



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 02:27 PM JST

PDB ID : 8ZSG / pdb_00008zsg
EMDB ID : EMD-60414
Title : CryoEM Helical Structure of resting KomBC complex
Authors : Hao, F.; Kai, S.; Eddie, T.; Bin, W.; Min, L.
Deposited on : 2024-06-05
Resolution : 3.66 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:

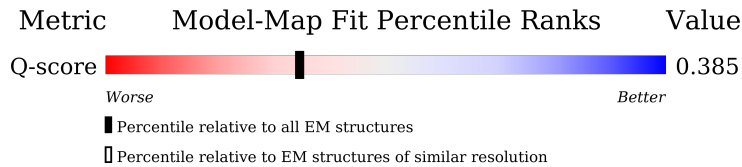
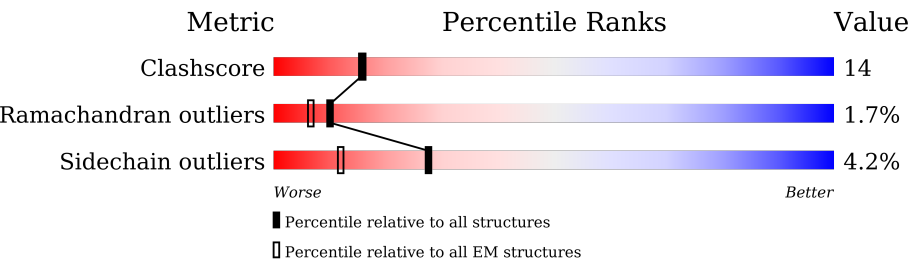
EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 3.66 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11491 (3.16 - 4.16)

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	264	<div>81%15%..</div>
1	B	264	<div>78%19%..</div>
1	C	264	<div>82%17%. </div>
1	D	264	<div>78%20%. </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	264	
1	L	264	
1	O	264	
1	P	264	
1	R	264	
1	T	264	
1	b	264	
1	f	264	
2	E	184	
2	F	184	
2	G	184	
2	H	184	
2	I	184	
2	J	184	
2	M	184	
2	N	184	
2	V	184	
2	X	184	
2	Z	184	
2	d	184	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43668 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 KomC, SIR2 domain protein, NADase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	T	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	b	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	f	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	A	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	C	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	K	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	O	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	B	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	D	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	L	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
1	P	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		

- Molecule 2 is a protein called KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	184	Total	C	N	O	S	0	0
			1473	946	249	272	6		
2	X	184	Total	C	N	O	S	0	0
			1473	946	249	272	6		

Continued on next page...

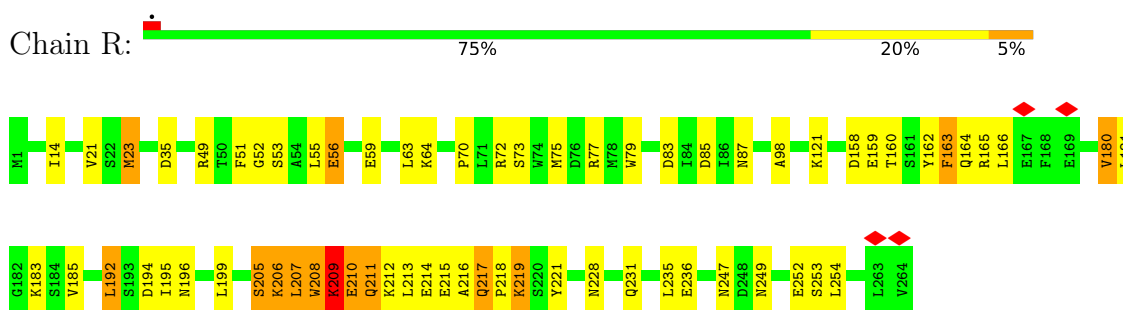
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	d	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	E	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	G	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	I	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	M	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	F	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	H	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	J	184	Total 1473	C 946	N 249	O 272	S 6	0	0
2	N	184	Total 1473	C 946	N 249	O 272	S 6	0	0

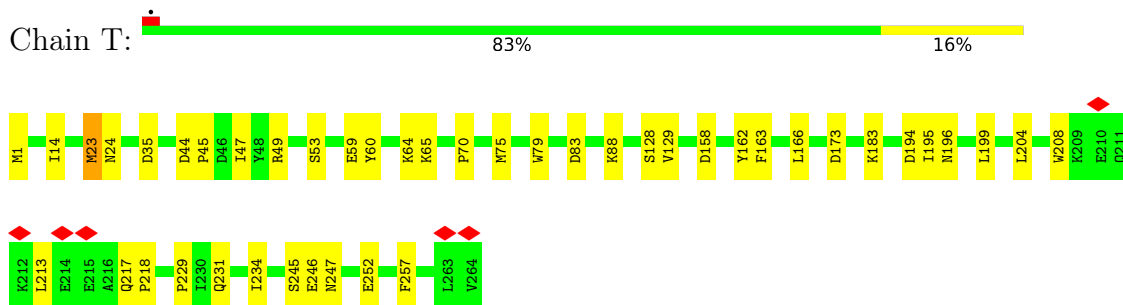
3 Residue-property plots

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.

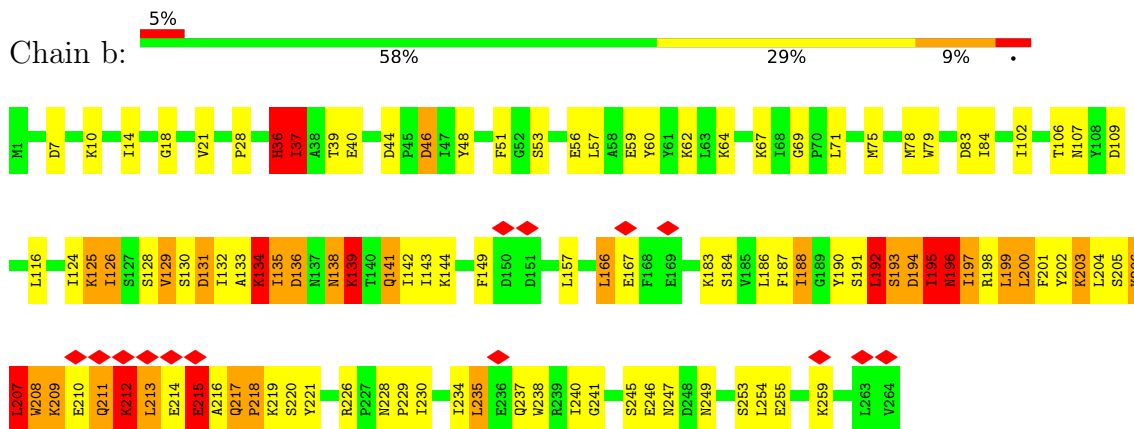
- Molecule 1: KomC, SIR2 domain protein, NADase



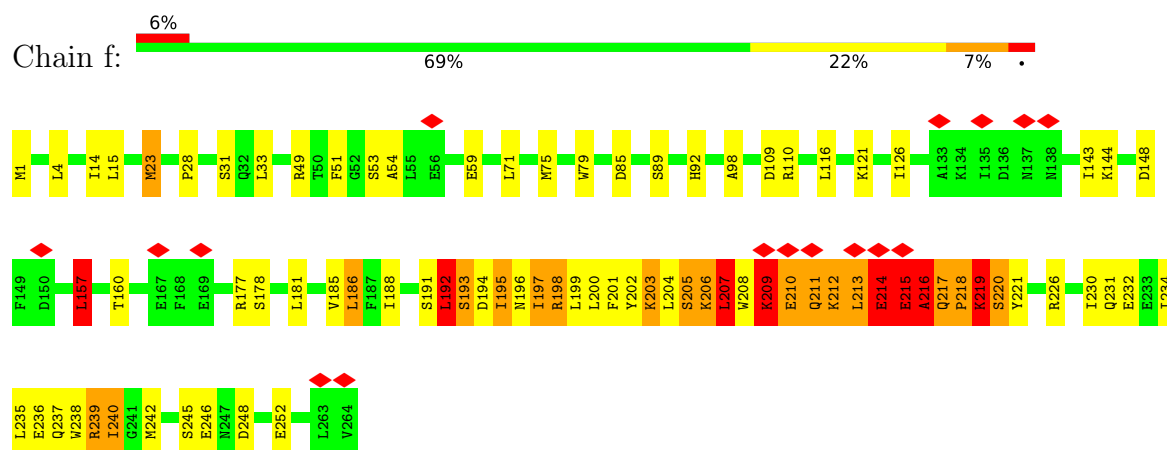
- Molecule 1: KomC, SIR2 domain protein, NADase



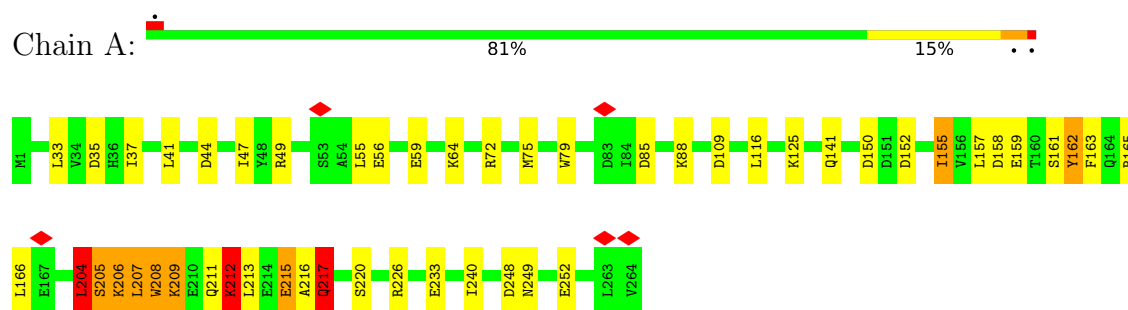
- Molecule 1: KomC, SIR2 domain protein, NADase



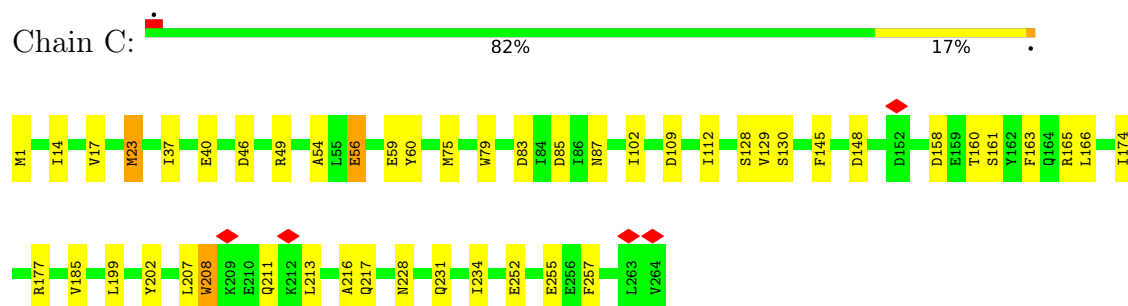
- Molecule 1: KomC, SIR2 domain protein, NADase



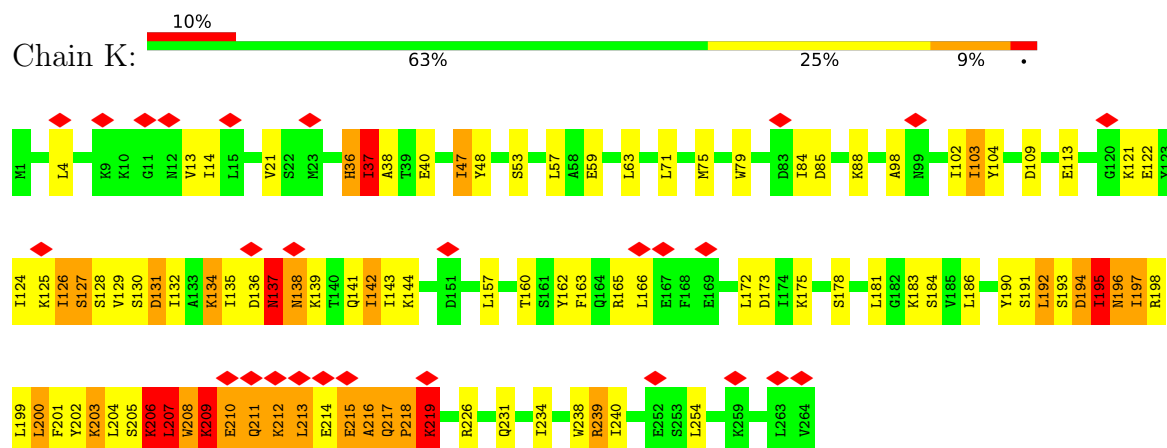
- Molecule 1: KomC, SIR2 domain protein, NADase



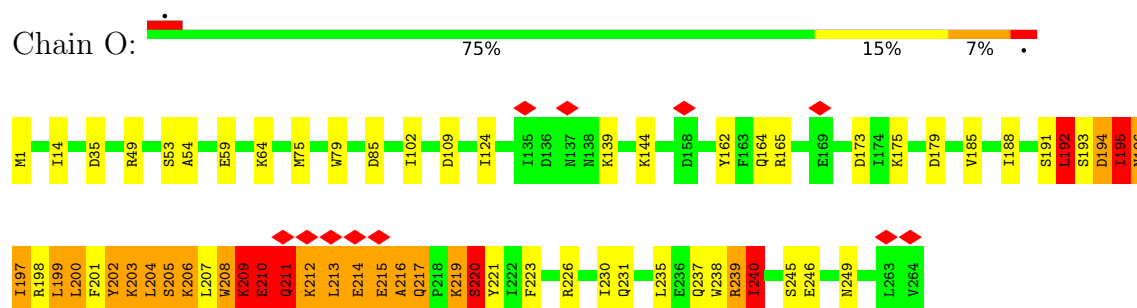
- Molecule 1: KomC, SIR2 domain protein, NADase



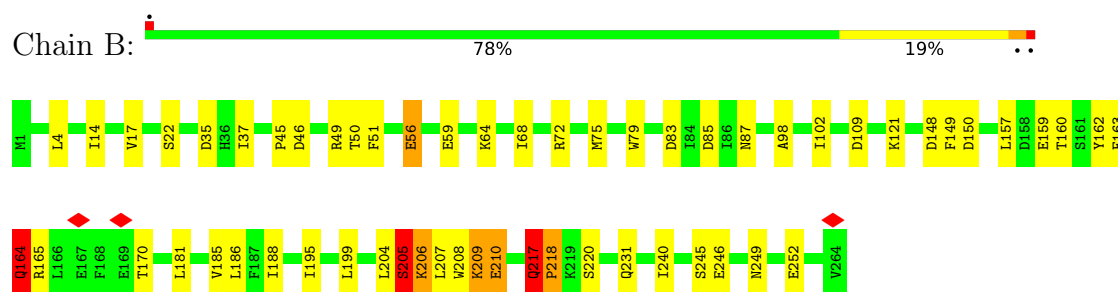
- Molecule 1: KomC, SIR2 domain protein, NADase



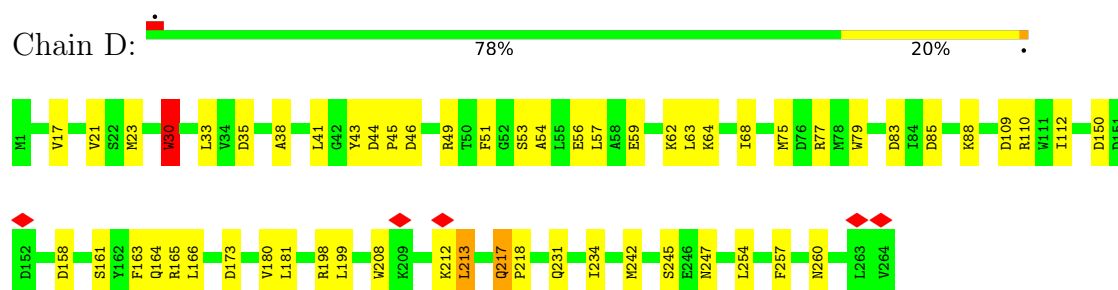
- Molecule 1: KomC, SIR2 domain protein, NADase



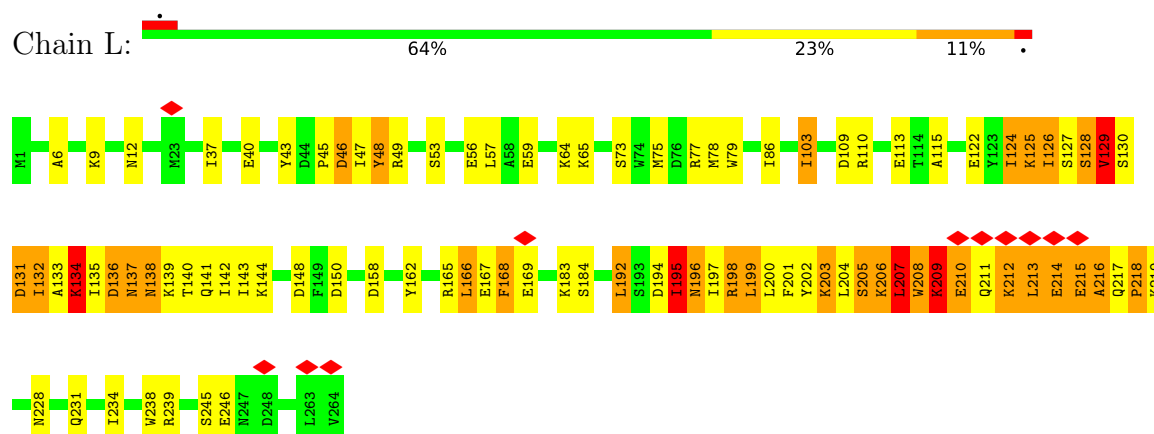
- Molecule 1: KomC, SIR2 domain protein, NADase



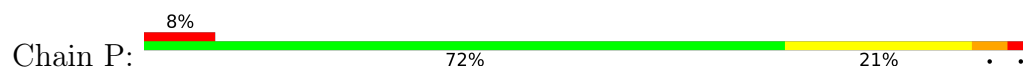
- Molecule 1: KomC, SIR2 domain protein, NADase

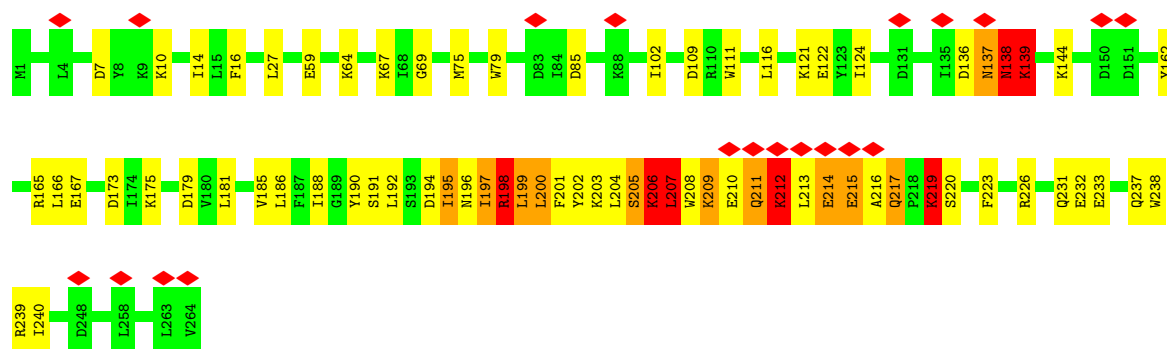


- Molecule 1: KomC, SIR2 domain protein, NADase

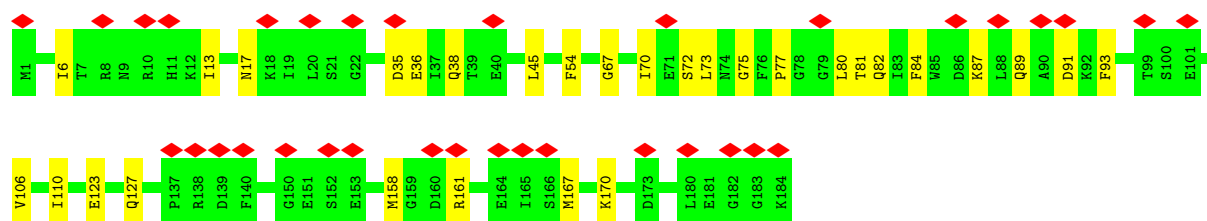
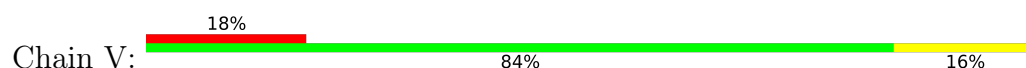


- Molecule 1: KomC, SIR2 domain protein, NADase

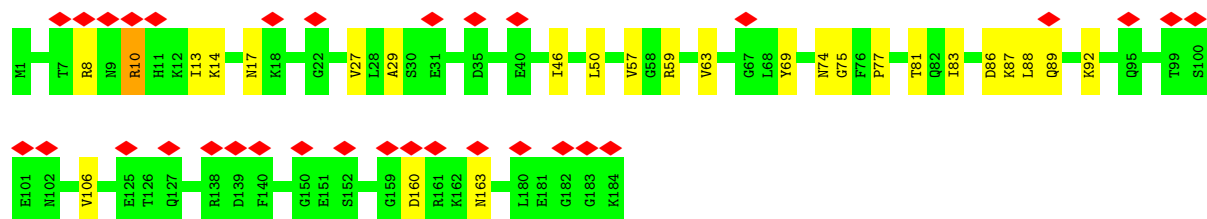
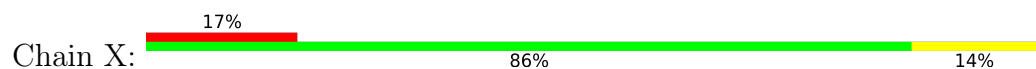




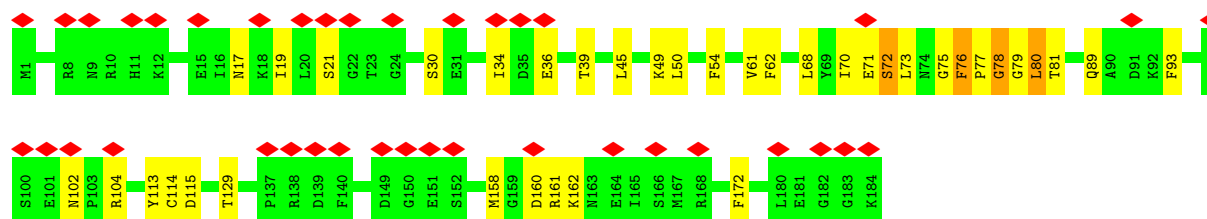
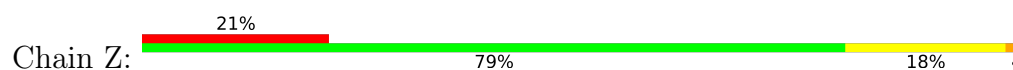
- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase



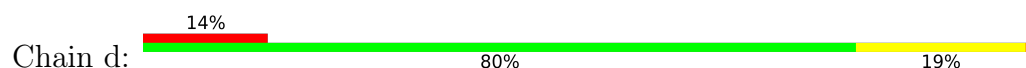
- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase

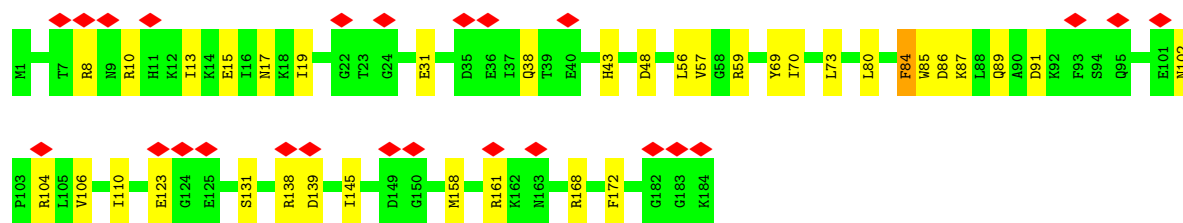


- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase

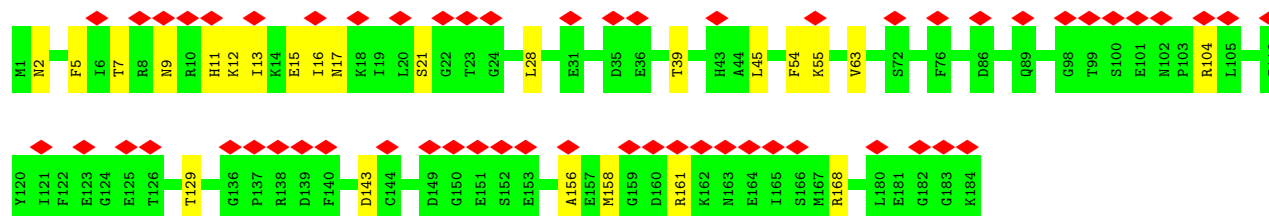
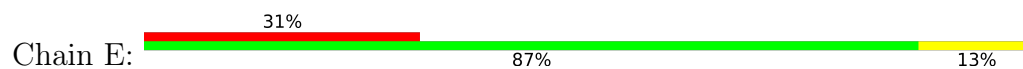


- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase

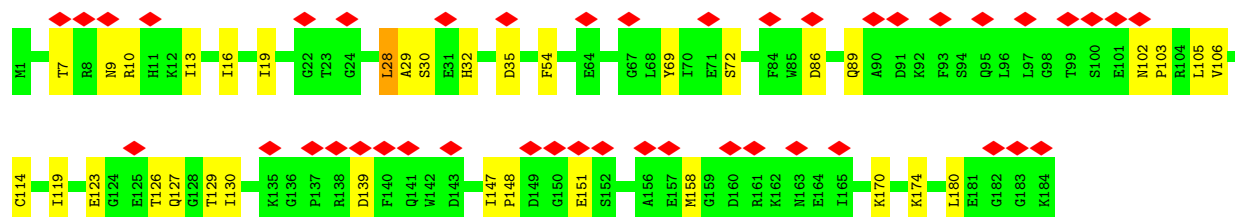
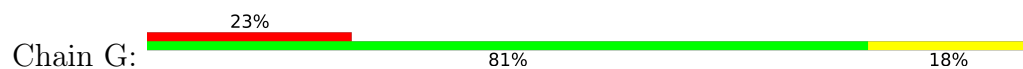




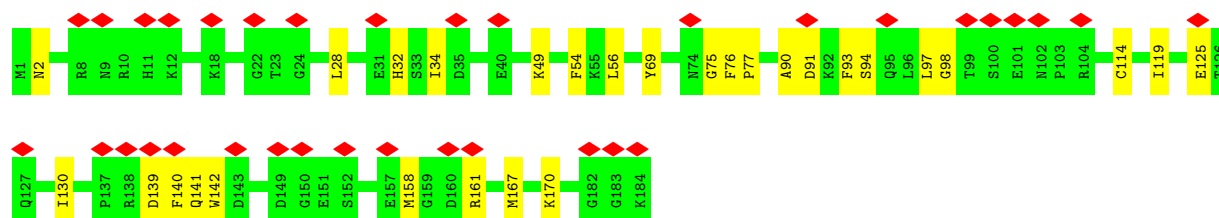
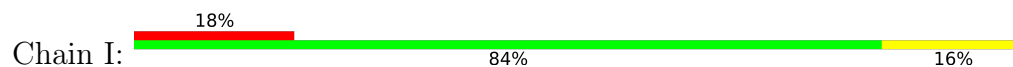
- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase



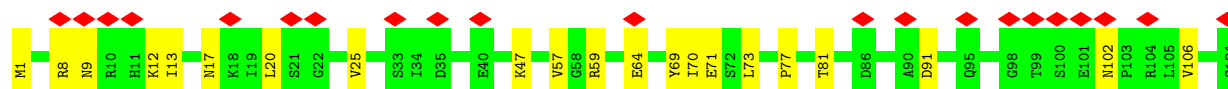
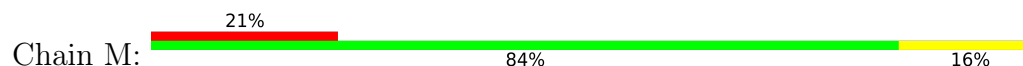
- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase

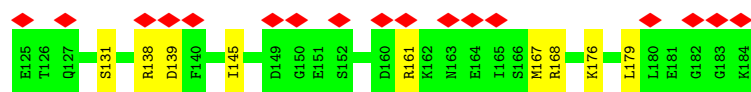


- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase

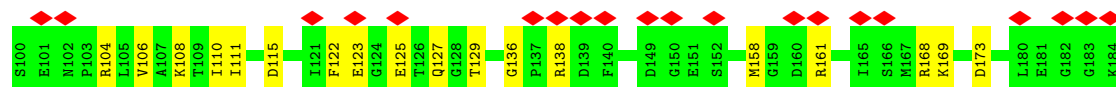
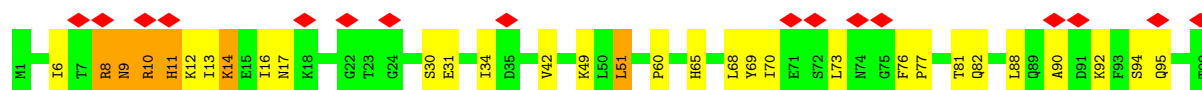
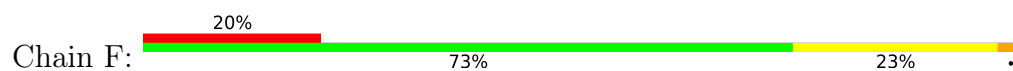


- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase

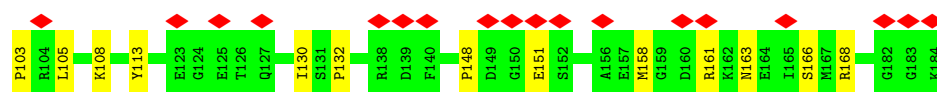
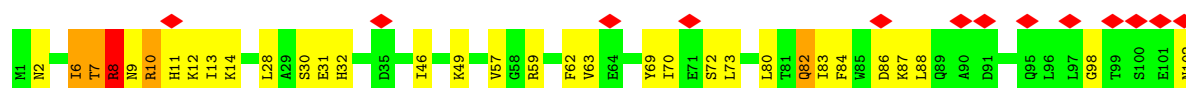
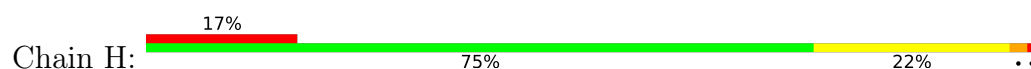




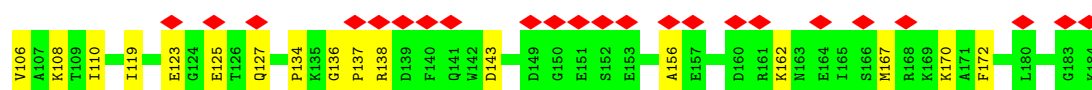
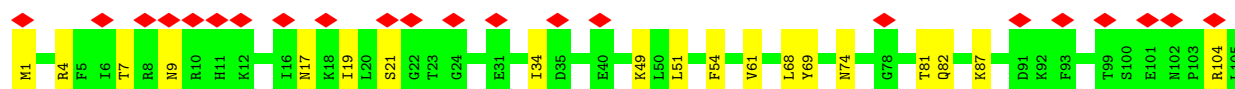
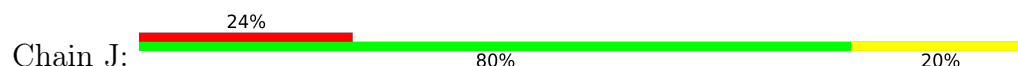
- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase



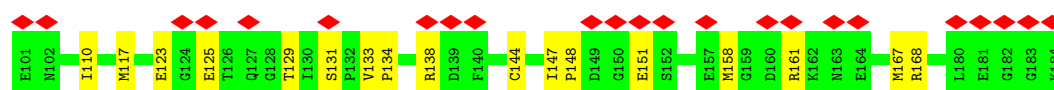
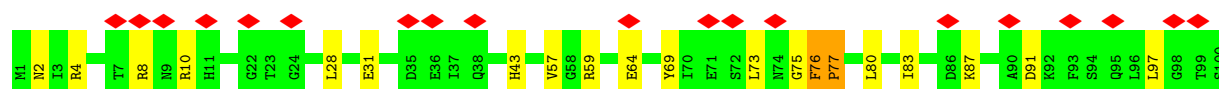
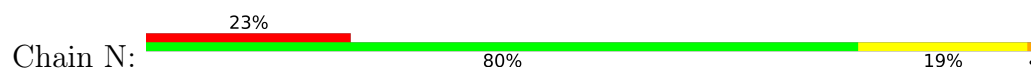
- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase



- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase



- Molecule 2: KomB, HAM-like protein, non-canonical purine NTP pyrophosphatase



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=68.32°, rise=47.11 Å, axial sym=C1	Depositor
Number of segments used	3	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.821	Depositor
Minimum map value	-0.333	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.47	1/2218 (0.0%)	0.65	1/2997 (0.0%)
1	B	0.48	1/2218 (0.0%)	0.66	2/2997 (0.1%)
1	C	0.37	0/2218	0.67	2/2997 (0.1%)
1	D	0.36	0/2218	0.70	7/2997 (0.2%)
1	K	0.53	0/2218	0.76	4/2997 (0.1%)
1	L	0.61	1/2218 (0.0%)	0.81	8/2997 (0.3%)
1	O	0.50	1/2218 (0.0%)	0.63	1/2997 (0.0%)
1	P	0.47	0/2218	0.73	3/2997 (0.1%)
1	R	0.49	1/2218 (0.0%)	0.66	2/2997 (0.1%)
1	T	0.33	0/2218	0.66	0/2997
1	b	0.59	0/2218	0.82	7/2997 (0.2%)
1	f	0.49	0/2218	0.67	4/2997 (0.1%)
2	E	0.28	0/1503	0.68	2/2018 (0.1%)
2	F	0.31	0/1503	0.70	3/2018 (0.1%)
2	G	0.22	0/1503	0.60	0/2018
2	H	0.30	0/1503	0.64	1/2018 (0.0%)
2	I	0.30	1/1503 (0.1%)	0.65	0/2018
2	J	0.27	0/1503	0.65	2/2018 (0.1%)
2	M	0.22	0/1503	0.58	0/2018
2	N	0.26	0/1503	0.63	2/2018 (0.1%)
2	V	0.28	0/1503	0.67	1/2018 (0.0%)
2	X	0.27	0/1503	0.66	1/2018 (0.0%)
2	Z	0.26	0/1503	0.65	2/2018 (0.1%)
2	d	0.31	0/1503	0.70	0/2018
All	All	0.41	6/44652 (0.0%)	0.68	55/60180 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	GLN	CA-C	-6.03	1.45	1.52
1	O	202	TYR	CA-C	-5.71	1.45	1.52
2	I	76	PHE	C-N	5.44	1.41	1.34
1	A	162	TYR	CA-C	-5.43	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	217	GLN	CA-C	-5.42	1.46	1.52
1	L	205	SER	CA-C	-5.18	1.46	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	GLN	N-CA-C	-9.07	89.76	109.81
1	P	166	LEU	CA-CB-CG	9.00	147.80	116.30
1	b	212	LYS	N-CA-C	-8.77	99.03	113.50
1	C	208	TRP	N-CA-C	-7.17	103.55	111.36
1	b	36	HIS	CA-C-N	6.82	134.25	121.97
1	b	36	HIS	C-N-CA	6.82	134.25	121.97
1	B	205	SER	N-CA-C	-6.63	103.75	110.97
2	J	82	GLN	CB-CG-CD	6.51	123.67	112.60
1	D	217	GLN	CA-C-N	-6.02	113.75	119.89
1	D	217	GLN	C-N-CA	-6.02	113.75	119.89
1	P	232	GLU	CA-CB-CG	5.99	126.09	114.10
1	P	198	ARG	N-CA-C	-5.96	103.96	111.11
1	f	157	LEU	N-CA-C	-5.95	107.83	114.62
2	Z	102	ASN	CA-C-N	-5.93	114.78	120.83
2	Z	102	ASN	C-N-CA	-5.93	114.78	120.83
1	D	212	LYS	CA-CB-CG	5.91	125.93	114.10
1	D	213	LEU	CA-CB-CG	5.90	136.94	116.30
1	D	30	TRP	N-CA-C	-5.80	105.03	111.36
1	b	53	SER	CA-C-N	5.73	132.48	121.54
1	b	53	SER	C-N-CA	5.73	132.48	121.54
1	D	212	LYS	CB-CG-CD	5.72	124.45	111.30
2	F	51	LEU	CA-CB-CG	5.68	136.18	116.30
2	E	158	MET	CB-CG-SD	5.64	129.62	112.70
1	L	53	SER	CA-C-N	5.62	132.27	121.54
1	L	53	SER	C-N-CA	5.62	132.27	121.54
1	A	204	LEU	N-CA-C	-5.62	104.85	110.97
1	K	53	SER	CA-C-N	5.60	132.24	121.54
1	K	53	SER	C-N-CA	5.60	132.24	121.54
2	H	82	GLN	CA-CB-CG	5.55	125.20	114.10
1	L	169	GLU	CA-CB-CG	5.51	125.13	114.10
2	X	10	ARG	CB-CG-CD	5.45	123.84	111.30
1	f	217	GLN	CA-C-O	-5.43	115.92	120.26
1	b	44	ASP	CB-CA-C	5.38	117.18	109.11
1	R	236	GLU	CA-CB-CG	5.37	124.84	114.10
1	K	47	ILE	CG1-CB-CG2	-5.36	94.61	110.70
1	L	205	SER	N-CA-C	-5.31	105.18	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	217	GLN	O-C-N	5.30	123.97	121.53
1	C	56	GLU	N-CA-C	-5.26	105.46	111.14
2	F	14	LYS	CA-CB-CG	5.26	124.61	114.10
1	K	36	HIS	N-CA-C	-5.25	103.76	110.53
2	E	161	ARG	CA-CB-CG	5.19	124.49	114.10
1	L	46	ASP	CA-C-N	5.17	131.28	121.97
1	L	46	ASP	C-N-CA	5.17	131.28	121.97
2	J	82	GLN	CA-CB-CG	5.15	124.39	114.10
2	F	11	HIS	N-CA-C	-5.14	105.65	112.34
1	b	69	GLY	N-CA-C	5.12	122.78	112.34
1	D	213	LEU	CB-CG-CD1	-5.11	95.37	110.70
1	L	238	TRP	CA-C-N	5.11	129.66	122.46
1	L	238	TRP	C-N-CA	5.11	129.66	122.46
1	R	163	PHE	N-CA-C	-5.10	105.91	111.82
1	f	216	ALA	N-CA-C	-5.09	99.96	110.80
1	O	204	LEU	N-CA-C	-5.07	105.44	110.97
2	N	117	MET	CB-CG-SD	5.06	127.89	112.70
2	N	125	GLU	CA-CB-CG	5.01	124.13	114.10
2	V	82	GLN	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2166	0	2150	57	0
1	B	2166	0	2150	62	0
1	C	2166	0	2150	43	0
1	D	2166	0	2150	43	0
1	K	2166	0	2150	132	0
1	L	2166	0	2150	128	0
1	O	2166	0	2150	111	0
1	P	2166	0	2150	106	0
1	R	2166	0	2150	72	0
1	T	2166	0	2150	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	2166	0	2150	147	0
1	f	2166	0	2150	101	0
2	E	1473	0	1494	13	0
2	F	1473	0	1494	42	0
2	G	1473	0	1494	23	0
2	H	1473	0	1494	50	0
2	I	1473	0	1494	19	0
2	J	1473	0	1494	20	0
2	M	1473	0	1494	18	0
2	N	1473	0	1494	27	0
2	V	1473	0	1494	16	0
2	X	1473	0	1494	18	0
2	Z	1473	0	1494	32	0
2	d	1473	0	1494	29	0
All	All	43668	0	43728	1253	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 14.

All (1253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD13	1:L:195:ILE:HG12	1.26	1.09
1:L:184:SER:HB2	1:L:218:PRO:HB2	1.38	1.02
1:R:208:TRP:CD1	1:R:217:GLN:HG2	1.98	0.98
1:K:219:LYS:HA	1:K:239:ARG:HH12	1.31	0.94
1:B:163:PHE:C	1:B:165:ARG:H	1.69	0.92
1:L:75:MET:O	1:L:79:TRP:HB2	1.69	0.92
1:b:184:SER:HB2	1:b:218:PRO:HB2	1.52	0.91
1:L:135:ILE:HG12	1:L:141:GLN:HE22	1.33	0.90
1:K:122:GLU:HB3	1:K:139:LYS:HD3	1.52	0.90
1:B:163:PHE:C	1:B:165:ARG:N	2.24	0.89
2:Z:76:PHE:HZ	2:d:84:PHE:HA	1.36	0.89
2:F:10:ARG:HA	2:F:13:ILE:HG13	1.52	0.89
1:A:75:MET:O	1:A:79:TRP:HB2	1.73	0.88
1:O:212:LYS:HZ3	1:O:213:LEU:H	1.20	0.87
1:C:75:MET:O	1:C:79:TRP:HB2	1.76	0.85
1:T:75:MET:O	1:T:79:TRP:HB2	1.77	0.84
2:Z:76:PHE:CZ	2:d:84:PHE:HA	2.12	0.84
1:b:124:ILE:HG12	1:b:139:LYS:HB2	1.58	0.84
1:b:207:LEU:O	1:b:210:GLU:HB2	1.76	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:43:TYR:HD2	1:L:48:TYR:CE1	1.96	0.84
1:b:126:ILE:HG23	1:b:143:ILE:HG12	1.58	0.83
1:L:125:LYS:HA	1:L:142:ILE:HG22	1.61	0.82
1:B:195:ILE:CD1	1:L:195:ILE:HG12	2.09	0.82
1:R:75:MET:O	1:R:79:TRP:HB2	1.80	0.81
1:K:184:SER:OG	1:K:218:PRO:HB2	1.80	0.81
2:H:10:ARG:HB3	2:H:14:LYS:NZ	1.95	0.80
1:O:205:SER:HA	1:O:208:TRP:CE2	2.18	0.79
1:R:208:TRP:HD1	1:R:217:GLN:HG2	1.42	0.78
1:K:208:TRP:CD1	1:K:209:LYS:HG2	2.20	0.78
1:b:209:LYS:HD3	1:b:238:TRP:HA	1.65	0.77
1:B:75:MET:O	1:B:79:TRP:HB2	1.83	0.77
1:P:208:TRP:CD1	1:P:209:LYS:H	2.03	0.77
1:O:211:GLN:HE22	1:O:213:LEU:HB3	1.51	0.76
1:f:194:ASP:O	1:f:195:ILE:C	2.28	0.76
1:C:160:THR:HG22	1:O:238:TRP:HE1	1.50	0.76
1:O:195:ILE:HG23	1:O:196:ASN:H	1.48	0.76
1:K:136:ASP:HB3	1:K:139:LYS:HB2	1.68	0.75
1:P:202:TYR:O	1:P:203:LYS:C	2.28	0.75
2:H:10:ARG:O	2:H:13:ILE:HG23	1.87	0.74
1:f:232:GLU:O	1:f:236:GLU:HB2	1.88	0.74
1:C:163:PHE:CE2	1:O:202:TYR:HB2	2.22	0.74
2:F:10:ARG:HA	2:F:13:ILE:CG1	2.16	0.74
1:P:206:LYS:C	1:P:210:GLU:HB2	2.13	0.74
1:P:202:TYR:CZ	1:P:206:LYS:HD3	2.22	0.73
2:F:6:ILE:HA	2:F:30:SER:HB3	1.69	0.73
1:P:195:ILE:HG23	1:P:196:ASN:H	1.52	0.73
1:b:138:ASN:O	1:b:139:LYS:C	2.30	0.73
1:K:216:ALA:O	1:K:217:GLN:C	2.30	0.73
2:N:75:GLY:C	2:N:77:PRO:HD3	2.14	0.73
1:L:209:LYS:O	1:L:210:GLU:C	2.32	0.73
1:L:195:ILE:HG23	1:L:196:ASN:H	1.54	0.73
2:Z:70:ILE:HG22	2:Z:72:SER:H	1.53	0.72
1:A:216:ALA:O	1:A:217:GLN:HB2	1.87	0.72
1:K:127:SER:O	1:K:172:LEU:HD11	1.88	0.72
1:L:208:TRP:O	1:L:209:LYS:C	2.30	0.72
1:A:56:GLU:HG2	1:A:159:GLU:HG3	1.70	0.72
1:T:163:PHE:HB3	1:f:202:TYR:CE2	2.25	0.72
1:O:209:LYS:HE3	1:O:210:GLU:HG3	1.72	0.72
1:L:135:ILE:HG12	1:L:141:GLN:NE2	2.05	0.72
1:f:205:SER:HA	1:f:208:TRP:CE2	2.25	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:LYS:HA	1:K:239:ARG:NH1	2.04	0.71
1:D:163:PHE:CE2	1:P:202:TYR:HB2	2.25	0.71
2:H:6:ILE:HD11	2:H:32:HIS:HB2	1.71	0.71
1:C:163:PHE:CD2	1:O:202:TYR:CG	2.78	0.71
1:f:195:ILE:O	1:f:196:ASN:C	2.34	0.71
1:b:195:ILE:O	1:b:196:ASN:C	2.31	0.71
1:K:208:TRP:HZ2	1:K:240:ILE:HD11	1.56	0.71
1:L:195:ILE:O	1:L:196:ASN:C	2.31	0.71
1:f:235:LEU:HD12	1:f:240:ILE:HG13	1.72	0.71
2:F:158:MET:HB3	2:F:161:ARG:HB2	1.73	0.71
1:B:163:PHE:O	1:B:165:ARG:N	2.24	0.71
1:f:197:ILE:HA	1:f:200:LEU:HD12	1.73	0.71
1:f:214:GLU:O	1:f:215:GLU:C	2.32	0.70
1:K:205:SER:HA	1:K:208:TRP:CZ2	2.26	0.70
1:L:205:SER:O	1:L:206:LYS:C	2.33	0.70
1:f:195:ILE:HG23	1:f:196:ASN:H	1.56	0.70
2:H:10:ARG:C	2:H:14:LYS:HZ3	1.98	0.70
1:b:217:GLN:O	1:b:218:PRO:C	2.35	0.70
1:O:201:PHE:HA	1:O:204:LEU:HD12	1.72	0.70
1:B:208:TRP:CD1	1:B:217:GLN:HG3	2.27	0.70
1:b:205:SER:O	1:b:206:LYS:C	2.33	0.69
1:K:208:TRP:CD1	1:K:209:LYS:H	2.10	0.69
1:O:202:TYR:O	1:O:203:LYS:C	2.34	0.69
1:R:209:LYS:O	1:R:210:GLU:C	2.35	0.69
1:f:199:LEU:O	1:f:200:LEU:C	2.32	0.69
1:K:131:ASP:HA	1:K:134:LYS:HD3	1.74	0.69
1:P:209:LYS:HG3	1:P:239:ARG:HG3	1.74	0.69
1:L:205:SER:HA	1:L:208:TRP:CZ2	2.27	0.69
1:f:201:PHE:O	1:f:202:TYR:C	2.34	0.69
1:R:195:ILE:HD13	1:b:195:ILE:HG12	1.73	0.69
2:Z:76:PHE:CE1	2:d:87:LYS:HB3	2.28	0.69
1:b:126:ILE:CG2	1:b:143:ILE:HG12	2.21	0.69
1:R:163:PHE:HB3	1:b:202:TYR:CD2	2.27	0.69
1:O:199:LEU:O	1:O:200:LEU:C	2.36	0.69
1:R:164:GLN:O	1:R:166:LEU:HG	1.93	0.68
1:K:113:GLU:HG3	1:K:142:ILE:HD12	1.74	0.68
1:b:194:ASP:O	1:b:195:ILE:C	2.36	0.68
1:K:209:LYS:O	1:K:210:GLU:C	2.36	0.68
1:K:192:LEU:HB2	1:K:231:GLN:NE2	2.08	0.68
1:L:200:LEU:O	1:L:201:PHE:C	2.33	0.68
1:L:129:VAL:HG13	1:L:130:SER:H	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:122:GLU:OE1	1:P:139:LYS:HB3	1.94	0.68
1:P:162:TYR:OH	1:P:196:ASN:HB2	1.93	0.68
1:L:122:GLU:HB2	1:L:139:LYS:HG2	1.76	0.68
1:R:180:VAL:HG12	1:R:208:TRP:CZ2	2.29	0.68
1:K:219:LYS:N	1:K:239:ARG:HH22	1.92	0.68
2:J:68:LEU:H	2:J:81:THR:HG21	1.59	0.67
1:O:200:LEU:O	1:O:201:PHE:C	2.35	0.67
1:f:205:SER:HA	1:f:208:TRP:CZ2	2.29	0.67
1:R:210:GLU:C	1:R:212:LYS:H	2.03	0.67
2:F:10:ARG:HA	2:F:13:ILE:CD1	2.24	0.67
1:L:135:ILE:CG1	1:L:141:GLN:HE22	2.07	0.67
1:f:200:LEU:O	1:f:201:PHE:C	2.37	0.67
1:O:195:ILE:O	1:O:196:ASN:C	2.35	0.67
1:K:192:LEU:HB2	1:K:231:GLN:HE22	1.60	0.67
2:d:158:MET:HB3	2:d:161:ARG:HB3	1.76	0.66
1:P:124:ILE:HD11	1:P:136:ASP:HB3	1.76	0.66
1:K:199:LEU:O	1:K:200:LEU:C	2.34	0.66
2:H:9:ASN:HD21	2:H:11:HIS:HB2	1.60	0.66
1:b:205:SER:HA	1:b:208:TRP:CE2	2.29	0.66
1:O:204:LEU:O	1:O:205:SER:C	2.37	0.66
1:b:203:LYS:O	1:b:206:LYS:HB2	1.96	0.66
1:P:209:LYS:HD3	1:P:238:TRP:HA	1.76	0.66
1:L:198:ARG:O	1:L:199:LEU:C	2.34	0.66
1:R:208:TRP:CE3	1:R:208:TRP:HA	2.30	0.66
2:M:57:VAL:HG12	2:M:59:ARG:H	1.61	0.66
1:b:102:ILE:HG23	1:b:141:GLN:HB2	1.77	0.66
1:b:196:ASN:O	1:b:197:ILE:C	2.39	0.66
1:L:122:GLU:HB3	1:L:139:LYS:HZ3	1.60	0.66
1:K:136:ASP:O	1:K:137:ASN:C	2.39	0.66
1:K:206:LYS:HB3	1:K:210:GLU:OE2	1.96	0.66
1:L:136:ASP:O	1:L:137:ASN:C	2.38	0.65
1:b:201:PHE:O	1:b:205:SER:N	2.24	0.65
1:K:75:MET:O	1:K:79:TRP:HB2	1.96	0.65
1:L:201:PHE:O	1:L:202:TYR:C	2.39	0.65
1:P:206:LYS:HA	1:P:206:LYS:HZ2	1.62	0.65
1:P:206:LYS:HD2	1:P:209:LYS:HZ1	1.61	0.65
1:A:220:SER:HB2	1:A:240:ILE:HG12	1.79	0.65
1:L:162:TYR:HE2	1:L:196:ASN:HB3	1.61	0.65
1:b:205:SER:HA	1:b:208:TRP:CZ2	2.30	0.65
1:P:194:ASP:O	1:P:195:ILE:C	2.36	0.65
1:P:204:LEU:O	1:P:206:LYS:N	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:199:LEU:O	1:b:200:LEU:C	2.40	0.65
1:K:219:LYS:HG2	1:K:239:ARG:NH2	2.11	0.65
1:O:201:PHE:O	1:O:205:SER:N	2.25	0.65
1:L:194:ASP:O	1:L:195:ILE:C	2.40	0.65
1:K:195:ILE:O	1:K:196:ASN:C	2.37	0.65
1:f:198:ARG:O	1:f:199:LEU:C	2.37	0.64
1:B:14:ILE:HB	1:B:185:VAL:HG23	1.79	0.64
1:A:207:LEU:C	1:A:209:LYS:H	2.06	0.64
1:b:195:ILE:HG23	1:b:196:ASN:H	1.62	0.64
1:K:206:LYS:HA	1:K:209:LYS:NZ	2.11	0.64
1:D:163:PHE:CD2	1:P:202:TYR:CG	2.85	0.64
2:J:34:ILE:HG21	2:J:49:LYS:HG3	1.80	0.64
1:b:209:LYS:O	1:b:210:GLU:C	2.40	0.64
1:P:206:LYS:HB3	1:P:210:GLU:CD	2.23	0.64
1:A:211:GLN:O	1:A:213:LEU:N	2.30	0.64
1:K:131:ASP:O	1:K:132:ILE:C	2.40	0.64
1:O:162:TYR:OH	1:O:196:ASN:HB2	1.97	0.64
1:O:205:SER:HA	1:O:208:TRP:CZ2	2.32	0.64
1:L:196:ASN:O	1:L:197:ILE:C	2.39	0.64
1:P:205:SER:HA	1:P:208:TRP:CZ2	2.33	0.64
1:f:196:ASN:O	1:f:197:ILE:C	2.38	0.64
1:K:195:ILE:HG23	1:K:196:ASN:H	1.62	0.64
1:K:202:TYR:O	1:K:203:LYS:C	2.38	0.64
1:K:206:LYS:HA	1:K:209:LYS:HZ2	1.62	0.64
1:T:163:PHE:HD1	1:f:202:TYR:CG	2.16	0.64
1:O:219:LYS:HG2	1:O:239:ARG:HD3	1.79	0.64
1:L:195:ILE:O	1:L:198:ARG:N	2.31	0.64
1:P:67:LYS:HG3	1:P:69:GLY:H	1.63	0.63
1:b:204:LEU:O	1:b:205:SER:C	2.41	0.63
1:f:197:ILE:HG23	1:f:201:PHE:HE1	1.62	0.63
1:f:205:SER:O	1:f:206:LYS:C	2.37	0.63
2:H:10:ARG:O	2:H:14:LYS:NZ	2.25	0.63
1:P:216:ALA:O	1:P:217:GLN:C	2.42	0.63
1:K:206:LYS:O	1:K:207:LEU:C	2.40	0.63
1:T:163:PHE:CD1	1:f:202:TYR:CG	2.87	0.63
1:O:198:ARG:O	1:O:199:LEU:C	2.41	0.63
1:B:209:LYS:O	1:B:210:GLU:C	2.40	0.63
1:P:136:ASP:O	1:P:137:ASN:C	2.41	0.63
1:P:195:ILE:O	1:P:196:ASN:C	2.41	0.63
1:P:206:LYS:O	1:P:207:LEU:C	2.40	0.63
1:R:209:LYS:O	1:R:212:LYS:N	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:217:GLN:O	1:K:218:PRO:C	2.39	0.63
1:O:212:LYS:NZ	1:O:213:LEU:H	1.96	0.63
1:D:234:ILE:HD13	1:P:59:GLU:HG2	1.79	0.63
1:K:208:TRP:O	1:K:209:LYS:C	2.41	0.62
2:H:10:ARG:HA	2:H:13:ILE:CG2	2.28	0.62
1:P:206:LYS:HA	1:P:209:LYS:HZ3	1.64	0.62
1:b:195:ILE:HA	1:b:198:ARG:CD	2.29	0.62
1:b:131:ASP:O	1:b:134:LYS:HG3	2.00	0.62
1:b:202:TYR:O	1:b:203:LYS:C	2.42	0.62
1:O:75:MET:O	1:O:79:TRP:HB2	1.99	0.62
1:R:53:SER:H	1:R:56:GLU:CG	2.12	0.62
1:O:194:ASP:O	1:O:195:ILE:C	2.43	0.62
1:P:209:LYS:HA	1:P:239:ARG:HE	1.64	0.62
1:O:191:SER:O	1:O:193:SER:N	2.32	0.62
1:L:199:LEU:O	1:L:200:LEU:C	2.38	0.62
2:Z:76:PHE:CZ	2:d:84:PHE:CD1	2.88	0.62
1:L:208:TRP:CD1	1:L:209:LYS:H	2.17	0.62
1:f:206:LYS:O	1:f:207:LEU:C	2.43	0.62
2:I:2:ASN:HD22	2:I:28:LEU:HD11	1.65	0.61
1:B:204:LEU:HD22	1:B:208:TRP:CZ2	2.35	0.61
2:Z:158:MET:HG3	2:Z:162:LYS:HB2	1.83	0.61
1:P:204:LEU:O	1:P:205:SER:C	2.43	0.61
1:L:205:SER:HA	1:L:208:TRP:CE2	2.36	0.61
1:C:163:PHE:HD2	1:O:202:TYR:CG	2.16	0.61
1:O:239:ARG:C	1:O:240:ILE:HG12	2.23	0.61
1:L:131:ASP:O	1:L:132:ILE:C	2.43	0.61
1:P:200:LEU:O	1:P:201:PHE:C	2.40	0.61
2:Z:79:GLY:C	2:Z:81:THR:H	2.09	0.61
1:A:44:ASP:HB3	1:A:47:ILE:HG12	1.83	0.61
2:N:76:PHE:N	2:N:77:PRO:HD3	2.16	0.61
1:L:122:GLU:O	1:L:139:LYS:HA	2.00	0.61
1:P:199:LEU:O	1:P:200:LEU:C	2.40	0.61
1:b:192:LEU:HD21	1:b:201:PHE:CE2	2.35	0.61
1:K:197:ILE:O	1:K:198:ARG:C	2.40	0.61
1:K:195:ILE:HA	1:K:198:ARG:CD	2.31	0.60
1:P:197:ILE:O	1:P:198:ARG:C	2.43	0.60
1:b:132:ILE:O	1:b:133:ALA:C	2.41	0.60
1:R:209:LYS:O	1:R:211:GLN:N	2.35	0.60
2:F:68:LEU:H	2:F:81:THR:HG21	1.66	0.60
2:H:7:THR:N	2:H:30:SER:O	2.34	0.60
1:L:133:ALA:C	1:L:135:ILE:H	2.09	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:180:VAL:HG12	1:R:208:TRP:HZ2	1.65	0.60
1:B:159:GLU:OE1	1:B:163:PHE:CZ	2.55	0.60
1:B:195:ILE:HD11	1:L:195:ILE:HG21	1.82	0.60
1:C:208:TRP:HA	1:C:208:TRP:CE3	2.35	0.60
1:f:191:SER:O	1:f:193:SER:N	2.34	0.60
2:F:10:ARG:CA	2:F:13:ILE:HG13	2.27	0.60
2:G:148:PRO:HG2	2:G:151:GLU:HB2	1.83	0.60
1:O:208:TRP:CD1	1:O:209:LYS:H	2.19	0.60
2:H:11:HIS:O	2:H:12:LYS:C	2.45	0.60
1:L:206:LYS:O	1:L:207:LEU:C	2.44	0.60
1:P:208:TRP:CG	1:P:209:LYS:H	2.18	0.60
1:P:206:LYS:HA	1:P:209:LYS:NZ	2.16	0.60
1:D:62:LYS:HD3	1:D:68:ILE:HG23	1.83	0.60
1:L:201:PHE:HD1	1:L:201:PHE:H	1.50	0.60
2:H:10:ARG:C	2:H:14:LYS:NZ	2.60	0.60
1:b:197:ILE:O	1:b:198:ARG:C	2.45	0.59
1:b:208:TRP:O	1:b:209:LYS:C	2.45	0.59
1:C:174:ILE:HD13	1:C:177:ARG:HH21	1.67	0.59
1:O:191:SER:O	1:O:192:LEU:C	2.45	0.59
1:O:205:SER:O	1:O:206:LYS:C	2.42	0.59
1:K:163:PHE:HA	1:K:166:LEU:HD23	1.83	0.59
1:O:201:PHE:O	1:O:202:TYR:C	2.41	0.59
1:B:207:LEU:O	1:B:208:TRP:C	2.42	0.59
1:L:201:PHE:O	1:L:205:SER:N	2.33	0.59
1:O:210:GLU:O	1:O:212:LYS:HG3	2.01	0.59
1:f:202:TYR:O	1:f:203:LYS:C	2.45	0.59
1:O:214:GLU:O	1:O:215:GLU:C	2.46	0.59
1:D:166:LEU:HD22	1:D:199:LEU:HD22	1.84	0.59
1:b:206:LYS:HB3	1:b:210:GLU:OE2	2.02	0.59
1:f:211:GLN:HB3	1:f:217:GLN:HG3	1.85	0.59
1:b:184:SER:HB2	1:b:218:PRO:CB	2.28	0.59
1:K:204:LEU:O	1:K:205:SER:C	2.42	0.59
1:O:196:ASN:OD1	1:O:196:ASN:N	2.36	0.59
1:P:206:LYS:O	1:P:208:TRP:N	2.36	0.59
2:V:54:PHE:O	1:b:226:ARG:NH2	2.35	0.59
1:b:201:PHE:O	1:b:202:TYR:C	2.44	0.59
1:C:234:ILE:HD13	1:O:59:GLU:HG2	1.83	0.59
2:H:103:PRO:HB3	2:H:130:ILE:HB	1.85	0.59
1:R:195:ILE:CD1	1:b:195:ILE:HG12	2.32	0.59
2:E:55:LYS:HA	1:K:226:ARG:HH21	1.67	0.59
2:d:69:TYR:HB2	2:d:106:VAL:HB	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:LEU:HD21	2:H:73:LEU:HD13	1.85	0.59
1:A:215:GLU:CG	1:C:130:SER:HA	2.33	0.58
1:K:201:PHE:O	1:K:202:TYR:C	2.46	0.58
1:L:217:GLN:O	1:L:218:PRO:C	2.47	0.58
1:L:131:ASP:O	1:L:134:LYS:N	2.36	0.58
1:R:215:GLU:CD	1:R:215:GLU:H	2.10	0.58
1:K:214:GLU:CD	1:K:215:GLU:H	2.11	0.58
1:B:205:SER:O	1:B:209:LYS:HG2	2.02	0.58
1:L:139:LYS:O	1:L:140:THR:C	2.47	0.58
1:b:206:LYS:O	1:b:207:LEU:C	2.46	0.58
1:L:126:ILE:HG23	1:L:142:ILE:O	2.02	0.58
2:N:158:MET:HE2	2:N:161:ARG:HH21	1.69	0.58
2:H:9:ASN:ND2	2:H:11:HIS:HB2	2.17	0.58
2:Z:76:PHE:O	2:Z:77:PRO:C	2.47	0.58
1:b:198:ARG:O	1:b:199:LEU:C	2.43	0.58
1:C:46:ASP:N	1:C:46:ASP:OD1	2.37	0.58
1:A:205:SER:O	1:A:206:LYS:C	2.43	0.58
1:O:210:GLU:C	1:O:212:LYS:H	2.12	0.58
1:L:128:SER:O	1:L:129:VAL:C	2.46	0.58
2:H:10:ARG:O	2:H:13:ILE:CG2	2.52	0.58
1:T:35:ASP:OD1	1:T:49:ARG:NH2	2.37	0.57
1:O:204:LEU:O	1:O:206:LYS:N	2.37	0.57
1:R:210:GLU:O	1:R:212:LYS:N	2.38	0.57
1:A:207:LEU:O	1:A:209:LYS:N	2.36	0.57
1:K:128:SER:O	1:K:129:VAL:C	2.47	0.57
1:K:206:LYS:O	1:K:210:GLU:HB2	2.05	0.57
1:P:196:ASN:O	1:P:197:ILE:C	2.47	0.57
1:A:204:LEU:HD13	1:A:208:TRP:HE1	1.68	0.57
1:C:208:TRP:HA	1:C:208:TRP:HE3	1.69	0.57
1:K:194:ASP:O	1:K:195:ILE:C	2.47	0.57
1:O:197:ILE:O	1:O:198:ARG:C	2.42	0.57
1:L:130:SER:O	1:L:131:ASP:C	2.48	0.57
1:b:75:MET:O	1:b:79:TRP:HB2	2.04	0.57
1:f:195:ILE:O	1:f:198:ARG:N	2.37	0.57
1:K:136:ASP:O	1:K:138:ASN:N	2.37	0.57
1:K:191:SER:O	1:K:193:SER:N	2.38	0.57
1:K:195:ILE:HA	1:K:198:ARG:HD3	1.85	0.57
1:K:213:LEU:O	1:K:214:GLU:C	2.48	0.57
1:R:181:LEU:HA	1:R:208:TRP:CZ2	2.40	0.57
1:b:195:ILE:HA	1:b:198:ARG:HD2	1.87	0.57
1:K:199:LEU:O	1:K:202:TYR:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:OD1	1:B:49:ARG:NH2	2.38	0.57
1:P:195:ILE:HA	1:P:198:ARG:HD2	1.86	0.57
1:P:209:LYS:NZ	1:P:209:LYS:HB3	2.19	0.57
1:R:35:ASP:OD1	1:R:49:ARG:NH2	2.38	0.57
2:M:71:GLU:HB3	2:M:102:ASN:HD21	1.70	0.57
2:H:6:ILE:O	2:H:7:THR:HB	2.03	0.57
2:M:69:TYR:HB2	2:M:106:VAL:HB	1.86	0.57
1:K:13:VAL:HG23	1:K:184:SER:HB2	1.86	0.57
1:R:205:SER:O	1:R:206:LYS:C	2.47	0.56
1:R:207:LEU:O	1:R:208:TRP:C	2.48	0.56
2:X:86:ASP:HA	2:X:89:GLN:HE22	1.70	0.56
1:f:192:LEU:HD12	1:f:197:ILE:CG2	2.35	0.56
1:K:219:LYS:CA	1:K:239:ARG:HH22	2.18	0.56
2:F:10:ARG:O	2:F:13:ILE:N	2.34	0.56
1:b:131:ASP:HA	1:b:134:LYS:HD2	1.87	0.56
1:b:191:SER:O	1:b:192:LEU:C	2.46	0.56
1:b:216:ALA:O	1:b:217:GLN:C	2.46	0.56
1:R:56:GLU:HG2	1:b:198:ARG:NH2	2.20	0.56
1:R:159:GLU:O	1:R:160:THR:C	2.49	0.56
1:f:201:PHE:O	1:f:205:SER:N	2.23	0.56
1:K:203:LYS:O	1:K:206:LYS:HB2	2.04	0.56
1:B:205:SER:O	1:B:206:LYS:C	2.45	0.56
1:L:197:ILE:O	1:L:198:ARG:C	2.48	0.56
1:K:136:ASP:OD2	1:K:139:LYS:HG3	2.06	0.56
1:O:205:SER:HA	1:O:208:TRP:NE1	2.19	0.56
1:P:202:TYR:O	1:P:205:SER:N	2.38	0.56
1:f:1:MET:SD	1:f:1:MET:N	2.74	0.56
2:H:57:VAL:HG12	2:H:59:ARG:H	1.71	0.56
1:b:195:ILE:O	1:b:198:ARG:N	2.38	0.56
1:f:231:GLN:O	1:f:235:LEU:HB2	2.05	0.56
1:P:208:TRP:O	1:P:211:GLN:N	2.39	0.56
1:A:204:LEU:O	1:A:205:SER:C	2.49	0.56
2:M:70:ILE:HB	2:M:73:LEU:HB2	1.88	0.56
1:B:59:GLU:HG2	1:L:234:ILE:HG12	1.86	0.56
1:R:14:ILE:HB	1:R:185:VAL:HG12	1.88	0.56
1:R:249:ASN:ND2	1:R:252:GLU:OE1	2.39	0.56
2:M:9:ASN:HD22	2:M:12:LYS:HE2	1.71	0.56
1:K:131:ASP:O	1:K:134:LYS:HG2	2.05	0.56
1:K:196:ASN:O	1:K:197:ILE:C	2.47	0.56
1:B:165:ARG:NH2	1:B:170:THR:OG1	2.39	0.56
1:R:207:LEU:O	1:R:209:LYS:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:PHE:O	1:K:226:ARG:NH2	2.37	0.56
1:O:206:LYS:O	1:O:207:LEU:C	2.49	0.56
2:N:167:MET:SD	2:N:167:MET:N	2.76	0.56
1:A:125:LYS:NZ	1:A:150:ASP:OD2	2.39	0.56
1:K:192:LEU:HD21	1:K:201:PHE:CE2	2.42	0.56
1:O:231:GLN:O	1:O:235:LEU:HB2	2.06	0.56
2:J:87:LYS:HG3	2:N:76:PHE:HD1	1.71	0.56
1:f:109:ASP:OD2	1:f:109:ASP:N	2.39	0.55
1:A:155:ILE:HG23	1:A:157:LEU:HD23	1.88	0.55
1:D:35:ASP:OD1	1:D:49:ARG:NH2	2.39	0.55
1:b:186:LEU:HG	1:b:188:ILE:HD11	1.88	0.55
1:b:109:ASP:O	1:b:144:LYS:NZ	2.39	0.55
1:B:159:GLU:OE1	1:B:163:PHE:CE1	2.59	0.55
1:T:163:PHE:CE1	1:f:202:TYR:HB2	2.42	0.55
1:L:167:GLU:N	1:L:167:GLU:OE1	2.39	0.55
1:R:56:GLU:OE2	1:b:230:ILE:HG21	2.06	0.55
1:b:218:PRO:O	1:b:219:LYS:C	2.49	0.55
1:f:238:TRP:O	1:f:239:ARG:HB2	2.06	0.55
1:K:129:VAL:O	1:K:130:SER:C	2.47	0.55
2:X:10:ARG:O	2:X:14:LYS:NZ	2.38	0.55
2:F:76:PHE:HB2	2:H:87:LYS:HB3	1.88	0.55
1:P:199:LEU:O	1:P:202:TYR:N	2.40	0.55
1:P:208:TRP:CD1	1:P:209:LYS:N	2.72	0.55
1:b:228:ASN:OD1	1:b:228:ASN:N	2.39	0.55
1:A:161:SER:C	1:A:163:PHE:H	2.15	0.55
1:b:215:GLU:HB2	1:b:217:GLN:OE1	2.06	0.55
1:f:15:LEU:HD11	1:f:188:ILE:HD13	1.89	0.55
1:P:124:ILE:HD11	1:P:139:LYS:HD2	1.89	0.55
1:f:220:SER:OG	1:f:221:TYR:N	2.39	0.55
1:O:191:SER:C	1:O:193:SER:N	2.62	0.55
1:b:149:PHE:O	1:A:72:ARG:NH2	2.40	0.55
1:C:60:TYR:HB2	1:O:230:ILE:HG23	1.89	0.55
1:O:209:LYS:HE3	1:O:210:GLU:H	1.72	0.55
1:B:249:ASN:ND2	1:B:252:GLU:OE1	2.40	0.55
1:D:247:ASN:OD1	1:D:247:ASN:N	2.40	0.55
2:N:158:MET:SD	2:N:158:MET:N	2.80	0.55
1:L:195:ILE:HG23	1:L:196:ASN:N	2.21	0.54
1:R:208:TRP:HA	1:R:208:TRP:HE3	1.70	0.54
1:P:208:TRP:O	1:P:211:GLN:HB3	2.06	0.54
1:b:194:ASP:OD1	1:b:194:ASP:N	2.40	0.54
1:A:56:GLU:O	1:A:59:GLU:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:O	1:B:207:LEU:C	2.49	0.54
1:O:194:ASP:OD2	1:O:197:ILE:HG12	2.07	0.54
1:O:209:LYS:O	1:O:210:GLU:C	2.48	0.54
1:D:161:SER:HA	1:D:164:GLN:HG2	1.90	0.54
1:R:162:TYR:HE1	1:R:196:ASN:HD22	1.53	0.54
1:b:197:ILE:O	1:b:200:LEU:HB2	2.07	0.54
1:f:194:ASP:N	1:f:194:ASP:OD1	2.41	0.54
2:H:82:GLN:NE2	2:H:86:ASP:OD2	2.40	0.54
2:H:163:ASN:HA	2:H:168:ARG:HH12	1.73	0.54
1:P:85:ASP:OD1	1:P:85:ASP:N	2.40	0.54
1:P:213:LEU:HA	1:P:217:GLN:NE2	2.22	0.54
2:I:158:MET:HG3	2:I:161:ARG:HE	1.73	0.54
1:f:214:GLU:HB3	1:f:215:GLU:OE1	2.08	0.54
1:L:148:ASP:OD1	1:L:148:ASP:N	2.41	0.54
1:f:194:ASP:OD1	1:f:197:ILE:HB	2.07	0.54
1:C:85:ASP:OD1	1:C:87:ASN:ND2	2.41	0.54
1:O:195:ILE:HG23	1:O:196:ASN:N	2.22	0.54
1:P:212:LYS:NZ	1:P:212:LYS:H	2.05	0.54
1:C:145:PHE:O	1:C:165:ARG:NH1	2.41	0.54
1:O:237:GLN:C	1:O:239:ARG:N	2.63	0.54
1:R:210:GLU:C	1:R:212:LYS:N	2.66	0.53
2:X:57:VAL:HG12	2:X:59:ARG:H	1.72	0.53
1:b:37:ILE:HG21	1:b:71:LEU:HD13	1.89	0.53
2:E:13:ILE:O	2:E:17:ASN:ND2	2.41	0.53
2:F:9:ASN:C	2:F:10:ARG:HG2	2.33	0.53
1:L:203:LYS:O	1:L:206:LYS:HB2	2.08	0.53
1:b:211:GLN:HG3	1:b:213:LEU:HD23	1.89	0.53
2:H:166:SER:OG	2:H:168:ARG:NH1	2.41	0.53
2:N:134:PRO:HB2	2:N:138:ARG:HH22	1.73	0.53
1:P:137:ASN:O	1:P:138:ASN:C	2.49	0.53
1:A:226:ARG:NH2	2:G:54:PHE:O	2.41	0.53
1:K:122:GLU:HB3	1:K:139:LYS:CD	2.32	0.53
2:d:10:ARG:O	2:d:10:ARG:NH1	2.33	0.53
1:A:56:GLU:CD	1:K:198:ARG:HH21	2.16	0.53
1:K:129:VAL:O	1:K:132:ILE:HB	2.09	0.53
1:L:137:ASN:CG	1:L:138:ASN:N	2.65	0.53
1:b:128:SER:C	1:b:130:SER:N	2.62	0.53
1:C:128:SER:OG	1:C:129:VAL:N	2.42	0.53
1:C:216:ALA:O	1:C:217:GLN:HB3	2.08	0.53
2:I:158:MET:HE3	2:I:158:MET:H	1.73	0.53
1:B:181:LEU:HG	1:B:208:TRP:CZ3	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7:ASP:HA	1:P:10:LYS:HD2	1.91	0.53
1:b:124:ILE:HD11	1:b:139:LYS:HD2	1.90	0.53
1:D:51:PHE:HB3	1:P:226:ARG:HH21	1.73	0.53
1:L:202:TYR:O	1:L:203:LYS:C	2.49	0.53
1:P:214:GLU:CD	1:P:215:GLU:H	2.16	0.53
1:B:4:LEU:HD11	1:B:186:LEU:HD13	1.91	0.53
1:P:188:ILE:HG22	1:P:223:PHE:HB3	1.90	0.53
1:b:247:ASN:ND2	1:b:249:ASN:O	2.41	0.53
1:K:207:LEU:O	1:K:210:GLU:HB2	2.08	0.53
1:O:196:ASN:O	1:O:197:ILE:C	2.49	0.53
2:H:69:TYR:HE2	2:H:108:LYS:HB2	1.74	0.53
2:J:136:GLY:O	2:J:138:ARG:NH1	2.41	0.53
2:d:13:ILE:O	2:d:17:ASN:ND2	2.41	0.53
1:D:56:GLU:O	1:D:59:GLU:N	2.42	0.53
2:N:43:HIS:NE2	2:N:123:GLU:OE2	2.42	0.53
1:L:59:GLU:HG2	1:L:158:ASP:HB2	1.90	0.53
1:L:73:SER:OG	1:L:77:ARG:NH1	2.41	0.53
2:X:88:LEU:HD22	2:X:92:LYS:HG2	1.90	0.53
2:E:16:ILE:HD11	2:E:168:ARG:HH21	1.74	0.53
2:I:34:ILE:HG21	2:I:49:LYS:HG3	1.89	0.53
2:F:13:ILE:O	2:F:17:ASN:ND2	2.38	0.53
1:L:129:VAL:O	1:L:130:SER:C	2.50	0.53
2:d:15:GLU:HG3	2:d:168:ARG:HH22	1.74	0.52
1:C:56:GLU:O	1:C:59:GLU:N	2.41	0.52
1:K:178:SER:HA	1:K:181:LEU:HD23	1.90	0.52
1:B:208:TRP:CG	1:B:217:GLN:HG3	2.43	0.52
1:P:219:LYS:O	1:P:220:SER:OG	2.25	0.52
1:T:195:ILE:HG21	1:f:195:ILE:HG12	1.92	0.52
1:b:191:SER:O	1:b:193:SER:N	2.43	0.52
1:C:14:ILE:HB	1:C:185:VAL:HG22	1.91	0.52
1:R:159:GLU:HB3	1:R:163:PHE:CE2	2.45	0.52
2:d:43:HIS:NE2	2:d:123:GLU:OE2	2.41	0.52
1:b:195:ILE:HG13	1:b:196:ASN:N	2.22	0.52
1:P:198:ARG:O	1:P:199:LEU:C	2.52	0.52
2:V:13:ILE:O	2:V:17:ASN:ND2	2.41	0.52
1:b:48:TYR:CZ	1:b:57:LEU:HB2	2.44	0.52
2:I:54:PHE:O	1:O:226:ARG:NH2	2.42	0.52
1:R:206:LYS:O	1:R:210:GLU:HG2	2.08	0.52
2:X:69:TYR:HB2	2:X:106:VAL:HB	1.92	0.52
1:b:128:SER:O	1:b:129:VAL:C	2.51	0.52
1:K:124:ILE:HD11	1:K:139:LYS:HE3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:208:TRP:O	1:O:209:LYS:C	2.53	0.52
1:A:206:LYS:O	1:A:207:LEU:C	2.52	0.52
1:B:46:ASP:HB3	2:F:51:LEU:HD21	1.91	0.52
1:L:219:LYS:HD2	1:L:239:ARG:HB2	1.92	0.52
2:V:106:VAL:HG13	2:V:127:GLN:HG3	1.92	0.52
1:b:184:SER:CB	1:b:218:PRO:HB2	2.34	0.52
2:G:86:ASP:O	2:G:89:GLN:NE2	2.42	0.52
1:R:59:GLU:HG2	1:b:234:ILE:HG12	1.91	0.52
1:K:102:ILE:HG23	1:K:141:GLN:HG3	1.92	0.52
1:L:167:GLU:O	1:L:168:PHE:CB	2.57	0.52
1:L:197:ILE:O	1:L:200:LEU:HB2	2.10	0.52
1:R:73:SER:OG	1:R:77:ARG:NH1	2.43	0.52
2:I:90:ALA:O	2:I:94:SER:OG	2.25	0.52
1:R:208:TRP:CE3	1:R:208:TRP:CA	2.93	0.52
2:V:36:GLU:O	2:V:38:GLN:NE2	2.43	0.52
2:G:114:CYS:HB2	2:G:119:ILE:HG22	1.92	0.52
1:O:14:ILE:HB	1:O:185:VAL:HG22	1.92	0.52
1:B:98:ALA:O	1:B:121:LYS:NZ	2.43	0.52
1:D:41:LEU:HD11	1:D:64:LYS:HG3	1.91	0.52
1:P:122:GLU:OE1	1:P:139:LYS:HD3	2.10	0.52
1:O:191:SER:OG	1:O:193:SER:HB3	2.10	0.51
1:D:208:TRP:HA	1:D:208:TRP:CE3	2.45	0.51
1:L:165:ARG:O	1:L:167:GLU:N	2.44	0.51
1:L:167:GLU:O	1:L:168:PHE:HB2	2.09	0.51
1:f:219:LYS:HG3	1:f:219:LYS:O	2.10	0.51
1:O:195:ILE:O	1:O:198:ARG:HG3	2.10	0.51
2:H:80:LEU:HD23	2:H:83:ILE:HD12	1.92	0.51
1:P:195:ILE:HG23	1:P:196:ASN:N	2.24	0.51
2:F:65:HIS:HE1	2:F:82:GLN:HE22	1.59	0.51
1:L:43:TYR:CD2	1:L:48:TYR:CE1	2.87	0.51
1:L:122:GLU:HB3	1:L:139:LYS:NZ	2.25	0.51
1:f:110:ARG:HH22	1:D:77:ARG:HH12	1.57	0.51
1:f:213:LEU:O	1:f:214:GLU:C	2.53	0.51
2:E:7:THR:HG23	2:E:9:ASN:H	1.76	0.51
1:K:138:ASN:O	1:K:139:LYS:C	2.54	0.51
1:K:209:LYS:O	1:K:212:LYS:N	2.43	0.51
2:F:10:ARG:O	2:F:13:ILE:HG13	2.10	0.51
1:b:133:ALA:C	1:b:135:ILE:H	2.19	0.51
1:O:215:GLU:O	1:O:216:ALA:HB2	2.10	0.51
1:B:56:GLU:O	1:B:59:GLU:N	2.43	0.51
2:F:10:ARG:HB3	2:F:13:ILE:HD12	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:SER:HB3	2:H:102:ASN:HB3	1.92	0.51
2:J:74:ASN:ND2	2:N:87:LYS:O	2.42	0.51
1:L:200:LEU:O	1:L:203:LYS:N	2.43	0.51
1:T:163:PHE:HD1	1:f:202:TYR:CD1	2.28	0.51
2:I:114:CYS:HB2	2:I:119:ILE:HG22	1.93	0.51
1:P:213:LEU:HA	1:P:217:GLN:CD	2.35	0.51
1:f:197:ILE:O	1:f:198:ARG:C	2.53	0.51
2:F:8:ARG:HH11	2:F:31:GLU:CB	2.23	0.51
1:P:138:ASN:OD1	1:P:138:ASN:N	2.43	0.51
2:X:13:ILE:HD13	2:X:29:ALA:HB2	1.92	0.51
1:b:208:TRP:O	1:b:211:GLN:N	2.39	0.51
1:f:109:ASP:O	1:f:144:LYS:NZ	2.44	0.51
1:K:21:VAL:HG12	1:K:254:LEU:HD21	1.93	0.51
1:L:79:TRP:HD1	1:L:109:ASP:HB3	1.75	0.51
1:L:113:GLU:OE2	1:L:144:LYS:NZ	2.39	0.51
1:L:212:LYS:HA	1:L:215:GLU:OE1	2.11	0.51
1:O:207:LEU:HD22	1:O:207:LEU:H	1.75	0.51
1:B:163:PHE:O	1:B:164:GLN:C	2.52	0.51
1:L:205:SER:OG	1:L:206:LYS:N	2.39	0.51
1:R:207:LEU:HA	1:R:210:GLU:OE1	2.12	0.50
1:b:195:ILE:HD11	1:b:199:LEU:HD13	1.92	0.50
2:I:158:MET:HG2	2:I:161:ARG:HB3	1.93	0.50
2:M:13:ILE:O	2:M:17:ASN:ND2	2.44	0.50
1:B:85:ASP:OD1	1:B:87:ASN:ND2	2.43	0.50
1:D:163:PHE:CE2	1:P:202:TYR:CB	2.94	0.50
1:R:214:GLU:O	1:R:215:GLU:C	2.53	0.50
1:O:209:LYS:HB2	1:O:209:LYS:HZ2	1.76	0.50
2:G:35:ASP:OD1	2:G:35:ASP:N	2.38	0.50
2:I:69:TYR:HA	2:I:77:PRO:HD2	1.94	0.50
1:O:214:GLU:HB3	1:O:215:GLU:OE2	2.10	0.50
1:B:56:GLU:OE1	1:B:159:GLU:HG3	2.12	0.50
1:D:21:VAL:HG12	1:D:254:LEU:HD21	1.94	0.50
2:F:34:ILE:HG21	2:F:49:LYS:HG3	1.93	0.50
1:L:40:GLU:OE2	1:L:65:LYS:NZ	2.40	0.50
1:R:207:LEU:C	1:R:209:LYS:N	2.68	0.50
1:O:214:GLU:CD	1:O:215:GLU:HG3	2.36	0.50
1:L:133:ALA:O	1:L:135:ILE:N	2.43	0.50
1:P:209:LYS:O	1:P:210:GLU:C	2.54	0.50
1:D:63:LEU:HD13	1:P:233:GLU:HG3	1.93	0.50
2:N:148:PRO:HG2	2:N:151:GLU:HB2	1.93	0.50
1:b:136:ASP:OD2	1:b:139:LYS:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:204:LEU:O	1:b:207:LEU:HB2	2.12	0.50
1:C:166:LEU:HD12	1:C:199:LEU:HD13	1.93	0.50
1:L:45:PRO:O	1:L:49:ARG:NH1	2.45	0.50
1:P:194:ASP:N	1:P:194:ASP:OD1	2.44	0.50
1:R:211:GLN:O	1:R:212:LYS:C	2.54	0.50
1:b:196:ASN:N	1:b:196:ASN:OD1	2.44	0.50
1:b:245:SER:OG	1:b:246:GLU:N	2.45	0.50
1:K:214:GLU:O	1:K:215:GLU:C	2.55	0.50
1:L:195:ILE:HA	1:L:198:ARG:NH1	2.26	0.50
1:b:198:ARG:O	1:b:201:PHE:N	2.44	0.50
1:b:204:LEU:O	1:b:207:LEU:N	2.45	0.50
1:A:249:ASN:ND2	1:A:252:GLU:OE1	2.44	0.50
2:G:103:PRO:HB2	2:G:130:ILE:H	1.77	0.50
2:H:7:THR:O	2:H:31:GLU:HA	2.11	0.50
1:P:212:LYS:H	1:P:212:LYS:HZ3	1.58	0.50
1:R:247:ASN:HB3	1:R:253:SER:HB2	1.94	0.50
1:A:163:PHE:C	1:A:165:ARG:N	2.66	0.50
1:C:158:ASP:OD1	1:C:158:ASP:N	2.37	0.50
1:L:138:ASN:ND2	1:L:139:LYS:HG3	2.27	0.50
1:P:204:LEU:C	1:P:206:LYS:N	2.69	0.50
1:b:208:TRP:CD1	1:b:209:LYS:H	2.30	0.49
2:G:105:LEU:O	2:G:127:GLN:NE2	2.45	0.49
1:K:204:LEU:O	1:K:207:LEU:HB2	2.12	0.49
1:K:109:ASP:O	1:K:144:LYS:NZ	2.43	0.49
1:K:208:TRP:O	1:K:210:GLU:N	2.45	0.49
1:B:50:THR:OG1	1:B:51:PHE:N	2.45	0.49
1:B:181:LEU:HG	1:B:208:TRP:CH2	2.46	0.49
1:L:86:ILE:HD11	1:L:115:ALA:HB2	1.94	0.49
1:b:255:GLU:O	1:b:259:LYS:HB2	2.12	0.49
1:A:211:GLN:HB3	1:A:213:LEU:HD12	1.93	0.49
1:D:208:TRP:HA	1:D:208:TRP:HE3	1.77	0.49
2:F:8:ARG:HD2	2:F:31:GLU:HB2	1.94	0.49
2:N:91:ASP:N	2:N:91:ASP:OD1	2.45	0.49
1:b:106:THR:HG23	1:b:190:TYR:OH	2.12	0.49
2:G:69:TYR:N	2:G:106:VAL:O	2.46	0.49
2:G:158:MET:N	2:G:158:MET:SD	2.83	0.49
2:F:13:ILE:HB	2:F:14:LYS:HD3	1.95	0.49
1:L:184:SER:OG	1:L:219:LYS:O	2.28	0.49
2:Z:76:PHE:CZ	2:d:87:LYS:HB2	2.48	0.49
1:b:46:ASP:O	1:b:48:TYR:N	2.46	0.49
1:K:212:LYS:O	1:K:213:LEU:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:194:ASP:HB2	1:O:196:ASN:OD1	2.12	0.49
1:f:202:TYR:CE2	1:f:206:LYS:HE3	2.47	0.49
1:O:209:LYS:O	1:O:211:GLN:N	2.46	0.49
1:O:245:SER:OG	1:O:246:GLU:N	2.45	0.49
2:J:108:LYS:HG2	2:J:125:GLU:HB3	1.94	0.49
1:R:51:PHE:HE2	1:b:229:PRO:HD2	1.78	0.49
2:V:67:GLY:HA2	2:V:81:THR:HG21	1.94	0.49
1:C:1:MET:HE1	1:C:257:PHE:HE1	1.78	0.49
1:C:56:GLU:O	1:C:59:GLU:HB2	2.13	0.49
1:C:79:TRP:HD1	1:C:109:ASP:HB3	1.77	0.49
1:C:158:ASP:OD1	1:C:161:SER:OG	2.24	0.49
1:C:163:PHE:HD2	1:O:202:TYR:CD1	2.31	0.49
2:F:10:ARG:C	2:F:12:LYS:N	2.65	0.49
2:Z:34:ILE:HG21	2:Z:49:LYS:HG3	1.94	0.49
2:M:91:ASP:OD1	2:M:138:ARG:NH2	2.44	0.49
1:D:59:GLU:HG2	1:D:158:ASP:HB2	1.95	0.49
2:F:42:VAL:HG13	2:F:65:HIS:HD2	1.78	0.49
1:A:159:GLU:OE1	1:A:163:PHE:CZ	2.66	0.49
1:K:36:HIS:C	1:K:38:ALA:H	2.20	0.49
1:K:208:TRP:HB2	1:K:217:GLN:HG3	1.95	0.49
1:L:199:LEU:HD12	1:L:199:LEU:HA	1.63	0.49
1:P:124:ILE:CG1	1:P:139:LYS:HD2	2.43	0.48
1:P:196:ASN:O	1:P:199:LEU:N	2.46	0.48
2:V:158:MET:HB3	2:V:161:ARG:HB2	1.94	0.48
1:f:71:LEU:HD23	1:f:157:LEU:HD21	1.95	0.48
1:f:234:ILE:O	1:f:237:GLN:HB3	2.13	0.48
1:A:163:PHE:HB3	1:K:202:TYR:CE2	2.48	0.48
1:A:211:GLN:C	1:A:213:LEU:N	2.71	0.48
1:K:165:ARG:NH2	1:K:173:ASP:OD1	2.45	0.48
1:B:79:TRP:HD1	1:B:109:ASP:HB3	1.78	0.48
1:R:63:LEU:HD11	1:b:237:GLN:HE22	1.78	0.48
1:R:73:SER:OG	1:L:110:ARG:NH2	2.47	0.48
2:d:69:TYR:N	2:d:106:VAL:O	2.42	0.48
1:f:85:ASP:OD1	1:f:85:ASP:N	2.43	0.48
1:A:56:GLU:OE1	1:K:234:ILE:HG13	2.12	0.48
1:K:205:SER:HB2	1:K:238:TRP:HB3	1.95	0.48
1:O:205:SER:OG	1:O:206:LYS:N	2.46	0.48
2:H:9:ASN:C	2:H:11:HIS:N	2.69	0.48
2:V:89:GLN:O	2:V:93:PHE:HB2	2.13	0.48
2:Z:76:PHE:CZ	2:d:87:LYS:CB	2.95	0.48
1:A:163:PHE:O	1:A:166:LEU:N	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PHE:CE2	1:O:202:TYR:CB	2.96	0.48
1:K:194:ASP:N	1:K:194:ASP:OD1	2.45	0.48
1:L:122:GLU:CB	1:L:139:LYS:HG2	2.42	0.48
1:L:192:LEU:HD11	1:L:201:PHE:CE2	2.47	0.48
1:A:211:GLN:O	1:A:212:LYS:C	2.56	0.48
2:I:69:TYR:HB3	2:I:75:GLY:HA2	1.95	0.48
1:K:136:ASP:CG	1:K:138:ASN:HD22	2.22	0.48
2:H:7:THR:OG1	2:H:8:ARG:N	2.43	0.48
2:H:9:ASN:O	2:H:11:HIS:N	2.47	0.48
1:P:27:LEU:HD11	1:P:111:TRP:HE1	1.77	0.48
1:P:109:ASP:O	1:P:144:LYS:NZ	2.40	0.48
1:b:200:LEU:O	1:b:201:PHE:C	2.54	0.48
1:K:48:TYR:OH	1:K:57:LEU:N	2.47	0.48
2:J:17:ASN:O	2:J:21:SER:OG	2.31	0.48
1:T:1:MET:HE1	1:T:257:PHE:HE1	1.78	0.48
2:V:167:MET:HA	2:V:170:LYS:HD2	1.95	0.48
2:Z:89:GLN:O	2:Z:93:PHE:HB2	2.13	0.48
1:b:36:HIS:HA	1:b:39:THR:HG22	1.96	0.48
1:f:31:SER:OG	1:f:49:ARG:NH2	2.43	0.48
1:O:211:GLN:NE2	1:O:213:LEU:HB3	2.24	0.48
1:B:220:SER:HB2	1:B:240:ILE:HG12	1.96	0.48
2:N:129:THR:N	2:N:147:ILE:O	2.42	0.48
1:T:194:ASP:OD1	1:T:196:ASN:ND2	2.47	0.48
2:Z:54:PHE:O	1:f:226:ARG:NH2	2.43	0.48
1:f:194:ASP:O	1:f:196:ASN:N	2.47	0.48
1:A:207:LEU:HG	1:A:211:GLN:HE22	1.79	0.48
1:K:205:SER:O	1:K:206:LYS:C	2.56	0.48
1:O:194:ASP:OD1	1:O:194:ASP:N	2.43	0.48
1:O:237:GLN:C	1:O:239:ARG:H	2.20	0.48
2:d:8:ARG:NH1	2:d:31:GLU:OE1	2.47	0.48
2:d:85:TRP:HA	2:d:85:TRP:CE3	2.48	0.48
2:d:110:ILE:HG12	2:d:123:GLU:HG2	1.96	0.48
1:b:203:LYS:O	1:b:204:LEU:C	2.52	0.48
2:M:1:MET:HB3	2:M:25:VAL:HG12	1.95	0.48
1:K:136:ASP:C	1:K:138:ASN:N	2.71	0.48
2:J:7:THR:HG22	2:J:9:ASN:H	1.79	0.48
1:P:214:GLU:O	1:P:215:GLU:C	2.55	0.48
1:C:163:PHE:HE2	1:O:202:TYR:HB2	1.76	0.48
1:L:138:ASN:HD22	1:L:139:LYS:HG3	1.77	0.48
1:L:194:ASP:HB2	1:L:197:ILE:HG12	1.96	0.48
1:P:201:PHE:HA	1:P:204:LEU:HD12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:204:LEU:O	1:f:207:LEU:HB2	2.14	0.47
1:A:162:TYR:O	1:A:163:PHE:HD1	1.96	0.47
1:O:208:TRP:HD1	1:O:209:LYS:H	1.62	0.47
1:L:138:ASN:HD22	1:L:138:ASN:C	2.22	0.47
1:P:219:LYS:HB3	1:P:220:SER:H	1.54	0.47
1:f:192:LEU:HD11	1:f:201:PHE:CE1	2.49	0.47
1:A:215:GLU:HG2	1:C:130:SER:HA	1.96	0.47
2:F:106:VAL:HG13	2:F:127:GLN:HG3	1.95	0.47
2:J:110:ILE:HG12	2:J:123:GLU:HG2	1.96	0.47
2:N:64:GLU:OE2	2:N:168:ARG:NE	2.47	0.47
1:R:231:GLN:NE2	1:b:56:GLU:OE2	2.41	0.47
1:b:133:ALA:O	1:b:135:ILE:N	2.46	0.47
1:A:207:LEU:C	1:A:209:LYS:N	2.68	0.47
1:O:206:LYS:O	1:O:210:GLU:HG3	2.14	0.47
1:T:44:ASP:HB3	1:T:47:ILE:HG12	1.96	0.47
1:b:209:LYS:CD	1:b:238:TRP:HA	2.39	0.47
1:A:79:TRP:HD1	1:A:109:ASP:HB3	1.80	0.47
1:O:14:ILE:HG23	1:O:102:ILE:HB	1.96	0.47
1:L:194:ASP:OD1	1:L:194:ASP:N	2.47	0.47
2:Z:36:GLU:HB3	2:Z:45:LEU:HD11	1.95	0.47
2:Z:73:LEU:HB2	2:Z:76:PHE:HB2	1.96	0.47
1:f:205:SER:OG	1:f:206:LYS:N	2.46	0.47
1:f:209:LYS:HG3	1:f:210:GLU:N	2.29	0.47
1:A:233:GLU:HG3	1:K:63:LEU:HD23	1.95	0.47
1:K:211:GLN:C	1:K:213:LEU:N	2.72	0.47
1:T:166:LEU:HD22	1:T:199:LEU:HD13	1.96	0.47
2:Z:68:LEU:O	2:Z:78:GLY:N	2.45	0.47
2:d:102:ASN:OD1	2:d:104:ARG:NH1	2.47	0.47
1:B:208:TRP:HA	1:B:208:TRP:CE3	2.49	0.47
2:N:138:ARG:NH1	2:N:144:CYS:SG	2.88	0.47
1:L:133:ALA:C	1:L:135:ILE:N	2.73	0.47
1:L:201:PHE:N	1:L:201:PHE:CD1	2.82	0.47
2:X:160:ASP:HA	2:X:163:ASN:HD22	1.79	0.47
1:b:7:ASP:HA	1:b:10:LYS:HD2	1.97	0.47
1:K:208:TRP:C	1:K:210:GLU:N	2.73	0.47
1:K:213:LEU:O	1:K:213:LEU:HG	2.15	0.47
1:B:208:TRP:CE3	1:B:208:TRP:CA	2.97	0.47
1:D:163:PHE:CE1	1:P:199:LEU:HD22	2.50	0.47
2:F:108:LYS:HG2	2:F:125:GLU:HB3	1.97	0.47
1:L:12:ASN:OD1	1:L:183:LYS:NZ	2.44	0.47
1:L:138:ASN:O	1:L:139:LYS:HB2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:208:TRP:CD1	1:L:209:LYS:HG2	2.49	0.47
1:P:209:LYS:HA	1:P:239:ARG:NE	2.30	0.47
1:R:214:GLU:O	1:R:216:ALA:N	2.48	0.47
1:R:215:GLU:OE2	1:R:215:GLU:N	2.47	0.47
1:f:4:LEU:HD21	1:f:186:LEU:HD21	1.97	0.47
1:C:23:MET:HE2	1:C:23:MET:HB2	1.66	0.47
1:D:217:GLN:O	1:D:218:PRO:C	2.58	0.47
2:X:50:LEU:HD13	2:X:63:VAL:HG22	1.97	0.47
2:Z:80:LEU:HD13	2:d:80:LEU:HD13	1.97	0.47
1:b:201:PHE:O	1:b:204:LEU:HB2	2.15	0.47
2:F:70:ILE:HG22	2:F:73:LEU:H	1.80	0.47
1:T:60:TYR:HB2	1:f:230:ILE:HG23	1.95	0.47
1:f:217:GLN:O	1:f:218:PRO:C	2.57	0.47
2:G:126:THR:OG1	2:G:170:LYS:NZ	2.42	0.47
1:O:1:MET:SD	1:O:1:MET:N	2.78	0.47
1:B:35:ASP:HA	1:B:45:PRO:HB3	1.96	0.47
1:P:197:ILE:HG23	1:P:201:PHE:CE1	2.50	0.47
1:T:64:LYS:HA	1:T:64:LYS:HD3	1.77	0.46
1:b:209:LYS:HE3	1:b:238:TRP:HA	1.96	0.46
2:H:11:HIS:HA	2:H:14:LYS:HE2	1.97	0.46
1:P:197:ILE:HG22	1:P:198:ARG:N	2.29	0.46
2:V:35:ASP:OD1	2:V:35:ASP:N	2.38	0.46
1:f:215:GLU:HB2	1:f:216:ALA:H	1.48	0.46
1:K:85:ASP:HB3	1:K:88:LYS:HG2	1.96	0.46
1:O:214:GLU:OE1	1:O:215:GLU:HG3	2.14	0.46
2:J:104:ARG:NH2	2:J:127:GLN:OE1	2.47	0.46
2:N:8:ARG:NH1	2:N:31:GLU:OE1	2.48	0.46
2:F:136:GLY:O	2:F:138:ARG:NH1	2.48	0.46
2:H:62:PHE:HB3	2:H:113:TYR:HD1	1.81	0.46
1:R:159:GLU:O	1:R:163:PHE:N	2.35	0.46
1:R:208:TRP:CD1	1:R:217:GLN:CG	2.85	0.46
1:b:207:LEU:HA	1:b:210:GLU:CD	2.41	0.46
1:O:200:LEU:O	1:O:203:LYS:N	2.49	0.46
2:H:148:PRO:HG2	2:H:151:GLU:HB2	1.97	0.46
1:L:167:GLU:O	1:L:168:PHE:CD2	2.69	0.46
1:A:158:ASP:O	1:A:162:TYR:N	2.49	0.46
1:A:163:PHE:O	1:A:165:ARG:N	2.48	0.46
1:C:252:GLU:HA	1:C:255:GLU:HB3	1.97	0.46
2:G:30:SER:HG	2:G:32:HIS:HD1	1.60	0.46
1:K:202:TYR:O	1:K:205:SER:N	2.48	0.46
1:B:150:ASP:OD1	1:B:150:ASP:N	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:70:ILE:O	2:V:75:GLY:N	2.43	0.46
1:b:18:GLY:O	1:b:107:ASN:ND2	2.48	0.46
1:f:181:LEU:HD23	1:f:217:GLN:HE22	1.80	0.46
1:f:209:LYS:O	1:f:210:GLU:C	2.57	0.46
1:O:175:LYS:NZ	1:O:179:ASP:OD2	2.45	0.46
2:H:8:ARG:NH1	2:H:31:GLU:O	2.49	0.46
1:T:53:SER:OG	1:f:198:ARG:NH1	2.49	0.46
1:A:85:ASP:O	1:A:88:LYS:NZ	2.48	0.46
2:I:141:GLN:OE1	2:I:142:TRP:N	2.49	0.46
1:B:56:GLU:HG2	1:B:159:GLU:HG3	1.97	0.46
2:H:8:ARG:HB3	2:H:8:ARG:CZ	2.45	0.46
2:X:69:TYR:N	2:X:106:VAL:O	2.46	0.46
1:f:23:MET:HE3	1:f:23:MET:HB3	1.65	0.46
1:f:185:VAL:H	1:f:220:SER:HB2	1.81	0.46
1:K:14:ILE:HD12	1:K:102:ILE:HB	1.97	0.46
1:B:208:TRP:HA	1:B:208:TRP:HE3	1.80	0.46
2:J:54:PHE:O	1:P:226:ARG:NH1	2.40	0.46
1:R:21:VAL:HG23	1:R:254:LEU:HD21	1.98	0.46
2:d:86:ASP:HA	2:d:89:GLN:HE21	1.81	0.46
1:b:36:HIS:ND1	1:b:40:GLU:OE2	2.42	0.46
2:E:39:THR:H	2:E:45:LEU:HD21	1.81	0.46
1:O:212:LYS:HZ3	1:O:213:LEU:N	2.00	0.46
1:L:129:VAL:HG13	1:L:130:SER:N	2.28	0.46
1:L:184:SER:HB2	1:L:218:PRO:CB	2.28	0.46
1:L:216:ALA:O	1:L:217:GLN:C	2.58	0.46
1:P:195:ILE:O	1:P:198:ARG:N	2.49	0.46
1:f:178:SER:HA	1:f:181:LEU:HD12	1.98	0.45
1:B:209:LYS:HG2	1:B:209:LYS:H	1.44	0.45
2:H:11:HIS:O	2:H:13:ILE:N	2.50	0.45
1:P:165:ARG:NH2	1:P:173:ASP:OD1	2.49	0.45
1:b:57:LEU:HD12	1:b:60:TYR:HB3	1.98	0.45
1:b:249:ASN:O	1:b:253:SER:OG	2.32	0.45
1:A:248:ASP:HB2	2:G:32:HIS:HE1	1.80	0.45
1:L:135:ILE:HA	1:L:141:GLN:HE22	1.82	0.45
1:b:59:GLU:HA	1:b:62:LYS:HG2	1.98	0.45
2:E:17:ASN:O	2:E:21:SER:OG	2.34	0.45
1:K:109:ASP:OD1	1:K:109:ASP:N	2.37	0.45
1:K:198:ARG:O	1:K:201:PHE:HB2	2.16	0.45
1:O:109:ASP:O	1:O:144:LYS:NZ	2.39	0.45
1:B:181:LEU:HD21	1:B:208:TRP:CE3	2.52	0.45
1:b:75:MET:HE1	1:b:157:LEU:HD21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:91:ASP:N	2:I:91:ASP:OD1	2.46	0.45
1:O:85:ASP:OD1	1:O:85:ASP:N	2.48	0.45
1:D:35:ASP:HA	1:D:45:PRO:HB3	1.97	0.45
2:H:70:ILE:HB	2:H:73:LEU:HB2	1.98	0.45
1:L:78:MET:HE2	1:L:78:MET:HB3	1.75	0.45
1:T:162:TYR:OH	1:T:196:ASN:ND2	2.49	0.45
2:d:70:ILE:HB	2:d:73:LEU:HB2	1.98	0.45
1:A:162:TYR:O	1:A:163:PHE:CD1	2.70	0.45
2:E:5:PHE:HE1	2:E:63:VAL:HA	1.81	0.45
1:K:219:LYS:HA	1:K:239:ARG:HH22	1.81	0.45
1:O:204:LEU:C	1:O:206:LYS:N	2.74	0.45
1:B:231:GLN:NE2	1:L:56:GLU:OE2	2.50	0.45
1:D:75:MET:O	1:D:79:TRP:HB2	2.17	0.45
1:R:56:GLU:HB2	1:b:234:ILE:CD1	2.47	0.45
1:f:53:SER:OG	1:f:54:ALA:N	2.49	0.45
1:K:194:ASP:O	1:K:198:ARG:HG3	2.16	0.45
1:K:203:LYS:O	1:K:204:LEU:C	2.58	0.45
1:B:56:GLU:CD	1:L:234:ILE:HD13	2.42	0.45
1:P:215:GLU:HB2	1:P:216:ALA:H	1.49	0.45
1:P:217:GLN:HE21	1:P:239:ARG:HH12	1.65	0.45
1:f:195:ILE:HG13	1:f:196:ASN:N	2.32	0.45
1:f:199:LEU:O	1:f:202:TYR:N	2.50	0.45
1:K:206:LYS:HB3	1:K:210:GLU:CD	2.42	0.45
1:B:37:ILE:HD12	1:B:37:ILE:HA	1.88	0.45
1:B:64:LYS:HA	1:B:64:LYS:HD3	1.72	0.45
1:R:64:LYS:HD3	1:R:64:LYS:HA	1.77	0.45
1:R:83:ASP:OD1	1:R:83:ASP:N	2.49	0.45
1:T:204:LEU:HD22	1:T:208:TRP:CZ2	2.52	0.45
1:A:152:ASP:N	1:A:152:ASP:OD1	2.50	0.45
2:M:167:MET:SD	2:M:167:MET:N	2.79	0.45
1:P:14:ILE:O	1:P:186:LEU:N	2.50	0.45
1:P:208:TRP:CG	1:P:209:LYS:N	2.80	0.45
1:P:211:GLN:O	1:P:239:ARG:NH2	2.49	0.45
1:T:229:PRO:HD2	1:f:51:PHE:HE2	1.82	0.45
1:b:116:LEU:HD12	1:b:142:ILE:HD11	1.99	0.45
1:A:37:ILE:HD12	1:A:37:ILE:HA	1.70	0.45
2:G:139:ASP:OD1	2:G:139:ASP:N	2.45	0.45
1:K:125:LYS:HE3	1:K:125:LYS:HB3	1.73	0.45
1:K:195:ILE:HG23	1:K:196:ASN:N	2.30	0.45
2:H:11:HIS:O	2:H:14:LYS:N	2.50	0.45
2:J:167:MET:HA	2:J:170:LYS:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:14:ILE:HB	1:P:185:VAL:HG12	1.99	0.45
2:X:77:PRO:O	2:X:81:THR:OG1	2.35	0.45
1:b:37:ILE:H	1:b:40:GLU:HG3	1.82	0.45
1:f:75:MET:O	1:f:79:TRP:HB2	2.17	0.45
1:f:245:SER:OG	1:f:246:GLU:N	2.48	0.45
1:C:208:TRP:O	1:C:211:GLN:O	2.34	0.45
2:I:32:HIS:HD2	2:I:56:LEU:HD22	1.82	0.45
2:M:8:ARG:HD3	2:M:8:ARG:HA	1.78	0.45
2:M:64:GLU:OE2	2:M:168:ARG:NE	2.49	0.45
1:K:122:GLU:O	1:K:139:LYS:HB3	2.17	0.45
1:O:64:LYS:HA	1:O:64:LYS:HD3	1.77	0.45
1:B:160:THR:O	1:B:164:GLN:HG2	2.17	0.45
1:D:198:ARG:HH12	1:D:231:GLN:HE22	1.64	0.45
1:L:201:PHE:HD1	1:L:201:PHE:N	2.13	0.45
2:Z:30:SER:OG	1:f:248:ASP:OD2	2.33	0.44
2:Z:77:PRO:O	2:Z:78:GLY:C	2.60	0.44
1:A:217:GLN:HB2	1:A:217:GLN:HE21	1.48	0.44
1:C:14:ILE:HG23	1:C:102:ILE:HB	2.00	0.44
1:K:212:LYS:HE2	1:K:212:LYS:HB2	1.36	0.44
1:O:235:LEU:CD1	1:O:240:ILE:HG13	2.47	0.44
1:R:192:LEU:HD21	1:R:235:LEU:HD11	1.99	0.44
2:Z:19:ILE:HG21	2:Z:172:PHE:HB3	1.99	0.44
1:b:212:LYS:HB2	1:b:212:LYS:HE2	1.58	0.44
1:f:211:GLN:HA	1:f:212:LYS:HZ3	1.82	0.44
2:I:125:GLU:O	2:I:170:LYS:NZ	2.44	0.44
1:K:196:ASN:O	1:K:199:LEU:N	2.50	0.44
1:O:209:LYS:HA	1:O:239:ARG:NH1	2.32	0.44
1:O:215:GLU:HB2	1:O:216:ALA:H	1.54	0.44
2:H:10:ARG:C	2:H:13:ILE:CG2	2.90	0.44
1:L:46:ASP:O	1:L:48:TYR:N	2.40	0.44
1:L:135:ILE:HA	1:L:141:GLN:NE2	2.32	0.44
1:P:207:LEU:O	1:P:210:GLU:HB3	2.17	0.44
1:R:53:SER:H	1:R:56:GLU:HG3	1.82	0.44
1:R:70:PRO:HD3	1:L:150:ASP:HB3	1.99	0.44
2:d:19:ILE:HG21	2:d:172:PHE:HB3	1.99	0.44
2:E:2:ASN:HD22	2:E:28:LEU:HD11	1.83	0.44
1:B:162:TYR:CG	1:B:162:TYR:O	2.70	0.44
2:Z:77:PRO:HB3	2:Z:81:THR:HG23	1.99	0.44
2:Z:160:ASP:N	2:Z:160:ASP:OD1	2.47	0.44
1:b:199:LEU:HD12	1:b:199:LEU:HA	1.64	0.44
1:K:239:ARG:HD2	1:K:239:ARG:HA	1.62	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:ARG:NH2	1:O:173:ASP:OD1	2.47	0.44
1:B:68:ILE:HD11	1:B:157:LEU:HB2	2.00	0.44
1:D:83:ASP:OD1	1:D:83:ASP:N	2.51	0.44
1:L:199:LEU:O	1:L:202:TYR:N	2.50	0.44
1:P:212:LYS:HB3	1:P:213:LEU:HD23	1.99	0.44
1:R:228:ASN:HD21	1:b:51:PHE:HB3	1.83	0.44
2:Z:50:LEU:HD21	2:Z:114:CYS:HB3	1.98	0.44
1:b:205:SER:OG	1:b:206:LYS:N	2.49	0.44
1:b:220:SER:O	1:b:241:GLY:N	2.37	0.44
2:F:10:ARG:HA	2:F:13:ILE:HD11	1.98	0.44
2:F:104:ARG:HH11	2:F:129:THR:HG23	1.83	0.44
1:D:46:ASP:HB3	2:J:51:LEU:HD11	1.99	0.44
1:D:85:ASP:HB3	1:D:88:LYS:HG2	1.99	0.44
1:R:52:GLY:HA3	1:R:56:GLU:OE2	2.18	0.44
1:f:235:LEU:CD1	1:f:240:ILE:HG13	2.46	0.44
1:K:98:ALA:O	1:K:121:LYS:NZ	2.41	0.44
1:K:124:ILE:O	1:K:126:ILE:HD12	2.18	0.44
2:J:69:TYR:HB2	2:J:106:VAL:HG13	1.99	0.44
1:R:211:GLN:O	1:R:213:LEU:HG	2.17	0.44
1:R:219:LYS:O	1:R:221:TYR:CE2	2.71	0.44
1:T:245:SER:OG	1:T:246:GLU:N	2.51	0.44
1:b:197:ILE:HG22	1:b:201:PHE:CE1	2.53	0.44
1:f:177:ARG:HG3	1:f:207:LEU:HD12	1.99	0.44
1:f:204:LEU:HA	1:f:207:LEU:HD23	2.00	0.44
1:O:210:GLU:C	1:O:212:LYS:N	2.76	0.44
2:N:4:ARG:HG2	2:N:57:VAL:HG21	2.00	0.44
1:L:204:LEU:O	1:L:205:SER:C	2.60	0.44
1:L:213:LEU:O	1:L:214:GLU:HB3	2.18	0.44
1:P:16:PHE:HB3	1:P:190:TYR:OH	2.17	0.44
1:b:213:LEU:O	1:b:215:GLU:HG3	2.18	0.44
1:K:211:GLN:C	1:K:213:LEU:H	2.26	0.44
2:F:10:ARG:C	2:F:13:ILE:HG13	2.43	0.44
2:H:2:ASN:HD22	2:H:28:LEU:HD11	1.82	0.44
2:H:10:ARG:HA	2:H:13:ILE:HG21	1.99	0.44
2:H:10:ARG:HA	2:H:10:ARG:HD3	1.51	0.44
2:N:80:LEU:HB3	2:N:83:ILE:HB	2.00	0.44
1:L:165:ARG:C	1:L:167:GLU:N	2.75	0.44
1:P:219:LYS:HZ1	1:P:240:ILE:N	2.16	0.44
1:R:72:ARG:HA	1:R:75:MET:HG3	2.00	0.43
2:V:110:ILE:HG12	2:V:123:GLU:HG3	1.99	0.43
1:b:130:SER:C	1:b:132:ILE:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:OD1	1:A:49:ARG:NH2	2.39	0.43
1:P:210:GLU:O	1:P:211:GLN:C	2.61	0.43
1:T:217:GLN:HA	1:T:218:PRO:HD2	1.88	0.43
1:b:183:LYS:C	1:b:218:PRO:HG2	2.43	0.43
1:K:219:LYS:CA	1:K:239:ARG:HH12	2.15	0.43
1:O:201:PHE:CA	1:O:204:LEU:HD12	2.43	0.43
1:L:131:ASP:C	1:L:133:ALA:N	2.76	0.43
1:R:164:GLN:C	1:R:166:LEU:N	2.76	0.43
1:T:231:GLN:HA	1:T:234:ILE:HG22	2.00	0.43
2:V:36:GLU:HB3	2:V:45:LEU:HD11	2.00	0.43
2:X:8:ARG:HD2	2:X:8:ARG:HA	1.90	0.43
1:b:211:GLN:HB3	1:b:215:GLU:OE1	2.18	0.43
2:M:139:ASP:OD1	2:M:139:ASP:N	2.49	0.43
1:K:184:SER:HB3	1:K:219:LYS:O	2.18	0.43
1:B:22:SER:O	1:B:22:SER:OG	2.35	0.43
2:J:4:ARG:HB2	2:J:61:VAL:HG12	1.99	0.43
1:P:212:LYS:H	1:P:212:LYS:CE	2.30	0.43
1:f:212:LYS:HZ3	1:f:212:LYS:N	2.15	0.43
1:K:199:LEU:HD12	1:K:202:TYR:HB3	2.00	0.43
1:D:165:ARG:NH2	1:D:173:ASP:OD2	2.51	0.43
2:F:10:ARG:O	2:F:11:HIS:C	2.58	0.43
1:L:245:SER:OG	1:L:246:GLU:N	2.52	0.43
1:P:116:LEU:HD22	1:P:121:LYS:HB3	2.00	0.43
1:P:196:ASN:N	1:P:196:ASN:OD1	2.52	0.43
2:Z:158:MET:HB2	2:Z:161:ARG:HG2	2.00	0.43
1:f:210:GLU:H	1:f:210:GLU:HG3	1.51	0.43
1:f:212:LYS:HE2	1:f:213:LEU:H	1.84	0.43
2:G:72:SER:HB3	2:G:102:ASN:HB3	1.98	0.43
2:G:129:THR:N	2:G:147:ILE:O	2.45	0.43
1:D:44:ASP:OD1	2:J:119:ILE:N	2.52	0.43
2:F:169:LYS:NZ	2:F:173:ASP:OD1	2.49	0.43
1:L:126:ILE:HG23	1:L:143:ILE:HG12	2.00	0.43
1:L:210:GLU:HB3	1:L:211:GLN:H	1.59	0.43
1:A:59:GLU:HB3	1:K:234:ILE:HD11	2.00	0.43
1:C:83:ASP:OD1	1:C:83:ASP:N	2.52	0.43
1:C:228:ASN:HB3	1:C:231:GLN:HB2	2.01	0.43
1:K:4:LEU:HD11	1:K:186:LEU:HD22	2.00	0.43
1:K:207:LEU:HA	1:K:210:GLU:OE1	2.17	0.43
1:O:210:GLU:O	1:O:212:LYS:N	2.52	0.43
1:D:63:LEU:HD11	1:P:237:GLN:HE22	1.83	0.43
1:D:64:LYS:HA	1:D:64:LYS:HD3	1.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:LYS:HD3	1:L:65:LYS:HA	1.86	0.43
1:R:59:GLU:OE2	1:R:158:ASP:HB2	2.18	0.43
1:R:98:ALA:O	1:R:121:LYS:NZ	2.52	0.43
1:b:14:ILE:HG23	1:b:102:ILE:HB	2.01	0.43
1:b:28:PRO:HG2	1:b:78:MET:HB3	2.01	0.43
2:E:104:ARG:HH11	2:E:129:THR:HG23	1.84	0.43
1:K:195:ILE:O	1:K:198:ARG:N	2.51	0.43
2:F:92:LYS:HB3	2:F:92:LYS:HE3	1.81	0.43
1:P:212:LYS:HE2	1:P:212:LYS:HB2	1.56	0.43
1:b:209:LYS:C	1:b:211:GLN:N	2.73	0.43
1:f:98:ALA:O	1:f:121:LYS:NZ	2.51	0.43
1:A:205:SER:OG	1:A:206:LYS:N	2.50	0.43
1:O:212:LYS:O	1:O:213:LEU:C	2.62	0.43
2:F:8:ARG:HH11	2:F:31:GLU:HB2	1.84	0.43
1:T:24:ASN:O	1:T:88:LYS:NZ	2.43	0.43
2:d:38:GLN:N	2:d:38:GLN:OE1	2.51	0.43
1:b:21:VAL:HG12	1:b:254:LEU:HD21	2.01	0.43
1:b:124:ILE:CG1	1:b:139:LYS:HB2	2.39	0.43
1:b:186:LEU:HG	1:b:188:ILE:CD1	2.48	0.43
1:f:192:LEU:HD12	1:f:192:LEU:HA	1.78	0.43
1:A:64:LYS:HA	1:A:64:LYS:HD3	1.80	0.43
2:G:69:TYR:HB2	2:G:106:VAL:HB	2.01	0.43
2:I:98:GLY:HA2	2:I:130:ILE:HG23	2.01	0.43
1:L:194:ASP:O	1:L:197:ILE:N	2.52	0.43
1:L:203:LYS:O	1:L:204:LEU:C	2.61	0.43
1:T:247:ASN:ND2	1:T:252:GLU:OE1	2.52	0.43
2:Z:79:GLY:C	2:Z:81:THR:N	2.74	0.43
2:d:57:VAL:HG12	2:d:59:ARG:H	1.83	0.43
1:b:130:SER:C	1:b:132:ILE:N	2.76	0.43
1:b:195:ILE:HA	1:b:198:ARG:HD3	2.00	0.43
2:M:77:PRO:O	2:M:81:THR:OG1	2.37	0.43
2:M:161:ARG:H	2:M:161:ARG:HG3	1.60	0.43
1:K:162:TYR:CE2	1:K:196:ASN:HB3	2.53	0.43
1:K:200:LEU:O	1:K:201:PHE:C	2.60	0.43
1:K:219:LYS:HG2	1:K:239:ARG:CZ	2.49	0.43
1:B:148:ASP:OD1	1:B:149:PHE:N	2.44	0.43
2:N:73:LEU:HD13	2:N:97:LEU:HD21	2.01	0.43
1:L:131:ASP:HA	1:L:134:LYS:HG2	2.00	0.43
1:R:211:GLN:O	1:R:213:LEU:N	2.52	0.42
1:b:209:LYS:O	1:b:211:GLN:N	2.52	0.42
1:f:192:LEU:HD12	1:f:197:ILE:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:206:LYS:HA	1:f:209:LYS:HB3	2.01	0.42
1:f:242:MET:HE2	1:f:242:MET:HB3	1.80	0.42
2:M:47:LYS:HE2	2:M:47:LYS:HB2	1.93	0.42
1:K:138:ASN:ND2	1:K:138:ASN:H	2.16	0.42
1:O:53:SER:OG	1:O:54:ALA:N	2.50	0.42
1:O:195:ILE:O	1:O:198:ARG:N	2.52	0.42
2:F:90:ALA:O	2:F:94:SER:OG	2.32	0.42
2:V:87:LYS:NZ	2:X:74:ASN:O	2.42	0.42
1:b:128:SER:O	1:b:130:SER:N	2.51	0.42
1:f:116:LEU:HD22	1:f:121:LYS:HB3	2.02	0.42
1:f:214:GLU:OE1	1:f:215:GLU:HG3	2.20	0.42
1:C:75:MET:HE2	1:C:75:MET:HB3	1.89	0.42
2:G:13:ILE:HG21	2:G:29:ALA:HB2	2.01	0.42
1:D:53:SER:OG	1:P:198:ARG:NH2	2.53	0.42
2:N:2:ASN:HD22	2:N:28:LEU:HD11	1.84	0.42
1:L:165:ARG:O	1:L:166:LEU:C	2.62	0.42
1:L:228:ASN:ND2	1:L:231:GLN:OE1	2.52	0.42
1:P:231:GLN:OE1	1:P:231:GLN:N	2.52	0.42
1:R:164:GLN:NE2	1:b:202:TYR:OH	2.52	0.42
2:d:8:ARG:HD3	2:d:8:ARG:HA	1.80	0.42
1:b:214:GLU:CG	1:b:215:GLU:H	2.33	0.42
1:B:14:ILE:HG23	1:B:102:ILE:HB	2.02	0.42
1:D:17:VAL:HG11	1:D:112:ILE:HD11	2.01	0.42
2:N:8:ARG:HA	2:N:8:ARG:HD3	1.77	0.42
1:P:79:TRP:HE3	1:P:109:ASP:HB3	1.84	0.42
1:P:175:LYS:NZ	1:P:179:ASP:OD2	2.52	0.42
1:b:213:LEU:O	1:b:214:GLU:C	2.61	0.42
1:f:212:LYS:HZ2	1:f:212:LYS:HG3	1.60	0.42
1:B:83:ASP:N	1:B:83:ASP:OD1	2.50	0.42
1:D:38:ALA:O	1:D:43:TYR:N	2.46	0.42
1:D:56:GLU:O	1:D:57:LEU:C	2.62	0.42
2:H:10:ARG:C	2:H:13:ILE:HG22	2.44	0.42
2:N:87:LYS:HD3	2:N:87:LYS:HA	1.88	0.42
2:Z:115:ASP:OD1	2:Z:115:ASP:N	2.52	0.42
1:b:166:LEU:HD13	1:b:166:LEU:HA	1.72	0.42
1:b:216:ALA:O	1:b:217:GLN:HB2	2.18	0.42
1:b:221:TYR:HD1	1:b:241:GLY:HA3	1.84	0.42
1:b:235:LEU:HD22	1:b:240:ILE:HG21	2.01	0.42
1:A:33:LEU:O	1:A:37:ILE:HB	2.20	0.42
1:C:56:GLU:OE2	1:C:56:GLU:N	2.53	0.42
1:B:208:TRP:CE2	1:B:217:GLN:NE2	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:TYR:HD2	2:F:77:PRO:HB2	1.84	0.42
1:R:207:LEU:O	1:R:210:GLU:HG2	2.20	0.42
1:R:214:GLU:C	1:R:216:ALA:N	2.76	0.42
2:X:46:ILE:HD13	2:X:46:ILE:HA	1.90	0.42
1:b:201:PHE:N	1:b:201:PHE:CD1	2.88	0.42
1:b:202:TYR:O	1:b:205:SER:N	2.52	0.42
1:b:208:TRP:CZ2	1:b:240:ILE:HD11	2.53	0.42
1:A:161:SER:C	1:A:163:PHE:N	2.77	0.42
1:A:209:LYS:C	1:A:211:GLN:N	2.77	0.42
1:O:209:LYS:CE	1:O:210:GLU:H	2.32	0.42
1:D:257:PHE:O	1:D:260:ASN:ND2	2.46	0.42
2:H:8:ARG:HA	2:H:10:ARG:CZ	2.49	0.42
2:J:134:PRO:O	2:J:138:ARG:NH2	2.53	0.42
1:L:124:ILE:H	1:L:124:ILE:HG12	1.69	0.42
1:L:202:TYR:CZ	1:L:206:LYS:HE2	2.54	0.42
1:P:75:MET:O	1:P:79:TRP:HB2	2.20	0.42
1:P:208:TRP:O	1:P:209:LYS:C	2.61	0.42
1:T:14:ILE:HD11	1:T:183:LYS:HD2	2.02	0.42
1:b:206:LYS:HZ3	1:b:206:LYS:HG3	1.56	0.42
1:f:208:TRP:O	1:f:209:LYS:C	2.63	0.42
2:G:7:THR:O	2:G:10:ARG:NH2	2.53	0.42
2:G:16:ILE:HA	2:G:19:ILE:HB	2.01	0.42
1:D:181:LEU:HD11	1:D:213:LEU:HD11	2.01	0.42
2:F:60:PRO:HB3	2:F:115:ASP:HA	2.01	0.42
2:H:9:ASN:C	2:H:11:HIS:H	2.27	0.42
1:R:85:ASP:OD1	1:R:87:ASN:ND2	2.53	0.42
1:T:35:ASP:HA	1:T:45:PRO:HB3	2.02	0.42
1:b:67:LYS:HE2	1:b:67:LYS:HB2	1.92	0.42
1:b:228:ASN:HA	1:b:229:PRO:HD3	1.83	0.42
1:f:203:LYS:O	1:f:204:LEU:C	2.63	0.42
1:K:59:GLU:OE1	1:K:160:THR:OG1	2.34	0.42
1:D:30:TRP:O	1:D:33:LEU:N	2.52	0.42
2:H:158:MET:SD	2:H:161:ARG:NH2	2.92	0.42
1:L:128:SER:N	1:L:131:ASP:OD2	2.53	0.42
1:L:130:SER:O	1:L:132:ILE:N	2.53	0.42
1:P:197:ILE:HG23	1:P:201:PHE:CD1	2.55	0.42
1:R:23:MET:H	1:R:23:MET:HG3	1.58	0.42
1:b:83:ASP:OD1	1:b:83:ASP:N	2.47	0.42
1:b:183:LYS:HA	1:b:218:PRO:HG2	2.02	0.42
1:b:187:PHE:CD2	1:b:201:PHE:CE2	3.07	0.42
1:f:192:LEU:HD12	1:f:197:ILE:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:212:LYS:O	1:f:213:LEU:C	2.61	0.42
1:K:131:ASP:O	1:K:134:LYS:N	2.52	0.42
1:O:124:ILE:HD11	1:O:139:LYS:HD2	2.01	0.42
1:B:195:ILE:HG22	1:B:199:LEU:HD23	2.02	0.42
2:N:110:ILE:HG12	2:N:123:GLU:HG2	2.01	0.42
1:L:103:ILE:HG23	1:L:142:ILE:HA	2.00	0.42
1:L:211:GLN:HE21	1:L:211:GLN:HB2	1.60	0.42
2:V:72:SER:O	2:X:92:LYS:NZ	2.41	0.42
2:V:77:PRO:HB2	2:V:81:THR:HG22	2.02	0.42
1:O:197:ILE:HG23	1:O:201:PHE:CE1	2.55	0.42
1:D:56:GLU:O	1:D:59:GLU:HB2	2.20	0.42
1:D:245:SER:O	2:N:59:ARG:NH2	2.51	0.42
2:F:92:LYS:HA	2:F:95:GLN:HE21	1.84	0.42
2:F:110:ILE:HG12	2:F:123:GLU:HG3	2.02	0.42
1:L:131:ASP:OD1	1:L:131:ASP:N	2.50	0.42
1:C:163:PHE:CE1	1:O:199:LEU:HD22	2.55	0.41
1:K:37:ILE:HG21	1:K:71:LEU:HD13	2.02	0.41
1:K:204:LEU:HA	1:K:207:LEU:CD2	2.50	0.41
1:O:210:GLU:OE1	1:O:211:GLN:N	2.53	0.41
2:F:9:ASN:H	2:F:9:ASN:ND2	2.18	0.41
2:H:98:GLY:HA3	2:H:132:PRO:HA	2.02	0.41
2:J:19:ILE:HG21	2:J:172:PHE:HB3	2.01	0.41
2:N:10:ARG:O	2:N:10:ARG:NH1	2.44	0.41
1:P:202:TYR:HA	1:P:205:SER:HB3	2.02	0.41
2:Z:62:PHE:HA	2:Z:113:TYR:HA	2.02	0.41
1:b:129:VAL:O	1:b:132:ILE:HB	2.20	0.41
1:b:199:LEU:O	1:b:202:TYR:N	2.52	0.41
1:f:28:PRO:HG2	1:f:79:TRP:CD1	2.56	0.41
1:f:144:LYS:HE2	1:f:148:ASP:HB3	2.02	0.41
1:C:37:ILE:HA	1:C:40:GLU:HB2	2.02	0.41
1:C:163:PHE:CD2	1:O:202:TYR:CB	3.03	0.41
2:I:56:LEU:HD23	2:I:56:LEU:HA	1.92	0.41
1:K:104:TYR:CZ	1:K:143:ILE:HD12	2.55	0.41
1:O:219:LYS:NZ	1:O:219:LYS:HB3	2.33	0.41
2:H:84:PHE:O	2:H:88:LEU:HB2	2.20	0.41
1:L:64:LYS:HA	1:L:64:LYS:HD3	1.84	0.41
1:L:125:LYS:NZ	1:L:150:ASP:OD2	2.53	0.41
2:X:17:ASN:HD21	2:X:27:VAL:H	1.68	0.41
1:b:195:ILE:HG23	1:b:196:ASN:N	2.32	0.41
1:f:89:SER:OG	1:f:92:HIS:ND1	2.38	0.41
2:E:143:ASP:O	2:E:156:ALA:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:103:ILE:HG23	1:K:142:ILE:HA	2.02	0.41
1:B:245:SER:OG	1:B:246:GLU:N	2.53	0.41
2:N:158:MET:HB3	2:N:161:ARG:HB3	2.02	0.41
1:L:205:SER:HB2	1:L:209:LYS:HD3	2.02	0.41
1:P:167:GLU:N	1:P:167:GLU:OE2	2.53	0.41
1:P:203:LYS:HE2	1:P:203:LYS:HB2	1.81	0.41
1:T:23:MET:HE3	1:T:23:MET:HB3	1.65	0.41
1:T:59:GLU:HG2	1:T:158:ASP:HB2	2.02	0.41
2:Z:76:PHE:CE1	2:d:84:PHE:CD1	3.08	0.41
2:d:139:ASP:N	2:d:139:ASP:OD1	2.48	0.41
1:b:217:GLN:N	1:b:218:PRO:HD3	2.35	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.94	0.41
1:D:242:MET:HE2	1:D:242:MET:HB3	1.89	0.41
2:X:83:ILE:O	2:X:87:LYS:HB2	2.20	0.41
1:b:64:LYS:HD3	1:b:64:LYS:HA	1.82	0.41
1:f:14:ILE:HB	1:f:185:VAL:HG22	2.03	0.41
1:O:220:SER:O	1:O:221:TYR:CD2	2.74	0.41
1:O:249:ASN:OD1	1:O:249:ASN:N	2.46	0.41
2:V:80:LEU:O	2:V:84:PHE:HB2	2.20	0.41
2:G:180:LEU:HD23	2:G:180:LEU:HA	1.93	0.41
1:K:201:PHE:O	1:K:204:LEU:HB2	2.20	0.41
1:K:214:GLU:CD	1:K:215:GLU:N	2.78	0.41
2:J:143:ASP:OD2	2:J:162:LYS:NZ	2.47	0.41
1:T:173:ASP:OD1	1:T:173:ASP:N	2.53	0.41
1:C:217:GLN:O	1:C:217:GLN:HG3	2.21	0.41
2:I:167:MET:SD	2:I:167:MET:N	2.94	0.41
2:M:20:LEU:HD23	2:M:176:LYS:HD3	2.02	0.41
1:K:124:ILE:HG13	1:K:139:LYS:HD2	2.03	0.41
1:K:135:ILE:HD11	1:K:175:LYS:HE2	2.03	0.41
1:O:195:ILE:HG13	1:O:196:ASN:N	2.36	0.41
1:B:208:TRP:CE3	1:B:208:TRP:N	2.89	0.41
2:H:49:LYS:HG2	2:H:63:VAL:HG11	2.02	0.41
2:H:105:LEU:HD22	2:H:130:ILE:HG13	2.02	0.41
2:J:137:PRO:HD2	2:J:156:ALA:HB1	2.03	0.41
2:N:69:TYR:HA	2:N:77:PRO:HG2	2.03	0.41
1:R:23:MET:HE2	1:R:23:MET:HB2	1.77	0.41
2:Z:68:LEU:HB2	2:Z:77:PRO:HB2	2.02	0.41
2:d:131:SER:HB3	2:d:145:ILE:HA	2.03	0.41
1:b:214:GLU:C	1:b:215:GLU:HG3	2.46	0.41
1:f:59:GLU:OE1	1:f:160:THR:N	2.50	0.41
1:f:252:GLU:H	1:f:252:GLU:HG3	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:HIS:O	2:E:15:GLU:HB2	2.20	0.41
1:K:204:LEU:HA	1:K:207:LEU:HD23	2.03	0.41
1:O:197:ILE:HG23	1:O:201:PHE:HE1	1.86	0.41
1:B:17:VAL:HG22	1:B:188:ILE:HD11	2.01	0.41
1:B:199:LEU:HD13	1:B:199:LEU:HA	1.91	0.41
1:B:207:LEU:HA	1:B:207:LEU:HD12	1.71	0.41
1:D:79:TRP:HD1	1:D:109:ASP:HB3	1.86	0.41
1:L:129:VAL:O	1:L:132:ILE:HB	2.20	0.41
1:L:209:LYS:H	1:L:209:LYS:HG2	1.74	0.41
1:P:238:TRP:O	1:P:239:ARG:HB2	2.21	0.41
1:T:128:SER:OG	1:T:129:VAL:N	2.53	0.41
2:Z:17:ASN:O	2:Z:21:SER:OG	2.29	0.41
1:b:194:ASP:HB2	1:b:196:ASN:OD1	2.21	0.41
1:b:211:GLN:OE1	1:b:211:GLN:HA	2.19	0.41
1:f:212:LYS:HZ3	1:f:212:LYS:H	1.68	0.41
1:C:202:TYR:OH	1:O:164:GLN:OE1	2.27	0.41
2:I:139:ASP:OD2	2:I:140:PHE:N	2.54	0.41
1:K:130:SER:OG	1:K:131:ASP:N	2.53	0.41
1:O:188:ILE:HG22	1:O:223:PHE:HB3	2.03	0.41
1:O:204:LEU:O	1:O:207:LEU:N	2.54	0.41
1:O:214:GLU:CD	1:O:215:GLU:H	2.28	0.41
1:O:235:LEU:HD12	1:O:240:ILE:HG13	2.03	0.41
1:D:110:ARG:NH2	1:D:150:ASP:OD1	2.48	0.41
2:Z:76:PHE:CE1	2:d:87:LYS:CB	3.01	0.41
1:f:148:ASP:N	1:f:148:ASP:OD1	2.54	0.41
1:A:163:PHE:C	1:A:165:ARG:H	2.29	0.41
1:O:215:GLU:HB2	1:O:217:GLN:OE1	2.21	0.41
2:H:46:ILE:HD13	2:H:46:ILE:HA	1.94	0.41
1:L:6:ALA:HA	1:L:9:LYS:HE2	2.03	0.41
1:P:14:ILE:HG23	1:P:102:ILE:HB	2.02	0.41
1:b:131:ASP:HB3	1:b:134:LYS:HD2	2.02	0.40
1:f:206:LYS:HB2	1:f:206:LYS:HE2	1.46	0.40
1:A:55:LEU:HD23	1:A:159:GLU:HG2	2.03	0.40
2:G:28:LEU:HD13	2:G:28:LEU:HA	1.93	0.40
1:K:199:LEU:HD12	1:K:199:LEU:HA	1.82	0.40
1:O:200:LEU:HD23	1:O:200:LEU:HA	1.93	0.40
1:O:238:TRP:O	1:O:239:ARG:CB	2.69	0.40
1:D:180:VAL:O	1:D:217:GLN:NE2	2.54	0.40
1:R:55:LEU:HD23	1:R:159:GLU:HG2	2.03	0.40
2:X:13:ILE:HG21	2:X:29:ALA:HB2	2.03	0.40
2:Z:104:ARG:HH11	2:Z:129:THR:HG23	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:129:VAL:HA	1:b:132:ILE:CD1	2.51	0.40
1:b:211:GLN:O	1:b:212:LYS:HG3	2.20	0.40
1:C:17:VAL:HG11	1:C:112:ILE:HD11	2.04	0.40
2:G:123:GLU:O	2:G:174:LYS:NZ	2.38	0.40
2:I:93:PHE:HE1	2:I:97:LEU:HD12	1.86	0.40
1:K:200:LEU:HA	1:K:200:LEU:HD23	1.74	0.40
1:K:211:GLN:HG3	1:K:213:LEU:HD23	2.03	0.40
1:O:217:GLN:N	1:O:217:GLN:CD	2.80	0.40
1:B:56:GLU:OE1	1:L:234:ILE:HD13	2.21	0.40
2:H:9:ASN:O	2:H:10:ARG:C	2.64	0.40
1:P:194:ASP:O	1:P:197:ILE:N	2.54	0.40
1:T:65:LYS:HE3	1:T:70:PRO:HG2	2.04	0.40
1:f:126:ILE:HB	1:f:143:ILE:HG13	2.03	0.40
1:f:204:LEU:O	1:f:205:SER:C	2.64	0.40
1:K:183:LYS:HA	1:K:218:PRO:HG2	2.04	0.40
1:K:197:ILE:O	1:K:200:LEU:N	2.55	0.40
1:O:35:ASP:OD1	1:O:49:ARG:NH2	2.50	0.40
2:F:16:ILE:HD11	2:F:168:ARG:HH21	1.85	0.40
2:H:10:ARG:HA	2:H:13:ILE:HG22	2.00	0.40
2:N:131:SER:OG	2:N:133:VAL:O	2.33	0.40
1:L:202:TYR:O	1:L:205:SER:N	2.54	0.40
1:L:219:LYS:CD	1:L:239:ARG:HB2	2.51	0.40
1:P:64:LYS:HD3	1:P:64:LYS:HA	1.85	0.40
1:T:252:GLU:H	1:T:252:GLU:HG3	1.73	0.40
1:b:217:GLN:N	1:b:218:PRO:CD	2.82	0.40
1:A:211:GLN:C	1:A:213:LEU:H	2.28	0.40
2:E:12:LYS:HG2	2:E:168:ARG:HH22	1.85	0.40
2:G:105:LEU:HD22	2:G:130:ILE:HG13	2.02	0.40
1:O:202:TYR:O	1:O:205:SER:N	2.55	0.40
2:F:9:ASN:O	2:F:10:ARG:NE	2.53	0.40
2:F:111:ILE:HG22	2:F:122:PHE:HB2	2.02	0.40
1:R:213:LEU:O	1:R:214:GLU:C	2.63	0.40
1:T:83:ASP:OD1	1:T:83:ASP:N	2.54	0.40
2:X:69:TYR:HA	2:X:75:GLY:HA2	2.04	0.40
2:d:91:ASP:OD2	2:d:138:ARG:NH1	2.44	0.40
1:b:125:LYS:HE3	1:b:125:LYS:HB3	1.66	0.40
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.93	0.40
1:A:162:TYR:O	1:A:162:TYR:CD2	2.74	0.40
1:A:212:LYS:HA	1:A:212:LYS:HD2	1.96	0.40
1:C:46:ASP:HA	1:C:49:ARG:HG2	2.04	0.40
2:M:131:SER:HB3	2:M:145:ILE:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:179:LEU:HD23	2:M:179:LEU:HA	1.95	0.40
1:K:190:TYR:HB3	1:K:201:PHE:HZ	1.87	0.40
1:B:217:GLN:C	1:B:218:PRO:O	2.65	0.40
1:L:200:LEU:HB3	1:L:204:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/264 (99%)	245 (94%)	14 (5%)	3 (1%)	12	42
1	B	262/264 (99%)	244 (93%)	14 (5%)	4 (2%)	8	36
1	C	262/264 (99%)	253 (97%)	8 (3%)	1 (0%)	30	62
1	D	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	30	62
1	K	262/264 (99%)	220 (84%)	29 (11%)	13 (5%)	1	17
1	L	262/264 (99%)	220 (84%)	30 (12%)	12 (5%)	2	18
1	O	262/264 (99%)	224 (86%)	26 (10%)	12 (5%)	2	18
1	P	262/264 (99%)	233 (89%)	20 (8%)	9 (3%)	3	24
1	R	262/264 (99%)	242 (92%)	15 (6%)	5 (2%)	6	33
1	T	262/264 (99%)	252 (96%)	10 (4%)	0	100	100
1	b	262/264 (99%)	223 (85%)	26 (10%)	13 (5%)	1	17
1	f	262/264 (99%)	229 (87%)	23 (9%)	10 (4%)	2	21
2	E	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
2	F	182/184 (99%)	166 (91%)	16 (9%)	0	100	100
2	G	182/184 (99%)	173 (95%)	9 (5%)	0	100	100
2	H	182/184 (99%)	166 (91%)	14 (8%)	2 (1%)	12	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	182/184 (99%)	174 (96%)	8 (4%)	0	100	100
2	J	182/184 (99%)	170 (93%)	12 (7%)	0	100	100
2	M	182/184 (99%)	169 (93%)	13 (7%)	0	100	100
2	N	182/184 (99%)	169 (93%)	11 (6%)	2 (1%)	12	42
2	V	182/184 (99%)	173 (95%)	9 (5%)	0	100	100
2	X	182/184 (99%)	175 (96%)	7 (4%)	0	100	100
2	Z	182/184 (99%)	169 (93%)	9 (5%)	4 (2%)	5	30
2	d	182/184 (99%)	175 (96%)	7 (4%)	0	100	100
All	All	5328/5376 (99%)	4887 (92%)	350 (7%)	91 (2%)	10	34

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	210	GLU
1	b	37	ILE
1	b	195	ILE
1	f	195	ILE
1	f	215	GLU
1	f	216	ALA
1	f	218	PRO
1	f	219	LYS
1	f	239	ARG
1	A	212	LYS
1	A	217	GLN
1	K	37	ILE
1	K	207	LEU
1	K	208	TRP
1	K	216	ALA
1	K	219	LYS
1	O	208	TRP
1	O	209	LYS
1	O	216	ALA
1	B	217	GLN
1	D	54	ALA
2	H	8	ARG
2	N	77	PRO
1	L	168	PHE
1	L	195	ILE
1	L	210	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	206	LYS
1	P	207	LEU
1	P	212	LYS
2	Z	80	LEU
1	b	134	LYS
1	b	215	GLU
1	A	208	TRP
1	C	54	ALA
1	K	47	ILE
1	K	192	LEU
1	O	192	LEU
1	O	200	LEU
1	O	210	GLU
1	B	210	GLU
2	H	7	THR
1	L	134	LYS
1	L	208	TRP
1	L	209	LYS
1	L	216	ALA
1	L	218	PRO
1	P	137	ASN
1	P	195	ILE
1	P	205	SER
1	R	209	LYS
1	R	211	GLN
2	Z	78	GLY
1	b	138	ASN
1	b	139	LYS
1	b	196	ASN
1	b	207	LEU
1	b	208	TRP
1	f	192	LEU
1	f	214	GLU
1	K	137	ASN
1	O	195	ILE
1	B	164	GLN
1	B	218	PRO
2	N	76	PHE
1	P	138	ASN
1	P	139	LYS
1	P	219	LYS
1	R	165	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	46	ASP
1	b	192	LEU
1	f	207	LEU
1	f	209	LYS
1	K	218	PRO
1	O	205	SER
1	L	207	LEU
2	Z	75	GLY
2	Z	76	PHE
1	K	206	LYS
1	K	209	LYS
1	O	211	GLN
1	O	220	SER
1	O	240	ILE
1	b	193	SER
1	K	210	GLU
1	K	195	ILE
1	L	37	ILE
1	L	47	ILE
1	R	218	PRO
1	L	129	VAL
1	O	217	GLN
1	b	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/240 (100%)	230 (96%)	10 (4%)	25	50
1	B	240/240 (100%)	234 (98%)	6 (2%)	42	61
1	C	240/240 (100%)	236 (98%)	4 (2%)	56	73
1	D	240/240 (100%)	238 (99%)	2 (1%)	79	86
1	K	240/240 (100%)	212 (88%)	28 (12%)	4	21
1	L	240/240 (100%)	211 (88%)	29 (12%)	4	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	240/240 (100%)	221 (92%)	19 (8%)	10	34
1	P	240/240 (100%)	222 (92%)	18 (8%)	11	35
1	R	240/240 (100%)	227 (95%)	13 (5%)	18	45
1	T	240/240 (100%)	238 (99%)	2 (1%)	79	86
1	b	240/240 (100%)	208 (87%)	32 (13%)	3	17
1	f	240/240 (100%)	218 (91%)	22 (9%)	7	29
2	E	161/161 (100%)	161 (100%)	0	100	100
2	F	161/161 (100%)	158 (98%)	3 (2%)	52	69
2	G	161/161 (100%)	159 (99%)	2 (1%)	67	79
2	H	161/161 (100%)	158 (98%)	3 (2%)	52	69
2	I	161/161 (100%)	161 (100%)	0	100	100
2	J	161/161 (100%)	160 (99%)	1 (1%)	84	90
2	M	161/161 (100%)	161 (100%)	0	100	100
2	N	161/161 (100%)	161 (100%)	0	100	100
2	V	161/161 (100%)	158 (98%)	3 (2%)	52	69
2	X	161/161 (100%)	161 (100%)	0	100	100
2	Z	161/161 (100%)	157 (98%)	4 (2%)	42	61
2	d	161/161 (100%)	158 (98%)	3 (2%)	52	69
All	All	4812/4812 (100%)	4608 (96%)	204 (4%)	27	50

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	23	MET
1	R	56	GLU
1	R	180	VAL
1	R	183	LYS
1	R	192	LEU
1	R	194	ASP
1	R	199	LEU
1	R	205	SER
1	R	206	LYS
1	R	207	LEU
1	R	208	TRP
1	R	209	LYS
1	R	219	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	23	MET
1	T	213	LEU
2	V	6	ILE
2	V	73	LEU
2	V	91	ASP
2	Z	39	THR
2	Z	61	VAL
2	Z	71	GLU
2	Z	72	SER
2	d	48	ASP
2	d	56	LEU
2	d	84	PHE
1	b	36	HIS
1	b	37	ILE
1	b	84	ILE
1	b	125	LYS
1	b	126	ILE
1	b	129	VAL
1	b	131	ASP
1	b	134	LYS
1	b	135	ILE
1	b	136	ASP
1	b	139	LYS
1	b	141	GLN
1	b	166	LEU
1	b	167	GLU
1	b	188	ILE
1	b	192	LEU
1	b	194	ASP
1	b	195	ILE
1	b	196	ASN
1	b	197	ILE
1	b	199	LEU
1	b	200	LEU
1	b	203	LYS
1	b	206	LYS
1	b	207	LEU
1	b	209	LYS
1	b	211	GLN
1	b	212	LYS
1	b	213	LEU
1	b	215	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	217	GLN
1	b	235	LEU
1	f	23	MET
1	f	33	LEU
1	f	157	LEU
1	f	186	LEU
1	f	192	LEU
1	f	193	SER
1	f	197	ILE
1	f	198	ARG
1	f	203	LYS
1	f	205	SER
1	f	206	LYS
1	f	207	LEU
1	f	209	LYS
1	f	210	GLU
1	f	211	GLN
1	f	212	LYS
1	f	213	LEU
1	f	214	GLU
1	f	215	GLU
1	f	219	LYS
1	f	220	SER
1	f	240	ILE
1	A	141	GLN
1	A	155	ILE
1	A	204	LEU
1	A	205	SER
1	A	206	LYS
1	A	207	LEU
1	A	209	LYS
1	A	212	LYS
1	A	215	GLU
1	A	217	GLN
1	C	23	MET
1	C	148	ASP
1	C	207	LEU
1	C	213	LEU
2	G	9	ASN
2	G	28	LEU
1	K	37	ILE
1	K	40	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	84	ILE
1	K	103	ILE
1	K	126	ILE
1	K	127	SER
1	K	131	ASP
1	K	134	LYS
1	K	137	ASN
1	K	138	ASN
1	K	142	ILE
1	K	157	LEU
1	K	194	ASP
1	K	195	ILE
1	K	196	ASN
1	K	197	ILE
1	K	200	LEU
1	K	203	LYS
1	K	206	LYS
1	K	207	LEU
1	K	209	LYS
1	K	211	GLN
1	K	212	LYS
1	K	213	LEU
1	K	215	GLU
1	K	217	GLN
1	K	219	LYS
1	K	239	ARG
1	O	192	LEU
1	O	194	ASP
1	O	195	ILE
1	O	196	ASN
1	O	197	ILE
1	O	199	LEU
1	O	203	LYS
1	O	206	LYS
1	O	209	LYS
1	O	210	GLU
1	O	211	GLN
1	O	212	LYS
1	O	213	LEU
1	O	214	GLU
1	O	215	GLU
1	O	219	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	220	SER
1	O	239	ARG
1	O	240	ILE
1	B	56	GLU
1	B	72	ARG
1	B	164	GLN
1	B	205	SER
1	B	206	LYS
1	B	209	LYS
1	D	23	MET
1	D	30	TRP
2	F	8	ARG
2	F	9	ASN
2	F	10	ARG
2	H	6	ILE
2	H	8	ARG
2	H	10	ARG
2	J	1	MET
1	L	48	TYR
1	L	57	LEU
1	L	103	ILE
1	L	124	ILE
1	L	125	LYS
1	L	126	ILE
1	L	127	SER
1	L	128	SER
1	L	129	VAL
1	L	131	ASP
1	L	132	ILE
1	L	134	LYS
1	L	136	ASP
1	L	137	ASN
1	L	138	ASN
1	L	166	LEU
1	L	192	LEU
1	L	195	ILE
1	L	196	ASN
1	L	198	ARG
1	L	199	LEU
1	L	203	LYS
1	L	206	LYS
1	L	207	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	209	LYS
1	L	212	LYS
1	L	213	LEU
1	L	214	GLU
1	L	215	GLU
1	P	138	ASN
1	P	139	LYS
1	P	181	LEU
1	P	191	SER
1	P	192	LEU
1	P	197	ILE
1	P	198	ARG
1	P	199	LEU
1	P	200	LEU
1	P	206	LYS
1	P	207	LEU
1	P	209	LYS
1	P	211	GLN
1	P	212	LYS
1	P	214	GLU
1	P	215	GLU
1	P	217	GLN
1	P	219	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	217	GLN
1	R	228	ASN
1	T	24	ASN
1	T	196	ASN
1	T	211	GLN
1	T	217	GLN
1	T	237	GLN
2	V	9	ASN
2	V	38	GLN
2	V	43	HIS
2	V	89	GLN
2	X	17	ASN
2	X	38	GLN
2	X	89	GLN
2	X	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	X	163	ASN
2	Z	74	ASN
2	Z	82	GLN
2	Z	102	ASN
2	d	2	ASN
2	d	17	ASN
2	d	89	GLN
1	b	92	HIS
1	b	118	ASN
1	b	247	ASN
1	f	217	GLN
1	f	228	ASN
1	f	247	ASN
1	A	80	HIS
1	A	211	GLN
1	A	217	GLN
1	A	228	ASN
1	C	24	ASN
1	C	92	HIS
2	E	11	HIS
2	E	102	ASN
2	E	163	ASN
2	G	17	ASN
2	G	41	ASN
2	G	141	GLN
2	I	2	ASN
2	M	2	ASN
2	M	17	ASN
2	M	89	GLN
2	M	102	ASN
1	K	32	GLN
1	K	87	ASN
1	K	118	ASN
1	K	138	ASN
1	K	231	GLN
1	O	32	GLN
1	O	87	ASN
1	O	211	GLN
1	O	228	ASN
1	B	92	HIS
1	B	217	GLN
1	D	118	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	231	GLN
1	D	249	ASN
2	F	9	ASN
2	F	38	GLN
2	F	65	HIS
2	F	82	GLN
2	F	95	GLN
2	F	163	ASN
2	H	82	GLN
2	H	95	GLN
2	J	9	ASN
2	N	32	HIS
2	N	82	GLN
2	N	163	ASN
1	L	87	ASN
1	L	141	GLN
1	L	211	GLN
1	P	217	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

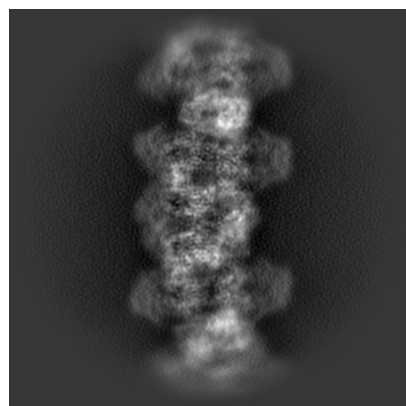
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60414. These allow visual inspection of the internal detail of the map and identification of artifacts.

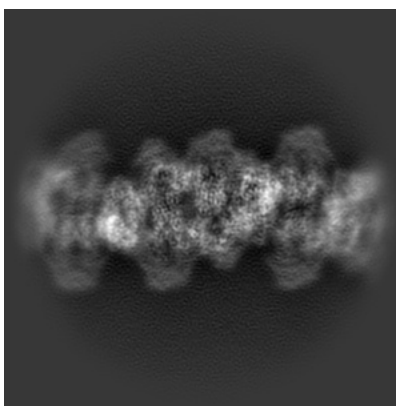
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

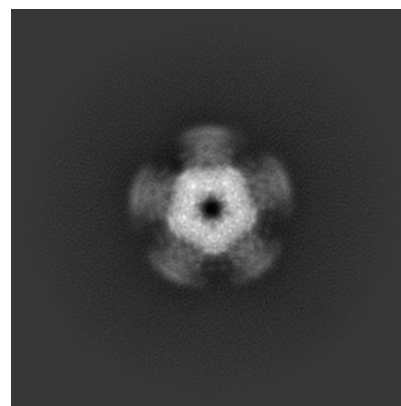
6.1.1 Primary map



X

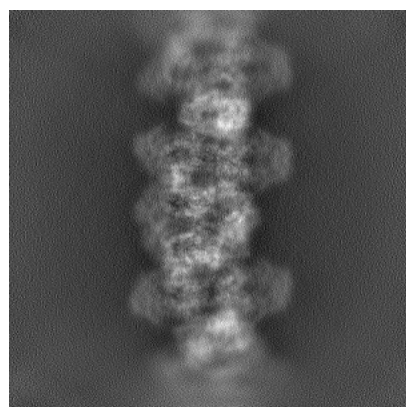


Y

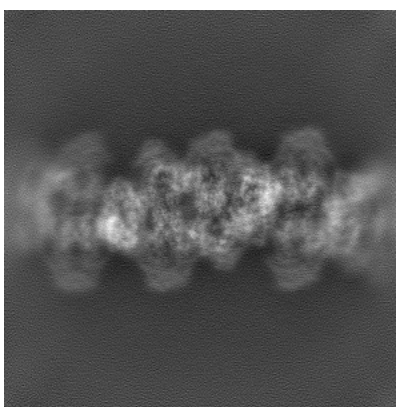


Z

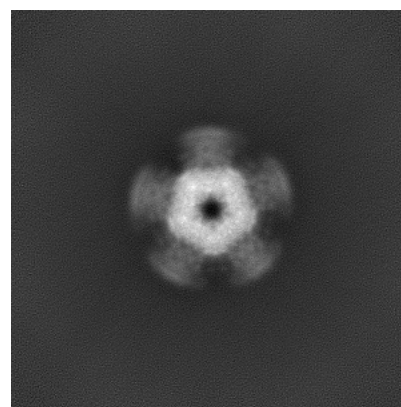
6.1.2 Raw map



X



Y

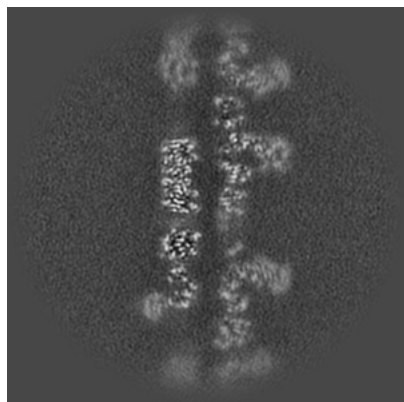


Z

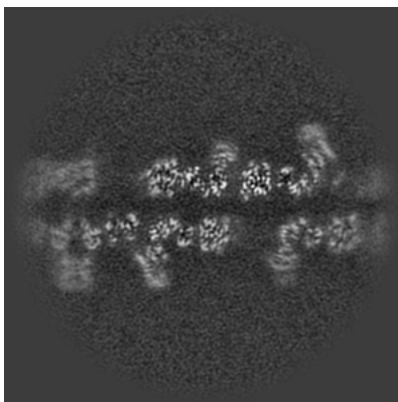
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

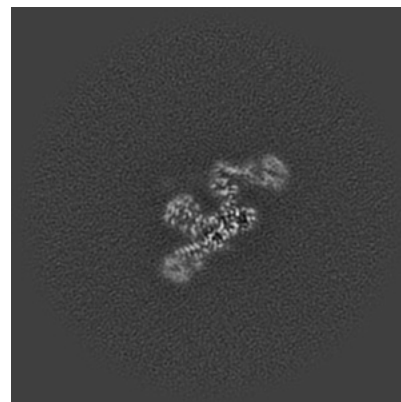
6.2.1 Primary map



X Index: 200

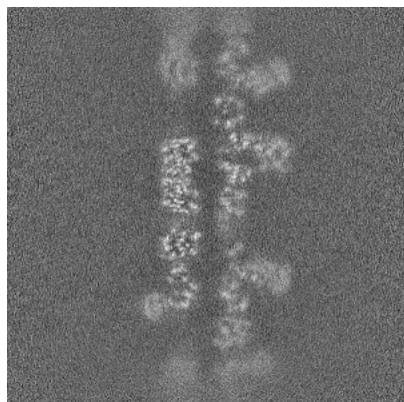


Y Index: 200

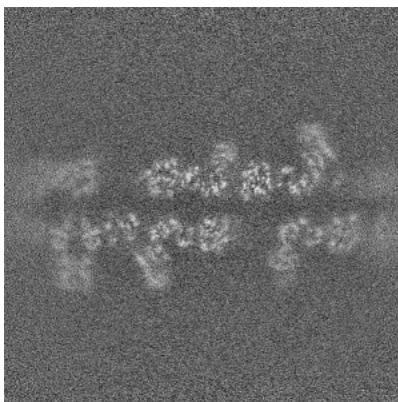


Z Index: 200

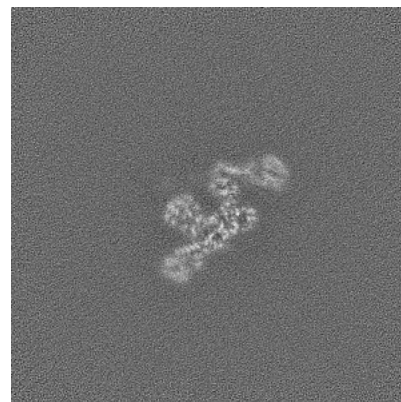
6.2.2 Raw map



X Index: 200



Y Index: 200

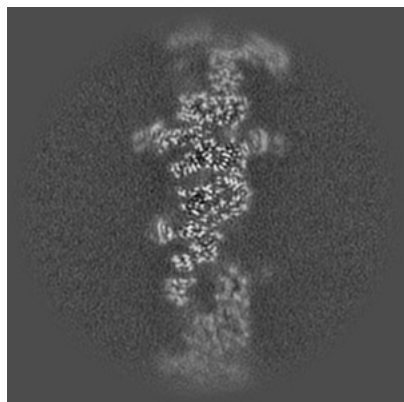


Z Index: 200

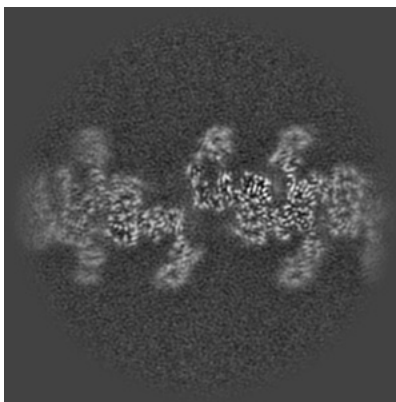
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

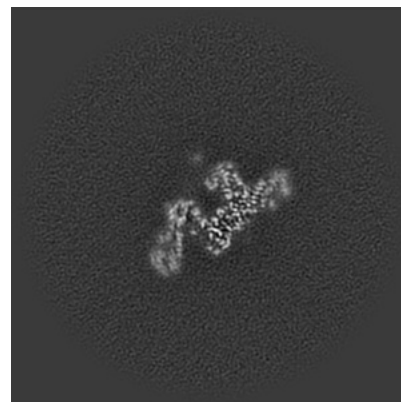
6.3.1 Primary map



X Index: 220

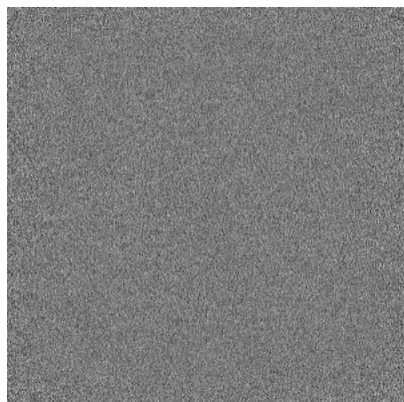


Y Index: 221

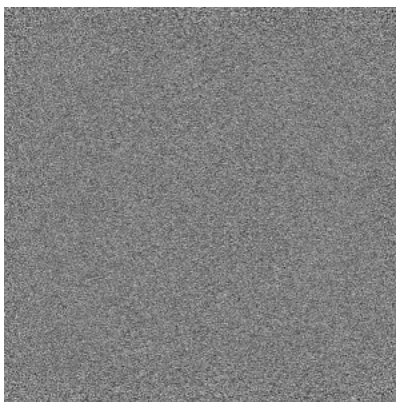


Z Index: 216

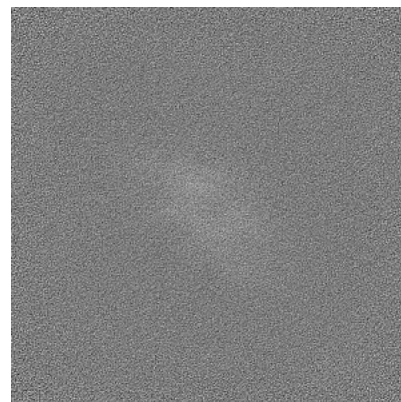
6.3.2 Raw map



X Index: 0



Y Index: 0

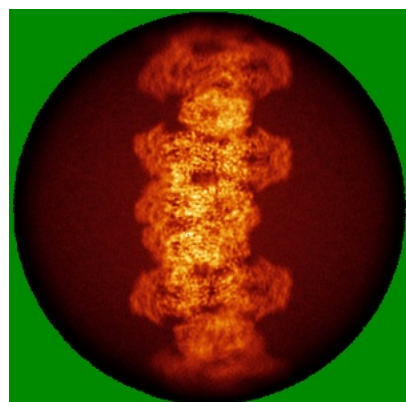


Z Index: 0

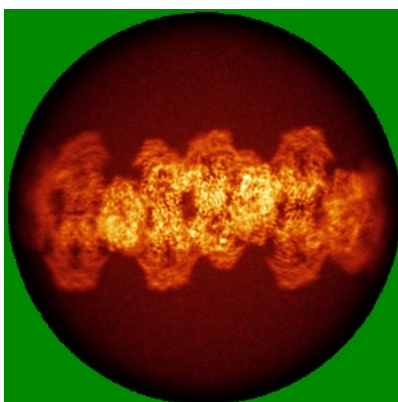
The images above show the largest variance slices of the map in three orthogonal directions.

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

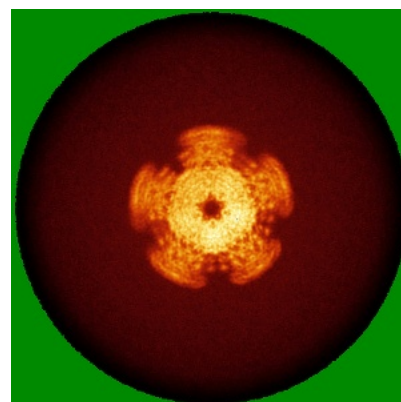
6.4.1 Primary map



X

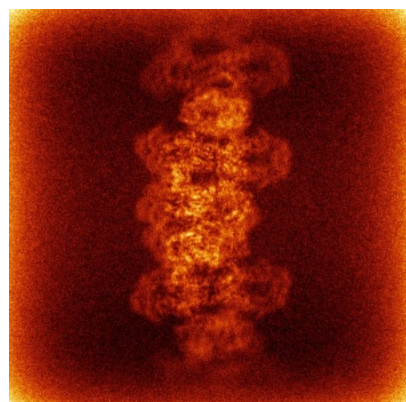


Y

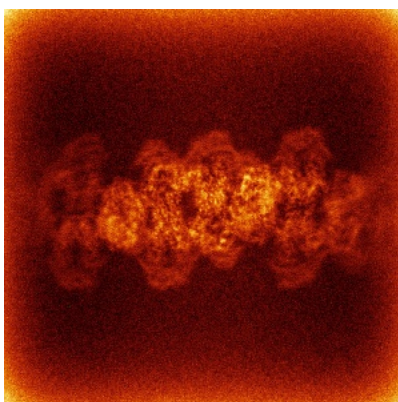


Z

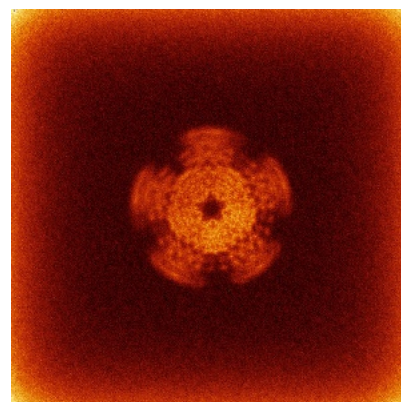
6.4.2 Raw map



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](#)

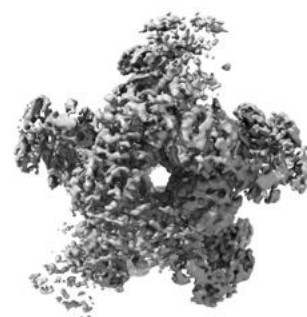
6.5.1 Primary map



X



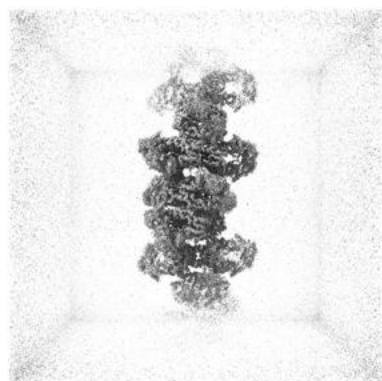
Y



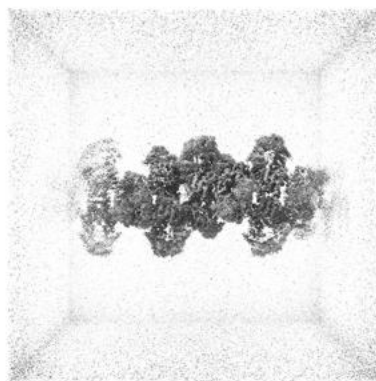
Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

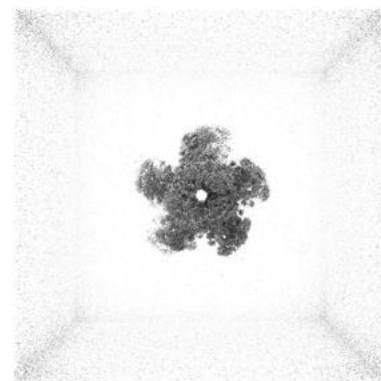
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

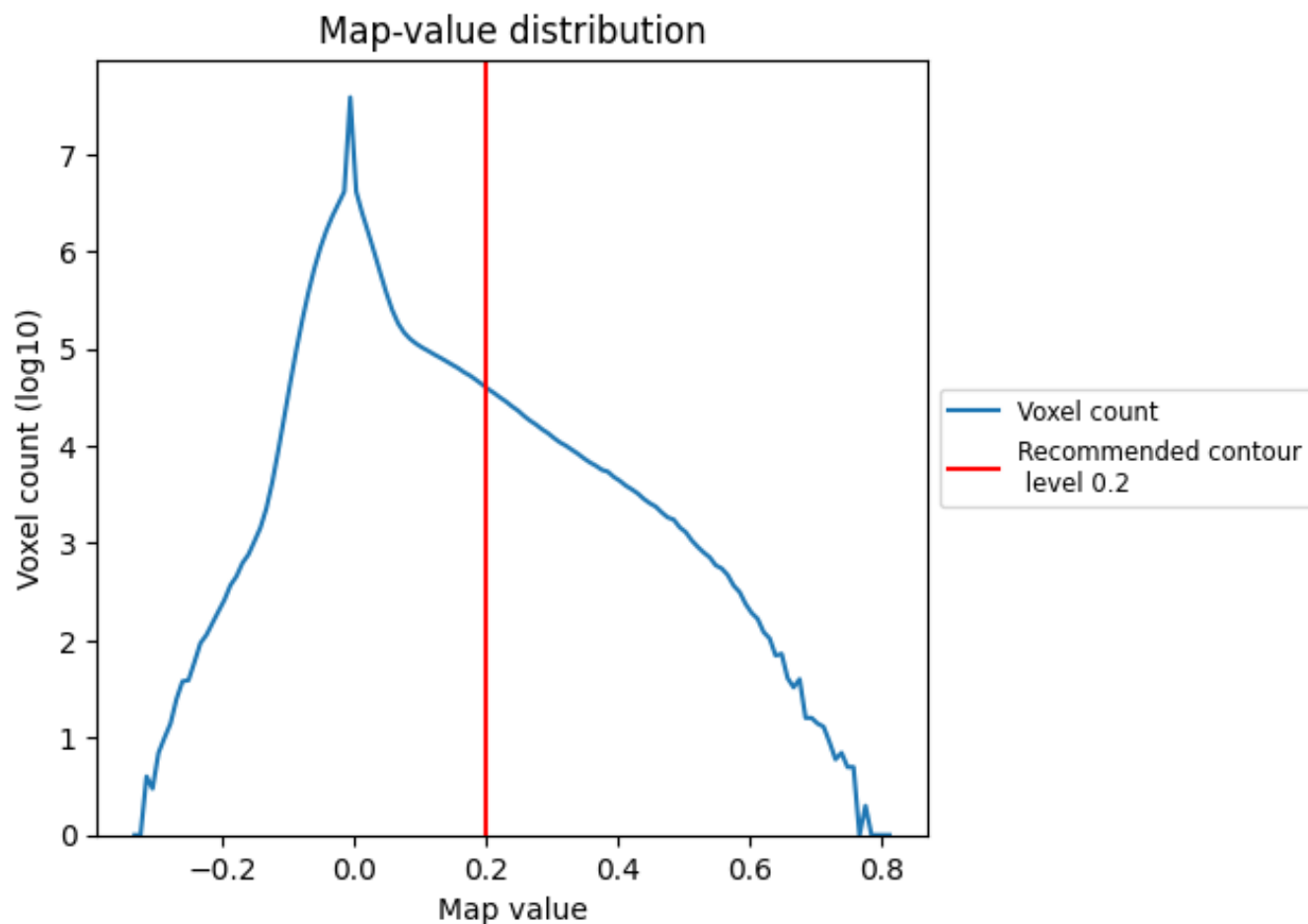
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

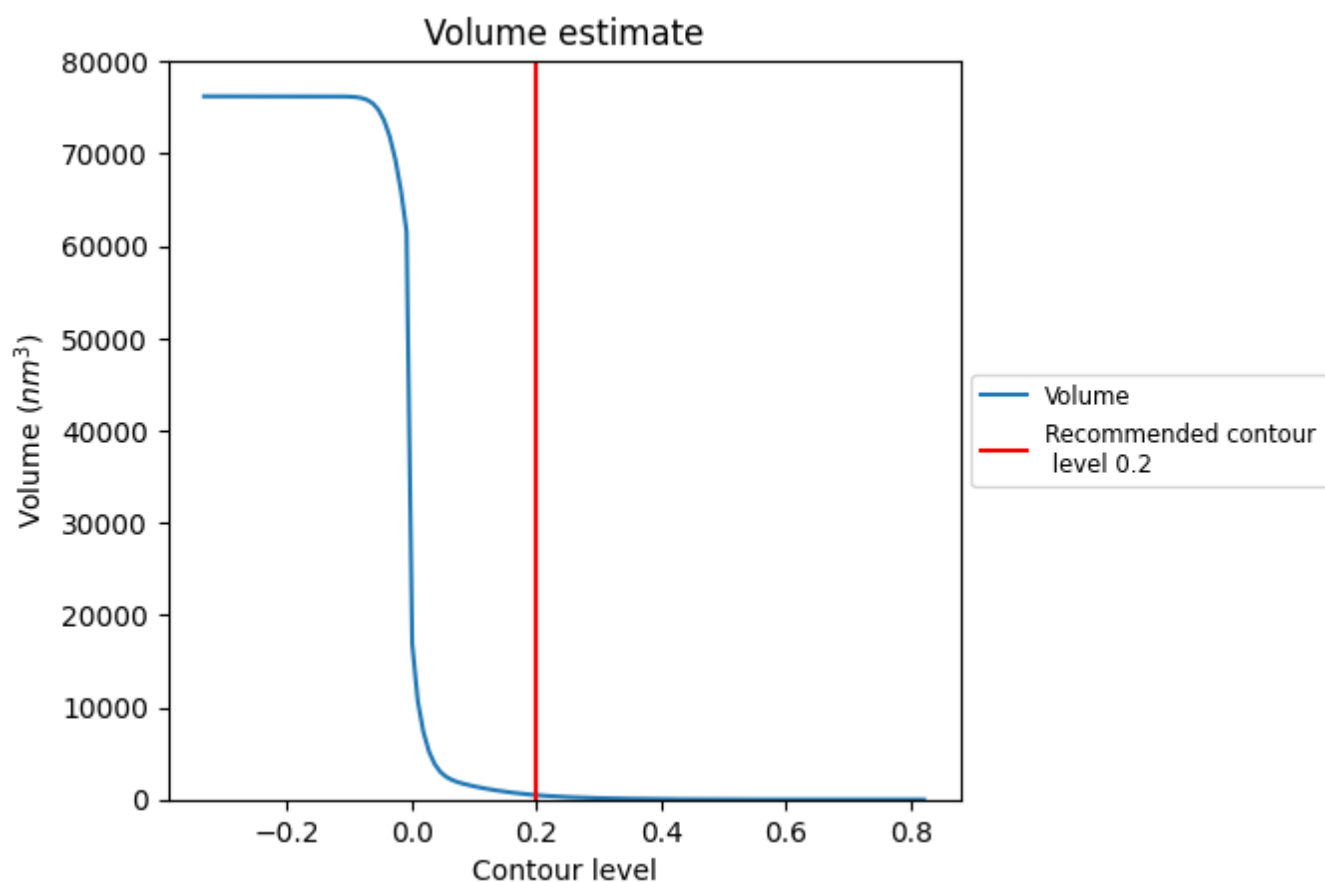
This section contains the results of statistical analysis of the map.

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.

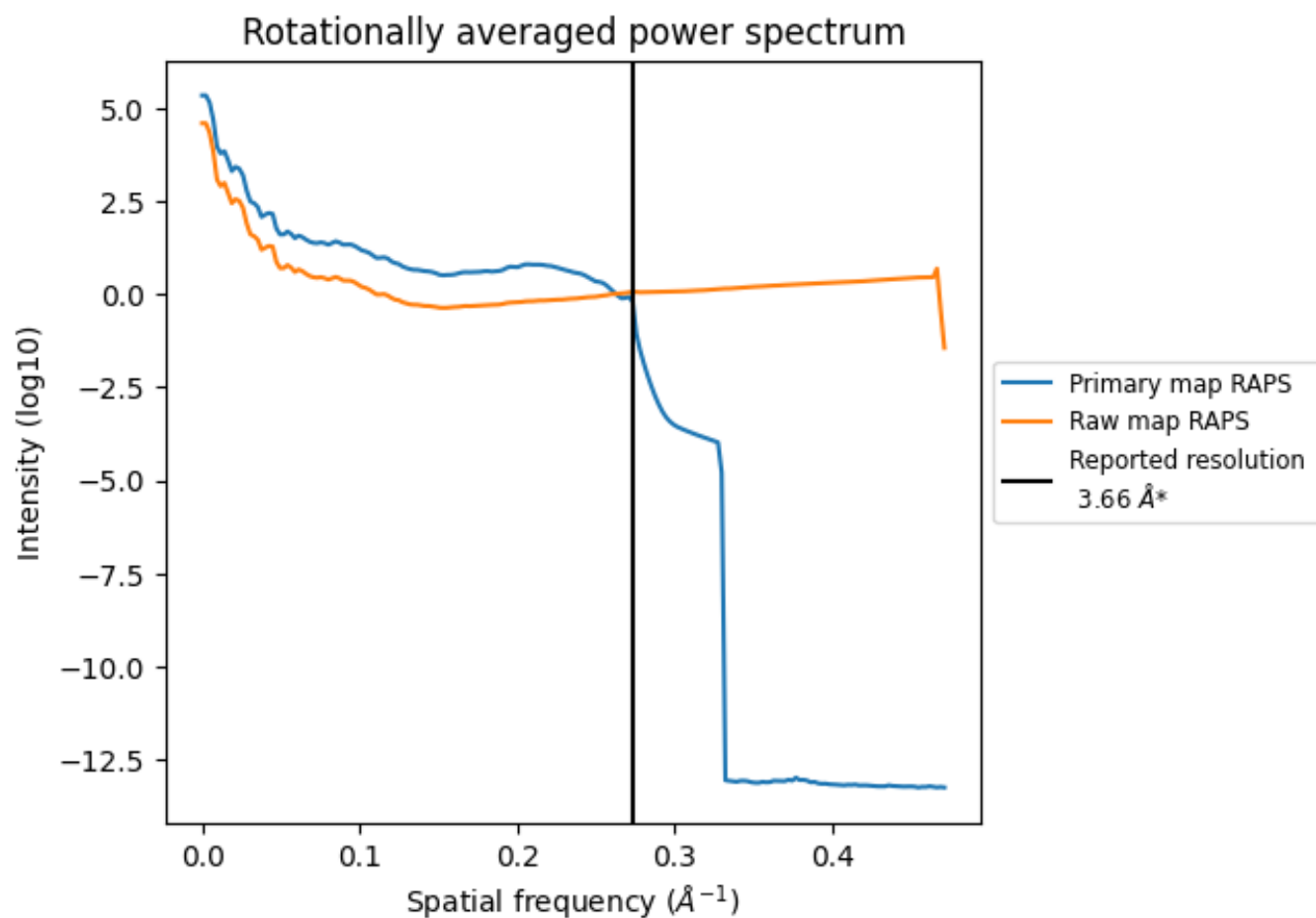
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 481 nm³; this corresponds to an approximate mass of 435 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 ⓘ

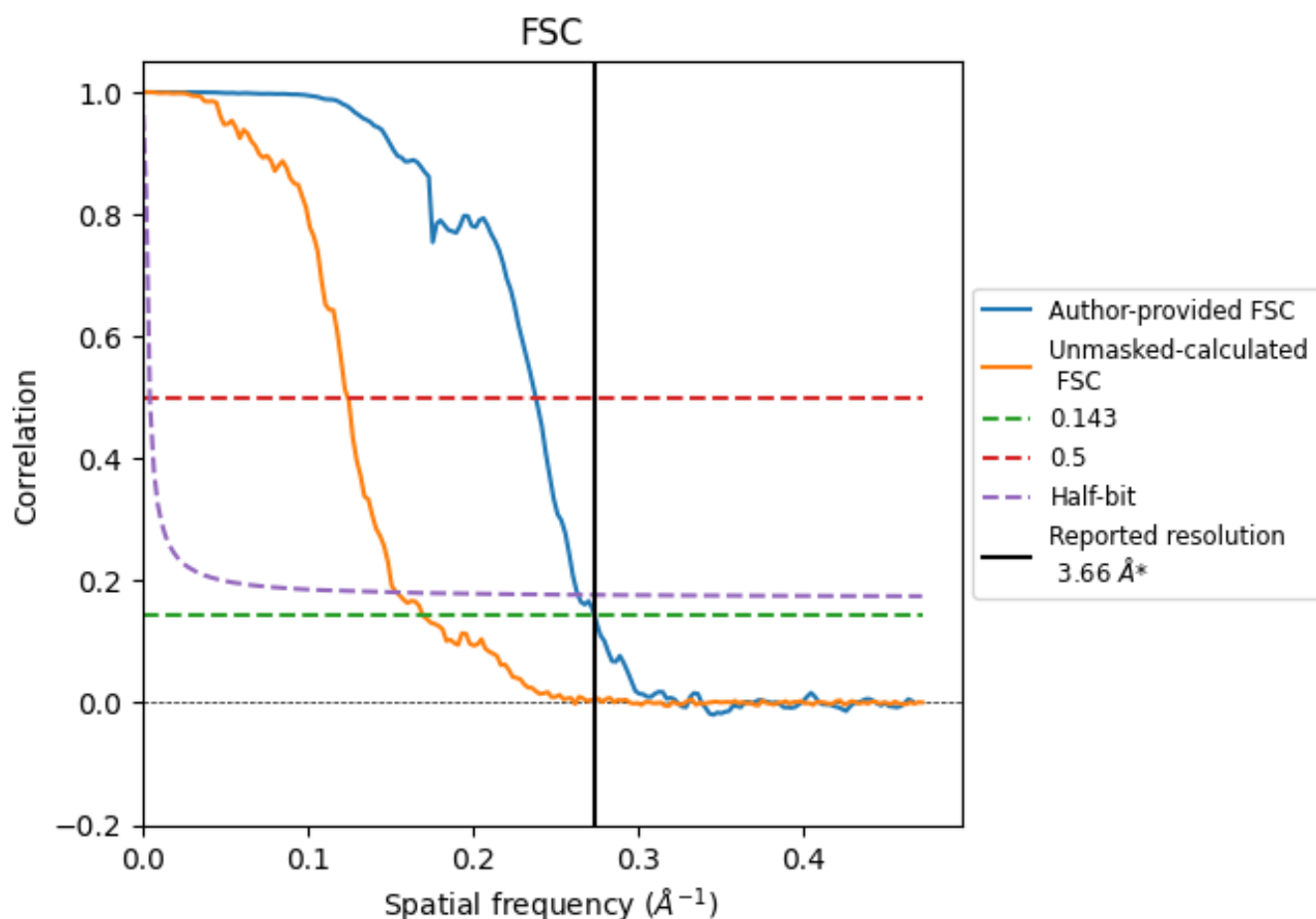


*Reported resolution corresponds to spatial frequency of 0.273 Å⁻¹

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 0.273 \AA^{-1}

8.2 Resolution estimates [i](#)

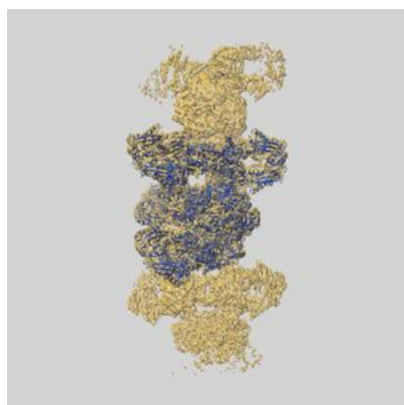
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.66	-	-
Author-provided FSC curve	3.66	4.20	3.80
Unmasked-calculated*	5.89	8.05	6.50

*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 5.89 differs from the reported value 3.66 by more than 10 %

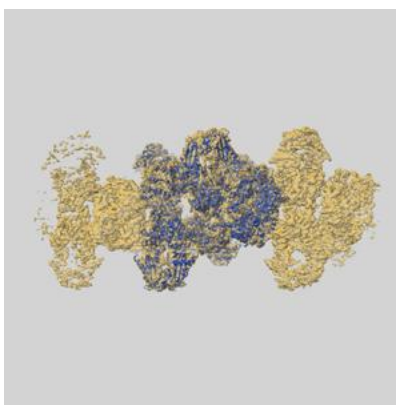
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60414 and PDB model 8ZSG. Per-residue inclusion information can be found in section [3](#) on page [6](#).

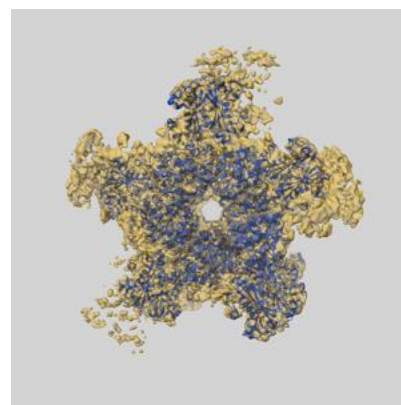
9.1 Map-model overlay [i](#)



X



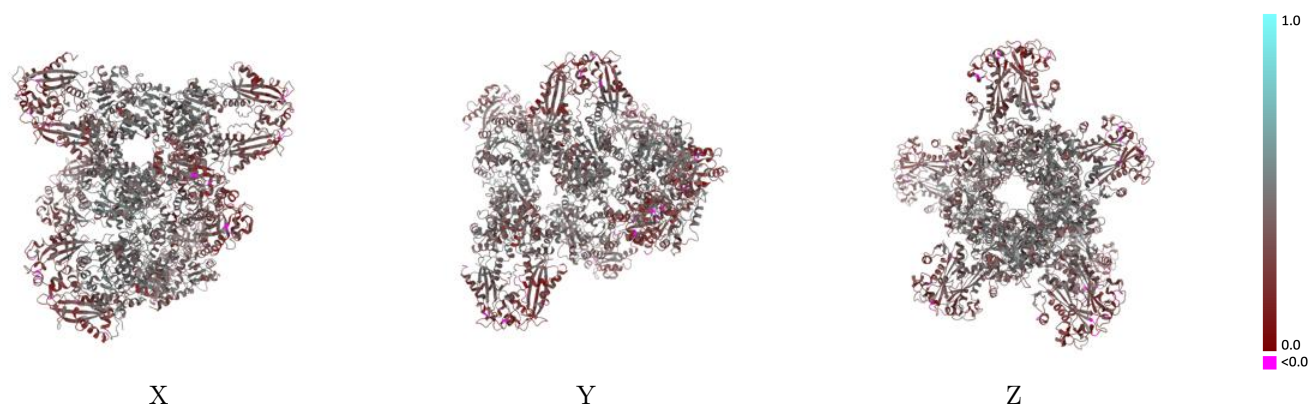
Y



Z

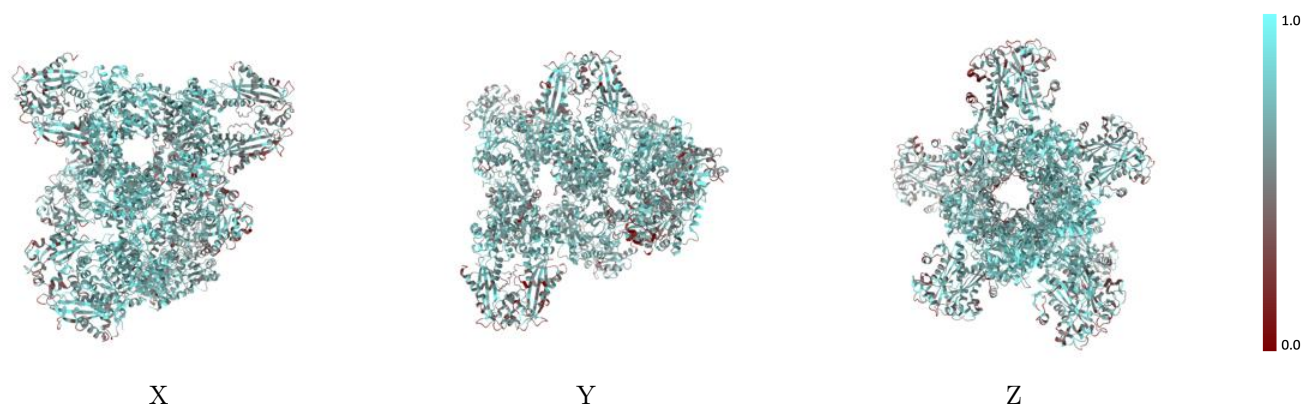
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



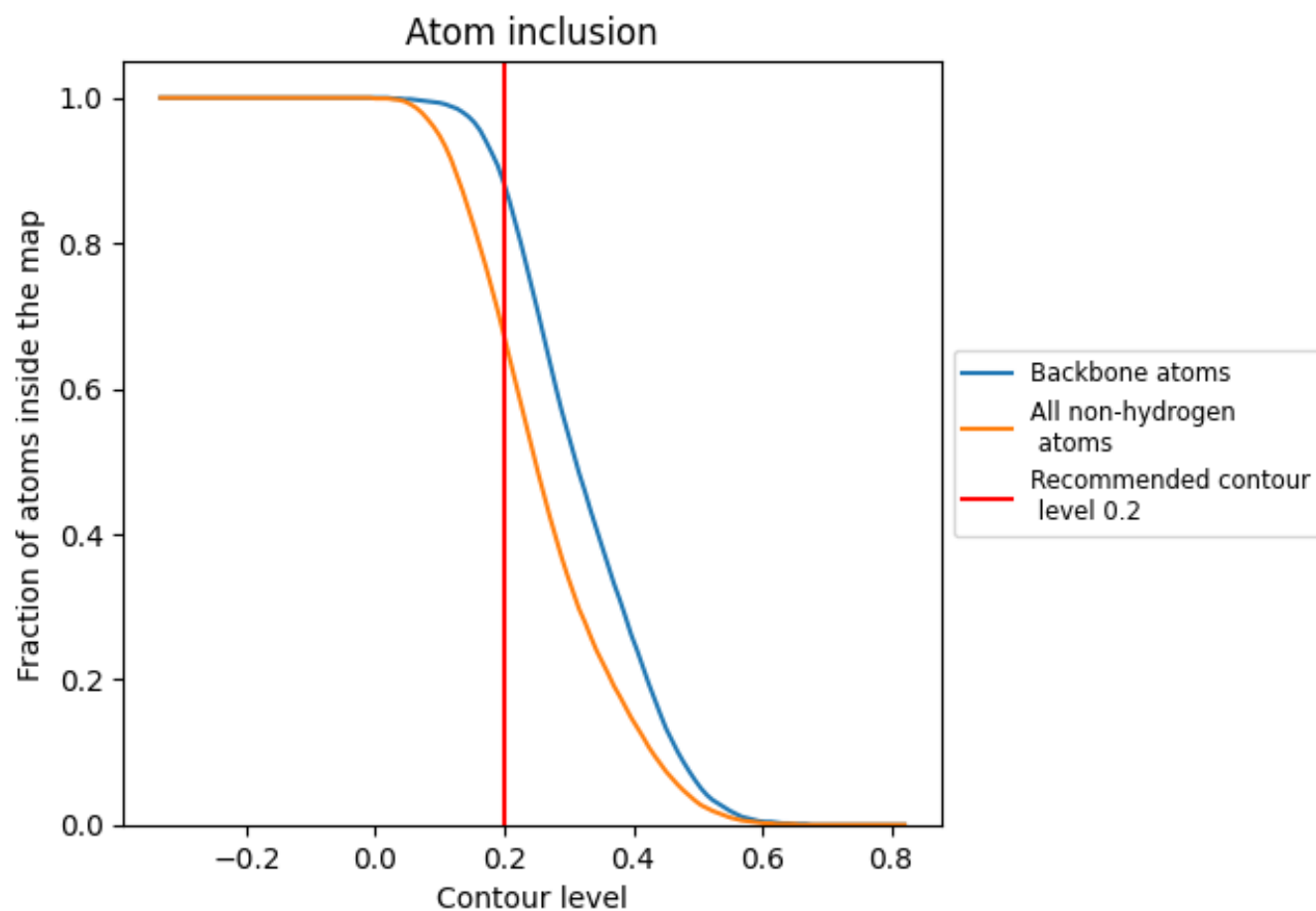
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 67% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.3850
A	 0.7410	 0.4420
B	 0.7750	 0.4500
C	 0.7740	 0.4480
D	 0.7530	 0.4430
E	 0.5020	 0.2910
F	 0.5960	 0.3240
G	 0.5590	 0.3220
H	 0.6250	 0.3450
I	 0.5960	 0.3120
J	 0.5110	 0.2810
K	 0.6440	 0.3860
L	 0.7370	 0.4230
M	 0.6010	 0.3310
N	 0.5620	 0.3280
O	 0.7330	 0.4270
P	 0.6460	 0.3940
R	 0.7710	 0.4550
T	 0.7790	 0.4510
V	 0.5980	 0.3090
X	 0.6070	 0.3310
Z	 0.5860	 0.3150
b	 0.7050	 0.4070
d	 0.6250	 0.3510
f	 0.7250	 0.4250

