-C	-9.78	89.97	110.80
13	M	87	GLY	N-CA-C	9.44	135.56	113.18
2	B	79	GLU	N-CA-C	9.32	130.65	110.80
1	A	269	SER	N-CA-C	-9.31	96.78	109.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	42	VAL	CA-C-N	-9.20	111.29	120.31
3	C	42	VAL	C-N-CA	-9.20	111.29	120.31
21	U	257	GLN	N-CA-C	9.12	130.22	110.80
2	B	79	GLU	CA-C-N	-9.11	110.36	122.56
2	B	79	GLU	C-N-CA	-9.11	110.36	122.56
1	A	49	GLY	N-CA-C	-9.07	91.68	113.18
2	B	897	ARG	N-CA-C	-9.03	97.75	111.56
9	I	58	ILE	N-CA-C	-8.96	99.50	112.04
21	U	256	THR	N-CA-C	-8.87	101.58	111.07
18	R	163	LEU	N-CA-C	-8.82	92.01	110.80
3	C	211	LEU	N-CA-C	-8.79	92.08	110.80
5	E	52	ARG	C-N-CD	-8.70	89.34	125.00
18	R	140	LYS	CA-C-N	-8.60	109.09	119.84
18	R	140	LYS	C-N-CA	-8.60	109.09	119.84
9	I	104	ALA	N-CA-C	-8.59	92.50	110.80
1	A	622	SER	N-CA-C	-8.53	90.97	109.81
20	T	181	GLN	N-CA-C	8.45	120.18	110.97
7	G	97	LEU	N-CA-C	8.35	122.52	108.90
2	B	62	ALA	CA-C-N	-8.20	111.94	120.38
2	B	62	ALA	C-N-CA	-8.20	111.94	120.38
13	M	121	ILE	N-CA-C	8.01	118.11	110.42
1	A	692	SER	N-CA-C	8.00	123.05	113.28
9	I	15	ARG	N-CA-C	-7.96	93.85	110.80
1	A	1314	THR	N-CA-C	-7.91	103.20	113.17
13	M	43	ASP	N-CA-C	-7.90	92.25	107.57
1	A	521	VAL	CB-CA-C	-7.83	106.05	114.35
10	J	63	ALA	CA-C-N	7.83	129.63	119.84
10	J	63	ALA	C-N-CA	7.83	129.63	119.84
9	I	84	HIS	CA-C-N	7.67	129.43	119.84
9	I	84	HIS	C-N-CA	7.67	129.43	119.84
20	T	177	ARG	N-CA-C	7.66	121.46	112.72
10	J	63	ALA	O-C-N	7.58	128.20	120.70
11	K	112	LYS	CA-C-N	-7.57	112.31	122.99
11	K	112	LYS	C-N-CA	-7.57	112.31	122.99
2	B	224	CYS	N-CA-C	7.46	119.72	108.46
4	D	127	LEU	N-CA-C	-7.39	103.22	111.28
1	A	204	HIS	N-CA-C	7.38	126.51	110.80
3	C	136	ASP	N-CA-C	7.36	120.47	108.55
2	B	288	ILE	N-CA-C	7.27	117.87	110.82
14	N	327	GLU	N-CA-C	-7.25	104.97	113.88
20	T	142	SER	N-CA-C	7.18	126.10	110.80
1	A	181	HIS	N-CA-C	-7.11	101.58	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	96	GLY	N-CA-C	7.07	122.54	111.08
2	B	58	ILE	N-CA-C	7.01	117.77	110.62
1	A	264	VAL	N-CA-C	6.98	123.86	109.34
5	E	126	ILE	N-CA-C	6.97	119.58	108.85
9	I	120	GLY	N-CA-C	-6.97	106.20	115.40
1	A	621	ILE	N-CA-C	6.96	123.83	109.34
13	M	38	GLY	N-CA-C	-6.96	96.68	113.18
1	A	910	LYS	CA-C-N	6.94	128.52	119.84
1	A	910	LYS	C-N-CA	6.94	128.52	119.84
14	N	319	ASP	N-CA-C	6.92	121.09	112.24
13	M	37	CYS	CA-C-N	-6.91	107.86	121.41
13	M	37	CYS	C-N-CA	-6.91	107.86	121.41
2	B	802	ASP	N-CA-C	6.85	118.75	111.28
20	T	211	VAL	N-CA-C	6.82	117.58	110.62
2	B	487	SER	CA-C-N	6.81	126.73	119.85
2	B	487	SER	C-N-CA	6.81	126.73	119.85
14	N	356	GLY	N-CA-C	6.81	129.33	113.18
1	A	614	ASP	N-CA-C	6.81	125.30	110.80
1	A	152	ASN	N-CA-C	6.79	119.54	107.80
9	I	84	HIS	N-CA-C	6.78	124.80	109.81
5	E	54	ARG	N-CA-C	-6.76	96.41	110.80
2	B	882	SER	N-CA-C	-6.73	103.56	112.72
2	B	879	GLU	N-CA-C	6.73	125.13	110.80
7	G	46	ILE	N-CA-C	6.72	117.51	110.72
1	A	1304	ILE	N-CA-C	-6.72	106.58	113.10
2	B	878	ASP	O-C-N	6.68	129.74	122.05
11	K	41	THR	N-CA-C	6.68	118.21	111.07
2	B	163	LEU	N-CA-C	6.66	121.00	112.34
2	B	598	VAL	N-CA-C	6.64	117.34	110.36
7	G	124	ASN	CA-C-N	-6.58	113.61	120.38
7	G	124	ASN	C-N-CA	-6.58	113.61	120.38
2	B	1076	GLU	N-CA-C	6.57	118.44	111.28
1	A	771	VAL	N-CA-C	6.56	117.31	110.62
13	M	93	PHE	N-CA-C	6.55	124.76	110.80
2	B	424	ASP	N-CA-C	-6.53	104.08	111.07
20	T	25	LYS	N-CA-C	6.51	118.38	111.28
2	B	408	PHE	N-CA-C	6.50	118.44	111.36
1	A	932	ARG	CA-C-N	-6.45	109.95	120.72
1	A	932	ARG	C-N-CA	-6.45	109.95	120.72
1	A	211	GLU	N-CA-C	-6.42	97.12	110.80
1	A	645	LEU	N-CA-C	6.40	120.92	113.18
1	A	622	SER	C-N-CD	-6.39	98.78	125.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	SER	N-CA-C	6.36	124.35	110.80
8	H	85	ALA	N-CA-C	-6.35	97.27	110.80
1	A	225	PHE	N-CA-C	6.29	118.14	111.28
2	B	978	ILE	N-CA-C	-6.28	103.49	112.35
13	M	51	GLU	N-CA-C	6.25	118.09	111.28
1	A	614	ASP	CA-C-N	-6.23	109.65	121.54
1	A	614	ASP	C-N-CA	-6.23	109.65	121.54
3	C	225	LYS	CA-C-N	-6.23	113.53	119.76
3	C	225	LYS	C-N-CA	-6.23	113.53	119.76
13	M	89	GLY	N-CA-C	-6.22	98.44	113.18
2	B	95	LYS	CA-C-N	6.14	126.50	119.93
2	B	95	LYS	C-N-CA	6.14	126.50	119.93
1	A	540	ASP	N-CA-C	6.13	117.97	111.28
11	K	82	SER	CA-C-N	6.12	125.80	119.56
11	K	82	SER	C-N-CA	6.12	125.80	119.56
1	A	213	LYS	N-CA-C	-6.10	97.80	110.80
1	A	48	GLU	N-CA-C	6.09	123.78	110.80
3	C	117	SER	N-CA-C	6.07	118.68	111.71
2	B	871	VAL	N-CA-C	6.05	115.07	106.53
3	C	199	LYS	CA-C-N	6.05	125.73	119.56
3	C	199	LYS	C-N-CA	6.05	125.73	119.56
8	H	113	SER	N-CA-C	6.04	118.36	108.52
17	Q	173	ALA	N-CA-C	6.02	117.64	111.14
5	E	132	GLN	N-CA-C	6.01	118.60	111.33
2	B	156	LEU	N-CA-C	6.00	119.05	110.10
9	I	73	SER	N-CA-C	5.99	120.12	112.34
1	A	1425	GLY	CA-C-N	5.98	125.69	119.05
1	A	1425	GLY	C-N-CA	5.98	125.69	119.05
13	M	42	GLY	N-CA-C	5.96	127.30	113.18
18	R	226	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	1035	GLU	N-CA-C	5.93	117.83	111.36
2	B	76	GLY	N-CA-C	5.93	127.23	113.18
9	I	85	PRO	N-CA-C	5.92	124.67	112.47
3	C	1	MET	CA-C-N	5.88	127.20	119.84
3	C	1	MET	C-N-CA	5.88	127.20	119.84
2	B	719	SER	CA-C-N	-5.87	113.57	119.56
2	B	719	SER	C-N-CA	-5.87	113.57	119.56
1	A	728	THR	CA-C-N	5.86	127.17	119.84
1	A	728	THR	C-N-CA	5.86	127.17	119.84
2	B	503	ASN	N-CA-C	5.85	118.44	111.71
1	A	476	ILE	N-CA-C	5.84	117.19	108.54
2	B	399	LEU	N-CA-C	5.83	117.31	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	145	VAL	N-CA-C	-5.83	107.61	113.20
6	F	126	THR	N-CA-C	-5.82	107.42	114.75
1	A	636	ILE	N-CA-C	5.81	116.46	110.82
17	Q	68	GLY	N-CA-C	5.79	120.18	112.77
1	A	785	ILE	N-CA-C	5.78	116.83	111.45
2	B	37	LYS	N-CA-C	-5.78	102.91	110.53
2	B	497	LYS	CA-C-N	-5.77	110.95	120.88
2	B	497	LYS	C-N-CA	-5.77	110.95	120.88
14	N	324	GLU	N-CA-C	5.76	120.38	111.56
21	U	252	LYS	N-CA-C	-5.74	98.57	110.80
2	B	759	VAL	CB-CA-C	-5.71	103.31	111.31
2	B	1065	GLY	CA-C-N	5.71	125.66	119.78
2	B	1065	GLY	C-N-CA	5.71	125.66	119.78
13	M	34	CYS	CA-C-N	5.70	125.82	119.32
13	M	34	CYS	C-N-CA	5.70	125.82	119.32
2	B	44	LEU	N-CA-C	5.69	117.28	111.14
2	B	77	GLU	N-CA-C	5.63	122.80	110.80
18	R	223	VAL	N-CA-C	5.63	121.06	109.34
9	I	14	ILE	N-CA-C	5.63	117.10	108.71
1	A	525	ILE	N-CA-C	5.59	115.78	110.53
1	A	890	ARG	N-CA-C	-5.57	100.24	108.99
1	A	1443	ALA	N-CA-C	5.57	117.03	111.07
1	A	256	PRO	CA-C-N	5.56	125.56	119.89
1	A	256	PRO	C-N-CA	5.56	125.56	119.89
7	G	107	PHE	N-CA-C	5.56	118.02	109.07
2	B	1024	GLY	N-CA-C	5.55	121.47	114.25
20	T	234	GLU	CG-CD-OE2	-5.55	105.64	118.40
1	A	418	TYR	N-CA-C	5.54	117.60	109.24
2	B	711	ILE	CA-C-N	5.54	126.01	120.14
2	B	711	ILE	C-N-CA	5.54	126.01	120.14
2	B	962	THR	CA-C-N	5.54	125.54	119.89
2	B	962	THR	C-N-CA	5.54	125.54	119.89
1	A	1376	LYS	N-CA-C	5.53	117.11	111.14
1	A	75	ALA	CB-CA-C	-5.53	110.18	116.54
11	K	110	LYS	O-C-N	5.49	127.72	122.07
20	T	142	SER	CA-C-N	-5.48	111.17	121.81
20	T	142	SER	C-N-CA	-5.48	111.17	121.81
20	T	234	GLU	CA-C-O	-5.47	114.71	121.11
13	M	90	ALA	N-CA-C	5.47	122.44	110.80
2	B	878	ASP	CA-C-N	5.46	131.97	121.54
2	B	878	ASP	C-N-CA	5.46	131.97	121.54
1	A	464	LEU	N-CA-C	5.45	117.30	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	753	TYR	CA-C-N	-5.45	114.01	120.11
2	B	753	TYR	C-N-CA	-5.45	114.01	120.11
17	Q	66	LEU	N-CA-C	5.43	117.20	111.28
2	B	983	GLU	CA-C-N	5.42	127.49	120.44
2	B	983	GLU	C-N-CA	5.42	127.49	120.44
9	I	35	LEU	N-CA-C	-5.41	102.47	110.48
1	A	539	GLN	CB-CA-C	-5.41	110.32	116.54
1	A	540	ASP	CB-CA-C	-5.41	101.81	110.79
2	B	1163	MET	N-CA-C	-5.41	105.55	111.82
6	F	84	GLU	CB-CA-C	-5.41	110.32	116.54
1	A	898	GLY	N-CA-C	5.40	120.61	114.67
1	A	620	HIS	N-CA-C	5.39	121.75	113.28
1	A	1405	MET	N-CA-C	5.37	118.05	111.82
2	B	953	ASP	N-CA-C	5.36	117.21	111.36
1	A	480	SER	N-CA-C	5.36	122.22	110.80
20	T	124	TYR	N-CA-C	5.36	122.22	110.80
20	T	233	TRP	N-CA-C	5.36	118.32	109.85
1	A	1386	ILE	N-CA-C	5.35	116.07	110.62
1	A	624	GLY	N-CA-C	5.34	125.84	113.18
1	A	683	GLU	N-CA-C	5.34	116.91	111.14
1	A	322	LEU	CA-C-N	5.32	126.49	119.84
1	A	322	LEU	C-N-CA	5.32	126.49	119.84
8	H	108	ALA	CB-CA-C	-5.31	110.43	116.54
1	A	565	MET	N-CA-C	5.30	117.06	111.28
3	C	260	GLN	CB-CA-C	-5.30	101.83	110.85
1	A	136	GLN	CA-C-N	5.30	125.11	119.28
1	A	136	GLN	C-N-CA	5.30	125.11	119.28
5	E	200	ALA	N-CA-C	-5.30	105.58	111.36
2	B	590	LEU	N-CA-C	5.29	117.13	111.36
7	G	14	HIS	CA-C-N	5.29	126.46	119.84
7	G	14	HIS	C-N-CA	5.29	126.46	119.84
3	C	221	ASP	CA-C-N	5.29	125.75	120.04
3	C	221	ASP	C-N-CA	5.29	125.75	120.04
3	C	267	ILE	N-CA-C	-5.28	107.58	112.43
13	M	15	CYS	CA-C-N	5.28	124.46	118.97
13	M	15	CYS	C-N-CA	5.28	124.46	118.97
2	B	986	GLN	CA-C-N	5.26	125.79	120.00
2	B	986	GLN	C-N-CA	5.26	125.79	120.00
3	C	240	ARG	CA-C-N	5.25	124.70	119.24
3	C	240	ARG	C-N-CA	5.25	124.70	119.24
2	B	162	LEU	N-CA-C	5.24	118.45	111.75
9	I	98	GLN	N-CA-C	5.24	117.44	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	69	THR	N-CA-C	-5.22	106.59	113.17
1	A	1470	CYS	N-CA-C	5.20	118.89	112.54
5	E	64	HIS	N-CA-C	5.20	121.88	110.80
3	C	61	ASP	N-CA-C	5.20	116.64	111.07
6	F	54	THR	CA-C-N	5.20	125.27	119.87
6	F	54	THR	C-N-CA	5.20	125.27	119.87
7	G	108	ILE	N-CA-C	5.19	115.05	107.37
1	A	220	ARG	N-CA-C	-5.17	105.55	111.14
1	A	1192	TRP	N-CA-CB	5.17	118.19	110.22
20	T	210	VAL	N-CA-C	5.17	116.64	111.00
11	K	9	SER	N-CA-C	5.16	119.07	112.87
2	B	855	ALA	CA-C-N	5.14	125.43	119.93
2	B	855	ALA	C-N-CA	5.14	125.43	119.93
2	B	972	ILE	N-CA-C	5.14	119.99	108.88
2	B	984	CYS	N-CA-C	5.14	116.57	111.07
1	A	1192	TRP	CA-CB-CG	5.12	123.34	113.60
1	A	13	CYS	CA-C-N	5.12	125.09	120.03
1	A	13	CYS	C-N-CA	5.12	125.09	120.03
2	B	106	SER	N-CA-C	5.12	114.18	108.25
8	H	83	SER	N-CA-C	-5.11	105.77	112.72
2	B	1044	GLY	CA-C-N	-5.11	114.72	120.14
2	B	1044	GLY	C-N-CA	-5.11	114.72	120.14
2	B	294	ASP	CA-C-N	5.10	124.89	119.28
2	B	294	ASP	C-N-CA	5.10	124.89	119.28
2	B	646	ARG	N-CA-C	5.10	118.60	112.38
13	M	273	GLU	N-CA-C	5.09	116.52	111.07
2	B	223	SER	N-CA-C	5.09	116.81	108.52
2	B	1072	ARG	N-CA-C	5.07	118.44	111.54
14	N	346	LYS	CB-CA-C	-5.07	110.75	116.63
2	B	1112	ASP	CA-C-N	-5.07	113.50	119.84
2	B	1112	ASP	C-N-CA	-5.07	113.50	119.84
2	B	1160	GLN	N-CA-C	5.06	116.87	111.36
2	B	643	LEU	N-CA-C	5.05	116.79	111.28
20	T	178	ALA	N-CA-C	-5.03	100.08	110.80
11	K	21	ILE	N-CA-C	5.03	115.09	107.80
1	A	669	TYR	N-CA-C	5.02	116.44	111.07
1	A	770	VAL	N-CA-C	5.02	115.25	110.53
2	B	704	LEU	N-CA-C	5.02	117.79	109.46
20	T	234	GLU	CG-CD-OE1	5.01	129.93	118.40
1	A	368	THR	CA-C-N	-5.01	114.83	120.14
1	A	368	THR	C-N-CA	-5.01	114.83	120.14
2	B	164	ASN	N-CA-C	5.01	117.47	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	218	PHE	N-CA-C	5.00	116.54	111.14

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	234	THR	Peptide
5	E	126	ILE	Peptide
8	H	111	ARG	Peptide
14	N	324	GLU	Peptide
14	N	355	ASP	Peptide
14	N	360	LEU	Mainchain
14	N	371	ILE	Peptide
18	R	146	ARG	Peptide
18	R	213	ASP	Sidechain
19	S	148	PRO	Peptide
20	T	123	ASN	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	11515	0	11606	544	0
2	B	9317	0	9306	396	0
3	C	2213	0	2153	70	0
4	D	1062	0	1042	10	0
5	E	1723	0	1745	67	0
6	F	689	0	715	18	0
7	G	1351	0	1358	33	0
8	H	1205	0	1168	62	0
9	I	1013	0	932	80	0
10	J	533	0	553	49	0
11	K	937	0	959	26	0
12	L	388	0	393	16	0
13	M	2391	0	2408	127	0
14	N	930	0	888	33	0
15	O	806	0	818	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1462	0	1549	64	0
17	Q	1484	0	1496	170	0
18	R	1357	0	1380	176	0
19	S	1138	0	1103	26	0
20	T	1788	0	1819	92	0
21	U	1343	0	1338	64	0
22	X	1553	0	843	32	0
23	Y	1517	0	843	26	0
24	A	1	0	0	0	0
24	U	1	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	47728	0	46415	1826	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1826) 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)
17:Q:14:LEU:CD1	17:Q:102:VAL:HG23	1.29	1.58
17:Q:180:PHE:CZ	18:R:211:SER:CB	1.91	1.52
17:Q:180:PHE:CZ	18:R:211:SER:HB2	1.39	1.52
8:H:65:TYR:CE2	8:H:70:LEU:HB3	1.02	1.51
17:Q:14:LEU:HD11	17:Q:102:VAL:CG2	1.47	1.45
10:J:62:TYR:C	10:J:64:PRO:HD2	1.36	1.44
2:B:92:TYR:CG	20:T:145:LEU:HD13	1.51	1.43
17:Q:109:HIS:CE1	18:R:224:THR:HG21	1.51	1.43
17:Q:14:LEU:CD1	17:Q:102:VAL:CG2	1.98	1.42
8:H:65:TYR:CE2	8:H:70:LEU:CB	1.99	1.41
1:A:927:GLU:HB3	1:A:931:ARG:CG	1.48	1.39
1:A:1319:LYS:HG2	1:A:1333:GLU:CD	1.48	1.39
17:Q:105:TYR:CE1	18:R:231:GLU:CD	2.02	1.38
8:H:65:TYR:HE2	8:H:70:LEU:CB	1.33	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:180:PHE:HZ	18:R:211:SER:CB	1.27	1.37
13:M:10:LEU:O	13:M:12:ARG:N	1.57	1.36
17:Q:23:ARG:CZ	18:R:209:GLN:N	1.88	1.36
13:M:47:ASP:O	13:M:49:GLY:N	1.56	1.35
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.52	1.34
1:A:1250:ASP:HB3	21:U:227:GLU:CD	1.22	1.34
9:I:103:ARG:O	9:I:105:GLU:N	1.61	1.33
1:A:1319:LYS:CG	1:A:1333:GLU:CD	2.01	1.33
17:Q:105:TYR:CE1	17:Q:109:HIS:NE2	1.95	1.33
1:A:152:ASN:O	1:A:153:ILE:CG1	1.75	1.33
1:A:197:GLU:OE2	13:M:93:PHE:CE2	1.82	1.31
17:Q:180:PHE:CE2	18:R:211:SER:HB2	1.67	1.30
5:E:27:LEU:H	5:E:64:HIS:CB	1.42	1.29
17:Q:23:ARG:CD	18:R:207:SER:O	1.79	1.29
1:A:199:TYR:CE1	13:M:93:PHE:HZ	1.50	1.28
1:A:199:TYR:CZ	13:M:93:PHE:HZ	1.52	1.28
18:R:196:ASP:O	18:R:198:LYS:N	1.66	1.28
17:Q:23:ARG:NH2	18:R:209:GLN:H	1.30	1.27
1:A:199:TYR:OH	13:M:93:PHE:CZ	1.86	1.27
5:E:47:LYS:HB2	5:E:48:PRO:CD	1.62	1.26
1:A:262:PRO:HG2	1:A:274:ASP:CG	1.59	1.26
17:Q:113:ARG:NH2	18:R:218:LYS:HE2	1.52	1.23
16:P:206:GLU:CG	16:P:236:LYS:HZ2	1.52	1.23
2:B:92:TYR:CD2	20:T:145:LEU:HD13	1.74	1.23
17:Q:113:ARG:HH22	18:R:218:LYS:CE	1.53	1.22
1:A:1319:LYS:HD3	1:A:1333:GLU:OE2	1.33	1.21
17:Q:23:ARG:NE	18:R:207:SER:O	1.72	1.21
17:Q:105:TYR:HE1	18:R:231:GLU:CG	1.51	1.21
1:A:1310:HIS:O	21:U:252:LYS:HG2	1.38	1.20
8:H:65:TYR:CZ	8:H:70:LEU:HB3	1.75	1.20
5:E:27:LEU:N	5:E:64:HIS:HB3	1.27	1.19
9:I:14:ILE:HG13	9:I:16:PHE:CE2	1.77	1.19
18:R:215:GLU:O	18:R:216:PHE:HB2	1.37	1.19
1:A:152:ASN:C	1:A:153:ILE:HG12	1.67	1.18
9:I:103:ARG:O	9:I:105:GLU:HG2	1.39	1.18
17:Q:109:HIS:CE1	18:R:224:THR:CG2	2.26	1.18
17:Q:109:HIS:ND1	18:R:224:THR:CG2	2.05	1.18
18:R:190:LEU:CD1	18:R:205:ASP:OD2	1.91	1.18
13:M:10:LEU:HD11	13:M:14:THR:HB	1.26	1.17
1:A:271:ARG:O	1:A:272:ASN:HB3	1.40	1.17
2:B:51:ILE:HG22	20:T:141:LEU:HD11	1.20	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:63:ALA:N	10:J:64:PRO:CD	2.06	1.16
1:A:202:TRP:CE3	1:A:212:LYS:HB3	1.80	1.16
1:A:157:GLY:N	1:A:181:HIS:NE2	1.93	1.15
16:P:206:GLU:HG3	16:P:236:LYS:NZ	1.60	1.15
13:M:178:LYS:O	20:T:154:LYS:HB3	1.46	1.15
1:A:1319:LYS:CD	1:A:1333:GLU:OE2	1.93	1.14
2:B:491:ARG:O	2:B:492:ASP:HB2	1.44	1.14
1:A:927:GLU:CB	1:A:931:ARG:HG2	1.77	1.14
10:J:62:TYR:C	10:J:64:PRO:CD	2.21	1.13
17:Q:23:ARG:HH12	18:R:209:GLN:HB2	1.01	1.13
1:A:1319:LYS:HG2	1:A:1333:GLU:CG	1.78	1.12
17:Q:180:PHE:CE2	18:R:211:SER:CB	2.26	1.12
17:Q:29:GLU:OE2	18:R:194:ARG:NH2	1.81	1.11
2:B:51:ILE:CG2	20:T:141:LEU:HD11	1.77	1.11
1:A:931:ARG:O	1:A:932:ARG:HB2	1.51	1.11
9:I:14:ILE:HG13	9:I:16:PHE:CZ	1.85	1.11
1:A:199:TYR:CZ	13:M:93:PHE:CZ	2.33	1.11
5:E:52:ARG:CB	5:E:53:PRO:HD2	1.75	1.11
1:A:1250:ASP:CB	21:U:227:GLU:CD	2.13	1.10
2:B:132:VAL:HB	2:B:141:GLN:CG	1.71	1.10
2:B:225:LEU:HB2	2:B:228:SER:HB3	1.11	1.10
17:Q:14:LEU:HD12	17:Q:102:VAL:CG2	1.79	1.10
1:A:199:TYR:CE1	13:M:93:PHE:CZ	2.39	1.10
17:Q:101:ASN:O	17:Q:102:VAL:HG12	1.52	1.10
1:A:927:GLU:HB3	1:A:931:ARG:HG2	1.24	1.10
9:I:103:ARG:O	9:I:105:GLU:CG	1.98	1.10
1:A:927:GLU:HB3	1:A:931:ARG:CD	1.83	1.09
17:Q:180:PHE:CZ	18:R:211:SER:HB3	1.84	1.09
1:A:202:TRP:CE3	1:A:212:LYS:CB	2.34	1.09
2:B:879:GLU:O	2:B:880:LEU:HB2	1.35	1.08
1:A:133:SER:OG	1:A:136:GLN:HB3	1.52	1.08
3:C:136:ASP:OD2	3:C:138:ASP:HB2	1.53	1.08
2:B:882:SER:O	2:B:887:TYR:CD1	2.06	1.08
17:Q:23:ARG:HD3	18:R:207:SER:O	1.43	1.08
1:A:1310:HIS:O	21:U:252:LYS:CG	2.02	1.07
1:A:611:ASP:OD2	1:A:627:LYS:HE3	1.51	1.07
17:Q:108:ASP:O	18:R:234:GLU:OE2	1.72	1.07
13:M:10:LEU:CD1	13:M:14:THR:HB	1.64	1.07
17:Q:105:TYR:CE1	18:R:231:GLU:CG	2.34	1.07
1:A:132:LYS:O	1:A:133:SER:HB2	1.25	1.06
17:Q:180:PHE:HZ	18:R:211:SER:CA	1.68	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LEU:HB2	2:B:228:SER:CB	1.85	1.06
1:A:197:GLU:OE2	13:M:93:PHE:CZ	2.08	1.06
1:A:152:ASN:O	1:A:153:ILE:HG12	0.89	1.05
21:U:230:SER:O	21:U:231:ASP:HB2	1.50	1.05
5:E:49:SER:O	5:E:54:ARG:NH1	1.89	1.05
1:A:205:VAL:O	1:A:206:ASN:HB2	1.54	1.05
2:B:880:LEU:O	2:B:881:GLU:HB2	1.26	1.04
21:U:226:GLU:O	21:U:227:GLU:HB2	1.57	1.04
2:B:92:TYR:HB3	20:T:145:LEU:HB2	1.38	1.04
9:I:103:ARG:C	9:I:105:GLU:N	2.01	1.04
1:A:927:GLU:CB	1:A:931:ARG:CG	2.34	1.03
13:M:94:ASP:OD1	13:M:99:SER:C	2.02	1.03
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.10	1.03
9:I:103:ARG:O	9:I:104:ALA:C	2.00	1.03
2:B:51:ILE:HG22	20:T:141:LEU:CD1	1.87	1.03
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.07	1.03
2:B:225:LEU:CB	2:B:228:SER:CB	2.37	1.03
1:A:132:LYS:O	1:A:133:SER:CB	2.05	1.02
1:A:265:VAL:O	1:A:272:ASN:OD1	1.77	1.02
1:A:202:TRP:CZ3	1:A:212:LYS:CG	2.42	1.02
2:B:78:VAL:O	2:B:79:GLU:CB	2.03	1.02
2:B:52:GLN:HA	20:T:141:LEU:HD13	1.39	1.02
2:B:132:VAL:HB	2:B:141:GLN:HG3	1.06	1.02
2:B:225:LEU:CB	2:B:228:SER:HB3	1.89	1.01
10:J:64:PRO:C	10:J:66:GLU:H	1.66	1.01
16:P:297:LYS:CB	16:P:298:PRO:CD	2.36	1.01
9:I:103:ARG:O	9:I:105:GLU:CA	2.09	1.01
1:A:1319:LYS:CG	1:A:1333:GLU:OE2	2.08	1.00
9:I:105:GLU:O	9:I:106:ASP:HB2	1.60	1.00
17:Q:23:ARG:CZ	18:R:208:CYS:C	2.34	1.00
2:B:1066:PRO:HB3	13:M:46:ILE:HD13	1.39	1.00
17:Q:23:ARG:NH1	18:R:209:GLN:HB2	1.76	1.00
5:E:47:LYS:CB	5:E:48:PRO:HD2	1.91	0.99
5:E:27:LEU:N	5:E:64:HIS:CB	2.06	0.99
9:I:103:ARG:O	9:I:105:GLU:CB	2.10	0.99
1:A:199:TYR:OH	13:M:93:PHE:CE2	2.05	0.99
2:B:92:TYR:CG	20:T:145:LEU:CD1	2.44	0.99
5:E:52:ARG:CB	5:E:53:PRO:CD	2.40	0.99
20:T:154:LYS:HD2	20:T:154:LYS:H	1.28	0.99
16:P:206:GLU:HG3	16:P:236:LYS:HZ2	0.83	0.99
5:E:47:LYS:HB2	5:E:48:PRO:HD2	1.00	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:GLU:O	8:H:67:ASP:HB2	1.62	0.98
1:A:262:PRO:HG2	1:A:274:ASP:OD1	1.63	0.97
2:B:78:VAL:O	2:B:79:GLU:HB2	1.16	0.97
1:A:265:VAL:O	1:A:272:ASN:CG	2.07	0.97
5:E:47:LYS:CB	5:E:48:PRO:CD	2.42	0.97
17:Q:109:HIS:ND1	18:R:224:THR:HG23	1.77	0.97
17:Q:113:ARG:HH22	18:R:218:LYS:HE2	1.15	0.96
17:Q:14:LEU:HD12	17:Q:102:VAL:HG21	1.44	0.96
17:Q:105:TYR:O	17:Q:109:HIS:CD2	2.19	0.96
1:A:495:ASP:O	1:A:497:ASP:N	1.98	0.96
18:R:195:PRO:CB	18:R:199:LYS:HD2	1.96	0.96
18:R:225:VAL:HB	18:R:230:GLU:HG3	1.46	0.95
1:A:1319:LYS:HG2	1:A:1333:GLU:OE2	1.64	0.95
18:R:215:GLU:O	18:R:216:PHE:CB	2.10	0.95
20:T:177:ARG:C	20:T:179:ASP:H	1.74	0.95
2:B:74:ALA:HB2	20:T:201:ASP:HB3	1.47	0.95
17:Q:101:ASN:O	17:Q:102:VAL:CG1	2.13	0.95
21:U:231:ASP:O	21:U:232:GLU:CG	2.14	0.95
13:M:94:ASP:OD1	13:M:99:SER:O	1.85	0.95
15:O:3:TYR:O	15:O:5:LEU:N	2.01	0.94
2:B:225:LEU:HB3	2:B:228:SER:HB2	1.48	0.94
1:A:157:GLY:N	1:A:181:HIS:CD2	2.34	0.94
1:A:265:VAL:O	1:A:272:ASN:ND2	2.01	0.94
10:J:63:ALA:N	10:J:64:PRO:HD2	1.74	0.94
10:J:63:ALA:N	10:J:64:PRO:HD3	1.79	0.94
18:R:190:LEU:HD11	18:R:205:ASP:OD2	1.65	0.94
16:P:162:VAL:O	16:P:164:GLN:NE2	2.01	0.93
5:E:52:ARG:HB3	5:E:53:PRO:CD	1.94	0.93
1:A:1319:LYS:CD	1:A:1356:ARG:HH12	1.80	0.93
17:Q:105:TYR:CD1	18:R:231:GLU:OE2	2.21	0.93
2:B:92:TYR:HB3	20:T:145:LEU:CB	1.97	0.93
17:Q:23:ARG:HH12	18:R:209:GLN:CB	1.80	0.93
16:P:297:LYS:HE2	16:P:297:LYS:HA	1.48	0.93
2:B:132:VAL:CB	2:B:141:GLN:HG3	1.97	0.92
16:P:297:LYS:HA	16:P:297:LYS:CE	1.97	0.92
17:Q:113:ARG:HH22	18:R:218:LYS:HE3	1.34	0.92
1:A:927:GLU:HB3	1:A:931:ARG:CB	2.00	0.92
1:A:927:GLU:CB	1:A:931:ARG:HD3	1.98	0.92
2:B:490:GLY:O	2:B:491:ARG:HB2	1.66	0.92
17:Q:23:ARG:NH2	18:R:209:GLN:N	2.03	0.92
5:E:52:ARG:O	5:E:53:PRO:O	1.87	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:TRP:HE3	1:A:212:LYS:HB3	1.25	0.92
13:M:10:LEU:HD11	13:M:14:THR:CB	1.99	0.92
18:R:196:ASP:C	18:R:198:LYS:H	1.78	0.92
17:Q:105:TYR:CD1	18:R:231:GLU:CD	2.46	0.91
21:U:230:SER:O	21:U:231:ASP:CB	2.18	0.91
13:M:10:LEU:C	13:M:12:ARG:N	2.19	0.91
2:B:92:TYR:CD2	20:T:145:LEU:CD1	2.54	0.91
16:P:206:GLU:CG	16:P:236:LYS:NZ	2.26	0.91
17:Q:23:ARG:CZ	18:R:209:GLN:H	1.66	0.91
1:A:931:ARG:O	1:A:932:ARG:CB	2.18	0.90
1:A:210:GLN:OE1	1:A:212:LYS:HD3	1.70	0.90
13:M:94:ASP:HB3	13:M:97:GLY:O	1.71	0.90
1:A:1250:ASP:HB3	21:U:227:GLU:OE2	1.70	0.90
1:A:197:GLU:OE2	13:M:93:PHE:CD2	2.25	0.90
2:B:721:ARG:HG3	2:B:977:THR:HG22	1.52	0.89
2:B:254:GLN:HG3	2:B:303:PRO:HG2	1.51	0.89
2:B:880:LEU:O	2:B:881:GLU:CB	2.13	0.89
1:A:261:ARG:O	1:A:263:ALA:N	2.06	0.89
2:B:52:GLN:HA	20:T:141:LEU:CD1	2.01	0.89
1:A:1319:LYS:HG2	1:A:1333:GLU:HG2	1.52	0.89
5:E:48:PRO:O	5:E:49:SER:HB2	1.73	0.89
13:M:179:GLU:HA	20:T:154:LYS:HG2	1.55	0.89
1:A:203:LYS:O	1:A:204:HIS:HB2	1.71	0.88
2:B:491:ARG:O	2:B:492:ASP:CB	2.20	0.88
1:A:608:THR:C	1:A:610:PRO:HD2	1.98	0.88
1:A:212:LYS:HA	1:A:212:LYS:CE	2.02	0.87
20:T:177:ARG:NH1	20:T:209:PRO:O	2.07	0.87
17:Q:54:PHE:CD2	18:R:194:ARG:HD2	2.09	0.87
2:B:225:LEU:CB	2:B:228:SER:HB2	2.02	0.87
9:I:85:PRO:O	9:I:86:CYS:C	2.11	0.87
9:I:105:GLU:O	9:I:106:ASP:CB	2.22	0.86
17:Q:105:TYR:HE1	18:R:231:GLU:HG3	1.40	0.86
17:Q:113:ARG:NH2	18:R:218:LYS:CE	2.23	0.86
15:O:3:TYR:C	15:O:5:LEU:H	1.83	0.86
9:I:15:ARG:O	9:I:16:PHE:O	1.94	0.86
17:Q:24:GLY:CA	18:R:210:PHE:CE2	2.58	0.86
1:A:355:MET:SD	2:B:1091:ARG:NH1	2.48	0.86
1:A:202:TRP:CZ3	1:A:212:LYS:HB3	2.10	0.86
2:B:751:LEU:HD12	2:B:808:SER:HB3	1.56	0.86
13:M:11:PRO:O	13:M:12:ARG:HB3	1.73	0.86
1:A:271:ARG:O	1:A:272:ASN:CB	2.19	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1066:PRO:CB	13:M:46:ILE:HD13	2.05	0.85
10:J:62:TYR:O	10:J:64:PRO:HD2	1.74	0.85
18:R:225:VAL:CB	18:R:230:GLU:HG3	2.06	0.85
13:M:37:CYS:SG	13:M:39:LEU:HD22	2.17	0.85
1:A:210:GLN:NE2	1:A:212:LYS:HG2	1.91	0.85
17:Q:23:ARG:NE	18:R:208:CYS:C	2.34	0.85
3:C:136:ASP:OD2	3:C:138:ASP:CB	2.24	0.85
1:A:202:TRP:CZ3	1:A:212:LYS:HG3	2.11	0.85
15:O:3:TYR:HB3	15:O:98:CYS:SG	2.16	0.85
1:A:1319:LYS:HD3	1:A:1356:ARG:HH12	1.39	0.85
1:A:1319:LYS:HG3	1:A:1333:GLU:CD	2.01	0.85
1:A:927:GLU:HB3	1:A:931:ARG:HD3	1.55	0.85
1:A:1313:GLN:HE22	1:A:1318:LYS:HD2	1.42	0.85
5:E:49:SER:O	5:E:54:ARG:CZ	2.24	0.85
2:B:879:GLU:O	2:B:880:LEU:CB	2.24	0.84
13:M:44:ARG:HE	13:M:46:ILE:CG2	1.89	0.84
21:U:231:ASP:O	21:U:232:GLU:HG2	1.77	0.84
1:A:202:TRP:CZ3	1:A:212:LYS:CB	2.61	0.84
1:A:477:LEU:HD11	1:A:483:ARG:HD3	1.58	0.84
17:Q:109:HIS:HA	18:R:234:GLU:OE1	1.76	0.84
1:A:609:HIS:N	1:A:610:PRO:CD	2.41	0.83
2:B:179:LEU:HD11	2:B:771:GLU:HG2	1.59	0.83
1:A:927:GLU:CB	1:A:931:ARG:CD	2.50	0.83
2:B:92:TYR:CB	20:T:145:LEU:HD13	2.08	0.83
17:Q:105:TYR:CD1	17:Q:109:HIS:NE2	2.32	0.83
18:R:162:GLY:O	18:R:163:LEU:HB2	1.78	0.83
18:R:195:PRO:HB2	18:R:199:LYS:HD2	1.60	0.83
21:U:256:THR:O	21:U:257:GLN:HB2	1.76	0.83
17:Q:24:GLY:CA	18:R:210:PHE:HE2	1.92	0.83
2:B:1117:HIS:HB2	2:B:1127:ILE:HD13	1.61	0.83
9:I:57:LYS:O	9:I:59:THR:HG23	1.78	0.83
1:A:927:GLU:CG	1:A:931:ARG:HD3	2.08	0.82
16:P:297:LYS:HB3	16:P:298:PRO:HD2	1.55	0.82
3:C:209:SER:O	3:C:212:ASP:OD1	1.97	0.82
1:A:1313:GLN:NE2	1:A:1318:LYS:HB2	1.95	0.82
5:E:52:ARG:HG2	5:E:53:PRO:HD3	1.59	0.82
13:M:107:MET:HG2	23:Y:63:DG:H22	1.41	0.82
8:H:100:GLU:HG3	8:H:101:GLY:H	1.45	0.81
17:Q:23:ARG:HB2	18:R:207:SER:OG	1.80	0.81
21:U:231:ASP:O	21:U:232:GLU:HG3	1.79	0.81
9:I:103:ARG:C	9:I:105:GLU:H	1.89	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:64:PRO:C	10:J:66:GLU:N	2.34	0.81
2:B:290:TYR:HB3	2:B:562:ALA:HB1	1.62	0.81
2:B:591:ARG:NH1	2:B:663:GLU:OE2	2.12	0.81
14:N:332:GLU:HG2	15:O:92:LYS:HB3	1.63	0.81
9:I:14:ILE:HG12	9:I:16:PHE:CG	2.16	0.81
1:A:595:ILE:HG21	1:A:675:VAL:HG21	1.62	0.80
1:A:999:ARG:HE	8:H:99:ILE:HD12	1.43	0.80
17:Q:180:PHE:CE2	18:R:211:SER:HB3	2.09	0.80
1:A:927:GLU:HG2	1:A:931:ARG:HD3	1.64	0.80
1:A:1251:ASN:HA	21:U:234:LYS:HE3	1.62	0.80
1:A:1113:SER:O	1:A:1114:ALA:HB3	1.82	0.80
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.64	0.80
1:A:202:TRP:HE3	1:A:212:LYS:CB	1.84	0.80
11:K:111:ASP:O	11:K:112:LYS:HB2	1.80	0.80
17:Q:105:TYR:CE1	17:Q:109:HIS:CE1	2.70	0.80
1:A:1319:LYS:CD	1:A:1356:ARG:NH1	2.45	0.80
17:Q:24:GLY:C	18:R:210:PHE:HE2	1.89	0.80
1:A:1022:ILE:H	1:A:1034:GLN:HE22	1.29	0.79
1:A:1123:ARG:NH2	1:A:1381:GLU:OE1	2.15	0.79
2:B:27:TRP:CE2	2:B:762:ARG:HG2	2.18	0.79
20:T:177:ARG:C	20:T:179:ASP:N	2.37	0.79
2:B:874:PRO:O	2:B:875:GLU:HB3	1.82	0.79
2:B:631:GLN:HB3	2:B:685:LYS:HE2	1.64	0.79
2:B:1068:GLN:O	2:B:1072:ARG:N	2.15	0.79
4:D:54:GLU:OE2	7:G:28:GLN:NE2	2.15	0.79
1:A:262:PRO:CG	1:A:274:ASP:CG	2.52	0.78
17:Q:23:ARG:NH1	18:R:209:GLN:N	2.31	0.78
1:A:624:GLY:O	1:A:626:THR:N	2.16	0.78
1:A:1251:ASN:ND2	21:U:227:GLU:O	2.12	0.78
9:I:85:PRO:O	9:I:86:CYS:O	2.00	0.78
17:Q:108:ASP:C	18:R:234:GLU:OE2	2.25	0.78
2:B:52:GLN:CA	20:T:141:LEU:HD13	2.05	0.78
17:Q:111:ARG:NH1	17:Q:188:TYR:OH	2.16	0.78
20:T:177:ARG:O	20:T:179:ASP:N	2.14	0.78
2:B:882:SER:O	2:B:887:TYR:CE1	2.35	0.78
1:A:648:SER:O	1:A:651:SER:OG	2.02	0.78
21:U:231:ASP:C	21:U:232:GLU:HG2	2.09	0.78
3:C:212:ASP:O	3:C:214:ASP:N	2.16	0.78
1:A:261:ARG:C	1:A:263:ALA:H	1.91	0.78
17:Q:70:LYS:NZ	18:R:226:ASP:O	2.16	0.78
1:A:609:HIS:N	1:A:610:PRO:HD2	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:316:SER:OG	16:P:235:ARG:NH1	2.17	0.78
1:A:205:VAL:O	1:A:206:ASN:CB	2.31	0.77
2:B:483:ARG:HH11	2:B:526:LEU:HB2	1.48	0.77
8:H:65:TYR:HE2	8:H:70:LEU:CA	1.98	0.77
2:B:225:LEU:HD13	2:B:228:SER:OG	1.84	0.77
9:I:14:ILE:HG13	9:I:16:PHE:CD2	2.19	0.77
17:Q:54:PHE:HA	18:R:194:ARG:HD2	1.67	0.77
17:Q:23:ARG:NE	18:R:208:CYS:CA	2.48	0.77
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.17	0.77
5:E:61:LEU:HD13	5:E:73:PHE:HD1	1.49	0.77
1:A:608:THR:CB	1:A:610:PRO:HD2	2.14	0.76
2:B:803:ARG:NH2	2:B:951:GLN:OE1	2.16	0.76
11:K:39:ASP:OD1	11:K:39:ASP:N	2.18	0.76
2:B:133:ILE:HD13	2:B:139:GLN:HB3	1.66	0.76
7:G:111:HIS:NE2	17:Q:124:ARG:O	2.18	0.76
9:I:14:ILE:CG1	9:I:16:PHE:CE2	2.65	0.76
13:M:47:ASP:C	13:M:49:GLY:N	2.39	0.76
17:Q:23:ARG:NH1	18:R:209:GLN:CB	2.43	0.76
17:Q:39:ARG:NH2	18:R:159:ASP:OD2	2.18	0.76
17:Q:101:ASN:C	17:Q:102:VAL:HG12	2.10	0.76
17:Q:105:TYR:O	17:Q:109:HIS:HD2	1.69	0.76
13:M:182:ALA:HB2	20:T:154:LYS:HG3	1.68	0.76
17:Q:23:ARG:HE	18:R:208:CYS:CA	1.97	0.76
2:B:462:ALA:HB2	22:X:39:DT:H5”	1.67	0.76
2:B:761:THR:H	2:B:764:MET:HE3	1.51	0.76
17:Q:105:TYR:CE1	18:R:231:GLU:HG3	2.14	0.76
8:H:65:TYR:CZ	8:H:70:LEU:CB	2.50	0.75
13:M:11:PRO:O	13:M:12:ARG:CB	2.33	0.75
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.69	0.75
17:Q:29:GLU:CD	18:R:194:ARG:NH2	2.44	0.75
1:A:117:LEU:N	1:A:232:GLU:OE2	2.19	0.75
1:A:1319:LYS:HD3	1:A:1356:ARG:NH1	2.00	0.75
13:M:44:ARG:HE	13:M:46:ILE:HG22	1.52	0.75
17:Q:52:LEU:HB3	17:Q:54:PHE:HD1	1.50	0.75
17:Q:109:HIS:NE2	18:R:224:THR:HG21	2.00	0.75
17:Q:23:ARG:HE	18:R:208:CYS:HA	1.51	0.75
17:Q:24:GLY:HA3	18:R:210:PHE:CE2	2.21	0.75
3:C:212:ASP:C	3:C:214:ASP:H	1.93	0.75
5:E:55:ARG:HB3	5:E:78:GLU:OE2	1.87	0.75
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.69	0.75
14:N:320:VAL:HG11	16:P:236:LYS:HG2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:14:LEU:HD11	17:Q:102:VAL:CB	2.15	0.75
18:R:162:GLY:O	18:R:163:LEU:CB	2.32	0.75
5:E:27:LEU:H	5:E:64:HIS:HB3	0.74	0.75
17:Q:105:TYR:HE1	18:R:231:GLU:CB	2.00	0.75
1:A:331:LYS:NZ	23:Y:63:DG:O6	2.19	0.74
1:A:522:PRO:HA	1:A:666:ARG:HH21	1.52	0.74
1:A:1319:LYS:HD2	1:A:1356:ARG:HH12	1.52	0.74
2:B:735:VAL:HG22	2:B:750:VAL:HG13	1.67	0.74
5:E:40:PHE:CE2	5:E:46:ASP:OD2	2.40	0.74
13:M:15:CYS:SG	13:M:39:LEU:HD23	2.26	0.74
9:I:14:ILE:CG1	9:I:16:PHE:CD2	2.69	0.74
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.13	0.74
1:A:153:ILE:O	1:A:154:CYS:C	2.31	0.74
1:A:206:ASN:O	1:A:207:GLU:HB2	1.85	0.74
2:B:914:GLU:OE1	2:B:914:GLU:N	2.21	0.74
1:A:202:TRP:HZ3	1:A:212:LYS:HG3	1.52	0.74
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.17	0.74
8:H:65:TYR:OH	8:H:70:LEU:HB2	1.88	0.74
2:B:529:MET:HE2	2:B:623:ARG:HB2	1.68	0.74
13:M:10:LEU:H	13:M:11:PRO:HD3	1.52	0.74
1:A:212:LYS:HA	1:A:212:LYS:HE3	1.68	0.73
1:A:611:ASP:OD2	1:A:627:LYS:CE	2.35	0.73
17:Q:23:ARG:NH1	18:R:209:GLN:CA	2.51	0.73
17:Q:14:LEU:CD1	17:Q:102:VAL:HG21	1.99	0.73
17:Q:14:LEU:HD11	17:Q:102:VAL:HG23	0.74	0.73
18:R:225:VAL:CG1	18:R:230:GLU:HG3	2.18	0.73
1:A:1319:LYS:CD	1:A:1333:GLU:CD	2.56	0.73
17:Q:105:TYR:CZ	17:Q:109:HIS:NE2	2.53	0.73
9:I:104:ALA:O	9:I:105:GLU:HB2	1.86	0.73
1:A:264:VAL:O	1:A:266:MET:HG2	1.89	0.73
1:A:1177:TYR:H	9:I:51:SER:HB3	1.53	0.73
2:B:52:GLN:CA	20:T:141:LEU:CD1	2.61	0.73
13:M:10:LEU:CD1	13:M:14:THR:CB	2.57	0.73
17:Q:14:LEU:CG	17:Q:102:VAL:HG23	2.16	0.73
1:A:210:GLN:CD	1:A:212:LYS:HD3	2.13	0.73
3:C:274:ILE:HD12	11:K:84:GLN:HB3	1.69	0.73
3:C:40:ALA:HB1	3:C:171:LYS:HB3	1.70	0.72
9:I:14:ILE:HG12	9:I:16:PHE:CD1	2.23	0.72
13:M:37:CYS:SG	13:M:39:LEU:CD2	2.77	0.72
18:R:194:ARG:HG2	18:R:201:LEU:HD12	1.71	0.72
16:P:167:ASN:ND2	23:Y:79:DT:O2	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.71	0.72
10:J:64:PRO:O	10:J:66:GLU:N	2.21	0.72
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.71	0.72
21:U:252:LYS:O	21:U:253:THR:OG1	2.06	0.72
1:A:181:HIS:CD2	1:A:181:HIS:H	2.06	0.72
1:A:210:GLN:CD	1:A:212:LYS:CD	2.63	0.72
3:C:67:ARG:HH12	10:J:2:ILE:HG13	1.55	0.72
3:C:240:ARG:NH1	3:C:242:GLU:OE2	2.23	0.72
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.71	0.72
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.70	0.72
17:Q:23:ARG:HE	18:R:207:SER:C	1.98	0.72
5:E:1:MET:HE3	5:E:3:ASP:HB3	1.71	0.71
21:U:226:GLU:O	21:U:227:GLU:CB	2.36	0.71
1:A:269:SER:O	1:A:270:ALA:HB3	1.91	0.71
8:H:146:LYS:HE2	8:H:147:LYS:HG3	1.71	0.71
17:Q:102:VAL:O	17:Q:104:LYS:N	2.23	0.71
1:A:265:VAL:C	1:A:272:ASN:ND2	2.49	0.71
2:B:1085:ARG:NH2	23:Y:53:DG:OP2	2.24	0.71
8:H:66:GLU:O	8:H:67:ASP:CB	2.38	0.71
13:M:7:LEU:HD11	13:M:10:LEU:HD13	1.72	0.71
5:E:48:PRO:O	5:E:49:SER:CB	2.39	0.71
20:T:154:LYS:HD2	20:T:154:LYS:N	2.06	0.71
3:C:212:ASP:C	3:C:214:ASP:N	2.47	0.70
5:E:64:HIS:O	5:E:65:ASN:C	2.24	0.70
17:Q:23:ARG:HH21	18:R:208:CYS:HA	1.55	0.70
4:D:90:LYS:HE2	4:D:130:ILE:HD11	1.72	0.70
5:E:46:ASP:OD1	5:E:54:ARG:HG2	1.92	0.70
1:A:199:TYR:HE1	13:M:93:PHE:CZ	2.03	0.70
2:B:490:GLY:O	2:B:491:ARG:CB	2.37	0.70
2:B:777:ASN:O	10:J:47:ARG:NH1	2.24	0.70
17:Q:23:ARG:NH2	18:R:208:CYS:HA	2.05	0.70
18:R:190:LEU:HD12	18:R:205:ASP:OD2	1.86	0.70
1:A:960:ARG:NH2	1:A:961:GLU:OE2	2.24	0.70
2:B:48:ASP:OD1	2:B:159:THR:OG1	2.09	0.70
1:A:1319:LYS:HD2	1:A:1356:ARG:NH1	2.07	0.70
2:B:69:ALA:HB2	2:B:423:ILE:HB	1.74	0.70
1:A:632:ASN:HA	1:A:992:LYS:HD2	1.74	0.70
1:A:1251:ASN:ND2	21:U:227:GLU:HB3	2.07	0.69
2:B:988:LYS:NZ	2:B:1026:GLU:OE2	2.17	0.69
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.72	0.69
1:A:1192:TRP:HE3	1:A:1192:TRP:H	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:47:ASP:O	13:M:49:GLY:CA	2.40	0.69
17:Q:180:PHE:HZ	18:R:211:SER:HA	1.55	0.69
2:B:295:PRO:HB2	9:I:11:PHE:HD2	1.58	0.69
1:A:262:PRO:O	1:A:263:ALA:HB3	1.93	0.69
13:M:178:LYS:O	20:T:154:LYS:CB	2.34	0.69
2:B:313:GLU:OE2	19:S:153:ARG:NH2	2.26	0.69
2:B:331:THR:HB	2:B:334:LYS:HB2	1.75	0.69
1:A:197:GLU:OE1	1:A:308:LYS:NZ	2.26	0.68
1:A:1313:GLN:NE2	1:A:1316:ASN:OD1	2.25	0.68
11:K:111:ASP:O	11:K:112:LYS:CB	2.41	0.68
18:R:190:LEU:CD1	18:R:205:ASP:CG	2.65	0.68
2:B:225:LEU:HD13	2:B:228:SER:CB	2.24	0.68
2:B:323:SER:OG	2:B:335:ARG:NH1	2.27	0.68
17:Q:52:LEU:HB3	17:Q:54:PHE:CD1	2.28	0.68
1:A:271:ARG:HH12	2:B:821:LYS:HE2	1.58	0.68
21:U:251:ALA:O	21:U:252:LYS:HB2	1.92	0.68
2:B:591:ARG:NH2	2:B:601:VAL:O	2.27	0.68
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.76	0.68
8:H:65:TYR:CE2	8:H:70:LEU:CG	2.77	0.68
18:R:194:ARG:CG	18:R:201:LEU:HD12	2.23	0.68
1:A:540:ASP:HB2	2:B:790:GLN:NE2	2.09	0.68
2:B:13:ASP:OD1	2:B:636:LYS:NZ	2.27	0.67
8:H:84:ARG:O	8:H:86:ASP:N	2.24	0.67
17:Q:23:ARG:NE	18:R:208:CYS:HA	2.09	0.67
1:A:207:GLU:O	1:A:209:SER:N	2.27	0.67
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.77	0.67
17:Q:110:MET:HE1	18:R:222:SER:OG	1.94	0.67
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.67
22:X:44:DC:H42	23:Y:48:DC:H42	1.41	0.67
2:B:839:GLY:HA3	2:B:891:ASP:HB3	1.76	0.67
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.25	0.67
2:B:73:HIS:O	2:B:75:SER:N	2.28	0.67
2:B:132:VAL:CB	2:B:141:GLN:CG	2.51	0.67
2:B:1066:PRO:HB3	13:M:46:ILE:CD1	2.21	0.67
21:U:153:ARG:NH2	21:U:166:GLU:OE2	2.28	0.67
14:N:324:GLU:HA	16:P:188:ARG:HH12	1.58	0.67
20:T:140:ARG:O	20:T:142:SER:N	2.27	0.67
1:A:608:THR:OG1	1:A:610:PRO:HD2	1.94	0.67
21:U:231:ASP:C	21:U:232:GLU:CG	2.67	0.67
15:O:3:TYR:CD1	15:O:98:CYS:SG	2.87	0.67
1:A:202:TRP:CE3	1:A:212:LYS:HB2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:206:GLU:C	16:P:208:ARG:H	2.02	0.66
2:B:896:LEU:CD2	2:B:901:THR:HG21	2.25	0.66
1:A:1180:ASN:HB3	9:I:33:ARG:HH22	1.59	0.66
1:A:1319:LYS:CG	1:A:1333:GLU:CG	2.61	0.66
2:B:225:LEU:O	2:B:227:ASN:N	2.28	0.66
13:M:44:ARG:NE	13:M:46:ILE:CG2	2.58	0.66
16:P:203:ARG:HH21	16:P:203:ARG:HG3	1.59	0.66
17:Q:24:GLY:CA	18:R:210:PHE:CD2	2.79	0.66
20:T:177:ARG:NH2	20:T:212:TYR:HB2	2.10	0.66
1:A:133:SER:O	1:A:135:GLY:N	2.29	0.66
1:A:202:TRP:CZ3	1:A:212:LYS:HG2	2.29	0.66
1:A:460:ARG:NH2	1:A:493:ASN:HB2	2.10	0.66
9:I:60:HIS:CD2	9:I:62:VAL:HG12	2.31	0.66
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.77	0.66
17:Q:54:PHE:CD2	18:R:194:ARG:CD	2.77	0.66
2:B:312:GLN:OE1	19:S:153:ARG:NH1	2.30	0.65
1:A:1113:SER:O	1:A:1114:ALA:CB	2.44	0.65
1:A:1196:TYR:OH	1:A:1247:PHE:O	2.11	0.65
9:I:84:HIS:H	9:I:84:HIS:CD2	2.15	0.65
17:Q:57:LYS:NZ	22:X:27:DG:OP1	2.29	0.65
17:Q:180:PHE:HE2	18:R:211:SER:CB	2.01	0.65
18:R:225:VAL:HB	18:R:230:GLU:CG	2.22	0.65
14:N:363:ARG:HD3	14:N:365:TYR:OH	1.97	0.65
17:Q:103:VAL:O	17:Q:106:LYS:N	2.29	0.65
1:A:133:SER:O	1:A:134:LYS:C	2.36	0.65
8:H:65:TYR:OH	8:H:70:LEU:CB	2.43	0.65
13:M:89:GLY:O	13:M:90:ALA:HB3	1.95	0.65
2:B:1040:GLN:H	2:B:1040:GLN:CD	2.05	0.65
9:I:14:ILE:CG1	9:I:16:PHE:CG	2.80	0.65
2:B:98:HIS:HB2	2:B:108:MET:HE2	1.79	0.65
2:B:952:GLU:OE1	2:B:952:GLU:N	2.25	0.65
3:C:84:TYR:CZ	3:C:167:LYS:HE3	2.32	0.65
10:J:63:ALA:O	10:J:65:LEU:N	2.26	0.65
18:R:138:ALA:C	18:R:140:LYS:H	2.05	0.65
3:C:132:SER:HB3	3:C:147:ASP:HB2	1.79	0.65
1:A:152:ASN:O	1:A:153:ILE:CB	2.42	0.64
1:A:385:ALA:HA	1:A:450:MET:HE3	1.79	0.64
1:A:622:SER:O	1:A:623:PRO:C	2.41	0.64
2:B:595:ASP:OD1	20:T:129:ARG:NH1	2.30	0.64
13:M:47:ASP:O	13:M:48:VAL:C	2.38	0.64
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:52:ARG:CG	5:E:53:PRO:HD3	2.27	0.64
7:G:97:LEU:HB3	7:G:108:ILE:HB	1.78	0.64
2:B:74:ALA:CB	20:T:201:ASP:HB3	2.22	0.64
6:F:65:VAL:HG13	6:F:104:ILE:HD11	1.80	0.64
16:P:206:GLU:CB	16:P:236:LYS:HZ2	2.08	0.64
17:Q:24:GLY:HA2	18:R:210:PHE:CD2	2.33	0.64
20:T:154:LYS:H	20:T:154:LYS:CD	2.03	0.64
1:A:22:GLN:HE22	1:A:1448:SER:HB2	1.63	0.64
1:A:863:ARG:NH2	1:A:1415:THR:OG1	2.31	0.64
17:Q:103:VAL:HG23	17:Q:107:LEU:HD12	1.80	0.64
1:A:522:PRO:CA	1:A:666:ARG:HH21	2.10	0.64
2:B:92:TYR:CB	20:T:145:LEU:HB2	2.24	0.64
3:C:78:ILE:HD11	3:C:81:LYS:HE3	1.80	0.64
1:A:271:ARG:HH22	2:B:821:LYS:NZ	1.95	0.64
10:J:62:TYR:HB3	10:J:64:PRO:CD	2.28	0.64
17:Q:36:ILE:O	17:Q:41:SER:OG	2.16	0.64
18:R:142:LYS:NZ	18:R:172:GLU:OE2	2.26	0.64
1:A:609:HIS:O	1:A:610:PRO:O	2.17	0.63
2:B:141:GLN:HG3	2:B:141:GLN:O	1.96	0.63
13:M:178:LYS:NZ	13:M:279:GLY:O	2.27	0.63
16:P:298:PRO:O	16:P:300:ILE:HG12	1.97	0.63
18:R:190:LEU:CD1	18:R:205:ASP:HB2	2.28	0.63
1:A:133:SER:OG	1:A:136:GLN:CB	2.36	0.63
1:A:927:GLU:HB2	1:A:931:ARG:HG2	1.78	0.63
1:A:1027:ASP:OD1	5:E:162:ARG:NH1	2.31	0.63
1:A:1114:ALA:C	1:A:1116:ASN:H	2.07	0.63
1:A:1179:PRO:HG2	9:I:33:ARG:HG3	1.80	0.63
13:M:178:LYS:C	20:T:154:LYS:HB3	2.22	0.63
18:R:190:LEU:HD11	18:R:205:ASP:HB2	1.79	0.63
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.32	0.63
2:B:958:CYS:SG	2:B:959:GLU:N	2.72	0.63
9:I:84:HIS:CG	9:I:85:PRO:CD	2.70	0.63
20:T:177:ARG:HH22	20:T:212:TYR:HB2	1.63	0.63
2:B:1120:ASN:HB3	2:B:1145:GLN:HB3	1.81	0.63
13:M:108:SER:HB3	13:M:112:ARG:HH11	1.64	0.63
1:A:460:ARG:HH21	1:A:493:ASN:HB2	1.61	0.63
8:H:84:ARG:C	8:H:86:ASP:N	2.56	0.63
9:I:14:ILE:CG1	9:I:16:PHE:CZ	2.72	0.63
11:K:56:VAL:HA	11:K:77:THR:HG22	1.81	0.63
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.81	0.63
1:A:326:PRO:HB3	13:M:87:GLY:CA	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:ASN:OD1	2:B:553:LEU:N	2.33	0.62
4:D:70:ARG:NH1	7:G:140:ASP:OD1	2.31	0.62
2:B:249:LYS:O	2:B:250:SER:HB2	1.99	0.62
14:N:321:SER:OG	16:P:243:LYS:NZ	2.26	0.62
9:I:14:ILE:HG13	9:I:16:PHE:CE1	2.33	0.62
23:Y:56:DG:H2"	23:Y:57:DA:H5'	1.80	0.62
1:A:1112:VAL:HG12	1:A:1311:LEU:HD21	1.81	0.62
2:B:309:PHE:CE2	9:I:40:ARG:HD2	2.34	0.62
13:M:10:LEU:N	13:M:11:PRO:HD3	2.14	0.62
2:B:225:LEU:C	2:B:227:ASN:N	2.54	0.62
1:A:923:ASP:O	1:A:932:ARG:NH1	2.32	0.62
1:A:950:ASN:OD1	1:A:954:ARG:NH1	2.33	0.62
2:B:422:PHE:O	2:B:426:GLY:N	2.28	0.62
20:T:202:LEU:HD12	20:T:205:ILE:HD11	1.81	0.62
9:I:89:CYS:HB3	9:I:119:CYS:SG	2.39	0.62
1:A:244:ARG:HG2	1:A:245:PRO:HD2	1.81	0.62
1:A:339:LEU:HD11	2:B:1161:GLU:HG2	1.81	0.62
20:T:139:VAL:HG13	20:T:142:SER:OG	1.99	0.62
2:B:873:LEU:HB3	2:B:874:PRO:CD	2.30	0.62
17:Q:103:VAL:O	17:Q:104:LYS:C	2.43	0.62
17:Q:103:VAL:CG2	17:Q:104:LYS:N	2.62	0.62
1:A:93:PRO:HB3	1:A:251:THR:HG22	1.82	0.62
1:A:540:ASP:HB2	2:B:790:GLN:HE21	1.63	0.62
2:B:761:THR:H	2:B:764:MET:CE	2.13	0.62
9:I:14:ILE:CG1	9:I:16:PHE:CE1	2.83	0.62
1:A:779:ILE:O	1:A:783:GLN:HG3	2.00	0.61
1:A:896:LEU:HD23	1:A:1080:ILE:HD12	1.82	0.61
7:G:78:ARG:NH1	7:G:79:PRO:O	2.33	0.61
8:H:88:PHE:HD2	8:H:144:LEU:HB3	1.65	0.61
16:P:162:VAL:O	16:P:162:VAL:HG23	2.00	0.61
19:S:111:LYS:HE3	19:S:149:LEU:HD21	1.82	0.61
2:B:924:ARG:NH1	3:C:60:HIS:HB2	2.16	0.61
1:A:1102:MET:HB2	1:A:1389:ASP:OD1	2.00	0.61
1:A:1313:GLN:HE22	1:A:1318:LYS:CD	2.11	0.61
13:M:44:ARG:NE	13:M:46:ILE:HG22	2.15	0.61
1:A:1298:LEU:O	1:A:1300:GLY:N	2.31	0.61
20:T:145:LEU:O	20:T:145:LEU:HG	2.00	0.61
1:A:152:ASN:C	1:A:153:ILE:CG1	2.47	0.61
1:A:611:ASP:CG	1:A:626:THR:HG1	2.09	0.61
10:J:3:ILE:HD12	10:J:15:GLY:HA2	1.81	0.61
14:N:344:ARG:NH2	23:Y:79:DT:OP2	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:236:LYS:NZ	20:T:238:GLU:O	2.33	0.61
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.82	0.61
1:A:927:GLU:H	1:A:931:ARG:HG2	1.65	0.61
1:A:611:ASP:CG	1:A:626:THR:OG1	2.43	0.61
1:A:890:ARG:CZ	1:A:1023:VAL:HB	2.30	0.61
17:Q:23:ARG:CB	18:R:207:SER:OG	2.48	0.61
20:T:144:GLN:O	20:T:145:LEU:HB2	1.99	0.61
2:B:901:THR:OG1	2:B:902:GLY:N	2.31	0.61
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.83	0.61
5:E:71:GLN:HE21	5:E:99:ILE:HA	1.66	0.61
18:R:190:LEU:HD11	18:R:205:ASP:CB	2.31	0.61
18:R:190:LEU:HD13	18:R:205:ASP:OD2	1.97	0.61
3:C:67:ARG:HH21	3:C:148:ILE:HD11	1.65	0.60
6:F:62:ARG:NH1	6:F:127:ASP:O	2.27	0.60
1:A:603:ILE:HD11	1:A:988:TRP:CE2	2.35	0.60
1:A:1192:TRP:O	1:A:1196:TYR:N	2.34	0.60
8:H:23:ASP:O	8:H:25:VAL:N	2.32	0.60
17:Q:54:PHE:HA	18:R:194:ARG:CD	2.31	0.60
2:B:883:THR:O	2:B:884:ASN:C	2.41	0.60
1:A:267:GLN:H	13:M:49:GLY:HA2	1.66	0.60
1:A:927:GLU:HB3	1:A:931:ARG:HB2	1.82	0.60
3:C:56:SER:HG	3:C:158:GLU:H	1.46	0.60
1:A:364:ARG:HE	1:A:500:GLU:CD	2.10	0.60
1:A:857:THR:HG21	1:A:1100:THR:HA	1.84	0.60
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.84	0.60
11:K:62:LYS:HE2	11:K:72:ILE:HD11	1.82	0.60
21:U:227:GLU:O	21:U:228:MET:C	2.44	0.60
1:A:621:ILE:HG22	1:A:621:ILE:O	2.02	0.60
14:N:22:ILE:HD11	14:N:43:LYS:HB2	1.83	0.60
1:A:841:MET:HE1	2:B:503:ASN:CG	2.27	0.60
1:A:1319:LYS:CG	1:A:1333:GLU:HG2	2.29	0.60
18:R:144:ASN:ND2	18:R:173:GLU:OE2	2.28	0.60
1:A:95:PHE:CE2	1:A:218:PRO:HG3	2.37	0.60
1:A:929:ALA:C	1:A:931:ARG:H	2.07	0.60
17:Q:35:ASP:OD1	18:R:161:ARG:NH2	2.33	0.60
22:X:47:DG:H2"	22:X:48:DA:H5"	1.84	0.60
1:A:65:ILE:HD11	1:A:263:ALA:O	2.02	0.59
5:E:45:GLY:C	5:E:47:LYS:H	2.10	0.59
13:M:10:LEU:O	13:M:11:PRO:C	2.34	0.59
2:B:838:GLN:HB3	2:B:890:ARG:HA	1.84	0.59
3:C:117:SER:HB3	3:C:130:VAL:HG21	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:LEU:HD21	5:E:167:GLU:HG3	1.84	0.59
8:H:65:TYR:CE2	8:H:70:LEU:HD23	2.37	0.59
1:A:298:ALA:HB1	1:A:303:ILE:HD11	1.85	0.59
8:H:95:LYS:HB3	8:H:139:SER:HA	1.85	0.59
1:A:65:ILE:CD1	1:A:263:ALA:O	2.51	0.59
1:A:643:LYS:HD3	21:U:301:CYS:SG	2.43	0.59
17:Q:117:ASP:OD1	17:Q:174:ARG:NH1	2.35	0.59
18:R:93:ASP:O	18:R:140:LYS:NZ	2.35	0.59
22:X:50:DC:H2"	22:X:51:DG:C8	2.37	0.59
1:A:375:ILE:HD11	1:A:669:TYR:HB3	1.85	0.59
1:A:522:PRO:HA	1:A:666:ARG:NH2	2.17	0.59
18:R:190:LEU:HD11	18:R:205:ASP:CG	2.25	0.59
16:P:206:GLU:OE2	16:P:206:GLU:HA	2.02	0.59
17:Q:23:ARG:CZ	18:R:208:CYS:HA	2.32	0.59
17:Q:54:PHE:CD2	18:R:194:ARG:NE	2.70	0.59
1:A:202:TRP:CE3	1:A:212:LYS:CG	2.81	0.59
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.85	0.59
1:A:375:ILE:HG13	1:A:666:ARG:HH11	1.67	0.59
1:A:565:MET:HE2	11:K:61:TYR:HA	1.85	0.59
1:A:948:ILE:HG23	1:A:1007:ILE:HD11	1.85	0.59
1:A:1021:VAL:HA	1:A:1034:GLN:NE2	2.18	0.59
8:H:84:ARG:HB3	8:H:86:ASP:HB2	1.84	0.59
13:M:44:ARG:HE	13:M:46:ILE:HG23	1.65	0.59
17:Q:103:VAL:O	17:Q:105:TYR:N	2.36	0.59
20:T:142:SER:OG	20:T:143:GLN:OE1	2.17	0.59
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.34	0.59
2:B:297:MET:SD	2:B:373:LEU:HD22	2.42	0.59
13:M:44:ARG:NE	13:M:46:ILE:HG23	2.18	0.59
1:A:800:PHE:CZ	1:A:815:TYR:HE1	2.21	0.58
2:B:883:THR:O	2:B:885:ARG:N	2.36	0.58
10:J:62:TYR:CA	10:J:64:PRO:HD2	2.30	0.58
17:Q:23:ARG:CZ	18:R:208:CYS:CA	2.80	0.58
18:R:225:VAL:HG12	18:R:227:SER:H	1.67	0.58
1:A:720:ALA:HB1	9:I:108:MET:HG2	1.84	0.58
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.85	0.58
13:M:41:VAL:O	13:M:41:VAL:HG23	2.03	0.58
14:N:42:LEU:HB2	15:O:22:LEU:HD11	1.84	0.58
21:U:132:ARG:N	21:U:167:GLU:OE2	2.36	0.58
20:T:4:ARG:NE	20:T:102:ASP:OD2	2.35	0.58
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.38	0.58
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1016:SER:HB3	2:B:1022:LEU:HB3	1.86	0.58
1:A:133:SER:C	1:A:135:GLY:N	2.60	0.58
19:S:49:ARG:NH1	19:S:96:GLN:O	2.36	0.58
20:T:26:TYR:HE2	20:T:124:TYR:HH	1.52	0.58
1:A:353:ASN:HD21	2:B:1071:ASN:HD21	1.50	0.58
1:A:364:ARG:NH2	1:A:500:GLU:OE1	2.37	0.58
2:B:471:ASN:OD1	2:B:472:ARG:N	2.37	0.58
9:I:103:ARG:C	9:I:105:GLU:HG2	2.25	0.58
16:P:206:GLU:C	16:P:208:ARG:N	2.60	0.58
1:A:69:GLY:HA2	1:A:77:ASN:HA	1.85	0.58
1:A:1416:ARG:HB3	1:A:1433:GLU:OE1	2.03	0.58
2:B:289:ILE:O	2:B:291:ASP:N	2.35	0.58
9:I:14:ILE:CG1	9:I:16:PHE:CD1	2.86	0.58
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.85	0.58
2:B:73:HIS:C	2:B:75:SER:H	2.11	0.58
7:G:31:PHE:HE1	7:G:48:VAL:HB	1.68	0.58
8:H:106:THR:O	8:H:108:ALA:N	2.33	0.58
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	2.38	0.58
1:A:417:LYS:HG2	1:A:449:HIS:CE1	2.39	0.58
1:A:521:VAL:C	1:A:666:ARG:HH21	2.12	0.58
1:A:624:GLY:C	1:A:626:THR:H	2.11	0.58
1:A:799:PRO:O	1:A:806:THR:HG22	2.02	0.58
2:B:724:TYR:HB3	2:B:728:MET:HE3	1.85	0.58
13:M:10:LEU:N	13:M:11:PRO:CD	2.67	0.57
18:R:144:ASN:OD1	18:R:145:VAL:N	2.36	0.57
17:Q:54:PHE:CG	18:R:194:ARG:HD2	2.39	0.57
1:A:156:GLY:N	1:A:181:HIS:CE1	2.73	0.57
2:B:45:ASP:HB3	2:B:534:VAL:HG11	1.87	0.57
2:B:834:ARG:O	2:B:885:ARG:NH1	2.38	0.57
17:Q:23:ARG:NE	18:R:207:SER:C	2.56	0.57
17:Q:29:GLU:CD	18:R:194:ARG:HH21	2.09	0.57
2:B:685:LYS:HA	2:B:688:ALA:HB3	1.85	0.57
17:Q:180:PHE:CZ	18:R:211:SER:CA	2.61	0.57
18:R:99:LEU:HD12	18:R:124:LEU:HD12	1.86	0.57
18:R:195:PRO:HB3	18:R:199:LYS:HD2	1.86	0.57
1:A:480:SER:HB3	2:B:1059:ILE:HD12	1.86	0.57
1:A:1310:HIS:O	21:U:252:LYS:HG3	2.00	0.57
2:B:755:GLN:HB2	2:B:777:ASN:ND2	2.19	0.57
22:X:13:DA:H2"	22:X:14:DA:C8	2.40	0.57
2:B:228:SER:O	2:B:405:ARG:NH1	2.36	0.57
1:A:35:SER:OG	1:A:37:THR:HG22	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HG23	20:T:141:LEU:HD11	1.80	0.57
2:B:468:GLN:OE1	2:B:481:HIS:NE2	2.38	0.57
17:Q:42:CYS:O	17:Q:95:ASN:ND2	2.38	0.57
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.37	0.57
1:A:181:HIS:CD2	1:A:181:HIS:N	2.73	0.57
1:A:1251:ASN:OD1	21:U:197:ASN:ND2	2.35	0.57
2:B:895:PHE:N	2:B:895:PHE:CD1	2.73	0.57
5:E:27:LEU:N	5:E:64:HIS:HB2	2.12	0.57
3:C:212:ASP:O	3:C:213:GLU:C	2.48	0.56
17:Q:28:ILE:HG21	18:R:190:LEU:HD13	1.85	0.56
18:R:84:TYR:OH	18:R:88:ARG:NH1	2.38	0.56
2:B:326:ALA:HB2	2:B:338:TYR:CE2	2.40	0.56
2:B:483:ARG:NH1	2:B:526:LEU:HB2	2.20	0.56
16:P:162:VAL:C	16:P:164:GLN:HE21	2.05	0.56
20:T:129:ARG:HA	20:T:132:ILE:HD12	1.87	0.56
1:A:631:GLU:HG3	1:A:988:TRP:CH2	2.40	0.56
1:A:1085:GLU:OE2	6:F:59:LYS:HE2	2.05	0.56
1:A:1223:ASP:OD2	1:A:1224:ARG:NH1	2.38	0.56
2:B:1129:ASN:HA	2:B:1135:TYR:HD1	1.69	0.56
1:A:264:VAL:HG23	1:A:265:VAL:N	2.20	0.56
2:B:882:SER:O	2:B:887:TYR:CG	2.56	0.56
5:E:52:ARG:CB	5:E:53:PRO:HD3	2.34	0.56
1:A:279:LYS:HB2	1:A:336:LEU:HD21	1.88	0.56
1:A:1299:GLN:HG2	1:A:1300:GLY:N	2.21	0.56
2:B:496:ALA:HB3	2:B:498:PRO:HD2	1.87	0.56
3:C:148:ILE:HG12	10:J:5:VAL:HG22	1.86	0.56
7:G:93:ASN:OD1	7:G:94:LYS:N	2.38	0.56
9:I:75:ASP:HB3	9:I:78:LEU:HD12	1.86	0.56
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.39	0.56
2:B:74:ALA:HB2	20:T:201:ASP:CB	2.29	0.56
3:C:142:TYR:O	3:C:144:GLU:N	2.39	0.56
17:Q:24:GLY:HA2	18:R:210:PHE:CE2	2.40	0.56
19:S:115:LYS:NZ	19:S:117:GLY:O	2.32	0.56
2:B:800:ALA:O	2:B:805:PHE:HB3	2.05	0.56
2:B:1022:LEU:HD12	2:B:1023:ARG:HG3	1.87	0.56
14:N:333:ASN:OD1	14:N:361:ASN:N	2.26	0.56
21:U:291:CYS:SG	21:U:293:GLU:HB2	2.45	0.56
1:A:294:GLU:HA	1:A:298:ALA:HB2	1.88	0.56
1:A:464:LEU:HD21	1:A:1100:THR:HG21	1.88	0.56
2:B:720:PRO:O	2:B:724:TYR:HD2	1.88	0.56
12:L:26:ASN:HB3	12:L:28:ILE:HG13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:190:LEU:HD12	18:R:205:ASP:CG	2.29	0.56
1:A:631:GLU:HG3	1:A:988:TRP:HH2	1.69	0.56
2:B:225:LEU:O	2:B:228:SER:N	2.39	0.56
2:B:329:GLY:H	2:B:335:ARG:HH21	1.54	0.56
1:A:269:SER:O	1:A:270:ALA:CB	2.55	0.55
3:C:130:VAL:O	3:C:134:ASN:ND2	2.39	0.55
13:M:44:ARG:HG3	13:M:46:ILE:HG23	1.88	0.55
15:O:3:TYR:C	15:O:5:LEU:N	2.51	0.55
17:Q:16:ARG:HD2	17:Q:19:LYS:HB2	1.86	0.55
2:B:704:LEU:HD22	2:B:708:ALA:CB	2.36	0.55
3:C:154:ARG:N	3:C:157:GLN:OE1	2.38	0.55
1:A:212:LYS:HA	1:A:212:LYS:NZ	2.20	0.55
1:A:606:HIS:HB2	1:A:627:LYS:HA	1.87	0.55
1:A:800:PHE:HZ	1:A:815:TYR:HE1	1.53	0.55
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.87	0.55
1:A:1313:GLN:CD	1:A:1318:LYS:HB2	2.31	0.55
2:B:92:TYR:HE1	20:T:143:GLN:HE21	1.54	0.55
3:C:117:SER:OG	3:C:147:ASP:OD2	2.16	0.55
10:J:10:CYS:SG	10:J:11:GLY:N	2.79	0.55
17:Q:109:HIS:HE1	18:R:231:GLU:CB	2.19	0.55
19:S:172:ASN:OD1	19:S:173:HIS:N	2.38	0.55
7:G:107:PHE:CZ	17:Q:127:PHE:HZ	2.24	0.55
9:I:84:HIS:CG	9:I:85:PRO:HD3	1.92	0.55
1:A:611:ASP:O	1:A:612:ASP:HB2	2.05	0.55
1:A:1307:VAL:HG11	1:A:1339:ASP:OD2	2.06	0.55
12:L:19:CYS:SG	12:L:20:GLY:N	2.80	0.55
15:O:64:THR:HG21	16:P:188:ARG:HD2	1.89	0.55
1:A:138:LYS:HB2	1:A:1445:HIS:CE1	2.41	0.55
1:A:875:TYR:O	6:F:53:THR:HG22	2.06	0.55
2:B:728:MET:HE2	2:B:942:LYS:HE2	1.88	0.55
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.39	0.55
13:M:89:GLY:O	13:M:90:ALA:CB	2.55	0.55
17:Q:113:ARG:HB2	18:R:222:SER:O	2.07	0.55
18:R:151:LEU:HD13	18:R:154:LEU:HD13	1.89	0.55
19:S:110:PHE:HD1	19:S:148:PRO:HA	1.70	0.55
21:U:226:GLU:OE1	21:U:226:GLU:N	2.39	0.55
2:B:77:GLU:CG	2:B:78:VAL:H	2.15	0.55
23:Y:48:DC:H2"	23:Y:49:DG:C8	2.41	0.55
5:E:55:ARG:CB	5:E:78:GLU:OE2	2.55	0.55
13:M:94:ASP:OD2	13:M:100:LYS:N	2.39	0.55
1:A:180:GLY:C	1:A:182:GLY:H	2.15	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE3	1:A:1431:SER:HB2	1.88	0.55
1:A:460:ARG:NE	1:A:492:TYR:O	2.32	0.55
2:B:151:LYS:N	2:B:441:SER:OG	2.38	0.55
19:S:126:ILE:O	19:S:137:ALA:HA	2.07	0.55
1:A:121:SER:HA	1:A:126:ILE:HG21	1.87	0.54
1:A:1111:GLY:HA2	21:U:254:GLY:HA2	1.90	0.54
1:A:1310:HIS:HB3	21:U:252:LYS:HD3	1.88	0.54
5:E:185:ILE:HG13	5:E:189:GLN:OE1	2.07	0.54
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.36	0.54
1:A:208:ASP:OD1	1:A:209:SER:N	2.41	0.54
1:A:678:ASN:O	1:A:681:LEU:HB3	2.06	0.54
1:A:685:HIS:HB3	2:B:784:SER:OG	2.07	0.54
2:B:704:LEU:HD22	2:B:708:ALA:HB1	1.89	0.54
5:E:177:ASP:OD1	5:E:178:PRO:HD2	2.08	0.54
16:P:206:GLU:O	16:P:208:ARG:N	2.40	0.54
17:Q:103:VAL:HG23	17:Q:104:LYS:N	2.21	0.54
19:S:47:LEU:HD23	20:T:104:LEU:HD13	1.89	0.54
21:U:251:ALA:O	21:U:252:LYS:CB	2.53	0.54
1:A:262:PRO:O	1:A:263:ALA:CB	2.55	0.54
1:A:266:MET:C	1:A:272:ASN:ND2	2.64	0.54
1:A:870:SER:HB2	1:A:882:SER:HB3	1.90	0.54
2:B:35:ASP:CG	2:B:646:ARG:HH12	2.15	0.54
2:B:879:GLU:O	2:B:879:GLU:HG2	2.07	0.54
9:I:15:ARG:O	9:I:15:ARG:HG3	2.07	0.54
13:M:290:ARG:NH1	22:X:4:DG:OP1	2.39	0.54
19:S:103:ASN:HB2	19:S:107:GLY:HA3	1.89	0.54
1:A:219:GLU:O	1:A:222:HIS:HB3	2.08	0.54
1:A:1250:ASP:C	21:U:227:GLU:HG3	2.33	0.54
2:B:240:LEU:O	2:B:253:GLY:HA2	2.07	0.54
9:I:85:PRO:C	9:I:86:CYS:O	2.49	0.54
18:R:78:LEU:HD11	18:R:124:LEU:HD21	1.89	0.54
1:A:924:TYR:OH	1:A:949:GLN:HA	2.08	0.54
2:B:747:LEU:HD21	2:B:810:PHE:HE1	1.71	0.54
13:M:290:ARG:HH12	22:X:4:DG:P	2.31	0.54
16:P:206:GLU:CD	16:P:236:LYS:NZ	2.66	0.54
1:A:230:ASP:OD1	1:A:244:ARG:NH1	2.40	0.54
1:A:1103:THR:HG23	1:A:1106:THR:H	1.71	0.54
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.90	0.54
1:A:624:GLY:C	1:A:626:THR:N	2.66	0.54
2:B:116:ARG:HH12	12:L:42:ARG:HH11	1.54	0.54
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:323:GLU:HG3	14:N:325:GLY:HA3	1.89	0.54
1:A:549:THR:HG21	1:A:640:LEU:HG	1.90	0.54
1:A:603:ILE:HD11	1:A:988:TRP:NE1	2.23	0.54
1:A:1132:LYS:N	22:X:46:DC:OP1	2.37	0.54
1:A:1316:ASN:HA	21:U:292:ASN:O	2.07	0.54
1:A:1341:VAL:O	1:A:1343:LEU:N	2.38	0.54
8:H:65:TYR:CE2	8:H:70:LEU:CD2	2.91	0.54
13:M:179:GLU:CA	20:T:154:LYS:HG2	2.33	0.54
18:R:225:VAL:HG11	18:R:230:GLU:HG3	1.90	0.54
1:A:137:PRO:HB2	1:A:1445:HIS:NE2	2.23	0.54
2:B:649:ASN:OD1	2:B:650:ASN:N	2.41	0.54
8:H:88:PHE:CE1	8:H:146:LYS:HD2	2.42	0.54
17:Q:109:HIS:HE1	18:R:231:GLU:HA	1.73	0.54
1:A:266:MET:O	1:A:272:ASN:ND2	2.41	0.53
1:A:430:ARG:NH2	13:M:26:ASP:OD2	2.40	0.53
1:A:597:PRO:O	1:A:599:HIS:N	2.40	0.53
2:B:1152:PRO:HG2	2:B:1155:CYS:HB2	1.90	0.53
3:C:262:GLN:HG3	11:K:18:LYS:HG2	1.90	0.53
12:L:27:GLU:O	12:L:29:LYS:N	2.41	0.53
13:M:94:ASP:CG	13:M:99:SER:C	2.76	0.53
1:A:156:GLY:CA	1:A:181:HIS:NE2	2.72	0.53
1:A:203:LYS:O	1:A:204:HIS:CB	2.51	0.53
2:B:853:LEU:HD12	12:L:46:LYS:HE3	1.91	0.53
8:H:108:ALA:O	8:H:109:ALA:C	2.52	0.53
13:M:7:LEU:CD1	13:M:10:LEU:HD13	2.39	0.53
20:T:147:LYS:HG2	20:T:147:LYS:O	2.07	0.53
1:A:389:THR:HB	1:A:417:LYS:HD3	1.90	0.53
1:A:602:CYS:HB2	1:A:655:ILE:HD12	1.91	0.53
2:B:92:TYR:HE2	2:B:146:LYS:NZ	2.06	0.53
17:Q:105:TYR:CE1	18:R:231:GLU:HB2	2.43	0.53
2:B:874:PRO:O	2:B:875:GLU:CB	2.50	0.53
4:D:112:LYS:NZ	4:D:124:ASP:OD2	2.28	0.53
17:Q:23:ARG:HH22	18:R:209:GLN:H	1.40	0.53
18:R:140:LYS:HB3	18:R:141:PRO:HD3	1.89	0.53
1:A:535:MET:O	1:A:669:TYR:OH	2.25	0.53
17:Q:23:ARG:NH2	18:R:208:CYS:CA	2.72	0.53
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.43	0.53
13:M:7:LEU:HD11	13:M:10:LEU:CD1	2.39	0.53
13:M:44:ARG:HH11	13:M:46:ILE:HG22	1.74	0.53
20:T:228:ILE:O	20:T:230:LYS:N	2.38	0.53
1:A:220:ARG:O	1:A:221:VAL:C	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.90	0.53
2:B:289:ILE:HG21	2:B:298:MET:HE1	1.91	0.53
2:B:739:ASN:HB3	10:J:62:TYR:CZ	2.44	0.53
16:P:161:ILE:O	16:P:161:ILE:HG12	2.08	0.53
2:B:195:ILE:HD11	2:B:481:HIS:HE2	1.74	0.53
2:B:225:LEU:C	2:B:227:ASN:H	2.17	0.53
2:B:939:HIS:NE2	2:B:980:HIS:HA	2.24	0.53
5:E:15:LYS:NZ	5:E:33:LEU:O	2.40	0.53
5:E:112:PRO:HA	5:E:115:LYS:HE2	1.91	0.53
9:I:14:ILE:HA	9:I:16:PHE:CE1	2.43	0.53
2:B:160:TYR:HE1	20:T:144:GLN:HG2	1.74	0.53
2:B:248:LYS:O	2:B:249:LYS:HB2	2.07	0.53
2:B:1029:TYR:HA	2:B:1036:LYS:HA	1.91	0.53
3:C:58:VAL:HG21	10:J:59:LEU:HB3	1.90	0.53
8:H:108:ALA:O	8:H:110:THR:N	2.42	0.53
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.91	0.53
20:T:12:ALA:HB2	20:T:106:LEU:HD23	1.91	0.53
21:U:290:VAL:HG22	21:U:297:ARG:HG2	1.90	0.52
1:A:428:ASP:OD1	1:A:430:ARG:N	2.37	0.52
1:A:1248:ASN:HD21	1:A:1255:LEU:HA	1.75	0.52
1:A:1319:LYS:HG3	1:A:1333:GLU:OE1	2.09	0.52
2:B:27:TRP:CD2	2:B:762:ARG:HG2	2.43	0.52
7:G:94:LYS:HG3	7:G:95:VAL:HG23	1.90	0.52
9:I:60:HIS:CD2	9:I:62:VAL:CG1	2.92	0.52
1:A:516:GLN:HG3	1:A:520:MET:HE2	1.90	0.52
2:B:225:LEU:O	2:B:226:GLU:C	2.50	0.52
2:B:489:ILE:HG13	2:B:490:GLY:H	1.74	0.52
10:J:62:TYR:CB	10:J:64:PRO:CD	2.87	0.52
21:U:215:ILE:HG23	21:U:219:LEU:HD23	1.92	0.52
8:H:17:PRO:C	8:H:19:GLY:H	2.17	0.52
8:H:92:MET:HE2	8:H:143:LEU:HD22	1.91	0.52
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.35	0.52
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.91	0.52
1:A:11:SER:O	1:A:13:CYS:N	2.43	0.52
1:A:522:PRO:HG3	1:A:666:ARG:HG2	1.89	0.52
9:I:84:HIS:ND1	9:I:85:PRO:HD3	2.23	0.52
16:P:269:ARG:HB3	16:P:335:PHE:HB3	1.92	0.52
1:A:1172:ASN:OD1	1:A:1173:THR:N	2.43	0.52
2:B:225:LEU:CD1	2:B:228:SER:HB3	2.39	0.52
2:B:289:ILE:HD13	2:B:297:MET:SD	2.50	0.52
2:B:733:MET:HE1	2:B:1054:MET:HE3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:927:ARG:HG3	2:B:1054:MET:HE2	1.92	0.52
1:A:271:ARG:HH22	2:B:821:LYS:CE	2.21	0.52
1:A:476:ILE:HD12	1:A:476:ILE:N	2.25	0.52
1:A:927:GLU:N	1:A:931:ARG:HG2	2.24	0.52
2:B:133:ILE:HD13	2:B:139:GLN:CB	2.39	0.52
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.45	0.52
2:B:628:VAL:HG22	2:B:694:THR:C	2.35	0.52
18:R:194:ARG:CG	18:R:201:LEU:CD1	2.88	0.52
1:A:156:GLY:C	1:A:181:HIS:CD2	2.87	0.52
1:A:1162:GLU:HA	1:A:1304:ILE:HD11	1.92	0.52
17:Q:102:VAL:O	17:Q:102:VAL:HG13	2.10	0.52
1:A:625:ASP:OD2	8:H:22:PHE:CE1	2.63	0.52
2:B:952:GLU:HG3	3:C:39:ILE:HG23	1.91	0.52
14:N:359:ASN:ND2	14:N:364:ASP:OD1	2.43	0.52
17:Q:69:ASP:O	17:Q:70:LYS:HB2	2.10	0.52
1:A:126:ILE:HD13	1:A:129:ILE:HD12	1.92	0.51
2:B:329:GLY:H	2:B:335:ARG:NH2	2.07	0.51
1:A:581:LYS:NZ	8:H:88:PHE:O	2.38	0.51
2:B:160:TYR:CE1	20:T:144:GLN:HG2	2.46	0.51
2:B:906:GLN:HG2	12:L:45:TYR:HE1	1.75	0.51
2:B:991:ALA:HB1	10:J:43:TYR:HB2	1.90	0.51
2:B:1125:MET:H	2:B:1163:MET:HE1	1.75	0.51
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.75	0.51
1:A:264:VAL:CG2	1:A:265:VAL:N	2.73	0.51
1:A:927:GLU:CA	1:A:931:ARG:HG2	2.40	0.51
2:B:92:TYR:HB3	20:T:145:LEU:CG	2.41	0.51
17:Q:101:ASN:C	17:Q:102:VAL:CG1	2.77	0.51
1:A:156:GLY:HA2	1:A:181:HIS:CD2	2.46	0.51
1:A:489:THR:OG1	1:A:494:ALA:O	2.28	0.51
1:A:520:MET:HG3	1:A:522:PRO:HD2	1.93	0.51
2:B:72:GLN:NE2	2:B:77:GLU:O	2.44	0.51
2:B:116:ARG:NH1	12:L:42:ARG:HH11	2.09	0.51
16:P:297:LYS:C	16:P:299:ARG:H	2.17	0.51
18:R:190:LEU:CD1	18:R:205:ASP:CB	2.88	0.51
19:S:29:MET:HE2	19:S:146:PHE:HE2	1.75	0.51
1:A:689:ILE:HD13	2:B:985:LEU:HD22	1.93	0.51
18:R:177:ASN:HD22	18:R:177:ASN:C	2.19	0.51
22:X:39:DT:H2”	22:X:40:DT:H5”	1.92	0.51
1:A:1036:ASN:C	1:A:1036:ASN:HD22	2.18	0.51
2:B:45:ASP:OD2	2:B:531:TYR:OH	2.25	0.51
5:E:29:THR:HG22	5:E:31:ASP:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:66:ARG:HB3	15:O:73:THR:HB	1.93	0.51
17:Q:110:MET:SD	18:R:222:SER:HB2	2.50	0.51
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.91	0.51
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.93	0.51
3:C:4:ALA:HB2	11:K:93:ASP:OD2	2.11	0.51
5:E:47:LYS:NZ	5:E:52:ARG:O	2.41	0.51
9:I:15:ARG:C	9:I:16:PHE:O	2.53	0.51
8:H:10:PHE:CE2	8:H:39:LEU:HD13	2.46	0.51
1:A:153:ILE:O	1:A:154:CYS:O	2.29	0.51
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.51	0.51
2:B:193:VAL:N	2:B:468:GLN:O	2.41	0.51
13:M:17:ASN:OD1	13:M:18:HIS:N	2.44	0.51
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.46	0.51
1:A:271:ARG:HH12	2:B:821:LYS:CE	2.24	0.50
1:A:281:ALA:O	1:A:285:LYS:HG3	2.12	0.50
1:A:1181:PRO:C	1:A:1183:SER:H	2.18	0.50
2:B:92:TYR:CD1	20:T:145:LEU:HD13	2.30	0.50
2:B:714:PRO:O	2:B:717:ASN:HB2	2.11	0.50
7:G:151:ARG:HB2	7:G:158:PHE:CE1	2.46	0.50
8:H:106:THR:O	8:H:107:GLU:HB2	2.09	0.50
10:J:28:GLU:HG2	10:J:30:THR:HG22	1.93	0.50
17:Q:108:ASP:OD1	17:Q:111:ARG:NH2	2.19	0.50
1:A:202:TRP:HZ3	1:A:212:LYS:CG	2.09	0.50
2:B:733:MET:HE3	2:B:1051:LEU:O	2.12	0.50
1:A:924:TYR:HH	1:A:949:GLN:HA	1.77	0.50
1:A:1427:LEU:HD23	1:A:1456:GLU:HB3	1.93	0.50
2:B:513:GLU:HG3	2:B:726:SER:HB3	1.94	0.50
2:B:746:THR:HG22	2:B:812:ARG:NH1	2.27	0.50
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.93	0.50
22:X:13:DA:N6	23:Y:80:DT:O4	2.44	0.50
1:A:131:ALA:O	1:A:133:SER:N	2.45	0.50
2:B:866:ILE:HG13	2:B:867:ILE:N	2.25	0.50
2:B:157:ARG:N	2:B:161:CYS:SG	2.71	0.50
2:B:225:LEU:CD1	2:B:228:SER:CB	2.89	0.50
2:B:380:ARG:HE	2:B:609:GLU:CD	2.19	0.50
2:B:387:HIS:CD2	2:B:504:THR:HG21	2.46	0.50
2:B:738:THR:HG22	2:B:772:LEU:HD21	1.93	0.50
7:G:10:GLU:HB3	7:G:67:LEU:HD11	1.92	0.50
19:S:100:LEU:HD23	19:S:110:PHE:HD2	1.75	0.50
20:T:177:ARG:HE	20:T:208:GLN:HB2	1.77	0.50
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.76	0.50
1:A:595:ILE:C	1:A:595:ILE:HD12	2.37	0.50
2:B:499:ARG:HH11	2:B:520:VAL:HG22	1.76	0.50
2:B:803:ARG:HH12	2:B:951:GLN:HE22	1.59	0.50
13:M:103:ASN:HB3	13:M:105:ARG:HH22	1.77	0.50
16:P:242:GLN:HG3	16:P:248:ALA:HB3	1.94	0.50
17:Q:23:ARG:CD	18:R:207:SER:C	2.76	0.50
17:Q:180:PHE:CZ	18:R:211:SER:HA	2.39	0.50
1:A:614:ASP:O	1:A:615:SER:OG	2.21	0.50
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.42	0.50
2:B:628:VAL:HG12	2:B:633:LEU:HD23	1.94	0.50
2:B:838:GLN:O	2:B:891:ASP:N	2.40	0.50
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.47	0.50
2:B:1069:ILE:HG12	13:M:48:VAL:CG1	2.42	0.50
2:B:1124:ILE:HD12	2:B:1124:ILE:H	1.76	0.50
1:A:924:TYR:CE1	1:A:949:GLN:HG2	2.47	0.50
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.93	0.50
3:C:67:ARG:HH22	10:J:2:ILE:HG13	1.77	0.50
7:G:44:PHE:CD2	7:G:103:PRO:HG2	2.47	0.50
13:M:52:TRP:CD1	13:M:67:VAL:HG22	2.47	0.50
20:T:160:GLN:HA	20:T:163:ILE:HD12	1.94	0.50
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.76	0.49
13:M:60:ALA:O	13:M:62:LYS:N	2.45	0.49
16:P:203:ARG:HG3	16:P:203:ARG:NH2	2.25	0.49
1:A:980:PRO:HB2	1:A:981:CYS:SG	2.51	0.49
2:B:1117:HIS:O	2:B:1127:ILE:HG12	2.11	0.49
7:G:91:GLN:HG2	17:Q:145:PHE:CE1	2.47	0.49
8:H:17:PRO:O	8:H:19:GLY:N	2.45	0.49
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.59	0.49
8:H:103:GLU:HA	8:H:108:ALA:HB1	1.95	0.49
1:A:138:LYS:HB2	1:A:1445:HIS:HE1	1.76	0.49
1:A:326:PRO:HB3	13:M:87:GLY:N	2.27	0.49
1:A:691:ASP:HB3	1:A:766:PHE:HB2	1.94	0.49
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.45	0.49
19:S:125:TYR:CD1	19:S:139:PRO:HA	2.47	0.49
1:A:133:SER:O	1:A:136:GLN:N	2.35	0.49
3:C:44:ILE:HD11	3:C:238:SER:HB2	1.94	0.49
5:E:40:PHE:HE2	5:E:46:ASP:OD2	1.95	0.49
13:M:179:GLU:HA	20:T:154:LYS:CG	2.36	0.49
22:X:46:DC:H42	23:Y:47:DG:H22	1.59	0.49
1:A:800:PHE:HZ	1:A:815:TYR:CE1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:TRP:HE1	1:A:1248:ASN:HB3	1.77	0.49
1:A:1392:TYR:OH	1:A:1394:ASN:HA	2.13	0.49
2:B:77:GLU:HB3	2:B:78:VAL:HG23	1.93	0.49
2:B:968:ASN:CG	2:B:969:PRO:HD2	2.37	0.49
13:M:79:ASP:OD1	13:M:79:ASP:N	2.46	0.49
17:Q:35:ASP:CG	18:R:161:ARG:HH22	2.18	0.49
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.48	0.49
1:A:362:SER:HB3	2:B:1084:LEU:HD12	1.95	0.49
2:B:35:ASP:OD2	2:B:646:ARG:NH1	2.37	0.49
2:B:563:ASP:OD1	2:B:610:ARG:NH1	2.45	0.49
7:G:98:PHE:CZ	17:Q:152:PHE:HE1	2.31	0.49
16:P:311:VAL:HG11	23:Y:81:DA:C2	2.47	0.49
16:P:311:VAL:HG11	23:Y:81:DA:H2	1.78	0.49
19:S:118:VAL:HG13	19:S:120:GLU:HG3	1.95	0.49
1:A:361:PHE:HD1	1:A:388:MET:HE3	1.78	0.49
2:B:20:ASP:OD1	2:B:21:LEU:N	2.45	0.49
2:B:509:VAL:HG11	2:B:524:LYS:HB3	1.94	0.49
2:B:905:ASP:OD1	2:B:924:ARG:NH1	2.46	0.49
3:C:7:PRO:HG3	11:K:97:GLU:HG2	1.94	0.49
5:E:192:LYS:HE3	5:E:194:ILE:HD11	1.93	0.49
13:M:57:ASN:ND2	23:Y:54:DA:OP2	2.44	0.49
13:M:128:ILE:HG23	13:M:183:VAL:HG11	1.95	0.49
13:M:297:PRO:HG3	13:M:310:VAL:HG11	1.93	0.49
14:N:332:GLU:CD	15:O:92:LYS:HD3	2.38	0.49
1:A:262:PRO:CG	1:A:274:ASP:OD1	2.50	0.49
2:B:351:VAL:HG11	2:B:361:LYS:HA	1.94	0.49
3:C:267:ILE:HG21	3:C:274:ILE:HD13	1.93	0.49
22:X:40:DT:H1'	22:X:41:DT:H3'	1.95	0.49
1:A:27:SER:O	1:A:31:LEU:N	2.42	0.49
1:A:632:ASN:CA	1:A:992:LYS:HD2	2.43	0.49
2:B:191:GLU:OE2	2:B:472:ARG:NH1	2.46	0.49
2:B:223:SER:O	2:B:224:CYS:HB3	2.12	0.49
3:C:68:LEU:O	3:C:71:ILE:HG12	2.13	0.49
8:H:37:MET:HG2	8:H:127:GLY:HA3	1.95	0.49
17:Q:103:VAL:HG23	17:Q:107:LEU:CD1	2.43	0.49
1:A:210:GLN:CD	1:A:212:LYS:HG2	2.37	0.48
1:A:460:ARG:HB2	1:A:501:MET:SD	2.52	0.48
1:A:1408:ARG:NH2	1:A:1421:ARG:O	2.45	0.48
2:B:81:PRO:HD2	2:B:135:GLU:HG3	1.94	0.48
9:I:61:GLU:O	9:I:63:ASP:N	2.45	0.48
13:M:94:ASP:OD1	13:M:100:LYS:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:C	1:A:181:HIS:NE2	2.68	0.48
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.48	0.48
1:A:817:PRO:HG2	1:A:818:GLU:OE1	2.12	0.48
1:A:873:VAL:HB	1:A:1083:PRO:HA	1.93	0.48
11:K:61:TYR:HA	11:K:72:ILE:O	2.14	0.48
14:N:312:GLU:HB3	14:N:313:PRO:HD3	1.95	0.48
17:Q:101:ASN:O	17:Q:102:VAL:HG13	2.08	0.48
17:Q:102:VAL:O	17:Q:102:VAL:HG22	2.11	0.48
17:Q:105:TYR:CE1	18:R:231:GLU:OE1	2.59	0.48
1:A:484:LEU:N	1:A:484:LEU:HD23	2.28	0.48
1:A:809:HIS:CE1	2:B:697:GLU:OE2	2.67	0.48
4:D:40:LEU:HD13	7:G:75:ILE:HD11	1.95	0.48
5:E:11:TRP:O	5:E:15:LYS:HG2	2.14	0.48
5:E:47:LYS:HB2	5:E:48:PRO:HD3	1.78	0.48
1:A:924:TYR:CZ	1:A:949:GLN:HA	2.48	0.48
2:B:73:HIS:C	2:B:75:SER:N	2.71	0.48
2:B:549:SER:OG	2:B:577:HIS:NE2	2.44	0.48
3:C:136:ASP:CG	3:C:138:ASP:HB2	2.34	0.48
12:L:27:GLU:O	12:L:28:ILE:C	2.57	0.48
13:M:178:LYS:NZ	23:Y:86:DC:OP1	2.45	0.48
17:Q:28:ILE:HG21	18:R:205:ASP:OD2	2.13	0.48
1:A:1188:GLU:O	1:A:1192:TRP:HZ3	1.97	0.48
5:E:52:ARG:CG	5:E:53:PRO:CD	2.87	0.48
8:H:111:ARG:HB3	8:H:127:GLY:O	2.13	0.48
18:R:88:ARG:NH1	18:R:105:GLU:OE2	2.42	0.48
18:R:138:ALA:C	18:R:140:LYS:N	2.69	0.48
20:T:37:ARG:HH22	20:T:62:LEU:HB2	1.78	0.48
21:U:292:ASN:O	21:U:294:CYS:N	2.47	0.48
1:A:272:ASN:O	1:A:273:GLN:C	2.54	0.48
1:A:1155:LYS:HD3	21:U:249:GLN:OE1	2.13	0.48
2:B:1040:GLN:CD	2:B:1040:GLN:N	2.71	0.48
3:C:155:LYS:HB3	10:J:65:LEU:HD22	1.95	0.48
17:Q:113:ARG:HH12	18:R:218:LYS:HG3	1.79	0.48
1:A:546:ARG:HB3	1:A:640:LEU:O	2.13	0.48
1:A:1186:VAL:HG12	1:A:1188:GLU:HG2	1.96	0.48
18:R:93:ASP:HB3	18:R:95:HIS:CE1	2.47	0.48
1:A:379:GLY:HA2	1:A:475:ARG:O	2.14	0.48
2:B:26:CYS:SG	2:B:27:TRP:N	2.87	0.48
13:M:235:ILE:HD11	13:M:300:PHE:CE1	2.49	0.48
17:Q:28:ILE:CG2	18:R:205:ASP:OD2	2.61	0.48
1:A:138:LYS:NZ	1:A:1441:GLU:OE2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:HG22	1:A:468:SER:HB3	1.94	0.48
1:A:1036:ASN:ND2	1:A:1037:ALA:N	2.62	0.48
1:A:1213:ARG:NH2	1:A:1215:GLU:OE2	2.46	0.48
1:A:1410:HIS:N	5:E:174:GLN:HE22	2.12	0.48
2:B:202:THR:O	2:B:204:THR:N	2.47	0.48
7:G:114:PRO:HB2	7:G:116:GLU:HG2	1.95	0.48
17:Q:36:ILE:HD13	17:Q:52:LEU:HD21	1.96	0.48
21:U:290:VAL:HG13	21:U:297:ARG:HG2	1.96	0.48
1:A:1313:GLN:NE2	1:A:1318:LYS:HD2	2.20	0.48
2:B:1022:LEU:CD1	2:B:1023:ARG:HG3	2.44	0.48
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.95	0.48
20:T:177:ARG:CZ	20:T:212:TYR:HB2	2.44	0.48
1:A:297:GLY:HA3	17:Q:57:LYS:HG3	1.96	0.47
2:B:232:THR:OG1	2:B:233:SER:N	2.46	0.47
9:I:15:ARG:NH1	9:I:46:GLN:OE1	2.47	0.47
18:R:157:GLN:OE1	18:R:162:GLY:HA2	2.14	0.47
18:R:161:ARG:C	18:R:163:LEU:H	2.22	0.47
22:X:38:DT:H2'	22:X:39:DT:C6	2.49	0.47
1:A:155:GLU:C	1:A:181:HIS:CE1	2.92	0.47
1:A:1109:TYR:O	21:U:256:THR:HG22	2.14	0.47
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.96	0.47
8:H:56:PHE:HA	8:H:148:LEU:HA	1.96	0.47
13:M:289:TYR:HA	13:M:292:ILE:HG12	1.96	0.47
19:S:174:PHE:O	19:S:178:GLN:HG2	2.14	0.47
20:T:94:THR:HG22	20:T:109:ILE:HA	1.96	0.47
1:A:58:MET:HE3	1:A:258:LEU:HD21	1.96	0.47
1:A:490:THR:HG23	21:U:282:ASP:HB3	1.96	0.47
5:E:52:ARG:O	5:E:53:PRO:C	2.57	0.47
16:P:298:PRO:O	16:P:299:ARG:C	2.56	0.47
19:S:25:LYS:HD3	19:S:141:HIS:CD2	2.49	0.47
20:T:139:VAL:CG1	20:T:142:SER:OG	2.62	0.47
1:A:90:LEU:O	1:A:291:ARG:NH2	2.47	0.47
2:B:200:MET:HE1	2:B:220:GLU:OE2	2.14	0.47
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.49	0.47
13:M:235:ILE:HD11	13:M:300:PHE:HE1	1.79	0.47
16:P:239:ARG:HA	16:P:239:ARG:HD2	1.57	0.47
1:A:689:ILE:O	1:A:692:SER:OG	2.29	0.47
2:B:474:THR:HG23	2:B:477:SER:H	1.78	0.47
2:B:936:ALA:HB2	2:B:942:LYS:HA	1.97	0.47
3:C:143:VAL:HG23	3:C:144:GLU:H	1.80	0.47
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:22:ILE:HG23	13:M:35:PRO:HG2	1.96	0.47
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.96	0.47
15:O:50:GLN:O	15:O:53:ARG:NH1	2.47	0.47
1:A:117:LEU:HD23	1:A:119:VAL:H	1.80	0.47
1:A:766:PHE:CE1	1:A:781:ILE:HG12	2.49	0.47
2:B:119:THR:HG23	2:B:187:ILE:HA	1.97	0.47
2:B:414:GLU:HG2	2:B:436:LYS:HD3	1.95	0.47
2:B:715:ASP:OD1	2:B:715:ASP:N	2.46	0.47
2:B:1069:ILE:HA	2:B:1072:ARG:HE	1.80	0.47
3:C:61:ASP:OD2	12:L:48:ARG:NH1	2.48	0.47
10:J:44:CYS:O	10:J:47:ARG:HG3	2.15	0.47
1:A:206:ASN:C	1:A:208:ASP:H	2.22	0.47
1:A:220:ARG:HD2	1:A:223:GLU:OE1	2.14	0.47
1:A:406:VAL:HG21	1:A:440:LEU:HD11	1.97	0.47
1:A:522:PRO:HG3	1:A:666:ARG:HE	1.79	0.47
1:A:1251:ASN:HD21	21:U:227:GLU:HB3	1.79	0.47
2:B:101:ARG:O	13:M:175:ARG:NH2	2.45	0.47
2:B:127:ASP:OD2	2:B:144:HIS:NE2	2.47	0.47
3:C:242:GLU:OE1	3:C:242:GLU:N	2.46	0.47
8:H:128:ASP:N	8:H:128:ASP:OD1	2.46	0.47
9:I:57:LYS:C	9:I:59:THR:N	2.68	0.47
9:I:93:GLU:O	9:I:115:THR:HG22	2.15	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.15	0.47
15:O:66:ARG:N	15:O:73:THR:O	2.48	0.47
16:P:157:GLU:CD	16:P:333:LYS:HD3	2.40	0.47
16:P:206:GLU:CB	16:P:236:LYS:NZ	2.75	0.47
16:P:206:GLU:OE1	16:P:236:LYS:NZ	2.47	0.47
17:Q:109:HIS:HE1	18:R:231:GLU:CA	2.28	0.47
18:R:193:ASN:HB3	18:R:197:LYS:HA	1.95	0.47
18:R:213:ASP:C	18:R:215:GLU:H	2.22	0.47
21:U:252:LYS:HD2	21:U:252:LYS:HA	1.44	0.47
1:A:1177:TYR:N	9:I:51:SER:HB3	2.27	0.47
2:B:274:ARG:HE	2:B:308:ALA:HB1	1.79	0.47
2:B:1115:GLN:OE1	2:B:1115:GLN:N	2.47	0.47
1:A:641:CYS:SG	1:A:643:LYS:N	2.86	0.47
1:A:691:ASP:OD1	1:A:765:ASN:N	2.48	0.47
1:A:1450:PRO:O	1:A:1452:LYS:HG3	2.15	0.47
2:B:854:ILE:O	2:B:907:VAL:HG21	2.15	0.47
10:J:63:ALA:H	10:J:64:PRO:HD3	1.75	0.47
13:M:10:LEU:O	13:M:12:ARG:CA	2.53	0.47
13:M:86:LYS:NZ	22:X:35:DT:H3	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:205:SER:OG	16:P:278:GLN:NE2	2.43	0.47
1:A:532:ARG:HB3	1:A:649:ALA:HB2	1.96	0.47
1:A:809:HIS:HE1	2:B:697:GLU:OE2	1.98	0.47
1:A:929:ALA:C	1:A:931:ARG:N	2.73	0.47
2:B:41:ARG:HA	2:B:41:ARG:HD2	1.68	0.47
7:G:110:ARG:HA	7:G:113:ILE:HD12	1.97	0.47
13:M:169:ARG:HH11	13:M:206:VAL:HG21	1.79	0.47
22:X:44:DC:H2'	22:X:45:DG:C8	2.49	0.47
23:Y:71:DA:H2'	23:Y:71:DA:OP2	2.15	0.47
3:C:171:LYS:HE3	11:K:10:PHE:HB3	1.96	0.46
6:F:56:TYR:CD1	6:F:124:ILE:HB	2.50	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.80	0.46
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.50	0.46
16:P:161:ILE:O	16:P:161:ILE:HG23	2.15	0.46
1:A:246:GLU:HG2	1:A:247:TRP:CD1	2.49	0.46
1:A:606:HIS:O	1:A:608:THR:N	2.45	0.46
1:A:625:ASP:OD2	8:H:22:PHE:HE1	1.98	0.46
2:B:298:MET:O	2:B:301:VAL:HG12	2.16	0.46
2:B:1028:LEU:HA	2:B:1028:LEU:HD12	1.51	0.46
10:J:7:CYS:SG	10:J:48:MET:HE3	2.54	0.46
13:M:12:ARG:NH1	13:M:23:LEU:O	2.48	0.46
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.15	0.46
2:B:101:ARG:HB3	13:M:131:PRO:HG2	1.96	0.46
2:B:911:LEU:HD13	2:B:915:GLY:HA2	1.96	0.46
1:A:890:ARG:NH2	1:A:1023:VAL:HB	2.30	0.46
1:A:1013:VAL:HG11	1:A:1046:ARG:HG2	1.97	0.46
1:A:1192:TRP:HA	1:A:1195:VAL:HB	1.98	0.46
1:A:1199:MET:SD	1:A:1200:PRO:HD2	2.55	0.46
2:B:187:ILE:HD11	2:B:448:LEU:HD23	1.98	0.46
2:B:646:ARG:HA	2:B:649:ASN:HB3	1.98	0.46
3:C:49:TRP:O	3:C:163:ALA:HA	2.16	0.46
9:I:119:CYS:C	9:I:121:HIS:H	2.24	0.46
18:R:196:ASP:C	18:R:198:LYS:N	2.45	0.46
16:P:207:PRO:O	16:P:208:ARG:O	2.34	0.46
19:S:165:GLU:HA	19:S:168:ASN:HB2	1.97	0.46
22:X:31:DG:H2"	22:X:32:DA:O5'	2.16	0.46
1:A:561:MET:HG2	11:K:58:PHE:CD1	2.50	0.46
1:A:581:LYS:NZ	8:H:86:ASP:O	2.49	0.46
1:A:1408:ARG:HD2	1:A:1422:GLN:HE22	1.80	0.46
2:B:163:LEU:HD12	2:B:163:LEU:N	2.31	0.46
2:B:613:ARG:HD3	2:B:615:TYR:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:GLN:NE2	9:I:108:MET:SD	2.89	0.46
12:L:26:ASN:C	12:L:28:ILE:H	2.24	0.46
17:Q:24:GLY:O	18:R:210:PHE:HE2	1.99	0.46
18:R:149:LYS:HD2	18:R:175:LEU:H	1.81	0.46
20:T:179:ASP:O	20:T:181:GLN:N	2.48	0.46
22:X:37:DT:H4'	22:X:38:DT:H4'	1.98	0.46
1:A:1484:MET:CE	7:G:20:PRO:HD3	2.45	0.46
3:C:6:GLN:HG3	3:C:6:GLN:O	2.16	0.46
9:I:84:HIS:HB2	9:I:85:PRO:HD3	0.85	0.46
13:M:37:CYS:SG	13:M:39:LEU:HB2	2.55	0.46
18:R:138:ALA:O	18:R:140:LYS:N	2.49	0.46
1:A:133:SER:C	1:A:135:GLY:H	2.23	0.46
1:A:197:GLU:OE2	13:M:93:PHE:CE1	2.66	0.46
1:A:1128:ILE:HD11	1:A:1401:LEU:HD21	1.97	0.46
2:B:800:ALA:C	2:B:805:PHE:HB3	2.41	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HE3	1.98	0.46
3:C:262:GLN:O	3:C:266:GLU:HG2	2.16	0.46
13:M:182:ALA:CB	20:T:154:LYS:HG3	2.42	0.46
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.33	0.46
22:X:38:DT:C5	22:X:39:DT:H72	2.51	0.46
1:A:533:PRO:CG	1:A:654:HIS:HB2	2.46	0.46
1:A:592:PHE:CZ	1:A:595:ILE:HD11	2.50	0.46
2:B:195:ILE:HG21	2:B:486:ASN:HB2	1.97	0.46
2:B:529:MET:HE2	2:B:623:ARG:CB	2.42	0.46
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.79	0.46
5:E:172:ARG:HD2	5:E:210:GLN:HB3	1.98	0.46
8:H:7:GLU:OE2	8:H:57:ARG:NH2	2.48	0.46
8:H:108:ALA:C	8:H:110:THR:N	2.74	0.46
13:M:44:ARG:NH1	13:M:46:ILE:HG22	2.30	0.46
20:T:191:PHE:HA	20:T:197:TYR:HE2	1.81	0.46
1:A:777:SER:OG	1:A:779:ILE:HG22	2.15	0.46
2:B:285:LEU:O	2:B:289:ILE:HG22	2.16	0.46
2:B:897:ARG:O	2:B:898:THR:C	2.59	0.46
2:B:992:ASN:O	10:J:46:ARG:NH2	2.48	0.46
3:C:149:LEU:HD23	10:J:2:ILE:HD13	1.98	0.46
14:N:21:VAL:HG21	15:O:40:PHE:HD1	1.81	0.46
1:A:609:HIS:N	1:A:610:PRO:HD3	2.29	0.45
1:A:693:ILE:HG21	2:B:1023:ARG:NE	2.32	0.45
1:A:1050:CYS:HB3	1:A:1053:ARG:HG2	1.98	0.45
2:B:646:ARG:O	2:B:646:ARG:HG2	2.16	0.45
2:B:754:PRO:HB2	2:B:773:PRO:CG	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:GLN:HG2	12:L:45:TYR:CE1	2.51	0.45
18:R:120:MET:SD	18:R:137:TYR:OH	2.69	0.45
1:A:546:ARG:HE	1:A:546:ARG:HB2	1.59	0.45
1:A:1319:LYS:H	1:A:1356:ARG:HH22	1.64	0.45
5:E:14:ARG:NH1	5:E:58:LEU:O	2.49	0.45
5:E:25:GLY:O	5:E:65:ASN:HA	2.16	0.45
5:E:55:ARG:HD2	5:E:78:GLU:OE1	2.17	0.45
13:M:10:LEU:H	13:M:11:PRO:CD	2.24	0.45
15:O:3:TYR:CB	15:O:98:CYS:SG	2.98	0.45
18:R:78:LEU:HB2	18:R:119:LEU:HD22	1.98	0.45
19:S:125:TYR:HD1	19:S:139:PRO:HA	1.81	0.45
1:A:364:ARG:NE	1:A:500:GLU:CD	2.73	0.45
1:A:546:ARG:HG3	1:A:547:LYS:H	1.82	0.45
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.98	0.45
1:A:999:ARG:HE	8:H:99:ILE:CD1	2.22	0.45
2:B:422:PHE:CD1	2:B:422:PHE:C	2.92	0.45
2:B:487:SER:HA	2:B:488:PRO:HD3	1.67	0.45
2:B:898:THR:OG1	2:B:899:SER:N	2.49	0.45
8:H:24:ARG:O	8:H:45:ILE:N	2.49	0.45
19:S:143:TRP:C	19:S:143:TRP:CD1	2.95	0.45
21:U:280:SER:HB2	21:U:284:PRO:HA	1.98	0.45
2:B:739:ASN:HB3	10:J:62:TYR:OH	2.16	0.45
2:B:758:LEU:O	2:B:996:ILE:HG23	2.16	0.45
6:F:109:TYR:CD1	6:F:115:TYR:HB3	2.51	0.45
8:H:81:ARG:C	8:H:83:SER:H	2.25	0.45
13:M:91:ALA:O	13:M:92:SER:C	2.58	0.45
1:A:97:VAL:HG21	1:A:322:LEU:HD21	1.99	0.45
1:A:728:THR:HG23	1:A:736:THR:HG23	1.99	0.45
1:A:1036:ASN:C	1:A:1036:ASN:ND2	2.73	0.45
1:A:1112:VAL:HB	21:U:253:THR:HB	1.99	0.45
1:A:1408:ARG:HD2	1:A:1422:GLN:NE2	2.30	0.45
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.39	0.45
1:A:1484:MET:HE1	7:G:20:PRO:HG3	1.99	0.45
2:B:250:SER:HB3	2:B:251:ALA:H	1.40	0.45
2:B:1062:ARG:HH11	2:B:1082:GLY:HA2	1.80	0.45
2:B:1066:PRO:HA	13:M:46:ILE:HG21	1.98	0.45
3:C:44:ILE:HD11	3:C:238:SER:CB	2.46	0.45
8:H:75:TYR:HD1	8:H:75:TYR:H	1.65	0.45
13:M:86:LYS:HZ2	22:X:35:DT:H3	1.64	0.45
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.99	0.45
20:T:26:TYR:HE2	20:T:124:TYR:OH	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:177:ARG:HH22	20:T:212:TYR:CB	2.29	0.45
21:U:255:GLY:HA3	21:U:257:GLN:OE1	2.16	0.45
22:X:12:DT:H2"	22:X:13:DA:H8	1.81	0.45
1:A:210:GLN:HB2	1:A:212:LYS:HD2	1.99	0.45
2:B:900:GLU:OE1	11:K:1:MET:N	2.43	0.45
4:D:26:PHE:HE2	7:G:78:ARG:HG2	1.82	0.45
8:H:23:ASP:OD1	8:H:23:ASP:N	2.49	0.45
9:I:66:THR:C	9:I:68:ILE:H	2.24	0.45
18:R:225:VAL:HB	18:R:230:GLU:CB	2.47	0.45
1:A:527:THR:HG22	1:A:532:ARG:O	2.17	0.45
2:B:51:ILE:HG23	2:B:51:ILE:HD12	1.64	0.45
2:B:201:ALA:HB3	2:B:206:TYR:OH	2.16	0.45
2:B:651:TYR:HA	2:B:655:ASP:OD2	2.16	0.45
10:J:62:TYR:CB	10:J:64:PRO:HD2	2.46	0.45
13:M:37:CYS:SG	13:M:39:LEU:HD23	2.56	0.45
16:P:171:THR:HG22	16:P:220:VAL:HG22	1.98	0.45
2:B:225:LEU:HD13	2:B:228:SER:HB3	1.98	0.45
3:C:146:ASP:O	3:C:148:ILE:N	2.49	0.45
13:M:246:PRO:HB2	16:P:306:VAL:HG21	1.99	0.45
23:Y:80:DT:H2"	23:Y:81:DA:C8	2.52	0.45
1:A:522:PRO:N	1:A:666:ARG:HH21	2.15	0.45
1:A:611:ASP:OD2	1:A:627:LYS:HG3	2.17	0.45
2:B:51:ILE:HG22	20:T:141:LEU:HD13	1.89	0.45
2:B:514:THR:HG21	2:B:521:GLY:HA2	1.99	0.45
2:B:952:GLU:HG3	3:C:39:ILE:CG2	2.46	0.45
5:E:172:ARG:CD	5:E:210:GLN:HB3	2.47	0.45
9:I:14:ILE:HA	9:I:16:PHE:CD1	2.52	0.45
13:M:108:SER:HB3	13:M:112:ARG:NH1	2.31	0.45
14:N:324:GLU:HA	16:P:188:ARG:NH1	2.29	0.45
1:A:931:ARG:O	1:A:932:ARG:CG	2.65	0.45
2:B:100:GLU:O	2:B:103:GLY:N	2.40	0.45
2:B:295:PRO:HB2	9:I:11:PHE:CD2	2.46	0.45
2:B:453:TRP:CG	2:B:463:ARG:HB2	2.52	0.45
2:B:1101:GLN:OE1	6:F:64:ARG:NH1	2.50	0.45
15:O:3:TYR:HD1	15:O:98:CYS:SG	2.38	0.45
20:T:152:ASN:OD1	20:T:152:ASN:N	2.49	0.45
23:Y:56:DG:C2'	23:Y:57:DA:H5'	2.46	0.45
1:A:37:THR:O	1:A:39:GLY:N	2.50	0.44
1:A:107:LEU:HD23	1:A:191:ILE:HD13	1.99	0.44
1:A:267:GLN:H	13:M:49:GLY:CA	2.29	0.44
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASP:HB3	2:B:792:ASP:OD2	2.16	0.44
1:A:1195:VAL:HG12	21:U:192:ARG:HD3	1.98	0.44
2:B:250:SER:O	2:B:251:ALA:C	2.60	0.44
2:B:319:ASN:OD1	2:B:332:LYS:HG3	2.18	0.44
3:C:45:ILE:HG22	3:C:73:LEU:HD12	1.98	0.44
3:C:149:LEU:HD23	10:J:2:ILE:CD1	2.47	0.44
6:F:64:ARG:HH22	7:G:61:PRO:HB3	1.82	0.44
11:K:29:ASN:ND2	11:K:78:THR:O	2.50	0.44
18:R:77:VAL:HA	18:R:80:LYS:HE3	1.99	0.44
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.83	0.44
20:T:177:ARG:NH1	20:T:212:TYR:HB2	2.32	0.44
1:A:477:LEU:HB2	1:A:478:PRO:HD2	2.00	0.44
1:A:666:ARG:HA	1:A:666:ARG:HD3	1.28	0.44
1:A:1274:GLU:O	1:A:1276:VAL:N	2.48	0.44
2:B:403:LEU:O	2:B:407:MET:HG2	2.17	0.44
2:B:896:LEU:HD23	2:B:901:THR:HG21	1.97	0.44
8:H:130:ASN:O	8:H:134:GLY:N	2.50	0.44
10:J:6:ARG:H	10:J:14:VAL:H	1.65	0.44
10:J:21:TYR:CG	10:J:49:LEU:HD21	2.52	0.44
15:O:64:THR:CG2	16:P:188:ARG:HB3	2.47	0.44
17:Q:71:PHE:CE1	17:Q:106:LYS:HE3	2.52	0.44
1:A:610:PRO:O	1:A:612:ASP:N	2.50	0.44
1:A:797:ARG:NH2	1:A:820:ARG:HB2	2.33	0.44
1:A:908:THR:C	1:A:910:LYS:H	2.23	0.44
1:A:1191:GLU:O	1:A:1195:VAL:HG23	2.17	0.44
3:C:71:ILE:HG13	3:C:71:ILE:O	2.16	0.44
6:F:62:ARG:HH12	6:F:127:ASP:C	2.20	0.44
7:G:97:LEU:HD23	7:G:108:ILE:HD12	1.97	0.44
14:N:11:PRO:HA	14:N:14:TYR:HD2	1.81	0.44
14:N:32:ASP:HB3	14:N:34:VAL:HG23	2.00	0.44
14:N:354:LYS:HA	14:N:369:LYS:HA	1.99	0.44
18:R:153:ARG:O	18:R:157:GLN:N	2.46	0.44
1:A:156:GLY:CA	1:A:181:HIS:CD2	3.00	0.44
1:A:416:ALA:HA	1:A:448:ARG:HA	2.00	0.44
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.47	0.44
10:J:67:LYS:HB3	12:L:23:HIS:HE1	1.82	0.44
20:T:168:LYS:C	20:T:170:LYS:H	2.24	0.44
1:A:19:LYS:HD3	2:B:1174:VAL:HG23	1.98	0.44
1:A:275:ASP:HA	1:A:278:HIS:HB2	1.99	0.44
1:A:932:ARG:HD2	1:A:939:VAL:HG21	1.99	0.44
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:LEU:HD22	3:C:151:VAL:HG23	1.99	0.44
7:G:152:VAL:HG22	7:G:157:ILE:HG13	1.98	0.44
10:J:21:TYR:HB2	10:J:38:LEU:CD1	2.47	0.44
13:M:94:ASP:CG	13:M:100:LYS:N	2.75	0.44
13:M:252:SER:OG	23:Y:85:DG:OP1	2.30	0.44
14:N:315:ASN:HA	16:P:239:ARG:HH12	1.82	0.44
14:N:349:TRP:HB3	14:N:351:PHE:CE1	2.53	0.44
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.99	0.44
18:R:163:LEU:HD12	18:R:163:LEU:HA	1.76	0.44
1:A:19:LYS:HD2	2:B:1173:SER:H	1.82	0.44
1:A:51:ARG:NH2	2:B:878:ASP:OD1	2.51	0.44
1:A:264:VAL:O	1:A:265:VAL:C	2.60	0.44
1:A:389:THR:HB	1:A:417:LYS:CD	2.48	0.44
1:A:522:PRO:CA	1:A:666:ARG:HE	2.31	0.44
1:A:1319:LYS:HD2	1:A:1319:LYS:HA	1.37	0.44
2:B:87:LYS:NZ	2:B:89:GLU:OE2	2.51	0.44
2:B:302:LYS:HE2	9:I:23:MET:SD	2.57	0.44
3:C:67:ARG:NH1	10:J:2:ILE:HG13	2.28	0.44
5:E:27:LEU:H	5:E:64:HIS:CA	2.20	0.44
8:H:113:SER:OG	8:H:126:GLN:HG2	2.17	0.44
16:P:165:LEU:HD23	16:P:168:ILE:HD11	1.99	0.44
2:B:62:ALA:N	2:B:63:PRO:HD3	2.33	0.44
2:B:380:ARG:NE	2:B:609:GLU:OE1	2.48	0.44
9:I:35:LEU:HB3	9:I:48:ALA:HB3	1.99	0.44
15:O:84:VAL:HG23	15:O:85:THR:HG23	1.99	0.44
17:Q:51:LEU:HD11	18:R:163:LEU:HD11	1.99	0.44
1:A:608:THR:OG1	1:A:610:PRO:CD	2.63	0.44
1:A:608:THR:OG1	1:A:610:PRO:HG2	2.18	0.44
1:A:623:PRO:CB	8:H:122:LEU:HD13	2.48	0.44
1:A:1187:ALA:HB3	9:I:1:MET:HE1	2.00	0.44
2:B:80:GLU:OE1	2:B:134:LYS:HB3	2.17	0.44
2:B:291:ASP:C	2:B:293:GLU:H	2.26	0.44
9:I:57:LYS:HB3	9:I:59:THR:HG22	2.00	0.44
13:M:99:SER:HG	22:X:33:DA:H61	1.66	0.44
18:R:157:GLN:HG2	18:R:160:GLN:HB3	1.99	0.44
20:T:8:ASP:HB3	20:T:105:SER:HA	1.99	0.44
1:A:505:LEU:HA	1:A:506:PRO:HD2	1.83	0.44
1:A:521:VAL:O	1:A:666:ARG:NH2	2.50	0.44
1:A:686:THR:OG1	1:A:687:ILE:N	2.49	0.44
1:A:927:GLU:O	1:A:931:ARG:CB	2.66	0.44
1:A:1372:GLU:CD	5:E:193:ILE:HD13	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:GLY:O	1:A:1470:CYS:HB2	2.17	0.44
2:B:42:GLN:HG2	2:B:526:LEU:HD11	2.00	0.44
2:B:116:ARG:O	2:B:117:ASN:HB2	2.18	0.44
2:B:243:GLY:N	2:B:252:ILE:HG21	2.32	0.44
2:B:872:THR:HG23	2:B:888:THR:O	2.18	0.44
3:C:56:SER:OG	3:C:158:GLU:N	2.27	0.44
13:M:75:LEU:O	13:M:114:MET:HE3	2.18	0.44
1:A:326:PRO:HB3	13:M:87:GLY:HA2	1.99	0.43
8:H:34:SER:HB2	8:H:36:LYS:NZ	2.33	0.43
8:H:85:ALA:HB1	8:H:144:LEU:CD2	2.48	0.43
9:I:119:CYS:HB3	9:I:121:HIS:H	1.82	0.43
17:Q:109:HIS:CE1	18:R:231:GLU:HG3	2.52	0.43
21:U:224:THR:HG22	21:U:228:MET:HE3	1.99	0.43
23:Y:64:DC:N4	23:Y:65:DG:O6	2.51	0.43
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.53	0.43
1:A:1249:ASP:HB2	21:U:196:SER:HB2	2.00	0.43
2:B:803:ARG:HH21	3:C:177:ASN:HD22	1.66	0.43
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.99	0.43
10:J:62:TYR:HB2	10:J:64:PRO:HG2	2.00	0.43
13:M:86:LYS:HD3	13:M:86:LYS:HA	1.75	0.43
16:P:298:PRO:HB2	16:P:320:GLU:HB3	1.99	0.43
17:Q:23:ARG:CZ	18:R:209:GLN:HB2	2.45	0.43
20:T:177:ARG:NE	20:T:208:GLN:HB2	2.33	0.43
2:B:698:ILE:O	2:B:699:HIS:HB2	2.17	0.43
3:C:147:ASP:OD2	3:C:148:ILE:HG22	2.17	0.43
3:C:259:LEU:HD22	11:K:42:LEU:HD11	2.00	0.43
7:G:98:PHE:CZ	17:Q:145:PHE:HB2	2.53	0.43
18:R:195:PRO:CG	18:R:199:LYS:HD2	2.47	0.43
20:T:165:TYR:O	20:T:169:LYS:HG2	2.18	0.43
21:U:257:GLN:NE2	21:U:257:GLN:HA	2.33	0.43
1:A:640:LEU:HD13	1:A:645:LEU:HD13	2.00	0.43
1:A:1301:ILE:HG21	1:A:1345:ARG:CZ	2.48	0.43
2:B:22:TRP:O	2:B:24:GLU:N	2.51	0.43
2:B:184:TYR:HE2	2:B:191:GLU:HG2	1.84	0.43
17:Q:54:PHE:CA	18:R:194:ARG:HD2	2.42	0.43
21:U:225:ALA:HB3	21:U:228:MET:HA	1.99	0.43
1:A:350:VAL:HG11	1:A:1431:SER:HA	1.99	0.43
1:A:486:LEU:HD12	1:A:496:PHE:CE2	2.54	0.43
1:A:922:PHE:CE2	1:A:932:ARG:NH1	2.86	0.43
2:B:871:VAL:HG13	2:B:890:ARG:HB2	2.01	0.43
2:B:1069:ILE:HG12	13:M:48:VAL:HG11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:158:PHE:CE1	17:Q:139:LEU:HB2	2.53	0.43
12:L:26:ASN:C	12:L:28:ILE:N	2.76	0.43
13:M:32:MET:O	13:M:40:VAL:HA	2.19	0.43
1:A:368:THR:OG1	1:A:483:ARG:NH1	2.51	0.43
2:B:225:LEU:HB3	2:B:228:SER:CB	2.18	0.43
3:C:260:GLN:O	3:C:260:GLN:HG3	2.17	0.43
4:D:71:PHE:HE1	7:G:142:GLU:HG2	1.83	0.43
10:J:66:GLU:HB3	12:L:23:HIS:CE1	2.54	0.43
17:Q:109:HIS:CE1	18:R:231:GLU:HB2	2.54	0.43
17:Q:128:LYS:N	17:Q:163:GLU:O	2.51	0.43
1:A:485:ASN:OD1	1:A:486:LEU:N	2.52	0.43
1:A:510:GLU:HG2	6:F:67:GLY:C	2.44	0.43
1:A:868:MET:HE1	1:A:1400:LEU:HG	2.00	0.43
1:A:1168:LYS:HD3	1:A:1306:LYS:HG2	2.01	0.43
2:B:953:ASP:O	2:B:1031:GLY:HA3	2.19	0.43
10:J:44:CYS:SG	10:J:45:CYS:N	2.92	0.43
11:K:5:PRO:HD2	11:K:8:GLU:OE1	2.19	0.43
1:A:220:ARG:O	1:A:223:GLU:N	2.52	0.43
1:A:371:PRO:HD2	2:B:788:TYR:CZ	2.54	0.43
1:A:1410:HIS:HB2	5:E:174:GLN:NE2	2.34	0.43
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.92	0.43
2:B:707:CYS:C	2:B:709:SER:H	2.27	0.43
2:B:1005:ALA:O	2:B:1007:ASN:N	2.52	0.43
5:E:18:MET:HE3	5:E:32:GLU:OE2	2.19	0.43
8:H:66:GLU:O	8:H:66:GLU:HG2	2.17	0.43
9:I:35:LEU:HD12	9:I:35:LEU:HA	1.84	0.43
9:I:61:GLU:C	9:I:63:ASP:N	2.75	0.43
11:K:112:LYS:O	11:K:112:LYS:HD3	2.19	0.43
14:N:22:ILE:HG13	14:N:43:LYS:HD2	2.00	0.43
17:Q:109:HIS:HE1	18:R:231:GLU:HB2	1.83	0.43
19:S:23:THR:O	20:T:100:SER:OG	2.23	0.43
20:T:159:HIS:O	20:T:162:ASN:HB3	2.18	0.43
21:U:247:GLU:HA	21:U:250:MET:HG2	2.00	0.43
1:A:359:VAL:HA	2:B:1111:SER:HB3	2.00	0.43
1:A:566:PHE:HB3	1:A:674:THR:HG22	2.01	0.43
2:B:51:ILE:HD13	2:B:51:ILE:HA	1.89	0.43
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.83	0.43
23:Y:46:DC:H2"	23:Y:47:DG:C8	2.53	0.43
23:Y:89:DC:H2"	23:Y:90:DC:C5	2.54	0.43
1:A:613:GLU:HG2	21:U:262:THR:HB	2.01	0.43
2:B:437:THR:OG1	13:M:126:ASP:OD2	2.35	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:CYS:SG	2:B:730:LYS:NZ	2.92	0.43
2:B:711:ILE:HD13	2:B:711:ILE:HG21	1.76	0.43
2:B:819:SER:H	2:B:827:GLU:HB2	1.84	0.43
5:E:45:GLY:C	5:E:47:LYS:N	2.77	0.43
6:F:121:ASP:OD1	6:F:121:ASP:N	2.51	0.43
9:I:16:PHE:HB3	9:I:22:ASN:O	2.19	0.43
12:L:38:GLU:O	13:M:226:LYS:NZ	2.32	0.43
14:N:28:ILE:HD13	15:O:35:GLN:HG2	2.01	0.43
16:P:325:PHE:HA	16:P:328:ILE:HG22	2.01	0.43
17:Q:110:MET:CE	18:R:222:SER:OG	2.66	0.43
19:S:45:ALA:HA	19:S:102:VAL:HA	2.00	0.43
21:U:158:TYR:O	21:U:162:GLY:N	2.47	0.43
22:X:44:DC:N4	23:Y:48:DC:H42	2.14	0.43
1:A:865:ILE:HD12	1:A:866:LYS:N	2.34	0.42
1:A:936:GLU:HB2	1:A:939:VAL:HG23	2.00	0.42
1:A:1282:ASP:OD1	1:A:1283:VAL:HG23	2.19	0.42
2:B:235:ILE:HD11	2:B:347:MET:HG3	1.99	0.42
2:B:875:GLU:OE1	2:B:875:GLU:HA	2.19	0.42
2:B:1114:TYR:HE2	2:B:1156:LYS:HD3	1.84	0.42
9:I:58:ILE:C	9:I:60:HIS:H	2.27	0.42
12:L:35:ARG:NH1	12:L:42:ARG:HE	2.17	0.42
1:A:197:GLU:HG3	1:A:199:TYR:HE1	1.84	0.42
1:A:366:VAL:HB	1:A:481:THR:HG22	2.01	0.42
1:A:561:MET:SD	11:K:51:LEU:HD21	2.59	0.42
2:B:475:PHE:CE2	2:B:479:LEU:HD22	2.55	0.42
2:B:771:GLU:OE2	10:J:58:LYS:HE3	2.20	0.42
8:H:100:GLU:HG3	8:H:101:GLY:N	2.25	0.42
17:Q:35:ASP:HA	17:Q:38:ILE:HD12	2.01	0.42
20:T:98:GLU:HA	20:T:104:LEU:HD23	2.01	0.42
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.74	0.42
1:A:689:ILE:HG13	1:A:690:GLY:N	2.34	0.42
1:A:1050:CYS:SG	1:A:1051:SER:N	2.92	0.42
2:B:798:ARG:NH2	3:C:172:GLU:O	2.49	0.42
2:B:1119:CYS:HB3	2:B:1122:CYS:O	2.18	0.42
4:D:126:GLU:O	4:D:130:ILE:N	2.43	0.42
5:E:61:LEU:HD11	5:E:71:GLN:HG3	2.00	0.42
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.20	0.42
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.54	0.42
1:A:927:GLU:O	1:A:931:ARG:HB3	2.19	0.42
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.02	0.42
2:B:1162:LEU:HA	2:B:1162:LEU:HD23	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:PHE:CE1	7:G:48:VAL:HB	2.52	0.42
20:T:25:LYS:HA	20:T:25:LYS:HD2	1.82	0.42
20:T:34:ALA:C	20:T:35:SER:HG	2.26	0.42
1:A:546:ARG:HG3	1:A:547:LYS:N	2.34	0.42
1:A:780:ASN:ND2	2:B:976:MET:SD	2.89	0.42
1:A:1161:LEU:HD11	1:A:1346:VAL:HG22	2.02	0.42
2:B:17:ILE:HG23	2:B:18:THR:HG23	2.01	0.42
2:B:757:PRO:HA	2:B:1047:TYR:CD2	2.54	0.42
2:B:961:ILE:H	2:B:961:ILE:HG13	1.55	0.42
2:B:1022:LEU:HD11	2:B:1023:ARG:NH1	2.34	0.42
2:B:1043:ILE:HG21	2:B:1043:ILE:HD13	1.74	0.42
5:E:11:TRP:CZ2	5:E:36:THR:HA	2.54	0.42
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.55	0.42
16:P:204:ILE:HD12	16:P:206:GLU:HB2	2.00	0.42
17:Q:172:ASP:O	17:Q:176:LEU:N	2.39	0.42
1:A:522:PRO:CG	1:A:666:ARG:HE	2.33	0.42
1:A:1112:VAL:HG22	1:A:1309:MET:HE3	2.00	0.42
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.55	0.42
2:B:282:ARG:HH11	9:I:21:ASN:HD21	1.67	0.42
2:B:751:LEU:HD12	2:B:751:LEU:HA	1.81	0.42
3:C:84:TYR:CE1	3:C:167:LYS:HE3	2.55	0.42
9:I:68:ILE:HG23	9:I:122:ARG:HD2	2.00	0.42
17:Q:105:TYR:CE1	18:R:231:GLU:CB	2.86	0.42
22:X:15:DA:H2"	22:X:16:DA:C8	2.55	0.42
1:A:483:ARG:NH2	2:B:788:TYR:CE2	2.87	0.42
2:B:453:TRP:HB2	2:B:463:ARG:HB2	2.01	0.42
2:B:501:LEU:CD1	2:B:505:LEU:HD22	2.50	0.42
2:B:873:LEU:CB	2:B:874:PRO:CD	2.96	0.42
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.34	0.42
9:I:28:GLU:HG3	9:I:29:ASP:N	2.34	0.42
22:X:0:DG:H2"	22:X:1:DA:C8	2.55	0.42
23:Y:80:DT:H6	23:Y:80:DT:H2'	1.71	0.42
1:A:24:GLY:O	2:B:1166:SER:HB3	2.20	0.42
1:A:693:ILE:HG21	2:B:1023:ARG:HE	1.85	0.42
1:A:1130:ILE:HD12	1:A:1411:LEU:HD13	2.02	0.42
1:A:1158:LEU:HD21	1:A:1308:TYR:CE2	2.54	0.42
13:M:35:PRO:HB2	13:M:36:GLU:OE1	2.19	0.42
13:M:106:THR:HA	23:Y:63:DG:H21	1.84	0.42
1:A:67:ARG:HH21	13:M:45:VAL:HB	1.85	0.42
1:A:118:LEU:HD12	1:A:148:CYS:HB3	2.02	0.42
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD23	1:A:1459:MET:HE3	2.02	0.42
1:A:624:GLY:O	1:A:625:ASP:C	2.63	0.42
1:A:1176:TYR:HE1	9:I:52:CYS:HB2	1.85	0.42
2:B:414:GLU:HA	2:B:417:ILE:HG22	2.02	0.42
2:B:761:THR:N	2:B:764:MET:HE3	2.29	0.42
2:B:1125:MET:HG3	2:B:1163:MET:HE1	2.02	0.42
7:G:91:GLN:HG2	17:Q:145:PHE:CZ	2.54	0.42
14:N:314:LEU:HD12	16:P:242:GLN:NE2	2.34	0.42
14:N:333:ASN:HB3	14:N:359:ASN:O	2.20	0.42
16:P:295:MET:HG3	16:P:297:LYS:H	1.85	0.42
17:Q:30:HIS:CE1	17:Q:62:VAL:HG22	2.54	0.42
1:A:136:GLN:HG3	1:A:139:LYS:H	1.85	0.42
1:A:542:LEU:O	1:A:545:VAL:HG12	2.20	0.42
1:A:1130:ILE:HD11	1:A:1405:MET:HE1	2.02	0.42
1:A:1178:ASP:HB3	1:A:1260:ARG:HH22	1.85	0.42
1:A:1311:LEU:HA	1:A:1312:PRO:HD2	1.97	0.42
2:B:728:MET:SD	2:B:940:GLY:HA2	2.59	0.42
8:H:85:ALA:CB	8:H:144:LEU:CD2	2.98	0.42
21:U:225:ALA:O	21:U:227:GLU:N	2.51	0.42
1:A:478:PRO:O	1:A:479:TRP:HB2	2.20	0.41
1:A:522:PRO:CB	1:A:666:ARG:HE	2.33	0.41
1:A:692:SER:O	1:A:828:LEU:HD22	2.20	0.41
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.84	0.41
1:A:1098:PRO:HA	1:A:1101:GLN:OE1	2.20	0.41
10:J:5:VAL:HG12	10:J:6:ARG:HG3	2.02	0.41
11:K:63:VAL:HA	11:K:64:PRO:HD3	1.95	0.41
14:N:308:GLN:NE2	14:N:313:PRO:O	2.46	0.41
17:Q:136:PHE:HD1	17:Q:140:GLU:OE1	2.03	0.41
18:R:133:ILE:HG13	18:R:136:LYS:HG3	2.02	0.41
20:T:121:SER:OG	20:T:122:GLU:N	2.52	0.41
22:X:58:DC:H2"	22:X:59:DG:C8	2.54	0.41
1:A:525:ILE:HA	1:A:535:MET:HE3	2.02	0.41
1:A:1029:LEU:H	5:E:162:ARG:NH1	2.17	0.41
1:A:1251:ASN:HD21	21:U:227:GLU:C	2.17	0.41
1:A:1413:ALA:O	1:A:1418:GLY:HA3	2.19	0.41
2:B:65:ILE:O	2:B:85:LEU:HD12	2.20	0.41
2:B:74:ALA:CB	20:T:201:ASP:CB	2.96	0.41
2:B:92:TYR:CD1	20:T:145:LEU:CD1	2.96	0.41
3:C:27:ASP:OD1	3:C:28:LEU:N	2.53	0.41
5:E:73:PHE:HD2	5:E:90:TYR:OH	2.02	0.41
8:H:96:VAL:HB	8:H:137:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:255:ILE:HG21	16:P:258:MET:HE3	2.01	0.41
16:P:288:PHE:HA	16:P:289:PRO:HD3	1.96	0.41
17:Q:154:CYS:SG	17:Q:155:THR:N	2.93	0.41
1:A:84:HIS:C	1:A:257:PRO:HG3	2.45	0.41
1:A:261:ARG:C	1:A:263:ALA:N	2.60	0.41
1:A:823:VAL:HG13	1:A:835:GLU:HB3	2.02	0.41
1:A:924:TYR:OH	1:A:952:LEU:HB2	2.21	0.41
1:A:1473:LEU:HB3	7:G:59:ILE:HD12	2.01	0.41
2:B:92:TYR:HE1	20:T:143:GLN:NE2	2.15	0.41
2:B:251:ALA:O	2:B:254:GLN:NE2	2.53	0.41
2:B:529:MET:HB2	2:B:624:PRO:HD2	2.03	0.41
2:B:1068:GLN:HA	13:M:51:GLU:CD	2.46	0.41
5:E:11:TRP:HZ2	5:E:36:THR:HA	1.86	0.41
17:Q:23:ARG:HG2	18:R:207:SER:C	2.45	0.41
18:R:167:LEU:HD22	18:R:200:ILE:HB	2.02	0.41
19:S:16:VAL:O	20:T:39:GLU:HA	2.19	0.41
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.55	0.41
20:T:179:ASP:OD1	20:T:183:VAL:HG23	2.21	0.41
21:U:233:LEU:HB3	21:U:234:LYS:H	1.77	0.41
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.55	0.41
1:A:601:ASN:CG	1:A:988:TRP:HZ3	2.29	0.41
2:B:451:GLY:HA2	2:B:467:SER:HB3	2.01	0.41
2:B:849:ASP:OD1	2:B:850:ASP:N	2.53	0.41
3:C:52:ILE:HG21	3:C:55:ASN:HB2	2.01	0.41
3:C:71:ILE:HG22	3:C:148:ILE:HG21	2.02	0.41
9:I:84:HIS:CD2	9:I:84:HIS:N	2.85	0.41
13:M:11:PRO:O	13:M:12:ARG:CG	2.68	0.41
13:M:95:GLU:O	13:M:96:PHE:HD1	2.02	0.41
14:N:360:LEU:O	14:N:361:ASN:CB	2.69	0.41
16:P:283:TYR:CD2	16:P:285:PRO:HD3	2.55	0.41
17:Q:24:GLY:O	18:R:210:PHE:CE2	2.73	0.41
19:S:26:TYR:CD2	19:S:138:PHE:HB3	2.55	0.41
1:A:592:PHE:CZ	1:A:640:LEU:HD11	2.55	0.41
1:A:608:THR:OG1	1:A:610:PRO:CG	2.68	0.41
1:A:927:GLU:HG3	1:A:929:ALA:H	1.86	0.41
2:B:274:ARG:HA	2:B:278:PHE:O	2.20	0.41
2:B:674:MET:HE2	2:B:690:CYS:SG	2.60	0.41
2:B:747:LEU:HD23	2:B:747:LEU:C	2.45	0.41
3:C:42:VAL:CB	3:C:178:PRO:HG3	2.45	0.41
3:C:148:ILE:HD13	10:J:15:GLY:HA3	2.03	0.41
9:I:11:PHE:CD1	9:I:55:VAL:HG22	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ASP:CG	9:I:50:ASN:H	2.28	0.41
17:Q:23:ARG:CG	18:R:208:CYS:O	2.69	0.41
21:U:133:ALA:HA	21:U:134:PRO:HD3	1.89	0.41
1:A:265:VAL:HG23	1:A:266:MET:H	1.85	0.41
1:A:366:VAL:O	1:A:481:THR:HB	2.21	0.41
1:A:378:VAL:O	1:A:475:ARG:N	2.53	0.41
1:A:546:ARG:NH2	1:A:550:LYS:HD2	2.35	0.41
1:A:623:PRO:HB3	8:H:122:LEU:HD13	2.03	0.41
1:A:974:ASP:HB2	1:A:1317:LYS:NZ	2.36	0.41
1:A:1432:PHE:HD1	1:A:1433:GLU:HB2	1.84	0.41
9:I:96:PHE:HB3	9:I:112:TYR:CD1	2.56	0.41
15:O:79:VAL:HG21	15:O:93:VAL:HG12	2.01	0.41
20:T:143:GLN:OE1	20:T:143:GLN:N	2.54	0.41
22:X:13:DA:H2"	22:X:14:DA:H8	1.83	0.41
23:Y:38:DT:H2"	23:Y:39:DG:C8	2.56	0.41
1:A:271:ARG:NH1	2:B:821:LYS:HE2	2.31	0.41
1:A:483:ARG:HH21	2:B:788:TYR:HE2	1.68	0.41
1:A:1024:ASN:OD1	1:A:1025:GLY:N	2.54	0.41
1:A:1179:PRO:HA	1:A:1209:PRO:HA	2.03	0.41
1:A:1299:GLN:HG2	1:A:1300:GLY:H	1.85	0.41
2:B:128:ILE:HG21	2:B:431:LEU:HD21	2.03	0.41
2:B:479:LEU:HD12	2:B:479:LEU:HA	1.84	0.41
2:B:908:MET:HE2	2:B:908:MET:HB3	1.95	0.41
8:H:78:THR:HG21	11:K:78:THR:CG2	2.51	0.41
13:M:200:LYS:HE2	13:M:200:LYS:HB3	1.75	0.41
16:P:190:ALA:HB2	16:P:202:MET:HG2	2.01	0.41
17:Q:113:ARG:HH21	18:R:218:LYS:HE2	1.68	0.41
20:T:155:PRO:O	20:T:156:VAL:HG22	2.21	0.41
20:T:159:HIS:ND1	20:T:160:GLN:N	2.65	0.41
1:A:598:GLY:HA2	1:A:633:GLY:HA3	2.02	0.41
1:A:902:GLU:CD	1:A:982:ASN:HB2	2.46	0.41
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.51	0.41
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.21	0.41
2:B:181:PRO:HD3	2:B:475:PHE:HE1	1.86	0.41
2:B:631:GLN:HE21	2:B:685:LYS:HD2	1.86	0.41
2:B:895:PHE:HB2	2:B:896:LEU:H	1.67	0.41
4:D:73:ARG:HD3	4:D:141:GLN:HE22	1.86	0.41
5:E:197:SER:HB3	5:E:201:GLY:H	1.85	0.41
13:M:25:GLU:HG2	13:M:32:MET:SD	2.61	0.41
15:O:17:GLU:O	15:O:21:GLU:HG2	2.21	0.41
16:P:268:ILE:O	16:P:337:LYS:HE3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:278:THR:HG22	21:U:285:MET:SD	2.60	0.41
1:A:256:PRO:HG2	1:A:261:ARG:HD3	2.02	0.41
1:A:297:GLY:HA3	17:Q:57:LYS:CG	2.50	0.41
1:A:576:GLN:HB2	8:H:73:GLY:O	2.20	0.41
1:A:608:THR:HB	1:A:610:PRO:HD2	1.97	0.41
1:A:1464:ALA:O	1:A:1466:ALA:N	2.52	0.41
2:B:38:GLY:H	2:B:41:ARG:HG2	1.85	0.41
2:B:38:GLY:H	2:B:41:ARG:CG	2.34	0.41
2:B:237:VAL:HG12	2:B:372:LEU:HD22	2.02	0.41
2:B:268:PRO:HD2	2:B:271:ILE:HD12	2.02	0.41
2:B:422:PHE:CZ	2:B:429:PHE:HB2	2.55	0.41
2:B:527:ALA:HA	2:B:705:GLY:HA2	2.02	0.41
2:B:877:GLU:OE1	2:B:877:GLU:N	2.54	0.41
4:D:103:LEU:HD13	4:D:114:LEU:HD13	2.02	0.41
5:E:8:TYR:HD1	5:E:37:LEU:HD22	1.86	0.41
5:E:111:THR:HG23	22:X:56:DC:H4'	2.02	0.41
6:F:68:THR:HG21	7:G:59:ILE:HG21	2.02	0.41
6:F:71:LEU:HA	6:F:71:LEU:HD12	1.81	0.41
18:R:151:LEU:HB3	18:R:154:LEU:HB3	2.03	0.41
18:R:194:ARG:HG3	18:R:201:LEU:CD1	2.50	0.41
20:T:161:TYR:O	20:T:164:GLU:HB3	2.21	0.41
21:U:194:ARG:HH12	21:U:223:MET:HE2	1.86	0.41
21:U:226:GLU:CD	21:U:226:GLU:H	2.27	0.41
22:X:43:DT:H2"	22:X:44:DC:C4'	2.51	0.41
23:Y:77:DT:C6	23:Y:78:DT:H72	2.56	0.41
1:A:367:ILE:HG21	1:A:367:ILE:HD13	1.87	0.41
1:A:616:GLY:O	1:A:619:LYS:HB2	2.21	0.41
2:B:166:LEU:HB3	2:B:170:ASP:HB2	2.02	0.41
2:B:191:GLU:CD	2:B:743:ARG:HH22	2.28	0.41
2:B:280:SER:HB2	2:B:283:ASP:OD2	2.21	0.41
2:B:496:ALA:CB	2:B:498:PRO:HD2	2.50	0.41
2:B:561:ILE:HD12	2:B:561:ILE:HA	1.95	0.41
2:B:927:ARG:NH2	2:B:1057:ASP:OD1	2.54	0.41
3:C:1:MET:HB3	3:C:3:TYR:CE2	2.56	0.41
5:E:61:LEU:HD12	5:E:72:MET:O	2.21	0.41
5:E:116:GLN:O	5:E:119:VAL:HB	2.21	0.41
13:M:15:CYS:SG	13:M:39:LEU:CD2	3.04	0.41
13:M:36:GLU:OE1	13:M:36:GLU:N	2.54	0.41
17:Q:109:HIS:CE1	18:R:231:GLU:CB	3.02	0.41
2:B:191:GLU:OE1	2:B:472:ARG:HD2	2.21	0.40
2:B:299:GLU:OE2	2:B:302:LYS:HE3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:LEU:HG	2:B:698:ILE:HG22	2.03	0.40
5:E:171:PRO:HB2	5:E:207:ARG:HD2	2.02	0.40
7:G:128:TYR:O	7:G:137:ILE:N	2.53	0.40
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.86	0.40
16:P:171:THR:HG23	16:P:256:GLN:HG3	2.02	0.40
18:R:194:ARG:HB2	18:R:201:LEU:HG	2.02	0.40
18:R:194:ARG:HD3	18:R:194:ARG:HA	1.61	0.40
21:U:247:GLU:OE1	21:U:250:MET:HG3	2.22	0.40
21:U:252:LYS:HB3	21:U:253:THR:H	1.67	0.40
1:A:210:GLN:CD	1:A:212:LYS:CG	2.93	0.40
1:A:823:VAL:HA	1:A:835:GLU:HG2	2.03	0.40
1:A:1473:LEU:HD23	6:F:104:ILE:HD12	2.02	0.40
2:B:751:LEU:CD1	2:B:808:SER:HB3	2.39	0.40
5:E:80:PRO:HA	5:E:107:GLN:HB3	2.03	0.40
9:I:44:TYR:OH	9:I:46:GLN:NE2	2.47	0.40
10:J:8:PHE:CD2	10:J:48:MET:HE1	2.56	0.40
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.86	0.40
18:R:194:ARG:HG3	18:R:201:LEU:HD12	2.03	0.40
1:A:539:GLN:HB3	2:B:790:GLN:HG2	2.03	0.40
1:A:595:ILE:HD12	1:A:596:ILE:N	2.36	0.40
1:A:921:ARG:HG3	1:A:956:PHE:CZ	2.57	0.40
2:B:229:SER:HA	2:B:405:ARG:HH22	1.84	0.40
2:B:406:GLY:HA2	2:B:409:LYS:HE2	2.04	0.40
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.86	0.40
2:B:957:THR:HG21	2:B:1026:GLU:OE1	2.22	0.40
8:H:85:ALA:HB3	8:H:144:LEU:HD21	2.04	0.40
16:P:206:GLU:HB3	16:P:236:LYS:NZ	2.36	0.40
19:S:29:MET:HE2	19:S:146:PHE:CE2	2.55	0.40
20:T:23:VAL:HA	20:T:24:PRO:HD3	1.94	0.40
20:T:174:LYS:HG2	22:X:19:DG:H4'	2.02	0.40
1:A:320:ASN:HB2	1:A:338:SER:HB3	2.03	0.40
1:A:387:ASN:O	1:A:387:ASN:CG	2.64	0.40
1:A:604:ARG:HG2	1:A:605:THR:H	1.87	0.40
2:B:853:LEU:HB3	2:B:867:ILE:HG12	2.03	0.40
10:J:62:TYR:HB3	10:J:64:PRO:HD3	2.00	0.40
16:P:229:GLN:HA	16:P:232:LEU:HB3	2.03	0.40
17:Q:149:THR:HG23	17:Q:151:THR:H	1.86	0.40
22:X:31:DG:H2"	22:X:32:DA:C5'	2.52	0.40
22:X:64:DG:H2"	22:X:65:DA:C8	2.57	0.40
1:A:369:PRO:HB3	1:A:486:LEU:CD1	2.52	0.40
1:A:485:ASN:OD1	1:A:487:SER:N	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:TYR:C	1:A:926:ASN:H	2.29	0.40
1:A:1376:LYS:HD2	1:A:1379:GLU:OE2	2.22	0.40
1:A:1471:PHE:HZ	6:F:61:GLU:HA	1.87	0.40
2:B:499:ARG:NH2	2:B:522:LEU:HD11	2.37	0.40
3:C:4:ALA:HB2	11:K:93:ASP:CG	2.47	0.40
8:H:62:SER:O	8:H:140:ARG:NH2	2.54	0.40
9:I:88:LYS:HD3	9:I:119:CYS:SG	2.61	0.40
17:Q:113:ARG:NH1	18:R:218:LYS:HG3	2.37	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	1450/1970 (74%)	1258 (87%)	126 (9%)	66 (5%)	2 19
2	B	1163/1174 (99%)	1012 (87%)	109 (9%)	42 (4%)	2 23
3	C	273/275 (99%)	241 (88%)	23 (8%)	9 (3%)	3 24
4	D	127/142 (89%)	118 (93%)	9 (7%)	0	100 100
5	E	208/210 (99%)	188 (90%)	14 (7%)	6 (3%)	3 26
6	F	84/127 (66%)	78 (93%)	6 (7%)	0	100 100
7	G	169/172 (98%)	164 (97%)	5 (3%)	0	100 100
8	H	148/150 (99%)	117 (79%)	23 (16%)	8 (5%)	1 17
9	I	123/125 (98%)	91 (74%)	19 (15%)	13 (11%)	0 6
10	J	65/67 (97%)	51 (78%)	8 (12%)	6 (9%)	0 9
11	K	115/117 (98%)	110 (96%)	1 (1%)	4 (4%)	3 23
12	L	44/58 (76%)	31 (70%)	8 (18%)	5 (11%)	0 5
13	M	308/316 (98%)	266 (86%)	28 (9%)	14 (4%)	2 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	N	109/376 (29%)	99 (91%)	8 (7%)	2 (2%)	6 34
15	O	97/109 (89%)	92 (95%)	4 (4%)	1 (1%)	12 45
16	P	183/339 (54%)	170 (93%)	9 (5%)	4 (2%)	5 31
17	Q	176/439 (40%)	151 (86%)	17 (10%)	8 (4%)	2 19
18	R	163/291 (56%)	126 (77%)	26 (16%)	11 (7%)	1 14
19	S	134/517 (26%)	123 (92%)	8 (6%)	3 (2%)	5 31
20	T	218/249 (88%)	189 (87%)	19 (9%)	10 (5%)	2 19
21	U	168/301 (56%)	145 (86%)	10 (6%)	13 (8%)	1 12
All	All	5525/7524 (73%)	4820 (87%)	480 (9%)	225 (4%)	4 20

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	A	48	GLU
1	A	133	SER
1	A	153	ILE
1	A	204	HIS
1	A	208	ASP
1	A	262	PRO
1	A	272	ASN
1	A	295	GLN
1	A	344	LYS
1	A	496	PHE
1	A	598	GLY
1	A	605	THR
1	A	607	SER
1	A	610	PRO
1	A	623	PRO
1	A	625	ASP
1	A	911	PRO
1	A	1117	VAL
1	A	1200	PRO
1	A	1299	GLN
1	A	1342	SER
2	B	61	ASP
2	B	63	PRO
2	B	74	ALA
2	B	78	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	79	GLU
2	B	141	GLN
2	B	203	ASN
2	B	231	PRO
2	B	249	LYS
2	B	251	ALA
2	B	491	ARG
2	B	492	ASP
2	B	880	LEU
2	B	881	GLU
2	B	898	THR
2	B	901	THR
2	B	1136	GLU
2	B	1166	SER
3	C	143	VAL
5	E	47	LYS
5	E	49	SER
5	E	53	PRO
5	E	54	ARG
8	H	18	GLU
8	H	65	TYR
8	H	67	ASP
9	I	15	ARG
9	I	16	PHE
9	I	85	PRO
9	I	86	CYS
9	I	99	SER
9	I	104	ALA
9	I	106	ASP
9	I	118	HIS
10	J	64	PRO
12	L	28	ILE
13	M	10	LEU
13	M	11	PRO
13	M	12	ARG
13	M	48	VAL
13	M	87	GLY
14	N	355	ASP
15	O	4	GLN
16	P	207	PRO
16	P	208	ARG
17	Q	25	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	103	VAL
17	Q	118	GLU
18	R	140	LYS
18	R	163	LEU
18	R	195	PRO
18	R	197	LYS
20	T	124	TYR
20	T	142	SER
20	T	145	LEU
21	U	227	GLU
21	U	231	ASP
21	U	257	GLN
21	U	277	GLN
21	U	293	GLU
1	A	77	ASN
1	A	134	LYS
1	A	154	CYS
1	A	195	GLY
1	A	206	ASN
1	A	213	LYS
1	A	299	ALA
1	A	452	ASP
1	A	531	ASN
1	A	611	ASP
1	A	929	ALA
1	A	931	ARG
1	A	932	ARG
1	A	1275	VAL
1	A	1315	ASP
2	B	23	GLN
2	B	250	SER
2	B	428	ASP
2	B	518	HIS
2	B	527	ALA
2	B	549	SER
2	B	561	ILE
2	B	879	GLU
3	C	5	ASN
3	C	213	GLU
5	E	48	PRO
8	H	109	ALA
8	H	149	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	92	LYS
9	I	103	ARG
10	J	2	ILE
12	L	25	GLU
13	M	90	ALA
13	M	92	SER
13	M	93	PHE
16	P	297	LYS
16	P	299	ARG
17	Q	70	LYS
17	Q	104	LYS
17	Q	125	ALA
18	R	147	ASP
18	R	216	PHE
20	T	141	LEU
20	T	155	PRO
20	T	156	VAL
20	T	171	GLU
20	T	180	LYS
20	T	229	HIS
21	U	226	GLU
21	U	252	LYS
21	U	253	THR
1	A	184	CYS
1	A	210	GLN
1	A	374	SER
1	A	599	HIS
1	A	624	GLY
1	A	894	ASP
1	A	1102	MET
1	A	1103	THR
1	A	1265	ASP
1	A	1435	THR
2	B	77	GLU
2	B	513	GLU
2	B	685	LYS
2	B	873	LEU
2	B	884	ASN
8	H	24	ARG
10	J	6	ARG
10	J	65	LEU
11	K	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	80	ASP
11	K	111	ASP
13	M	56	SER
13	M	61	THR
13	M	306	PHE
17	Q	158	HIS
18	R	149	LYS
18	R	174	ALA
18	R	226	ASP
19	S	154	THR
21	U	228	MET
21	U	250	MET
21	U	279	ARG
21	U	294	CYS
1	A	261	ARG
1	A	265	VAL
1	A	300	ALA
1	A	615	SER
1	A	1113	SER
2	B	118	LEU
2	B	226	GLU
2	B	839	GLY
2	B	1006	VAL
3	C	7	PRO
3	C	138	ASP
11	K	112	LYS
12	L	16	ILE
12	L	27	GLU
13	M	101	TYR
14	N	312	GLU
17	Q	126	SER
18	R	156	ASP
19	S	151	ARG
20	T	178	ALA
21	U	233	LEU
1	A	65	ILE
1	A	132	LYS
1	A	485	ASN
1	A	612	ASP
1	A	817	PRO
1	A	935	GLN
1	A	1114	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1274	GLU
2	B	290	TYR
2	B	460	HIS
2	B	521	GLY
2	B	1129	ASN
3	C	147	ASP
9	I	12	VAL
10	J	30	THR
13	M	41	VAL
13	M	60	ALA
18	R	139	PHE
19	S	160	ALA
1	A	650	GLY
1	A	726	GLU
1	A	729	PRO
2	B	1025	ASN
3	C	74	ILE
8	H	21	LYS
8	H	139	SER
9	I	67	GLN
1	A	687	ILE
2	B	253	GLY
3	C	218	ALA
9	I	68	ILE
12	L	20	GLY
1	A	621	ILE
1	A	622	SER
2	B	136	GLY
3	C	151	VAL
5	E	51	GLY
10	J	5	VAL

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1279/1748 (73%)	1230 (96%)	49 (4%)	29	52
2	B	1020/1028 (99%)	983 (96%)	37 (4%)	31	54
3	C	252/252 (100%)	248 (98%)	4 (2%)	55	69
4	D	119/126 (94%)	118 (99%)	1 (1%)	73	77
5	E	192/192 (100%)	183 (95%)	9 (5%)	23	48
6	F	74/111 (67%)	73 (99%)	1 (1%)	59	71
7	G	152/153 (99%)	150 (99%)	2 (1%)	61	71
8	H	131/131 (100%)	127 (97%)	4 (3%)	35	57
9	I	112/112 (100%)	106 (95%)	6 (5%)	20	46
10	J	56/56 (100%)	54 (96%)	2 (4%)	31	54
11	K	106/106 (100%)	100 (94%)	6 (6%)	18	44
12	L	43/55 (78%)	40 (93%)	3 (7%)	14	40
13	M	263/268 (98%)	254 (97%)	9 (3%)	32	55
14	N	105/324 (32%)	105 (100%)	0	100	100
15	O	90/98 (92%)	90 (100%)	0	100	100
16	P	159/293 (54%)	156 (98%)	3 (2%)	50	66
17	Q	164/373 (44%)	157 (96%)	7 (4%)	26	49
18	R	150/261 (58%)	145 (97%)	5 (3%)	33	56
19	S	121/448 (27%)	118 (98%)	3 (2%)	42	62
20	T	196/218 (90%)	189 (96%)	7 (4%)	31	54
21	U	148/266 (56%)	140 (95%)	8 (5%)	20	46
All	All	4932/6619 (74%)	4766 (97%)	166 (3%)	33	55

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	72	GLN
1	A	87	HIS
1	A	117	LEU
1	A	132	LYS
1	A	133	SER
1	A	181	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	204	HIS
1	A	205	VAL
1	A	212	LYS
1	A	220	ARG
1	A	261	ARG
1	A	264	VAL
1	A	277	THR
1	A	343	LEU
1	A	449	HIS
1	A	463	THR
1	A	477	LEU
1	A	488	VAL
1	A	500	GLU
1	A	508	SER
1	A	546	ARG
1	A	587	THR
1	A	595	ILE
1	A	611	ASP
1	A	619	LYS
1	A	625	ASP
1	A	666	ARG
1	A	849	ASP
1	A	908	THR
1	A	954	ARG
1	A	981	CYS
1	A	1036	ASN
1	A	1050	CYS
1	A	1066	ASP
1	A	1075	LYS
1	A	1115	LYS
1	A	1139	LEU
1	A	1192	TRP
1	A	1203	ASP
1	A	1282	ASP
1	A	1298	LEU
1	A	1309	MET
1	A	1318	LYS
1	A	1319	LYS
1	A	1337	GLU
1	A	1339	ASP
1	A	1379	GLU
1	A	1420	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	73	HIS
2	B	77	GLU
2	B	79	GLU
2	B	129	THR
2	B	133	ILE
2	B	146	LYS
2	B	156	LEU
2	B	161	CYS
2	B	168	ASP
2	B	225	LEU
2	B	250	SER
2	B	287	HIS
2	B	302	LYS
2	B	422	PHE
2	B	491	ARG
2	B	548	TRP
2	B	591	ARG
2	B	666	ASP
2	B	711	ILE
2	B	737	ILE
2	B	782	ILE
2	B	785	TYR
2	B	790	GLN
2	B	793	SER
2	B	853	LEU
2	B	880	LEU
2	B	881	GLU
2	B	895	PHE
2	B	896	LEU
2	B	897	ARG
2	B	921	ILE
2	B	941	GLN
2	B	957	THR
2	B	1022	LEU
2	B	1054	MET
2	B	1069	ILE
2	B	1127	ILE
3	C	5	ASN
3	C	137	ASN
3	C	195	THR
3	C	273	THR
4	D	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	46	ASP
5	E	47	LYS
5	E	50	GLU
5	E	52	ARG
5	E	54	ARG
5	E	55	ARG
5	E	64	HIS
5	E	69	THR
5	E	127	LEU
6	F	121	ASP
7	G	22	LEU
7	G	128	TYR
8	H	38	ASP
8	H	70	LEU
8	H	84	ARG
8	H	107	GLU
9	I	14	ILE
9	I	15	ARG
9	I	60	HIS
9	I	61	GLU
9	I	66	THR
9	I	84	HIS
10	J	36	ASP
10	J	47	ARG
11	K	39	ASP
11	K	48	SER
11	K	63	VAL
11	K	67	LEU
11	K	111	ASP
11	K	112	LYS
12	L	19	CYS
12	L	27	GLU
12	L	28	ILE
13	M	10	LEU
13	M	14	THR
13	M	39	LEU
13	M	47	ASP
13	M	86	LYS
13	M	93	PHE
13	M	129	ASN
13	M	133	ASN
13	M	200	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	P	203	ARG
16	P	239	ARG
16	P	297	LYS
17	Q	97	ARG
17	Q	103	VAL
17	Q	128	LYS
17	Q	135	THR
17	Q	139	LEU
17	Q	177	LEU
17	Q	202	GLU
18	R	194	ARG
18	R	205	ASP
18	R	206	LYS
18	R	215	GLU
18	R	223	VAL
19	S	35	ASP
19	S	166	ARG
19	S	177	MET
20	T	147	LYS
20	T	154	LYS
20	T	156	VAL
20	T	177	ARG
20	T	185	ASP
20	T	201	ASP
20	T	204	ASP
21	U	226	GLU
21	U	233	LEU
21	U	252	LYS
21	U	257	GLN
21	U	276	VAL
21	U	292	ASN
21	U	299	LYS
21	U	301	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	96	HIS
1	A	122	ASN
1	A	136	GLN
1	A	181	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	GLN
1	A	273	GLN
1	A	372	ASN
1	A	493	ASN
1	A	502	ASN
1	A	590	GLN
1	A	677	ASN
1	A	731	ASN
1	A	746	ASN
1	A	765	ASN
1	A	783	GLN
1	A	1034	GLN
1	A	1036	ASN
1	A	1093	GLN
1	A	1190	GLN
1	A	1313	GLN
1	A	1316	ASN
1	A	1445	HIS
2	B	175	ASN
2	B	631	GLN
2	B	725	GLN
2	B	749	HIS
2	B	1021	HIS
2	B	1071	ASN
2	B	1117	HIS
3	C	5	ASN
3	C	66	HIS
3	C	137	ASN
3	C	173	HIS
3	C	260	GLN
4	D	102	ASN
5	E	22	HIS
5	E	132	GLN
5	E	148	HIS
7	G	9	HIS
7	G	24	ASN
7	G	124	ASN
8	H	126	GLN
8	H	133	HIS
9	I	60	HIS
9	I	84	HIS
10	J	61	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	40	HIS
12	L	23	HIS
13	M	129	ASN
13	M	148	GLN
15	O	45	ASN
16	P	256	GLN
16	P	327	ASN
18	R	95	HIS
18	R	188	GLN
19	S	27	ASN
19	S	53	ASN
19	S	141	HIS
19	S	173	HIS
20	T	181	GLN
21	U	205	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

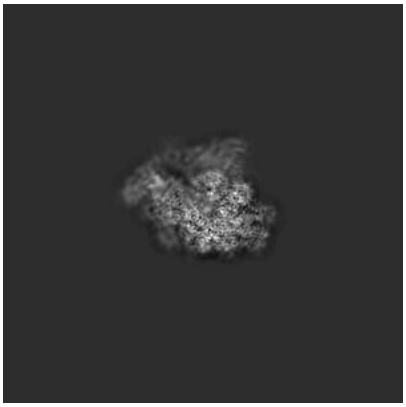
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8136. These allow visual inspection of the internal detail of the map and identification of artifacts.

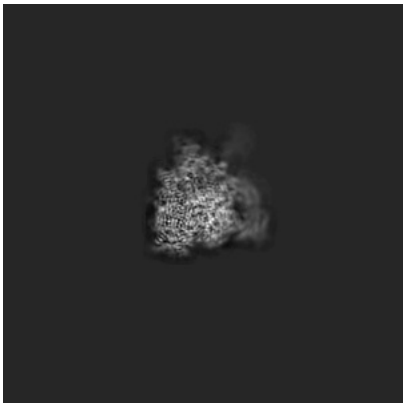
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

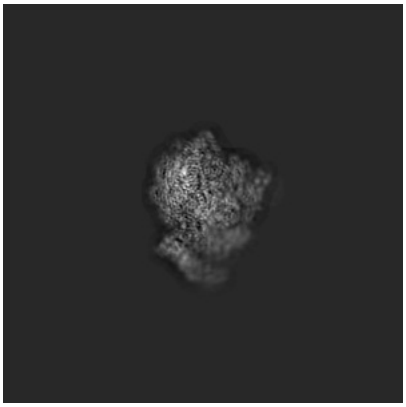
6.1.1 Primary map



X



Y

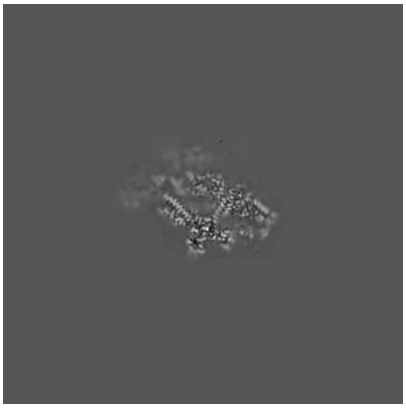


Z

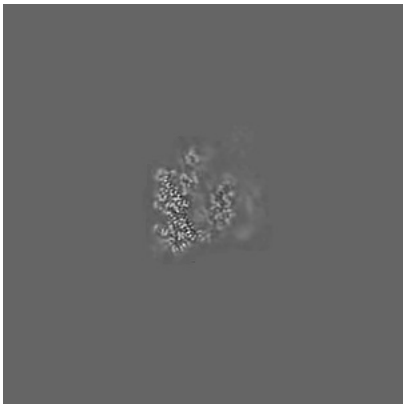
The images above show the map projected in three orthogonal directions.

6.2 Central slices

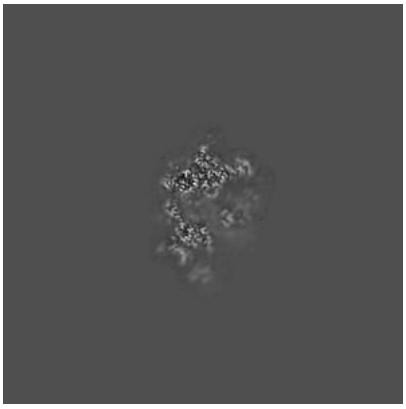
6.2.1 Primary map



X Index: 192



Y Index: 192

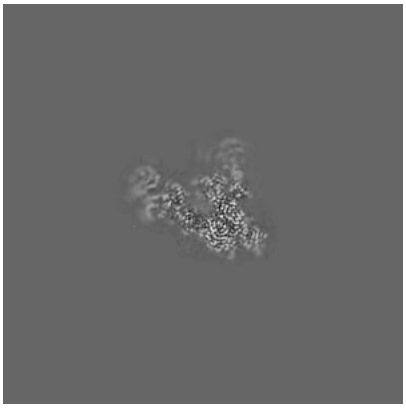


Z Index: 192

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

6.3 Largest variance slices (i)

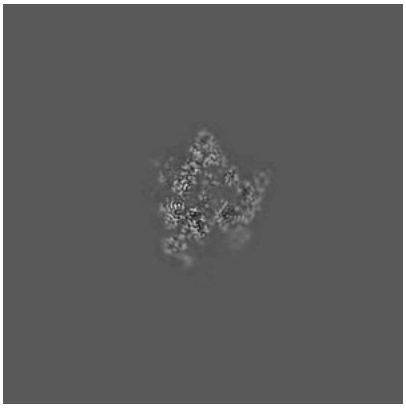
6.3.1 Primary map



X Index: 175



Y Index: 210

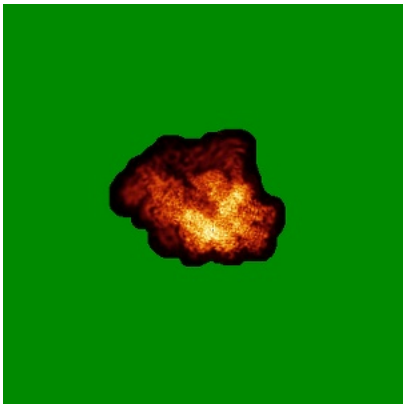


Z Index: 180

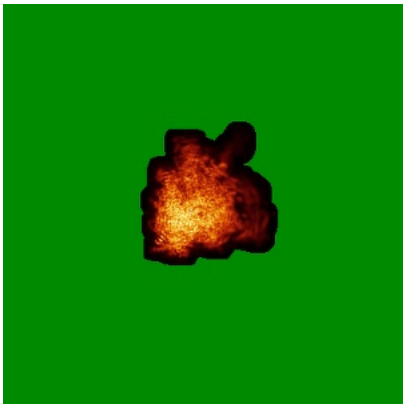
The images above show the largest variance slices of the map in three orthogonal directions.

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

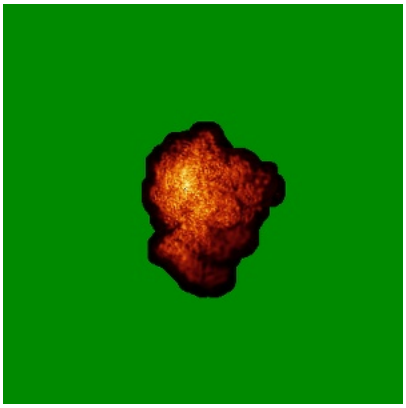
6.4.1 Primary map



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)

This section was not generated.

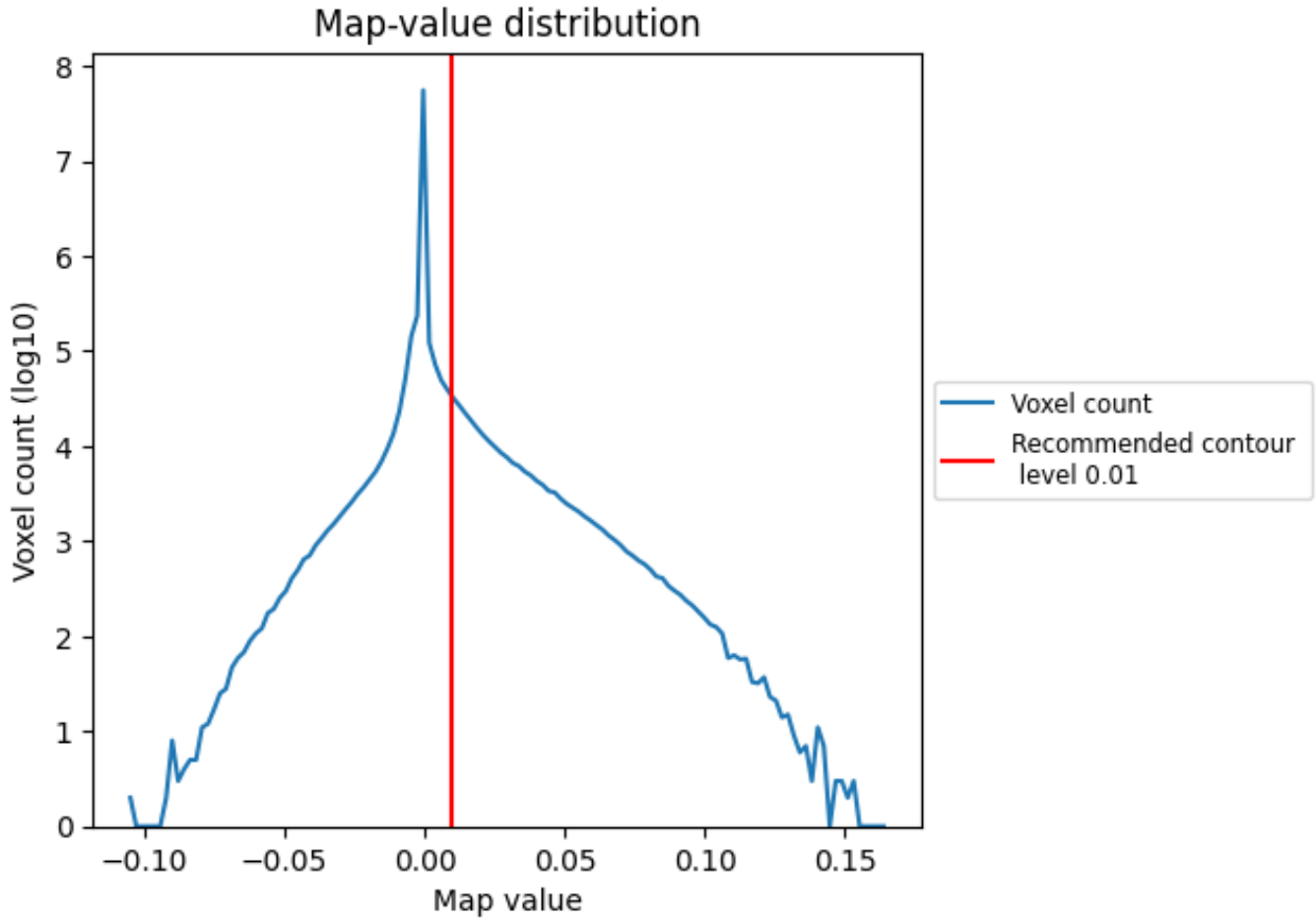
6.6 Mask visualisation (i)

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

7 Map analysis

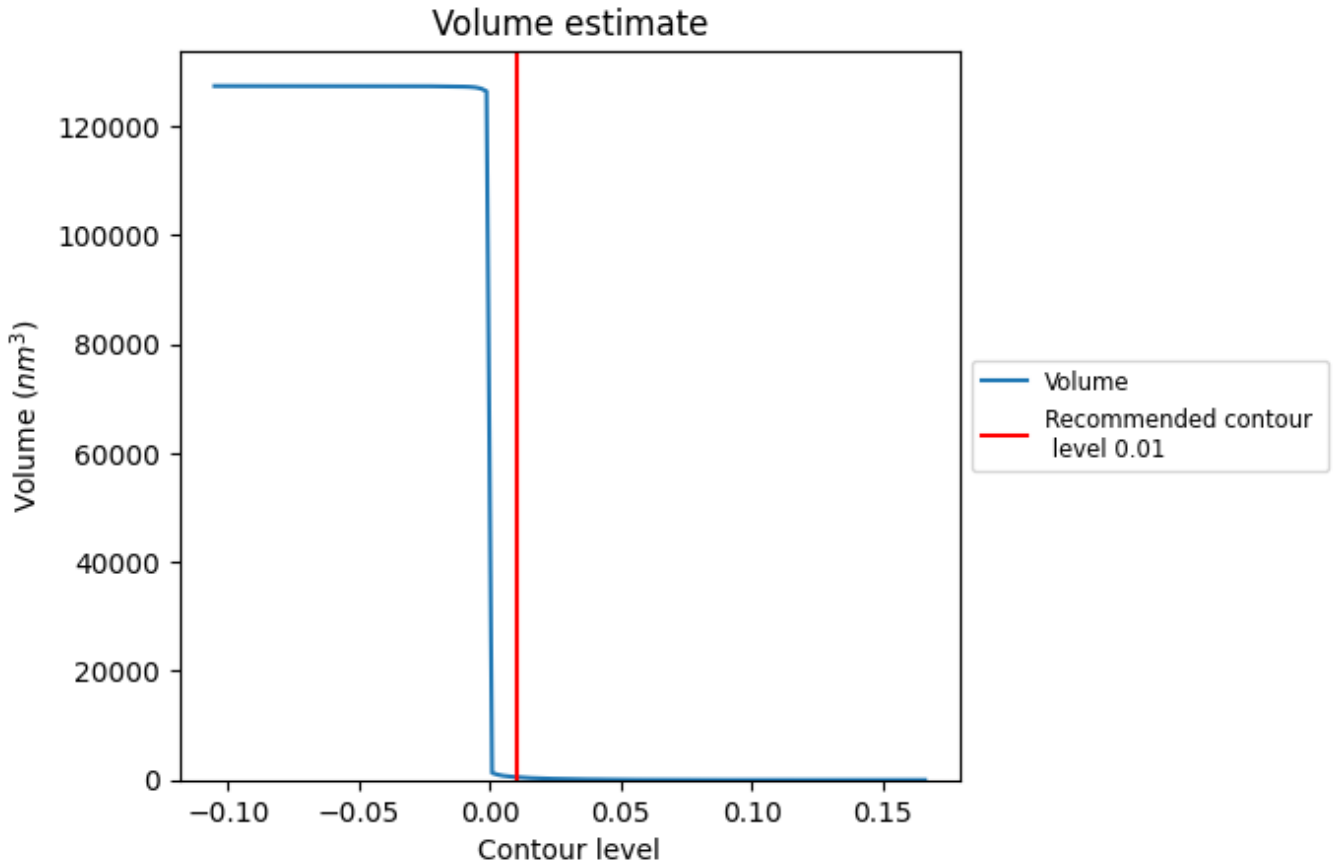
This section contains the results of statistical analysis of the map.

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.

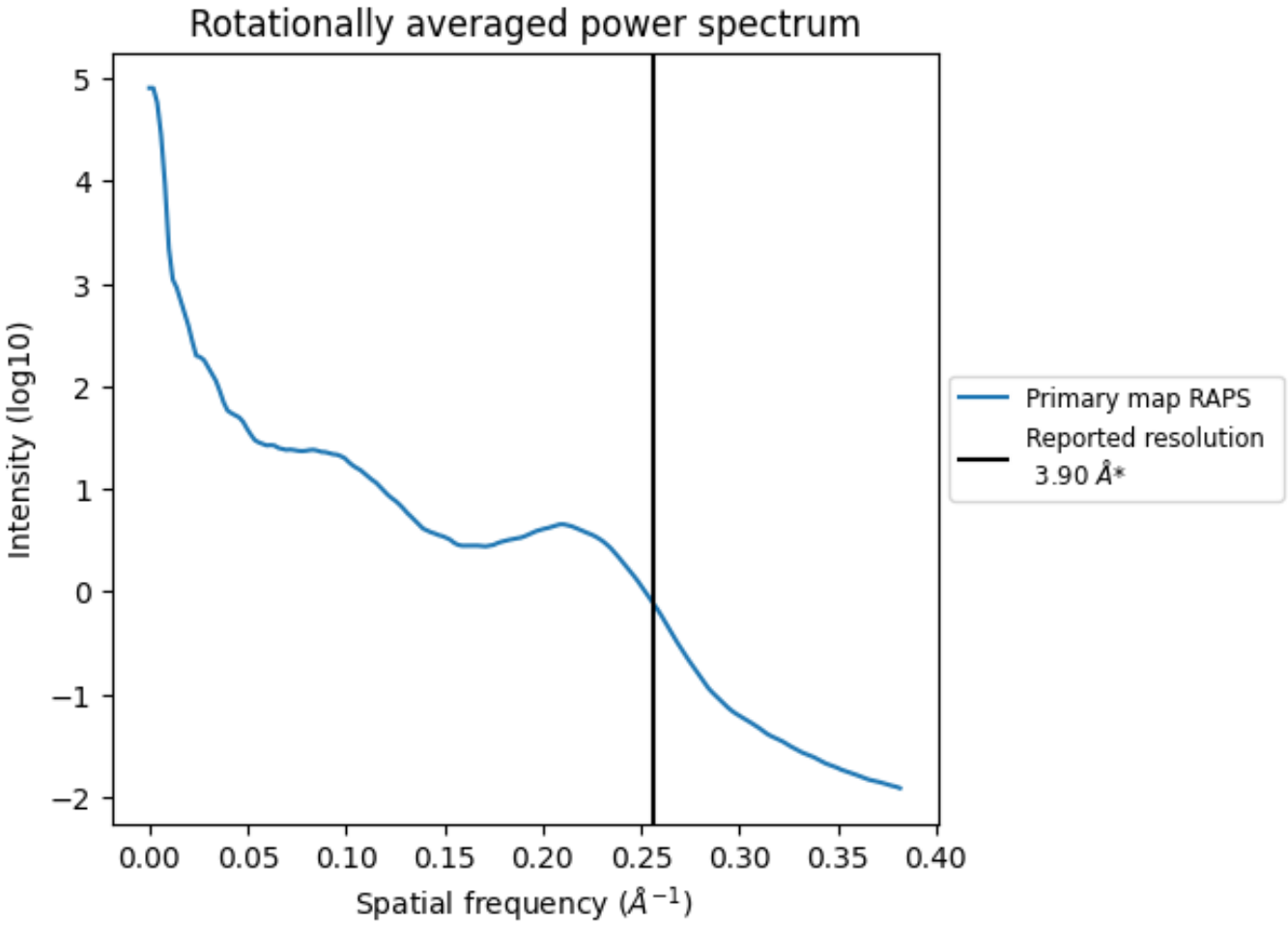
7.2 Volume estimate



The volume at the recommended contour level is 527 nm^3; this corresponds to an approximate mass of 476 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)

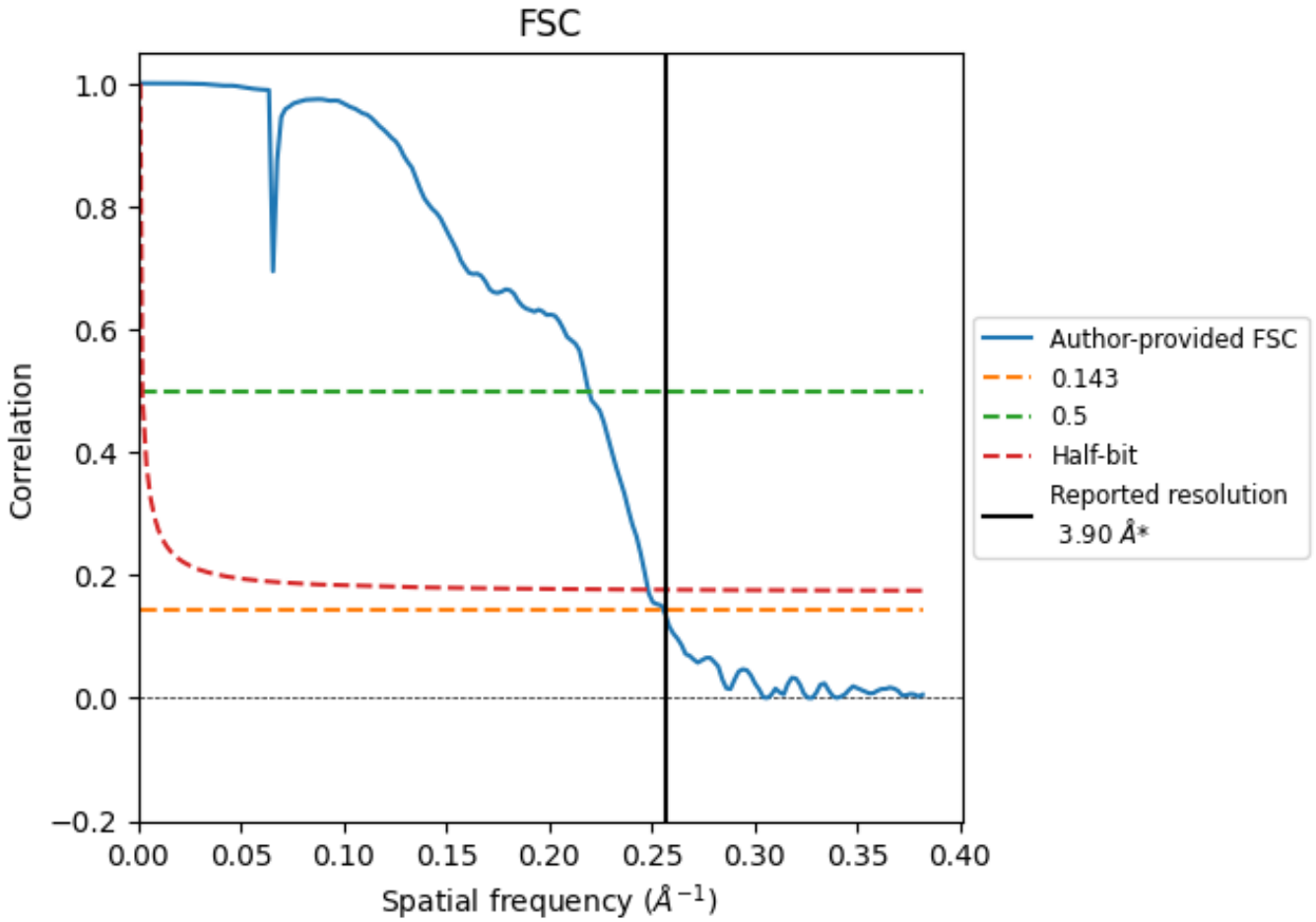


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

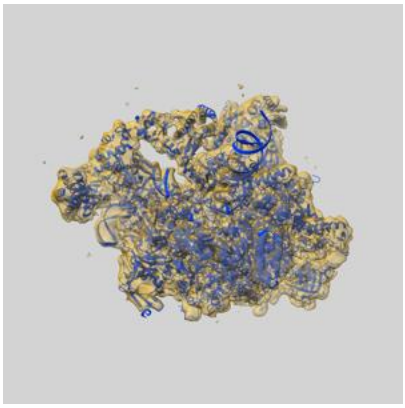
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.91	4.56	4.03
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

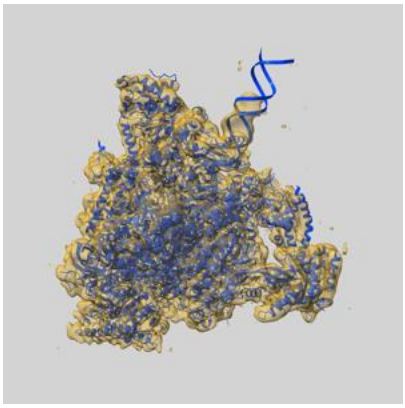
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8136 and PDB model 5IYB. Per-residue inclusion information can be found in section 3 on page 9.

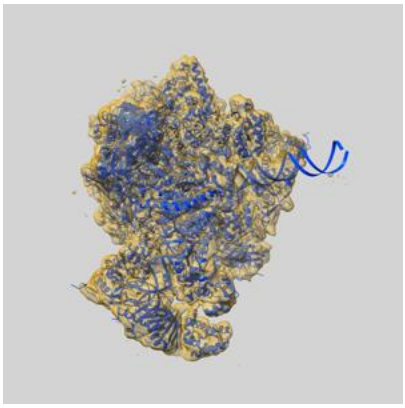
9.1 Map-model overlay



X



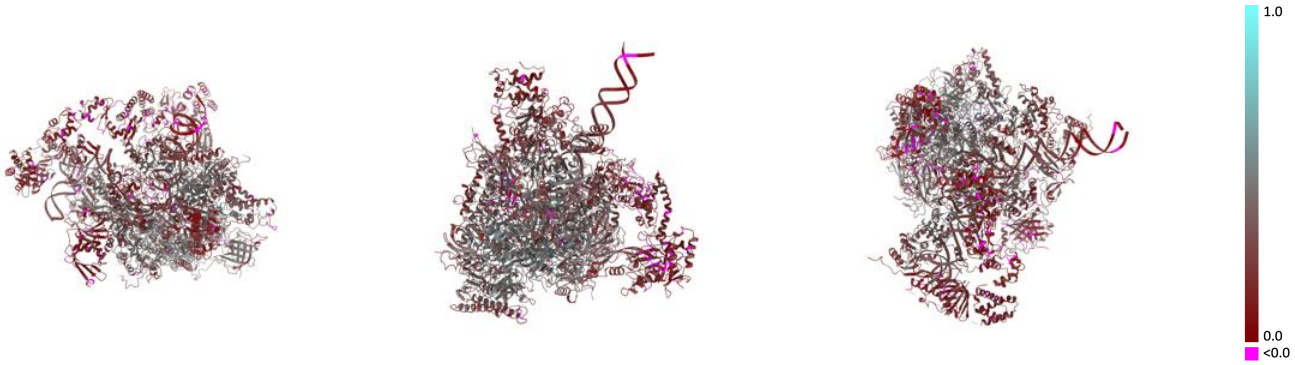
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

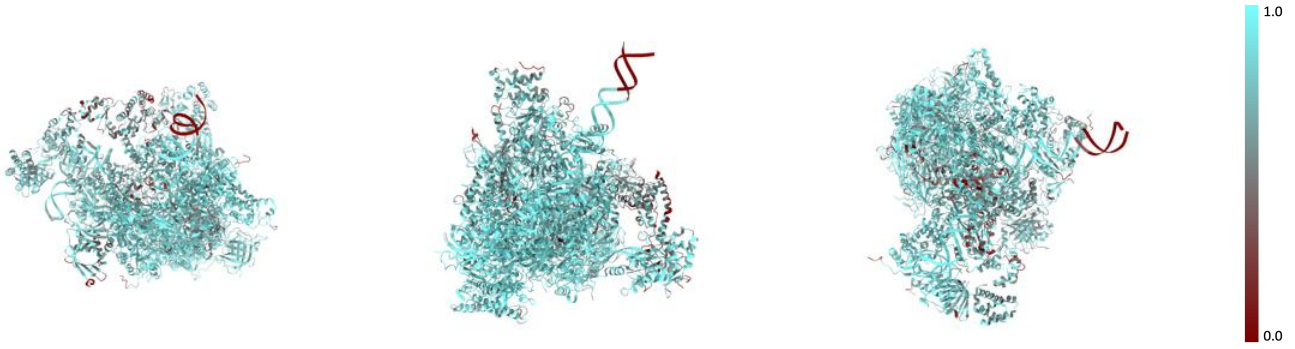
9.2 Q-score mapped to coordinate model (i)



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.

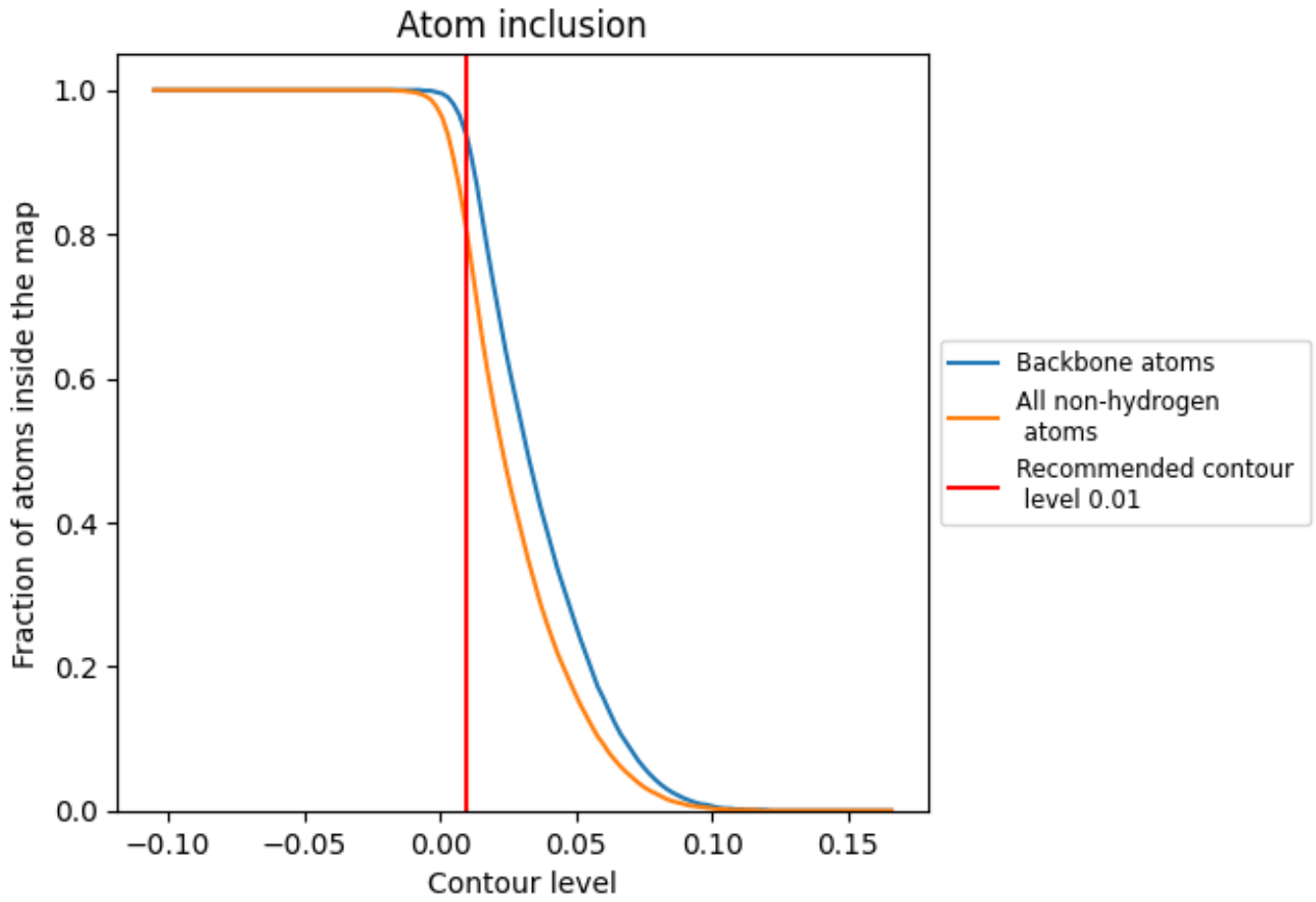
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.3070
A	0.8550	0.3670
B	0.8580	0.3980
C	0.8730	0.3800
D	0.7630	0.1680
E	0.8350	0.3290
F	0.8230	0.3910
G	0.7650	0.2070
H	0.8410	0.3310
I	0.8110	0.2800
J	0.8620	0.3750
K	0.8770	0.3820
L	0.8630	0.3470
M	0.8000	0.3090
N	0.7280	0.1550
O	0.7500	0.1720
P	0.8350	0.2550
Q	0.5500	0.1300
R	0.5530	0.1280
S	0.6820	0.1650
T	0.6890	0.1750
U	0.5750	0.1590
X	0.7710	0.2380
Y	0.7960	0.2480

