



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:02 AM UTC

PDB ID : 8QZ0 / pdb_00008qz0
EMDB ID : EMD-18769
Title : SWR1-hexasome-dimer complex
Authors : Jalal, A.S.B.; Wigley, D.B.
Deposited on : 2023-10-26
Resolution : 3.80 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

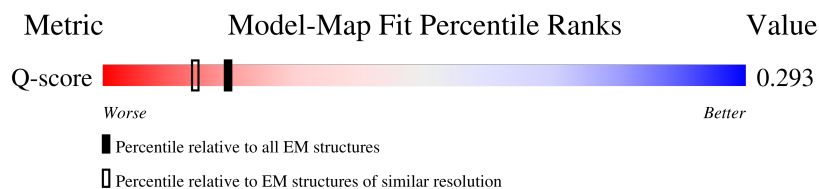
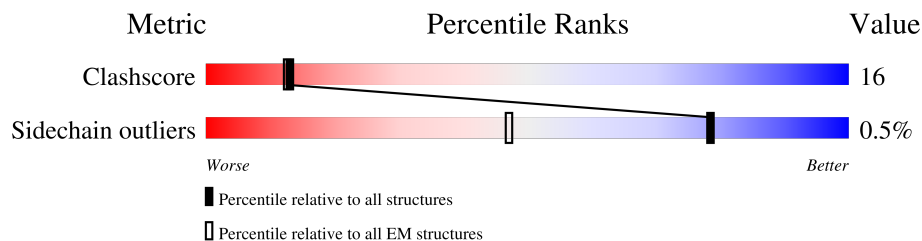
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



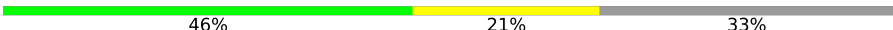
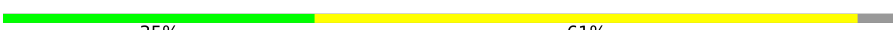
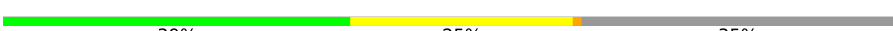
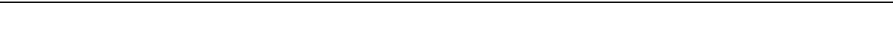
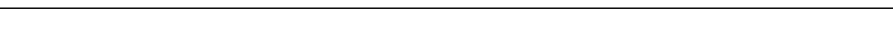
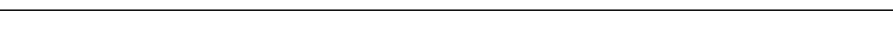
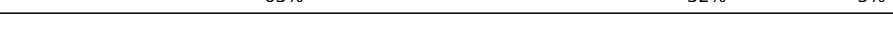
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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 $\leq 5\%$. 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	136	46% 33% 21%
1	B	136	55% 25% • 19%
2	C	103	39% 35% 26%
2	D	103	45% 24% 31%
3	E	132	59% 18% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	131	
5	H	131	
6	I	118	
7	J	118	
8	L	134	
9	P	303	
10	R	438	
11	S	280	
12	U	471	
12	W	471	
12	Y	471	
13	T	463	
13	V	463	
13	X	463	
14	Z	795	
15	M	1514	
16	K	153	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	BEF	M	1602	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 44167 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	108	Total	C	N	O	S	0	0
			864	546	165	152	1		
1	B	110	Total	C	N	O	S	0	0
			850	538	166	145	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	GLN	engineered mutation	UNP P61830
A	121	PRO	LYS	engineered mutation	UNP P61830
A	123	GLU	ASP	conflict	UNP P61830
A	125	GLN	LYS	engineered mutation	UNP P61830
B	120	MET	GLN	engineered mutation	UNP P61830
B	121	PRO	LYS	engineered mutation	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830
B	125	GLN	LYS	engineered mutation	UNP P61830

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	76	Total	C	N	O	0	0
			558	356	101	101		
2	D	71	Total	C	N	O	0	0
			527	329	103	95		

- Molecule 3 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	102	Total	C	N	O	0	0
			715	454	129	132		

- Molecule 4 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	88	Total	C	N	O	S	0	0
			640	396	112	131	1		

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	91	Total	C	N	O	S	0	0
			712	449	125	136	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	115	CYS	SER	engineered mutation	UNP P02293

- Molecule 6 is a DNA chain called DNA (113-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	113	Total	C	N	O	P	0	0
			2300	1090	419	678	113		

- Molecule 7 is a DNA chain called DNA (113-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	113	Total	C	N	O	P	0	0
			2333	1101	441	678	113		

- Molecule 8 is a protein called Histone H2A.Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	87	Total	C	N	O	0	0
			675	423	131	121		

- Molecule 9 is a protein called SWR1-complex protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	114	Total	C	N	O	0	0
			901	557	175	169		

- Molecule 10 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	385	Total	C	N	O	S	0	0
			3118	2024	507	572	15		

- Molecule 11 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	188	Total	C	N	O	S	0	0
			1500	940	270	281	9		

- Molecule 12 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	446	Total	C	N	O	S	0	0
			3430	2143	595	680	12		
12	W	433	Total	C	N	O	S	0	0
			3307	2076	569	651	11		
12	Y	443	Total	C	N	O	S	0	0
			3342	2091	581	659	11		

- Molecule 13 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	427	Total	C	N	O	S	0	0
			3257	2058	560	629	10		
13	X	441	Total	C	N	O	S	0	0
			3371	2128	581	653	9		
13	T	439	Total	C	N	O	S	0	0
			3304	2084	574	637	9		

- Molecule 14 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	173	Total	C	N	O	S	0	0
			1400	875	259	262	4		

- Molecule 15 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	794	Total	C	N	O	S	0	0
			6223	3929	1098	1170	26		

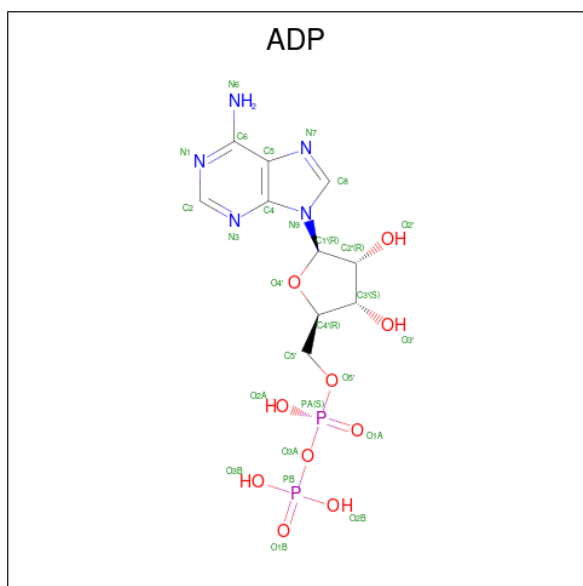
- Molecule 16 is a protein called Histone H2A.Z-specific chaperone CHZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	76	Total	C	N	O	S	0	0
			606	356	95	152	3		

There is a discrepancy between the modelled and reference sequences:

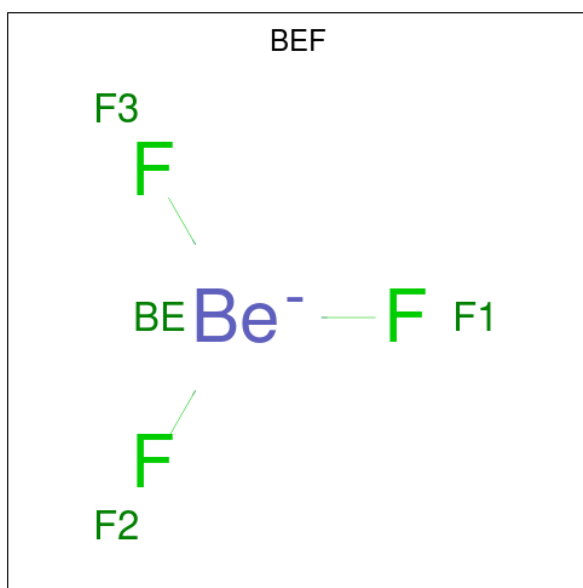
Chain	Residue	Modelled	Actual	Comment	Reference
K	98	CYS	SER	engineered mutation	UNP P40019

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
18	R	1	Total	Be	F	0
			4	1	3	
18	M	1	Total	Be	F	0
			4	1	3	

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	R	1	Total	Mg	0
			1	1	
19	U	1	Total	Mg	0
			1	1	
19	V	1	Total	Mg	0
			1	1	
19	W	1	Total	Mg	0
			1	1	
19	X	1	Total	Mg	0
			1	1	
19	Y	1	Total	Mg	0
			1	1	
19	T	1	Total	Mg	0
			1	1	
19	M	1	Total	Mg	0
			1	1	

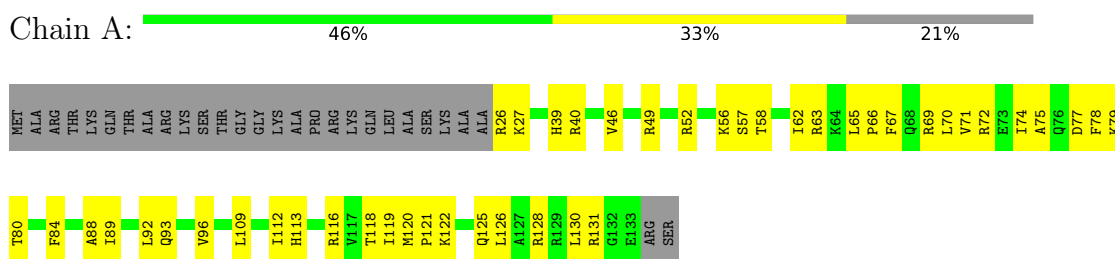
- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	S	2	Total 2	Zn 2	0

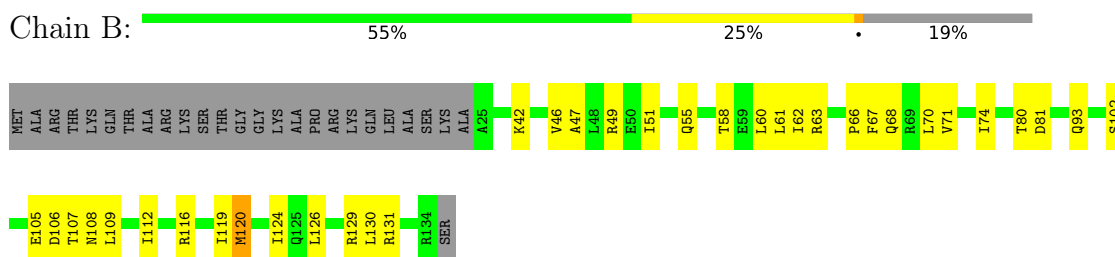
3 Residue-property plots

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.

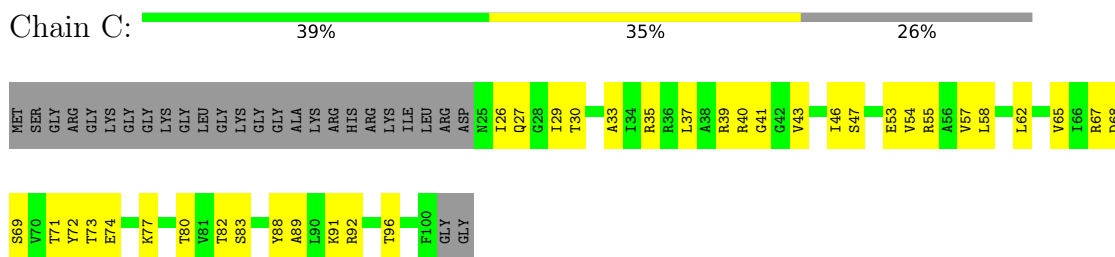
• Molecule 1: Histone H3



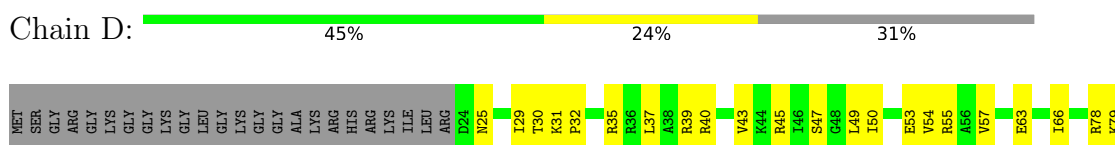
• Molecule 1: Histone H3



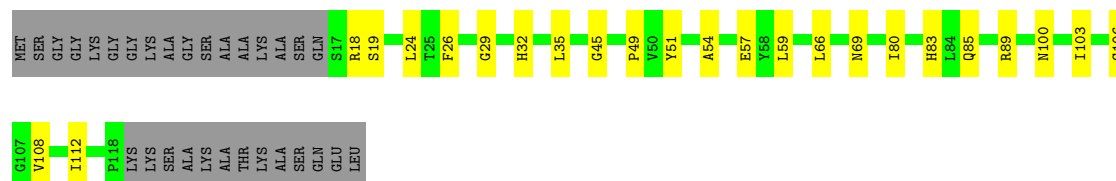
• Molecule 2: Histone H4



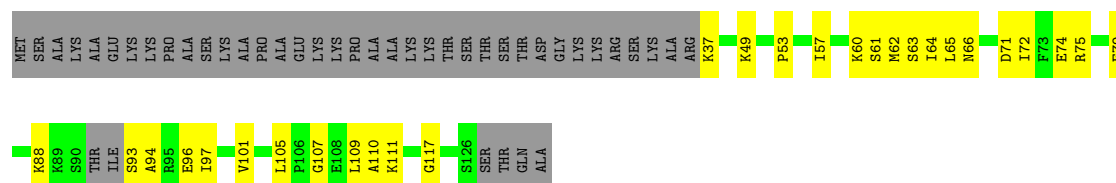
• Molecule 2: Histone H4



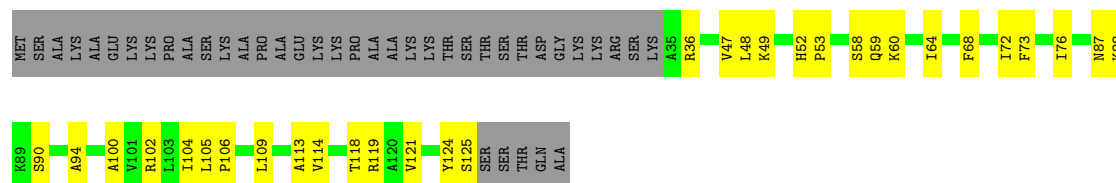
- Molecule 3: Histone H2A.1



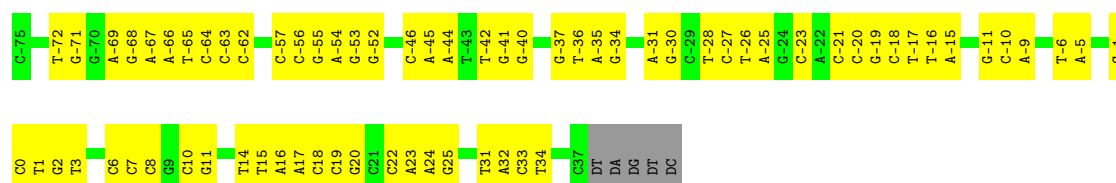
- Molecule 4: Histone H2B.1



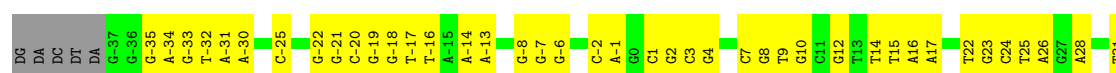
- Molecule 5: Histone H2B.1

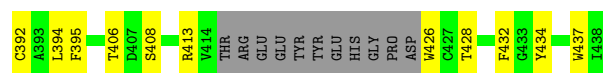


- Molecule 6: DNA (113-MER)

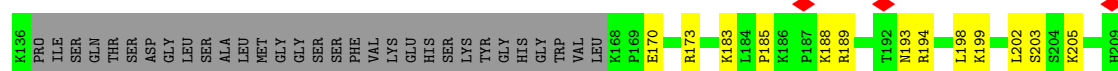
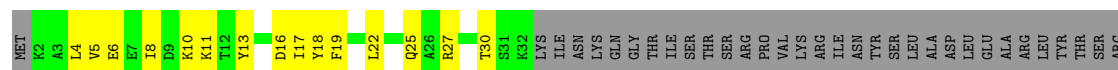


- Molecule 7: DNA (113-MER)

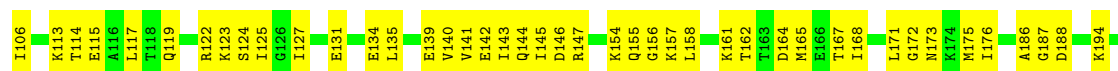




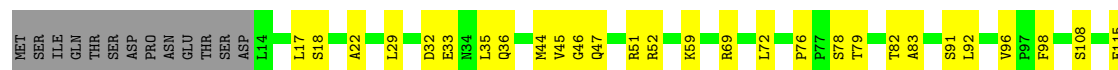
• Molecule 11: Vacuolar protein sorting-associated protein 71

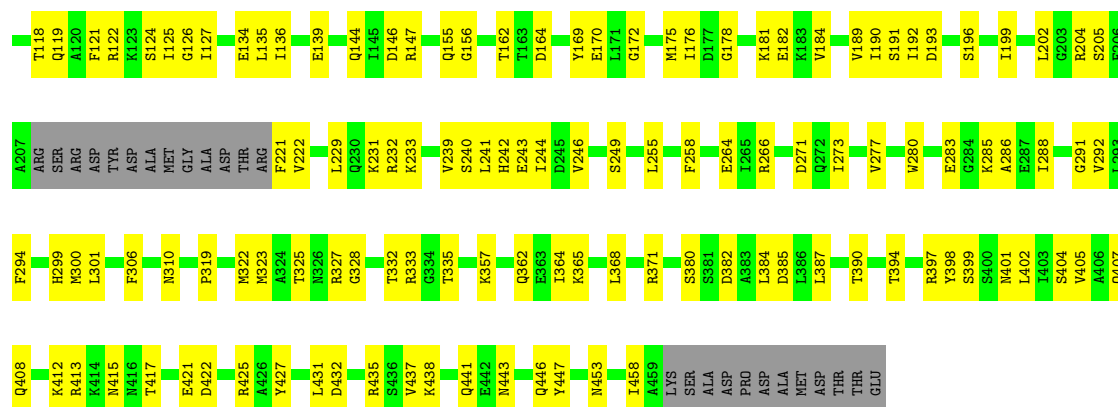


• Molecule 12: RuvB-like protein 2



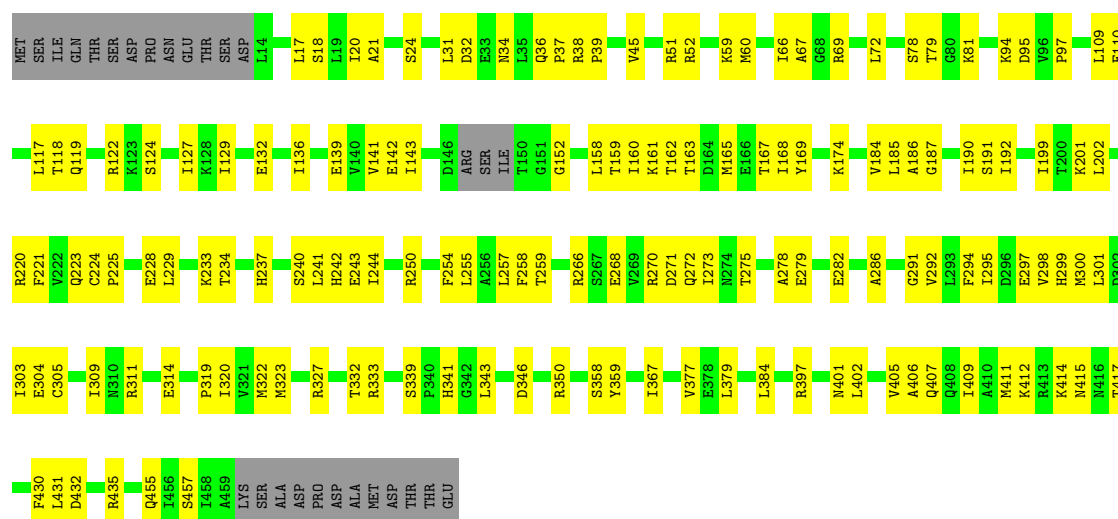
• Molecule 12: RuvB-like protein 2





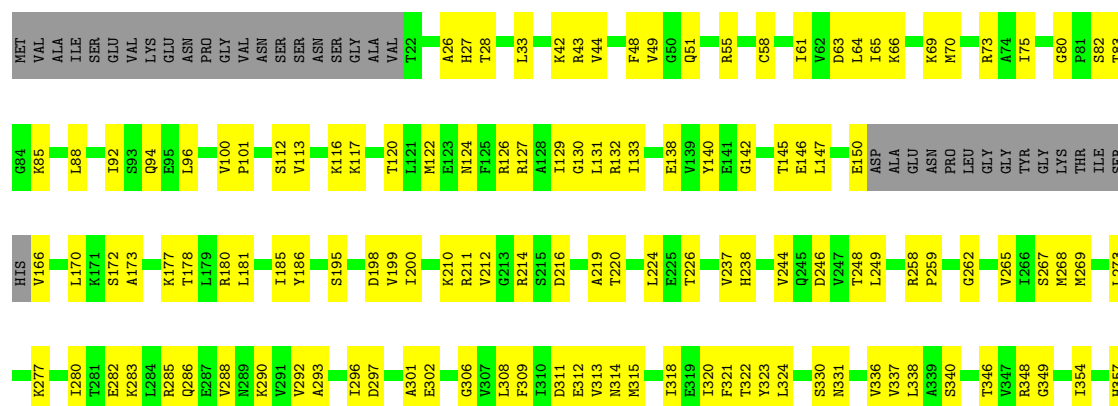
• Molecule 12: RuvB-like protein 2

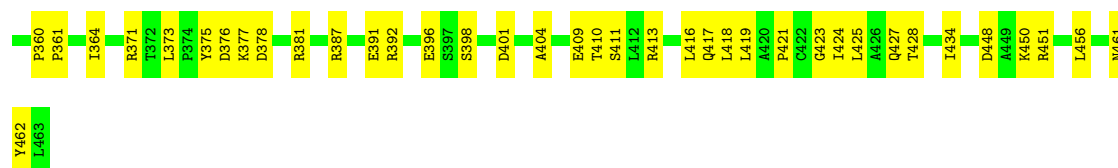
Chain Y: 63% 31% 6%



• Molecule 13: RuvB-like protein 1

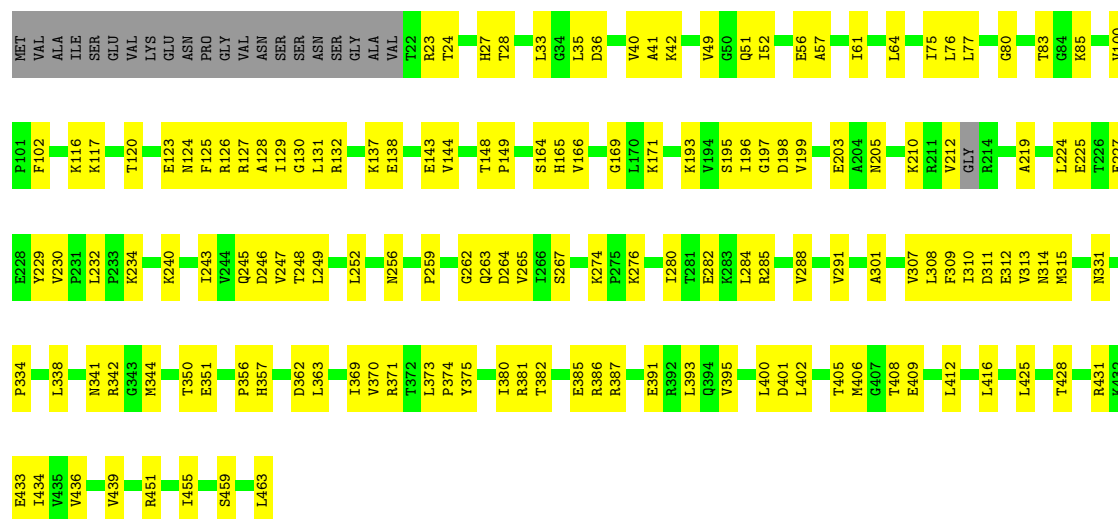
Chain V: 56% 36% 8%





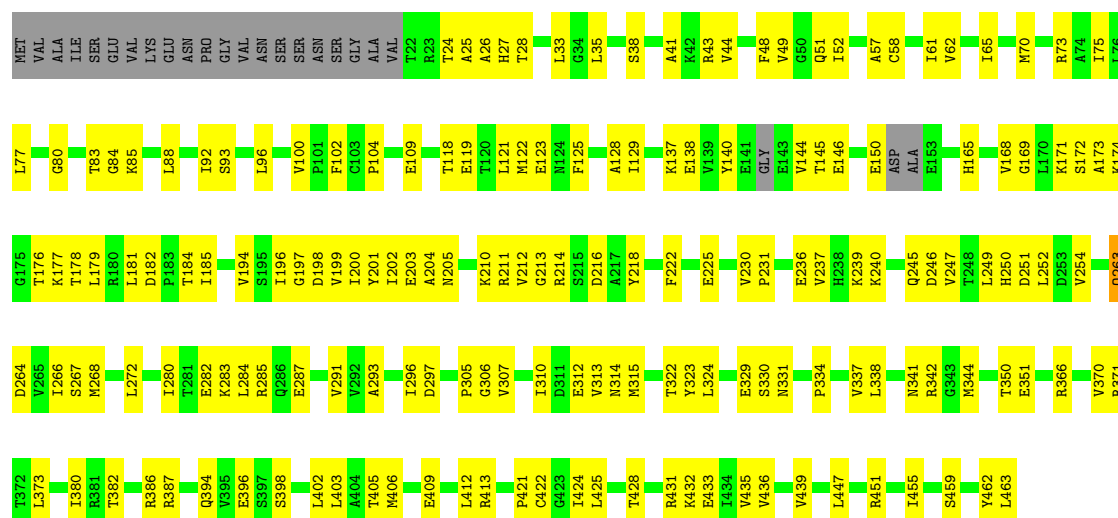
• Molecule 13: RuvB-like protein 1

Chain X: 63% 32% 5%



• Molecule 13: RuvB-like protein 1

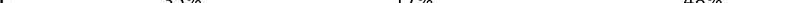
Chain T: 57% 37% 5%



• Molecule 14: Vacuolar protein sorting-associated protein 72

Chain Z: 16% 5% 78%

- Molecule 15: Helicase SWR1

Chain M: 

ARG	LYS	ALA	ALA	MET
LEU	PRO	GLU	PRO	ARG
LEU	ARG	GLU	LEU	THR
LYS	ILE	LYS	VAL	THR
GLY	LYS	TYR	ARG	HIS
ILE	LEU	ASP	ASN	LEU
GLU	VAL	HIS	LYS	SER
ASN	VAL	ILE	CYS	LEU
GLY	HIS	ALA	GLU	HIS
ALA	PRO	ALA	GLU	LYS
LEU	PRO	VAL	LEU	ASP
LYS	GLN	GLU	LEU	GLY
TYR	THR	GLU	TYR	LYS
ASP	THR	PRO	LYS	ALA
LYS	ILE	SER	LEU	GLY
GLU	THR	GLU	SER	THR
THR	ASN	ALA	ASP	GLU
ASP	PRO	PHE	HIS	ASP
SER	LEU	THR	SER	GLN
GLN	HIS	ILE	ASN	VAL
LEU	LEU	ILE	ASN	ALA
GLN	VAL	CYS	ARG	LYS
VAL	VAL	LYS	LYS	LYS
ILE	PRO	PRO	SER	GLY
THR	PRO	SER	ILE	THR
SER	GLY	ASP	VAL	ASN
LYS	GLU	ASP	PRO	ASP
ILE	SER	SER	GLN	TYR
GLU	GLU	GLU	LYS	LEU
ILE	SER	PHE	ARG	THR
THR	HIS	GLU	PRO	ARG
ILE	GLU	ASN	ILE	ARG
ILE	ILE	THR	GLN	ASN
THR	ILE	SER	HIS	GLU
TYR	ALA	GLU	LEU	LEU
LYS	SER	HIS	LYS	PHE
PRO	PHE	TYR	LYS	HIS
ASP	LYS	SER	ARG	LEU
PRO	SER	ASP	GLU	THR
ILE	LEU	ASN	ALA	SER
SER	GLU	PHE	LYS	PHE
TYR	ASP	TYR	ALA	VAL
PHE	ASP	PHE	SER	SER
TYR	LEU	THR	LEU	SER
LYS	THR	THR	LYS	VAL
GLN	LEU	SER	PHE	THR
GLN	GLU	GLU	GLU	PRO
ILE	ASN	GLU	ARG	LYS
THR	THR	GLU	LYS	GLY
HIS	TYR	ILE	GLU	PHE
ASP	ILE	LYS	ASN	ASN
ASP	ASP	LYS	PRO	ASP
HIS	GLU	LYS	LEU	SER
LEU	GLN	ARG	PRO	GLU
ILE	ARG	GLY	LEU	LYS
ASN	ARG	ARG	HIS	SER
GLN	LEU	GLU	GLU	GLN
GLY	SER	LYS	HIS	THR

- Molecule 16: Histone H2A.Z-specific chaperone CHZ1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00126	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/877	0.42	0/1178
1	B	0.12	0/862	0.38	0/1159
2	C	0.16	0/564	0.41	0/763
2	D	0.13	0/531	0.35	0/716
3	E	0.12	0/725	0.32	0/992
4	G	0.10	0/646	0.28	0/873
5	H	0.13	0/722	0.35	0/972
6	I	0.18	0/2576	0.39	0/3969
7	J	0.17	0/2620	0.33	0/4046
8	L	0.09	0/682	0.24	0/917
9	P	0.16	0/914	0.58	2/1232 (0.2%)
10	R	0.15	0/3206	0.39	2/4351 (0.0%)
11	S	0.17	0/1521	0.46	0/2047
12	U	0.12	0/3468	0.34	0/4674
12	W	0.12	0/3343	0.30	0/4508
12	Y	0.10	0/3378	0.30	0/4561
13	T	0.14	0/3342	0.36	0/4527
13	V	0.11	0/3294	0.30	0/4458
13	X	0.11	0/3412	0.32	0/4618
14	Z	0.12	0/1419	0.38	2/1899 (0.1%)
15	M	0.11	0/6330	0.34	0/8561
16	K	0.12	0/606	0.40	0/806
All	All	0.13	0/45038	0.35	6/61827 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	R	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
15	M	0	2
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	233	PRO	CA-C-N	7.76	136.36	121.54
9	P	233	PRO	C-N-CA	7.76	136.36	121.54
14	Z	299	PRO	CA-C-N	6.01	132.51	121.70
14	Z	299	PRO	C-N-CA	6.01	132.51	121.70
10	R	264	PHE	CA-C-N	-5.06	112.82	122.53
10	R	264	PHE	C-N-CA	-5.06	112.82	122.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	M	1159	ASP	Peptide
15	M	871	MET	Peptide
10	R	220	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	864	0	903	41	0
1	B	850	0	878	36	0
2	C	558	0	542	36	0
2	D	527	0	536	27	0
3	E	715	0	692	24	0
4	G	640	0	617	23	0
5	H	712	0	736	35	0
6	I	2300	0	1266	78	0
7	J	2333	0	1266	84	0
8	L	675	0	718	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	901	0	898	35	0
10	R	3118	0	3058	107	0
11	S	1500	0	1537	68	0
12	U	3430	0	3505	137	0
12	W	3307	0	3388	119	0
12	Y	3342	0	3364	112	0
13	T	3304	0	3389	137	0
13	V	3257	0	3385	127	0
13	X	3371	0	3487	109	0
14	Z	1400	0	1393	35	0
15	M	6223	0	6066	209	0
16	K	606	0	536	20	0
17	M	27	0	10	2	0
17	R	27	0	11	5	0
17	T	27	0	12	4	0
17	U	27	0	12	2	0
17	V	27	0	12	5	0
17	W	27	0	10	4	0
17	X	27	0	12	4	0
17	Y	27	0	11	1	0
18	M	4	0	0	2	0
18	R	4	0	0	1	0
19	M	1	0	0	0	0
19	R	1	0	0	0	0
19	T	1	0	0	0	0
19	U	1	0	0	0	0
19	V	1	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
20	S	2	0	0	0	0
All	All	44167	0	42250	1417	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 16.

All (1417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-55:DG:N2	7:J:55:DC:O2	1.97	0.95
10:R:220:GLY:O	10:R:222:PHE:N	2.01	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:374:GLN:HE22	13:T:174:LYS:HA	1.34	0.93
13:T:58:CYS:HB3	13:T:92:ILE:HD11	1.53	0.87
8:L:34:VAL:HA	8:L:60:THR:HG21	1.60	0.84
10:R:375:ARG:HE	10:R:376:GLN:H	1.22	0.84
6:I:20:DG:N2	7:J:-20:DC:O2	2.12	0.83
6:I:-52:DG:N2	7:J:52:DC:O2	2.11	0.81
12:U:156:GLY:HA3	12:U:171:LEU:HD23	1.61	0.81
6:I:-41:DG:H1	7:J:42:DA:N6	1.78	0.81
10:R:226:LEU:HD23	11:S:105:LEU:HD13	1.61	0.81
15:M:1138:LYS:O	15:M:1139:ASN:ND2	2.14	0.80
15:M:980:MET:HE1	15:M:983:VAL:HG22	1.64	0.80
5:H:105:LEU:HD11	5:H:109:LEU:HB2	1.63	0.80
4:G:88:LYS:HZ1	6:I:-34:DG:H8	1.29	0.79
12:U:154:LYS:HD3	12:U:176:ILE:HD13	1.64	0.79
12:U:432:ASP:HB3	12:U:435:ARG:HD3	1.65	0.78
6:I:-52:DG:N1	7:J:52:DC:N3	2.31	0.78
6:I:-55:DG:N1	7:J:55:DC:N3	2.31	0.78
1:A:69:ARG:HH22	2:D:29:ILE:HG12	1.49	0.77
6:I:25:DG:N2	7:J:-25:DC:O2	2.18	0.77
15:M:1082:ASN:HD21	15:M:1116:VAL:HG21	1.48	0.76
13:T:406:MET:HA	13:T:409:GLU:HB2	1.66	0.76
6:I:-53:DG:N1	7:J:53:DC:N3	2.28	0.75
6:I:-41:DG:N1	7:J:42:DA:N6	2.34	0.75
6:I:20:DG:N1	7:J:-20:DC:N3	2.30	0.75
12:W:135:LEU:H	12:W:232:ARG:HH21	1.33	0.75
11:S:170:GLU:HG2	11:S:173:ARG:HE	1.51	0.75
10:R:262:ASP:OD1	10:R:263:SER:N	2.21	0.74
1:B:60:LEU:HD21	1:B:93:GLN:HG2	1.70	0.73
13:T:26:ALA:HA	13:T:387:ARG:HH12	1.53	0.73
1:A:131:ARG:HH12	1:B:130:LEU:HB3	1.53	0.73
14:Z:595:THR:HG23	14:Z:596:LEU:HB3	1.71	0.73
6:I:-46:DC:N3	7:J:46:DG:N1	2.28	0.73
15:M:960:LEU:HB3	15:M:991:LYS:HZ3	1.52	0.73
13:X:265:VAL:HG23	15:M:1220:VAL:HG11	1.68	0.72
15:M:1200:ASN:O	15:M:1210:ARG:NH2	2.22	0.72
2:C:74:GLU:HA	2:C:77:LYS:HA	1.71	0.72
13:V:181:LEU:HD13	13:V:185:ILE:HG13	1.70	0.72
15:M:1078:LEU:HB3	15:M:1116:VAL:HG23	1.69	0.72
12:U:157:LYS:HB3	12:U:168:ILE:HD11	1.72	0.72
13:T:344:MET:HE3	13:T:344:MET:HA	1.71	0.72
12:U:99:THR:HG1	12:U:124:SER:HG	1.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:103:MET:HG2	11:S:120:LEU:HB3	1.72	0.71
6:I:-46:DC:O2	7:J:46:DG:N2	2.17	0.71
15:M:970:THR:HG23	15:M:971:LYS:HD2	1.73	0.71
12:U:408:GLN:HG2	13:V:64:LEU:HD22	1.73	0.71
13:T:145:THR:HG22	13:T:171:LYS:HG2	1.73	0.71
6:I:31:DT:O2	6:I:32:DA:N6	2.24	0.70
10:R:223:LEU:HA	10:R:313:ILE:HG13	1.73	0.70
12:Y:38:ARG:O	12:Y:51:ARG:NH2	2.24	0.70
12:U:175:MET:SD	12:U:175:MET:N	2.65	0.69
13:T:181:LEU:HD13	13:T:185:ILE:HB	1.75	0.69
12:W:189:VAL:C	12:W:190:ILE:HD13	2.17	0.69
13:X:51:GLN:NE2	13:X:373:LEU:O	2.25	0.69
9:P:238:LEU:O	9:P:242:GLN:NE2	2.26	0.69
12:W:135:LEU:HD21	12:W:191:SER:HB2	1.73	0.69
10:R:375:ARG:NE	10:R:376:GLN:H	1.91	0.69
11:S:263:ILE:HB	11:S:269:PHE:HA	1.75	0.69
15:M:873:GLN:HB2	15:M:882:SER:H	1.57	0.69
13:T:177:LYS:HB3	13:T:237:VAL:HG21	1.76	0.68
6:I:-20:DC:N4	6:I:-19:DG:O6	2.26	0.68
12:U:141:VAL:HG22	12:U:142:GLU:HG2	1.74	0.68
1:B:55:GLN:NE2	3:E:108:VAL:O	2.25	0.68
5:H:90:SER:OG	8:L:48:ARG:NH1	2.26	0.68
9:P:226:ILE:O	9:P:232:ARG:NH2	2.27	0.68
13:V:70:MET:SD	13:V:70:MET:N	2.66	0.68
6:I:-53:DG:N2	7:J:53:DC:O2	2.18	0.68
6:I:6:DC:O2	7:J:-6:DG:N2	2.26	0.68
10:R:273:GLU:HG3	10:R:305:THR:HA	1.76	0.68
12:U:387:LEU:HD21	12:U:403:ILE:HB	1.74	0.68
13:T:181:LEU:HB2	13:T:185:ILE:HD13	1.75	0.68
10:R:375:ARG:HE	10:R:376:GLN:N	1.90	0.68
4:G:62:MET:SD	4:G:62:MET:N	2.61	0.67
5:H:121:VAL:HG13	8:L:54:LYS:HZ2	1.60	0.67
13:X:24:THR:OG1	13:X:27:HIS:O	2.12	0.67
13:X:263:GLN:NE2	15:M:1216:ASN:O	2.27	0.67
10:R:255:VAL:HG13	10:R:314:PRO:HB3	1.77	0.67
8:L:39:ARG:NH2	16:K:74:ASP:OD1	2.28	0.67
12:U:407:GLN:HG3	12:U:411:MET:HE1	1.77	0.67
12:W:18:SER:HA	13:X:331:ASN:HD21	1.60	0.67
13:V:124:ASN:OD1	13:V:127:ARG:NH2	2.27	0.66
13:X:406:MET:HA	13:X:409:GLU:HB2	1.77	0.66
12:Y:127:ILE:HD11	12:Y:286:ALA:HB1	1.75	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:261:PHE:O	10:R:265:LYS:NZ	2.28	0.66
12:Y:60:MET:HE1	12:Y:66:ILE:HB	1.77	0.66
5:H:119:ARG:HH22	16:K:106:ARG:HH22	1.41	0.66
13:T:51:GLN:NE2	13:T:373:LEU:O	2.28	0.66
13:X:282:GLU:HA	13:X:285:ARG:HG3	1.76	0.66
12:W:29:LEU:H	12:W:91:SER:HB2	1.60	0.66
12:U:300:MET:O	12:U:333:ARG:NH1	2.29	0.66
11:S:18:TYR:HB3	12:U:145:ILE:HD11	1.77	0.65
12:W:397:ARG:O	12:W:401:ASN:ND2	2.28	0.65
12:Y:18:SER:OG	13:T:331:ASN:OD1	2.13	0.65
13:X:311:ASP:OD2	12:Y:311:ARG:NH2	2.30	0.65
12:Y:258:PHE:HB3	13:T:284:LEU:HD21	1.78	0.65
15:M:990:ARG:O	15:M:994:ASN:HB3	1.96	0.65
10:R:314:PRO:O	10:R:368:ARG:NH1	2.30	0.65
13:V:43:ARG:HG3	13:V:44:VAL:HG23	1.76	0.65
13:X:143:GLU:HB2	13:X:171:LYS:HB3	1.79	0.65
15:M:1082:ASN:ND2	15:M:1116:VAL:HG21	2.11	0.65
13:T:199:VAL:HG13	13:T:212:VAL:HB	1.79	0.65
12:W:365:LYS:HE3	12:W:384:LEU:HB3	1.79	0.65
10:R:266:THR:HB	10:R:269:LYS:HE3	1.78	0.65
13:T:329:GLU:OE1	13:T:366:ARG:NH1	2.30	0.65
12:U:327:ARG:NH1	13:T:462:TYR:OH	2.30	0.64
10:R:428:THR:O	11:S:194:ARG:NH1	2.30	0.64
6:I:31:DT:H1'	6:I:32:DA:N7	2.13	0.64
6:I:53:DG:O6	7:J:53:DC:N4	2.28	0.64
13:V:312:GLU:OE2	13:V:314:ASN:ND2	2.31	0.64
15:M:747:PRO:HD2	15:M:819:GLN:HE22	1.62	0.64
12:Y:119:GLN:OE1	12:Y:270:ARG:NH2	2.30	0.64
13:T:137:LYS:HZ1	13:T:204:ALA:H	1.44	0.64
15:M:1089:PHE:O	15:M:1092:ALA:N	2.31	0.64
2:D:30:THR:O	2:D:55:ARG:NH2	2.29	0.64
13:V:265:VAL:HA	13:V:268:MET:HE1	1.78	0.64
13:X:252:LEU:O	13:X:256:ASN:ND2	2.30	0.64
14:Z:241:ARG:HH12	15:M:740:CYS:HA	1.61	0.64
13:T:129:ILE:HG13	13:T:334:PRO:HB3	1.78	0.64
8:L:33:PRO:HG2	8:L:36:ARG:HD2	1.80	0.64
11:S:266:VAL:HG12	11:S:267:SER:H	1.62	0.64
15:M:1079:ARG:HA	15:M:1082:ASN:HD22	1.63	0.64
1:A:130:LEU:HD12	1:B:130:LEU:HD12	1.80	0.63
15:M:1007:SER:HB2	15:M:1188:VAL:HG12	1.78	0.63
2:C:27:GLN:OE1	2:C:55:ARG:NH1	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:311:ARG:HH12	13:T:104:PRO:HB2	1.64	0.63
15:M:1350:GLN:O	15:M:1354:ARG:NH1	2.31	0.63
13:T:80:GLY:O	13:T:85:LYS:NZ	2.32	0.63
9:P:272:PHE:HA	9:P:275:ARG:HE	1.64	0.63
12:W:22:ALA:HA	12:W:371:ARG:HH22	1.64	0.62
12:W:422:ASP:OD1	12:W:425:ARG:NH2	2.32	0.62
11:S:268:CYS:HA	11:S:271:LEU:HG	1.81	0.62
12:Y:132:GLU:HA	12:Y:234:THR:HA	1.81	0.62
15:M:1051:ASP:OD2	15:M:1133:ARG:NH2	2.32	0.62
7:J:31:DT:H2'	7:J:32:DG:C8	2.34	0.62
6:I:-17:DT:H2''	6:I:-16:DT:C5	2.34	0.62
15:M:1138:LYS:HD2	15:M:1138:LYS:H	1.65	0.62
9:P:269:ARG:HG3	13:V:244:VAL:HG11	1.80	0.62
15:M:691:LEU:HD11	15:M:770:GLY:HA3	1.80	0.62
12:U:188:ASP:HB3	12:U:204:ARG:HD2	1.80	0.62
13:T:451:ARG:O	13:T:455:ILE:HG12	2.00	0.62
15:M:956:ARG:NH2	15:M:996:PRO:O	2.32	0.62
11:S:205:LYS:HE2	11:S:214:SER:HA	1.80	0.62
13:X:232:LEU:O	13:X:234:LYS:NZ	2.32	0.62
12:Y:34:ASN:O	12:Y:36:GLN:NE2	2.33	0.62
2:D:37:LEU:HD13	2:D:40:ARG:HE	1.64	0.62
7:J:9:DT:H2''	7:J:10:DG:C8	2.35	0.62
13:T:197:GLY:O	13:T:214:ARG:NH1	2.33	0.62
13:X:33:LEU:HG	13:X:35:LEU:HD23	1.82	0.62
12:Y:163:THR:HG23	12:Y:224:CYS:HB3	1.82	0.62
13:V:265:VAL:O	13:V:269:MET:HB3	1.99	0.61
13:V:330:SER:OG	13:V:331:ASN:N	2.33	0.61
11:S:17:ILE:HD11	12:U:147:ARG:HB2	1.81	0.61
12:Y:161:LYS:NZ	12:Y:224:CYS:SG	2.73	0.61
12:W:175:MET:SD	12:W:175:MET:N	2.72	0.61
11:S:19:PHE:HB3	12:U:144:GLN:HA	1.81	0.61
12:Y:31:LEU:O	12:Y:38:ARG:NH2	2.32	0.61
12:Y:271:ASP:OD1	12:Y:271:ASP:N	2.33	0.61
13:T:402:LEU:O	13:T:405:THR:OG1	2.10	0.61
5:H:76:ILE:HG12	5:H:104:ILE:HD11	1.81	0.61
13:V:288:VAL:O	13:V:292:VAL:HG12	2.00	0.61
12:W:244:ILE:HD12	12:W:244:ILE:H	1.65	0.61
13:X:144:VAL:HG13	13:X:169:GLY:H	1.64	0.61
15:M:1174:ARG:O	15:M:1177:ILE:HG13	2.00	0.61
7:J:3:DC:H2''	7:J:4:DG:C8	2.35	0.61
13:T:198:ASP:OD1	13:T:214:ARG:NH1	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:48:LEU:HD13	8:L:71:LEU:HB3	1.81	0.61
11:S:220:MET:HA	11:S:223:ASN:HD22	1.66	0.61
12:U:115:GLU:OE2	12:U:270:ARG:NH2	2.34	0.61
12:U:408:GLN:HG3	13:V:63:ASP:OD1	2.01	0.61
12:W:446:GLN:HE22	13:X:374:PRO:HG3	1.66	0.61
14:Z:298:THR:C	14:Z:300:ALA:HA	2.25	0.61
13:T:245:GLN:HB2	15:M:1038:VAL:HG21	1.83	0.61
5:H:105:LEU:HD12	5:H:106:PRO:HD2	1.81	0.61
12:W:231:LYS:HG3	12:W:233:LYS:HE3	1.82	0.60
12:Y:233:LYS:NZ	15:M:1057:TYR:OH	2.24	0.60
6:I:-42:DT:O4	6:I:-41:DG:O6	2.19	0.60
10:R:256:SER:HB2	10:R:368:ARG:HH11	1.66	0.60
2:D:47:SER:H	2:D:50:ILE:HD12	1.67	0.60
13:V:85:LYS:NZ	17:V:501:ADP:O2B	2.35	0.60
13:V:308:LEU:HB3	13:V:336:VAL:HG12	1.82	0.60
13:T:24:THR:OG1	13:T:27:HIS:O	2.18	0.60
13:V:96:LEU:HB3	13:V:100:VAL:HG11	1.81	0.60
13:T:83:THR:N	17:T:501:ADP:O1A	2.34	0.60
1:A:66:PRO:HA	1:A:69:ARG:HE	1.67	0.60
6:I:22:DC:H2'	6:I:23:DA:C8	2.36	0.60
15:M:685:ASP:OD1	15:M:701:LYS:NZ	2.35	0.60
13:X:264:ASP:HA	15:M:1220:VAL:HG13	1.84	0.60
15:M:759:ASN:OD1	15:M:1302:GLN:NE2	2.34	0.60
15:M:995:HIS:O	15:M:997:ASN:N	2.34	0.60
16:K:112:ILE:HD11	16:K:121:LEU:HD11	1.81	0.60
2:C:29:ILE:H	2:C:29:ILE:HD12	1.67	0.60
12:U:375:GLU:OE2	13:V:73:ARG:NH2	2.35	0.60
8:L:83:VAL:HG12	8:L:85:ARG:H	1.66	0.60
10:R:254:PHE:HE1	10:R:257:PRO:HD3	1.66	0.60
12:W:280:TRP:HB3	12:W:286:ALA:HB3	1.83	0.60
13:V:220:THR:OG1	14:Z:277:GLN:OE1	2.20	0.59
12:W:184:VAL:HG13	12:W:190:ILE:HD11	1.83	0.59
12:W:408:GLN:O	12:W:412:LYS:NZ	2.31	0.59
4:G:57:ILE:HD11	6:I:-54:DA:H3'	1.83	0.59
5:H:48:LEU:O	5:H:52:HIS:N	2.34	0.59
13:V:129:ILE:HD11	13:V:249:LEU:HD12	1.83	0.59
15:M:1108:ASN:O	15:M:1112:LEU:HG	2.02	0.59
7:J:22:DT:H2''	7:J:23:DG:C8	2.37	0.59
12:U:266:ARG:NH2	12:U:268:GLU:OE2	2.35	0.59
13:V:49:VAL:H	17:V:501:ADP:HN62	1.50	0.59
12:W:380:SER:OG	12:W:382:ASP:OD1	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-14:DA:H2''	7:J:-13:DA:C8	2.37	0.59
15:M:1081:THR:HB	15:M:1112:LEU:HD22	1.84	0.59
13:V:315:MET:O	13:V:348:ARG:NH1	2.27	0.59
12:Y:124:SER:HB3	12:Y:319:PRO:HG3	1.84	0.59
15:M:1080:GLU:HA	15:M:1083:LYS:HD2	1.83	0.59
12:U:105:GLU:HG2	13:V:323:TYR:HE1	1.66	0.59
12:Y:78:SER:N	17:Y:501:ADP:O3B	2.35	0.59
6:I:-41:DG:N1	7:J:42:DA:C6	2.71	0.59
12:Y:257:LEU:H	12:Y:257:LEU:HD12	1.66	0.59
10:R:220:GLY:C	10:R:222:PHE:H	2.10	0.59
12:W:382:ASP:OD1	12:W:382:ASP:N	2.36	0.59
10:R:187:PHE:O	10:R:352:ASN:ND2	2.31	0.59
5:H:100:ALA:O	5:H:104:ILE:HG12	2.03	0.58
15:M:826:ALA:HB3	15:M:852:THR:HB	1.86	0.58
1:B:80:THR:HG22	1:B:81:ASP:H	1.68	0.58
12:U:243:GLU:N	12:U:243:GLU:OE1	2.34	0.58
13:V:375:TYR:OH	17:V:501:ADP:N7	2.30	0.58
12:W:46:GLY:O	12:W:51:ARG:NE	2.35	0.58
13:X:80:GLY:O	13:X:85:LYS:NZ	2.37	0.58
13:T:150:GLU:N	13:T:165:HIS:O	2.34	0.58
13:T:313:VAL:HG11	13:T:338:LEU:HG	1.85	0.58
12:W:204:ARG:O	12:W:221:PHE:N	2.37	0.58
15:M:755:SER:HB2	15:M:1326:LEU:HD11	1.85	0.58
6:I:-21:DC:H2'	6:I:-20:DC:C6	2.39	0.58
2:C:72:TYR:OH	2:C:92:ARG:HD3	2.03	0.58
2:D:32:PRO:HB3	2:D:35:ARG:HH21	1.68	0.58
13:V:199:VAL:HG13	13:V:212:VAL:HB	1.85	0.58
15:M:665:ILE:O	15:M:669:GLU:HG2	2.04	0.58
15:M:1380:LEU:O	15:M:1384:ASN:ND2	2.33	0.58
10:R:127:SER:OG	10:R:413:ARG:NH2	2.37	0.58
12:U:364:ILE:HG13	12:U:396:LEU:HD12	1.85	0.58
14:Z:289:GLN:N	14:Z:595:THR:O	2.37	0.58
8:L:87:THR:HG22	8:L:89:ARG:H	1.69	0.58
10:R:80:LEU:HD21	10:R:91:LEU:HD23	1.85	0.58
12:Y:279:GLU:OE1	15:M:1151:LYS:NZ	2.35	0.58
10:R:217:ASP:HB3	11:S:102:PHE:HZ	1.68	0.58
12:U:20:ILE:HB	13:V:70:MET:HA	1.86	0.58
13:T:264:ASP:O	13:T:267:SER:OG	2.14	0.58
15:M:960:LEU:HB3	15:M:991:LYS:NZ	2.18	0.58
7:J:40:DC:H2'	7:J:41:DC:C4	2.39	0.58
10:R:13:TYR:HA	10:R:59:ARG:HH21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:140:VAL:O	12:U:161:LYS:NZ	2.36	0.58
12:U:370:ILE:O	12:U:373:GLN:NE2	2.36	0.58
13:V:273:LEU:HD13	13:T:272:LEU:HD13	1.86	0.58
13:T:239:LYS:NZ	13:T:240:LYS:O	2.37	0.58
1:A:131:ARG:NH1	1:B:130:LEU:O	2.37	0.57
13:V:172:SER:OG	13:V:173:ALA:N	2.37	0.57
12:Y:314:GLU:OE2	12:Y:350:ARG:NH2	2.37	0.57
15:M:875:VAL:HG23	15:M:878:GLY:H	1.69	0.57
8:L:41:LEU:HG	8:L:51:VAL:HG21	1.86	0.57
12:U:310:ASN:ND2	12:U:346:ASP:OD2	2.37	0.57
12:Y:339:SER:OG	12:Y:343:LEU:O	2.22	0.57
5:H:102:ARG:HH11	5:H:114:VAL:HG21	1.67	0.57
11:S:117:PRO:HA	11:S:120:LEU:HG	1.87	0.57
13:T:201:TYR:HE1	13:T:210:LYS:HG2	1.69	0.57
10:R:43:SER:HB3	10:R:75:ILE:HG12	1.85	0.57
10:R:254:PHE:CE1	10:R:257:PRO:HD3	2.39	0.57
13:X:120:THR:O	13:X:124:ASN:ND2	2.33	0.57
12:U:38:ARG:O	12:U:51:ARG:NH1	2.35	0.57
12:W:306:PHE:O	12:W:310:ASN:ND2	2.37	0.57
13:X:127:ARG:HD3	12:Y:266:ARG:HH22	1.69	0.57
13:X:425:LEU:O	13:X:428:THR:OG1	2.21	0.57
13:T:174:LYS:HB3	13:T:236:GLU:HA	1.87	0.57
15:M:720:ALA:HB3	15:M:931:ARG:HA	1.87	0.57
15:M:1275:LEU:HA	15:M:1278:LEU:HD12	1.86	0.57
10:R:11:GLY:H	10:R:15:ILE:HG12	1.69	0.57
10:R:115:ALA:O	10:R:119:ILE:HG12	2.04	0.57
11:S:8:ILE:O	13:V:178:THR:OG1	2.22	0.57
13:T:122:MET:HA	13:T:122:MET:HE2	1.86	0.57
2:C:67:ARG:O	2:C:71:THR:HG23	2.03	0.57
5:H:124:TYR:O	8:L:27:ARG:NH2	2.37	0.57
9:P:260:LEU:HD11	13:V:94:GLN:HG2	1.86	0.57
10:R:110:GLU:O	10:R:114:HIS:ND1	2.35	0.57
13:T:70:MET:HE1	13:T:73:ARG:HG2	1.86	0.57
12:U:131:GLU:OE2	12:U:237:HIS:ND1	2.37	0.57
15:M:1256:GLN:NE2	15:M:1260:ASP:OD1	2.37	0.57
12:U:300:MET:HE3	12:U:300:MET:HA	1.86	0.57
13:X:42:LYS:H	13:X:42:LYS:HZ3	1.53	0.57
13:X:129:ILE:HG13	13:X:334:PRO:HB3	1.87	0.57
12:Y:184:VAL:HG13	12:Y:186:ALA:H	1.68	0.57
13:T:168:VAL:O	13:T:179:LEU:N	2.33	0.57
1:A:75:ALA:HB2	2:D:66:ILE:HD11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:THR:HG21	7:J:-13:DA:H5''	1.87	0.56
13:X:341:ASN:OD1	13:X:342:ARG:NH1	2.38	0.56
15:M:1262:GLY:O	15:M:1263:HIS:ND1	2.38	0.56
3:E:18:ARG:HD2	6:I:-44:DA:H4'	1.85	0.56
9:P:292:LEU:O	9:P:296:LEU:HG	2.05	0.56
13:V:258:ARG:HH22	13:V:277:LYS:HD2	1.70	0.56
13:X:83:THR:N	17:X:501:ADP:O1A	2.38	0.56
13:X:131:LEU:HD11	13:X:301:ALA:HB1	1.88	0.56
12:Y:36:GLN:OE1	12:Y:52:ARG:NH2	2.32	0.56
12:Y:295:ILE:HG22	12:Y:298:VAL:HG22	1.87	0.56
12:W:273:ILE:O	12:W:277:VAL:HG22	2.05	0.56
13:T:75:ILE:HG23	13:T:337:VAL:HG23	1.87	0.56
15:M:902:ILE:HG21	15:M:1389:LEU:HA	1.87	0.56
12:U:86:MET:HE3	12:U:86:MET:HA	1.88	0.56
13:X:164:SER:O	13:X:165:HIS:ND1	2.38	0.56
13:T:177:LYS:NZ	13:T:178:THR:O	2.39	0.56
15:M:956:ARG:NH2	15:M:1000:GLU:O	2.39	0.56
15:M:966:SER:HA	15:M:969:GLN:HE21	1.69	0.56
16:K:115:LYS:HG3	16:K:116:LYS:H	1.70	0.56
1:B:55:GLN:O	2:C:40:ARG:NH1	2.38	0.56
1:B:58:THR:OG1	3:E:106:GLY:O	2.19	0.56
4:G:93:SER:OG	4:G:94:ALA:N	2.38	0.56
11:S:22:LEU:HB3	12:U:142:GLU:HB2	1.88	0.56
13:V:210:LYS:NZ	13:V:211:ARG:O	2.36	0.56
3:E:80:ILE:HG23	3:E:83:HIS:H	1.71	0.56
12:W:437:VAL:O	12:W:441:GLN:NE2	2.33	0.56
13:X:280:ILE:O	13:X:285:ARG:NH2	2.39	0.56
4:G:93:SER:N	4:G:96:GLU:OE1	2.39	0.56
15:M:1242:GLN:HA	15:M:1248:LEU:HD23	1.87	0.56
1:A:77:ASP:OD1	1:A:78:PHE:N	2.39	0.56
1:B:108:ASN:ND2	2:C:41:GLY:O	2.38	0.56
10:R:256:SER:O	10:R:368:ARG:HD3	2.05	0.56
12:U:17:LEU:HD22	13:V:293:ALA:HB2	1.88	0.56
15:M:1279:GLU:OE1	15:M:1291:ARG:NH1	2.38	0.56
12:U:413:ARG:NH2	12:U:421:GLU:OE2	2.39	0.55
10:R:243:ILE:O	10:R:247:ASN:ND2	2.39	0.55
13:V:371:ARG:HH11	13:V:373:LEU:HD21	1.70	0.55
13:V:423:GLY:HA2	13:V:434:ILE:HD11	1.88	0.55
13:T:58:CYS:O	13:T:62:VAL:HG23	2.06	0.55
2:C:35:ARG:NH2	2:C:46:ILE:O	2.40	0.55
6:I:-69:DA:H2''	6:I:-68:DG:C8	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:33:LEU:HG	13:T:35:LEU:HD23	1.88	0.55
13:T:341:ASN:OD1	13:T:342:ARG:NH1	2.39	0.55
11:S:91:THR:OG1	11:S:92:GLN:N	2.36	0.55
12:U:38:ARG:HD2	12:U:41:SER:HB3	1.87	0.55
12:W:408:GLN:HG2	13:X:64:LEU:HB2	1.89	0.55
13:X:431:ARG:HH12	13:X:434:ILE:HA	1.72	0.55
13:T:75:ILE:HD11	13:T:370:VAL:HG23	1.89	0.55
15:M:956:ARG:NH1	15:M:1244:ASP:OD2	2.34	0.55
7:J:41:DC:C4	7:J:42:DA:N6	2.75	0.55
13:T:57:ALA:O	13:T:61:ILE:HG12	2.06	0.55
16:K:97:THR:HG21	16:K:101:ILE:HD13	1.89	0.55
10:R:434:TYR:HA	10:R:437:TRP:CD1	2.42	0.55
13:V:33:LEU:O	13:V:55:ARG:NH1	2.36	0.55
12:W:390:THR:O	12:W:394:THR:OG1	2.18	0.55
13:X:148:THR:HG23	14:Z:606:LEU:HD11	1.89	0.55
10:R:60:PRO:HD3	10:R:71:LEU:HD23	1.89	0.55
10:R:92:LYS:HG3	10:R:93:GLU:CD	2.31	0.55
11:S:17:ILE:HG12	12:U:147:ARG:HH21	1.72	0.55
14:Z:241:ARG:HD2	15:M:745:TRP:HZ2	1.72	0.55
13:T:129:ILE:HG12	13:T:305:PRO:HA	1.89	0.55
1:A:89:ILE:O	1:A:93:GLN:NE2	2.39	0.55
13:X:36:ASP:HB3	13:X:40:VAL:HG23	1.88	0.55
12:U:165:MET:C	12:U:165:MET:HE3	2.31	0.54
2:C:77:LYS:HZ2	15:M:621:SER:HB3	1.72	0.54
11:S:203:SER:O	11:S:203:SER:OG	2.23	0.54
12:W:427:TYR:O	12:W:435:ARG:NH2	2.32	0.54
6:I:-67:DA:N1	7:J:68:DC:N4	2.55	0.54
6:I:-1:DG:H2'	6:I:0:DC:C6	2.41	0.54
8:L:34:VAL:O	8:L:38:LYS:HG3	2.07	0.54
12:U:186:ALA:O	12:U:204:ARG:NH2	2.32	0.54
15:M:1078:LEU:HA	15:M:1081:THR:HG23	1.89	0.54
4:G:107:GLY:HA2	4:G:110:ALA:HB3	1.89	0.54
13:V:416:LEU:HA	13:V:419:LEU:HD23	1.89	0.54
13:X:402:LEU:HG	13:X:406:MET:HE1	1.89	0.54
13:X:459:SER:OG	13:X:463:LEU:O	2.25	0.54
13:T:252:LEU:HD21	15:M:1045:LEU:HD13	1.89	0.54
2:C:69:SER:O	2:C:73:THR:OG1	2.21	0.54
5:H:48:LEU:HD22	8:L:71:LEU:HD22	1.89	0.54
10:R:256:SER:OG	10:R:314:PRO:HB2	2.06	0.54
12:U:375:GLU:O	13:V:69:LYS:NZ	2.40	0.54
13:X:85:LYS:NZ	17:X:501:ADP:O1B	2.31	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:249:LEU:HD12	13:T:249:LEU:H	1.73	0.54
15:M:1276:ASP:N	15:M:1276:ASP:OD1	2.40	0.54
10:R:41:TYR:HB3	10:R:45:HIS:HB3	1.89	0.54
10:R:313:ILE:HA	10:R:316:THR:HG23	1.90	0.54
13:X:77:LEU:HD11	13:X:85:LYS:HB3	1.90	0.54
12:Y:397:ARG:O	12:Y:401:ASN:ND2	2.30	0.54
1:B:68:GLN:HA	1:B:71:VAL:HG12	1.90	0.54
1:B:124:ILE:HD11	2:C:53:GLU:HG3	1.89	0.54
13:X:274:LYS:HZ3	12:Y:250:ARG:HD3	1.72	0.54
13:T:315:MET:HE3	13:T:315:MET:HA	1.89	0.54
15:M:1059:ALA:HB2	15:M:1134:PRO:HB2	1.90	0.54
15:M:1192:MET:N	15:M:1192:MET:HE2	2.23	0.54
1:B:106:ASP:OD2	1:B:131:ARG:NH2	2.38	0.54
12:U:299:HIS:HD2	12:U:325:THR:HB	1.71	0.54
12:W:35:LEU:O	12:W:52:ARG:NH1	2.36	0.54
12:W:36:GLN:OE1	12:W:52:ARG:NH1	2.41	0.54
13:T:282:GLU:HA	13:T:285:ARG:HG3	1.90	0.54
15:M:1226:GLN:OE1	15:M:1226:GLN:N	2.37	0.54
1:A:72:ARG:NH2	6:I:-23:DC:OP1	2.35	0.54
4:G:62:MET:O	4:G:66:ASN:ND2	2.33	0.54
11:S:117:PRO:HB2	11:S:128:ARG:HD2	1.90	0.54
12:W:431:LEU:HB3	13:X:369:ILE:HB	1.89	0.54
13:X:195:SER:OG	13:X:196:ILE:N	2.39	0.54
12:Y:379:LEU:HD23	12:Y:384:LEU:HD12	1.90	0.54
15:M:1360:GLN:NE2	15:M:1363:ASP:O	2.41	0.54
4:G:71:ASP:OD1	4:G:72:ILE:N	2.42	0.53
13:X:126:ARG:NH2	13:X:285:ARG:HD3	2.23	0.53
6:I:-45:DA:H2''	6:I:-44:DA:N7	2.24	0.53
6:I:2:DG:H2'	6:I:3:DT:H71	1.90	0.53
12:U:243:GLU:HG3	12:U:257:LEU:HD11	1.89	0.53
13:V:417:GLN:O	12:W:69:ARG:NH2	2.40	0.53
12:W:178:GLY:HA3	12:W:199:ILE:HD13	1.89	0.53
13:X:288:VAL:HA	13:X:291:VAL:HG12	1.90	0.53
6:I:-31:DA:H2''	6:I:-30:DG:H5'	1.88	0.53
6:I:20:DG:O6	7:J:-20:DC:N4	2.36	0.53
7:J:3:DC:H2''	7:J:4:DG:N7	2.23	0.53
9:P:210:ARG:HG3	9:P:226:ILE:HG23	1.90	0.53
10:R:262:ASP:O	10:R:266:THR:OG1	2.11	0.53
12:W:332:THR:OG1	12:W:335:THR:OG1	2.26	0.53
13:T:146:GLU:HA	13:T:196:ILE:HD11	1.90	0.53
10:R:202:PRO:HG2	10:R:209:TYR:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:8:ILE:HG13	11:S:10:LYS:H	1.73	0.53
1:B:120:MET:N	1:B:120:MET:SD	2.81	0.53
10:R:391:ASP:OD2	10:R:394:LEU:HD13	2.09	0.53
12:U:122:ARG:HH12	12:U:270:ARG:HB3	1.72	0.53
12:Y:20:ILE:HG12	13:T:70:MET:HG2	1.90	0.53
13:T:396:GLU:OE1	13:T:398:SER:N	2.41	0.53
3:E:45:GLY:HA3	4:G:93:SER:HB2	1.91	0.53
12:U:105:GLU:O	13:V:116:LYS:NZ	2.37	0.53
13:V:131:LEU:HD11	13:V:301:ALA:HB1	1.91	0.53
6:I:-69:DA:H2''	6:I:-68:DG:H8	1.72	0.53
12:U:64:GLY:HA2	12:U:290:PRO:HG3	1.91	0.53
13:V:133:ILE:HD13	13:V:301:ALA:HB2	1.90	0.53
13:V:387:ARG:HG2	13:V:416:LEU:HD22	1.91	0.53
15:M:1161:GLU:HG2	15:M:1164:LYS:HD3	1.91	0.53
1:A:116:ARG:NH2	1:A:118:THR:OG1	2.42	0.53
3:E:32:HIS:HA	3:E:35:LEU:HD12	1.89	0.53
7:J:33:DT:H2''	7:J:34:DC:C5	2.43	0.53
9:P:230:GLY:HA3	9:P:232:ARG:HH21	1.74	0.53
10:R:260:TYR:HD1	10:R:315:GLU:HG3	1.74	0.53
12:U:69:ARG:HH12	13:T:25:ALA:HA	1.73	0.53
7:J:-18:DG:H2''	7:J:-17:DT:H5''	1.89	0.53
13:X:24:THR:OG1	13:X:28:THR:OG1	2.25	0.53
13:T:24:THR:OG1	13:T:28:THR:OG1	2.23	0.53
4:G:101:VAL:HG13	4:G:105:LEU:HD22	1.90	0.53
5:H:49:LYS:HA	5:H:53:PRO:HA	1.91	0.53
7:J:56:DG:H2''	7:J:57:DG:N7	2.23	0.53
13:T:264:ASP:OD2	13:T:266:ILE:HG12	2.09	0.53
13:V:42:LYS:O	13:V:55:ARG:NH2	2.42	0.52
13:X:313:VAL:HG11	13:X:338:LEU:HG	1.91	0.52
15:M:843:PHE:O	15:M:848:ARG:NH2	2.42	0.52
15:M:1138:LYS:C	15:M:1139:ASN:HD22	2.10	0.52
2:D:45:ARG:HA	7:J:7:DC:H4'	1.90	0.52
12:W:362:GLN:CD	12:W:362:GLN:H	2.17	0.52
14:Z:260:LYS:O	14:Z:264:VAL:HG13	2.08	0.52
13:T:216:ASP:HB2	13:T:231:PRO:HA	1.92	0.52
1:A:126:LEU:HD22	1:B:109:LEU:HD13	1.91	0.52
2:D:43:VAL:HG12	2:D:45:ARG:H	1.73	0.52
7:J:44:DT:H2''	7:J:45:DT:C5	2.44	0.52
9:P:231:LEU:O	9:P:231:LEU:HD23	2.10	0.52
10:R:33:ALA:HB1	10:R:55:ILE:HD11	1.92	0.52
12:Y:266:ARG:CZ	12:Y:268:GLU:HB2	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:447:LEU:HD22	13:T:451:ARG:HE	1.74	0.52
15:M:967:ARG:O	15:M:967:ARG:NH1	2.41	0.52
15:M:982:ILE:HG13	15:M:983:VAL:HG13	1.91	0.52
15:M:832:PHE:O	15:M:838:GLN:NE2	2.43	0.52
15:M:911:ASP:O	15:M:916:LYS:NZ	2.42	0.52
15:M:981:SER:HA	15:M:984:ASN:HD22	1.73	0.52
10:R:130:LYS:HE3	10:R:432:PHE:HB3	1.92	0.52
13:X:259:PRO:HA	15:M:1166:LEU:HD22	1.90	0.52
12:Y:377:VAL:HG22	12:Y:407:GLN:HG3	1.90	0.52
15:M:1340:ASP:OD1	15:M:1340:ASP:N	2.43	0.52
6:I:-15:DA:H2	7:J:15:DT:H3	1.55	0.52
9:P:224:GLU:O	9:P:228:SER:OG	2.22	0.52
12:W:156:GLY:HA3	12:W:176:ILE:HD11	1.92	0.52
12:W:178:GLY:HA2	12:W:181:LYS:HZ2	1.75	0.52
12:Y:405:VAL:HG21	12:Y:430:PHE:CE2	2.45	0.52
13:T:213:GLY:HA3	13:T:230:VAL:HG21	1.90	0.52
13:T:447:LEU:HA	13:T:451:ARG:HH21	1.75	0.52
15:M:961:TYR:HB2	15:M:991:LYS:HE2	1.91	0.52
15:M:1020:ASP:N	15:M:1020:ASP:OD1	2.43	0.52
1:A:57:SER:OG	1:A:58:THR:N	2.43	0.52
6:I:-57:DC:H2''	6:I:-56:DC:C2	2.44	0.52
11:S:96:LEU:HB3	11:S:135:THR:HG21	1.91	0.52
13:T:26:ALA:O	17:T:501:ADP:O3'	2.20	0.52
13:T:48:PHE:HZ	13:T:88:LEU:HD22	1.75	0.52
15:M:1124:MET:N	15:M:1124:MET:HE2	2.25	0.52
15:M:1362:ARG:HH22	15:M:1365:HIS:CG	2.26	0.52
7:J:1:DC:H2''	7:J:2:DG:C8	2.45	0.52
9:P:244:ASP:OD1	9:P:245:TRP:N	2.43	0.52
10:R:256:SER:HB2	10:R:368:ARG:NH1	2.24	0.52
12:W:44:MET:SD	12:W:45:VAL:N	2.83	0.52
17:M:1601:ADP:O3A	18:M:1602:BEF:F2	2.18	0.52
1:A:62:ILE:HD12	1:A:62:ILE:H	1.74	0.52
2:D:31:LYS:HA	2:D:55:ARG:HH12	1.74	0.52
6:I:7:DC:H1'	6:I:8:DC:H5'	1.92	0.52
10:R:230:THR:O	10:R:234:ARG:HG2	2.09	0.52
13:T:93:SER:HA	13:T:96:LEU:HD12	1.92	0.52
15:M:1158:ILE:H	15:M:1158:ILE:HD12	1.74	0.52
7:J:34:DC:H2''	7:J:35:DT:C5	2.45	0.52
10:R:53:SER:HB2	10:R:279:PHE:HB3	1.91	0.52
15:M:960:LEU:HD23	15:M:996:PRO:HG3	1.92	0.52
1:B:47:ALA:O	1:B:51:ILE:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:HG22	2:C:33:ALA:HB1	1.91	0.51
4:G:105:LEU:HD21	4:G:109:LEU:HB2	1.91	0.51
5:H:59:GLN:HA	16:K:151:PHE:HE1	1.75	0.51
11:S:205:LYS:HE3	11:S:210:SER:HB3	1.91	0.51
6:I:16:DA:H2"	6:I:17:DA:C8	2.45	0.51
9:P:242:GLN:HG2	15:M:969:GLN:HB2	1.92	0.51
11:S:237:VAL:HG23	13:T:222:PHE:HA	1.93	0.51
12:U:69:ARG:HB2	12:U:320:ILE:HD12	1.92	0.51
12:U:310:ASN:O	12:U:350:ARG:NH2	2.39	0.51
12:W:134:GLU:HA	12:W:232:ARG:HE	1.75	0.51
12:W:271:ASP:OD1	12:W:271:ASP:N	2.40	0.51
13:T:182:ASP:OD1	13:T:184:THR:HG23	2.11	0.51
15:M:619:ASP:OD1	15:M:619:ASP:N	2.40	0.51
7:J:15:DT:H2"	7:J:16:DA:N7	2.24	0.51
12:U:402:LEU:HA	12:U:405:VAL:HG12	1.92	0.51
13:V:448:ASP:OD2	13:V:451:ARG:NH1	2.43	0.51
12:W:92:LEU:HD21	12:W:96:VAL:HB	1.92	0.51
13:T:280:ILE:HG23	13:T:284:LEU:HD12	1.92	0.51
15:M:1270:GLN:N	15:M:1270:GLN:OE1	2.43	0.51
2:C:96:THR:OG1	3:E:100:ASN:O	2.23	0.51
10:R:61:HIS:HA	10:R:66:LEU:HA	1.93	0.51
13:X:130:GLY:HA2	13:X:248:THR:HA	1.91	0.51
12:Y:220:ARG:NH1	12:Y:221:PHE:O	2.44	0.51
13:T:459:SER:OG	13:T:463:LEU:O	2.27	0.51
15:M:984:ASN:HA	15:M:987:MET:HE1	1.90	0.51
3:E:18:ARG:HG3	3:E:29:GLY:H	1.76	0.51
9:P:209:SER:HB2	9:P:232:ARG:HE	1.75	0.51
6:I:-41:DG:C6	6:I:-40:DG:C6	2.99	0.51
10:R:249:LYS:HA	10:R:253:LEU:HD13	1.92	0.51
10:R:406:THR:HG23	10:R:408:SER:H	1.76	0.51
13:X:102:PHE:HD1	13:X:307:VAL:HG13	1.76	0.51
12:Y:109:LEU:H	12:Y:109:LEU:HD23	1.75	0.51
12:Y:141:VAL:HG22	12:Y:142:GLU:HG2	1.92	0.51
13:T:96:LEU:HB3	13:T:100:VAL:HG11	1.93	0.51
15:M:1052:LYS:HA	15:M:1141:ILE:HB	1.93	0.51
7:J:-22:DG:C2	7:J:-21:DG:C2	2.98	0.51
13:X:401:ASP:O	13:X:405:THR:HG23	2.11	0.51
13:T:121:LEU:HD21	13:T:324:LEU:HD13	1.93	0.51
13:T:263:GLN:O	13:T:268:MET:HE2	2.10	0.51
1:A:131:ARG:HH22	1:B:130:LEU:HD22	1.75	0.51
9:P:218:LYS:HG2	9:P:219:ARG:H	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:192:ASP:OD1	10:R:356:THR:OG1	2.28	0.51
10:R:359:ASN:HA	17:R:501:ADP:N3	2.25	0.51
11:S:16:ASP:HB3	12:U:147:ARG:CZ	2.41	0.51
12:U:58:LEU:O	12:U:62:GLN:HG2	2.10	0.51
12:U:146:ASP:HB3	12:U:155:GLN:H	1.76	0.51
12:U:382:ASP:N	12:U:382:ASP:OD1	2.43	0.51
12:W:82:THR:N	17:W:501:ADP:O2A	2.43	0.51
12:W:136:ILE:HG23	12:W:229:LEU:HD12	1.92	0.51
12:W:258:PHE:HB3	13:X:284:LEU:HD21	1.91	0.51
13:X:144:VAL:HB	13:X:197:GLY:HA3	1.93	0.51
15:M:750:ILE:HD11	15:M:800:ILE:HG12	1.93	0.51
15:M:1264:ARG:N	15:M:1334:ASP:OD2	2.43	0.51
1:B:119:ILE:HG22	2:C:46:ILE:HA	1.92	0.51
15:M:992:VAL:HG11	15:M:1376:GLU:HG3	1.93	0.51
3:E:32:HIS:CG	3:E:49:PRO:HB3	2.46	0.51
11:S:22:LEU:HD22	12:U:142:GLU:HB2	1.92	0.51
12:U:167:THR:OG1	12:U:168:ILE:N	2.43	0.51
13:X:143:GLU:HG3	13:X:171:LYS:HD2	1.93	0.51
12:Y:159:THR:HA	12:Y:168:ILE:HA	1.93	0.51
14:Z:267:LYS:O	14:Z:270:ARG:HG2	2.10	0.51
15:M:1301:ARG:O	15:M:1305:THR:OG1	2.28	0.51
2:C:82:THR:HG22	2:C:83:SER:H	1.76	0.50
6:I:-46:DC:H2"	6:I:-45:DA:C8	2.46	0.50
12:W:108:SER:HA	13:X:116:LYS:HG2	1.93	0.50
13:X:315:MET:HE2	13:X:315:MET:HA	1.93	0.50
12:Y:304:GLU:OE1	12:Y:304:GLU:N	2.42	0.50
15:M:1328:ILE:H	15:M:1354:ARG:HE	1.59	0.50
1:A:71:VAL:HG13	1:A:84:PHE:HE2	1.76	0.50
11:S:199:LYS:HA	11:S:203:SER:HB3	1.93	0.50
12:U:145:ILE:HG22	12:U:176:ILE:HG23	1.93	0.50
13:V:224:LEU:HD22	12:W:169:TYR:HB3	1.93	0.50
12:Y:430:PHE:HE1	13:T:57:ALA:HB1	1.76	0.50
9:P:242:GLN:NE2	15:M:969:GLN:O	2.44	0.50
2:C:77:LYS:NZ	15:M:621:SER:HB3	2.27	0.50
12:W:192:ILE:HD13	12:W:199:ILE:HG13	1.93	0.50
15:M:995:HIS:ND1	15:M:1245:CYS:HA	2.26	0.50
15:M:1077:LYS:O	15:M:1081:THR:HG23	2.11	0.50
15:M:1150:VAL:HG12	15:M:1152:TYR:H	1.76	0.50
12:U:300:MET:HG3	13:V:322:THR:HG21	1.94	0.50
10:R:375:ARG:O	10:R:377:LEU:N	2.43	0.50
12:U:106:ILE:HD11	12:U:301:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:80:GLY:O	13:V:83:THR:OG1	2.24	0.50
13:V:425:LEU:O	13:V:428:THR:OG1	2.27	0.50
1:A:69:ARG:NH2	2:D:29:ILE:HG12	2.23	0.50
1:A:121:PRO:HG3	2:D:49:LEU:HD13	1.93	0.50
2:C:80:THR:OG1	15:M:627:ASN:OD1	2.28	0.50
11:S:194:ARG:CZ	11:S:198:LEU:HD11	2.42	0.50
13:V:320:ILE:O	13:V:324:LEU:HD23	2.11	0.50
12:W:146:ASP:O	12:W:155:GLN:N	2.45	0.50
13:T:171:LYS:NZ	13:T:218:TYR:OH	2.41	0.50
1:B:126:LEU:O	1:B:130:LEU:HG	2.12	0.50
3:E:19:SER:OG	3:E:24:LEU:O	2.28	0.50
4:G:61:SER:HA	4:G:64:ILE:HD12	1.94	0.50
12:Y:165:MET:HE1	12:Y:167:THR:OG1	2.12	0.50
14:Z:271:LEU:HD11	15:M:1313:ARG:HH12	1.77	0.50
9:P:249:VAL:HG21	9:P:258:LEU:HD11	1.93	0.50
11:S:30:THR:HG23	11:S:236:LYS:HA	1.94	0.50
12:W:300:MET:HA	12:W:333:ARG:HD3	1.93	0.50
12:Y:255:LEU:O	12:Y:259:THR:N	2.34	0.50
14:Z:214:GLU:HG2	14:Z:218:LYS:HE2	1.93	0.50
2:D:63:GLU:HA	2:D:66:ILE:HG22	1.93	0.49
12:U:268:GLU:HA	12:U:271:ASP:OD2	2.11	0.49
13:V:376:ASP:OD1	13:V:377:LYS:N	2.34	0.49
13:X:433:GLU:N	13:X:433:GLU:OE1	2.44	0.49
13:T:144:VAL:HG21	13:T:200:ILE:HD12	1.93	0.49
15:M:863:LEU:HD12	15:M:863:LEU:H	1.77	0.49
15:M:1054:LEU:HB3	15:M:1134:PRO:HB3	1.94	0.49
7:J:-22:DG:N2	7:J:-21:DG:C2	2.80	0.49
8:L:38:LYS:HZ3	8:L:53:SER:HB2	1.77	0.49
12:W:364:ILE:O	12:W:368:LEU:HG	2.11	0.49
13:X:225:GLU:HG3	13:X:227:GLU:H	1.77	0.49
13:X:391:GLU:HG3	13:X:393:LEU:HG	1.94	0.49
15:M:830:LYS:HD2	15:M:856:LEU:HG	1.93	0.49
12:U:378:GLU:OE1	12:U:378:GLU:N	2.44	0.49
12:U:457:SER:OG	12:U:459:ALA:O	2.29	0.49
12:W:78:SER:HA	17:W:501:ADP:H5'1	1.94	0.49
13:T:137:LYS:HZ1	13:T:204:ALA:N	2.10	0.49
15:M:944:LYS:HE2	15:M:1352:GLN:HE22	1.76	0.49
15:M:954:SER:HB3	15:M:957:GLN:HB3	1.94	0.49
3:E:66:LEU:HA	3:E:69:ASN:ND2	2.26	0.49
12:U:114:THR:HG21	13:T:109:GLU:HA	1.95	0.49
13:V:396:GLU:OE1	13:V:398:SER:OG	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:44:MET:SD	12:W:51:ARG:HD3	2.53	0.49
12:W:413:ARG:NH1	12:W:422:ASP:OD2	2.45	0.49
12:W:415:ASN:ND2	12:W:417:THR:O	2.45	0.49
2:D:80:THR:N	7:J:28:DA:OP1	2.45	0.49
7:J:-17:DT:H2"	7:J:-16:DT:C2	2.48	0.49
10:R:315:GLU:OE2	10:R:319:HIS:ND1	2.46	0.49
12:U:127:ILE:HD13	12:U:288:ILE:HA	1.95	0.49
12:U:188:ASP:N	12:U:188:ASP:OD1	2.44	0.49
13:X:41:ALA:HB3	13:X:52:ILE:HG23	1.94	0.49
13:X:451:ARG:O	13:X:455:ILE:HD12	2.12	0.49
12:Y:299:HIS:CE1	12:Y:327:ARG:HD2	2.47	0.49
13:T:77:LEU:HD11	13:T:85:LYS:HB3	1.93	0.49
11:S:107:THR:HG22	11:S:109:ASN:H	1.76	0.49
12:U:139:GLU:O	12:U:161:LYS:N	2.36	0.49
13:V:259:PRO:HB2	15:M:1193:ARG:HG3	1.95	0.49
12:Y:241:LEU:O	12:Y:244:ILE:HG22	2.13	0.49
14:Z:193:THR:HA	14:Z:196:ARG:HD3	1.95	0.49
15:M:1275:LEU:HD23	15:M:1318:ILE:HD12	1.94	0.49
10:R:227:LEU:O	10:R:231:LEU:HG	2.12	0.49
11:S:11:LYS:O	11:S:13:TYR:N	2.44	0.49
13:X:402:LEU:O	13:X:405:THR:OG1	2.16	0.49
12:Y:411:MET:HE3	12:Y:411:MET:C	2.38	0.49
15:M:831:ASN:OD1	15:M:834:SER:N	2.46	0.49
15:M:1114:GLY:O	15:M:1118:MET:HG3	2.11	0.49
13:X:249:LEU:HD12	13:X:249:LEU:H	1.77	0.49
13:X:381:ARG:NE	13:X:401:ASP:OD1	2.43	0.49
15:M:827:HIS:HB3	15:M:856:LEU:HD21	1.94	0.49
7:J:-16:DT:OP1	15:M:804:GLN:NE2	2.46	0.49
9:P:291:GLN:O	9:P:295:GLN:HG2	2.12	0.49
12:W:136:ILE:HB	12:W:192:ILE:HG23	1.95	0.49
12:Y:97:PRO:HG2	12:Y:291:GLY:HA3	1.95	0.49
3:E:66:LEU:HA	3:E:69:ASN:HD21	1.76	0.49
4:G:75:ARG:O	4:G:79:GLU:HG2	2.12	0.49
10:R:275:VAL:HG23	10:R:288:ARG:HD3	1.94	0.49
12:U:146:ASP:OD1	12:U:147:ARG:N	2.45	0.49
13:V:101:PRO:HG2	13:V:306:GLY:HA3	1.95	0.49
12:W:387:LEU:HD12	12:W:399:SER:HB3	1.93	0.49
13:X:344:MET:HE2	13:X:344:MET:HA	1.95	0.49
13:T:84:GLY:HA2	17:T:501:ADP:H5'2	1.95	0.49
15:M:987:MET:HA	15:M:990:ARG:HD3	1.95	0.49
15:M:1178:ASP:O	15:M:1230:LYS:NZ	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:7:DC:H2"	7:J:8:DG:C8	2.48	0.48
12:U:37:PRO:HB3	12:U:51:ARG:HD2	1.94	0.48
12:W:398:TYR:OH	12:W:435:ARG:NH1	2.46	0.48
13:T:312:GLU:OE2	13:T:314:ASN:HB3	2.13	0.48
15:M:912:LYS:O	15:M:912:LYS:NZ	2.37	0.48
11:S:4:LEU:HD12	11:S:5:VAL:H	1.78	0.48
6:I:-53:DG:H2"	6:I:-52:DG:C8	2.48	0.48
10:R:58:ARG:NH1	10:R:70:GLU:OE2	2.46	0.48
12:U:134:GLU:HG3	12:U:194:LYS:HZ2	1.79	0.48
12:U:140:VAL:O	12:U:187:GLY:HA2	2.13	0.48
12:U:172:GLY:O	12:U:175:MET:HE2	2.13	0.48
13:T:49:VAL:O	17:T:501:ADP:N6	2.46	0.48
15:M:1126:ASN:O	15:M:1132:ARG:NH1	2.25	0.48
1:B:102:SER:HA	1:B:105:GLU:HG2	1.96	0.48
2:C:26:ILE:HG13	2:C:55:ARG:HH21	1.77	0.48
5:H:119:ARG:HH22	16:K:106:ARG:NH2	2.11	0.48
6:I:19:DC:H2"	6:I:20:DG:H5"	1.95	0.48
11:S:241:ILE:HG13	11:S:262:LYS:HB2	1.95	0.48
12:W:415:ASN:HD22	12:W:417:THR:HG22	1.77	0.48
13:X:375:TYR:OH	17:X:501:ADP:N7	2.37	0.48
13:T:70:MET:HE1	13:T:73:ARG:CG	2.43	0.48
15:M:697:ARG:HB2	15:M:700:GLN:HG3	1.96	0.48
3:E:85:GLN:NE2	3:E:106:GLY:HA2	2.29	0.48
9:P:284:TYR:HE1	12:U:216:GLY:HA2	1.79	0.48
12:U:329:VAL:H	12:U:341:HIS:H	1.61	0.48
13:V:262:GLY:HA3	13:V:267:SER:HB2	1.95	0.48
13:V:378:ASP:OD1	13:V:378:ASP:N	2.44	0.48
14:Z:603:PRO:HB3	14:Z:606:LEU:HB2	1.95	0.48
13:T:41:ALA:HB3	13:T:52:ILE:HG23	1.95	0.48
15:M:1293:ASP:OD1	15:M:1293:ASP:N	2.46	0.48
8:L:89:ARG:O	8:L:92:GLN:HG3	2.14	0.48
10:R:261:PHE:HA	10:R:264:PHE:CD1	2.49	0.48
14:Z:255:SER:HA	14:Z:258:LYS:HD3	1.95	0.48
15:M:1126:ASN:HA	15:M:1130:CYS:HB2	1.96	0.48
2:C:29:ILE:O	2:C:55:ARG:NH1	2.47	0.48
5:H:58:SER:HB3	8:L:85:ARG:HG3	1.96	0.48
9:P:285:LYS:O	9:P:289:ARG:HG2	2.14	0.48
11:S:241:ILE:HG13	11:S:242:THR:N	2.28	0.48
13:V:132:ARG:HG3	13:V:246:ASP:OD1	2.13	0.48
12:W:249:SER:O	12:W:266:ARG:NH2	2.47	0.48
13:T:380:ILE:HG12	13:T:412:LEU:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:1088:GLU:OE1	15:M:1105:LYS:HB2	2.14	0.48
16:K:72:MET:HE2	16:K:72:MET:N	2.29	0.48
12:W:127:ILE:HG22	12:W:288:ILE:HG22	1.95	0.48
13:X:125:PHE:CD2	13:X:334:PRO:HD2	2.48	0.48
4:G:88:LYS:NZ	6:I:34:DG:H2'	2.29	0.48
13:V:283:LYS:NZ	15:M:1018:TYR:OH	2.47	0.48
12:W:432:ASP:HB3	12:W:435:ARG:HD3	1.95	0.48
12:Y:358:SER:OG	12:Y:359:TYR:N	2.47	0.48
1:A:119:ILE:HG22	2:D:50:ILE:HG12	1.96	0.47
7:J:31:DA:H2''	7:J:30:DA:C8	2.49	0.47
7:J:41:DC:N3	7:J:42:DA:N6	2.61	0.47
10:R:106:MET:HA	11:S:202:LEU:HD21	1.96	0.47
12:U:175:MET:HE3	13:T:225:GLU:HA	1.95	0.47
13:V:26:ALA:O	13:V:27:HIS:ND1	2.47	0.47
13:V:145:THR:OG1	13:V:146:GLU:OE1	2.27	0.47
13:V:311:ASP:OD1	13:V:312:GLU:N	2.47	0.47
12:Y:174:LYS:H	12:Y:174:LYS:HG3	1.50	0.47
13:T:435:VAL:HG22	13:T:436:VAL:H	1.79	0.47
1:B:61:LEU:HD23	2:C:37:LEU:HD22	1.95	0.47
10:R:374:GLN:HE21	13:T:174:LYS:NZ	2.11	0.47
10:R:428:THR:HA	10:R:432:PHE:HB2	1.96	0.47
11:S:4:LEU:HG	11:S:5:VAL:HG23	1.96	0.47
12:U:18:SER:HB2	13:V:331:ASN:HB2	1.96	0.47
12:U:241:LEU:HA	12:U:244:ILE:HD12	1.96	0.47
12:W:76:PRO:O	12:W:79:THR:OG1	2.26	0.47
12:W:122:ARG:NH1	12:W:241:LEU:HG	2.30	0.47
14:Z:263:GLU:HA	14:Z:266:LYS:HE3	1.95	0.47
15:M:803:TYR:OH	15:M:824:ASP:O	2.29	0.47
15:M:875:VAL:HG11	15:M:880:LYS:HD3	1.95	0.47
15:M:994:ASN:HD21	15:M:999:PHE:H	1.61	0.47
1:A:88:ALA:HB2	2:D:83:SER:HA	1.95	0.47
9:P:212:HIS:CE1	9:P:226:ILE:HG21	2.49	0.47
10:R:231:LEU:O	10:R:235:HIS:ND1	2.33	0.47
10:R:358:GLY:H	17:R:501:ADP:H5'2	1.77	0.47
12:U:457:SER:OG	13:V:409:GLU:O	2.27	0.47
12:W:72:LEU:HD11	12:W:325:THR:HG22	1.96	0.47
12:W:121:PHE:O	12:W:124:SER:OG	2.19	0.47
12:Y:117:LEU:HD11	12:Y:305:CYS:HB3	1.97	0.47
12:Y:297:GLU:OE1	12:Y:299:HIS:NE2	2.47	0.47
13:T:424:ILE:O	13:T:428:THR:HG23	2.14	0.47
15:M:1040:LEU:HD12	15:M:1045:LEU:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:K:108:ARG:HD3	16:K:108:ARG:N	2.28	0.47
6:I:-65:DT:H1'	6:I:-64:DC:H5'	1.95	0.47
12:W:162:THR:HG23	12:W:164:ASP:H	1.79	0.47
12:W:193:ASP:OD1	12:W:196:SER:N	2.34	0.47
9:P:234:LYS:HD2	9:P:234:LYS:N	2.29	0.47
13:V:177:LYS:HB2	13:V:237:VAL:HG21	1.96	0.47
13:X:195:SER:HB3	13:X:198:ASP:HB2	1.96	0.47
12:Y:191:SER:HB3	12:Y:202:LEU:HD11	1.96	0.47
15:M:879:LYS:HA	15:M:879:LYS:HD3	1.65	0.47
7:J:14:DT:H2''	7:J:15:DT:H5'	1.95	0.47
9:P:286:GLU:OE2	9:P:290:GLN:HG2	2.14	0.47
12:W:32:ASP:OD1	12:W:33:GLU:N	2.48	0.47
12:W:98:PHE:HD1	12:W:292:VAL:HB	1.79	0.47
12:Y:457:SER:HB2	13:T:409:GLU:O	2.14	0.47
13:T:119:GLU:O	13:T:123:GLU:OE1	2.33	0.47
15:M:998:LEU:HD11	15:M:1273:LYS:HE3	1.96	0.47
15:M:1064:LYS:O	15:M:1068:VAL:HG12	2.14	0.47
2:D:37:LEU:O	2:D:40:ARG:HG3	2.15	0.47
9:P:270:GLN:O	9:P:274:GLN:HG2	2.14	0.47
12:U:70:ALA:HB2	12:U:313:LEU:HD11	1.97	0.47
13:V:61:ILE:O	13:V:65:ILE:HG22	2.15	0.47
12:W:115:GLU:O	12:W:118:THR:OG1	2.30	0.47
12:Y:415:ASN:ND2	12:Y:417:THR:O	2.45	0.47
15:M:1293:ASP:O	15:M:1296:THR:OG1	2.33	0.47
5:H:73:PHE:HE1	8:L:37:ILE:HG23	1.80	0.47
6:I:0:DC:H2'	6:I:1:DT:C6	2.50	0.47
6:I:6:DC:H1'	6:I:7:DC:C5	2.49	0.47
10:R:222:PHE:HB3	11:S:105:LEU:HD11	1.97	0.47
10:R:341:LEU:O	10:R:346:ARG:NE	2.47	0.47
12:U:407:GLN:O	12:U:410:ALA:N	2.47	0.47
13:X:144:VAL:HG13	13:X:169:GLY:N	2.30	0.47
12:Y:162:THR:HG22	12:Y:225:PRO:HG2	1.97	0.47
12:Y:294:PHE:CD1	12:Y:322:MET:HG2	2.50	0.47
13:T:310:ILE:HG22	13:T:313:VAL:HG12	1.97	0.47
2:C:35:ARG:O	2:C:39:ARG:HG2	2.15	0.47
7:J:-19:DG:H2''	7:J:-18:DG:C8	2.50	0.47
12:U:171:LEU:HD12	12:U:176:ILE:HG13	1.96	0.47
12:U:360:ASN:N	12:U:363:GLU:OE1	2.44	0.47
13:V:309:PHE:CZ	13:V:311:ASP:HB2	2.50	0.47
12:Y:119:GLN:HE21	12:Y:242:HIS:CE1	2.33	0.47
14:Z:272:ALA:O	14:Z:276:ARG:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:47:VAL:HG11	8:L:67:THR:HG23	1.97	0.46
9:P:210:ARG:HD3	9:P:226:ILE:HD12	1.95	0.46
9:P:221:PRO:HB2	9:P:223:LEU:HG	1.96	0.46
12:U:76:PRO:HD3	13:T:463:LEU:HD22	1.97	0.46
13:V:132:ARG:HB3	13:V:302:GLU:OE1	2.15	0.46
15:M:719:LEU:HD22	15:M:727:LYS:HD2	1.97	0.46
1:A:69:ARG:NH1	2:D:25:ASN:OD1	2.42	0.46
2:D:54:VAL:HA	2:D:57:VAL:HG22	1.97	0.46
6:I:14:DT:C6	6:I:15:DT:H72	2.50	0.46
9:P:234:LYS:C	9:P:236:THR:H	2.24	0.46
10:R:109:PRO:HG3	11:S:198:LEU:HD13	1.96	0.46
13:X:137:LYS:HD2	13:X:243:ILE:HD11	1.97	0.46
1:B:108:ASN:O	1:B:112:ILE:HG13	2.15	0.46
6:I:-18:DC:H2''	6:I:-17:DT:H5'	1.96	0.46
10:R:258:VAL:HG12	10:R:262:ASP:OD2	2.16	0.46
12:U:444:GLU:OE1	12:U:444:GLU:N	2.38	0.46
13:X:245:GLN:OE1	13:X:246:ASP:N	2.47	0.46
6:I:17:DA:H2''	6:I:18:DC:C6	2.51	0.46
8:L:81:LEU:HB3	8:L:83:VAL:HG23	1.98	0.46
10:R:17:PHE:HB2	10:R:89:PHE:CZ	2.50	0.46
12:U:276:LYS:NZ	12:U:280:TRP:HE1	2.13	0.46
12:W:144:GLN:HG2	14:Z:291:LEU:HD21	1.98	0.46
13:T:58:CYS:SG	13:T:88:LEU:HD12	2.55	0.46
13:T:194:VAL:HG13	13:T:211:ARG:HD2	1.97	0.46
13:T:250:HIS:O	13:T:254:VAL:HG13	2.16	0.46
15:M:762:MET:N	15:M:762:MET:SD	2.88	0.46
2:D:39:ARG:NE	7:J:8:DG:OP2	2.48	0.46
5:H:52:HIS:CD2	8:L:72:GLU:HA	2.50	0.46
9:P:214:ARG:NH1	9:P:250:ASP:OD2	2.49	0.46
9:P:283:ARG:HH22	9:P:284:TYR:HD1	1.64	0.46
10:R:33:ALA:HB3	10:R:41:TYR:HD2	1.81	0.46
13:V:280:ILE:HB	13:V:285:ARG:HH21	1.80	0.46
13:V:331:ASN:N	13:V:331:ASN:OD1	2.43	0.46
12:Y:37:PRO:HB2	12:Y:51:ARG:NH2	2.31	0.46
13:T:102:PHE:HD1	13:T:307:VAL:HG13	1.81	0.46
15:M:1002:ARG:NH1	15:M:1236:PRO:HB2	2.31	0.46
6:I:-67:DA:H1'	6:I:-66:DA:N7	2.31	0.46
7:J:-34:DA:H2''	7:J:-33:DG:N7	2.31	0.46
12:W:438:LYS:HA	12:W:441:GLN:HG2	1.97	0.46
12:Y:160:ILE:N	12:Y:167:THR:O	2.40	0.46
15:M:980:MET:O	15:M:984:ASN:ND2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-26:DT:H2''	6:I:-25:DA:N7	2.31	0.46
6:I:23:DA:H2''	6:I:24:DA:C8	2.51	0.46
10:R:5:PRO:HB3	10:R:98:HIS:HB2	1.98	0.46
10:R:65:GLN:NE2	10:R:111:LEU:HD22	2.30	0.46
11:S:25:GLN:O	11:S:27:ARG:N	2.45	0.46
11:S:259:CYS:HA	11:S:278:ARG:CZ	2.46	0.46
13:V:101:PRO:HG3	13:V:130:GLY:N	2.31	0.46
12:W:301:LEU:HD12	12:W:301:LEU:HA	1.87	0.46
13:X:193:LYS:HA	13:X:193:LYS:HD2	1.66	0.46
15:M:1079:ARG:NH1	15:M:1120:ASN:OD1	2.48	0.46
2:C:53:GLU:O	2:C:57:VAL:HG12	2.15	0.46
7:J:63:DG:H2''	7:J:64:DG:C8	2.51	0.46
8:L:66:LEU:O	8:L:70:VAL:HG22	2.16	0.46
10:R:195:PHE:HB2	17:R:501:ADP:H3'	1.89	0.46
10:R:221:ARG:O	11:S:106:ASN:HA	2.15	0.46
12:U:119:GLN:HG2	12:U:242:HIS:CE1	2.50	0.46
13:V:126:ARG:HG3	13:V:285:ARG:HH11	1.80	0.46
12:W:147:ARG:O	14:Z:289:GLN:HG3	2.16	0.46
12:Y:244:ILE:HD12	12:Y:244:ILE:HA	1.82	0.46
12:Y:258:PHE:CB	13:T:284:LEU:HD21	2.45	0.46
13:T:382:THR:O	13:T:386:ARG:HG2	2.15	0.46
12:U:135:LEU:H	12:U:135:LEU:HD23	1.80	0.46
12:W:243:GLU:HA	12:W:246:VAL:HG12	1.97	0.46
12:Y:432:ASP:OD2	12:Y:435:ARG:NE	2.48	0.46
1:A:67:PHE:HE2	1:A:96:VAL:HG21	1.81	0.46
12:U:140:VAL:HG12	12:U:188:ASP:H	1.81	0.46
13:V:216:ASP:HA	13:V:219:ALA:HB2	1.98	0.46
13:V:424:ILE:HD12	13:V:427:GLN:HB3	1.97	0.46
13:X:436:VAL:O	13:X:439:VAL:HG22	2.16	0.46
2:C:47:SER:HA	6:I:7:DC:H5''	1.98	0.45
7:J:35:DT:H2''	7:J:36:DA:N7	2.30	0.45
10:R:191:ILE:HG12	10:R:353:ILE:HD11	1.98	0.45
12:W:125:ILE:HG22	12:W:291:GLY:H	1.81	0.45
13:X:385:GLU:HG3	13:X:400:LEU:HD21	1.99	0.45
13:X:387:ARG:HD2	13:X:387:ARG:HA	1.80	0.45
13:T:287:GLU:O	13:T:291:VAL:HG23	2.17	0.45
15:M:954:SER:O	15:M:958:ARG:N	2.36	0.45
1:A:113:HIS:CD2	1:B:129:ARG:HH21	2.34	0.45
1:B:63:ARG:HB2	1:B:66:PRO:HD2	1.98	0.45
6:I:-42:DT:C4	6:I:-41:DG:O6	2.69	0.45
7:J:66:DT:H6	7:J:66:DT:H2'	1.61	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:290:GLN:HB3	12:U:221:PHE:CZ	2.51	0.45
12:U:56:VAL:O	12:U:60:MET:HG2	2.16	0.45
12:W:323:MET:HB2	12:W:323:MET:HE3	1.74	0.45
12:Y:21:ALA:HB3	12:Y:24:SER:HB3	1.97	0.45
15:M:606:PHE:CG	15:M:632:GLU:HG3	2.51	0.45
15:M:1288:LEU:HB3	15:M:1314:ILE:HA	1.97	0.45
1:B:63:ARG:H	1:B:63:ARG:HG2	1.57	0.45
2:C:39:ARG:NH1	2:C:43:VAL:O	2.49	0.45
5:H:36:ARG:NH2	16:K:66:GLU:O	2.50	0.45
7:J:61:DC:H2''	7:J:62:DG:C8	2.52	0.45
8:L:24:SER:HB3	16:K:78:ASP:HB3	1.98	0.45
9:P:285:LYS:O	9:P:285:LYS:HD2	2.16	0.45
10:R:378:PRO:HA	13:T:176:THR:H	1.82	0.45
12:U:173:ASN:O	12:U:176:ILE:HD12	2.17	0.45
12:W:231:LYS:H	12:W:232:ARG:NH2	2.14	0.45
12:Y:72:LEU:HD21	12:Y:341:HIS:CD2	2.50	0.45
4:G:111:LYS:HE3	14:Z:192:ARG:HA	1.98	0.45
6:I:66:DA:H2'	6:I:65:DT:H71	1.98	0.45
7:J:25:DT:H2''	7:J:26:DA:N7	2.31	0.45
12:U:432:ASP:OD1	12:U:433:SER:N	2.49	0.45
12:W:191:SER:HB3	12:W:202:LEU:HD11	1.98	0.45
13:X:312:GLU:OE2	13:X:314:ASN:HB3	2.16	0.45
12:Y:69:ARG:HB2	12:Y:320:ILE:HD12	1.98	0.45
13:T:129:ILE:HG12	13:T:306:GLY:H	1.81	0.45
15:M:750:ILE:HD11	15:M:800:ILE:HA	1.98	0.45
5:H:125:SER:OG	8:L:54:LYS:NZ	2.38	0.45
10:R:352:ASN:N	10:R:352:ASN:OD1	2.49	0.45
12:W:182:GLU:O	12:W:184:VAL:HG23	2.17	0.45
13:X:262:GLY:O	13:X:267:SER:OG	2.27	0.45
13:X:350:THR:OG1	13:X:351:GLU:N	2.50	0.45
13:X:382:THR:O	13:X:386:ARG:HG2	2.16	0.45
13:T:421:PRO:O	13:T:425:LEU:HG	2.17	0.45
2:D:29:ILE:HG22	2:D:55:ARG:CZ	2.46	0.45
6:I:20:DG:N1	7:J:19:DG:O6	2.50	0.45
6:I:32:DA:H61	7:J:31:DA:N6	2.15	0.45
10:R:192:ASP:HB2	10:R:199:TRP:HB2	1.99	0.45
12:U:146:ASP:O	12:U:154:LYS:HG2	2.17	0.45
13:V:122:MET:HE2	13:V:122:MET:HB2	1.87	0.45
13:V:340:SER:OG	13:V:357:HIS:HB3	2.17	0.45
13:V:361:PRO:HA	13:V:364:ILE:HB	1.97	0.45
12:W:44:MET:SD	12:W:44:MET:C	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:309:PHE:C	13:X:310:ILE:HD13	2.41	0.45
13:X:356:PRO:HB2	13:X:357:HIS:CE1	2.51	0.45
12:Y:79:THR:HG22	12:Y:81:LYS:HE3	1.98	0.45
15:M:941:MET:SD	15:M:941:MET:N	2.89	0.45
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.86	0.45
6:I:-42:DT:C4	6:I:-41:DG:C6	3.05	0.45
7:J:55:DC:H1'	7:J:56:DG:C4	2.52	0.45
10:R:60:PRO:HA	10:R:68:LEU:HD12	1.97	0.45
11:S:189:ARG:NH1	11:S:193:ASN:HD22	2.15	0.45
13:V:69:LYS:HB3	13:V:70:MET:SD	2.56	0.45
13:V:150:GLU:OE2	13:V:180:ARG:NH2	2.50	0.45
13:X:80:GLY:O	13:X:83:THR:OG1	2.34	0.45
14:Z:595:THR:HA	14:Z:596:LEU:HA	1.74	0.45
15:M:631:VAL:HA	15:M:635:GLU:HB2	1.99	0.45
15:M:1245:CYS:SG	15:M:1248:LEU:N	2.88	0.45
3:E:85:GLN:HE22	3:E:106:GLY:HA2	1.81	0.45
3:E:112:ILE:HA	3:E:112:ILE:HD12	1.79	0.45
12:W:294:PHE:HD1	12:W:322:MET:HG3	1.82	0.45
12:W:384:LEU:HD23	12:W:384:LEU:HA	1.86	0.45
13:X:380:ILE:HG12	13:X:412:LEU:HD12	1.99	0.45
12:Y:17:LEU:HB3	13:T:293:ALA:HB2	1.99	0.45
1:B:126:LEU:HA	1:B:129:ARG:NE	2.32	0.45
3:E:51:TYR:CZ	4:G:117:GLY:HA3	2.51	0.45
6:I:-11:DG:N1	7:J:12:DG:O6	2.50	0.45
7:J:66:DT:H1'	7:J:67:DT:O4'	2.16	0.45
13:V:166:VAL:HG11	13:V:186:TYR:CD1	2.52	0.45
12:W:127:ILE:HD11	15:M:1180:PHE:HE1	1.82	0.45
12:W:365:LYS:NZ	12:W:385:ASP:OD1	2.47	0.45
15:M:815:ARG:HD3	15:M:815:ARG:HA	1.72	0.45
15:M:926:ARG:HD3	15:M:1396:GLU:HG2	1.97	0.45
15:M:1288:LEU:HD12	15:M:1288:LEU:HA	1.75	0.45
8:L:101:LEU:HD23	8:L:104:LEU:HD23	1.99	0.45
10:R:210:TYR:HA	10:R:213:VAL:HG23	1.98	0.45
13:V:318:ILE:HG22	13:V:349:GLY:HA3	1.98	0.45
12:Y:141:VAL:HG11	12:Y:161:LYS:HB3	1.98	0.45
15:M:981:SER:HA	15:M:984:ASN:HB2	1.98	0.45
10:R:222:PHE:HD2	11:S:105:LEU:HG	1.82	0.44
12:W:283:GLU:CD	12:W:285:LYS:H	2.25	0.44
13:T:140:TYR:HB2	13:T:202:ILE:HG23	1.98	0.44
7:J:-32:DT:H2''	7:J:-31:DA:H8	1.81	0.44
7:J:64:DG:C5	7:J:65:DA:N6	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:197:GLN:HA	9:P:200:LYS:HE2	2.00	0.44
10:R:193:SER:HA	10:R:198:THR:HG23	1.99	0.44
11:S:170:GLU:CD	11:S:173:ARG:HH21	2.25	0.44
13:X:138:GLU:HG3	13:X:240:LYS:HG2	1.98	0.44
13:X:274:LYS:HA	13:X:274:LYS:HD3	1.76	0.44
15:M:794:ASP:OD1	15:M:794:ASP:N	2.48	0.44
15:M:1245:CYS:SG	15:M:1248:LEU:HB2	2.58	0.44
15:M:1267:ILE:HB	15:M:1318:ILE:HG22	1.98	0.44
15:M:1282:LEU:HD13	15:M:1289:TYR:HB3	1.99	0.44
2:C:82:THR:OG1	15:M:626:VAL:HG21	2.17	0.44
11:S:257:VAL:HG22	12:U:168:ILE:HG22	2.00	0.44
13:V:166:VAL:HG21	13:V:186:TYR:CD2	2.52	0.44
13:V:346:THR:HG23	13:V:354:ILE:HG12	2.00	0.44
13:V:448:ASP:OD1	13:V:450:LYS:N	2.49	0.44
12:W:422:ASP:O	12:W:425:ARG:NH2	2.50	0.44
12:Y:110:GLU:OE1	12:Y:110:GLU:N	2.50	0.44
13:T:198:ASP:OD2	13:T:211:ARG:NE	2.50	0.44
15:M:606:PHE:CD1	15:M:632:GLU:HG3	2.53	0.44
3:E:26:PHE:CD1	3:E:57:GLU:HG2	2.52	0.44
12:U:72:LEU:HB2	12:U:323:MET:HG3	2.00	0.44
12:U:297:GLU:HB2	12:U:299:HIS:CE1	2.53	0.44
13:V:88:LEU:O	13:V:92:ILE:HG22	2.17	0.44
12:W:190:ILE:HG22	12:W:191:SER:N	2.32	0.44
12:Y:38:ARG:HG3	12:Y:39:PRO:HD2	2.00	0.44
12:Y:141:VAL:HB	12:Y:161:LYS:HG2	1.99	0.44
13:T:61:ILE:O	13:T:65:ILE:HG13	2.18	0.44
15:M:1107:SER:O	15:M:1110:GLN:HG3	2.17	0.44
15:M:1296:THR:O	15:M:1301:ARG:NH2	2.46	0.44
1:A:66:PRO:HD3	7:J:17:DA:H5''	1.99	0.44
6:I:22:DC:H4'	15:M:1343:TRP:CD1	2.52	0.44
7:J:-35:DG:H2''	7:J:-34:DA:C8	2.52	0.44
12:U:271:ASP:OD1	12:U:272:GLN:N	2.51	0.44
13:V:296:ILE:HG13	13:V:297:ASP:N	2.32	0.44
12:Y:292:VAL:HG22	12:Y:320:ILE:HB	1.99	0.44
14:Z:583:GLU:HG2	14:Z:585:PRO:HD3	1.99	0.44
15:M:858:ASN:H	15:M:1389:LEU:HD21	1.83	0.44
1:A:79:LYS:NZ	1:A:80:THR:O	2.51	0.44
12:U:298:VAL:HG22	12:U:325:THR:HG22	2.00	0.44
12:W:119:GLN:OE1	12:W:242:HIS:NE2	2.49	0.44
12:W:205:SER:HA	12:W:222:VAL:HG12	1.99	0.44
12:W:404:SER:O	12:W:407:GLN:NE2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:59:LYS:HD2	12:Y:59:LYS:HA	1.70	0.44
12:Y:278:ALA:O	12:Y:282:GLU:HG2	2.17	0.44
12:Y:405:VAL:HG21	12:Y:430:PHE:HE2	1.83	0.44
15:M:718:ILE:O	15:M:930:LEU:N	2.37	0.44
2:C:62:LEU:HA	2:C:65:VAL:HG22	1.99	0.44
2:D:31:LYS:HD2	2:D:55:ARG:NH1	2.33	0.44
3:E:51:TYR:HB3	4:G:97:ILE:HG21	2.00	0.44
4:G:71:ASP:HA	4:G:74:GLU:HG3	1.99	0.44
6:I:-35:DA:H1'	6:I:-34:DG:C5	2.53	0.44
12:W:283:GLU:OE2	12:W:285:LYS:HG2	2.17	0.44
12:W:413:ARG:NH1	12:W:421:GLU:OE2	2.50	0.44
12:W:447:TYR:OH	13:X:371:ARG:NH2	2.47	0.44
13:X:203:GLU:OE1	13:X:205:ASN:N	2.51	0.44
12:Y:94:LYS:HD2	12:Y:94:LYS:HA	1.75	0.44
12:U:122:ARG:HE	12:U:241:LEU:HB3	1.83	0.44
12:U:125:ILE:HD11	12:U:319:PRO:HD3	1.99	0.44
12:U:359:TYR:OH	17:U:501:ADP:N7	2.37	0.44
13:V:391:GLU:O	13:V:392:ARG:HG2	2.17	0.44
12:W:17:LEU:O	13:X:331:ASN:ND2	2.49	0.44
12:W:327:ARG:HB2	12:W:327:ARG:HH11	1.83	0.44
13:X:387:ARG:HG2	13:X:416:LEU:HD22	2.00	0.44
12:Y:143:ILE:HG22	12:Y:158:LEU:HD22	2.00	0.44
12:Y:294:PHE:HD1	12:Y:322:MET:HG2	1.83	0.44
13:T:137:LYS:NZ	13:T:204:ALA:H	2.15	0.44
13:T:431:ARG:NH2	13:T:435:VAL:HB	2.33	0.44
15:M:823:LEU:HD12	15:M:850:LEU:HD22	2.00	0.44
1:A:56:LYS:HE3	1:A:56:LYS:HB3	1.79	0.44
5:H:68:PHE:O	5:H:72:ILE:HG12	2.18	0.44
11:S:10:LYS:HD2	11:S:10:LYS:HA	1.72	0.44
13:V:461:ASN:N	13:V:461:ASN:OD1	2.51	0.44
12:Y:118:THR:O	12:Y:122:ARG:HG2	2.17	0.44
14:Z:206:VAL:O	14:Z:209:LYS:HG2	2.18	0.44
13:T:169:GLY:HA2	13:T:178:THR:HA	2.00	0.44
13:T:330:SER:OG	13:T:331:ASN:N	2.51	0.44
13:T:402:LEU:HD11	13:T:439:VAL:HG21	1.99	0.44
7:J:46:DG:H2''	7:J:47:DA:C8	2.53	0.43
7:J:48:DG:H2''	7:J:49:DC:C5	2.53	0.43
11:S:112:ASP:O	11:S:116:VAL:HG23	2.17	0.43
12:U:350:ARG:HD3	13:T:413:ARG:CZ	2.47	0.43
13:V:421:PRO:HA	13:V:424:ILE:HG22	1.99	0.43
12:Y:190:ILE:HG23	12:Y:201:LYS:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:297:GLU:OE2	12:Y:300:MET:HG3	2.18	0.43
12:Y:455:GLN:OE1	12:Y:457:SER:N	2.39	0.43
15:M:965:MET:HG3	15:M:969:GLN:HB3	1.99	0.43
6:I:-72:DT:H2''	6:I:-71:DG:H8	1.83	0.43
6:I:-55:DG:N2	7:J:55:DC:C2	2.78	0.43
6:I:-36:DT:H2''	6:I:-35:DA:N7	2.34	0.43
7:J:-31:DA:H1'	7:J:-30:DA:H5'	2.00	0.43
8:L:35:GLY:O	8:L:39:ARG:HG3	2.18	0.43
13:V:48:PHE:HE1	13:V:51:GLN:HB2	1.82	0.43
13:V:456:LEU:HA	13:V:456:LEU:HD23	1.79	0.43
12:W:458:ILE:HD11	13:X:408:THR:HB	2.00	0.43
13:X:131:LEU:HD12	13:X:132:ARG:N	2.34	0.43
15:M:1078:LEU:HD23	15:M:1119:LEU:HD22	2.01	0.43
1:A:27:LYS:HA	1:A:27:LYS:HD3	1.79	0.43
1:B:42:LYS:HB3	1:B:42:LYS:HE3	1.68	0.43
5:H:60:LYS:HG3	8:L:88:PRO:HG2	2.00	0.43
8:L:37:ILE:HD12	8:L:60:THR:HG22	2.00	0.43
12:W:139:GLU:HA	12:W:189:VAL:HG22	2.01	0.43
13:T:283:LYS:HD2	13:T:283:LYS:HA	1.72	0.43
7:J:-22:DG:C2	7:J:-21:DG:N1	2.86	0.43
7:J:71:DC:H2''	7:J:72:DA:C8	2.52	0.43
10:R:187:PHE:CD2	10:R:348:LEU:HD21	2.53	0.43
10:R:375:ARG:NE	10:R:376:GLN:N	2.57	0.43
12:U:134:GLU:HG3	12:U:194:LYS:NZ	2.33	0.43
12:W:402:LEU:HA	12:W:405:VAL:HG22	1.99	0.43
13:X:127:ARG:HD3	12:Y:266:ARG:NH2	2.31	0.43
12:Y:297:GLU:HG2	13:T:322:THR:HB	2.00	0.43
4:G:61:SER:O	4:G:65:LEU:HG	2.18	0.43
9:P:215:ARG:HD2	9:P:215:ARG:HA	1.82	0.43
10:R:308:ASP:HB3	10:R:309:GLU:OE2	2.18	0.43
11:S:183:LYS:HZ2	11:S:185:PRO:HG3	1.83	0.43
13:T:203:GLU:HG2	13:T:205:ASN:H	1.83	0.43
15:M:1357:ARG:HD2	15:M:1357:ARG:HA	1.83	0.43
1:A:125:GLN:OE1	1:A:128:ARG:NH2	2.43	0.43
6:I:-62:DC:H5''	14:Z:218:LYS:HG2	2.01	0.43
12:U:188:ASP:HA	12:U:204:ARG:HA	2.01	0.43
13:V:321:PHE:CD2	13:V:360:PRO:HD3	2.53	0.43
13:X:131:LEU:N	13:X:247:VAL:O	2.52	0.43
13:X:274:LYS:O	13:X:276:LYS:N	2.51	0.43
14:Z:258:LYS:O	14:Z:261:GLU:HG3	2.19	0.43
13:T:138:GLU:HG2	13:T:240:LYS:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:721:ASP:O	18:M:1602:BEF:F1	2.26	0.43
15:M:772:LYS:HB2	15:M:796:PHE:HA	1.99	0.43
15:M:893:TRP:O	15:M:895:GLY:N	2.52	0.43
2:C:54:VAL:O	2:C:58:LEU:HG	2.19	0.43
3:E:59:LEU:HD21	4:G:109:LEU:HD13	2.01	0.43
10:R:191:ILE:HD12	10:R:200:ILE:HG12	1.99	0.43
12:U:203:GLY:N	12:U:223:GLN:HE22	2.16	0.43
13:V:88:LEU:HD12	13:V:88:LEU:HA	1.83	0.43
13:V:198:ASP:HA	13:V:214:ARG:HG3	1.99	0.43
13:V:381:ARG:NH1	13:V:401:ASP:OD1	2.51	0.43
15:M:607:GLY:O	15:M:629:SER:OG	2.28	0.43
15:M:752:VAL:HG12	15:M:824:ASP:HB3	2.01	0.43
6:I:-10:DC:H2''	6:I:-9:DA:N7	2.33	0.43
7:J:-22:DG:H2''	7:J:-21:DG:C8	2.53	0.43
8:L:65:TYR:OH	16:K:108:ARG:NH2	2.50	0.43
9:P:208:GLU:HG2	9:P:234:LYS:HE2	1.99	0.43
11:S:193:ASN:OD1	11:S:194:ARG:N	2.51	0.43
12:U:300:MET:HE3	12:U:333:ARG:HD2	2.01	0.43
12:U:443:ASN:HB3	12:U:446:GLN:HG3	2.01	0.43
13:V:418:LEU:C	13:V:421:PRO:HD2	2.44	0.43
13:X:395:VAL:HG22	13:X:434:ILE:HD12	2.01	0.43
14:Z:194:SER:OG	14:Z:195:LYS:N	2.51	0.43
15:M:858:ASN:N	15:M:1389:LEU:HD21	2.33	0.43
15:M:1066:THR:HA	15:M:1070:ASN:HB3	1.99	0.43
10:R:195:PHE:HA	17:R:501:ADP:O2'	2.18	0.43
11:S:30:THR:HG21	12:U:155:GLN:HG2	2.01	0.43
11:S:194:ARG:HG2	11:S:198:LEU:HG	2.00	0.43
11:S:241:ILE:HG13	11:S:242:THR:H	1.83	0.43
12:Y:185:LEU:HG	12:Y:187:GLY:H	1.83	0.43
12:Y:192:ILE:HG23	12:Y:199:ILE:HG22	2.00	0.43
13:T:43:ARG:HG3	13:T:44:VAL:HG23	2.00	0.43
15:M:775:THR:HA	15:M:800:ILE:HB	2.00	0.43
2:C:72:TYR:HE2	2:C:89:ALA:HB2	1.84	0.43
12:U:117:LEU:HD11	12:U:305:CYS:HB3	2.00	0.43
12:U:171:LEU:CD1	12:U:176:ILE:HG13	2.48	0.43
12:W:155:GLN:HE22	12:W:170:GLU:HB2	1.84	0.43
13:X:362:ASP:OD1	13:X:363:LEU:N	2.52	0.43
12:Y:184:VAL:HG13	12:Y:186:ALA:N	2.33	0.43
12:Y:412:LYS:HA	12:Y:412:LYS:HD3	1.79	0.43
13:T:150:GLU:HB2	13:T:165:HIS:H	1.84	0.43
13:T:245:GLN:OE1	13:T:246:ASP:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:938:GLU:HA	15:M:941:MET:HE1	2.00	0.43
1:A:92:LEU:HD12	2:D:86:VAL:HG21	2.01	0.42
1:B:71:VAL:HA	1:B:74:ILE:HG22	2.01	0.42
2:D:39:ARG:HA	2:D:39:ARG:HD3	1.73	0.42
3:E:89:ARG:HE	3:E:89:ARG:HB2	1.53	0.42
10:R:392:CYS:HA	10:R:395:PHE:HB3	2.01	0.42
13:V:82:SER:H	13:V:413:ARG:NH2	2.17	0.42
13:V:249:LEU:HD23	13:V:249:LEU:HA	1.81	0.42
15:M:1164:LYS:O	15:M:1169:ARG:NH1	2.51	0.42
4:G:37:LYS:HE2	7:J:50:DG:H5'	2.00	0.42
5:H:94:ALA:HA	8:L:55:ALA:HA	2.01	0.42
10:R:60:PRO:O	10:R:67:THR:N	2.35	0.42
10:R:76:TRP:CH2	10:R:80:LEU:HD23	2.54	0.42
11:S:22:LEU:HD21	12:U:144:GLN:HB2	2.01	0.42
12:U:421:GLU:HG2	12:U:422:ASP:N	2.34	0.42
13:V:85:LYS:N	17:V:501:ADP:O2A	2.52	0.42
13:V:138:GLU:OE1	13:V:238:HIS:NE2	2.52	0.42
12:W:172:GLY:H	12:W:175:MET:CE	2.32	0.42
5:H:119:ARG:NH2	16:K:106:ARG:HH12	2.16	0.42
12:U:394:THR:OG1	12:U:395:SER:N	2.51	0.42
13:V:282:GLU:O	13:V:286:GLN:HG2	2.19	0.42
13:V:290:LYS:HB3	13:V:290:LYS:HE2	1.83	0.42
12:W:443:ASN:ND2	12:W:446:GLN:OE1	2.44	0.42
12:Y:191:SER:H	12:Y:202:LEU:HG	1.83	0.42
13:T:394:GLN:HB2	13:T:432:LYS:HE3	2.02	0.42
1:A:46:VAL:O	1:A:49:ARG:HG2	2.19	0.42
5:H:125:SER:HG	8:L:54:LYS:HZ1	1.63	0.42
10:R:135:VAL:O	10:R:138:PRO:HD2	2.18	0.42
10:R:318:PHE:HB2	10:R:319:HIS:ND1	2.34	0.42
12:U:331:LYS:HD3	12:U:338:LYS:HG3	2.01	0.42
12:W:190:ILE:HG21	12:W:199:ILE:HG23	2.01	0.42
13:X:199:VAL:HG21	13:X:230:VAL:HG23	2.01	0.42
12:Y:301:LEU:O	12:Y:333:ARG:HB2	2.18	0.42
13:T:263:GLN:HE21	13:T:263:GLN:HB3	1.65	0.42
15:M:1214:MET:HA	15:M:1217:CYS:HB2	2.02	0.42
8:L:34:VAL:HB	16:K:78:ASP:OD1	2.20	0.42
10:R:91:LEU:HD11	10:R:94:GLY:HA2	2.00	0.42
12:U:143:ILE:HG23	12:U:158:LEU:HD11	2.02	0.42
12:Y:412:LYS:HD2	13:T:38:SER:HA	2.01	0.42
15:M:655:VAL:HG23	15:M:656:HIS:ND1	2.34	0.42
15:M:699:TYR:HD2	15:M:937:VAL:HG11	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:1064:LYS:HD3	15:M:1064:LYS:HA	1.77	0.42
1:B:106:ASP:O	1:B:109:LEU:HG	2.19	0.42
3:E:26:PHE:HB2	3:E:57:GLU:OE2	2.19	0.42
6:I:37:DG:C8	6:I:36:DT:H72	2.55	0.42
6:I:0:DC:H3'	6:I:1:DT:H71	2.00	0.42
11:S:205:LYS:HB3	11:S:210:SER:HB2	2.02	0.42
12:U:101:ILE:O	12:U:295:ILE:HA	2.19	0.42
12:U:164:ASP:OD1	12:U:164:ASP:N	2.51	0.42
13:V:117:LYS:O	13:V:120:THR:OG1	2.35	0.42
12:W:59:LYS:HA	12:W:59:LYS:HD3	1.74	0.42
13:X:76:LEU:O	13:X:369:ILE:HA	2.19	0.42
13:T:245:GLN:HG3	13:T:247:VAL:HG13	2.01	0.42
13:T:350:THR:OG1	13:T:351:GLU:N	2.52	0.42
15:M:995:HIS:NE2	15:M:1247:LYS:HG3	2.34	0.42
15:M:1197:LEU:HD12	15:M:1197:LEU:HA	1.89	0.42
15:M:1327:GLY:HA2	15:M:1354:ARG:CZ	2.50	0.42
1:A:26:ARG:NH1	10:R:73:SER:OG	2.53	0.42
12:W:189:VAL:O	12:W:190:ILE:HD13	2.18	0.42
12:Y:45:VAL:HB	12:Y:367:ILE:HD11	2.02	0.42
13:T:44:VAL:HG22	13:T:49:VAL:HG12	2.00	0.42
15:M:608:LYS:HE2	15:M:610:GLU:HG3	2.00	0.42
15:M:1133:ARG:N	15:M:1134:PRO:HD2	2.35	0.42
1:A:65:LEU:HB2	7:J:17:DA:H5''	2.02	0.42
2:D:50:ILE:O	2:D:53:GLU:HG2	2.19	0.42
2:D:79:LYS:N	7:J:28:DA:OP1	2.49	0.42
6:I:33:DC:H2''	6:I:34:DT:C6	2.55	0.42
7:J:71:DC:H2''	7:J:72:DA:H8	1.85	0.42
10:R:113:LYS:HA	10:R:428:THR:HG21	2.01	0.42
10:R:126:ASP:OD1	10:R:126:ASP:N	2.51	0.42
11:S:30:THR:HA	11:S:235:PHE:O	2.19	0.42
12:U:141:VAL:HG13	12:U:142:GLU:H	1.84	0.42
12:W:115:GLU:OE2	12:W:264:GLU:N	2.53	0.42
12:Y:303:ILE:HD11	12:Y:332:THR:OG1	2.20	0.42
14:Z:240:GLU:H	14:Z:240:GLU:HG3	1.73	0.42
14:Z:256:LEU:HB3	14:Z:260:LYS:NZ	2.35	0.42
13:T:394:GLN:HB3	13:T:433:GLU:HA	2.02	0.42
15:M:1062:ILE:HG22	15:M:1130:CYS:SG	2.60	0.42
4:G:49:LYS:HA	4:G:53:PRO:HA	2.00	0.42
7:J:61:DC:O3'	15:M:787:ARG:NH2	2.52	0.42
11:S:109:ASN:HD21	11:S:111:SER:HB3	1.85	0.42
12:U:113:LYS:NZ	12:U:302:ASP:OD2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:123:LYS:HE3	12:U:242:HIS:CD2	2.55	0.42
12:U:162:THR:OG1	12:U:165:MET:O	2.37	0.42
12:U:410:ALA:HB2	12:U:418:VAL:HG12	2.01	0.42
13:V:75:ILE:O	13:V:337:VAL:HA	2.19	0.42
13:V:364:ILE:HD13	13:V:364:ILE:HA	1.89	0.42
13:X:52:ILE:O	13:X:56:GLU:HG2	2.19	0.42
12:Y:431:LEU:HD11	13:T:371:ARG:NE	2.35	0.42
1:A:39:HIS:CG	1:A:40:ARG:H	2.38	0.42
1:A:70:LEU:O	1:A:74:ILE:HG12	2.20	0.42
2:C:39:ARG:HA	2:C:39:ARG:HD2	1.91	0.42
10:R:95:LYS:HB2	10:R:95:LYS:HE2	1.83	0.42
11:S:103:MET:HG3	11:S:116:VAL:HG13	2.02	0.42
11:S:110:PHE:HA	11:S:113:LEU:HG	2.02	0.42
12:U:408:GLN:CG	13:V:64:LEU:HD22	2.47	0.42
12:W:47:GLN:NE2	12:W:357:LYS:O	2.52	0.42
13:X:210:LYS:HG2	13:X:212:VAL:HG13	2.02	0.42
13:X:219:ALA:HA	13:X:229:TYR:CE1	2.55	0.42
12:Y:298:VAL:HG21	12:Y:323:MET:HB3	2.02	0.42
14:Z:278:LYS:HE2	14:Z:278:LYS:HB3	1.86	0.42
15:M:955:LYS:HA	15:M:955:LYS:HD3	1.80	0.42
1:A:120:MET:HE1	1:A:122:LYS:CB	2.50	0.41
6:I:-16:DT:H2''	6:I:-15:DA:C8	2.55	0.41
7:J:-7:DG:H2''	7:J:-6:DG:C8	2.54	0.41
10:R:106:MET:HE3	10:R:106:MET:HB2	1.79	0.41
13:V:27:HIS:O	13:V:28:THR:OG1	2.27	0.41
13:V:58:CYS:SG	13:V:92:ILE:HB	2.60	0.41
13:V:200:ILE:HA	13:V:211:ARG:HA	2.00	0.41
13:V:377:LYS:HD2	13:V:404:ALA:HB1	2.01	0.41
12:W:78:SER:N	17:W:501:ADP:O1B	2.37	0.41
14:Z:241:ARG:HH22	15:M:740:CYS:HA	1.83	0.41
15:M:1083:LYS:O	15:M:1087:GLU:HG2	2.20	0.41
12:U:131:GLU:HG2	12:U:235:VAL:HB	2.02	0.41
12:U:212:TYR:O	12:U:215:MET:HE3	2.20	0.41
12:W:83:ALA:HB2	17:W:501:ADP:H2'	2.02	0.41
13:X:126:ARG:HH22	13:X:285:ARG:HD3	1.83	0.41
12:Y:152:GLY:HA3	14:Z:620:TYR:CD2	2.55	0.41
13:T:172:SER:OG	13:T:173:ALA:N	2.53	0.41
15:M:1066:THR:HA	15:M:1070:ASN:CB	2.51	0.41
15:M:1161:GLU:O	15:M:1164:LYS:HG2	2.20	0.41
2:C:39:ARG:HH11	2:C:43:VAL:HG13	1.85	0.41
6:I:-55:DG:H1'	6:I:-54:DA:C5	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-46:DC:N4	7:J:46:DG:O6	2.30	0.41
6:I:-28:DT:H2''	6:I:-27:DC:C6	2.56	0.41
7:J:-2:DC:H2''	7:J:-1:DA:H8	1.86	0.41
10:R:209:TYR:CZ	10:R:211:LYS:HB2	2.55	0.41
17:R:501:ADP:O2A	18:R:502:BEF:F1	2.29	0.41
12:W:299:HIS:HB3	12:W:325:THR:OG1	2.20	0.41
12:W:453:ASN:OD1	12:W:453:ASN:N	2.51	0.41
12:Y:139:GLU:CB	12:Y:160:ILE:HB	2.50	0.41
12:Y:272:GLN:O	12:Y:275:THR:OG1	2.33	0.41
12:Y:346:ASP:OD2	12:Y:346:ASP:C	2.63	0.41
13:T:403:LEU:HD23	13:T:403:LEU:HA	1.94	0.41
15:M:953:LEU:O	15:M:958:ARG:NH2	2.52	0.41
15:M:1140:LEU:O	15:M:1144:LEU:HD12	2.20	0.41
2:D:79:LYS:HE2	2:D:79:LYS:HB2	1.67	0.41
3:E:85:GLN:HE21	3:E:103:ILE:HG22	1.85	0.41
5:H:48:LEU:HB2	8:L:71:LEU:HD13	2.01	0.41
5:H:64:ILE:HD12	8:L:88:PRO:HB3	2.01	0.41
5:H:105:LEU:HD12	5:H:106:PRO:CD	2.48	0.41
6:I:-6:DT:H2''	6:I:-5:DA:N7	2.35	0.41
7:J:-8:DG:H1'	7:J:-7:DG:O4'	2.20	0.41
12:U:47:GLN:HE21	12:U:359:TYR:HE1	1.67	0.41
13:V:83:THR:N	17:V:501:ADP:O1B	2.49	0.41
12:W:294:PHE:CD1	12:W:322:MET:HG3	2.55	0.41
13:X:57:ALA:O	13:X:61:ILE:HG12	2.20	0.41
12:Y:223:GLN:CD	15:M:1065:LEU:HD23	2.45	0.41
13:T:144:VAL:N	13:T:198:ASP:O	2.54	0.41
1:A:63:ARG:HB3	7:J:17:DA:H4'	2.03	0.41
1:B:107:THR:HG22	1:B:124:ILE:HA	2.02	0.41
2:C:40:ARG:HH21	3:E:108:VAL:HG12	1.86	0.41
7:J:-21:DG:C2	7:J:-20:DC:C2	3.08	0.41
7:J:-19:DG:H5''	15:M:1272:THR:HB	2.02	0.41
9:P:190:GLN:HE22	9:P:195:PRO:HG3	1.85	0.41
11:S:100:ARG:NH1	11:S:104:GLU:OE2	2.54	0.41
12:U:92:LEU:HG	12:U:96:VAL:HB	2.03	0.41
13:V:112:SER:OG	13:V:113:VAL:N	2.54	0.41
13:V:211:ARG:HE	13:V:211:ARG:HB2	1.69	0.41
13:V:313:VAL:HG11	13:V:338:LEU:HD12	2.01	0.41
12:W:239:VAL:HG13	12:W:243:GLU:OE1	2.20	0.41
12:W:301:LEU:O	12:W:333:ARG:HB2	2.20	0.41
15:M:1110:GLN:HE22	15:M:1111:LYS:HE2	1.84	0.41
15:M:1158:ILE:HB	15:M:1162:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:1282:LEU:HD23	15:M:1287:TYR:HD2	1.85	0.41
15:M:1327:GLY:HA2	15:M:1354:ARG:NE	2.35	0.41
10:R:287:VAL:O	10:R:294:ASN:ND2	2.44	0.41
11:S:6:GLU:O	13:V:180:ARG:N	2.41	0.41
12:U:265:ILE:O	12:U:270:ARG:NH2	2.44	0.41
13:V:96:LEU:HD12	13:V:100:VAL:HG11	2.02	0.41
13:V:424:ILE:O	13:V:428:THR:HG23	2.21	0.41
12:W:124:SER:OG	12:W:319:PRO:HG3	2.21	0.41
13:X:149:PRO:HB3	13:X:166:VAL:HG22	2.03	0.41
12:Y:129:ILE:HG22	12:Y:237:HIS:HB2	2.03	0.41
12:Y:240:SER:HB3	12:Y:243:GLU:OE2	2.20	0.41
12:Y:431:LEU:HD23	12:Y:431:LEU:HA	1.84	0.41
1:A:120:MET:CE	1:A:122:LYS:H	2.33	0.41
2:C:68:ASP:O	2:C:71:THR:OG1	2.24	0.41
5:H:36:ARG:HH22	16:K:70:SER:N	2.19	0.41
5:H:59:GLN:HA	16:K:151:PHE:CE1	2.55	0.41
5:H:118:THR:HG22	16:K:94:GLU:CD	2.45	0.41
12:U:157:LYS:HE2	12:U:157:LYS:HB2	1.78	0.41
12:U:399:SER:O	12:U:403:ILE:HG22	2.20	0.41
13:V:285:ARG:H	13:V:285:ARG:HG2	1.69	0.41
13:V:410:THR:OG1	13:V:411:SER:N	2.53	0.41
13:V:462:TYR:HB2	12:W:328:GLY:HA3	2.02	0.41
12:W:29:LEU:HD12	12:W:29:LEU:HA	1.94	0.41
12:Y:406:ALA:HA	12:Y:409:ILE:HG22	2.03	0.41
14:Z:318:LYS:HD3	14:Z:318:LYS:HA	1.91	0.41
15:M:837:TRP:HB3	15:M:838:GLN:HE21	1.85	0.41
15:M:1237:ASP:OD1	15:M:1238:LYS:N	2.44	0.41
2:D:78:ARG:HE	7:J:28:DA:P	2.44	0.41
10:R:426:TRP:HB3	11:S:188:LYS:HD3	2.01	0.41
12:U:127:ILE:HD13	12:U:127:ILE:HA	1.89	0.41
13:V:195:SER:HG	13:V:198:ASP:CG	2.25	0.41
13:X:196:ILE:HA	14:Z:613:LEU:HD21	2.02	0.41
13:X:224:LEU:HD11	12:Y:169:TYR:HB3	2.02	0.41
12:Y:412:LYS:O	12:Y:414:LYS:NZ	2.43	0.41
15:M:856:LEU:HB2	15:M:862:GLU:CD	2.46	0.41
15:M:994:ASN:CG	15:M:998:LEU:HB3	2.46	0.41
15:M:1113:GLU:O	15:M:1116:VAL:HG12	2.21	0.41
1:A:52:ARG:HD2	1:A:52:ARG:HA	1.91	0.41
1:A:109:LEU:HA	1:A:112:ILE:HG12	2.02	0.41
1:A:113:HIS:ND1	1:B:126:LEU:HD22	2.36	0.41
1:B:46:VAL:HA	1:B:49:ARG:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLN:OE1	2:C:40:ARG:NH2	2.54	0.41
1:B:67:PHE:O	1:B:70:LEU:HG	2.20	0.41
2:C:88:TYR:O	2:C:91:LYS:HG2	2.20	0.41
3:E:54:ALA:HA	3:E:57:GLU:OE1	2.21	0.41
4:G:60:LYS:O	4:G:63:SER:OG	2.39	0.41
10:R:36:LYS:HG3	10:R:54:SER:C	2.46	0.41
10:R:209:TYR:CE2	10:R:211:LYS:HB2	2.55	0.41
10:R:226:LEU:HD23	11:S:105:LEU:CD1	2.42	0.41
10:R:434:TYR:H	11:S:194:ARG:NH2	2.18	0.41
12:U:204:ARG:HG2	12:U:219:THR:HG21	2.02	0.41
12:U:345:LEU:HD23	12:U:345:LEU:HA	1.85	0.41
12:U:448:ILE:HG12	12:U:454:VAL:HG22	2.03	0.41
13:V:127:ARG:HG3	13:V:248:THR:HG21	2.02	0.41
12:W:255:LEU:HD11	15:M:1166:LEU:HD12	2.03	0.41
13:X:75:ILE:HD11	13:X:370:VAL:HG23	2.03	0.41
13:X:77:LEU:CD1	13:X:85:LYS:HB3	2.50	0.41
12:Y:243:GLU:OE1	12:Y:243:GLU:N	2.50	0.41
12:Y:299:HIS:ND1	12:Y:327:ARG:HD2	2.36	0.41
12:Y:305:CYS:O	12:Y:309:ILE:HG12	2.21	0.41
13:T:125:PHE:CE2	13:T:334:PRO:HD2	2.55	0.41
13:T:201:TYR:CE1	13:T:210:LYS:HG2	2.54	0.41
15:M:727:LYS:HG3	17:M:1601:ADP:O2B	2.21	0.41
15:M:871:MET:HG3	15:M:884:PHE:H	1.86	0.41
15:M:1082:ASN:OD1	15:M:1116:VAL:HG11	2.21	0.41
15:M:1146:LYS:HA	15:M:1146:LYS:HD3	1.71	0.41
15:M:1292:LEU:HD12	15:M:1292:LEU:HA	1.95	0.41
2:C:77:LYS:NZ	15:M:622:GLU:HG3	2.36	0.41
6:I:24:DA:H2''	6:I:25:DG:C8	2.56	0.41
8:L:101:LEU:HD23	8:L:101:LEU:HA	1.97	0.41
10:R:215:LYS:HG2	11:S:211:PHE:CD1	2.56	0.41
11:S:241:ILE:CG1	11:S:262:LYS:H	2.34	0.41
12:U:72:LEU:HD23	12:U:353:ILE:HG12	2.02	0.41
13:X:120:THR:O	13:X:123:GLU:HG2	2.20	0.41
13:X:124:ASN:CG	13:X:127:ARG:HH21	2.28	0.41
13:T:402:LEU:HD11	13:T:439:VAL:CG2	2.50	0.41
6:I:-64:DC:H1'	6:I:-63:DC:O4'	2.22	0.40
6:I:10:DC:H2''	6:I:11:DG:H8	1.86	0.40
10:R:106:MET:HB3	10:R:199:TRP:CZ2	2.55	0.40
10:R:336:GLU:HB2	11:S:222:LYS:HD2	2.03	0.40
12:U:23:HIS:NE2	17:U:501:ADP:H3'	2.36	0.40
12:U:414:LYS:HB2	12:U:414:LYS:HE2	1.92	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:387:ARG:HA	13:V:387:ARG:HD2	1.94	0.40
13:X:128:ALA:HB3	13:X:334:PRO:HG3	2.03	0.40
12:Y:244:ILE:HD11	15:M:1147:ASP:CG	2.46	0.40
14:Z:209:LYS:O	14:Z:212:LYS:HG2	2.21	0.40
13:T:198:ASP:OD1	13:T:214:ARG:HA	2.20	0.40
13:T:402:LEU:HD12	13:T:406:MET:HE1	2.03	0.40
13:T:422:CYS:SG	13:T:439:VAL:HG12	2.61	0.40
15:M:845:THR:OG1	15:M:846:GLN:N	2.54	0.40
1:A:113:HIS:CE1	1:B:126:LEU:HD22	2.57	0.40
7:J:39:DA:C5	7:J:40:DC:C4	3.09	0.40
8:L:52:GLY:HA3	16:K:89:GLU:OE2	2.21	0.40
8:L:87:THR:HG22	8:L:89:ARG:N	2.34	0.40
12:U:20:ILE:HD13	12:U:20:ILE:HA	1.91	0.40
12:U:361:GLU:O	12:U:364:ILE:HG22	2.22	0.40
13:V:66:LYS:HE3	13:V:66:LYS:HB3	1.83	0.40
12:W:126:GLY:HA2	12:W:240:SER:HA	2.03	0.40
14:Z:299:PRO:HD3	14:Z:303:LEU:HD13	2.03	0.40
13:T:128:ALA:HB3	13:T:334:PRO:HG3	2.02	0.40
15:M:1113:GLU:HA	15:M:1116:VAL:HG12	2.03	0.40
10:R:360:PHE:HB3	10:R:365:PHE:CD2	2.56	0.40
13:V:146:GLU:O	13:V:147:LEU:HD13	2.22	0.40
13:V:226:THR:HG23	12:W:175:MET:SD	2.61	0.40
13:X:49:VAL:O	17:X:501:ADP:N6	2.55	0.40
12:Y:241:LEU:HD12	12:Y:241:LEU:HA	1.85	0.40
13:T:118:THR:HB	13:T:323:TYR:CD2	2.56	0.40
13:T:194:VAL:HG11	13:T:200:ILE:HD11	2.03	0.40
13:T:296:ILE:HG13	13:T:297:ASP:N	2.36	0.40
13:T:387:ARG:HA	13:T:387:ARG:HD2	1.75	0.40
15:M:671:ASP:HA	15:M:674:THR:HG22	2.03	0.40
15:M:832:PHE:CD1	15:M:833:ARG:HG2	2.56	0.40
15:M:1310:THR:OG1	15:M:1311:ASP:N	2.54	0.40
1:B:116:ARG:HE	1:B:116:ARG:HB2	1.69	0.40
5:H:60:LYS:HE3	5:H:60:LYS:HB3	1.79	0.40
5:H:87:ASN:O	5:H:88:LYS:HG2	2.21	0.40
8:L:87:THR:HG23	16:K:139:LYS:HG2	2.02	0.40
10:R:289:ASN:OD1	10:R:292:LYS:HG3	2.21	0.40
13:V:117:LYS:HB2	13:V:320:ILE:HD11	2.03	0.40
13:V:140:TYR:HA	13:V:237:VAL:O	2.20	0.40
13:V:198:ASP:HA	13:V:214:ARG:HA	2.03	0.40
12:W:431:LEU:HD12	12:W:431:LEU:HA	1.88	0.40
13:X:402:LEU:HD12	13:X:405:THR:OG1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:431:ARG:NH1	13:X:433:GLU:O	2.54	0.40
12:Y:94:LYS:NZ	12:Y:95:ASP:H	2.20	0.40
12:Y:244:ILE:HG23	12:Y:273:ILE:CD1	2.51	0.40
12:Y:402:LEU:HA	12:Y:405:VAL:HG12	2.03	0.40
15:M:687:PRO:HB3	15:M:701:LYS:HE2	2.04	0.40
15:M:1065:LEU:HD12	15:M:1065:LEU:HA	1.92	0.40
5:H:113:ALA:HB1	8:L:62:VAL:HG22	2.04	0.40
7:J:24:DC:H2''	7:J:25:DT:O5'	2.21	0.40
8:L:78:ALA:HA	8:L:90:HIS:CE1	2.57	0.40
9:P:230:GLY:O	9:P:231:LEU:HB3	2.21	0.40
10:R:234:ARG:NH1	11:S:245:SER:O	2.54	0.40
11:S:263:ILE:HD12	11:S:269:PHE:CD1	2.57	0.40
13:V:142:GLY:HA3	13:V:170:LEU:HG	2.03	0.40
13:X:23:ARG:NH2	12:Y:67:ALA:HB2	2.36	0.40
12:Y:228:GLU:OE1	12:Y:229:LEU:N	2.55	0.40
14:Z:287:ILE:HD12	14:Z:288:LEU:H	1.87	0.40
15:M:840:LEU:HA	15:M:843:PHE:HD1	1.85	0.40
15:M:934:LYS:HE2	15:M:1356:HIS:HE1	1.87	0.40
15:M:1054:LEU:HD13	15:M:1134:PRO:HD3	2.04	0.40
15:M:1183:LEU:HD12	15:M:1184:THR:H	1.86	0.40
16:K:115:LYS:C	16:K:117:THR:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	77/113 (68%)	77 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	80/113 (71%)	79 (99%)	1 (1%)	61	71
2	C	50/81 (62%)	50 (100%)	0	100	100
2	D	52/81 (64%)	52 (100%)	0	100	100
3	E	65/99 (66%)	65 (100%)	0	100	100
4	G	66/109 (61%)	66 (100%)	0	100	100
5	H	78/109 (72%)	78 (100%)	0	100	100
8	L	69/103 (67%)	68 (99%)	1 (1%)	59	70
9	P	93/262 (36%)	93 (100%)	0	100	100
10	R	349/396 (88%)	348 (100%)	1 (0%)	86	84
11	S	176/261 (67%)	174 (99%)	2 (1%)	65	73
12	U	379/403 (94%)	378 (100%)	1 (0%)	86	84
12	W	365/403 (91%)	365 (100%)	0	100	100
12	Y	359/403 (89%)	356 (99%)	3 (1%)	73	76
13	T	344/391 (88%)	342 (99%)	2 (1%)	78	79
13	V	356/391 (91%)	356 (100%)	0	100	100
13	X	368/391 (94%)	365 (99%)	3 (1%)	73	76
14	Z	148/732 (20%)	148 (100%)	0	100	100
15	M	662/1376 (48%)	657 (99%)	5 (1%)	73	76
16	K	67/136 (49%)	67 (100%)	0	100	100
All	All	4203/6353 (66%)	4184 (100%)	19 (0%)	78	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	120	MET
8	L	37	ILE
10	R	325	ILE
11	S	106	ASN
11	S	130	ARG
12	U	352	ILE
13	X	100	VAL
13	X	117	LYS
13	X	308	LEU
12	Y	32	ASP
12	Y	136	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Y	254	PHE
13	T	251	ASP
13	T	263	GLN
15	M	723	MET
15	M	754	THR
15	M	811	HIS
15	M	1139	ASN
15	M	1214	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	27	GLN
9	P	212	HIS
10	R	185	HIS
10	R	247	ASN
10	R	374	GLN
11	S	223	ASN
12	U	47	GLN
12	U	223	GLN
13	V	94	GLN
13	V	263	GLN
12	W	252	GLN
12	W	326	ASN
13	X	286	GLN
12	Y	25	HIS
12	Y	326	ASN
12	Y	408	GLN
13	T	29	HIS
13	T	286	GLN
15	M	661	ASN
15	M	695	ASN
15	M	712	ASN
15	M	838	GLN
15	M	844	ASN
15	M	984	ASN
15	M	1036	ASN
15	M	1082	ASN
15	M	1084	GLN
15	M	1222	ASN
15	M	1228	GLN
15	M	1280	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	1385	GLN

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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	ADP	R	501	19	28,29,29	1.44	4 (14%)	43,45,45	1.90	11 (25%)
17	ADP	W	501	19	28,29,29	1.43	4 (14%)	43,45,45	1.80	9 (20%)
17	ADP	X	501	19	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
17	ADP	M	1601	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	10 (23%)
17	ADP	T	501	19	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
17	ADP	V	501	19	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
18	BEF	R	502	-	0,3,3	-	-	-	-	-
17	ADP	Y	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
18	BEF	M	1602	-	0,3,3	-	-	-	-	-
17	ADP	U	501	19	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	R	501	19	-	0/16/32/32	0/3/3/3
17	ADP	W	501	19	-	1/16/32/32	0/3/3/3
17	ADP	X	501	19	-	3/16/32/32	0/3/3/3
17	ADP	M	1601	-	-	6/16/32/32	0/3/3/3
17	ADP	T	501	19	-	2/16/32/32	0/3/3/3
17	ADP	V	501	19	-	7/16/32/32	0/3/3/3
17	ADP	Y	501	-	-	3/16/32/32	0/3/3/3
17	ADP	U	501	19	-	2/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	501	ADP	C5-C4	4.82	1.47	1.39
17	W	501	ADP	C5-C4	4.78	1.47	1.39
17	T	501	ADP	C5-C4	4.73	1.47	1.39
17	X	501	ADP	C5-C4	4.72	1.47	1.39
17	Y	501	ADP	C5-C4	4.71	1.47	1.39
17	M	1601	ADP	C5-C4	4.70	1.47	1.39
17	U	501	ADP	C5-C4	4.68	1.47	1.39
17	V	501	ADP	C5-C4	4.61	1.47	1.39
17	R	501	ADP	C5-C6	2.82	1.48	1.41
17	W	501	ADP	C5-C6	2.79	1.48	1.41
17	M	1601	ADP	C5-C6	2.72	1.48	1.41
17	T	501	ADP	C5-C6	2.67	1.48	1.41
17	X	501	ADP	C5-C6	2.65	1.48	1.41
17	V	501	ADP	C5-C6	2.64	1.48	1.41
17	U	501	ADP	C5-C6	2.63	1.48	1.41
17	Y	501	ADP	C5-C6	2.63	1.48	1.41
17	R	501	ADP	C8-N7	2.55	1.36	1.31
17	W	501	ADP	C8-N7	2.43	1.36	1.31
17	T	501	ADP	C5-N7	-2.42	1.34	1.39
17	Y	501	ADP	C5-N7	-2.41	1.34	1.39
17	U	501	ADP	C5-N7	-2.38	1.34	1.39
17	V	501	ADP	C5-N7	-2.35	1.34	1.39
17	X	501	ADP	C5-N7	-2.34	1.34	1.39
17	M	1601	ADP	C8-N7	2.33	1.36	1.31
17	U	501	ADP	C8-N7	2.26	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	501	ADP	C8-N7	2.25	1.36	1.31
17	V	501	ADP	C8-N7	2.23	1.36	1.31
17	R	501	ADP	C5-N7	-2.22	1.35	1.39
17	X	501	ADP	C8-N7	2.21	1.35	1.31
17	M	1601	ADP	C5-N7	-2.20	1.35	1.39
17	Y	501	ADP	C8-N7	2.19	1.35	1.31
17	W	501	ADP	C5-N7	-2.18	1.35	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	501	ADP	C5-C4-N3	-6.08	118.34	126.72
17	U	501	ADP	C5-C4-N3	-6.06	118.37	126.72
17	T	501	ADP	C5-C4-N3	-6.01	118.45	126.72
17	Y	501	ADP	C5-C4-N3	-5.95	118.52	126.72
17	R	501	ADP	C5-C4-N3	-5.94	118.54	126.72
17	V	501	ADP	C5-C4-N3	-5.83	118.69	126.72
17	M	1601	ADP	C5-C4-N3	-5.81	118.72	126.72
17	W	501	ADP	C5-C4-N3	-5.78	118.76	126.72
17	X	501	ADP	N3-C4-N9	4.95	135.59	127.17
17	U	501	ADP	N3-C4-N9	4.88	135.46	127.17
17	T	501	ADP	N3-C4-N9	4.88	135.46	127.17
17	Y	501	ADP	N3-C4-N9	4.83	135.39	127.17
17	V	501	ADP	N3-C4-N9	4.70	135.16	127.17
17	M	1601	ADP	N3-C4-N9	4.59	134.98	127.17
17	W	501	ADP	N3-C4-N9	4.46	134.75	127.17
17	R	501	ADP	N3-C4-N9	4.42	134.68	127.17
17	X	501	ADP	C2-N3-C4	3.76	121.01	111.83
17	R	501	ADP	C2-N3-C4	3.75	120.99	111.83
17	T	501	ADP	C2-N3-C4	3.73	120.94	111.83
17	U	501	ADP	C2-N3-C4	3.70	120.88	111.83
17	M	1601	ADP	C2-N3-C4	3.70	120.87	111.83
17	W	501	ADP	C2-N3-C4	3.66	120.77	111.83
17	V	501	ADP	C2-N3-C4	3.64	120.73	111.83
17	R	501	ADP	C4-C5-N7	-3.63	106.44	110.58
17	Y	501	ADP	C2-N3-C4	3.60	120.61	111.83
17	M	1601	ADP	C4-C5-N7	-3.53	106.55	110.58
17	W	501	ADP	C4-C5-N7	-3.52	106.56	110.58
17	Y	501	ADP	C4-C5-N7	-3.47	106.62	110.58
17	V	501	ADP	C4-C5-N7	-3.36	106.74	110.58
17	U	501	ADP	C4-C5-N7	-3.32	106.79	110.58
17	X	501	ADP	C4-C5-N7	-3.29	106.81	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	501	ADP	C4-C5-N7	-3.27	106.84	110.58
17	R	501	ADP	N3-C2-N1	-3.27	123.63	128.58
17	M	1601	ADP	N3-C2-N1	-3.26	123.65	128.58
17	W	501	ADP	N3-C2-N1	-3.22	123.70	128.58
17	X	501	ADP	N3-C2-N1	-3.22	123.71	128.58
17	T	501	ADP	N3-C2-N1	-3.18	123.76	128.58
17	U	501	ADP	N3-C2-N1	-3.18	123.77	128.58
17	V	501	ADP	N3-C2-N1	-3.15	123.82	128.58
17	Y	501	ADP	N3-C2-N1	-2.99	124.06	128.58
17	Y	501	ADP	C4-N9-C8	2.76	108.63	105.74
17	V	501	ADP	C4-N9-C8	2.75	108.63	105.74
17	M	1601	ADP	C4-N9-C8	2.68	108.56	105.74
17	Y	501	ADP	C5-N7-C8	2.65	107.61	103.45
17	M	1601	ADP	C5-N7-C8	2.59	107.53	103.45
17	U	501	ADP	C4-N9-C8	2.58	108.45	105.74
17	X	501	ADP	C4-N9-C8	2.57	108.44	105.74
17	R	501	ADP	C5-N7-C8	2.54	107.44	103.45
17	U	501	ADP	C3'-C2'-C1'	2.53	106.26	101.46
17	T	501	ADP	C4-N9-C8	2.53	108.40	105.74
17	R	501	ADP	C3'-C2'-C1'	2.52	106.23	101.46
17	V	501	ADP	C5-N7-C8	2.52	107.41	103.45
17	X	501	ADP	C5-N7-C8	2.50	107.39	103.45
17	U	501	ADP	C5-N7-C8	2.47	107.34	103.45
17	T	501	ADP	C5-N7-C8	2.47	107.34	103.45
17	W	501	ADP	C5-N7-C8	2.45	107.31	103.45
17	R	501	ADP	O4'-C1'-N9	2.45	112.79	108.09
17	W	501	ADP	C4-N9-C8	2.42	108.28	105.74
17	T	501	ADP	C3'-C2'-C1'	2.42	106.04	101.46
17	Y	501	ADP	C3'-C2'-C1'	2.27	105.76	101.46
17	M	1601	ADP	C3'-C2'-C1'	2.27	105.76	101.46
17	R	501	ADP	O2'-C2'-C3'	-2.25	104.60	111.82
17	X	501	ADP	C3'-C2'-C1'	2.24	105.70	101.46
17	V	501	ADP	C3'-C2'-C1'	2.21	105.64	101.46
17	R	501	ADP	C6-C5-N7	2.13	136.20	132.09
17	M	1601	ADP	C6-C5-N7	2.13	136.19	132.09
17	W	501	ADP	C6-C5-N7	2.09	136.12	132.09
17	W	501	ADP	C3'-C2'-C1'	2.04	105.32	101.46
17	R	501	ADP	C4-N9-C8	2.04	107.88	105.74
17	Y	501	ADP	N9-C8-N7	-2.03	111.05	113.94
17	M	1601	ADP	N9-C8-N7	-2.02	111.07	113.94
17	V	501	ADP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	U	501	ADP	C5'-O5'-PA-O3A
17	V	501	ADP	C5'-O5'-PA-O1A
17	V	501	ADP	C5'-O5'-PA-O2A
17	V	501	ADP	C5'-O5'-PA-O3A
17	W	501	ADP	C5'-O5'-PA-O1A
17	X	501	ADP	C5'-O5'-PA-O1A
17	X	501	ADP	C5'-O5'-PA-O2A
17	X	501	ADP	C5'-O5'-PA-O3A
17	Y	501	ADP	C5'-O5'-PA-O1A
17	Y	501	ADP	C5'-O5'-PA-O2A
17	Y	501	ADP	C5'-O5'-PA-O3A
17	T	501	ADP	C5'-O5'-PA-O3A
17	M	1601	ADP	PB-O3A-PA-O5'
17	M	1601	ADP	C5'-O5'-PA-O1A
17	M	1601	ADP	C5'-O5'-PA-O2A
17	M	1601	ADP	C5'-O5'-PA-O3A
17	M	1601	ADP	O4'-C4'-C5'-O5'
17	V	501	ADP	O4'-C4'-C5'-O5'
17	V	501	ADP	C3'-C4'-C5'-O5'
17	M	1601	ADP	C3'-C4'-C5'-O5'
17	U	501	ADP	C5'-O5'-PA-O1A
17	T	501	ADP	C5'-O5'-PA-O1A
17	V	501	ADP	PB-O3A-PA-O1A
17	V	501	ADP	PB-O3A-PA-O2A

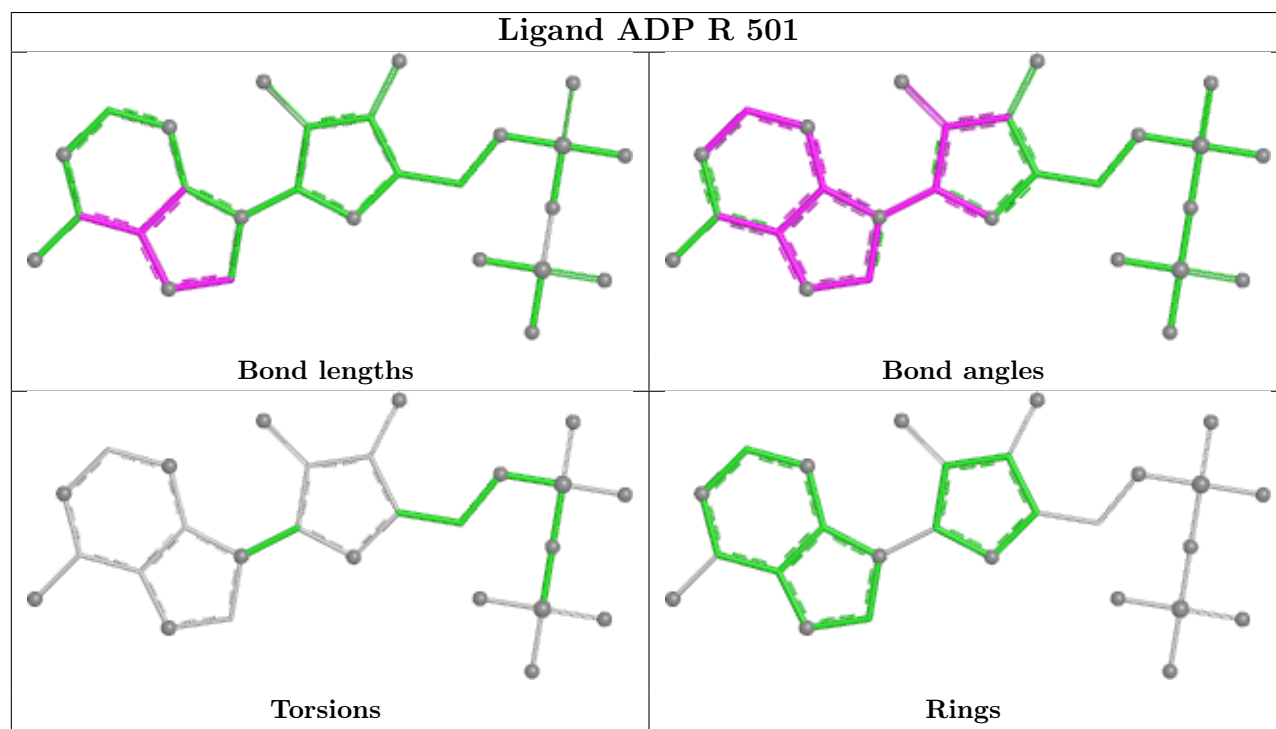
There are no ring outliers.

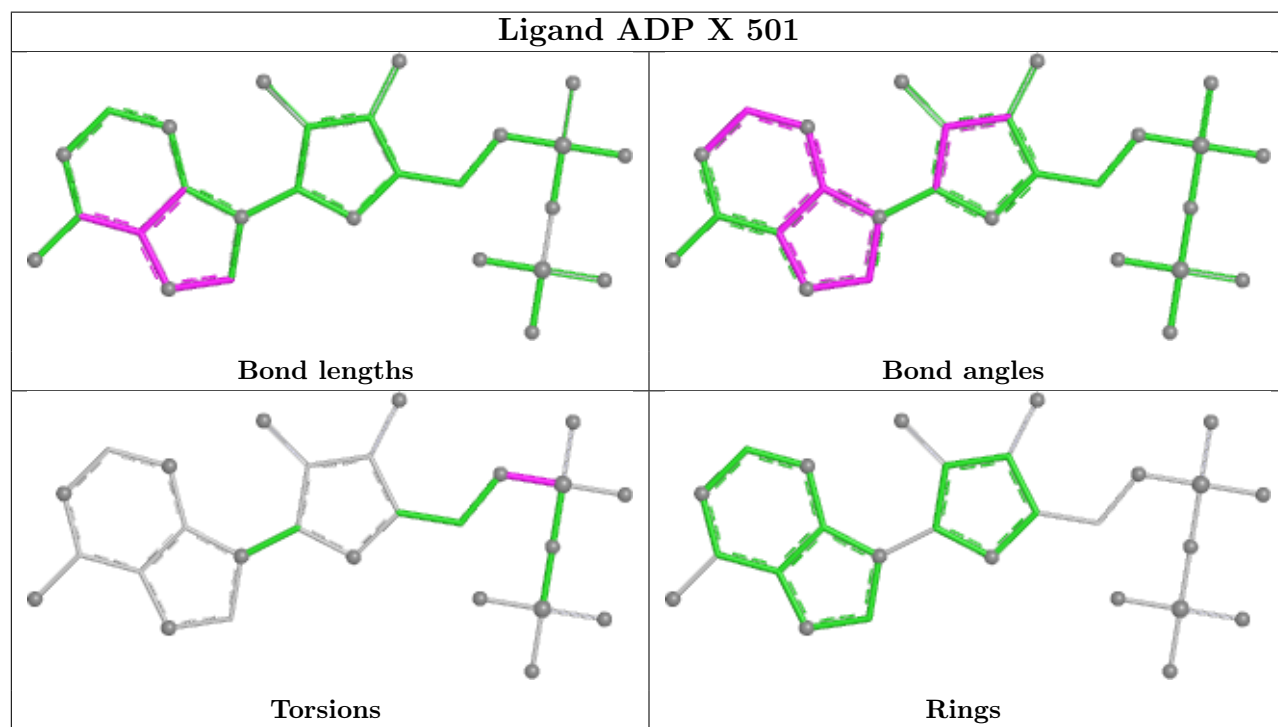
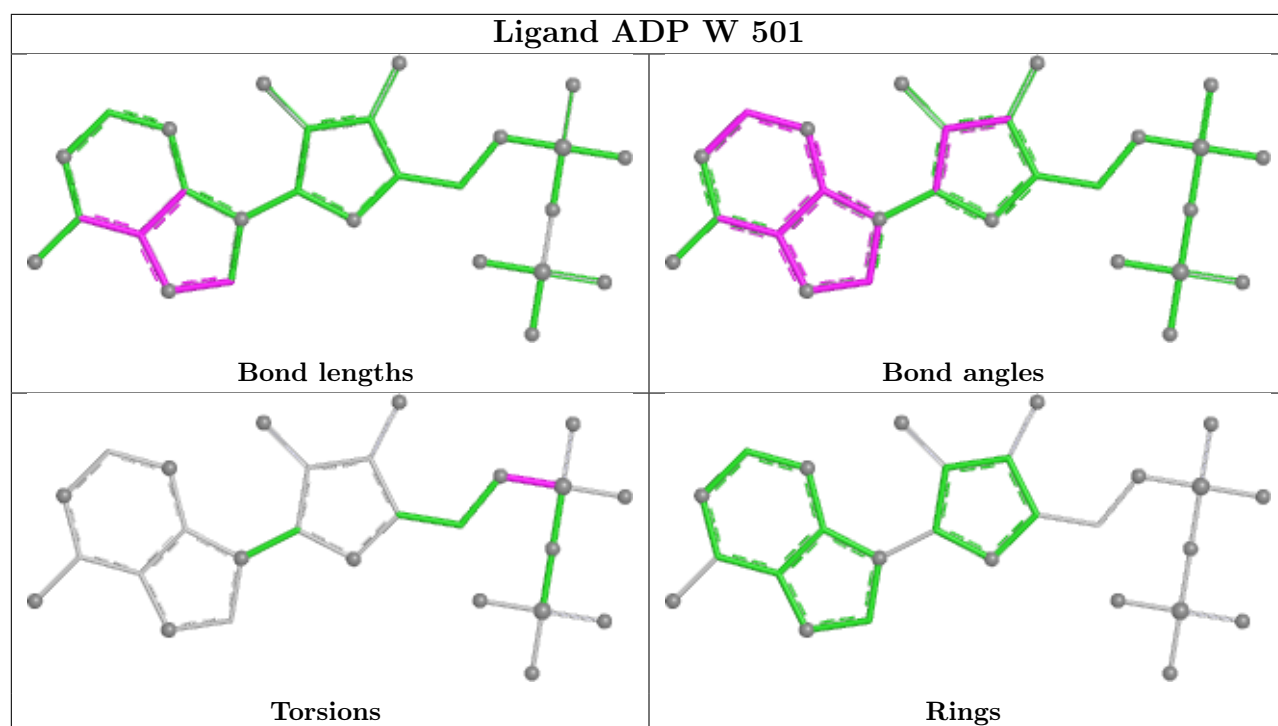
10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	R	501	ADP	5	0
17	W	501	ADP	4	0
17	X	501	ADP	4	0
17	M	1601	ADP	2	0
17	T	501	ADP	4	0
17	V	501	ADP	5	0
18	R	502	BEF	1	0
17	Y	501	ADP	1	0
18	M	1602	BEF	2	0
17	U	501	ADP	2	0

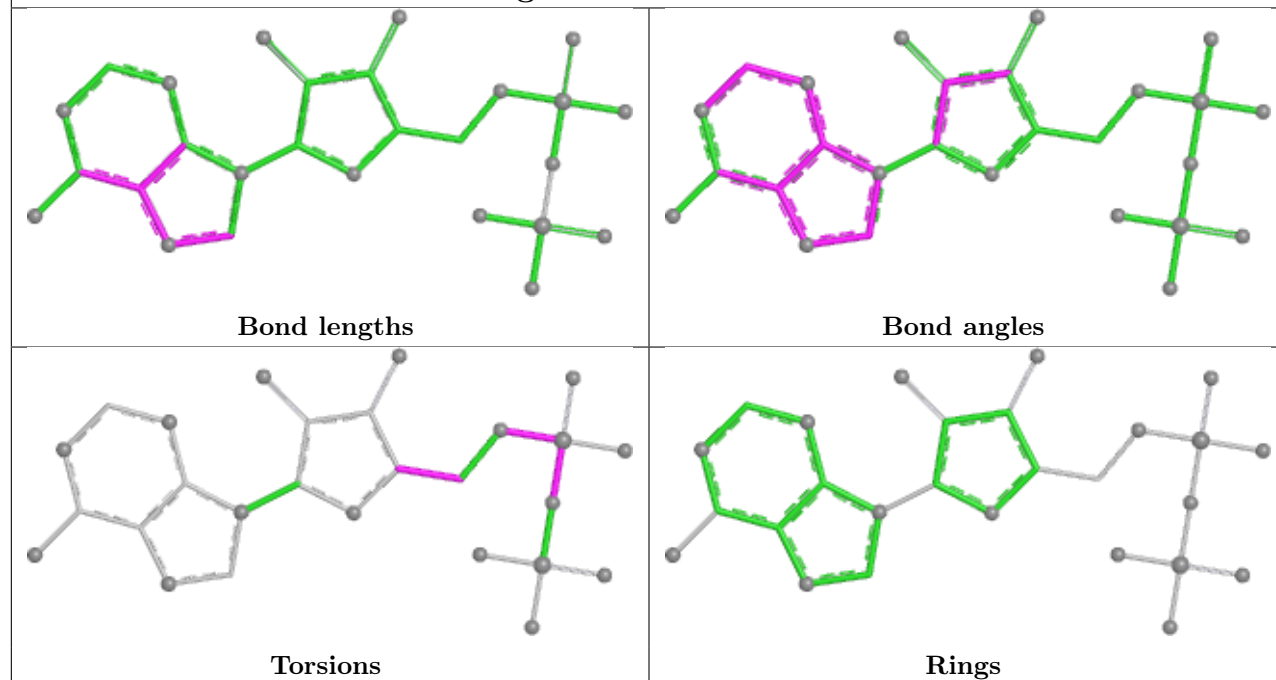
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

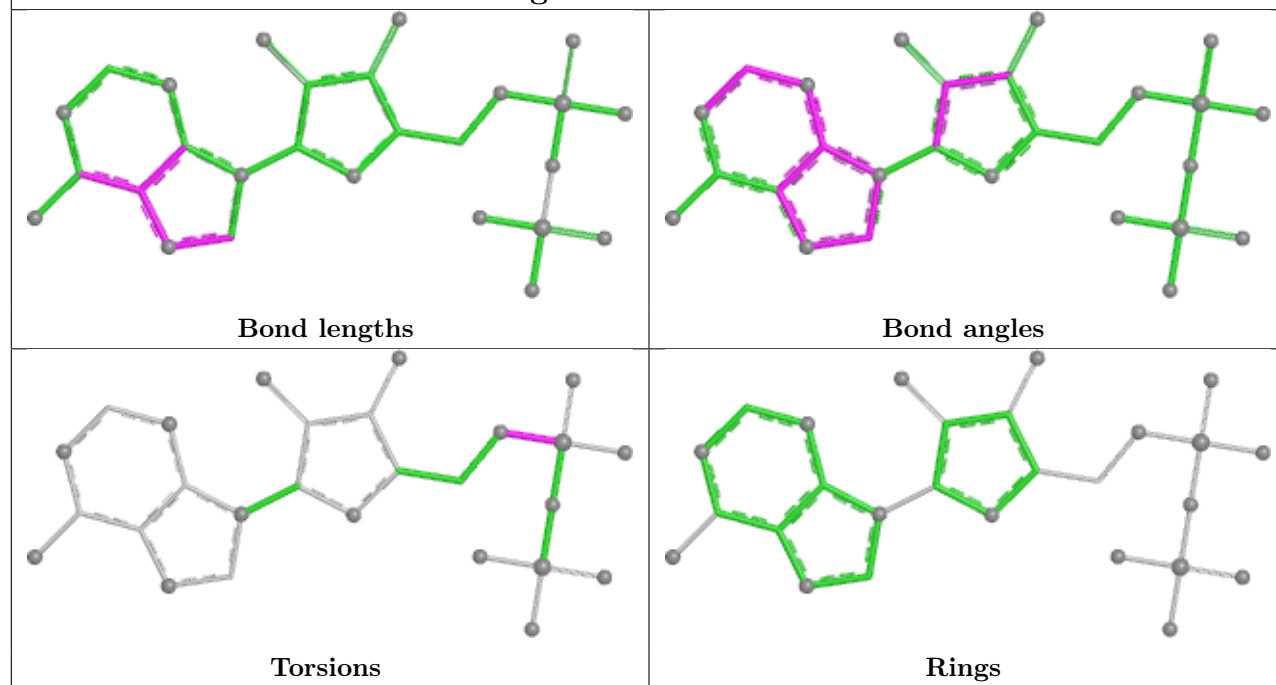


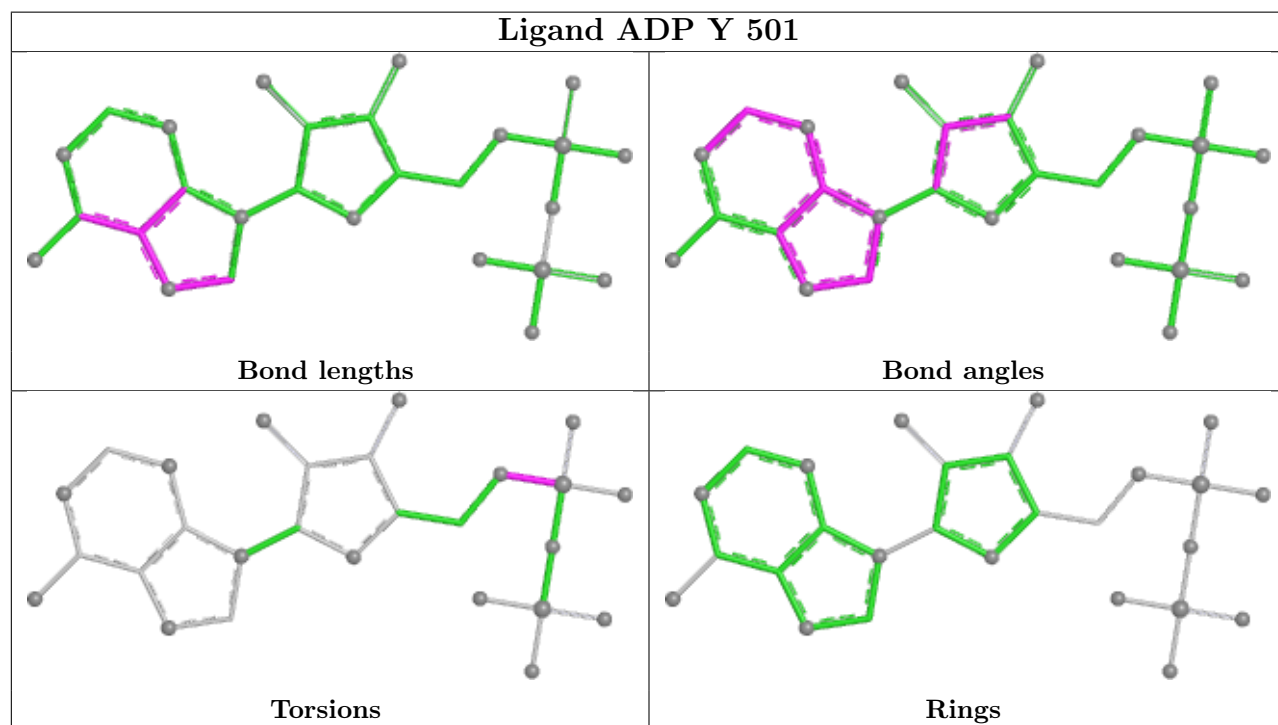
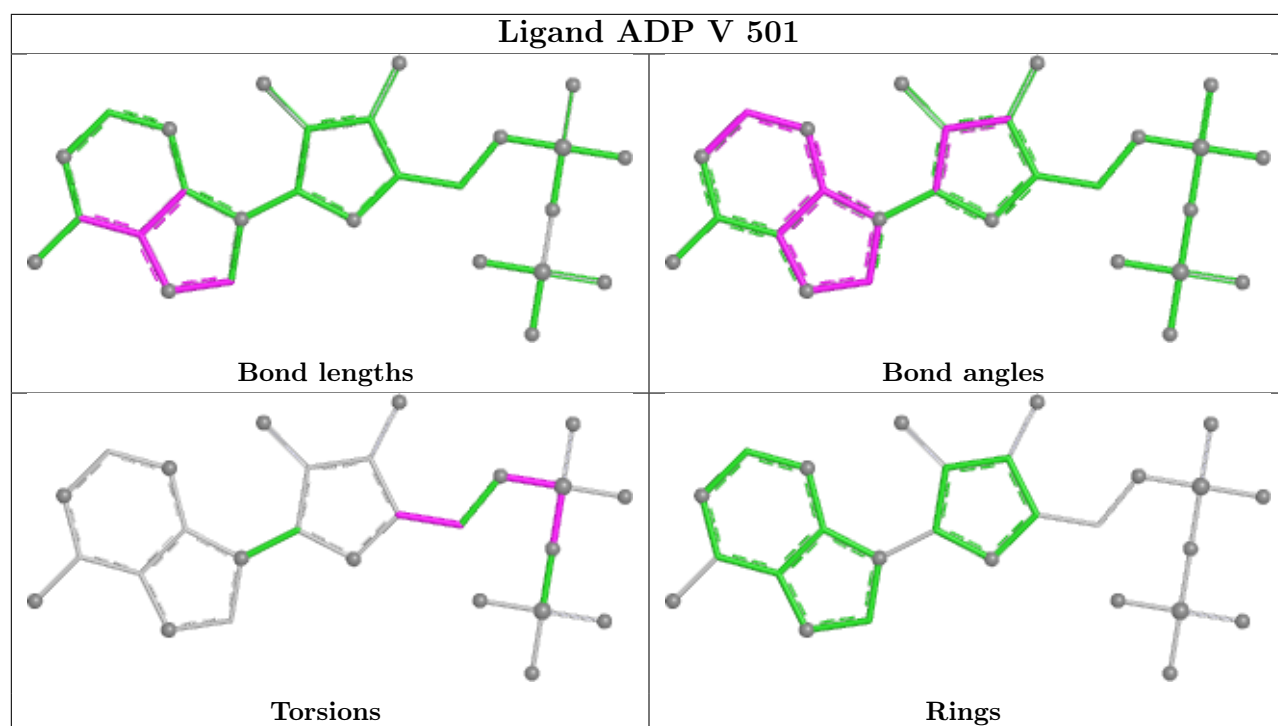


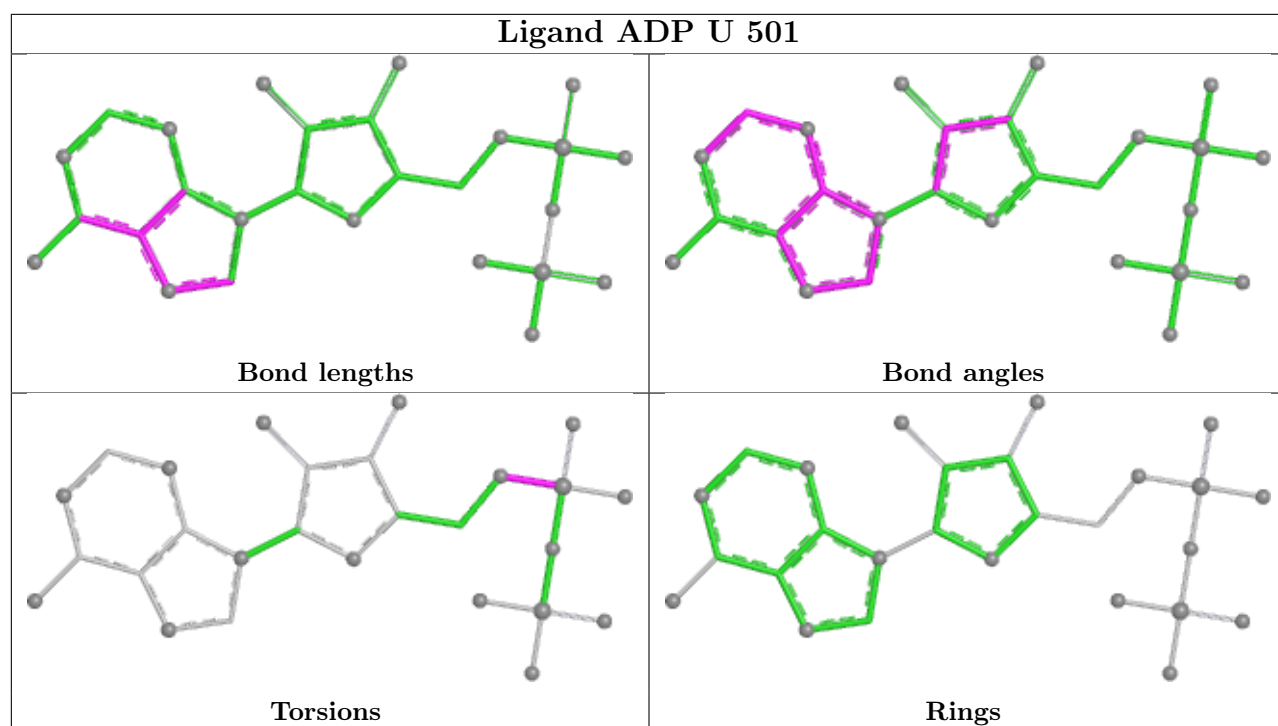
Ligand ADP M 1601



Ligand ADP T 501







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.

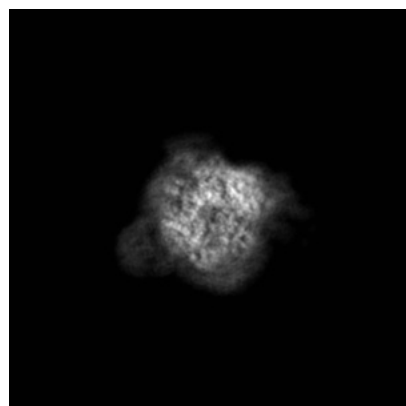
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18769. These allow visual inspection of the internal detail of the map and identification of artifacts.

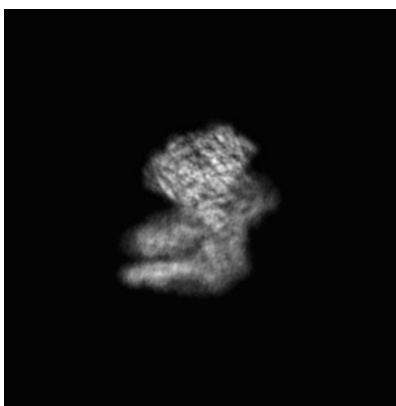
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

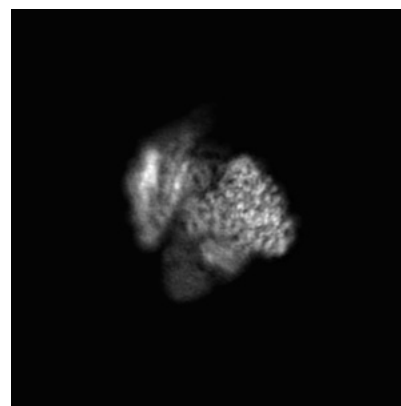
6.1.1 Primary map



X

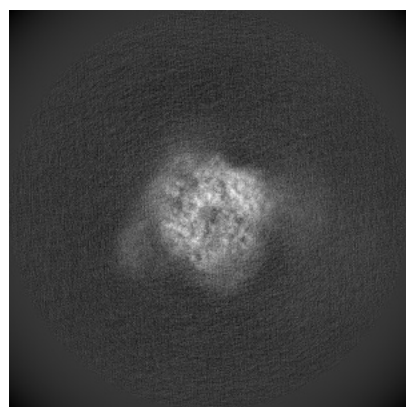


Y

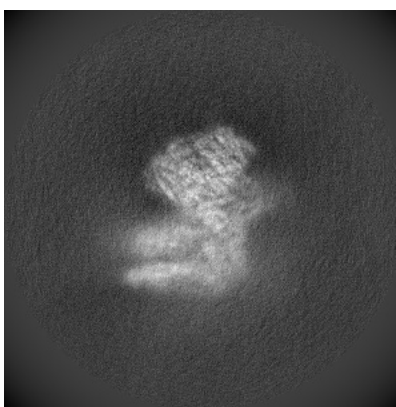


Z

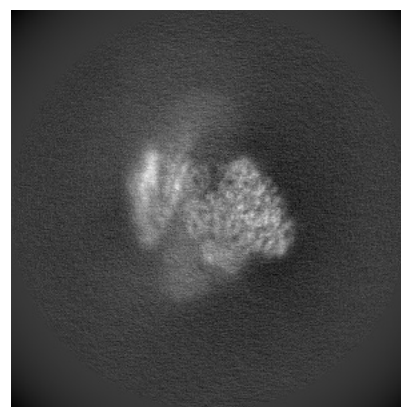
6.1.2 Raw map



X



Y

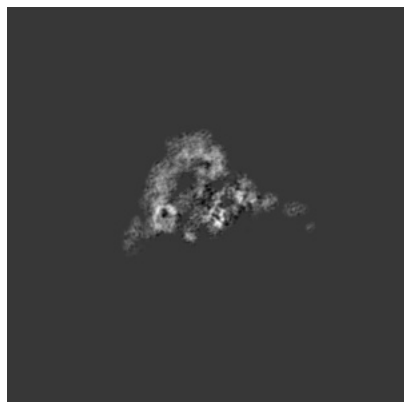


Z

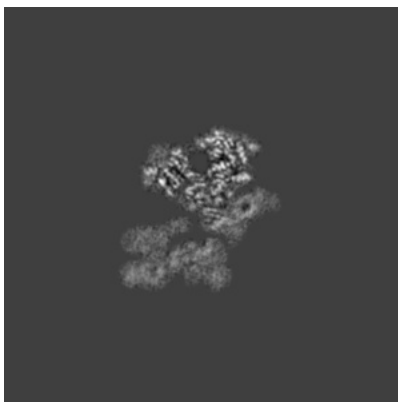
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

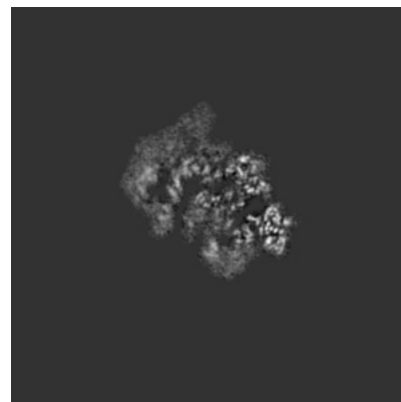
6.2.1 Primary map



X Index: 240

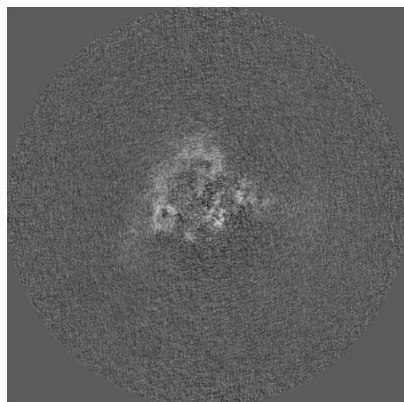


Y Index: 240

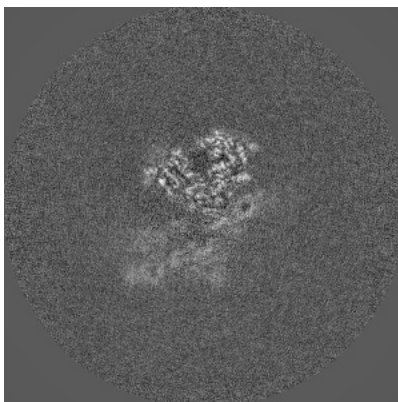


Z Index: 240

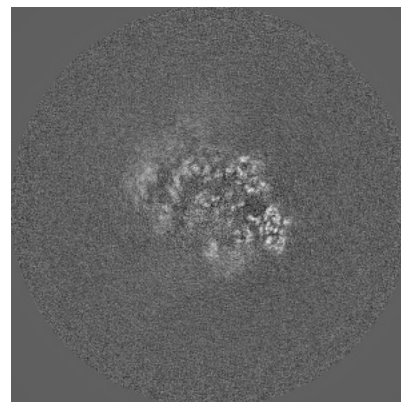
6.2.2 Raw map



X Index: 240



Y Index: 240

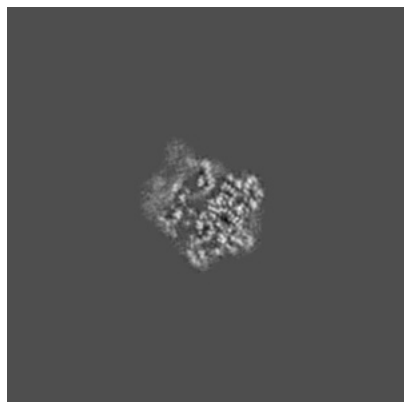


Z Index: 240

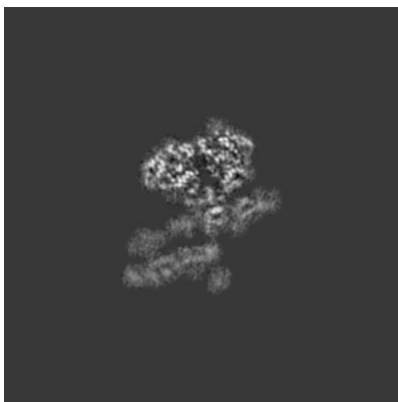
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

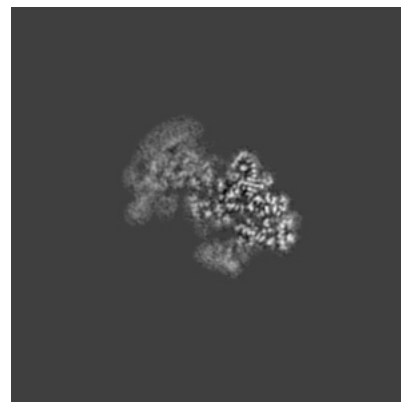
6.3.1 Primary map



X Index: 276

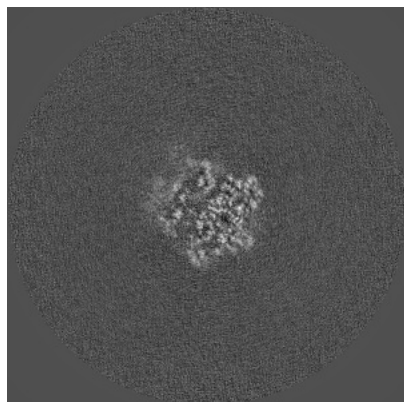


Y Index: 231

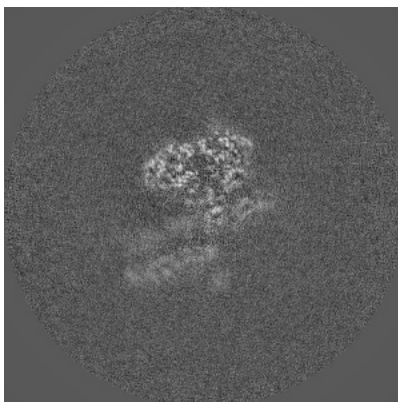


Z Index: 258

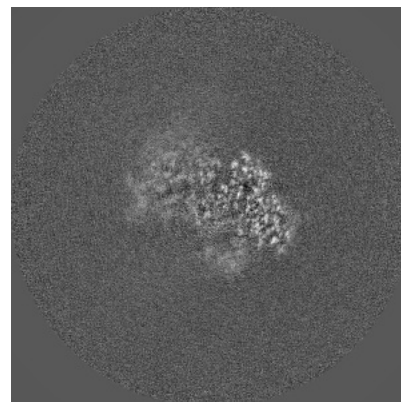
6.3.2 Raw map



X Index: 276



Y Index: 231

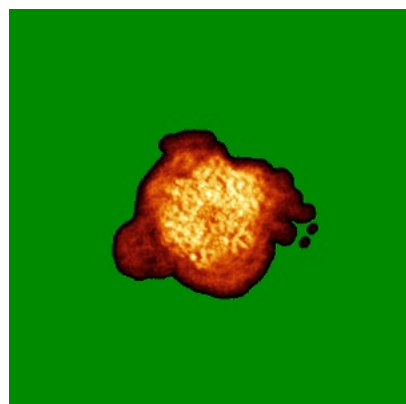


Z Index: 252

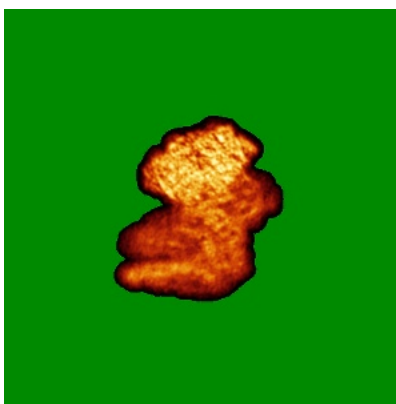
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

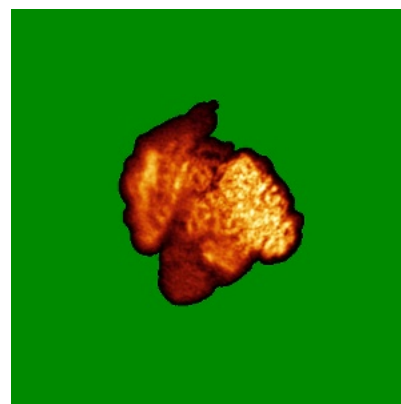
6.4.1 Primary map



X

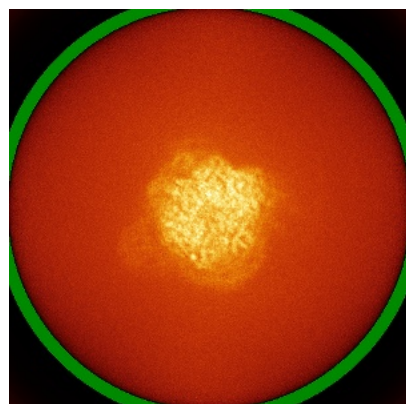


Y

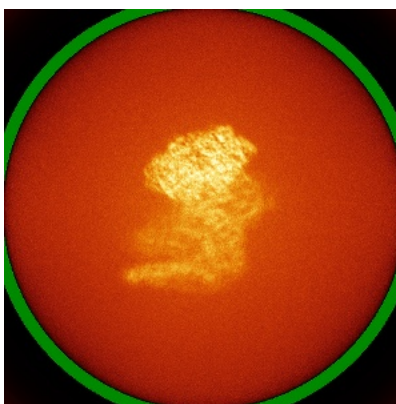


Z

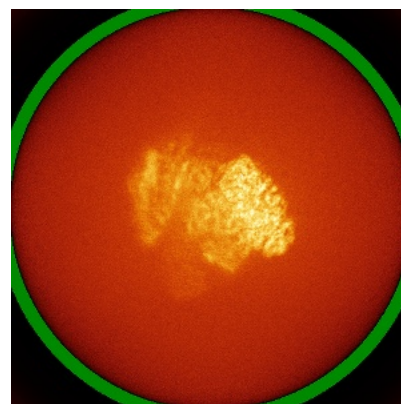
6.4.2 Raw map



X



Y

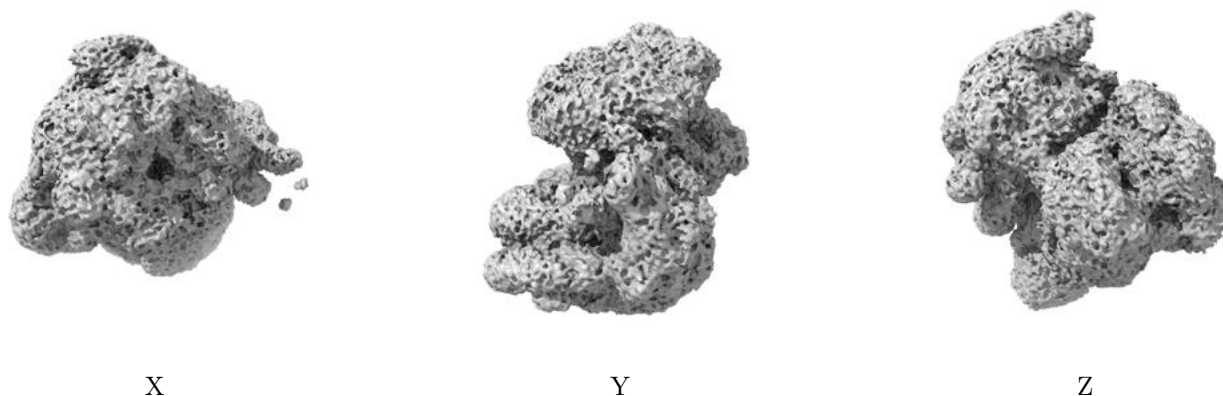


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

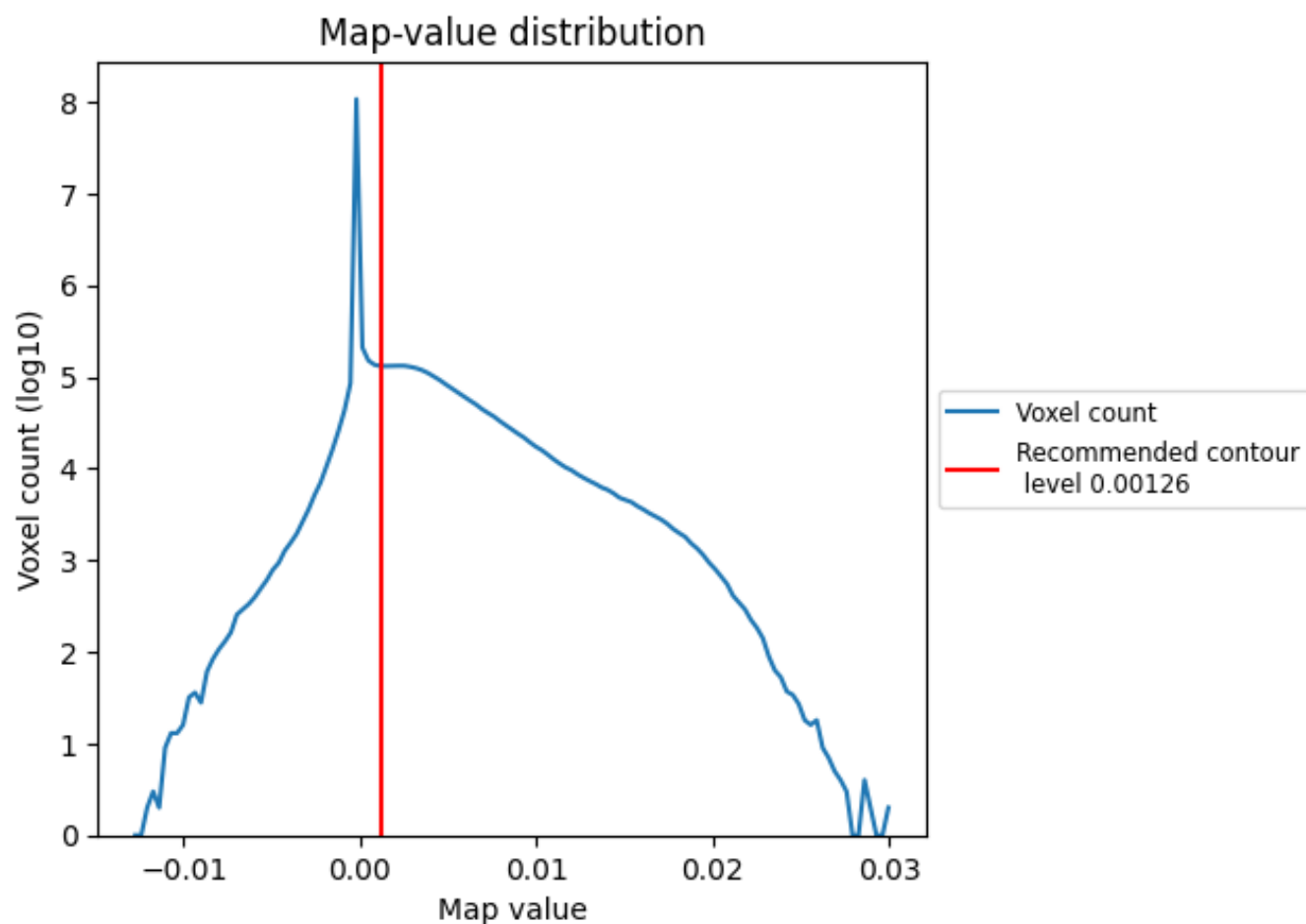
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

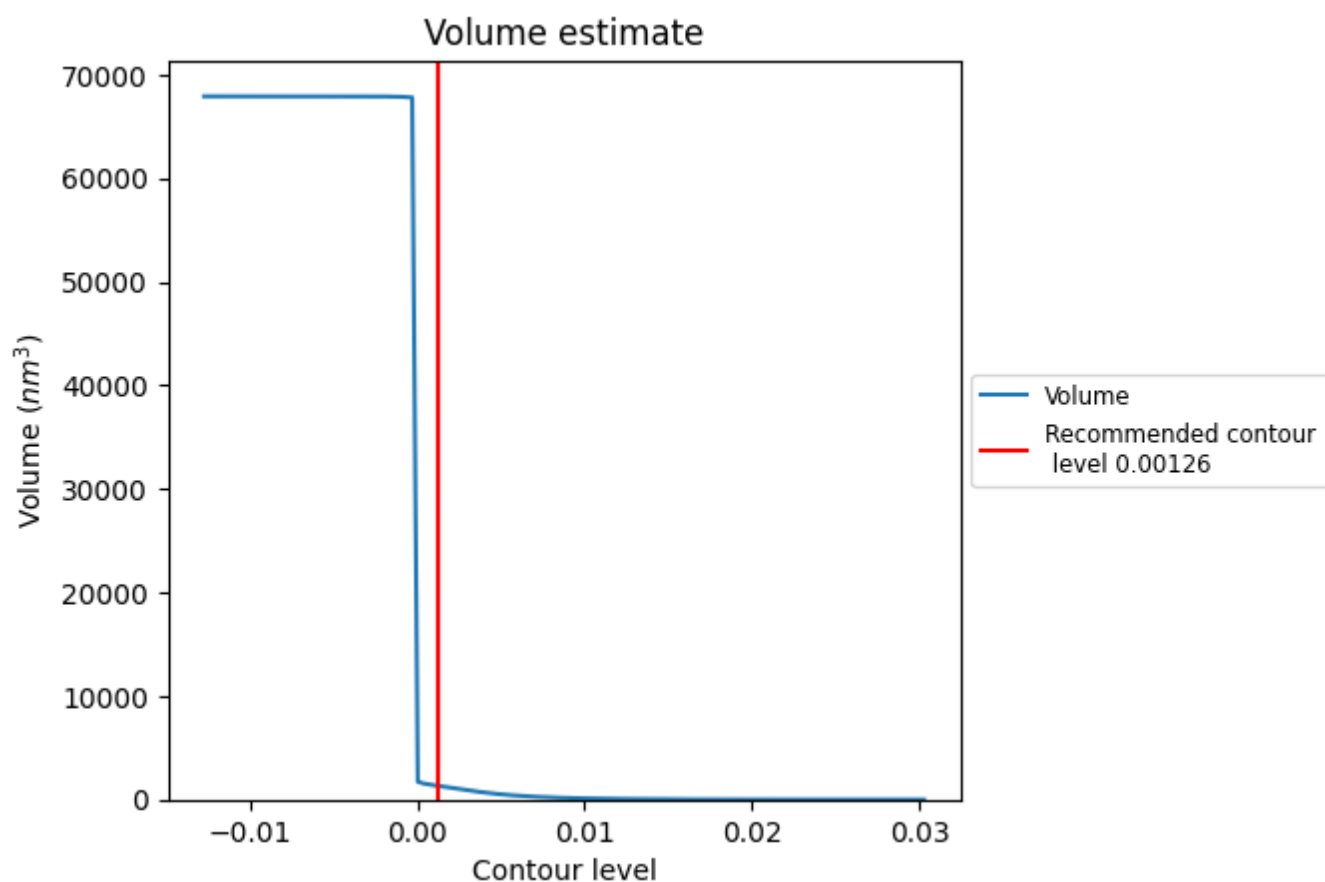
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

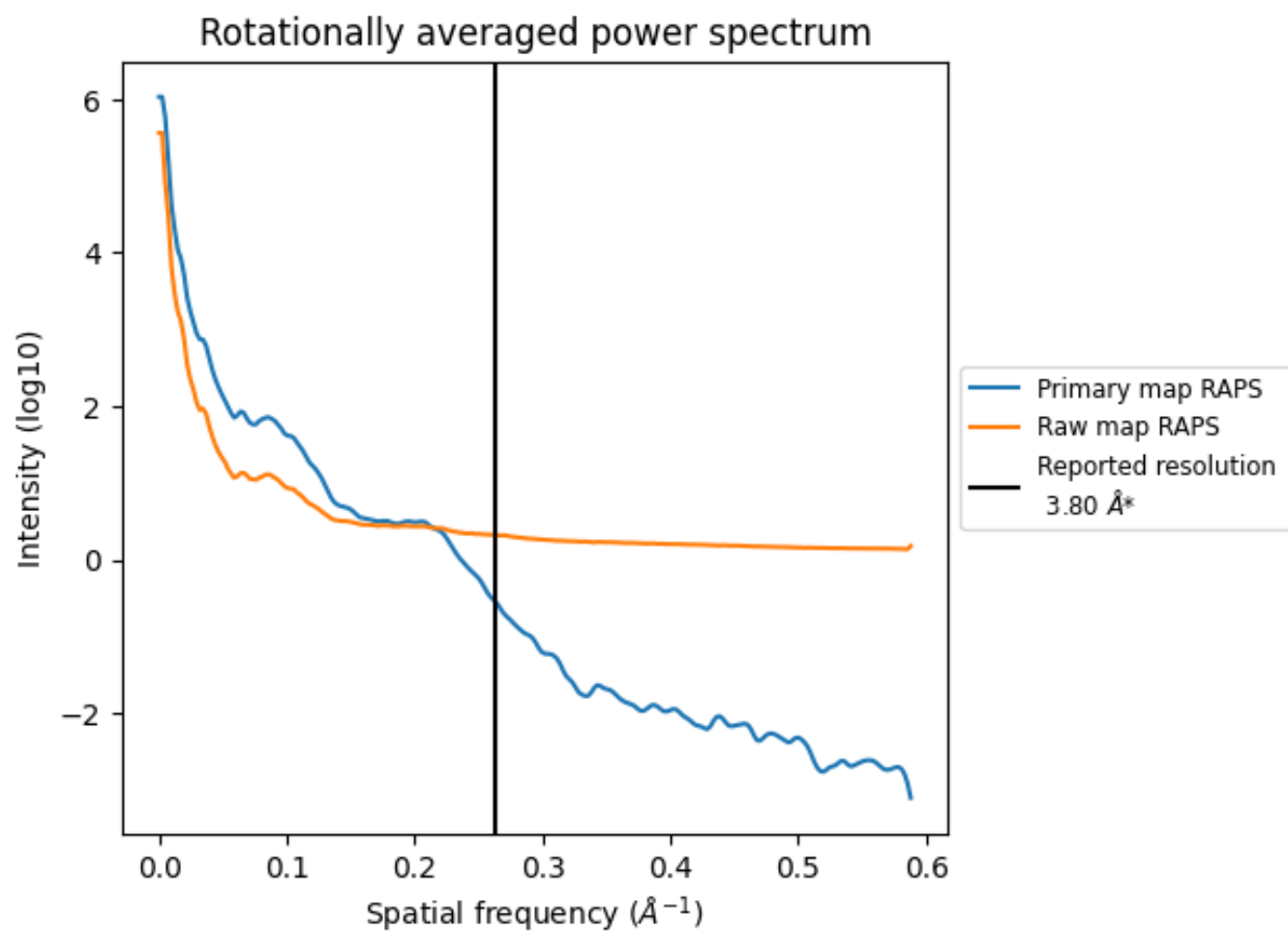
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1321 nm³; this corresponds to an approximate mass of 1193 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 ⓘ

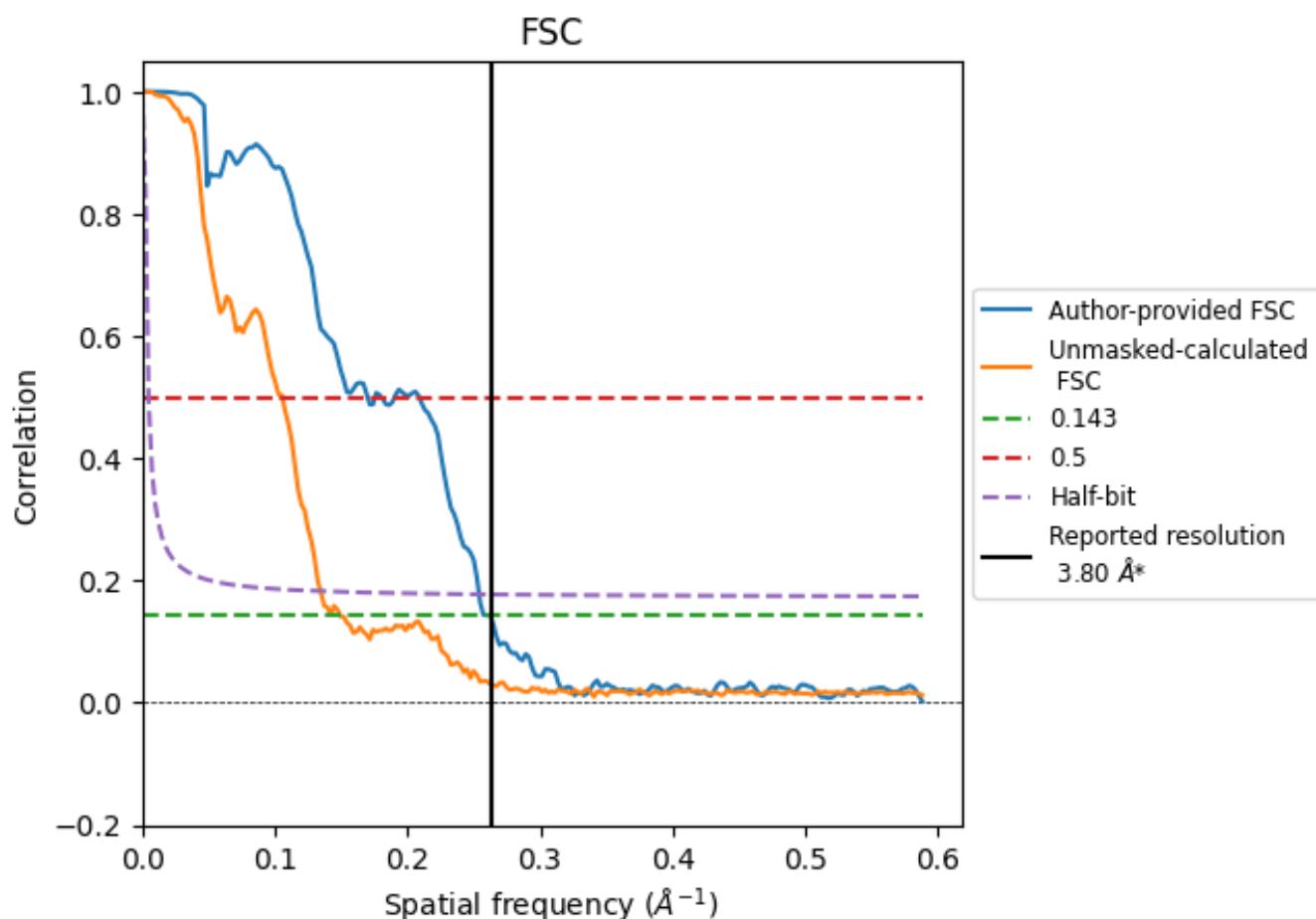


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

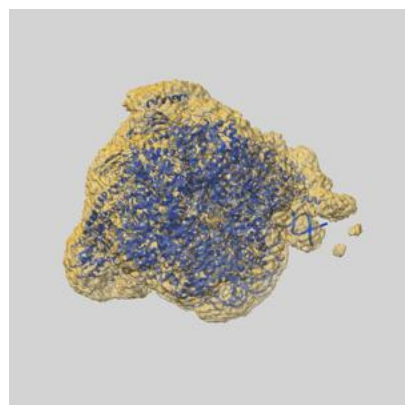
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	5.88	3.94
Unmasked-calculated*	6.71	9.46	7.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.71 differs from the reported value 3.8 by more than 10 %

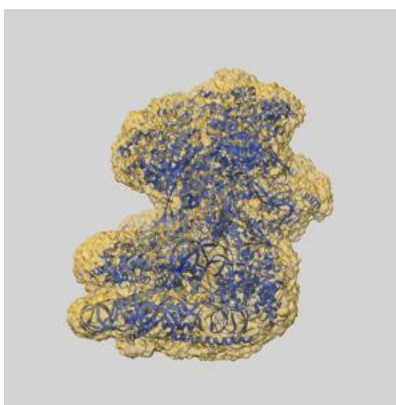
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18769 and PDB model 8QZ0. Per-residue inclusion information can be found in section [3](#) on page [10](#).

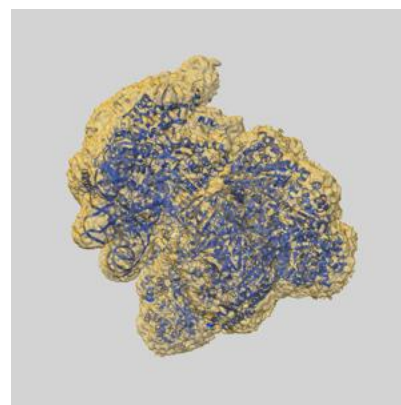
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00126 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](#)



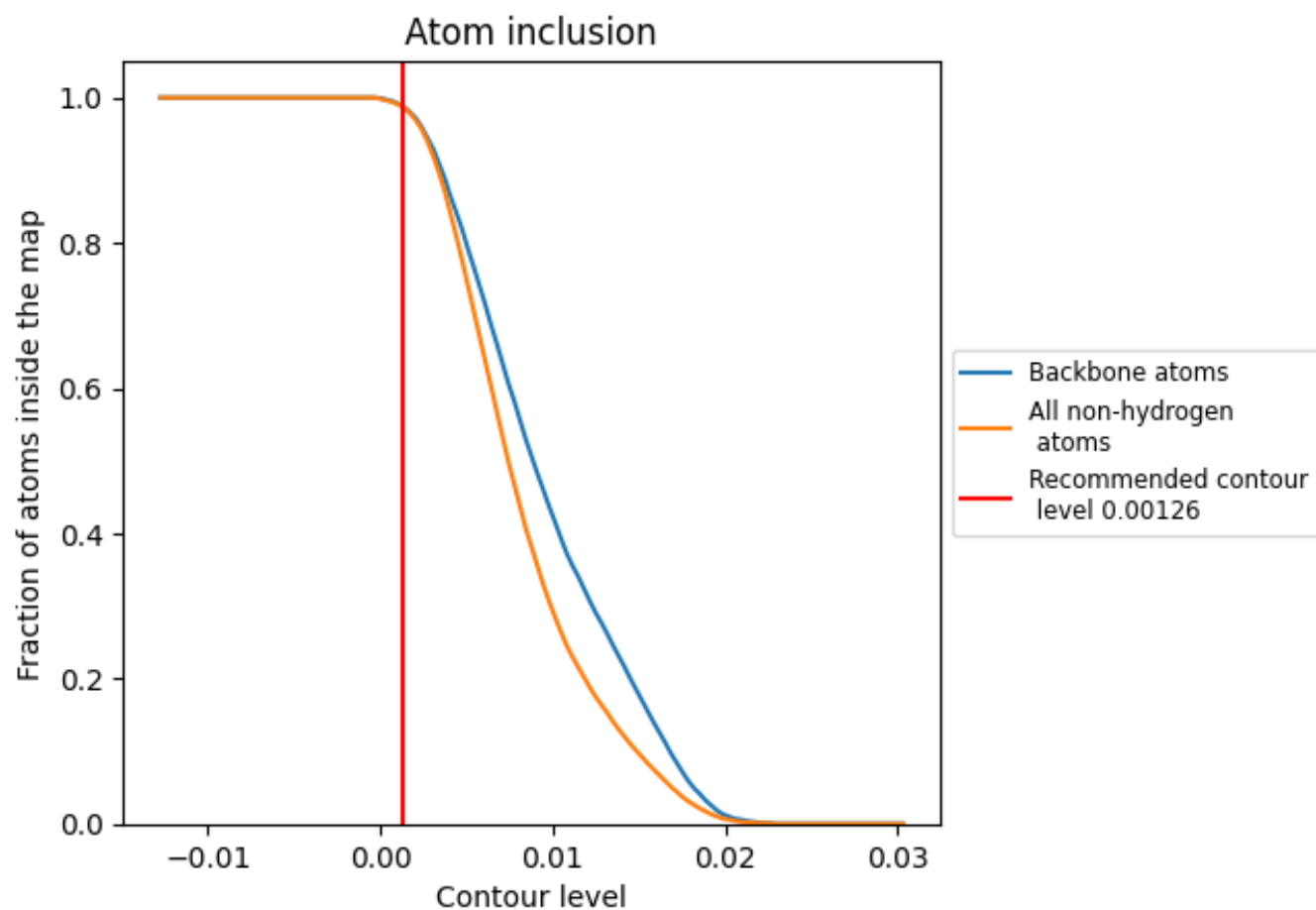
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.00126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.00126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.2930
A	 0.9810	 0.1980
B	 0.9790	 0.2680
C	 0.9910	 0.2440
D	 0.9980	 0.1990
E	 1.0000	 0.2110
G	 1.0000	 0.2280
H	 0.9930	 0.1740
I	 0.9900	 0.1960
J	 0.9880	 0.1900
K	 0.9480	 0.1350
L	 0.9880	 0.1420
M	 0.9880	 0.2750
P	 0.9790	 0.2670
R	 0.9620	 0.1580
S	 0.9060	 0.1520
T	 0.9990	 0.3730
U	 0.9860	 0.3760
V	 1.0000	 0.4200
W	 1.0000	 0.3980
X	 1.0000	 0.3790
Y	 0.9990	 0.3840
Z	 0.9990	 0.2230

