



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:54 AM UTC

PDB ID : 8H37 / pdb_00008h37
EMDB ID : EMD-34453
Title : Cryo-EM Structure of the KBTBD2-CUL3-Rbx1-p85a tetrameric complex
Authors : Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on : 2022-10-08
Resolution : 7.52 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

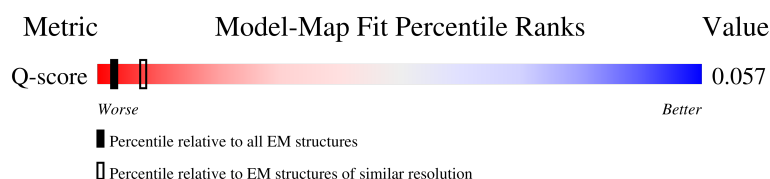
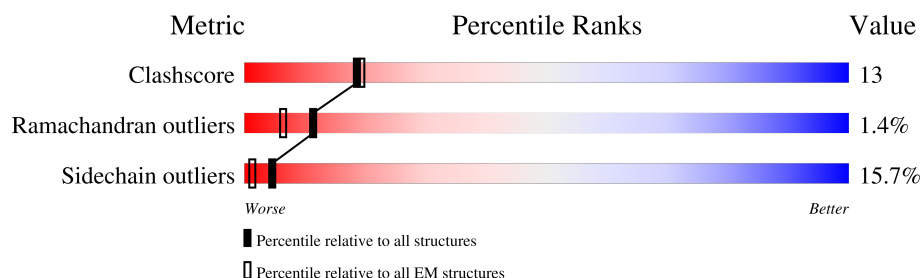
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.52 Å.

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



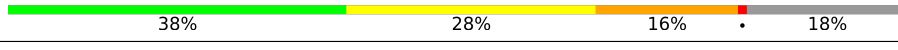
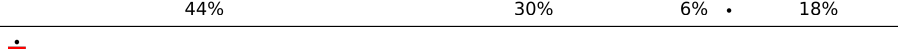
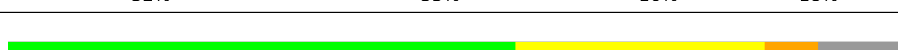
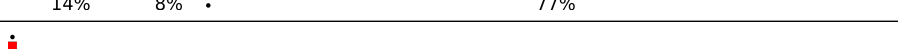
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	377 (7.02 - 8.01)

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	C	768	
1	F	768	
1	M	768	
1	O	768	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	108	
2	E	108	
2	Q	108	
2	R	108	
3	A	623	
3	B	623	
3	N	623	
3	P	623	
4	G	724	
4	H	724	
4	I	724	
4	J	724	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 49321 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 Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	720	Total	C	N	O	S	0	0
			5791	3633	1024	1095	39		
1	F	720	Total	C	N	O	S	0	0
			5677	3558	1010	1073	36		
1	M	720	Total	C	N	O	S	0	0
			5672	3553	1008	1074	37		
1	O	720	Total	C	N	O	S	0	0
			5767	3620	1017	1091	39		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	D	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	R	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	Q	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

- Molecule 3 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	567	Total	C	N	O	S	0	0
			4559	2918	750	853	38		
3	B	564	Total	C	N	O	S	0	0
			4510	2884	746	842	38		
3	N	564	Total	C	N	O	S	0	0
			4510	2880	746	846	38		
3	P	557	Total	C	N	O	S	0	0
			4423	2833	725	831	34		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ASP	SER	engineered mutation	UNP Q8IY47
B	252	ASP	SER	engineered mutation	UNP Q8IY47
N	252	ASP	SER	engineered mutation	UNP Q8IY47
P	252	ASP	SER	engineered mutation	UNP Q8IY47

- Molecule 4 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	168	Total	C	N	O	S	0	0
			1424	885	256	278	5		
4	H	168	Total	C	N	O	S	0	0
			1341	828	246	263	4		
4	I	168	Total	C	N	O	S	0	0
			1360	840	250	266	4		
4	J	168	Total	C	N	O	S	0	0
			1327	816	244	263	4		

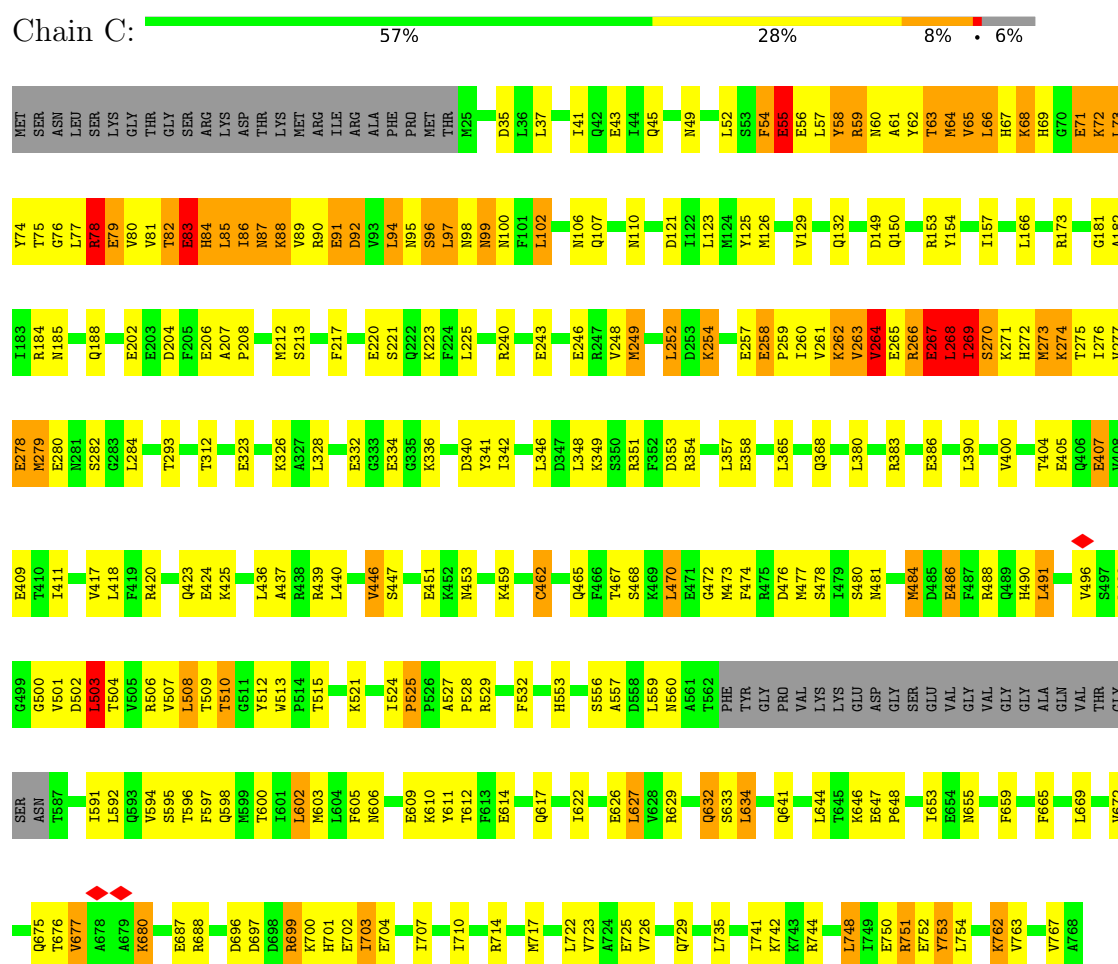
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	E	3	Total	Zn	0
			3	3	
5	D	3	Total	Zn	0
			3	3	
5	R	3	Total	Zn	0
			3	3	
5	Q	3	Total	Zn	0
			3	3	

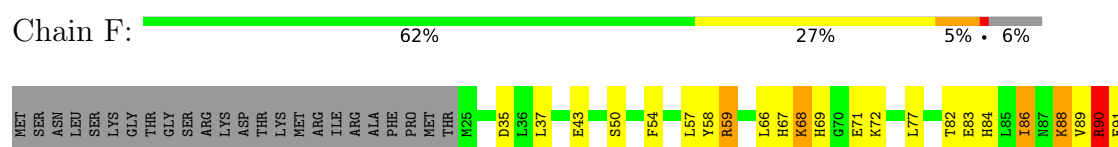
3 Residue-property plots

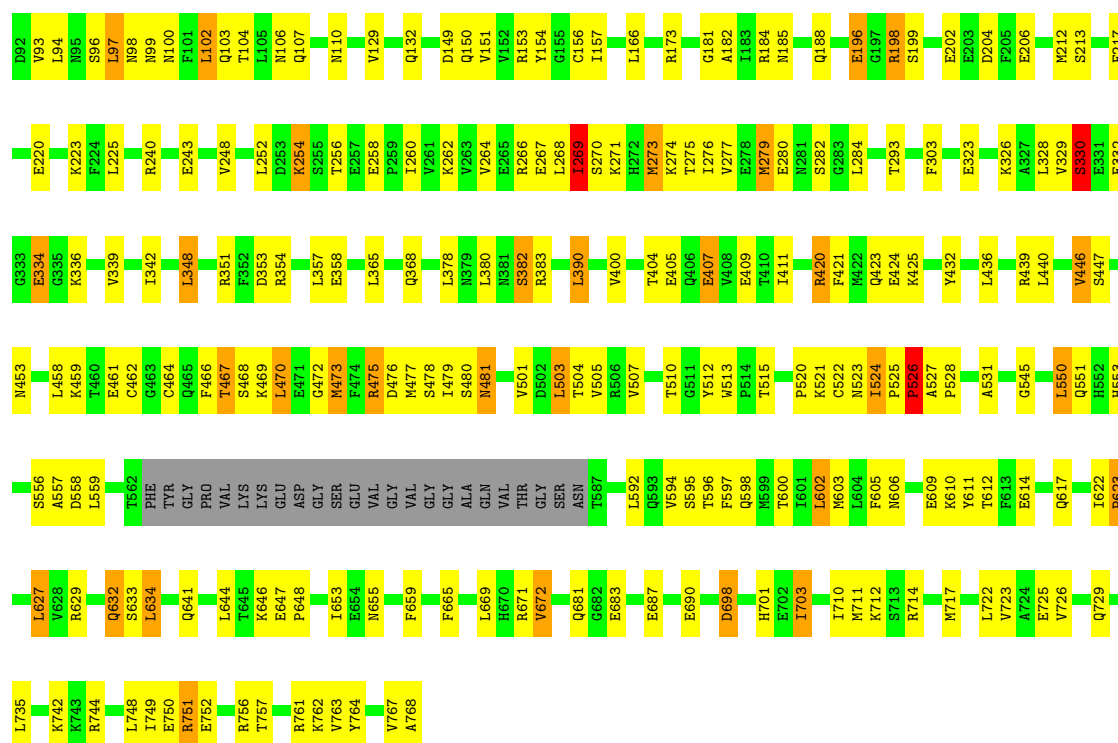
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cullin-3

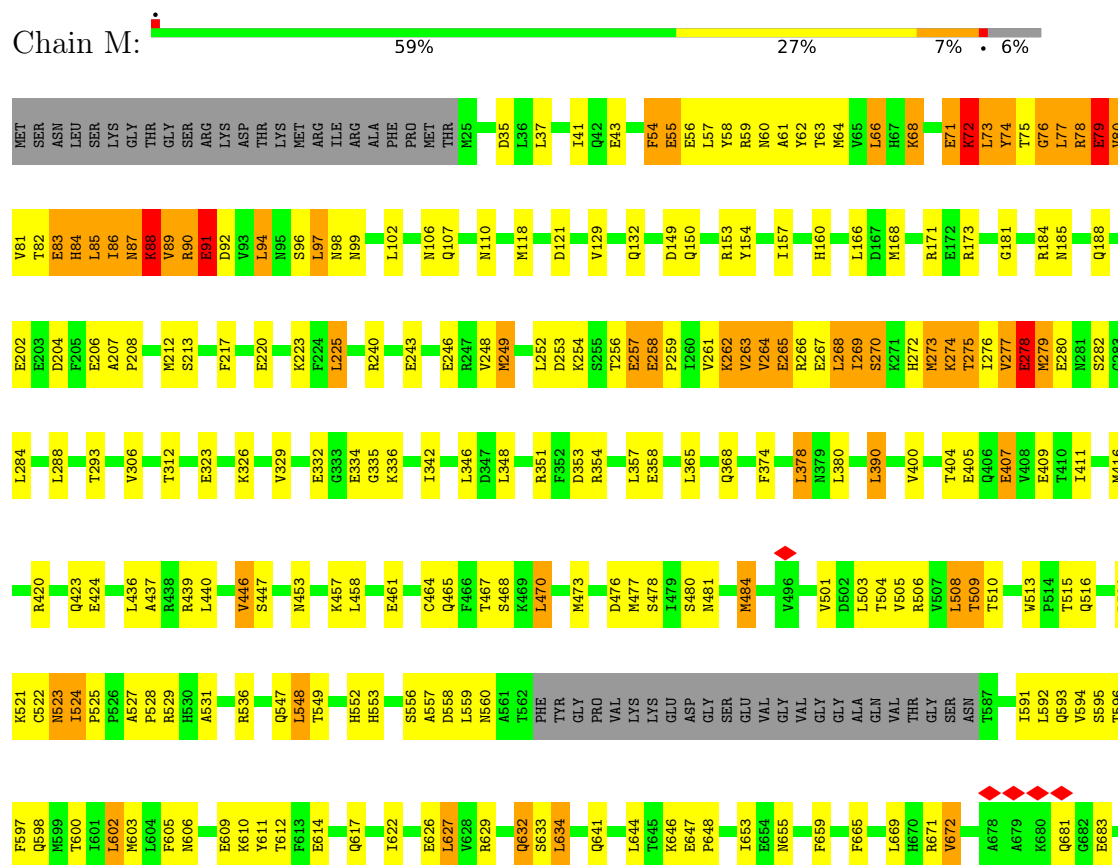


• Molecule 1: Cullin-3





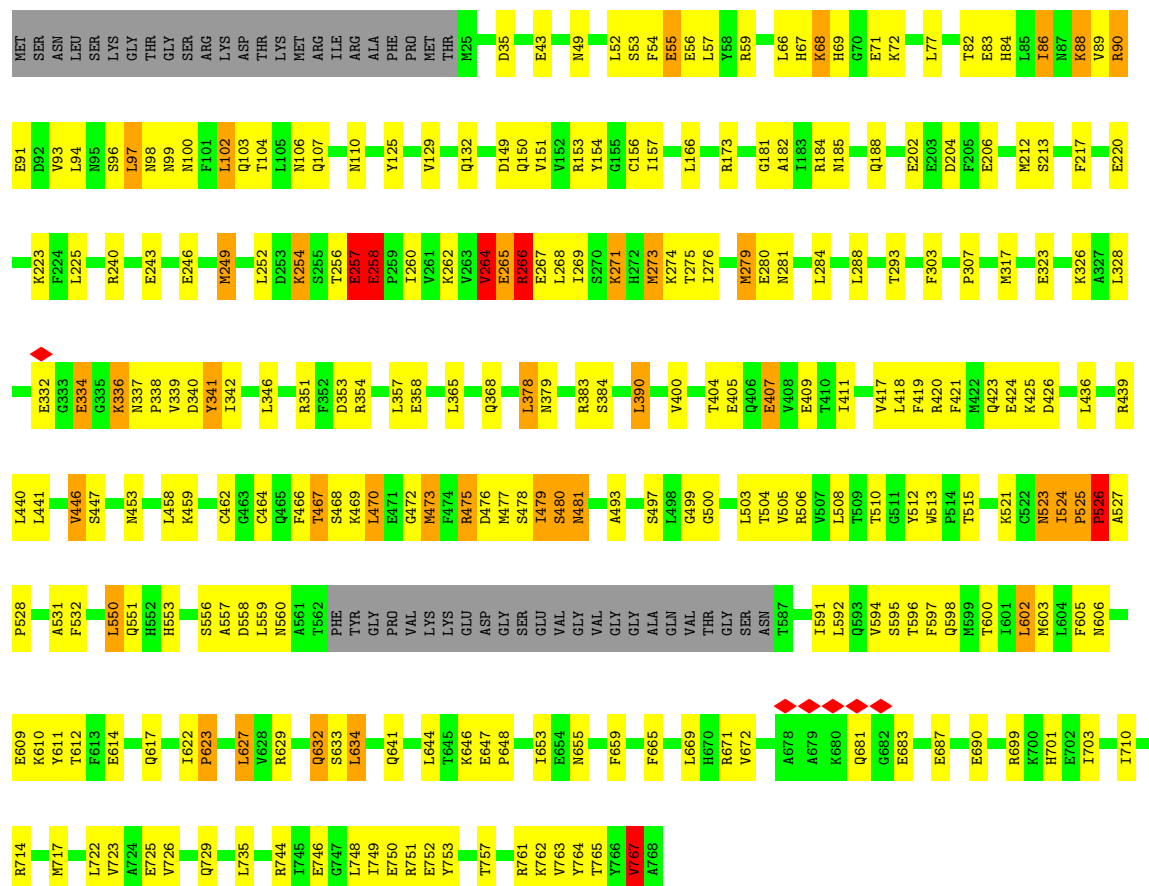
- Molecule 1: Cullin-3





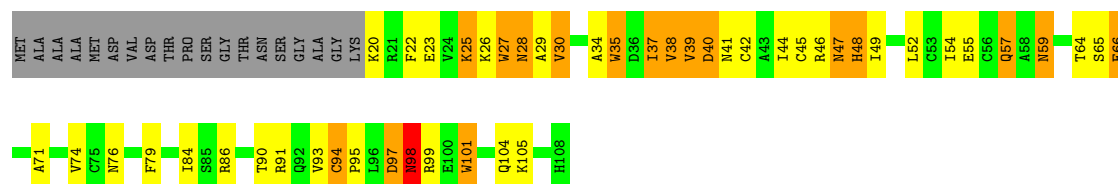
• Molecule 1: Cullin-3

Chain O: 60% 28% 5% • 6%



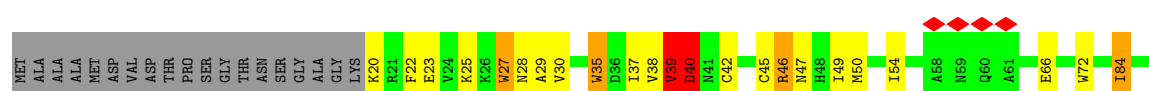
• Molecule 2: E3 ubiquitin-protein ligase RBX1

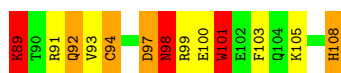
Chain E: 38% 28% 16% • 18%



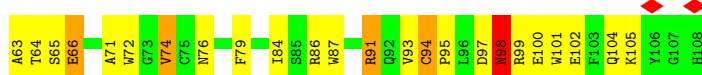
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain D: 49% 21% 7% 5% 18%

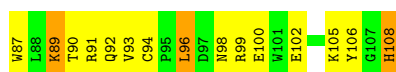




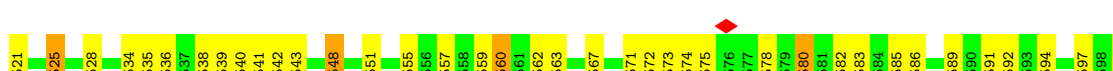
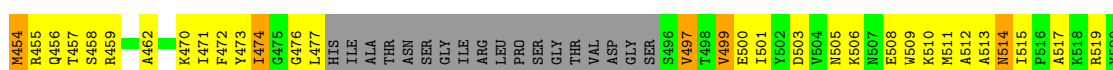
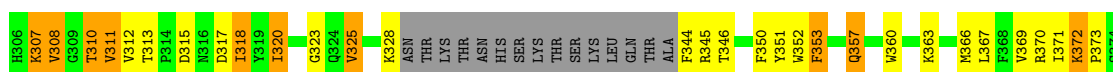
• Molecule 2: E3 ubiquitin-protein ligase RBX1



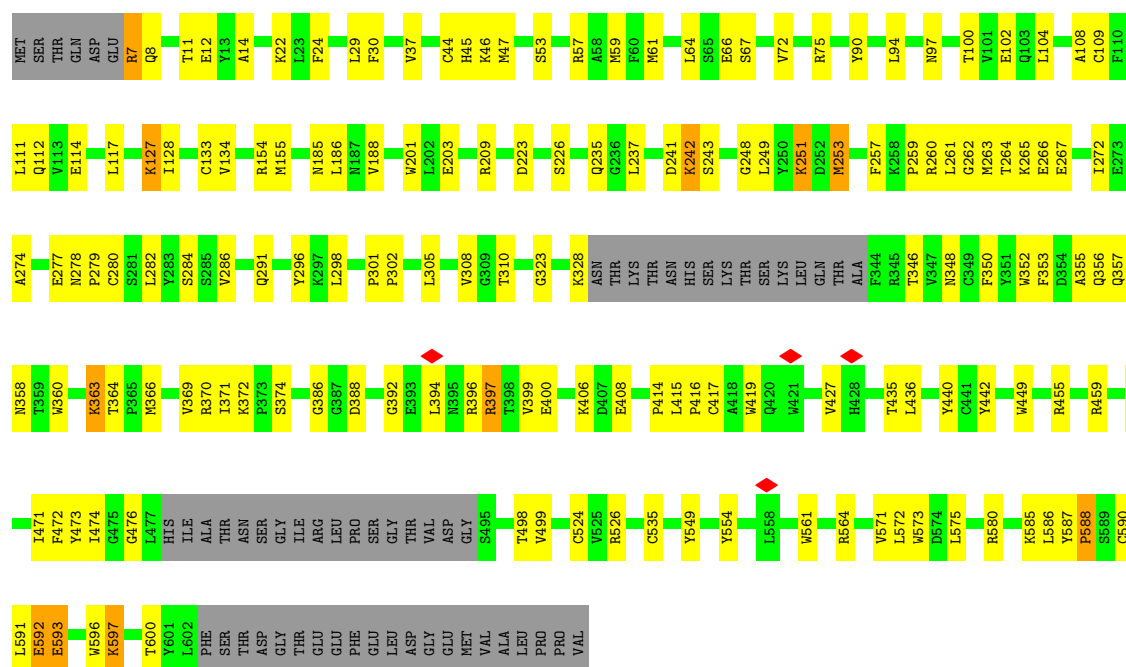
• Molecule 2: E3 ubiquitin-protein ligase RBX1



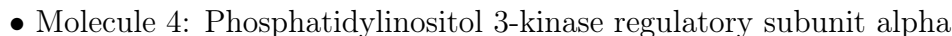
• Molecule 3: Kelch repeat and BTB domain-containing protein 2



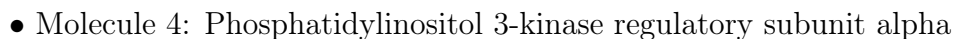
Chain B: 64% 25% 9%

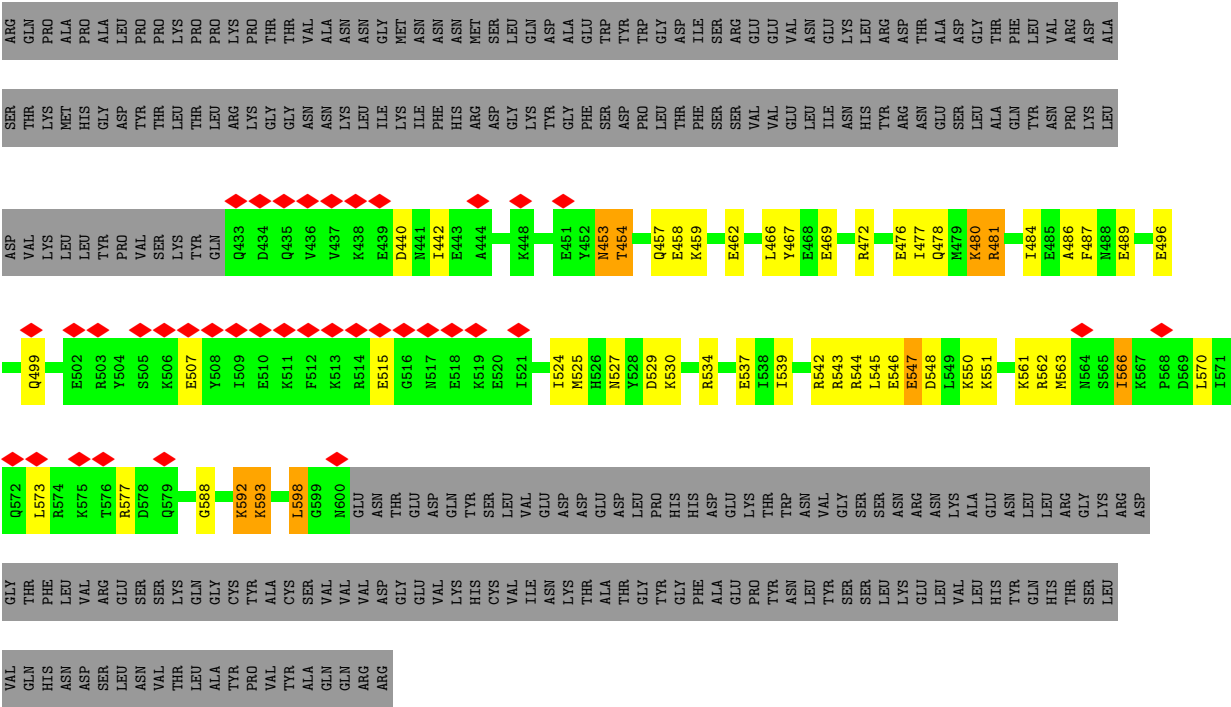


Chain P: 68% 20% • 11%

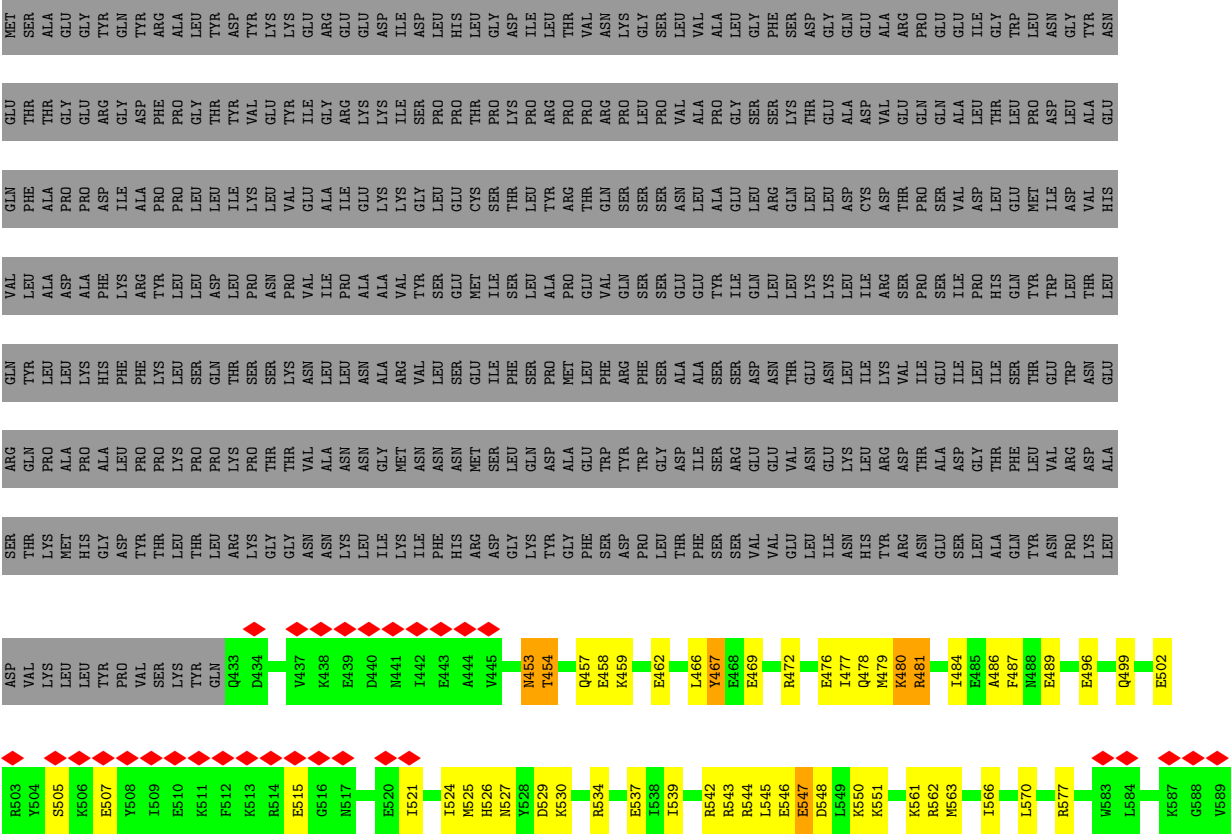
[illegible]

Chain H: 16% 6% 77%





• Molecule 4: Phosphatidylinositol 3-kinase regulatory subunit alpha



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	239068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.603	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.664, 2.664, 2.664	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C	0.63	12/5879 (0.2%)	0.78	15/7905 (0.2%)
1	F	0.56	1/5760 (0.0%)	0.75	8/7752 (0.1%)
1	M	0.81	30/5753 (0.5%)	0.78	13/7743 (0.2%)
1	O	0.56	2/5854 (0.0%)	0.76	11/7873 (0.1%)
2	D	0.81	1/759 (0.1%)	1.02	2/1029 (0.2%)
2	E	0.85	1/759 (0.1%)	1.06	1/1029 (0.1%)
2	Q	0.89	1/759 (0.1%)	1.04	1/1029 (0.1%)
2	R	0.83	1/759 (0.1%)	1.05	1/1029 (0.1%)
3	A	0.76	0/4667	0.86	1/6335 (0.0%)
3	B	0.42	0/4616	0.56	2/6268 (0.0%)
3	N	0.39	0/4616	0.53	2/6266 (0.0%)
3	P	0.43	0/4527	0.58	2/6151 (0.0%)
4	G	0.51	0/1443	0.69	0/1926
4	H	0.56	0/1356	0.75	0/1813
4	I	0.56	0/1376	0.77	0/1839
4	J	0.52	0/1342	0.70	0/1797
All	All	0.61	49/50225 (0.1%)	0.74	59/67784 (0.1%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	84	HIS	CA-C	-8.46	1.42	1.52
1	M	78	ARG	CA-C	-8.24	1.42	1.52
1	M	62	TYR	CA-C	-7.80	1.42	1.52
1	M	58	TYR	CA-C	-7.78	1.42	1.52
1	C	62	TYR	CA-C	-7.76	1.42	1.52
1	O	525	PRO	C-O	-7.68	1.15	1.24
1	C	58	TYR	CA-C	-7.62	1.42	1.52
1	M	74	TYR	CA-C	-7.59	1.43	1.52
1	M	54	PHE	CA-C	-7.57	1.42	1.52
1	C	54	PHE	CA-C	-7.53	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	80	VAL	CA-C	-7.01	1.43	1.52
1	M	77	LEU	CA-C	-6.98	1.43	1.52
1	M	55	GLU	CA-C	-6.85	1.44	1.52
1	C	61	ALA	CA-C	-6.82	1.44	1.52
1	C	55	GLU	CA-C	-6.79	1.44	1.52
1	M	61	ALA	CA-C	-6.75	1.44	1.52
1	M	63	THR	CA-C	-6.60	1.44	1.52
1	M	57	LEU	N-CA	-6.58	1.38	1.46
1	C	57	LEU	N-CA	-6.56	1.38	1.46
1	C	63	THR	CA-C	-6.45	1.44	1.52
1	M	85	LEU	CA-C	-6.29	1.44	1.52
1	M	72	LYS	CA-C	-6.17	1.44	1.52
1	M	88	LYS	CA-C	-6.13	1.44	1.52
1	M	91	GLU	CA-C	-6.01	1.44	1.52
1	C	55	GLU	N-CA	-5.94	1.39	1.46
1	M	73	LEU	CA-C	-5.88	1.45	1.52
1	M	87	ASN	N-CA	-5.79	1.38	1.46
2	R	30	VAL	CA-CB	-5.73	1.47	1.54
1	M	55	GLU	N-CA	-5.73	1.39	1.46
2	E	30	VAL	CA-CB	-5.70	1.47	1.54
2	D	30	VAL	CA-CB	-5.66	1.47	1.54
2	Q	30	VAL	CA-CB	-5.66	1.47	1.54
1	M	80	VAL	N-CA	-5.63	1.39	1.46
1	M	63	THR	N-CA	-5.51	1.39	1.46
1	M	75	THR	CA-C	-5.50	1.45	1.52
1	M	84	HIS	N-CA	-5.48	1.40	1.46
1	C	63	THR	N-CA	-5.42	1.39	1.46
1	C	64	MET	CA-C	-5.41	1.45	1.52
1	O	481	ASN	C-O	5.39	1.30	1.24
1	M	87	ASN	CA-C	-5.35	1.45	1.52
1	F	481	ASN	C-O	5.34	1.30	1.24
1	C	59	ARG	CA-C	-5.31	1.46	1.52
1	M	59	ARG	CA-C	-5.30	1.46	1.52
1	M	75	THR	N-CA	-5.26	1.39	1.46
1	M	64	MET	CA-C	-5.25	1.45	1.52
1	M	83	GLU	CA-C	-5.10	1.46	1.52
1	M	79	GLU	CA-C	-5.09	1.46	1.52
1	M	56	GLU	CA-C	-5.05	1.46	1.52
1	C	56	GLU	CA-C	-5.02	1.46	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	PRO	O-C-N	-14.29	114.74	121.31
1	O	67	HIS	N-CA-C	-11.57	100.70	112.97
1	F	67	HIS	N-CA-C	-11.54	100.74	112.97
1	M	55	GLU	N-CA-C	-10.55	99.86	111.36
1	C	55	GLU	N-CA-C	-10.54	99.88	111.36
1	O	466	PHE	N-CA-C	-9.55	102.43	114.56
1	F	466	PHE	N-CA-C	-9.49	102.51	114.56
1	F	90	ARG	N-CA-C	-8.46	102.02	111.07
1	O	90	ARG	N-CA-C	-8.45	102.03	111.07
1	M	91	GLU	N-CA-C	-7.61	102.64	112.23
1	M	72	LYS	N-CA-C	-7.36	102.27	111.11
1	M	62	TYR	N-CA-C	-6.63	104.13	111.82
1	C	62	TYR	N-CA-C	-6.62	104.14	111.82
2	D	27	TRP	O-C-N	-6.45	116.05	123.33
2	Q	27	TRP	O-C-N	-6.38	116.13	123.33
2	R	27	TRP	O-C-N	-6.26	116.00	123.27
1	O	69	HIS	N-CA-C	-6.23	103.36	111.71
3	P	523	PRO	CA-C-N	-6.22	113.73	123.13
3	P	523	PRO	C-N-CA	-6.22	113.73	123.13
1	F	69	HIS	N-CA-C	-6.21	103.39	111.71
2	E	27	TRP	O-C-N	-6.19	116.09	123.27
1	C	503	LEU	CA-C-O	-6.08	114.69	121.51
1	M	89	VAL	N-CA-C	6.04	119.54	111.44
2	D	89	LYS	N-CA-C	-5.86	106.18	113.38
1	C	95	ASN	N-CA-C	-5.85	105.85	112.87
1	C	92	ASP	N-CA-C	-5.85	104.81	111.07
1	C	62	TYR	CA-C-N	-5.80	112.55	120.44
1	C	62	TYR	C-N-CA	-5.80	112.55	120.44
1	M	76	GLY	N-CA-C	-5.80	105.77	112.73
1	F	467	THR	N-CA-C	-5.80	105.47	112.54
1	M	62	TYR	CA-C-N	-5.79	112.56	120.44
1	M	62	TYR	C-N-CA	-5.79	112.56	120.44
1	O	467	THR	N-CA-C	-5.79	105.48	112.54
1	C	58	TYR	N-CA-C	-5.74	105.17	111.82
1	M	58	TYR	N-CA-C	-5.73	105.17	111.82
3	A	323	GLY	CA-C-O	-5.73	118.19	122.37
1	O	523	ASN	CB-CA-C	5.57	118.96	109.72
1	M	265	GLU	N-CA-C	-5.50	106.62	113.38
1	O	623	PRO	CA-C-N	-5.42	115.99	122.44
1	O	623	PRO	C-N-CA	-5.42	115.99	122.44
1	F	623	PRO	CA-C-N	-5.40	116.02	122.44
1	F	623	PRO	C-N-CA	-5.40	116.02	122.44
1	C	762	LYS	N-CA-C	-5.36	107.39	114.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	78	ARG	N-CA-C	-5.36	104.67	111.11
1	C	264	VAL	N-CA-C	-5.36	105.28	110.42
3	N	588	PRO	N-CA-C	-5.34	106.10	113.53
3	B	588	PRO	N-CA-C	-5.32	106.14	113.53
3	B	242	LYS	N-CA-C	-5.25	106.14	112.54
3	N	242	LYS	N-CA-C	-5.19	106.20	112.54
1	O	525	PRO	N-CA-C	5.19	117.03	110.70
1	O	475	ARG	N-CA-C	-5.17	105.56	111.14
1	F	475	ARG	N-CA-C	-5.11	105.62	111.14
1	C	97	LEU	N-CA-C	-5.09	105.63	111.07
1	O	264	VAL	N-CA-CB	5.06	115.93	110.62
1	C	99	ASN	N-CA-C	5.02	117.44	109.50
1	M	54	PHE	CA-C-N	-5.01	113.18	120.29
1	M	54	PHE	C-N-CA	-5.01	113.18	120.29
1	C	54	PHE	CA-C-N	-5.01	113.18	120.29
1	C	54	PHE	C-N-CA	-5.01	113.18	120.29

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	C	5791	0	5773	215	0
1	F	5677	0	5575	138	0
1	M	5672	0	5583	158	0
1	O	5767	0	5730	150	0
2	D	737	0	686	23	0
2	E	737	0	686	45	0
2	Q	737	0	686	16	0
2	R	737	0	686	59	0
3	A	4559	0	4441	108	0
3	B	4510	0	4385	124	0
3	N	4510	0	4373	136	0
3	P	4423	0	4245	110	0
4	G	1424	0	1387	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1341	0	1243	23	0
4	I	1360	0	1276	29	0
4	J	1327	0	1203	25	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
All	All	49321	0	47958	1265	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 13.

All (1265) 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)
3:B:154:ARG:HD3	3:B:357:GLN:NE2	1.43	1.33
3:N:154:ARG:HD3	3:N:357:GLN:NE2	1.43	1.30
1:M:531:ALA:HB3	2:R:27:TRP:CZ3	1.76	1.20
3:N:298:LEU:HD23	3:N:591:LEU:HD21	1.26	1.18
3:N:14:ALA:HB2	3:P:18:LEU:HD22	1.21	1.15
3:P:298:LEU:CD2	3:P:591:LEU:HD21	1.76	1.13
3:B:298:LEU:HD23	3:B:591:LEU:HD21	1.26	1.11
3:P:298:LEU:HD23	3:P:591:LEU:HD21	1.14	1.10
3:N:185:ASN:CG	3:N:356:GLN:HE22	1.59	1.10
3:B:185:ASN:CG	3:B:356:GLN:HE22	1.59	1.08
1:O:54:PHE:HB2	3:N:59:MET:HE1	1.29	1.06
1:C:54:PHE:HB2	3:A:59:MET:HE1	1.07	1.04
2:D:39:VAL:O	2:D:40:ASP:HB3	1.56	1.04
1:O:54:PHE:CB	3:N:59:MET:HE1	1.86	1.03
1:F:68:LYS:HE3	3:B:142:LEU:HD12	1.40	1.03
3:N:154:ARG:HD3	3:N:357:GLN:HE21	0.94	1.03
3:P:154:ARG:HD3	3:P:357:GLN:NE2	1.74	1.03
2:Q:39:VAL:O	2:Q:40:ASP:HB3	1.56	1.02
3:B:154:ARG:CD	3:B:357:GLN:NE2	2.22	1.02
3:N:154:ARG:CD	3:N:357:GLN:NE2	2.22	1.02
1:F:525:PRO:HA	1:F:603:MET:HE2	1.40	1.01
2:E:37:ILE:HD11	2:E:39:VAL:HG22	1.44	0.99
3:B:154:ARG:HD3	3:B:357:GLN:HE21	0.94	0.99
1:O:525:PRO:HA	1:O:603:MET:HE2	1.44	0.98
1:C:480:SER:HB2	1:C:506:ARG:HB3	1.40	0.97
1:C:440:LEU:HB3	1:C:477:MET:SD	2.04	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:HA	1:C:88:LYS:HB3	1.46	0.96
1:C:440:LEU:HD13	1:C:477:MET:HG3	1.47	0.96
1:C:54:PHE:CB	3:A:59:MET:HE1	1.94	0.96
2:R:37:ILE:HD11	2:R:39:VAL:HG22	1.44	0.95
1:F:768:ALA:HB1	2:D:89:LYS:HB3	1.47	0.95
1:M:531:ALA:HB3	2:R:27:TRP:HZ3	1.14	0.95
3:P:154:ARG:HH11	3:P:357:GLN:HE22	1.13	0.95
1:F:68:LYS:NZ	3:B:142:LEU:HA	1.81	0.95
1:C:54:PHE:HB2	3:A:59:MET:CE	1.95	0.95
3:N:57:ARG:CZ	3:P:24:PHE:HZ	1.79	0.94
1:C:349:LYS:NZ	1:C:417:VAL:HG12	1.82	0.94
3:N:298:LEU:CD2	3:N:591:LEU:HD21	1.98	0.94
3:N:14:ALA:CB	3:P:18:LEU:HD22	1.97	0.93
1:C:484:MET:SD	1:C:504:THR:HG22	2.09	0.93
3:P:297:LYS:HB3	3:P:592:GLU:OE1	1.70	0.91
3:B:298:LEU:CD2	3:B:591:LEU:HD21	1.99	0.91
2:R:79:PHE:CD2	2:R:84:ILE:HG21	2.06	0.91
3:N:30:PHE:HE1	3:P:60:PHE:CB	1.84	0.90
1:O:59:ARG:CZ	3:N:75:ARG:HD2	2.01	0.90
3:N:30:PHE:CE1	3:P:60:PHE:CB	2.55	0.90
1:O:96:SER:HB3	1:O:104:THR:HG21	1.54	0.89
3:A:308:VAL:HB	3:A:320:ILE:HG13	1.53	0.89
3:P:185:ASN:CG	3:P:356:GLN:HE22	1.82	0.88
1:F:96:SER:HB3	1:F:104:THR:HG21	1.54	0.88
3:A:497:VAL:HG23	3:A:514:ASN:ND2	1.87	0.87
1:M:531:ALA:CB	2:R:27:TRP:CZ3	2.56	0.87
2:R:71:ALA:CB	2:R:84:ILE:HD11	2.05	0.86
2:E:71:ALA:CB	2:E:84:ILE:HD11	2.04	0.86
1:C:484:MET:CE	1:C:504:THR:HG22	2.05	0.86
1:C:349:LYS:HZ3	1:C:417:VAL:HG12	1.39	0.85
1:M:531:ALA:CB	2:R:27:TRP:HZ3	1.87	0.85
3:P:154:ARG:HD3	3:P:357:GLN:HE21	1.39	0.84
1:F:531:ALA:CB	2:D:27:TRP:CZ3	2.62	0.82
3:N:185:ASN:CG	3:N:356:GLN:NE2	2.37	0.82
3:A:61:MET:HE3	3:B:30:PHE:CZ	2.13	0.82
1:O:53:SER:HA	3:N:66:GLU:OE2	1.79	0.82
1:O:440:LEU:HD13	1:O:477:MET:HG3	1.61	0.82
1:F:440:LEU:HD13	1:F:477:MET:HG3	1.61	0.81
3:B:185:ASN:CG	3:B:356:GLN:NE2	2.37	0.80
2:R:39:VAL:HG12	2:R:39:VAL:O	1.82	0.80
3:P:154:ARG:NH1	3:P:357:GLN:NE2	2.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:14:ALA:HB2	3:P:18:LEU:CD2	2.07	0.80
1:O:55:GLU:OE2	3:N:72:VAL:HG13	1.81	0.80
2:E:71:ALA:HB3	2:E:84:ILE:HD11	1.63	0.79
3:N:61:MET:SD	3:P:29:LEU:HD22	2.22	0.79
3:P:154:ARG:NH1	3:P:357:GLN:HE22	1.79	0.79
2:R:71:ALA:HB3	2:R:84:ILE:HD11	1.63	0.79
1:C:484:MET:SD	1:C:504:THR:HA	2.22	0.78
1:F:68:LYS:HZ1	3:B:142:LEU:HA	1.43	0.78
1:F:89:VAL:HG11	1:F:151:VAL:HG22	1.65	0.78
1:M:525:PRO:HB2	1:M:528:PRO:HD2	1.64	0.78
3:N:154:ARG:HH11	3:N:357:GLN:NE2	1.82	0.78
1:O:89:VAL:HG11	1:O:151:VAL:HG22	1.65	0.78
2:E:39:VAL:HG12	2:E:39:VAL:O	1.82	0.78
1:O:59:ARG:HD2	3:N:75:ARG:HB2	1.67	0.77
1:M:277:VAL:HG21	1:M:312:THR:HB	1.65	0.77
3:B:154:ARG:HH11	3:B:357:GLN:NE2	1.82	0.76
1:C:58:TYR:HH	3:A:112:GLN:CD	1.93	0.76
1:F:531:ALA:HB1	2:D:27:TRP:CZ3	2.22	0.75
3:N:265:LYS:HD3	3:N:587:TYR:CE1	2.22	0.75
1:C:91:GLU:HA	1:C:94:LEU:HB2	1.67	0.75
1:O:49:ASN:ND2	3:N:64:LEU:HD21	2.02	0.75
3:N:24:PHE:HZ	3:P:57:ARG:NE	1.83	0.75
3:B:265:LYS:HD3	3:B:587:TYR:CE1	2.22	0.75
3:A:253:MET:HB3	3:A:258:LYS:HG3	1.69	0.74
1:C:125:TYR:HD1	3:A:112:GLN:HE21	1.35	0.74
1:M:531:ALA:HB3	2:R:27:TRP:CE3	2.22	0.74
3:B:297:LYS:HB3	3:B:592:GLU:OE1	1.87	0.74
3:A:308:VAL:HB	3:A:320:ILE:CG1	2.17	0.74
1:F:37:LEU:HD13	1:F:57:LEU:HD12	1.68	0.74
3:N:358:ASN:ND2	3:N:591:LEU:O	2.21	0.74
3:A:427:VAL:HG23	3:A:432:TYR:HB2	1.70	0.74
3:P:253:MET:HB3	3:P:258:LYS:HG3	1.69	0.74
1:C:58:TYR:OH	3:A:112:GLN:CD	2.31	0.73
1:F:93:VAL:HG11	1:F:156:CYS:SG	2.28	0.73
1:F:531:ALA:HB1	2:D:27:TRP:CE3	2.24	0.73
3:P:185:ASN:CG	3:P:356:GLN:NE2	2.47	0.73
3:B:358:ASN:ND2	3:B:591:LEU:O	2.21	0.73
1:F:531:ALA:HB3	2:D:27:TRP:CZ3	2.24	0.73
1:F:68:LYS:CE	3:B:142:LEU:HD12	2.19	0.72
1:M:480:SER:HB2	1:M:506:ARG:HB3	1.69	0.72
1:O:93:VAL:HG11	1:O:156:CYS:SG	2.29	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:297:LYS:HB3	3:P:592:GLU:CD	2.14	0.71
3:P:298:LEU:HD23	3:P:591:LEU:CD2	2.08	0.71
3:B:261:LEU:HG	3:B:587:TYR:CE1	2.25	0.71
3:B:266:GLU:HG3	3:B:588:PRO:HG3	1.73	0.71
3:N:261:LEU:HG	3:N:587:TYR:CE1	2.25	0.71
3:P:154:ARG:CD	3:P:357:GLN:NE2	2.53	0.71
1:C:274:LYS:HA	1:C:277:VAL:HG22	1.72	0.71
1:O:59:ARG:NH2	3:N:75:ARG:HD2	2.06	0.71
3:A:61:MET:HE3	3:B:30:PHE:CE2	2.25	0.71
2:R:34:ALA:HA	2:R:76:ASN:ND2	2.05	0.70
1:O:54:PHE:HB2	3:N:59:MET:CE	2.16	0.70
1:M:262:LYS:HB3	1:M:266:ARG:NH1	2.07	0.70
2:R:71:ALA:HB3	2:R:84:ILE:CD1	2.22	0.70
2:R:79:PHE:CD2	2:R:84:ILE:CG2	2.74	0.70
1:F:378:LEU:HD23	1:F:421:PHE:O	1.92	0.70
2:E:71:ALA:HB3	2:E:84:ILE:CD1	2.22	0.69
3:P:459:ARG:HB3	3:P:476:GLY:HA2	1.74	0.69
4:G:466:LEU:HD13	4:G:563:MET:HG2	1.75	0.69
3:N:266:GLU:HG3	3:N:588:PRO:HG3	1.73	0.69
3:B:397:ARG:HB3	3:B:415:LEU:HB2	1.74	0.69
3:P:372:LYS:HD3	3:P:580:ARG:HH21	1.58	0.69
3:N:397:ARG:HB3	3:N:415:LEU:HB2	1.74	0.68
1:M:89:VAL:HA	1:M:92:ASP:HB2	1.75	0.68
1:M:622:ILE:HG12	1:M:627:LEU:HD13	1.75	0.68
4:J:466:LEU:HD13	4:J:563:MET:HG2	1.75	0.68
1:C:259:PRO:HA	1:C:262:LYS:HG2	1.75	0.68
4:H:466:LEU:HD13	4:H:563:MET:HG2	1.75	0.68
3:N:185:ASN:ND2	3:N:356:GLN:HE22	1.92	0.68
3:N:436:LEU:O	3:N:455:ARG:NH2	2.26	0.68
1:C:506:ARG:HB2	2:E:30:VAL:HG22	1.76	0.68
1:M:68:LYS:HE3	3:P:141:ASP:O	1.93	0.68
1:O:54:PHE:CZ	3:N:64:LEU:CD1	2.76	0.68
1:O:323:GLU:HA	1:O:326:LYS:HZ3	1.58	0.68
1:F:323:GLU:HA	1:F:326:LYS:HZ3	1.58	0.68
1:O:66:LEU:C	1:O:68:LYS:H	2.02	0.68
3:A:302:PRO:HD2	3:A:305:LEU:HB2	1.74	0.67
3:B:185:ASN:ND2	3:B:356:GLN:HE22	1.92	0.67
1:F:622:ILE:HG12	1:F:627:LEU:HD13	1.77	0.67
3:B:436:LEU:O	3:B:455:ARG:NH2	2.26	0.67
4:I:466:LEU:HD13	4:I:563:MET:HG2	1.75	0.67
1:C:622:ILE:HG12	1:C:627:LEU:HD13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:57:ARG:CZ	3:P:24:PHE:CZ	2.71	0.67
1:C:58:TYR:OH	3:A:112:GLN:NE2	2.27	0.67
3:B:372:LYS:HD3	3:B:580:ARG:HH21	1.60	0.67
1:O:532:PHE:HB2	2:Q:27:TRP:HH2	1.59	0.66
1:C:323:GLU:HA	1:C:326:LYS:HZ3	1.58	0.66
1:F:66:LEU:C	1:F:68:LYS:H	2.02	0.66
1:F:425:LYS:HZ2	1:F:462:CYS:HB2	1.58	0.66
1:O:425:LYS:HZ2	1:O:462:CYS:HB2	1.58	0.66
3:N:154:ARG:CD	3:N:357:GLN:HE22	2.07	0.66
1:M:66:LEU:HD21	3:P:143:PHE:CE1	2.31	0.66
1:C:277:VAL:HG21	1:C:312:THR:HB	1.77	0.66
3:A:427:VAL:CG2	3:A:432:TYR:HB2	2.25	0.66
1:O:54:PHE:CZ	3:N:64:LEU:HD11	2.30	0.66
3:N:372:LYS:HD3	3:N:580:ARG:HH21	1.60	0.66
1:O:525:PRO:HD2	1:O:528:PRO:HB2	1.78	0.66
1:C:488:ARG:HD3	1:C:503:LEU:O	1.96	0.66
1:C:75:THR:HA	1:C:78:ARG:HD2	1.77	0.65
1:M:81:VAL:O	1:M:84:HIS:HB3	1.96	0.65
1:C:697:ASP:HA	1:C:700:LYS:HD2	1.77	0.65
1:F:531:ALA:CB	2:D:27:TRP:CE3	2.78	0.65
3:B:154:ARG:CD	3:B:357:GLN:HE22	2.07	0.65
3:B:301:PRO:HD2	3:B:360:TRP:HD1	1.61	0.65
3:A:517:ALA:HB1	3:A:521:SER:CB	2.27	0.65
3:N:301:PRO:HD2	3:N:360:TRP:HD1	1.61	0.65
1:C:59:ARG:NH2	3:A:75:ARG:HD2	2.12	0.65
4:J:459:LYS:HB3	4:J:570:LEU:HD13	1.79	0.65
3:P:300:SER:HA	3:P:360:TRP:HE1	1.62	0.65
1:O:622:ILE:HG12	1:O:627:LEU:HD13	1.77	0.65
3:A:17:LEU:CD1	3:B:51:THR:HB	2.27	0.65
1:M:525:PRO:HA	1:M:603:MET:HE2	1.79	0.65
4:G:453:ASN:HA	4:G:577:ARG:HH12	1.61	0.65
4:G:459:LYS:HB3	4:G:570:LEU:HD13	1.79	0.65
1:F:54:PHE:HA	1:F:57:LEU:HD23	1.79	0.64
1:O:525:PRO:HB2	1:O:528:PRO:HD2	1.78	0.64
1:M:504:THR:O	2:R:28:ASN:HA	1.98	0.64
3:A:325:VAL:HG12	3:A:345:ARG:HB3	1.78	0.64
3:N:459:ARG:NH1	3:N:498:THR:OG1	2.30	0.64
1:C:504:THR:O	2:E:28:ASN:HA	1.98	0.64
3:B:459:ARG:NH1	3:B:498:THR:OG1	2.30	0.64
2:E:37:ILE:HD11	2:E:39:VAL:CG2	2.25	0.64
4:G:449:LEU:HD21	4:G:594:LEU:CD2	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:37:ILE:HD11	2:R:39:VAL:CG2	2.25	0.64
3:A:109:CYS:O	3:A:112:GLN:NE2	2.31	0.64
4:H:459:LYS:HB3	4:H:570:LEU:HD13	1.79	0.64
3:N:57:ARG:NH2	3:P:24:PHE:HZ	1.95	0.64
1:C:556:SER:HA	1:C:595:SER:HA	1.80	0.63
1:M:531:ALA:CB	2:R:27:TRP:CE3	2.81	0.63
1:M:248:VAL:HG11	1:M:257:GLU:HB2	1.81	0.63
4:I:459:LYS:HB3	4:I:570:LEU:HD13	1.79	0.63
3:P:109:CYS:O	3:P:112:GLN:NE2	2.31	0.63
3:P:268:MET:HE1	3:P:588:PRO:HB3	1.79	0.63
2:E:94:CYS:HB2	2:E:101:TRP:HB2	1.79	0.63
1:C:437:ALA:HA	1:C:513:TRP:HZ3	1.63	0.63
1:O:266:ARG:HG2	1:O:307:PRO:HD3	1.80	0.63
1:F:102:LEU:O	1:F:106:ASN:ND2	2.32	0.63
3:N:301:PRO:HD2	3:N:360:TRP:CD1	2.34	0.63
1:C:102:LEU:O	1:C:106:ASN:ND2	2.32	0.63
1:F:556:SER:HA	1:F:595:SER:HA	1.80	0.63
1:O:556:SER:HA	1:O:595:SER:HA	1.80	0.63
1:C:74:TYR:HA	1:C:77:LEU:HD12	1.81	0.62
1:M:503:LEU:HD11	1:M:531:ALA:HB1	1.79	0.62
2:E:44:ILE:CD1	2:E:84:ILE:HG22	2.28	0.62
1:C:525:PRO:HB2	1:C:528:PRO:HD2	1.82	0.62
1:O:102:LEU:O	1:O:106:ASN:ND2	2.32	0.62
2:R:44:ILE:CD1	2:R:84:ILE:HG22	2.28	0.62
1:C:703:ILE:HB	1:C:741:ILE:HD13	1.80	0.62
3:P:436:LEU:O	3:P:455:ARG:NH2	2.31	0.62
1:C:221:SER:HB3	1:C:268:LEU:HD22	1.81	0.62
1:C:267:GLU:O	1:C:268:LEU:C	2.42	0.62
3:B:301:PRO:HD2	3:B:360:TRP:CD1	2.34	0.62
3:B:352:TRP:HB3	3:B:363:LYS:HE3	1.82	0.62
3:A:243:SER:HB2	3:A:292:ALA:HB2	1.80	0.62
3:N:154:ARG:HH11	3:N:357:GLN:HE22	1.48	0.61
1:M:556:SER:HA	1:M:595:SER:HA	1.80	0.61
1:M:83:GLU:HA	1:M:86:ILE:HG22	1.82	0.61
3:P:154:ARG:HH11	3:P:357:GLN:NE2	1.85	0.61
1:M:323:GLU:HA	1:M:326:LYS:HZ3	1.65	0.61
3:N:154:ARG:NH1	3:N:357:GLN:NE2	2.49	0.61
1:F:86:ILE:HA	1:F:150:GLN:HE22	1.66	0.61
1:F:459:LYS:HZ2	1:F:467:THR:HB	1.66	0.60
1:M:84:HIS:O	1:M:88:LYS:HB2	2.01	0.60
1:M:87:ASN:O	1:M:88:LYS:C	2.43	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:526:PRO:HD2	1:O:603:MET:SD	2.41	0.60
3:N:24:PHE:HZ	3:P:57:ARG:CD	2.13	0.60
1:F:459:LYS:NZ	1:F:467:THR:HB	2.16	0.60
3:N:352:TRP:HB3	3:N:363:LYS:HE3	1.82	0.60
1:O:459:LYS:NZ	1:O:467:THR:HB	2.16	0.60
2:R:79:PHE:HB2	2:R:84:ILE:HG23	1.82	0.60
3:B:154:ARG:HH11	3:B:357:GLN:HE22	1.48	0.60
3:B:154:ARG:NH1	3:B:357:GLN:NE2	2.49	0.60
1:F:527:ALA:HB3	1:F:528:PRO:HD3	1.82	0.60
1:O:86:ILE:HA	1:O:150:GLN:HE22	1.66	0.60
3:N:370:ARG:NH1	3:N:386:GLY:O	2.34	0.60
2:R:34:ALA:HA	2:R:76:ASN:HD21	1.65	0.60
3:A:517:ALA:CB	3:A:521:SER:CB	2.80	0.60
1:C:524:ILE:HG22	1:C:529:ARG:HG3	1.84	0.60
1:O:273:MET:HB2	1:O:303:PHE:CZ	2.36	0.60
3:B:370:ARG:NH1	3:B:386:GLY:O	2.34	0.60
4:J:453:ASN:HA	4:J:577:ARG:HH12	1.65	0.60
3:P:267:GLU:HG2	3:P:585:LYS:HG2	1.84	0.60
3:P:459:ARG:NH1	3:P:498:THR:OG1	2.35	0.59
1:M:86:ILE:HA	1:M:150:GLN:HE22	1.66	0.59
1:M:523:ASN:HD21	1:M:603:MET:HE1	1.66	0.59
2:D:72:TRP:HE1	2:D:108:HIS:HA	1.68	0.59
1:C:99:ASN:O	1:C:100:ASN:C	2.44	0.59
1:F:106:ASN:O	1:F:110:ASN:ND2	2.36	0.59
2:E:44:ILE:HD12	2:E:84:ILE:CG2	2.33	0.59
4:I:547:GLU:HA	4:I:550:LYS:HG2	1.84	0.59
3:N:44:CYS:SG	3:N:45:HIS:N	2.75	0.59
1:C:106:ASN:O	1:C:110:ASN:ND2	2.36	0.59
1:C:349:LYS:NZ	1:C:417:VAL:CG1	2.62	0.59
1:F:703:ILE:HD11	1:F:744:ARG:HD3	1.84	0.59
3:P:397:ARG:NH1	3:P:415:LEU:O	2.36	0.59
1:M:276:ILE:C	1:M:278:GLU:H	2.10	0.59
3:A:350:PHE:CD1	3:A:352:TRP:CH2	2.91	0.59
1:C:87:ASN:O	1:C:88:LYS:C	2.46	0.59
1:C:748:LEU:HA	1:C:751:ARG:HG3	1.84	0.59
1:M:106:ASN:O	1:M:110:ASN:ND2	2.36	0.59
2:Q:72:TRP:HE1	2:Q:108:HIS:HA	1.68	0.59
3:B:297:LYS:HB3	3:B:592:GLU:CD	2.28	0.58
3:B:535:CYS:SG	3:B:564:ARG:NH1	2.75	0.58
3:N:30:PHE:CZ	3:P:60:PHE:CB	2.85	0.58
3:P:396:ARG:HD2	3:P:397:ARG:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:458:LEU:HB3	1:F:467:THR:HG22	1.86	0.58
2:R:44:ILE:HD12	2:R:84:ILE:CG2	2.33	0.58
3:A:573:TRP:HD1	3:A:597:LYS:HG2	1.67	0.58
3:B:44:CYS:SG	3:B:45:HIS:N	2.75	0.58
3:P:185:ASN:ND2	3:P:356:GLN:HE22	2.01	0.58
1:M:68:LYS:NZ	3:P:142:LEU:O	2.31	0.58
1:O:106:ASN:O	1:O:110:ASN:ND2	2.36	0.58
3:N:535:CYS:SG	3:N:564:ARG:NH1	2.75	0.58
1:C:92:ASP:O	1:C:96:SER:HB2	2.03	0.58
3:P:154:ARG:HD3	3:P:357:GLN:HE22	1.63	0.58
3:P:535:CYS:SG	3:P:564:ARG:NH1	2.77	0.58
1:C:85:LEU:CA	1:C:88:LYS:HB3	2.27	0.58
1:F:525:PRO:HD2	1:F:528:PRO:HB2	1.85	0.58
1:O:703:ILE:HD11	1:O:744:ARG:HD3	1.85	0.58
3:A:373:PRO:HA	3:A:387:GLY:HA3	1.84	0.58
3:N:22:LYS:HE2	3:N:90:TYR:HB3	1.85	0.58
4:H:547:GLU:HA	4:H:550:LYS:HG2	1.84	0.58
1:C:77:LEU:O	1:C:78:ARG:C	2.46	0.58
2:R:94:CYS:HB2	2:R:101:TRP:HB2	1.85	0.58
4:G:547:GLU:HA	4:G:550:LYS:HG2	1.85	0.58
1:C:274:LYS:CA	1:C:277:VAL:HG22	2.34	0.58
3:B:355:ALA:O	3:B:587:TYR:HD2	1.87	0.57
4:J:547:GLU:HA	4:J:550:LYS:HG2	1.85	0.57
1:M:71:GLU:O	1:M:72:LYS:C	2.44	0.57
1:O:458:LEU:HB3	1:O:467:THR:HG22	1.86	0.57
1:O:503:LEU:HD11	1:O:531:ALA:HB1	1.86	0.57
2:R:79:PHE:HD2	2:R:84:ILE:HG21	1.61	0.57
1:C:265:GLU:HA	1:C:269:ILE:HG13	1.87	0.57
1:C:202:GLU:HA	1:C:206:GLU:HB3	1.87	0.57
1:O:93:VAL:HA	1:O:97:LEU:HG	1.87	0.57
3:N:355:ALA:O	3:N:587:TYR:HD2	1.87	0.57
1:C:703:ILE:HD11	1:C:744:ARG:HD3	1.87	0.56
1:M:202:GLU:HA	1:M:206:GLU:HB3	1.87	0.56
1:O:202:GLU:HA	1:O:206:GLU:HB3	1.87	0.56
3:B:201:TRP:O	3:B:209:ARG:NH1	2.36	0.56
1:C:121:ASP:HB3	3:A:58:ALA:HB1	1.86	0.56
1:F:220:GLU:HA	1:F:223:LYS:HG2	1.87	0.56
3:A:497:VAL:HG23	3:A:514:ASN:HD22	1.69	0.56
1:C:125:TYR:CD1	3:A:112:GLN:NE2	2.71	0.56
1:C:274:LYS:HA	1:C:277:VAL:CG2	2.36	0.56
1:F:612:THR:OG1	1:F:655:ASN:O	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:612:THR:OG1	1:O:655:ASN:O	2.24	0.56
3:A:201:TRP:O	3:A:209:ARG:NH1	2.38	0.56
1:F:557:ALA:HB3	1:F:594:VAL:HG23	1.88	0.56
3:A:285:SER:HB3	3:A:300:SER:HB3	1.87	0.56
3:B:353:PHE:HB2	3:B:360:TRP:CZ2	2.41	0.56
3:N:201:TRP:O	3:N:209:ARG:NH1	2.36	0.56
3:N:274:ALA:N	3:N:284:SER:O	2.32	0.56
1:O:220:GLU:HA	1:O:223:LYS:HG2	1.87	0.56
3:B:392:GLY:HA2	3:B:396:ARG:HG2	1.88	0.56
3:P:297:LYS:O	3:P:592:GLU:HB3	2.06	0.56
1:C:274:LYS:O	1:C:275:THR:C	2.49	0.56
2:Q:27:TRP:CZ2	2:Q:29:ALA:HB2	2.41	0.56
1:C:63:THR:HA	1:C:66:LEU:HD22	1.87	0.56
1:M:220:GLU:HA	1:M:223:LYS:HG2	1.87	0.56
1:O:532:PHE:HB2	2:Q:27:TRP:CH2	2.39	0.56
2:R:27:TRP:CZ2	2:R:29:ALA:HB2	2.40	0.56
3:A:603:PHE:HB3	4:G:467:TYR:HE2	1.71	0.56
3:A:350:PHE:HE2	3:A:366:MET:HB2	1.70	0.56
3:N:353:PHE:HB2	3:N:360:TRP:CZ2	2.41	0.56
1:F:93:VAL:HA	1:F:97:LEU:HG	1.87	0.55
1:M:557:ALA:HB3	1:M:594:VAL:HG23	1.88	0.55
1:O:557:ALA:HB3	1:O:594:VAL:HG23	1.88	0.55
1:C:612:THR:OG1	1:C:655:ASN:O	2.24	0.55
4:I:453:ASN:HA	4:I:577:ARG:HH12	1.70	0.55
3:N:267:GLU:HG2	3:N:585:LYS:HG2	1.89	0.55
1:F:202:GLU:HA	1:F:206:GLU:HB3	1.87	0.55
1:M:83:GLU:O	1:M:84:HIS:C	2.45	0.55
1:O:49:ASN:HA	1:O:52:LEU:HD13	1.88	0.55
1:O:100:ASN:HB3	1:O:103:GLN:HB2	1.89	0.55
2:E:27:TRP:CZ2	2:E:29:ALA:HB2	2.40	0.55
1:C:480:SER:HA	1:C:507:VAL:H	1.72	0.55
1:M:129:VAL:O	1:M:132:GLN:NE2	2.40	0.55
1:C:409:GLU:OE2	1:C:453:ASN:ND2	2.40	0.55
1:F:100:ASN:HB3	1:F:103:GLN:HB2	1.89	0.55
1:M:478:SER:HA	1:M:481:ASN:HD21	1.72	0.55
2:D:27:TRP:CZ2	2:D:29:ALA:HB2	2.41	0.55
3:A:528:VAL:HG23	3:A:535:CYS:SG	2.46	0.55
1:M:506:ARG:HB2	2:R:30:VAL:HG22	1.88	0.55
4:G:449:LEU:HD21	4:G:594:LEU:HD22	1.89	0.55
4:G:496:GLU:HG2	4:G:499:GLN:HE21	1.72	0.55
3:N:392:GLY:HA2	3:N:396:ARG:HG2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:717:MET:HB3	1:O:722:LEU:HG	1.89	0.55
3:N:524:CYS:SG	3:N:526:ARG:NH1	2.80	0.55
1:C:129:VAL:O	1:C:132:GLN:NE2	2.40	0.55
1:C:557:ALA:HB3	1:C:594:VAL:HG23	1.88	0.55
1:C:704:GLU:O	1:C:707:ILE:HG22	2.06	0.55
1:M:717:MET:HB3	1:M:722:LEU:HG	1.89	0.55
1:O:409:GLU:OE2	1:O:453:ASN:ND2	2.40	0.55
3:P:397:ARG:HB3	3:P:415:LEU:HB2	1.89	0.55
1:C:49:ASN:HA	1:C:52:LEU:HD13	1.88	0.55
1:M:520:PRO:HG2	1:M:552:HIS:H	1.72	0.55
3:A:397:ARG:HG2	3:A:418:ALA:HA	1.89	0.55
3:B:185:ASN:OD1	3:B:356:GLN:NE2	2.40	0.55
3:B:188:VAL:HG23	3:B:263:MET:HE2	1.89	0.55
4:H:496:GLU:HG2	4:H:499:GLN:HE21	1.72	0.55
1:F:129:VAL:O	1:F:132:GLN:NE2	2.40	0.55
1:O:54:PHE:HB3	3:N:59:MET:HE1	1.83	0.55
3:N:188:VAL:HG23	3:N:263:MET:HE2	1.89	0.55
1:M:261:VAL:HA	1:M:264:VAL:HB	1.89	0.54
1:M:365:LEU:HD12	1:M:368:GLN:HE21	1.72	0.54
4:H:453:ASN:HA	4:H:577:ARG:HH12	1.72	0.54
4:I:496:GLU:HG2	4:I:499:GLN:HE21	1.72	0.54
1:C:220:GLU:HA	1:C:223:LYS:HG2	1.87	0.54
1:M:612:THR:OG1	1:M:655:ASN:O	2.24	0.54
2:R:52:LEU:HD21	2:R:59:ASN:HA	1.89	0.54
1:C:478:SER:HA	1:C:481:ASN:HD21	1.72	0.54
1:F:409:GLU:OE2	1:F:453:ASN:ND2	2.40	0.54
2:R:79:PHE:CB	2:R:84:ILE:HG23	2.38	0.54
3:A:47:MET:HE1	3:B:47:MET:HE1	1.88	0.54
4:I:534:ARG:HH22	3:N:253:MET:HE2	1.73	0.54
3:N:185:ASN:OD1	3:N:356:GLN:NE2	2.40	0.54
1:C:94:LEU:C	1:C:96:SER:H	2.16	0.54
1:F:525:PRO:HB2	1:F:528:PRO:HD2	1.88	0.54
1:O:129:VAL:O	1:O:132:GLN:NE2	2.40	0.54
2:E:44:ILE:HD11	2:E:84:ILE:HG22	1.89	0.54
3:B:267:GLU:HG2	3:B:585:LYS:HG2	1.89	0.54
3:P:298:LEU:HD21	3:P:591:LEU:HD21	1.84	0.54
2:E:34:ALA:HA	2:E:76:ASN:ND2	2.23	0.54
4:G:484:ILE:HD11	4:G:542:ARG:HG3	1.89	0.54
1:M:409:GLU:OE2	1:M:453:ASN:ND2	2.40	0.54
1:O:365:LEU:HD12	1:O:368:GLN:HE21	1.73	0.54
3:P:201:TRP:O	3:P:209:ARG:NH1	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:VAL:O	2:D:40:ASP:CB	2.42	0.54
1:F:365:LEU:HD12	1:F:368:GLN:HE21	1.72	0.54
4:J:496:GLU:HG2	4:J:499:GLN:HE21	1.72	0.54
1:F:248:VAL:HA	1:F:252:LEU:HB2	1.89	0.54
1:F:378:LEU:CD2	1:F:421:PHE:O	2.56	0.54
1:O:273:MET:HB2	1:O:303:PHE:HZ	1.72	0.54
1:C:76:GLY:O	1:C:77:LEU:C	2.51	0.53
1:O:614:GLU:OE1	1:O:617:GLN:NE2	2.41	0.53
3:P:414:PRO:O	3:P:449:TRP:NE1	2.41	0.53
1:C:437:ALA:HA	1:C:513:TRP:CZ3	2.43	0.53
1:C:717:MET:HB3	1:C:722:LEU:HG	1.89	0.53
1:F:717:MET:HB3	1:F:722:LEU:HG	1.89	0.53
1:M:614:GLU:OE1	1:M:617:GLN:NE2	2.41	0.53
2:Q:39:VAL:O	2:Q:40:ASP:CB	2.42	0.53
1:F:68:LYS:HZ3	3:B:142:LEU:HA	1.70	0.53
1:F:614:GLU:OE1	1:F:617:GLN:NE2	2.42	0.53
1:M:85:LEU:O	1:M:86:ILE:C	2.51	0.53
1:C:488:ARG:NH2	1:C:502:ASP:HA	2.23	0.53
3:A:462:ALA:HB1	3:A:473:TYR:HB3	1.89	0.53
4:J:484:ILE:HD11	4:J:542:ARG:HG3	1.89	0.53
3:A:17:LEU:CD1	3:B:51:THR:CB	2.87	0.53
3:A:555:ASP:HB2	3:A:560:ARG:H	1.73	0.53
3:B:253:MET:HE2	4:H:534:ARG:HH22	1.73	0.53
4:H:484:ILE:HD11	4:H:542:ARG:HG3	1.90	0.53
1:C:58:TYR:OH	1:C:125:TYR:HB2	2.08	0.53
1:C:79:GLU:O	1:C:80:VAL:C	2.52	0.53
1:C:217:PHE:HB3	1:C:268:LEU:HD23	1.91	0.53
2:R:39:VAL:O	2:R:39:VAL:CG1	2.53	0.53
1:C:59:ARG:CZ	3:A:75:ARG:HD2	2.39	0.53
1:C:425:LYS:HD2	1:C:462:CYS:HB2	1.91	0.53
3:P:370:ARG:NH1	3:P:386:GLY:O	2.39	0.53
1:C:94:LEU:C	1:C:96:SER:N	2.66	0.53
1:F:66:LEU:C	1:F:68:LYS:N	2.67	0.53
1:F:390:LEU:HG	1:F:681:GLN:HG2	1.91	0.53
3:A:270:ILE:HD13	3:A:318:ILE:HG12	1.90	0.53
3:A:375:LEU:HD23	3:A:384:ALA:HA	1.90	0.53
4:G:469:GLU:HA	4:G:472:ARG:HG2	1.91	0.53
4:G:487:PHE:HE2	4:G:545:LEU:HG	1.74	0.53
3:B:524:CYS:SG	3:B:526:ARG:NH1	2.80	0.53
3:N:350:PHE:HD1	3:N:363:LYS:HB2	1.74	0.53
1:C:365:LEU:HD12	1:C:368:GLN:HE21	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:GLU:OE1	1:C:617:GLN:NE2	2.41	0.53
4:H:469:GLU:HA	4:H:472:ARG:HG2	1.91	0.53
1:C:166:LEU:HD22	1:C:212:MET:HG2	1.91	0.52
1:F:166:LEU:HD22	1:F:212:MET:HG2	1.92	0.52
1:M:76:GLY:O	1:M:77:LEU:C	2.51	0.52
3:A:350:PHE:HD1	3:A:352:TRP:CH2	2.27	0.52
3:P:435:THR:OG1	3:P:436:LEU:N	2.41	0.52
1:C:82:THR:O	1:C:83:GLU:C	2.51	0.52
1:O:102:LEU:HD13	1:O:182:ALA:HB1	1.91	0.52
1:O:404:THR:OG1	1:O:407:GLU:OE2	2.20	0.52
4:H:487:PHE:HE2	4:H:545:LEU:HG	1.74	0.52
3:P:297:LYS:HB2	3:P:594:SER:OG	2.09	0.52
1:C:85:LEU:O	1:C:86:ILE:C	2.52	0.52
1:C:467:THR:HA	1:C:470:LEU:HB2	1.90	0.52
1:O:508:LEU:HD13	1:O:513:TRP:CE2	2.45	0.52
4:I:484:ILE:HD11	4:I:542:ARG:HG3	1.89	0.52
1:C:246:GLU:HA	1:C:249:MET:HE2	1.92	0.52
1:F:526:PRO:HD2	1:F:603:MET:HE2	1.91	0.52
1:O:459:LYS:HZ2	1:O:467:THR:HB	1.73	0.52
2:R:63:ALA:HB1	2:R:66:GLU:HA	1.92	0.52
3:B:346:THR:HG22	3:B:369:VAL:HB	1.92	0.52
1:C:274:LYS:O	1:C:277:VAL:HG22	2.09	0.52
1:M:118:MET:HE1	3:P:62:SER:O	2.09	0.52
3:B:274:ALA:HB1	3:B:575:LEU:HD22	1.92	0.52
3:B:296:TYR:HB3	3:B:591:LEU:HD22	1.92	0.52
3:N:94:LEU:HD11	3:N:104:LEU:HD21	1.91	0.52
1:O:426:ASP:OD2	1:O:699:ARG:NH2	2.42	0.52
2:R:44:ILE:HD11	2:R:84:ILE:HG22	1.89	0.52
3:A:393:GLU:HA	3:A:397:ARG:HD2	1.92	0.52
3:B:350:PHE:HD1	3:B:363:LYS:HB2	1.74	0.52
1:C:77:LEU:O	1:C:81:VAL:HG22	2.09	0.52
1:F:102:LEU:HD13	1:F:182:ALA:HB1	1.91	0.52
1:F:149:ASP:HA	1:F:153:ARG:HB2	1.92	0.52
1:M:548:LEU:HD21	2:R:31:ALA:HB1	1.92	0.52
3:A:108:ALA:O	3:A:112:GLN:N	2.43	0.52
4:G:502:GLU:O	4:G:505:SER:OG	2.24	0.52
3:B:53:SER:OG	3:B:111:LEU:O	2.28	0.52
1:O:240:ARG:NH1	1:O:243:GLU:OE2	2.43	0.52
3:N:346:THR:HG22	3:N:369:VAL:HB	1.92	0.52
3:N:467:PHE:HB3	3:N:472:PHE:HE2	1.75	0.52
1:C:248:VAL:HA	1:C:252:LEU:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASN:HD21	2:E:22:PHE:HD2	1.57	0.52
1:M:149:ASP:HA	1:M:153:ARG:HB2	1.92	0.52
1:M:166:LEU:HD22	1:M:212:MET:HG2	1.92	0.52
1:O:166:LEU:HD22	1:O:212:MET:HG2	1.91	0.52
3:A:61:MET:HE3	3:B:30:PHE:CE1	2.45	0.52
3:A:285:SER:HB2	3:A:298:LEU:HB3	1.92	0.52
1:M:246:GLU:HA	1:M:249:MET:HE2	1.92	0.51
3:B:22:LYS:HE2	3:B:90:TYR:HB3	1.91	0.51
3:B:186:LEU:HB2	3:B:260:ARG:HD3	1.92	0.51
3:N:47:MET:HE3	3:P:21:LEU:HD13	1.91	0.51
3:N:53:SER:OG	3:N:111:LEU:O	2.28	0.51
3:P:108:ALA:O	3:P:112:GLN:N	2.43	0.51
1:M:240:ARG:NH1	1:M:243:GLU:OE2	2.43	0.51
1:O:149:ASP:HA	1:O:153:ARG:HB2	1.92	0.51
1:O:472:GLY:HA3	1:O:512:TYR:CZ	2.45	0.51
3:B:155:MET:HE1	3:B:352:TRP:CZ3	2.45	0.51
3:B:549:TYR:OH	3:B:575:LEU:N	2.40	0.51
3:N:186:LEU:HB2	3:N:260:ARG:HD3	1.92	0.51
4:J:469:GLU:HA	4:J:472:ARG:HG2	1.91	0.51
3:P:154:ARG:CD	3:P:357:GLN:HE22	2.21	0.51
1:F:240:ARG:NH1	1:F:243:GLU:OE2	2.43	0.51
3:N:155:MET:HE1	3:N:352:TRP:CZ3	2.45	0.51
4:J:487:PHE:HE2	4:J:545:LEU:HG	1.74	0.51
1:C:64:MET:O	1:C:69:HIS:HB2	2.11	0.51
1:C:125:TYR:HD1	3:A:112:GLN:NE2	2.06	0.51
4:I:469:GLU:HA	4:I:472:ARG:HG2	1.91	0.51
3:N:459:ARG:NH2	3:N:473:TYR:O	2.44	0.51
1:C:59:ARG:HD2	3:A:76:ASN:OD1	2.10	0.51
1:O:441:LEU:HD21	1:O:508:LEU:HD11	1.91	0.51
3:P:305:LEU:HB3	3:P:325:VAL:HG12	1.93	0.51
1:O:55:GLU:OE2	3:N:72:VAL:CG1	2.56	0.51
3:B:371:ILE:HB	3:B:388:ASP:HB2	1.92	0.51
3:B:573:TRP:HB3	3:B:597:LYS:HD3	1.92	0.51
1:C:102:LEU:HD13	1:C:182:ALA:HB1	1.91	0.51
1:C:240:ARG:NH1	1:C:243:GLU:OE2	2.43	0.51
1:F:472:GLY:HA3	1:F:512:TYR:CZ	2.46	0.51
1:F:531:ALA:CB	2:D:27:TRP:HZ3	2.17	0.51
3:B:226:SER:HB3	3:B:259:PRO:HB3	1.93	0.51
4:H:543:ARG:HH21	4:H:546:GLU:HG3	1.76	0.51
1:C:149:ASP:HA	1:C:153:ARG:HB2	1.92	0.51
1:O:440:LEU:HB3	1:O:477:MET:SD	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:274:ALA:N	3:B:284:SER:O	2.38	0.51
1:F:58:TYR:O	1:F:59:ARG:C	2.54	0.50
1:O:606:ASN:HD21	2:Q:22:PHE:HD2	1.57	0.50
3:A:10:ASN:HD21	3:B:119:ARG:HH22	1.59	0.50
3:A:44:CYS:SG	3:A:45:HIS:N	2.84	0.50
3:B:467:PHE:HB3	3:B:472:PHE:HE2	1.75	0.50
4:I:487:PHE:HE2	4:I:545:LEU:HG	1.74	0.50
3:N:188:VAL:H	3:N:262:GLY:HA3	1.76	0.50
1:F:348:LEU:HA	1:F:351:ARG:HG2	1.93	0.50
1:F:404:THR:OG1	1:F:407:GLU:OE2	2.20	0.50
2:R:71:ALA:HB1	2:R:84:ILE:HD11	1.93	0.50
1:C:45:GLN:HB3	1:C:84:HIS:CD2	2.47	0.50
1:F:528:PRO:HA	1:F:531:ALA:HB3	1.94	0.50
2:R:61:ALA:O	2:R:62:SER:C	2.53	0.50
2:Q:20:LYS:HE3	2:Q:23:GLU:HG2	1.93	0.50
3:A:119:ARG:HH22	3:B:10:ASN:HD22	1.59	0.50
3:N:348:ASN:ND2	3:N:366:MET:O	2.32	0.50
3:P:44:CYS:SG	3:P:45:HIS:N	2.84	0.50
3:P:385:ILE:HG21	3:P:433:VAL:HG21	1.93	0.50
1:C:86:ILE:HG12	1:C:150:GLN:NE2	2.25	0.50
1:C:349:LYS:HE2	1:C:418:LEU:HB2	1.92	0.50
1:M:404:THR:OG1	1:M:407:GLU:OE2	2.20	0.50
2:R:44:ILE:HD12	2:R:84:ILE:HG23	1.93	0.50
4:I:459:LYS:HA	4:I:462:GLU:HG3	1.93	0.50
3:N:435:THR:OG1	3:N:436:LEU:N	2.42	0.50
1:C:269:ILE:O	1:C:270:SER:C	2.54	0.50
1:C:451:GLU:HB3	1:C:474:PHE:CE1	2.47	0.50
1:M:606:ASN:HD21	2:R:22:PHE:HD2	1.57	0.50
4:I:543:ARG:HH21	4:I:546:GLU:HG3	1.76	0.50
1:M:632:GLN:HG3	1:M:633:SER:N	2.27	0.50
2:E:45:CYS:HB2	2:E:54:ILE:HG12	1.93	0.50
3:P:459:ARG:NH1	3:P:475:GLY:O	2.45	0.50
1:F:440:LEU:HB3	1:F:477:MET:SD	2.51	0.50
2:E:44:ILE:HD12	2:E:84:ILE:HG23	1.93	0.50
4:G:543:ARG:HH21	4:G:546:GLU:HG3	1.76	0.50
3:N:235:GLN:HG3	3:N:242:LYS:HZ3	1.76	0.50
3:P:22:LYS:HE2	3:P:90:TYR:HB3	1.93	0.50
1:C:41:ILE:HD12	1:C:80:VAL:HG11	1.94	0.50
1:C:632:GLN:HG3	1:C:633:SER:N	2.27	0.50
3:B:235:GLN:HG3	3:B:242:LYS:HZ3	1.77	0.50
3:B:459:ARG:NH2	3:B:473:TYR:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:301:PRO:N	3:N:302:PRO:HD2	2.27	0.50
1:F:526:PRO:HD2	1:F:603:MET:SD	2.52	0.50
1:F:606:ASN:HD21	2:D:22:PHE:HD2	1.57	0.50
1:M:270:SER:HA	1:M:273:MET:HB3	1.93	0.50
4:H:459:LYS:HA	4:H:462:GLU:HG3	1.93	0.50
1:C:476:ASP:HB3	1:C:508:LEU:HB3	1.94	0.49
1:C:524:ILE:CG2	1:C:529:ARG:HG3	2.41	0.49
3:N:301:PRO:HB2	3:N:360:TRP:HB2	1.94	0.49
1:C:524:ILE:HB	1:C:529:ARG:CG	2.42	0.49
1:M:66:LEU:HD21	3:P:143:PHE:CD1	2.46	0.49
1:M:527:ALA:HB3	1:M:528:PRO:HD3	1.94	0.49
1:M:559:LEU:O	1:M:592:LEU:N	2.39	0.49
1:O:473:MET:HG3	1:O:513:TRP:CZ2	2.46	0.49
4:H:502:GLU:O	4:H:505:SER:OG	2.25	0.49
1:C:274:LYS:O	1:C:278:GLU:HG2	2.12	0.49
1:C:451:GLU:HB3	1:C:474:PHE:CZ	2.47	0.49
1:M:440:LEU:HD13	1:M:477:MET:HG3	1.93	0.49
1:M:723:VAL:HG11	1:M:742:LYS:HZ3	1.77	0.49
3:A:47:MET:CE	3:B:47:MET:HE1	2.42	0.49
3:A:542:HIS:H	3:A:548:LYS:HG2	1.77	0.49
3:B:353:PHE:HB2	3:B:360:TRP:CH2	2.47	0.49
3:N:353:PHE:HB2	3:N:360:TRP:CH2	2.47	0.49
4:J:459:LYS:HD2	4:J:570:LEU:HD13	1.95	0.49
3:B:301:PRO:N	3:B:302:PRO:HD2	2.27	0.49
4:I:453:ASN:HD21	4:I:598:LEU:HG	1.77	0.49
3:P:186:LEU:HB2	3:P:260:ARG:HD3	1.94	0.49
1:M:264:VAL:O	1:M:268:LEU:HB3	2.13	0.49
3:B:435:THR:OG1	3:B:436:LEU:N	2.42	0.49
1:O:598:GLN:HG2	1:O:634:LEU:HG	1.94	0.49
2:D:20:LYS:HE3	2:D:23:GLU:HG2	1.93	0.49
3:A:170:MET:O	3:A:209:ARG:NH2	2.37	0.49
3:N:371:ILE:HB	3:N:388:ASP:HB2	1.93	0.49
4:J:543:ARG:HH21	4:J:546:GLU:HG3	1.76	0.49
3:P:24:PHE:CD1	3:P:29:LEU:HD12	2.48	0.49
1:M:523:ASN:HD22	1:M:529:ARG:NH1	2.10	0.49
1:O:265:GLU:O	1:O:269:ILE:HG13	2.12	0.49
2:E:20:LYS:HE3	2:E:23:GLU:HG2	1.93	0.49
2:E:84:ILE:HD12	2:E:101:TRP:HZ2	1.77	0.49
3:A:24:PHE:CD1	3:A:29:LEU:HD12	2.48	0.49
3:N:226:SER:HB3	3:N:259:PRO:HB3	1.93	0.49
1:C:440:LEU:HD13	1:C:477:MET:CG	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:186:LEU:HB2	3:A:260:ARG:HD3	1.94	0.49
3:A:226:SER:HB3	3:A:259:PRO:HB3	1.95	0.49
3:B:188:VAL:H	3:B:262:GLY:HA3	1.77	0.49
3:P:370:ARG:NH2	3:P:398:THR:O	2.38	0.49
1:C:107:GLN:HA	1:C:110:ASN:HD21	1.78	0.48
1:C:217:PHE:HA	1:C:220:GLU:HG2	1.95	0.48
1:O:508:LEU:HD13	1:O:513:TRP:CD2	2.48	0.48
2:E:71:ALA:HB1	2:E:84:ILE:HD11	1.93	0.48
3:N:274:ALA:O	3:N:284:SER:N	2.38	0.48
3:P:366:MET:HG2	3:P:409:TRP:CZ2	2.48	0.48
1:F:68:LYS:HE3	3:B:142:LEU:CD1	2.28	0.48
1:F:198:ARG:HE	1:F:198:ARG:HB2	1.44	0.48
1:O:217:PHE:HA	1:O:220:GLU:HG2	1.95	0.48
4:G:459:LYS:HD2	4:G:570:LEU:HD13	1.95	0.48
4:I:566:ILE:HD12	4:I:566:ILE:HA	1.74	0.48
4:J:454:THR:O	4:J:458:GLU:HG2	2.13	0.48
1:M:107:GLN:HA	1:M:110:ASN:HD21	1.79	0.48
1:O:107:GLN:HA	1:O:110:ASN:HD21	1.78	0.48
3:B:261:LEU:HG	3:B:587:TYR:CZ	2.48	0.48
3:N:399:VAL:HG12	3:N:414:PRO:HA	1.96	0.48
1:C:503:LEU:O	1:C:504:THR:HG23	2.14	0.48
1:C:644:LEU:HD11	1:C:659:PHE:HB3	1.96	0.48
1:F:598:GLN:HG2	1:F:634:LEU:HG	1.94	0.48
1:O:644:LEU:HD11	1:O:659:PHE:HB3	1.96	0.48
2:R:20:LYS:HE3	2:R:23:GLU:HG2	1.93	0.48
3:B:301:PRO:HB2	3:B:360:TRP:HB2	1.94	0.48
1:F:107:GLN:HA	1:F:110:ASN:HD21	1.78	0.48
1:M:559:LEU:HD11	2:R:22:PHE:HB3	1.95	0.48
1:O:497:SER:C	1:O:499:GLY:H	2.21	0.48
2:E:44:ILE:HD12	2:E:84:ILE:HG22	1.96	0.48
3:A:265:LYS:HG2	3:A:585:LYS:HB3	1.96	0.48
1:C:54:PHE:HB3	3:A:59:MET:SD	2.54	0.48
1:C:491:LEU:HD11	1:C:500:GLY:HA3	1.95	0.48
1:F:644:LEU:HD11	1:F:659:PHE:HB3	1.96	0.48
2:D:45:CYS:HB2	2:D:54:ILE:HG12	1.96	0.48
2:Q:27:TRP:CE2	2:Q:29:ALA:HB2	2.49	0.48
4:I:527:ASN:HA	4:I:530:LYS:HE3	1.94	0.48
1:C:459:LYS:HG3	1:C:467:THR:HG21	1.95	0.48
1:F:524:ILE:H	1:F:524:ILE:HG12	1.50	0.48
1:M:83:GLU:O	1:M:86:ILE:HG22	2.13	0.48
1:M:390:LEU:HG	1:M:681:GLN:HG2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:504:THR:OG1	2:R:27:TRP:O	2.31	0.48
1:O:559:LEU:HD11	2:Q:22:PHE:HB3	1.95	0.48
3:B:399:VAL:HG12	3:B:414:PRO:HA	1.96	0.48
3:P:371:ILE:N	3:P:387:GLY:O	2.40	0.48
1:C:263:VAL:O	1:C:267:GLU:HG3	2.14	0.48
1:C:614:GLU:HA	1:C:617:GLN:HG2	1.96	0.48
1:F:328:LEU:HD22	1:F:348:LEU:HD21	1.95	0.48
2:E:27:TRP:CE2	2:E:29:ALA:HB2	2.49	0.48
3:P:572:LEU:HD22	3:P:572:LEU:HA	1.75	0.48
1:C:264:VAL:O	1:C:265:GLU:C	2.56	0.48
1:C:267:GLU:HG3	1:C:267:GLU:H	1.49	0.48
1:C:504:THR:OG1	2:E:27:TRP:O	2.31	0.48
1:C:723:VAL:HG11	1:C:742:LYS:HZ3	1.79	0.48
1:O:614:GLU:HA	1:O:617:GLN:HG2	1.96	0.48
3:N:301:PRO:CG	3:N:360:TRP:HB2	2.44	0.48
3:N:549:TYR:OH	3:N:575:LEU:N	2.40	0.48
1:C:41:ILE:CD1	1:C:80:VAL:HG11	2.44	0.47
1:C:91:GLU:H	1:C:91:GLU:HG3	1.46	0.47
1:M:605:PHE:HE2	1:M:611:TYR:HB2	1.79	0.47
1:C:559:LEU:HD11	2:E:22:PHE:HB3	1.95	0.47
1:M:72:LYS:H	1:M:72:LYS:HG2	1.28	0.47
3:B:301:PRO:CG	3:B:360:TRP:HB2	2.44	0.47
1:M:265:GLU:HB2	1:M:306:VAL:HB	1.96	0.47
3:A:346:THR:HB	3:A:369:VAL:HG11	1.96	0.47
3:A:474:ILE:HG12	3:A:499:VAL:HG13	1.96	0.47
3:B:102:GLU:OE1	3:B:102:GLU:N	2.41	0.47
4:H:459:LYS:HD2	4:H:570:LEU:HD13	1.96	0.47
1:C:81:VAL:HG23	1:C:82:THR:H	1.79	0.47
1:C:386:GLU:OE1	1:C:386:GLU:N	2.44	0.47
1:C:696:ASP:HA	1:C:699:ARG:HD2	1.95	0.47
1:F:559:LEU:HD11	2:D:22:PHE:HB3	1.95	0.47
1:M:536:ARG:HA	1:M:548:LEU:HG	1.96	0.47
3:B:286:VAL:HG11	3:B:573:TRP:HH2	1.80	0.47
4:I:544:ARG:O	4:I:547:GLU:HG3	2.15	0.47
1:M:478:SER:HA	1:M:481:ASN:ND2	2.29	0.47
1:O:66:LEU:C	1:O:68:LYS:N	2.67	0.47
2:D:27:TRP:CE2	2:D:29:ALA:HB2	2.49	0.47
4:H:539:ILE:HD12	4:H:542:ARG:HH21	1.80	0.47
1:M:614:GLU:HA	1:M:617:GLN:HG2	1.96	0.47
1:O:605:PHE:HE2	1:O:611:TYR:HB2	1.80	0.47
1:O:646:LYS:HE3	1:O:659:PHE:HE1	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:27:TRP:CE2	2:R:29:ALA:HB2	2.49	0.47
3:A:394:LEU:H	3:A:394:LEU:HG	1.44	0.47
4:I:539:ILE:HD12	4:I:542:ARG:HH21	1.80	0.47
3:N:261:LEU:HG	3:N:587:TYR:CZ	2.49	0.47
3:N:442:TYR:HB2	3:N:449:TRP:CZ3	2.50	0.47
3:P:226:SER:HB3	3:P:259:PRO:HB3	1.95	0.47
3:P:431:ILE:HB	3:P:442:TYR:HB3	1.96	0.47
1:C:248:VAL:HG11	1:C:257:GLU:HG3	1.95	0.47
1:F:614:GLU:HA	1:F:617:GLN:HG2	1.96	0.47
3:A:253:MET:HG2	3:A:258:LYS:HA	1.97	0.47
3:B:155:MET:HE1	3:B:352:TRP:CH2	2.50	0.47
3:B:442:TYR:HB2	3:B:449:TRP:CZ3	2.50	0.47
4:I:459:LYS:HD2	4:I:570:LEU:HD13	1.96	0.47
3:P:297:LYS:O	3:P:592:GLU:CB	2.63	0.47
1:C:609:GLU:HG3	1:C:610:LYS:H	1.80	0.47
1:M:82:THR:O	1:M:83:GLU:C	2.55	0.47
1:M:121:ASP:O	3:P:58:ALA:HB1	2.15	0.47
1:M:217:PHE:HA	1:M:220:GLU:HG2	1.96	0.47
1:O:531:ALA:HB3	2:Q:27:TRP:CE3	2.49	0.47
3:A:61:MET:SD	3:B:29:LEU:HG	2.55	0.47
3:N:308:VAL:HG12	3:N:323:GLY:HA3	1.97	0.47
1:F:326:LYS:HA	1:F:329:VAL:HG22	1.97	0.47
1:O:59:ARG:CD	3:N:75:ARG:HB2	2.42	0.47
2:R:45:CYS:HB2	2:R:54:ILE:HG12	1.96	0.47
4:G:539:ILE:HD12	4:G:542:ARG:HH21	1.80	0.47
4:I:592:LYS:HD2	4:I:592:LYS:HA	1.43	0.47
3:N:24:PHE:CZ	3:P:57:ARG:NE	2.73	0.47
3:N:155:MET:HE1	3:N:352:TRP:CH2	2.50	0.47
3:N:301:PRO:HG2	3:N:360:TRP:HB2	1.97	0.47
1:C:348:LEU:HA	1:C:351:ARG:HG2	1.97	0.47
1:F:269:ILE:HG22	1:F:273:MET:HB2	1.97	0.47
1:F:559:LEU:O	1:F:592:LEU:N	2.39	0.47
1:F:687:GLU:O	1:F:690:GLU:HG3	2.15	0.47
1:O:93:VAL:CG1	1:O:156:CYS:SG	3.02	0.47
1:O:269:ILE:HG22	1:O:303:PHE:CE2	2.50	0.47
3:A:525:VAL:HG12	3:A:536:VAL:HG21	1.97	0.47
4:G:544:ARG:O	4:G:547:GLU:HG3	2.15	0.47
3:B:251:LYS:HA	3:B:251:LYS:HD3	1.53	0.47
3:P:427:VAL:HG11	3:P:504:VAL:HG21	1.95	0.47
1:C:125:TYR:CE1	3:A:109:CYS:O	2.68	0.46
1:C:532:PHE:CB	2:E:27:TRP:CH2	2.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:PHE:HA	1:F:220:GLU:HG2	1.96	0.46
1:M:89:VAL:O	1:M:90:ARG:C	2.55	0.46
1:C:532:PHE:CB	2:E:27:TRP:HH2	2.28	0.46
1:M:225:LEU:HD13	1:M:272:HIS:CG	2.49	0.46
1:M:609:GLU:HG3	1:M:610:LYS:H	1.80	0.46
1:M:644:LEU:HD11	1:M:659:PHE:HB3	1.96	0.46
2:D:94:CYS:HB2	2:D:101:TRP:HB2	1.96	0.46
3:B:586:LEU:HD13	3:B:591:LEU:HD11	1.97	0.46
3:N:274:ALA:HB1	3:N:575:LEU:HD22	1.96	0.46
3:N:296:TYR:HB3	3:N:591:LEU:HD22	1.97	0.46
3:P:300:SER:HA	3:P:360:TRP:NE1	2.30	0.46
1:C:478:SER:HA	1:C:481:ASN:ND2	2.29	0.46
1:F:273:MET:HG3	1:F:303:PHE:HE2	1.81	0.46
1:O:525:PRO:HB3	1:O:603:MET:HG3	1.97	0.46
4:G:482:THR:O	4:G:485:GLU:HG3	2.15	0.46
1:C:96:SER:O	1:C:97:LEU:C	2.56	0.46
1:C:605:PHE:HE2	1:C:611:TYR:HB2	1.80	0.46
1:C:646:LYS:HE3	1:C:659:PHE:HE1	1.80	0.46
1:F:88:LYS:HA	1:F:88:LYS:HD3	1.61	0.46
1:F:93:VAL:CG1	1:F:156:CYS:SG	3.02	0.46
1:M:68:LYS:HA	1:M:68:LYS:HD3	1.76	0.46
1:M:77:LEU:O	1:M:78:ARG:C	2.53	0.46
1:M:646:LYS:HE3	1:M:659:PHE:HE1	1.80	0.46
1:M:687:GLU:O	1:M:690:GLU:HG3	2.15	0.46
1:O:82:THR:O	1:O:86:ILE:HG23	2.16	0.46
1:C:80:VAL:O	1:C:83:GLU:HB3	2.15	0.46
1:C:254:LYS:H	1:C:254:LYS:HG3	1.47	0.46
1:M:83:GLU:HG2	1:M:87:ASN:HD21	1.80	0.46
1:M:476:ASP:HB3	1:M:508:LEU:HB3	1.96	0.46
2:R:98:ASN:HD22	2:R:98:ASN:HA	1.50	0.46
3:A:282:LEU:HD22	3:A:282:LEU:HA	1.75	0.46
3:B:280:CYS:HB3	3:B:281:SER:H	1.54	0.46
1:F:68:LYS:CE	3:B:142:LEU:HA	2.44	0.46
1:M:91:GLU:H	1:M:91:GLU:HG3	1.36	0.46
1:O:609:GLU:HG3	1:O:610:LYS:H	1.80	0.46
3:B:459:ARG:HB3	3:B:476:GLY:HA3	1.98	0.46
3:N:416:PRO:HG2	3:N:440:TYR:CD1	2.50	0.46
3:P:154:ARG:CZ	3:P:357:GLN:NE2	2.79	0.46
1:C:513:TRP:H	1:C:513:TRP:CD1	2.33	0.46
1:F:254:LYS:H	1:F:254:LYS:HG3	1.50	0.46
4:H:544:ARG:O	4:H:547:GLU:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:H	1:C:85:LEU:HG	1.45	0.46
1:C:269:ILE:O	1:C:273:MET:N	2.48	0.46
1:C:486:GLU:HG3	1:C:490:HIS:CE1	2.51	0.46
1:F:605:PHE:HE2	1:F:611:TYR:HB2	1.79	0.46
1:O:260:ILE:O	1:O:264:VAL:HG12	2.16	0.46
1:O:753:TYR:HA	1:O:767:VAL:HG23	1.96	0.46
4:G:453:ASN:HA	4:G:577:ARG:NH1	2.29	0.46
3:N:352:TRP:HB3	3:N:363:LYS:CE	2.46	0.46
4:J:544:ARG:O	4:J:547:GLU:HG3	2.15	0.46
3:P:253:MET:HG2	3:P:258:LYS:HA	1.97	0.46
1:C:259:PRO:O	1:C:262:LYS:HB2	2.16	0.46
1:M:703:ILE:HD11	1:M:744:ARG:HD3	1.98	0.46
1:O:550:LEU:H	1:O:550:LEU:HG	1.51	0.46
3:A:499:VAL:HB	3:A:512:ALA:HB3	1.98	0.46
3:P:526:ARG:NH2	3:P:577:ARG:O	2.39	0.46
1:C:54:PHE:CB	3:A:59:MET:CE	2.75	0.46
1:F:646:LYS:HE3	1:F:659:PHE:HE1	1.80	0.46
1:O:55:GLU:OE1	3:N:66:GLU:HG3	2.16	0.46
2:Q:96:LEU:HD13	2:Q:96:LEU:HA	1.76	0.46
3:B:308:VAL:HG12	3:B:323:GLY:HA3	1.97	0.46
3:N:286:VAL:HG11	3:N:573:TRP:HH2	1.80	0.46
1:F:82:THR:O	1:F:86:ILE:HG23	2.16	0.45
1:M:269:ILE:O	1:M:270:SER:C	2.58	0.45
1:M:560:ASN:HD22	2:R:25:LYS:HD2	1.81	0.45
1:M:723:VAL:HA	1:M:726:VAL:HG12	1.98	0.45
1:O:531:ALA:HB3	2:Q:27:TRP:CZ3	2.51	0.45
3:B:416:PRO:HG2	3:B:440:TYR:CD1	2.50	0.45
3:N:188:VAL:N	3:N:262:GLY:HA3	2.31	0.45
1:F:473:MET:HG3	1:F:513:TRP:CZ2	2.51	0.45
1:F:526:PRO:HD2	1:F:603:MET:CE	2.45	0.45
1:F:609:GLU:HG3	1:F:610:LYS:H	1.80	0.45
2:R:41:ASN:HD21	2:R:46:ARG:HG2	1.81	0.45
3:A:272:ILE:HB	3:A:580:ARG:HB2	1.97	0.45
3:B:188:VAL:N	3:B:262:GLY:HA3	2.31	0.45
3:B:261:LEU:HD12	3:B:264:THR:OG1	2.17	0.45
3:B:363:LYS:O	3:B:364:THR:C	2.59	0.45
3:P:297:LYS:CB	3:P:592:GLU:OE1	2.55	0.45
1:M:97:LEU:HD22	1:M:160:HIS:CD2	2.51	0.45
1:M:467:THR:HA	1:M:470:LEU:HB2	1.98	0.45
1:O:632:GLN:HG3	1:O:633:SER:N	2.30	0.45
1:O:687:GLU:O	1:O:690:GLU:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:311:VAL:HG11	3:A:382:ILE:HG23	1.98	0.45
3:B:291:GLN:H	3:B:291:GLN:HG3	1.55	0.45
4:H:454:THR:O	4:H:458:GLU:HG2	2.16	0.45
3:N:57:ARG:NH2	3:P:24:PHE:CZ	2.79	0.45
4:J:481:ARG:HA	4:J:484:ILE:HG22	1.99	0.45
3:P:237:LEU:HB3	3:P:241:ASP:HB2	1.99	0.45
1:C:68:LYS:HE2	1:C:68:LYS:HB2	1.44	0.45
1:M:365:LEU:O	1:M:368:GLN:HG3	2.17	0.45
1:O:390:LEU:HD13	1:O:390:LEU:HA	1.72	0.45
1:O:419:PHE:HZ	1:O:425:LYS:HG3	1.82	0.45
1:O:88:LYS:HD3	1:O:88:LYS:HA	1.61	0.45
3:A:283:TYR:HD1	3:A:283:TYR:HA	1.71	0.45
3:B:301:PRO:HG2	3:B:360:TRP:HB2	1.97	0.45
3:B:571:VAL:HA	3:B:597:LYS:HG3	1.99	0.45
4:J:539:ILE:HD12	4:J:542:ARG:HH21	1.80	0.45
1:F:632:GLN:HG3	1:F:633:SER:N	2.30	0.45
3:A:352:TRP:HH2	3:A:409:TRP:HH2	1.65	0.45
3:N:251:LYS:HD3	3:N:251:LYS:HA	1.53	0.45
3:N:459:ARG:HB3	3:N:476:GLY:HA3	1.98	0.45
3:P:274:ALA:HB1	3:P:575:LEU:HD22	1.97	0.45
1:C:488:ARG:NH2	1:C:503:LEU:H	2.14	0.45
1:F:723:VAL:HA	1:F:726:VAL:HG12	1.99	0.45
4:G:454:THR:O	4:G:458:GLU:HG2	2.17	0.45
4:G:581:LEU:HD12	4:G:581:LEU:HA	1.74	0.45
3:B:455:ARG:HH22	3:B:459:ARG:H	1.65	0.45
4:I:529:ASP:OD1	4:I:529:ASP:N	2.50	0.45
3:N:261:LEU:HD12	3:N:264:THR:OG1	2.17	0.45
1:C:265:GLU:O	1:C:270:SER:N	2.47	0.45
1:O:54:PHE:CE2	3:N:64:LEU:HD12	2.52	0.45
1:O:273:MET:HE3	1:O:273:MET:HB3	1.61	0.45
3:B:237:LEU:HB3	3:B:241:ASP:HB2	1.99	0.45
3:N:127:LYS:HA	3:N:127:LYS:HD3	1.42	0.45
1:C:560:ASN:HD22	2:E:25:LYS:HD2	1.81	0.45
1:C:714:ARG:NH1	1:C:725:GLU:OE2	2.50	0.45
1:F:365:LEU:O	1:F:368:GLN:HG3	2.17	0.45
1:M:71:GLU:H	1:M:71:GLU:HG2	1.51	0.45
1:O:365:LEU:O	1:O:368:GLN:HG3	2.16	0.45
1:O:436:LEU:HD23	1:O:439:ARG:HH11	1.82	0.45
3:A:497:VAL:HG23	3:A:514:ASN:HD21	1.78	0.45
3:B:366:MET:HE1	3:B:370:ARG:HB2	1.99	0.45
4:H:480:LYS:HD3	4:H:480:LYS:HA	1.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:LEU:HD23	1:F:439:ARG:HH11	1.82	0.45
1:F:559:LEU:HD22	1:F:602:LEU:HD23	1.99	0.45
1:M:54:PHE:O	1:M:55:GLU:C	2.57	0.45
1:M:714:ARG:NH1	1:M:725:GLU:OE2	2.50	0.45
1:O:714:ARG:NH1	1:O:725:GLU:OE2	2.50	0.45
2:E:98:ASN:HD22	2:E:98:ASN:HA	1.50	0.45
3:A:573:TRP:CD1	3:A:597:LYS:HG2	2.50	0.45
4:G:529:ASP:OD1	4:G:529:ASP:N	2.50	0.45
3:P:307:LYS:HD3	3:P:372:LYS:HE3	1.99	0.45
1:C:559:LEU:HD22	1:C:602:LEU:HD23	1.99	0.44
1:F:723:VAL:HG11	1:F:742:LYS:HZ3	1.81	0.44
1:M:73:LEU:O	1:M:74:TYR:C	2.54	0.44
1:M:76:GLY:O	1:M:80:VAL:HG23	2.17	0.44
1:M:258:GLU:HA	1:M:261:VAL:HG22	1.99	0.44
1:O:723:VAL:HA	1:O:726:VAL:HG12	1.99	0.44
4:H:529:ASP:OD1	4:H:529:ASP:N	2.50	0.44
3:N:237:LEU:HB3	3:N:241:ASP:HB2	1.99	0.44
3:N:455:ARG:HH22	3:N:459:ARG:H	1.65	0.44
3:N:586:LEU:HD13	3:N:591:LEU:HD11	1.97	0.44
3:P:316:ASN:ND2	3:P:585:LYS:O	2.39	0.44
1:C:502:ASP:O	2:E:26:LYS:HA	2.17	0.44
1:O:338:PRO:HA	1:O:341:TYR:HB3	1.99	0.44
3:N:102:GLU:OE1	3:N:102:GLU:N	2.41	0.44
4:J:529:ASP:OD1	4:J:529:ASP:N	2.50	0.44
1:C:87:ASN:O	1:C:89:VAL:N	2.51	0.44
1:F:185:ASN:HA	1:F:188:GLN:HG2	2.00	0.44
2:E:41:ASN:HD21	2:E:46:ARG:HG2	1.81	0.44
3:A:287:CYS:HB2	3:A:298:LEU:HG	2.00	0.44
4:G:459:LYS:HA	4:G:462:GLU:HG3	2.00	0.44
4:I:454:THR:O	4:I:458:GLU:HG2	2.17	0.44
4:J:486:ALA:O	4:J:489:GLU:HG3	2.18	0.44
3:P:374:SER:HB2	3:P:385:ILE:HB	2.00	0.44
1:C:81:VAL:O	1:C:82:THR:C	2.60	0.44
1:C:185:ASN:HA	1:C:188:GLN:HG2	1.99	0.44
1:M:265:GLU:HG3	1:M:306:VAL:HA	2.00	0.44
1:O:351:ARG:HA	1:O:354:ARG:HG2	1.99	0.44
1:O:479:ILE:HD13	1:O:479:ILE:HA	1.83	0.44
2:E:47:ASN:O	2:E:48:HIS:HB2	2.18	0.44
2:E:84:ILE:HD12	2:E:101:TRP:CZ2	2.52	0.44
2:R:79:PHE:HB2	2:R:84:ILE:CG2	2.46	0.44
3:B:474:ILE:HG23	3:B:499:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:474:ILE:HG23	3:N:499:VAL:HG22	1.99	0.44
1:C:72:LYS:O	1:C:76:GLY:N	2.50	0.44
1:C:436:LEU:HD23	1:C:439:ARG:HH11	1.82	0.44
1:F:712:LYS:NZ	1:F:767:VAL:O	2.40	0.44
1:M:436:LEU:HD23	1:M:439:ARG:HH11	1.82	0.44
1:O:185:ASN:HA	1:O:188:GLN:HG2	2.00	0.44
2:R:79:PHE:CG	2:R:84:ILE:CG2	3.00	0.44
3:B:348:ASN:ND2	3:B:366:MET:O	2.32	0.44
3:B:370:ARG:HH21	3:B:400:GLU:HG2	1.83	0.44
4:I:486:ALA:O	4:I:489:GLU:HG3	2.18	0.44
3:N:363:LYS:O	3:N:364:THR:C	2.59	0.44
1:C:265:GLU:HA	1:C:269:ILE:CG1	2.47	0.44
1:C:723:VAL:HA	1:C:726:VAL:HG12	1.99	0.44
1:O:279:MET:HE2	1:O:279:MET:HB2	1.81	0.44
3:B:96:MET:HE3	3:B:96:MET:HB3	1.72	0.44
1:C:73:LEU:HD12	1:C:73:LEU:HA	1.79	0.44
1:C:488:ARG:HH22	1:C:502:ASP:HA	1.83	0.44
1:F:714:ARG:NH1	1:F:725:GLU:OE2	2.50	0.44
1:M:41:ILE:HD12	1:M:80:VAL:HG11	2.00	0.44
3:A:310:THR:HG22	3:A:580:ARG:HD3	2.00	0.44
3:A:434:MET:HB2	3:A:439:MET:HE3	2.00	0.44
3:B:366:MET:HG2	3:B:409:TRP:CZ2	2.53	0.44
4:I:481:ARG:HA	4:I:484:ILE:HG22	1.99	0.44
4:I:548:ASP:O	4:I:551:LYS:HG3	2.18	0.44
3:N:370:ARG:HH21	3:N:400:GLU:HG2	1.83	0.44
3:N:596:TRP:O	3:N:597:LYS:C	2.61	0.44
4:J:548:ASP:O	4:J:551:LYS:HG3	2.18	0.44
1:C:472:GLY:HA3	1:C:512:TYR:CE2	2.52	0.44
1:M:263:VAL:HA	1:M:266:ARG:HB2	1.98	0.44
1:M:390:LEU:HD13	1:M:390:LEU:HA	1.72	0.44
2:Q:45:CYS:HB2	2:Q:54:ILE:HG12	1.98	0.44
4:G:486:ALA:O	4:G:489:GLU:HG3	2.18	0.44
3:N:265:LYS:HD3	3:N:587:TYR:CD1	2.53	0.44
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.78	0.44
1:C:365:LEU:O	1:C:368:GLN:HG3	2.17	0.44
1:M:262:LYS:O	1:M:265:GLU:HG2	2.18	0.44
1:M:351:ARG:HA	1:M:354:ARG:HG2	1.99	0.44
3:B:170:MET:O	3:B:209:ARG:NH2	2.38	0.44
3:B:272:ILE:HD12	3:B:310:THR:HG22	1.99	0.44
1:C:488:ARG:HH21	1:C:503:LEU:H	1.66	0.43
1:M:84:HIS:CE1	1:M:88:LYS:HG2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:559:LEU:HD22	1:M:602:LEU:HD23	1.99	0.43
2:R:47:ASN:O	2:R:48:HIS:HB2	2.18	0.43
3:B:247:GLN:H	3:B:247:GLN:HG2	1.69	0.43
3:N:272:ILE:HD12	3:N:310:THR:HG22	1.99	0.43
3:P:462:ALA:HA	3:P:475:GLY:HA3	2.00	0.43
1:F:553:HIS:HA	1:F:597:PHE:CE1	2.53	0.43
1:M:553:HIS:HA	1:M:597:PHE:CE1	2.53	0.43
1:O:647:GLU:HB2	1:O:648:PRO:HD3	2.01	0.43
2:R:72:TRP:HB2	2:R:105:LYS:O	2.17	0.43
3:B:109:CYS:O	3:B:112:GLN:NE2	2.52	0.43
3:N:154:ARG:NH1	3:N:357:GLN:CD	2.77	0.43
1:C:351:ARG:HA	1:C:354:ARG:HG2	1.99	0.43
1:C:446:VAL:HG23	1:C:447:SER:H	1.83	0.43
1:F:647:GLU:HB2	1:F:648:PRO:HD3	2.00	0.43
1:M:185:ASN:HA	1:M:188:GLN:HG2	1.99	0.43
1:M:277:VAL:HG11	1:M:312:THR:OG1	2.18	0.43
1:M:484:MET:SD	1:M:504:THR:HA	2.58	0.43
1:O:265:GLU:HG2	1:O:266:ARG:N	2.32	0.43
1:O:480:SER:HB2	1:O:506:ARG:HE	1.84	0.43
1:O:524:ILE:H	1:O:524:ILE:HG12	1.53	0.43
1:O:553:HIS:HA	1:O:597:PHE:CE1	2.53	0.43
3:A:503:ASP:HB2	3:A:508:GLU:H	1.84	0.43
3:B:154:ARG:HH11	3:B:357:GLN:CD	2.26	0.43
1:C:54:PHE:CB	3:A:59:MET:SD	3.07	0.43
1:C:527:ALA:HB3	1:C:528:PRO:HD3	2.00	0.43
1:F:390:LEU:HD13	1:F:390:LEU:HA	1.71	0.43
1:F:525:PRO:O	1:F:526:PRO:C	2.60	0.43
1:M:423:GLN:HG2	1:M:424:GLU:H	1.83	0.43
1:O:622:ILE:CG1	1:O:627:LEU:HB2	2.49	0.43
2:R:71:ALA:CB	2:R:84:ILE:CD1	2.86	0.43
4:H:548:ASP:O	4:H:551:LYS:HG3	2.18	0.43
3:N:366:MET:HE1	3:N:370:ARG:HB2	1.99	0.43
3:P:265:LYS:HB3	3:P:265:LYS:HE3	1.66	0.43
1:C:54:PHE:O	1:C:55:GLU:C	2.57	0.43
1:C:88:LYS:HG3	1:C:89:VAL:HG13	1.99	0.43
1:M:647:GLU:HB2	1:M:648:PRO:HD3	2.00	0.43
1:O:378:LEU:HD12	1:O:378:LEU:HA	1.73	0.43
1:O:527:ALA:HB3	1:O:528:PRO:HD3	2.00	0.43
2:R:100:GLU:O	2:R:101:TRP:HB3	2.18	0.43
3:B:94:LEU:HD21	3:B:116:VAL:HG13	2.00	0.43
3:B:154:ARG:NH1	3:B:357:GLN:CD	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:287:CYS:SG	3:B:296:TYR:HB2	2.58	0.43
3:N:24:PHE:CZ	3:P:57:ARG:CD	2.97	0.43
3:N:265:LYS:HA	3:N:265:LYS:HD2	1.88	0.43
4:J:459:LYS:HA	4:J:462:GLU:HG3	1.99	0.43
4:J:534:ARG:HD2	3:P:257:PHE:CD2	2.54	0.43
1:C:525:PRO:HB3	1:C:603:MET:HG3	2.01	0.43
1:C:647:GLU:HB2	1:C:648:PRO:HD3	2.00	0.43
1:O:54:PHE:CZ	3:N:64:LEU:HD12	2.52	0.43
1:O:423:GLN:HG2	1:O:424:GLU:H	1.83	0.43
1:O:559:LEU:HD22	1:O:602:LEU:HD23	1.99	0.43
3:A:8:GLN:H	3:A:8:GLN:HG2	1.49	0.43
3:A:225:LEU:HB3	3:A:229:THR:HG23	2.01	0.43
3:A:442:TYR:H	3:A:442:TYR:HD2	1.67	0.43
4:H:486:ALA:O	4:H:489:GLU:HG3	2.18	0.43
4:J:467:TYR:HD1	4:J:467:TYR:HA	1.73	0.43
3:P:22:LYS:HE3	3:P:91:THR:HG23	2.00	0.43
3:P:319:TYR:HB3	3:P:350:PHE:CE2	2.54	0.43
1:C:354:ARG:HA	1:C:357:LEU:HG	2.01	0.43
1:F:622:ILE:CG1	1:F:627:LEU:HB2	2.49	0.43
1:F:751:ARG:HD3	1:F:751:ARG:HA	1.88	0.43
1:M:86:ILE:HA	1:M:150:GLN:NE2	2.33	0.43
2:R:65:SER:O	2:R:66:GLU:C	2.62	0.43
3:A:257:PHE:CD2	4:G:534:ARG:HD2	2.54	0.43
3:A:403:ASP:HB2	3:A:408:GLU:H	1.84	0.43
4:G:436:VAL:HG11	4:G:445:VAL:HG13	2.01	0.43
3:P:392:GLY:HA3	3:P:395:ASN:HB3	2.00	0.43
1:C:553:HIS:HA	1:C:597:PHE:CE1	2.53	0.43
1:F:446:VAL:HG23	1:F:447:SER:H	1.84	0.43
1:F:756:ARG:HA	1:F:764:TYR:CE1	2.54	0.43
1:M:446:VAL:HG23	1:M:447:SER:H	1.84	0.43
1:O:526:PRO:HD2	1:O:603:MET:CE	2.49	0.43
3:N:97:ASN:OD1	3:N:100:THR:OG1	2.32	0.43
3:P:305:LEU:H	3:P:305:LEU:HD23	1.84	0.43
1:C:272:HIS:O	1:C:273:MET:C	2.62	0.43
1:C:480:SER:HB2	1:C:506:ARG:CB	2.28	0.43
1:F:354:ARG:HA	1:F:357:LEU:HG	2.01	0.43
1:M:72:LYS:O	1:M:73:LEU:C	2.61	0.43
1:M:509:THR:C	2:R:32:LEU:HD11	2.44	0.43
1:O:154:TYR:HB3	1:O:157:ILE:HG22	2.01	0.43
1:O:500:GLY:HA2	1:O:503:LEU:HD23	2.01	0.43
3:A:472:PHE:CD1	3:A:499:VAL:HG12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:480:LYS:HB3	4:G:549:LEU:HD21	2.00	0.43
3:B:265:LYS:HD3	3:B:587:TYR:CD1	2.53	0.43
4:J:502:GLU:O	4:J:505:SER:OG	2.24	0.43
1:C:181:GLY:HA2	1:C:184:ARG:HG2	2.01	0.43
1:C:279:MET:HE3	1:C:279:MET:HB3	1.71	0.43
1:C:559:LEU:O	1:C:592:LEU:N	2.39	0.43
1:C:598:GLN:HG2	1:C:634:LEU:HG	2.01	0.43
1:F:351:ARG:HA	1:F:354:ARG:HG2	1.99	0.43
1:F:545:GLY:HA2	1:O:493:ALA:HB2	2.00	0.43
1:M:274:LYS:O	1:M:275:THR:C	2.61	0.43
1:M:700:LYS:HG2	1:M:744:ARG:HD2	2.00	0.43
2:R:87:TRP:CZ2	2:R:91:ARG:HB3	2.54	0.43
3:N:109:CYS:O	3:N:112:GLN:NE2	2.52	0.43
3:N:154:ARG:HH11	3:N:357:GLN:CD	2.26	0.43
3:P:291:GLN:H	3:P:291:GLN:HG2	1.48	0.43
1:O:265:GLU:O	1:O:266:ARG:C	2.62	0.42
1:O:280:GLU:HB3	1:O:281:ASN:H	1.74	0.42
3:A:351:TYR:HB3	3:A:360:TRP:HB3	2.01	0.42
4:G:513:LYS:HZ3	4:G:514:ARG:NH1	2.17	0.42
3:P:251:LYS:H	3:P:251:LYS:HG2	1.66	0.42
1:C:63:THR:O	1:C:66:LEU:HB2	2.20	0.42
1:O:125:TYR:O	1:O:129:VAL:HG22	2.19	0.42
1:O:264:VAL:O	1:O:265:GLU:C	2.61	0.42
1:O:446:VAL:HG23	1:O:447:SER:H	1.83	0.42
1:O:467:THR:HA	1:O:470:LEU:HB2	2.01	0.42
4:G:548:ASP:O	4:G:551:LYS:HG3	2.18	0.42
3:B:352:TRP:HB3	3:B:363:LYS:CE	2.46	0.42
3:N:554:TYR:HB2	3:N:561:TRP:CZ3	2.54	0.42
3:P:391:GLY:H	3:P:396:ARG:HG3	1.84	0.42
1:C:486:GLU:O	1:C:490:HIS:ND1	2.35	0.42
1:F:248:VAL:HG23	1:F:252:LEU:HD22	2.00	0.42
1:M:154:TYR:HB3	1:M:157:ILE:HG22	2.02	0.42
1:M:259:PRO:O	1:M:262:LYS:HB2	2.19	0.42
1:O:254:LYS:H	1:O:254:LYS:HG3	1.48	0.42
3:B:437:ASN:O	3:B:455:ARG:N	2.40	0.42
1:C:85:LEU:C	1:C:87:ASN:N	2.77	0.42
1:C:125:TYR:O	1:C:129:VAL:HG22	2.19	0.42
1:C:524:ILE:HB	1:C:529:ARG:HG2	2.01	0.42
1:F:181:GLY:HA2	1:F:184:ARG:HG2	2.01	0.42
1:M:181:GLY:HA2	1:M:184:ARG:HG2	2.01	0.42
1:O:97:LEU:HD22	1:O:97:LEU:HA	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:559:LEU:O	1:O:592:LEU:N	2.39	0.42
1:O:622:ILE:HG13	1:O:627:LEU:HB2	2.01	0.42
2:R:74:VAL:C	2:R:76:ASN:H	2.26	0.42
3:A:57:ARG:NH2	3:B:20:GLN:NE2	2.67	0.42
3:P:442:TYR:HB2	3:P:449:TRP:CZ3	2.54	0.42
1:F:89:VAL:HG11	1:F:151:VAL:CG2	2.45	0.42
1:F:269:ILE:H	1:F:269:ILE:HG12	1.49	0.42
1:F:423:GLN:HG2	1:F:424:GLU:H	1.83	0.42
1:O:181:GLY:HA2	1:O:184:ARG:HG2	2.01	0.42
1:O:257:GLU:O	1:O:258:GLU:C	2.62	0.42
3:A:175:ASP:HA	3:A:178:ILE:HG12	2.01	0.42
4:H:459:LYS:HE2	4:H:573:LEU:HD12	2.02	0.42
4:I:524:ILE:HD12	4:I:524:ILE:HA	1.89	0.42
3:P:276:SER:HA	3:P:573:TRP:HE1	1.85	0.42
3:P:307:LYS:HB3	3:P:371:ILE:HG23	2.00	0.42
3:P:554:TYR:HB2	3:P:561:TRP:CE3	2.55	0.42
1:C:510:THR:HG23	2:E:76:ASN:HD21	1.84	0.42
1:C:532:PHE:N	2:E:27:TRP:HZ3	2.17	0.42
1:O:354:ARG:HA	1:O:357:LEU:HG	2.01	0.42
1:O:475:ARG:O	1:O:476:ASP:C	2.62	0.42
1:O:526:PRO:HD2	1:O:603:MET:HE2	2.01	0.42
2:D:84:ILE:HD13	2:D:84:ILE:O	2.20	0.42
4:G:480:LYS:HA	4:G:480:LYS:HD3	1.55	0.42
4:G:527:ASN:HA	4:G:530:LYS:HE3	2.02	0.42
3:B:223:ASP:HB2	3:B:257:PHE:HE1	1.84	0.42
1:C:37:LEU:HD21	1:C:60:ASN:CB	2.50	0.42
1:C:273:MET:HE3	1:C:273:MET:HB3	1.82	0.42
1:F:173:ARG:HH12	1:F:213:SER:HA	1.84	0.42
1:M:79:GLU:O	1:M:80:VAL:C	2.58	0.42
2:E:39:VAL:O	2:E:39:VAL:CG1	2.53	0.42
2:Q:50:MET:HB2	2:Q:51:ASP:H	1.67	0.42
3:A:431:ILE:H	3:A:431:ILE:HG13	1.56	0.42
3:A:500:GLU:HA	3:A:511:MET:HG2	2.01	0.42
4:G:521:ILE:HD12	4:G:521:ILE:HA	1.84	0.42
3:B:97:ASN:OD1	3:B:100:THR:OG1	2.32	0.42
3:B:261:LEU:HD11	3:B:590:CYS:SG	2.60	0.42
1:F:467:THR:HA	1:F:470:LEU:HB2	2.01	0.42
1:F:622:ILE:HG13	1:F:627:LEU:HB2	2.01	0.42
1:M:274:LYS:HD2	1:M:274:LYS:HA	1.32	0.42
1:M:548:LEU:HD22	2:R:32:LEU:O	2.20	0.42
1:O:390:LEU:HG	1:O:681:GLN:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:65:SER:O	2:E:66:GLU:C	2.62	0.42
3:A:298:LEU:HD22	3:A:353:PHE:CE2	2.55	0.42
3:A:320:ILE:HB	3:A:360:TRP:CZ3	2.55	0.42
4:G:438:LYS:HD2	4:G:438:LYS:HA	1.74	0.42
4:G:459:LYS:O	4:G:462:GLU:HG3	2.20	0.42
4:I:459:LYS:HE2	4:I:573:LEU:HD12	2.02	0.42
3:N:261:LEU:HD11	3:N:590:CYS:SG	2.60	0.42
1:C:65:VAL:HG11	1:C:125:TYR:CE2	2.54	0.42
1:C:404:THR:OG1	1:C:407:GLU:OE2	2.20	0.42
1:M:173:ARG:HH12	1:M:213:SER:HA	1.84	0.42
2:E:79:PHE:HB2	2:E:84:ILE:HG23	2.02	0.42
3:A:298:LEU:HA	3:A:298:LEU:HD23	1.80	0.42
3:N:223:ASP:HB2	3:N:257:PHE:HE1	1.84	0.42
1:M:592:LEU:HD23	1:M:672:VAL:HG13	2.02	0.42
1:O:173:ARG:HH12	1:O:213:SER:HA	1.84	0.42
1:O:266:ARG:O	1:O:267:GLU:C	2.63	0.42
2:E:38:VAL:C	2:E:40:ASP:H	2.28	0.42
2:R:52:LEU:HA	2:R:52:LEU:HD13	1.75	0.42
1:C:423:GLN:HG2	1:C:424:GLU:H	1.83	0.41
1:F:90:ARG:HA	1:F:90:ARG:HD3	1.50	0.41
1:F:154:TYR:HB3	1:F:157:ILE:HG22	2.01	0.41
1:M:598:GLN:HG2	1:M:634:LEU:HG	2.01	0.41
1:O:293:THR:HB	1:O:358:GLU:CD	2.45	0.41
1:O:464:CYS:HA	1:O:467:THR:OG1	2.20	0.41
2:E:52:LEU:HD11	2:E:59:ASN:HA	2.02	0.41
3:A:451:GLU:H	3:A:451:GLU:HG2	1.52	0.41
3:N:427:VAL:HG21	3:N:471:ILE:HG12	2.02	0.41
3:P:175:ASP:HA	3:P:178:ILE:HG12	2.01	0.41
3:P:225:LEU:HB3	3:P:229:THR:HG23	2.01	0.41
1:C:173:ARG:HH12	1:C:213:SER:HA	1.84	0.41
1:C:753:TYR:O	1:C:754:LEU:C	2.63	0.41
1:F:54:PHE:O	1:F:57:LEU:HB2	2.19	0.41
1:F:531:ALA:HB1	2:D:27:TRP:HZ3	1.75	0.41
1:M:94:LEU:HD12	1:M:94:LEU:HA	1.77	0.41
1:M:275:THR:O	1:M:279:MET:HB2	2.19	0.41
1:M:354:ARG:HA	1:M:357:LEU:HG	2.01	0.41
3:B:596:TRP:O	3:B:597:LYS:C	2.63	0.41
1:F:558:ASP:OD1	1:F:671:ARG:NH2	2.54	0.41
1:M:37:LEU:HD21	1:M:60:ASN:CB	2.50	0.41
1:M:293:THR:HB	1:M:358:GLU:CD	2.45	0.41
3:A:454:MET:H	3:A:454:MET:HG2	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:554:TYR:HB2	3:B:561:TRP:CZ3	2.54	0.41
1:C:71:GLU:O	1:C:72:LYS:C	2.62	0.41
1:C:680:LYS:HB3	1:C:680:LYS:HE3	1.32	0.41
1:F:475:ARG:O	1:F:476:ASP:C	2.62	0.41
1:M:265:GLU:O	1:M:269:ILE:HB	2.21	0.41
3:A:307:LYS:HA	3:A:372:LYS:HG3	2.02	0.41
4:I:480:LYS:HA	4:I:480:LYS:HD3	1.52	0.41
4:I:534:ARG:HA	4:I:537:GLU:HG2	2.03	0.41
4:J:527:ASN:HA	4:J:530:LYS:HE3	2.02	0.41
4:J:534:ARG:HA	4:J:537:GLU:HG2	2.03	0.41
1:F:710:ILE:HG21	1:F:729:GLN:HE22	1.86	0.41
1:M:326:LYS:HA	1:M:329:VAL:HG22	2.01	0.41
1:M:374:PHE:O	1:M:378:LEU:HB2	2.21	0.41
1:M:437:ALA:HA	1:M:513:TRP:HZ3	1.85	0.41
3:A:53:SER:HB2	3:A:113:VAL:HG22	2.03	0.41
3:A:297:LYS:HD2	3:A:297:LYS:HA	1.87	0.41
3:A:350:PHE:HD1	3:A:352:TRP:CZ3	2.39	0.41
4:J:459:LYS:O	4:J:462:GLU:HG3	2.20	0.41
3:P:127:LYS:HA	3:P:127:LYS:HD3	1.49	0.41
1:C:265:GLU:O	1:C:266:ARG:C	2.64	0.41
1:C:383:ARG:H	1:C:383:ARG:HG2	1.67	0.41
1:M:416:MET:HE2	1:M:461:GLU:HG2	2.02	0.41
1:O:52:LEU:O	3:N:66:GLU:OE2	2.38	0.41
2:E:94:CYS:HA	2:E:95:PRO:HD3	1.87	0.41
2:R:54:ILE:HA	2:R:57:GLN:HE21	1.85	0.41
3:N:46:LYS:NZ	3:N:67:SER:O	2.53	0.41
3:N:109:CYS:HA	3:N:117:LEU:HD11	2.03	0.41
3:P:390:VAL:HA	3:P:396:ARG:HG3	2.03	0.41
1:C:81:VAL:HG23	1:C:82:THR:N	2.35	0.41
1:C:154:TYR:HB3	1:C:157:ILE:HG22	2.01	0.41
1:C:484:MET:HE1	1:C:504:THR:HG22	1.94	0.41
1:F:329:VAL:O	1:F:330:SER:C	2.63	0.41
1:F:378:LEU:C	1:F:380:LEU:H	2.29	0.41
1:F:520:PRO:HG3	1:F:553:HIS:CE1	2.55	0.41
1:M:87:ASN:HB2	1:M:88:LYS:H	1.61	0.41
1:M:761:ARG:H	1:M:761:ARG:HG2	1.75	0.41
2:E:34:ALA:HA	2:E:76:ASN:HD22	1.86	0.41
3:A:46:LYS:NZ	3:A:67:SER:O	2.54	0.41
4:G:566:ILE:HD12	4:G:566:ILE:HA	1.74	0.41
1:C:64:MET:C	1:C:66:LEU:N	2.78	0.41
1:M:288:LEU:O	1:M:351:ARG:NH2	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:560:ASN:HA	1:O:591:ILE:HG13	2.03	0.41
3:B:427:VAL:HG21	3:B:471:ILE:HG12	2.02	0.41
4:H:481:ARG:HA	4:H:484:ILE:HG22	2.03	0.41
1:C:263:VAL:O	1:C:266:ARG:HB2	2.21	0.41
1:F:293:THR:HB	1:F:358:GLU:CD	2.45	0.41
1:F:698:ASP:HA	1:F:701:HIS:CD2	2.56	0.41
1:M:91:GLU:O	1:M:92:ASP:C	2.63	0.41
1:M:593:GLN:HE21	1:M:593:GLN:HB3	1.71	0.41
1:O:317:MET:HE2	1:O:317:MET:HB2	2.00	0.41
2:E:84:ILE:CD1	2:E:101:TRP:HZ2	2.33	0.41
2:R:37:ILE:HD13	2:R:72:TRP:CH2	2.56	0.41
2:R:38:VAL:C	2:R:40:ASP:H	2.28	0.41
3:A:352:TRP:CH2	3:A:409:TRP:HH2	2.39	0.41
3:A:352:TRP:HH2	3:A:409:TRP:CH2	2.38	0.41
3:A:519:ARG:HA	4:I:440:ASP:CB	2.50	0.41
4:H:534:ARG:HA	4:H:537:GLU:HG2	2.02	0.41
4:I:593:LYS:HD2	4:I:593:LYS:HA	1.35	0.41
3:N:7:ARG:HD3	3:P:93:ASN:HB2	2.03	0.41
3:N:57:ARG:NE	3:P:24:PHE:HZ	2.13	0.41
3:N:593:GLU:H	3:N:593:GLU:HG2	1.46	0.41
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.89	0.41
1:C:274:LYS:HA	1:C:274:LYS:HD2	1.47	0.41
1:C:675:GLN:C	1:C:677:VAL:H	2.28	0.41
1:M:348:LEU:HA	1:M:351:ARG:HG2	2.02	0.41
1:O:246:GLU:HA	1:O:249:MET:HE2	2.03	0.41
2:D:98:ASN:HD22	2:D:98:ASN:HA	1.71	0.41
3:N:61:MET:HE2	3:N:61:MET:HA	2.03	0.41
3:N:263:MET:H	3:N:263:MET:HG2	1.61	0.41
3:N:417:CYS:HB2	3:N:419:TRP:CZ2	2.56	0.41
3:P:459:ARG:HD2	3:P:476:GLY:HA3	2.03	0.41
1:C:484:MET:SD	1:C:504:THR:CG2	2.95	0.40
1:F:432:TYR:HE2	1:F:470:LEU:HD21	1.86	0.40
1:F:531:ALA:HB3	2:D:27:TRP:CE3	2.53	0.40
1:F:711:MET:HE3	1:F:722:LEU:HB3	2.04	0.40
1:M:524:ILE:HB	1:M:529:ARG:HG3	2.03	0.40
1:M:750:GLU:H	1:M:750:GLU:HG2	1.56	0.40
1:M:762:LYS:HZ2	1:M:762:LYS:HG3	1.75	0.40
1:O:336:LYS:HB2	1:O:337:ASN:H	1.64	0.40
2:E:97:ASP:N	2:E:97:ASP:OD1	2.54	0.40
3:B:108:ALA:O	3:B:112:GLN:N	2.54	0.40
3:B:417:CYS:HB2	3:B:419:TRP:CZ2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:108:ALA:O	3:N:112:GLN:N	2.53	0.40
3:P:353:PHE:HB2	3:P:360:TRP:CH2	2.56	0.40
1:C:64:MET:C	1:C:66:LEU:H	2.28	0.40
1:C:123:LEU:HB3	1:C:126:MET:HE2	2.03	0.40
1:C:207:ALA:HB3	1:C:208:PRO:HD3	2.04	0.40
1:C:293:THR:HB	1:C:358:GLU:CD	2.46	0.40
1:F:503:LEU:HD21	2:D:27:TRP:HE3	1.86	0.40
1:M:80:VAL:O	1:M:81:VAL:C	2.60	0.40
1:O:710:ILE:HG21	1:O:729:GLN:HE22	1.86	0.40
1:O:717:MET:HG2	1:O:764:TYR:HE2	1.85	0.40
1:O:744:ARG:C	1:O:746:GLU:H	2.30	0.40
2:E:54:ILE:HA	2:E:57:GLN:HE21	1.86	0.40
3:A:123:TYR:HA	3:A:126:LYS:HE2	2.03	0.40
3:A:271:PHE:HB3	3:A:274:ALA:HB2	2.02	0.40
3:P:435:THR:O	3:P:455:ARG:NH2	2.38	0.40
1:C:710:ILE:HG21	1:C:729:GLN:HE22	1.85	0.40
1:F:420:ARG:NH1	1:F:461:GLU:OE2	2.55	0.40
1:M:207:ALA:HB3	1:M:208:PRO:HD3	2.04	0.40
1:M:622:ILE:CG1	1:M:627:LEU:HB2	2.52	0.40
1:O:558:ASP:OD1	1:O:671:ARG:NH2	2.54	0.40
2:D:97:ASP:OD1	2:D:97:ASP:N	2.54	0.40
2:R:94:CYS:HA	2:R:95:PRO:HD3	1.87	0.40
2:Q:89:LYS:HD2	2:Q:89:LYS:HA	1.56	0.40
3:A:357:GLN:H	3:A:357:GLN:HG2	1.50	0.40
1:C:524:ILE:HB	1:C:529:ARG:HG3	2.03	0.40
1:C:556:SER:OG	2:E:28:ASN:ND2	2.55	0.40
1:C:560:ASN:HA	1:C:591:ILE:HG13	2.03	0.40
1:C:622:ILE:CG1	1:C:627:LEU:HB2	2.52	0.40
1:F:550:LEU:H	1:F:550:LEU:HG	1.41	0.40
1:F:592:LEU:HD23	1:F:672:VAL:HG13	2.02	0.40
1:M:560:ASN:HA	1:M:591:ILE:HG13	2.03	0.40
1:O:271:LYS:HE3	1:O:271:LYS:HB2	1.76	0.40
1:O:288:LEU:O	1:O:351:ARG:NH2	2.42	0.40
1:O:334:GLU:H	1:O:334:GLU:HG2	1.56	0.40
3:B:273:GLU:OE2	3:B:307:LYS:N	2.55	0.40
3:P:81:THR:HG21	3:P:103:GLN:HG3	2.04	0.40
3:P:272:ILE:HD12	3:P:310:THR:HG22	2.03	0.40
1:C:477:MET:HE3	1:C:513:TRP:CH2	2.56	0.40
1:C:524:ILE:O	1:C:529:ARG:NE	2.54	0.40
1:F:334:GLU:H	1:F:334:GLU:HG2	1.51	0.40
1:F:464:CYS:HA	1:F:467:THR:OG1	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:553:HIS:HA	1:F:597:PHE:HE1	1.87	0.40
1:M:168:MET:HA	1:M:171:ARG:HG2	2.04	0.40
1:M:548:LEU:HD22	1:M:548:LEU:HA	1.92	0.40
1:M:558:ASP:OD1	1:M:671:ARG:NH2	2.54	0.40
1:M:710:ILE:HG21	1:M:729:GLN:HE22	1.86	0.40
2:R:74:VAL:C	2:R:76:ASN:N	2.80	0.40
4:G:549:LEU:O	4:G:552:GLN:HG3	2.22	0.40
3:B:109:CYS:HA	3:B:117:LEU:HD11	2.03	0.40
4:J:480:LYS:HD3	4:J:480:LYS:HA	1.54	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	C	716/768 (93%)	628 (88%)	80 (11%)	8 (1%)	11	46
1	F	716/768 (93%)	633 (88%)	72 (10%)	11 (2%)	8	40
1	M	716/768 (93%)	648 (90%)	62 (9%)	6 (1%)	16	54
1	O	716/768 (93%)	646 (90%)	64 (9%)	6 (1%)	16	54
2	D	87/108 (81%)	60 (69%)	17 (20%)	10 (12%)	0	5
2	E	87/108 (81%)	57 (66%)	18 (21%)	12 (14%)	0	3
2	Q	87/108 (81%)	62 (71%)	19 (22%)	6 (7%)	1	11
2	R	87/108 (81%)	57 (66%)	20 (23%)	10 (12%)	0	5
3	A	561/623 (90%)	480 (86%)	76 (14%)	5 (1%)	14	51
3	B	558/623 (90%)	510 (91%)	44 (8%)	4 (1%)	18	56
3	N	558/623 (90%)	512 (92%)	42 (8%)	4 (1%)	18	56
3	P	547/623 (88%)	505 (92%)	40 (7%)	2 (0%)	30	67
4	G	166/724 (23%)	156 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	166/724 (23%)	156 (94%)	10 (6%)	0	100	100
4	I	166/724 (23%)	156 (94%)	8 (5%)	2 (1%)	10	44
4	J	166/724 (23%)	155 (93%)	11 (7%)	0	100	100
All	All	6100/8892 (69%)	5421 (89%)	593 (10%)	86 (1%)	11	40

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	88	LYS
1	C	268	LEU
1	F	526	PRO
2	D	40	ASP
2	Q	40	ASP
3	N	592	GLU
1	C	84	HIS
1	C	269	ILE
1	F	269	ILE
1	F	501	VAL
1	M	88	LYS
1	M	501	VAL
2	E	39	VAL
2	E	66	GLU
2	E	94	CYS
2	D	35	TRP
2	D	92	GLN
2	D	94	CYS
2	R	39	VAL
2	R	66	GLU
2	R	94	CYS
2	Q	35	TRP
3	A	302	PRO
3	A	391	GLY
3	A	599	PRO
4	I	442	ILE
1	C	78	ARG
1	C	83	GLU
1	C	258	GLU
1	F	50	SER
1	M	278	GLU
1	O	257	GLU
1	O	526	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	35	TRP
2	E	64	THR
2	E	98	ASN
2	R	35	TRP
2	R	64	THR
2	R	98	ASN
3	A	476	GLY
3	B	248	GLY
3	N	248	GLY
1	C	267	GLU
1	F	196	GLU
1	F	270	SER
1	F	279	MET
1	F	330	SER
1	M	277	VAL
1	O	258	GLU
2	E	40	ASP
2	E	97	ASP
2	D	97	ASP
2	D	98	ASN
2	R	40	ASP
2	R	97	ASP
2	Q	94	CYS
3	N	600	THR
1	F	382	SER
1	M	335	GLY
1	O	266	ARG
2	E	48	HIS
2	D	39	VAL
2	R	48	HIS
2	Q	46	ARG
3	A	513	ALA
1	F	59	ARG
2	E	57	GLN
2	E	101	TRP
2	D	46	ARG
2	D	101	TRP
2	Q	39	VAL
3	B	600	THR
1	O	767	VAL
2	E	38	VAL
2	R	38	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	588	GLY
3	P	516	PRO
3	P	571	VAL
3	B	279	PRO
3	B	595	PRO
3	N	279	PRO
1	F	623	PRO
1	M	269	ILE
1	O	623	PRO
2	D	38	VAL
2	Q	38	VAL

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	C	635/693 (92%)	522 (82%)	113 (18%)	2	9
1	F	603/693 (87%)	498 (83%)	105 (17%)	2	9
1	M	604/693 (87%)	501 (83%)	103 (17%)	2	10
1	O	628/693 (91%)	520 (83%)	108 (17%)	2	9
2	D	78/90 (87%)	54 (69%)	24 (31%)	0	2
2	E	78/90 (87%)	60 (77%)	18 (23%)	1	5
2	Q	78/90 (87%)	49 (63%)	29 (37%)	0	1
2	R	78/90 (87%)	61 (78%)	17 (22%)	1	6
3	A	504/560 (90%)	377 (75%)	127 (25%)	0	4
3	B	495/560 (88%)	460 (93%)	35 (7%)	13	35
3	N	496/560 (89%)	462 (93%)	34 (7%)	14	36
3	P	477/560 (85%)	446 (94%)	31 (6%)	15	37
4	G	151/654 (23%)	123 (82%)	28 (18%)	1	8
4	H	129/654 (20%)	110 (85%)	19 (15%)	3	13
4	I	134/654 (20%)	115 (86%)	19 (14%)	3	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	125/654 (19%)	105 (84%)	20 (16%)	2	11
All	All	5293/7988 (66%)	4463 (84%)	830 (16%)	4	12

All (830) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	35	ASP
1	C	43	GLU
1	C	55	GLU
1	C	65	VAL
1	C	66	LEU
1	C	67	HIS
1	C	68	LYS
1	C	71	GLU
1	C	72	LYS
1	C	73	LEU
1	C	78	ARG
1	C	79	GLU
1	C	82	THR
1	C	83	GLU
1	C	85	LEU
1	C	86	ILE
1	C	87	ASN
1	C	90	ARG
1	C	91	GLU
1	C	94	LEU
1	C	96	SER
1	C	98	ASN
1	C	102	LEU
1	C	204	ASP
1	C	225	LEU
1	C	249	MET
1	C	252	LEU
1	C	254	LYS
1	C	258	GLU
1	C	260	ILE
1	C	261	VAL
1	C	262	LYS
1	C	263	VAL
1	C	264	VAL
1	C	266	ARG
1	C	267	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	268	LEU
1	C	269	ILE
1	C	270	SER
1	C	271	LYS
1	C	273	MET
1	C	274	LYS
1	C	276	ILE
1	C	278	GLU
1	C	279	MET
1	C	280	GLU
1	C	282	SER
1	C	284	LEU
1	C	328	LEU
1	C	332	GLU
1	C	334	GLU
1	C	336	LYS
1	C	340	ASP
1	C	341	TYR
1	C	342	ILE
1	C	346	LEU
1	C	353	ASP
1	C	380	LEU
1	C	390	LEU
1	C	400	VAL
1	C	405	GLU
1	C	407	GLU
1	C	411	ILE
1	C	420	ARG
1	C	446	VAL
1	C	462	CYS
1	C	465	GLN
1	C	468	SER
1	C	470	LEU
1	C	473	MET
1	C	484	MET
1	C	486	GLU
1	C	491	LEU
1	C	496	VAL
1	C	498	LEU
1	C	501	VAL
1	C	503	LEU
1	C	508	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	509	THR
1	C	510	THR
1	C	515	THR
1	C	521	LYS
1	C	596	THR
1	C	600	THR
1	C	602	LEU
1	C	626	GLU
1	C	627	LEU
1	C	629	ARG
1	C	632	GLN
1	C	634	LEU
1	C	641	GLN
1	C	653	ILE
1	C	665	PHE
1	C	669	LEU
1	C	672	VAL
1	C	676	THR
1	C	677	VAL
1	C	680	LYS
1	C	687	GLU
1	C	688	ARG
1	C	699	ARG
1	C	701	HIS
1	C	702	GLU
1	C	703	ILE
1	C	735	LEU
1	C	748	LEU
1	C	750	GLU
1	C	751	ARG
1	C	752	GLU
1	C	753	TYR
1	C	762	LYS
1	C	763	VAL
1	C	767	VAL
1	F	35	ASP
1	F	43	GLU
1	F	68	LYS
1	F	71	GLU
1	F	72	LYS
1	F	77	LEU
1	F	83	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	84	HIS
1	F	86	ILE
1	F	88	LYS
1	F	90	ARG
1	F	91	GLU
1	F	94	LEU
1	F	97	LEU
1	F	98	ASN
1	F	99	ASN
1	F	102	LEU
1	F	196	GLU
1	F	198	ARG
1	F	199	SER
1	F	204	ASP
1	F	225	LEU
1	F	254	LYS
1	F	256	THR
1	F	258	GLU
1	F	260	ILE
1	F	262	LYS
1	F	264	VAL
1	F	266	ARG
1	F	267	GLU
1	F	268	LEU
1	F	269	ILE
1	F	271	LYS
1	F	273	MET
1	F	274	LYS
1	F	275	THR
1	F	276	ILE
1	F	277	VAL
1	F	279	MET
1	F	280	GLU
1	F	282	SER
1	F	284	LEU
1	F	330	SER
1	F	332	GLU
1	F	334	GLU
1	F	336	LYS
1	F	339	VAL
1	F	342	ILE
1	F	348	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	353	ASP
1	F	382	SER
1	F	383	ARG
1	F	390	LEU
1	F	400	VAL
1	F	405	GLU
1	F	407	GLU
1	F	411	ILE
1	F	420	ARG
1	F	446	VAL
1	F	468	SER
1	F	469	LYS
1	F	470	LEU
1	F	473	MET
1	F	478	SER
1	F	479	ILE
1	F	480	SER
1	F	481	ASN
1	F	503	LEU
1	F	504	THR
1	F	505	VAL
1	F	507	VAL
1	F	510	THR
1	F	515	THR
1	F	521	LYS
1	F	522	CYS
1	F	523	ASN
1	F	524	ILE
1	F	526	PRO
1	F	550	LEU
1	F	551	GLN
1	F	596	THR
1	F	600	THR
1	F	602	LEU
1	F	627	LEU
1	F	629	ARG
1	F	632	GLN
1	F	634	LEU
1	F	641	GLN
1	F	653	ILE
1	F	665	PHE
1	F	669	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	672	VAL
1	F	683	GLU
1	F	698	ASP
1	F	703	ILE
1	F	735	LEU
1	F	748	LEU
1	F	749	ILE
1	F	750	GLU
1	F	751	ARG
1	F	752	GLU
1	F	757	THR
1	F	761	ARG
1	F	762	LYS
1	F	763	VAL
1	M	35	ASP
1	M	43	GLU
1	M	66	LEU
1	M	68	LYS
1	M	71	GLU
1	M	72	LYS
1	M	79	GLU
1	M	86	ILE
1	M	88	LYS
1	M	90	ARG
1	M	91	GLU
1	M	94	LEU
1	M	96	SER
1	M	97	LEU
1	M	98	ASN
1	M	99	ASN
1	M	102	LEU
1	M	204	ASP
1	M	225	LEU
1	M	249	MET
1	M	252	LEU
1	M	253	ASP
1	M	254	LYS
1	M	256	THR
1	M	257	GLU
1	M	258	GLU
1	M	262	LYS
1	M	263	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	264	VAL
1	M	267	GLU
1	M	268	LEU
1	M	270	SER
1	M	273	MET
1	M	274	LYS
1	M	275	THR
1	M	278	GLU
1	M	279	MET
1	M	280	GLU
1	M	282	SER
1	M	284	LEU
1	M	332	GLU
1	M	334	GLU
1	M	336	LYS
1	M	342	ILE
1	M	346	LEU
1	M	353	ASP
1	M	378	LEU
1	M	380	LEU
1	M	390	LEU
1	M	400	VAL
1	M	405	GLU
1	M	407	GLU
1	M	411	ILE
1	M	420	ARG
1	M	446	VAL
1	M	457	LYS
1	M	458	LEU
1	M	464	CYS
1	M	465	GLN
1	M	468	SER
1	M	470	LEU
1	M	473	MET
1	M	484	MET
1	M	505	VAL
1	M	508	LEU
1	M	509	THR
1	M	510	THR
1	M	515	THR
1	M	516	GLN
1	M	521	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	522	CYS
1	M	523	ASN
1	M	524	ILE
1	M	547	GLN
1	M	548	LEU
1	M	549	THR
1	M	596	THR
1	M	600	THR
1	M	602	LEU
1	M	626	GLU
1	M	627	LEU
1	M	629	ARG
1	M	632	GLN
1	M	634	LEU
1	M	641	GLN
1	M	653	ILE
1	M	665	PHE
1	M	669	LEU
1	M	672	VAL
1	M	683	GLU
1	M	695	VAL
1	M	698	ASP
1	M	701	HIS
1	M	703	ILE
1	M	735	LEU
1	M	750	GLU
1	M	753	TYR
1	M	754	LEU
1	M	761	ARG
1	M	762	LYS
1	M	763	VAL
1	M	765	THR
1	M	767	VAL
1	O	35	ASP
1	O	43	GLU
1	O	55	GLU
1	O	56	GLU
1	O	57	LEU
1	O	68	LYS
1	O	71	GLU
1	O	72	LYS
1	O	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	83	GLU
1	O	84	HIS
1	O	86	ILE
1	O	88	LYS
1	O	90	ARG
1	O	91	GLU
1	O	94	LEU
1	O	97	LEU
1	O	98	ASN
1	O	99	ASN
1	O	102	LEU
1	O	204	ASP
1	O	225	LEU
1	O	249	MET
1	O	252	LEU
1	O	254	LYS
1	O	256	THR
1	O	257	GLU
1	O	258	GLU
1	O	262	LYS
1	O	264	VAL
1	O	265	GLU
1	O	266	ARG
1	O	268	LEU
1	O	271	LYS
1	O	273	MET
1	O	274	LYS
1	O	275	THR
1	O	276	ILE
1	O	279	MET
1	O	284	LEU
1	O	328	LEU
1	O	332	GLU
1	O	334	GLU
1	O	336	LYS
1	O	339	VAL
1	O	340	ASP
1	O	341	TYR
1	O	342	ILE
1	O	346	LEU
1	O	353	ASP
1	O	378	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	379	ASN
1	O	383	ARG
1	O	384	SER
1	O	390	LEU
1	O	400	VAL
1	O	405	GLU
1	O	407	GLU
1	O	411	ILE
1	O	417	VAL
1	O	418	LEU
1	O	420	ARG
1	O	421	PHE
1	O	446	VAL
1	O	468	SER
1	O	469	LYS
1	O	470	LEU
1	O	473	MET
1	O	478	SER
1	O	479	ILE
1	O	480	SER
1	O	481	ASN
1	O	504	THR
1	O	505	VAL
1	O	510	THR
1	O	515	THR
1	O	521	LYS
1	O	523	ASN
1	O	524	ILE
1	O	526	PRO
1	O	550	LEU
1	O	551	GLN
1	O	596	THR
1	O	600	THR
1	O	602	LEU
1	O	627	LEU
1	O	629	ARG
1	O	632	GLN
1	O	634	LEU
1	O	641	GLN
1	O	653	ILE
1	O	665	PHE
1	O	669	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	672	VAL
1	O	683	GLU
1	O	701	HIS
1	O	735	LEU
1	O	748	LEU
1	O	749	ILE
1	O	750	GLU
1	O	751	ARG
1	O	752	GLU
1	O	757	THR
1	O	761	ARG
1	O	762	LYS
1	O	763	VAL
1	O	765	THR
1	O	767	VAL
2	E	25	LYS
2	E	28	ASN
2	E	35	TRP
2	E	37	ILE
2	E	42	CYS
2	E	47	ASN
2	E	49	ILE
2	E	55	GLU
2	E	59	ASN
2	E	74	VAL
2	E	86	ARG
2	E	90	THR
2	E	91	ARG
2	E	93	VAL
2	E	98	ASN
2	E	99	ARG
2	E	104	GLN
2	E	105	LYS
2	D	25	LYS
2	D	28	ASN
2	D	35	TRP
2	D	37	ILE
2	D	39	VAL
2	D	40	ASP
2	D	42	CYS
2	D	46	ARG
2	D	47	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	49	ILE
2	D	50	MET
2	D	66	GLU
2	D	84	ILE
2	D	89	LYS
2	D	91	ARG
2	D	92	GLN
2	D	93	VAL
2	D	98	ASN
2	D	99	ARG
2	D	100	GLU
2	D	101	TRP
2	D	103	PHE
2	D	105	LYS
2	D	108	HIS
2	R	25	LYS
2	R	28	ASN
2	R	35	TRP
2	R	37	ILE
2	R	42	CYS
2	R	47	ASN
2	R	49	ILE
2	R	52	LEU
2	R	59	ASN
2	R	74	VAL
2	R	86	ARG
2	R	91	ARG
2	R	93	VAL
2	R	98	ASN
2	R	99	ARG
2	R	102	GLU
2	R	104	GLN
2	Q	25	LYS
2	Q	28	ASN
2	Q	35	TRP
2	Q	37	ILE
2	Q	39	VAL
2	Q	40	ASP
2	Q	42	CYS
2	Q	46	ARG
2	Q	47	ASN
2	Q	49	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	50	MET
2	Q	59	ASN
2	Q	66	GLU
2	Q	74	VAL
2	Q	84	ILE
2	Q	87	TRP
2	Q	89	LYS
2	Q	90	THR
2	Q	91	ARG
2	Q	92	GLN
2	Q	93	VAL
2	Q	96	LEU
2	Q	98	ASN
2	Q	99	ARG
2	Q	100	GLU
2	Q	102	GLU
2	Q	105	LYS
2	Q	106	TYR
2	Q	108	HIS
3	A	7	ARG
3	A	8	GLN
3	A	9	ILE
3	A	12	GLU
3	A	37	VAL
3	A	53	SER
3	A	54	SER
3	A	128	ILE
3	A	131	GLU
3	A	133	CYS
3	A	241	ASP
3	A	243	SER
3	A	253	MET
3	A	263	MET
3	A	270	ILE
3	A	275	SER
3	A	277	GLU
3	A	278	ASN
3	A	280	CYS
3	A	281	SER
3	A	282	LEU
3	A	283	TYR
3	A	286	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	291	GLN
3	A	297	LYS
3	A	298	LEU
3	A	300	SER
3	A	305	LEU
3	A	307	LYS
3	A	308	VAL
3	A	310	THR
3	A	311	VAL
3	A	312	VAL
3	A	313	THR
3	A	315	ASP
3	A	317	ASP
3	A	318	ILE
3	A	320	ILE
3	A	325	VAL
3	A	328	LYS
3	A	344	PHE
3	A	353	PHE
3	A	357	GLN
3	A	363	LYS
3	A	367	LEU
3	A	370	ARG
3	A	371	ILE
3	A	372	LYS
3	A	375	LEU
3	A	376	VAL
3	A	377	CYS
3	A	378	CYS
3	A	381	TYR
3	A	388	ASP
3	A	389	SER
3	A	393	GLU
3	A	394	LEU
3	A	396	ARG
3	A	397	ARG
3	A	398	THR
3	A	401	ARG
3	A	404	THR
3	A	406	LYS
3	A	410	THR
3	A	411	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	412	VAL
3	A	417	CYS
3	A	426	VAL
3	A	427	VAL
3	A	431	ILE
3	A	436	LEU
3	A	445	ARG
3	A	446	SER
3	A	447	ASP
3	A	451	GLU
3	A	452	MET
3	A	454	MET
3	A	455	ARG
3	A	456	GLN
3	A	457	THR
3	A	458	SER
3	A	459	ARG
3	A	470	LYS
3	A	471	ILE
3	A	474	ILE
3	A	477	LEU
3	A	497	VAL
3	A	499	VAL
3	A	501	ILE
3	A	505	ASN
3	A	506	LYS
3	A	509	TRP
3	A	510	LYS
3	A	514	ASN
3	A	515	ILE
3	A	525	VAL
3	A	534	LEU
3	A	538	MET
3	A	539	ARG
3	A	540	GLU
3	A	541	THR
3	A	543	LEU
3	A	548	LYS
3	A	551	THR
3	A	557	GLU
3	A	559	ASP
3	A	560	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	562	SER
3	A	563	LEU
3	A	567	ILE
3	A	571	VAL
3	A	572	LEU
3	A	574	ASP
3	A	575	LEU
3	A	578	ASP
3	A	580	ARG
3	A	582	THR
3	A	583	VAL
3	A	586	LEU
3	A	589	SER
3	A	591	LEU
3	A	592	GLU
3	A	594	SER
3	A	602	LEU
3	A	603	PHE
3	A	604	SER
3	A	605	THR
4	G	433	GLN
4	G	434	ASP
4	G	436	VAL
4	G	437	VAL
4	G	438	LYS
4	G	440	ASP
4	G	453	ASN
4	G	454	THR
4	G	457	GLN
4	G	467	TYR
4	G	476	GLU
4	G	477	ILE
4	G	479	MET
4	G	480	LYS
4	G	481	ARG
4	G	507	GLU
4	G	515	GLU
4	G	521	ILE
4	G	524	ILE
4	G	525	MET
4	G	526	HIS
4	G	547	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	561	LYS
4	G	562	ARG
4	G	566	ILE
4	G	581	LEU
4	G	598	LEU
4	G	600	ASN
3	B	7	ARG
3	B	8	GLN
3	B	9	ILE
3	B	19	GLU
3	B	29	LEU
3	B	37	VAL
3	B	61	MET
3	B	93	ASN
3	B	96	MET
3	B	114	GLU
3	B	127	LYS
3	B	133	CYS
3	B	134	VAL
3	B	203	GLU
3	B	243	SER
3	B	249	LEU
3	B	251	LYS
3	B	253	MET
3	B	275	SER
3	B	277	GLU
3	B	278	ASN
3	B	280	CYS
3	B	282	LEU
3	B	291	GLN
3	B	305	LEU
3	B	328	LYS
3	B	363	LYS
3	B	374	SER
3	B	394	LEU
3	B	397	ARG
3	B	408	GLU
3	B	568	SER
3	B	571	VAL
3	B	572	LEU
3	B	597	LYS
4	H	453	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	454	THR
4	H	457	GLN
4	H	467	TYR
4	H	476	GLU
4	H	477	ILE
4	H	478	GLN
4	H	480	LYS
4	H	481	ARG
4	H	507	GLU
4	H	515	GLU
4	H	521	ILE
4	H	524	ILE
4	H	525	MET
4	H	526	HIS
4	H	547	GLU
4	H	561	LYS
4	H	562	ARG
4	H	566	ILE
4	I	453	ASN
4	I	454	THR
4	I	457	GLN
4	I	467	TYR
4	I	476	GLU
4	I	477	ILE
4	I	478	GLN
4	I	480	LYS
4	I	481	ARG
4	I	507	GLU
4	I	515	GLU
4	I	525	MET
4	I	547	GLU
4	I	561	LYS
4	I	562	ARG
4	I	566	ILE
4	I	592	LYS
4	I	593	LYS
4	I	598	LEU
3	N	7	ARG
3	N	8	GLN
3	N	11	THR
3	N	12	GLU
3	N	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	37	VAL
3	N	114	GLU
3	N	127	LYS
3	N	128	ILE
3	N	133	CYS
3	N	134	VAL
3	N	203	GLU
3	N	243	SER
3	N	249	LEU
3	N	251	LYS
3	N	253	MET
3	N	277	GLU
3	N	278	ASN
3	N	280	CYS
3	N	282	LEU
3	N	291	GLN
3	N	305	LEU
3	N	328	LYS
3	N	363	LYS
3	N	374	SER
3	N	394	LEU
3	N	397	ARG
3	N	406	LYS
3	N	408	GLU
3	N	571	VAL
3	N	572	LEU
3	N	592	GLU
3	N	593	GLU
3	N	597	LYS
4	J	453	ASN
4	J	454	THR
4	J	457	GLN
4	J	467	TYR
4	J	476	GLU
4	J	477	ILE
4	J	478	GLN
4	J	479	MET
4	J	480	LYS
4	J	481	ARG
4	J	507	GLU
4	J	515	GLU
4	J	521	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	J	524	ILE
4	J	525	MET
4	J	526	HIS
4	J	547	GLU
4	J	561	LYS
4	J	562	ARG
4	J	566	ILE
3	P	8	GLN
3	P	11	THR
3	P	37	VAL
3	P	96	MET
3	P	127	LYS
3	P	128	ILE
3	P	131	GLU
3	P	133	CYS
3	P	134	VAL
3	P	243	SER
3	P	249	LEU
3	P	253	MET
3	P	263	MET
3	P	265	LYS
3	P	277	GLU
3	P	282	LEU
3	P	291	GLN
3	P	324	GLN
3	P	346	THR
3	P	390	VAL
3	P	396	ARG
3	P	406	LYS
3	P	407	ASP
3	P	408	GLU
3	P	540	GLU
3	P	567	ILE
3	P	568	SER
3	P	570	ARG
3	P	571	VAL
3	P	572	LEU
3	P	589	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	99	ASN
1	C	106	ASN
1	C	110	ASN
1	C	112	HIS
1	C	163	GLN
1	C	218	GLN
1	C	222	GLN
1	C	228	ASN
1	C	281	ASN
1	C	308	ASN
1	C	324	GLN
1	C	343	GLN
1	C	381	ASN
1	C	465	GLN
1	C	560	ASN
1	C	606	ASN
1	C	618	GLN
1	C	641	GLN
1	C	657	HIS
1	F	69	HIS
1	F	87	ASN
1	F	106	ASN
1	F	110	ASN
1	F	112	HIS
1	F	150	GLN
1	F	163	GLN
1	F	218	GLN
1	F	228	ASN
1	F	281	ASN
1	F	308	ASN
1	F	324	GLN
1	F	523	ASN
1	F	553	HIS
1	F	606	ASN
1	F	618	GLN
1	F	641	GLN
1	F	657	HIS
1	F	718	GLN
1	F	719	HIS
1	M	84	HIS
1	M	87	ASN
1	M	98	ASN
1	M	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	103	GLN
1	M	110	ASN
1	M	112	HIS
1	M	150	GLN
1	M	160	HIS
1	M	163	GLN
1	M	218	GLN
1	M	222	GLN
1	M	228	ASN
1	M	281	ASN
1	M	308	ASN
1	M	324	GLN
1	M	343	GLN
1	M	423	GLN
1	M	523	ASN
1	M	560	ASN
1	M	606	ASN
1	M	618	GLN
1	M	641	GLN
1	M	657	HIS
1	M	719	HIS
1	O	69	HIS
1	O	87	ASN
1	O	106	ASN
1	O	110	ASN
1	O	112	HIS
1	O	150	GLN
1	O	163	GLN
1	O	218	GLN
1	O	222	GLN
1	O	228	ASN
1	O	281	ASN
1	O	308	ASN
1	O	324	GLN
1	O	343	GLN
1	O	381	ASN
1	O	423	GLN
1	O	606	ASN
1	O	618	GLN
1	O	641	GLN
1	O	657	HIS
1	O	718	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	719	HIS
2	E	28	ASN
2	E	41	ASN
2	E	59	ASN
2	E	60	GLN
2	E	98	ASN
2	E	104	GLN
2	D	28	ASN
2	D	98	ASN
2	R	28	ASN
2	R	41	ASN
2	R	57	GLN
2	R	60	GLN
2	R	98	ASN
2	R	104	GLN
2	Q	28	ASN
2	Q	98	ASN
3	A	71	HIS
3	A	185	ASN
3	A	187	ASN
3	A	230	GLN
3	A	316	ASN
3	A	357	GLN
3	A	437	ASN
3	A	514	ASN
3	A	542	HIS
4	G	450	HIS
4	G	453	ASN
4	G	455	GLN
4	G	564	ASN
4	G	572	GLN
4	G	595	ASN
3	B	20	GLN
3	B	76	ASN
3	B	166	GLN
3	B	230	GLN
3	B	356	GLN
3	B	357	GLN
4	H	453	ASN
4	H	457	GLN
4	H	564	ASN
4	H	572	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	453	ASN
4	I	455	GLN
4	I	564	ASN
4	I	572	GLN
4	I	591	GLN
4	I	595	ASN
3	N	71	HIS
3	N	76	ASN
3	N	93	ASN
3	N	112	GLN
3	N	166	GLN
3	N	230	GLN
3	N	278	ASN
3	N	356	GLN
3	N	357	GLN
4	J	450	HIS
4	J	453	ASN
4	J	455	GLN
4	J	457	GLN
4	J	564	ASN
4	J	572	GLN
3	P	71	HIS
3	P	93	ASN
3	P	185	ASN
3	P	230	GLN
3	P	278	ASN
3	P	306	HIS
3	P	356	GLN
3	P	357	GLN
3	P	566	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34453. 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](#)

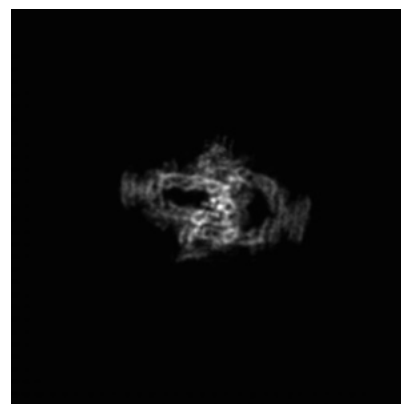
6.1.1 Primary map



X

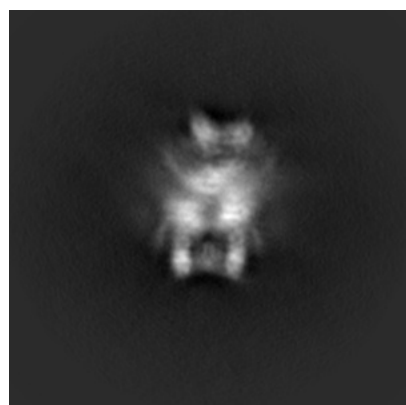


Y

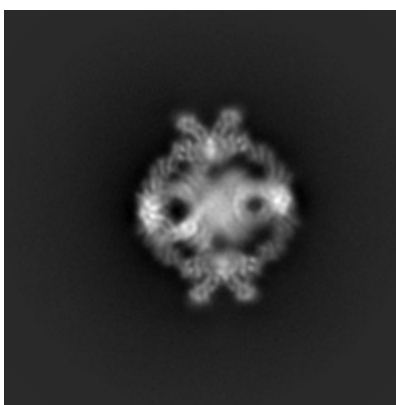


Z

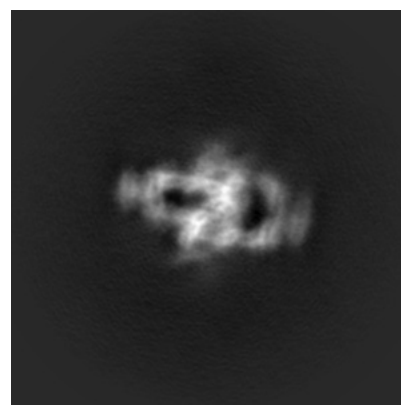
6.1.2 Raw map



X



Y



Z

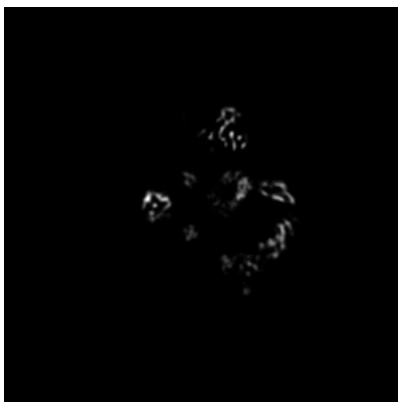
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 96

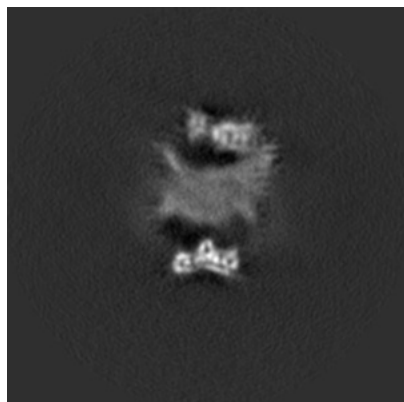


Y Index: 96

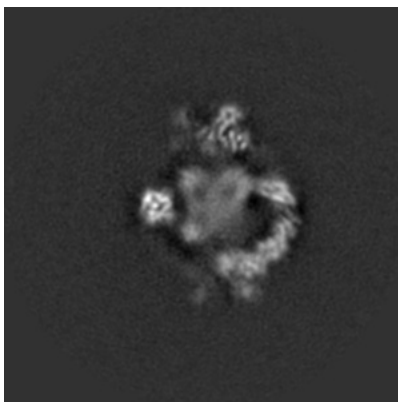


Z Index: 96

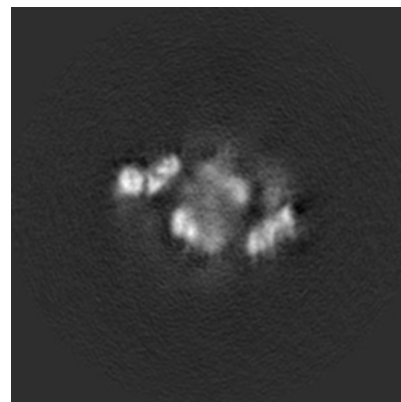
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

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

6.3 Largest variance slices [i](#)

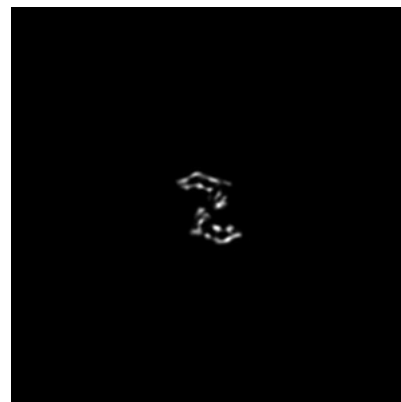
6.3.1 Primary map



X Index: 102

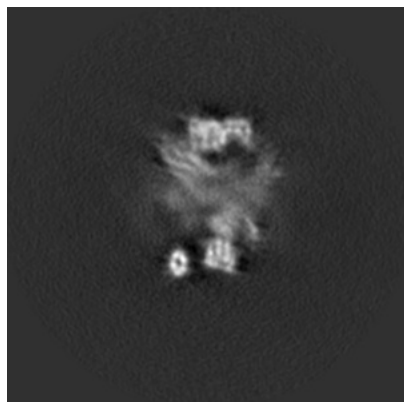


Y Index: 106

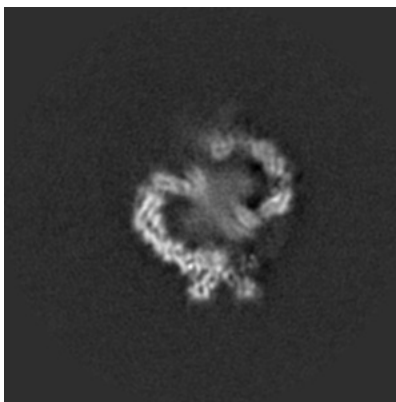


Z Index: 68

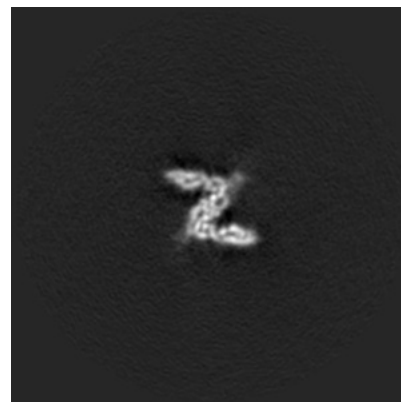
6.3.2 Raw map



X Index: 102



Y Index: 108

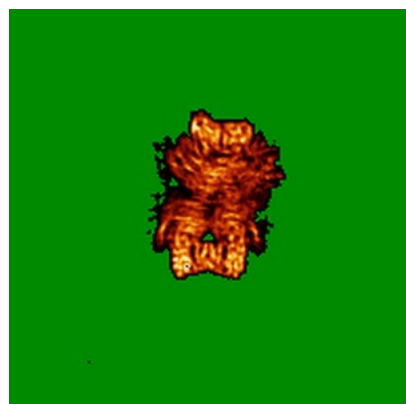


Z Index: 71

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

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

6.4.1 Primary map



X



Y

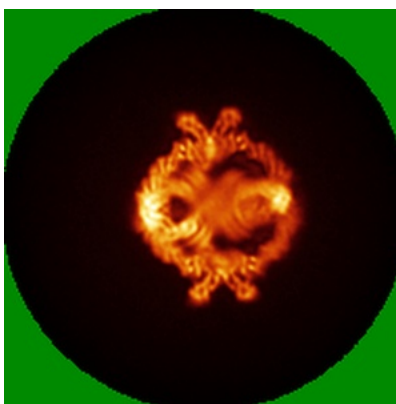


Z

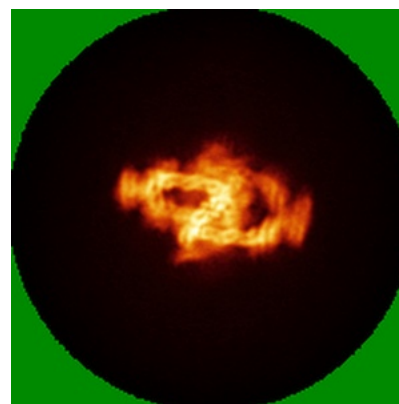
6.4.2 Raw map



X



Y

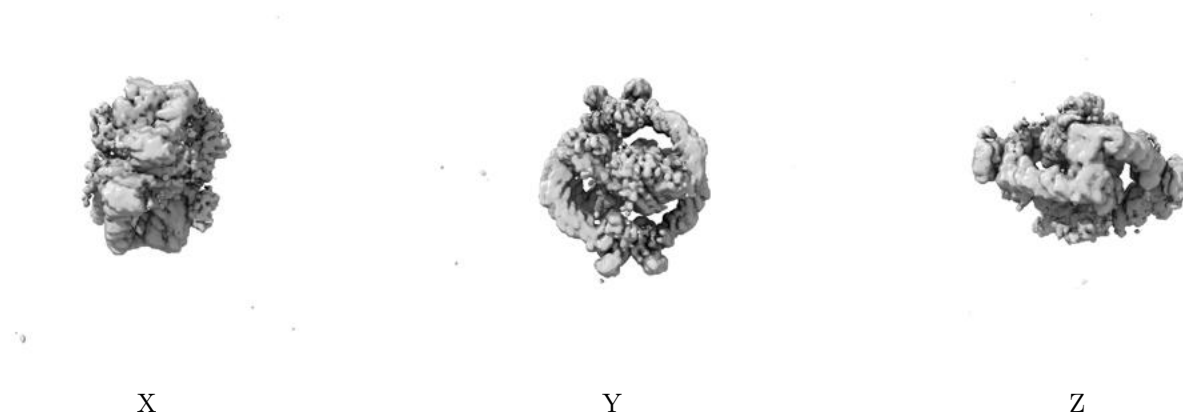


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. 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



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.

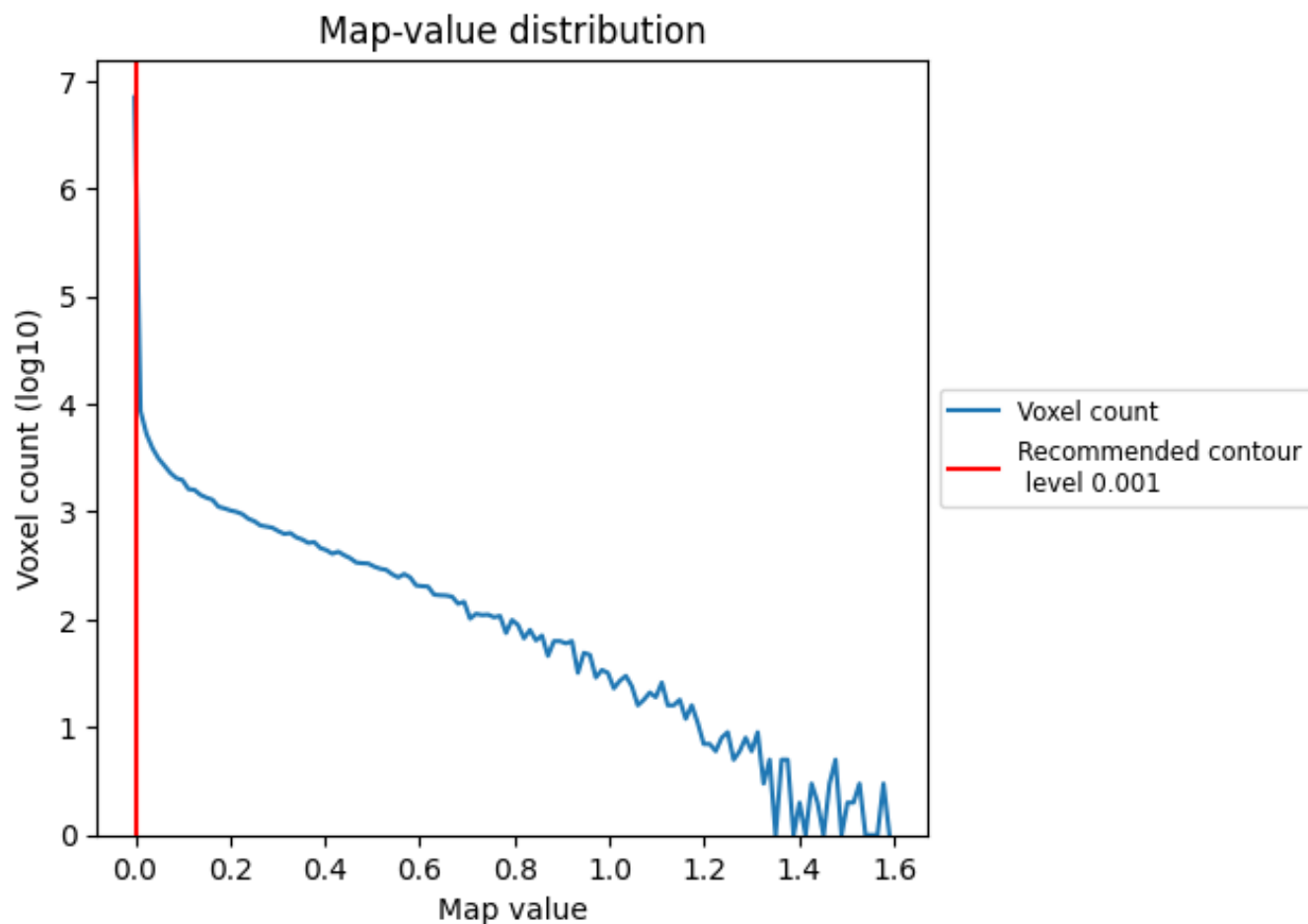
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

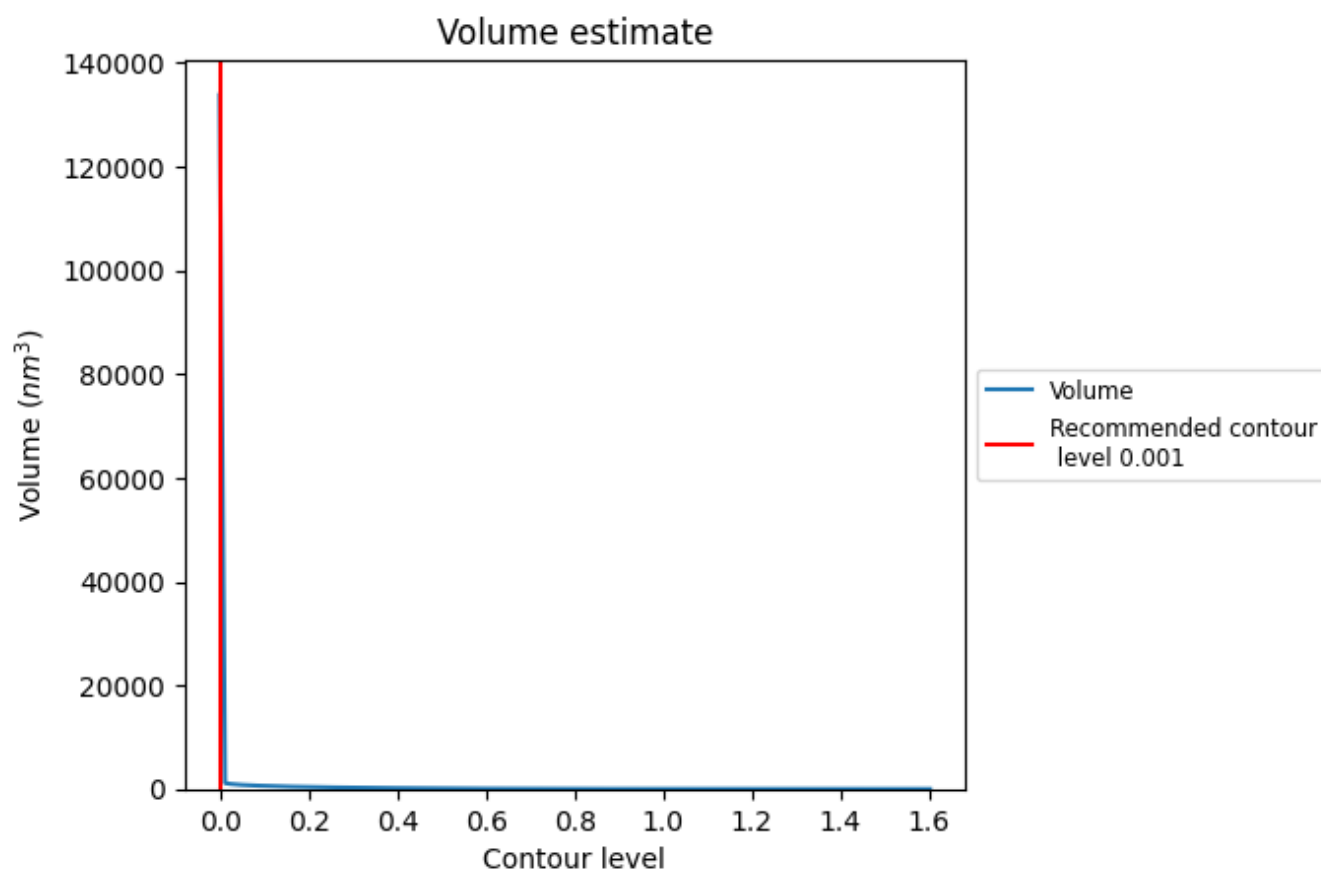
This section contains the results of statistical analysis of the map.

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.

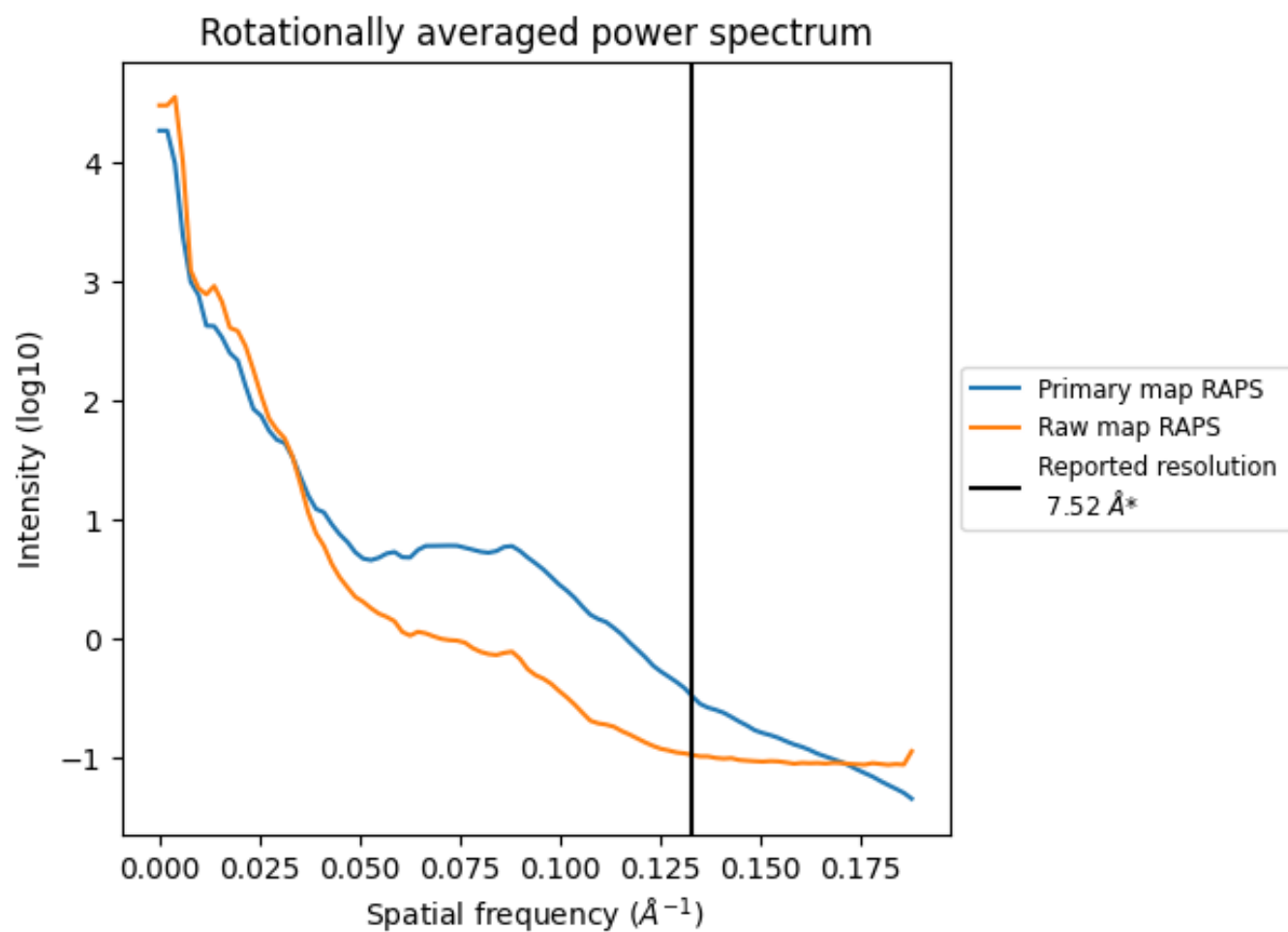
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108428 nm^3 ; this corresponds to an approximate mass of 97946 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 ⓘ

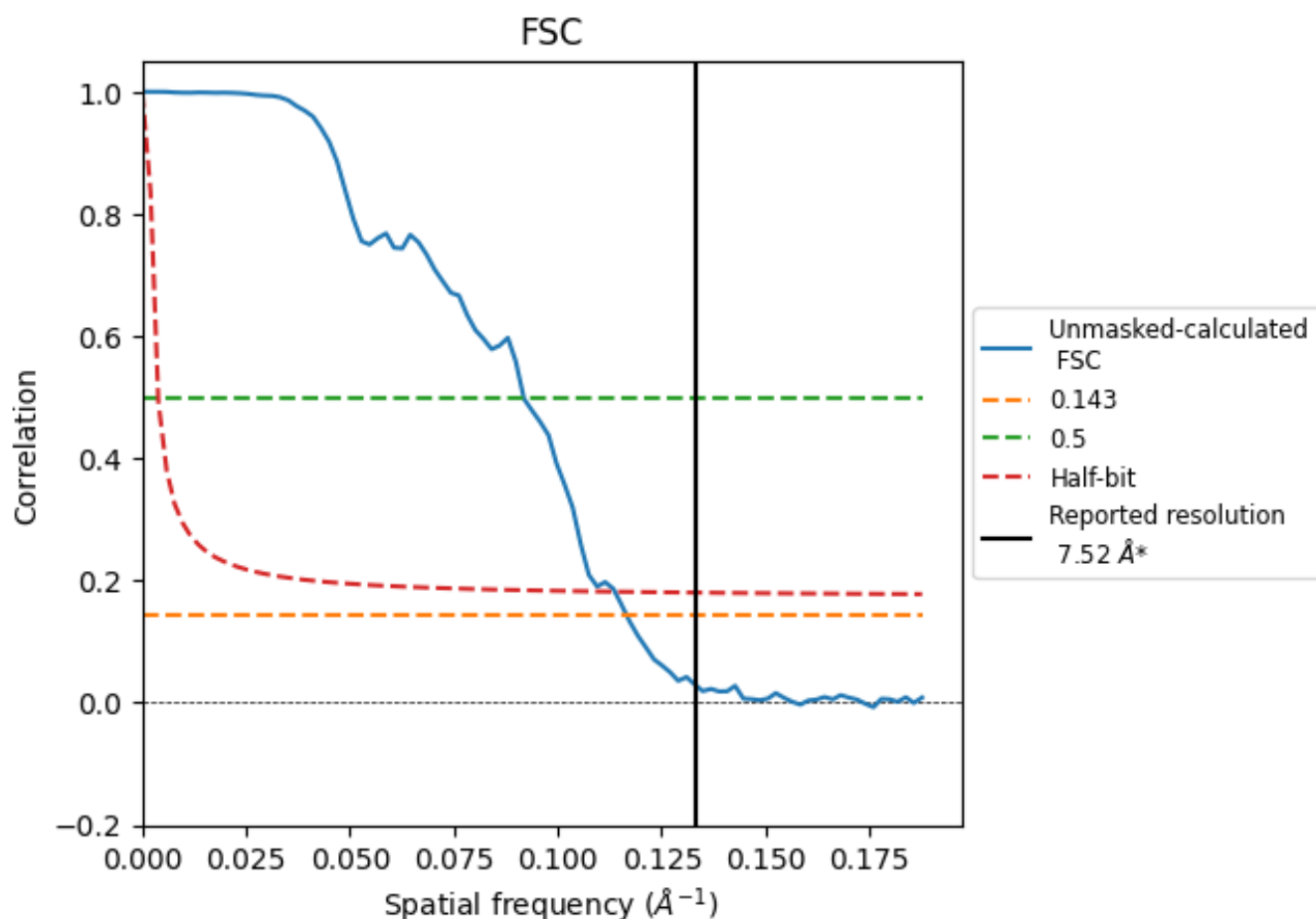


*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

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 0.133 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

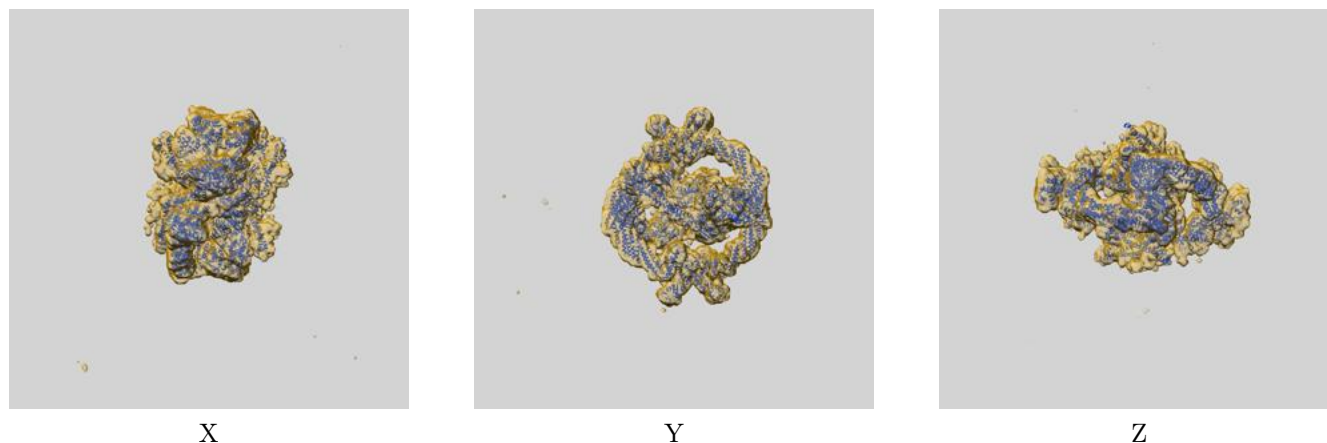
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.58	10.89	8.79

*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 8.58 differs from the reported value 7.52 by more than 10 %

9 Map-model fit [i](#)

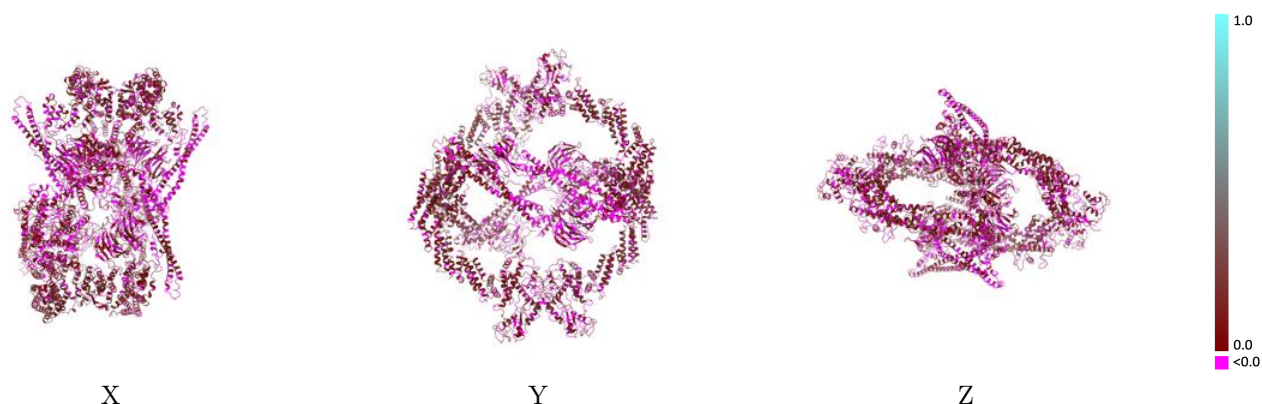
This section contains information regarding the fit between EMDB map EMD-34453 and PDB model 8H37. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



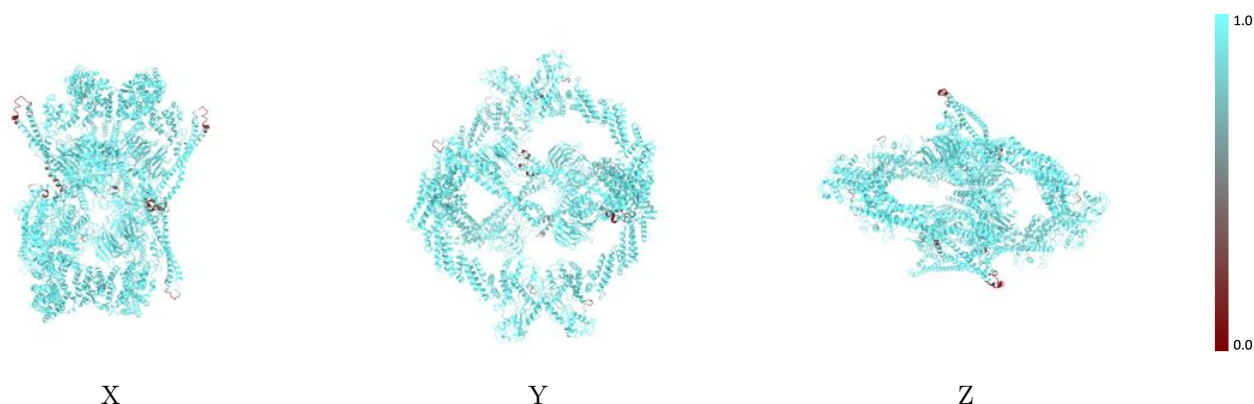
The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



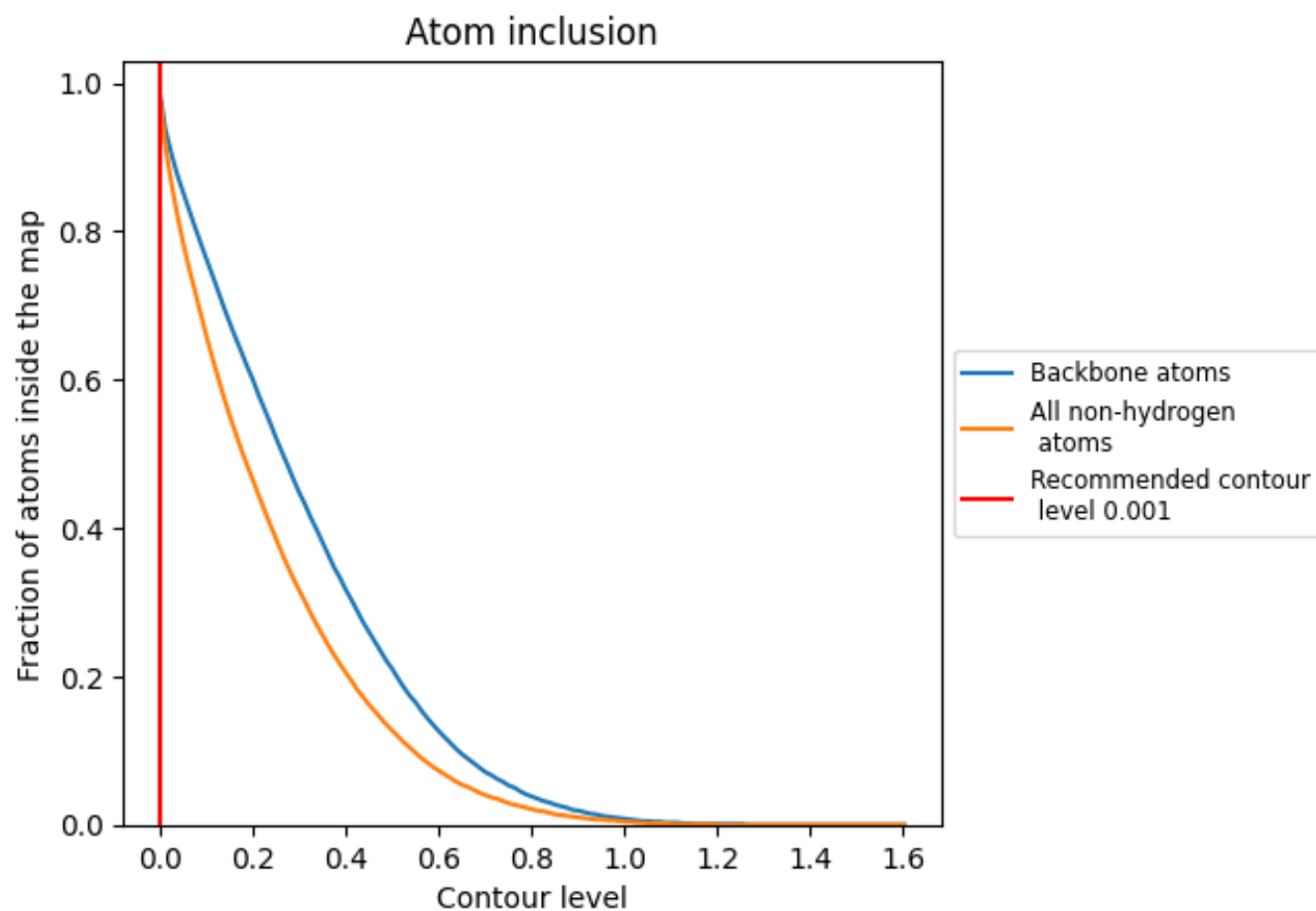
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.001).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9740	 0.0570
A	 0.9950	 0.0600
B	 0.9880	 0.0440
C	 0.9930	 0.1050
D	 0.9200	 0.0200
E	 0.9710	 0.0270
F	 0.9950	 0.0940
G	 0.9610	 0.0420
H	 0.9320	 0.0330
I	 0.7700	 -0.0150
J	 0.8140	 -0.0430
M	 0.9860	 0.0840
N	 0.9800	 0.0250
O	 0.9870	 0.0720
P	 0.9890	 0.0280
Q	 0.9810	 0.0150
R	 0.9490	 -0.0020

