



Full wwPDB EM Validation Report ⓘ

Aug 13, 2026 – 01:39 pm BST

PDB ID : 9SO9 / pdb_00009so9
EMDB ID : EMD-55053
Title : BRCA1-A complex bound to K63-oligoUbATA - closed form StateC*
Authors : Murachelli, A.G.; Sixma, T.K.
Deposited on : 2025-09-12
Resolution : 3.40 Å (reported)
Based on initial models : 1ubq, 6gvw

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

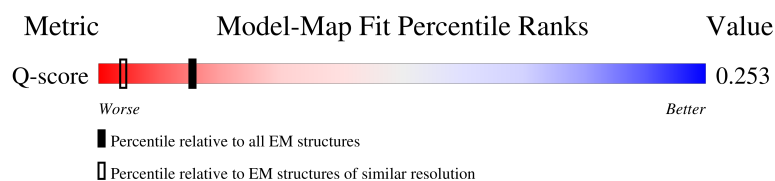
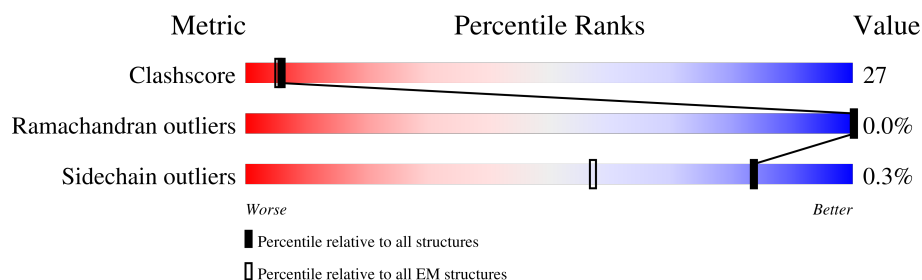
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

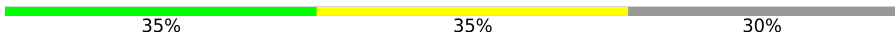
The reported resolution of this entry is 3.40 Å.

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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	409	
1	F	409	
2	B	316	
2	G	316	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	383	61% 38% ..
3	H	383	56% 44% .
4	D	349	31% 36% 32%
4	I	349	49% 19% 32% .
5	E	171	20% 13% 66%
5	J	171	18% 16% 66%
6	L	76	55% 43% .
7	M	76	67% 28% 5%
8	N	76	50% 47% .

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21051 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 BRCA1-A complex subunit Abraxas 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	285	Total	C	N	O	S	0	0
			2293	1451	400	430	12		
1	F	245	Total	C	N	O	S	0	0
			1970	1248	342	372	8		

- Molecule 2 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	260	Total	C	N	O	S	0	0
			2088	1306	371	397	14		
2	G	258	Total	C	N	O	S	0	0
			2069	1296	368	391	14		

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	380	Total	C	N	O	S	0	0
			3056	1979	500	563	14		
3	H	383	Total	C	N	O	S	0	0
			3078	1993	504	567	14		

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	237	Total	C	N	O	S	0	0
			1889	1206	306	359	18		
4	I	239	Total	C	N	O	S	0	0
			1901	1214	308	361	18		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q9NWV8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	ALA	-	expression tag	UNP Q9NWX8
D	-17	HIS	-	expression tag	UNP Q9NWX8
D	-16	HIS	-	expression tag	UNP Q9NWX8
D	-15	HIS	-	expression tag	UNP Q9NWX8
D	-14	HIS	-	expression tag	UNP Q9NWX8
D	-13	HIS	-	expression tag	UNP Q9NWX8
D	-12	HIS	-	expression tag	UNP Q9NWX8
D	-11	SER	-	expression tag	UNP Q9NWX8
D	-10	ALA	-	expression tag	UNP Q9NWX8
D	-9	ALA	-	expression tag	UNP Q9NWX8
D	-8	LEU	-	expression tag	UNP Q9NWX8
D	-7	GLU	-	expression tag	UNP Q9NWX8
D	-6	VAL	-	expression tag	UNP Q9NWX8
D	-5	LEU	-	expression tag	UNP Q9NWX8
D	-4	PHE	-	expression tag	UNP Q9NWX8
D	-3	GLN	-	expression tag	UNP Q9NWX8
D	-2	GLY	-	expression tag	UNP Q9NWX8
D	-1	PRO	-	expression tag	UNP Q9NWX8
D	0	GLY	-	expression tag	UNP Q9NWX8
I	-19	MET	-	initiating methionine	UNP Q9NWX8
I	-18	ALA	-	expression tag	UNP Q9NWX8
I	-17	HIS	-	expression tag	UNP Q9NWX8
I	-16	HIS	-	expression tag	UNP Q9NWX8
I	-15	HIS	-	expression tag	UNP Q9NWX8
I	-14	HIS	-	expression tag	UNP Q9NWX8
I	-13	HIS	-	expression tag	UNP Q9NWX8
I	-12	HIS	-	expression tag	UNP Q9NWX8
I	-11	SER	-	expression tag	UNP Q9NWX8
I	-10	ALA	-	expression tag	UNP Q9NWX8
I	-9	ALA	-	expression tag	UNP Q9NWX8
I	-8	LEU	-	expression tag	UNP Q9NWX8
I	-7	GLU	-	expression tag	UNP Q9NWX8
I	-6	VAL	-	expression tag	UNP Q9NWX8
I	-5	LEU	-	expression tag	UNP Q9NWX8
I	-4	PHE	-	expression tag	UNP Q9NWX8
I	-3	GLN	-	expression tag	UNP Q9NWX8
I	-2	GLY	-	expression tag	UNP Q9NWX8
I	-1	PRO	-	expression tag	UNP Q9NWX8
I	0	GLY	-	expression tag	UNP Q9NWX8

- Molecule 5 is a protein called BRCA1-A complex subunit RAP80.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	58	Total 466	C 305	N 78	O 80	S 3	0	0
5	J	58	Total 466	C 305	N 78	O 80	S 3	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	243	MET	-	initiating methionine	UNP Q96RL1
E	244	ALA	-	expression tag	UNP Q96RL1
E	245	SER	-	expression tag	UNP Q96RL1
E	246	TRP	-	expression tag	UNP Q96RL1
E	247	SER	-	expression tag	UNP Q96RL1
E	248	HIS	-	expression tag	UNP Q96RL1
E	249	PRO	-	expression tag	UNP Q96RL1
E	250	GLN	-	expression tag	UNP Q96RL1
E	251	PHE	-	expression tag	UNP Q96RL1
E	252	GLU	-	expression tag	UNP Q96RL1
E	253	LYS	-	expression tag	UNP Q96RL1
E	254	GLY	-	expression tag	UNP Q96RL1
E	255	ALA	-	expression tag	UNP Q96RL1
E	256	LEU	-	expression tag	UNP Q96RL1
E	257	GLU	-	expression tag	UNP Q96RL1
E	258	VAL	-	expression tag	UNP Q96RL1
E	259	LEU	-	expression tag	UNP Q96RL1
E	260	PHE	-	expression tag	UNP Q96RL1
E	261	GLN	-	expression tag	UNP Q96RL1
E	262	GLY	-	expression tag	UNP Q96RL1
E	263	PRO	-	expression tag	UNP Q96RL1
E	264	GLY	-	expression tag	UNP Q96RL1
J	243	MET	-	initiating methionine	UNP Q96RL1
J	244	ALA	-	expression tag	UNP Q96RL1
J	245	SER	-	expression tag	UNP Q96RL1
J	246	TRP	-	expression tag	UNP Q96RL1
J	247	SER	-	expression tag	UNP Q96RL1
J	248	HIS	-	expression tag	UNP Q96RL1
J	249	PRO	-	expression tag	UNP Q96RL1
J	250	GLN	-	expression tag	UNP Q96RL1
J	251	PHE	-	expression tag	UNP Q96RL1
J	252	GLU	-	expression tag	UNP Q96RL1
J	253	LYS	-	expression tag	UNP Q96RL1
J	254	GLY	-	expression tag	UNP Q96RL1
J	255	ALA	-	expression tag	UNP Q96RL1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	256	LEU	-	expression tag	UNP Q96RL1
J	257	GLU	-	expression tag	UNP Q96RL1
J	258	VAL	-	expression tag	UNP Q96RL1
J	259	LEU	-	expression tag	UNP Q96RL1
J	260	PHE	-	expression tag	UNP Q96RL1
J	261	GLN	-	expression tag	UNP Q96RL1
J	262	GLY	-	expression tag	UNP Q96RL1
J	263	PRO	-	expression tag	UNP Q96RL1
J	264	GLY	-	expression tag	UNP Q96RL1

- Molecule 6 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	75	Total	C	N	O	S	0	0
			597	376	104	116	1		

- Molecule 7 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	72	Total	C	N	O	S	0	0
			572	360	98	113	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	63A	DAB	LYS	engineered mutation	UNP P0CG48

- Molecule 8 is a protein called Polyubiquitin-C.

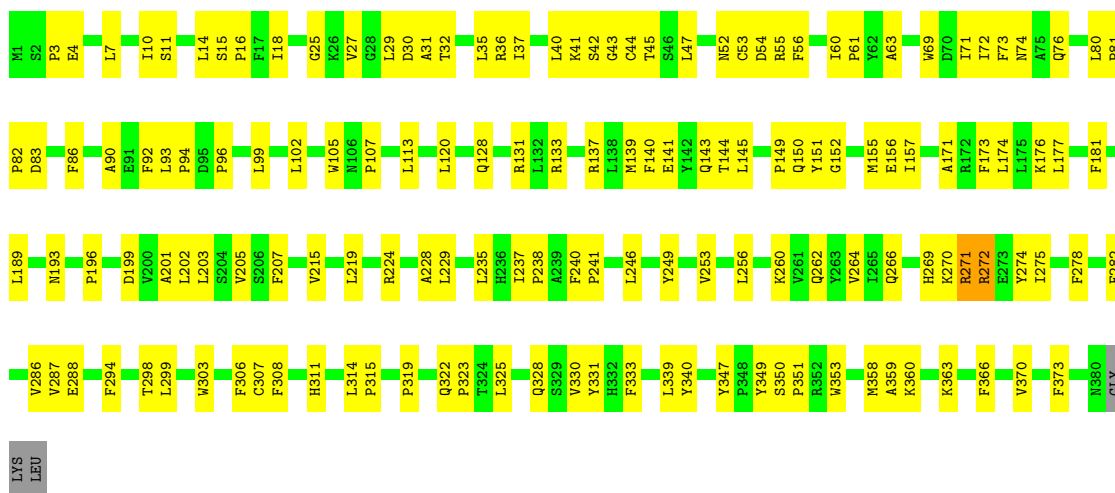
Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	76	Total	C	N	O	S	0	0
			604	380	105	117	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	77	A1JPL	GLY	engineered mutation	UNP P0CG48

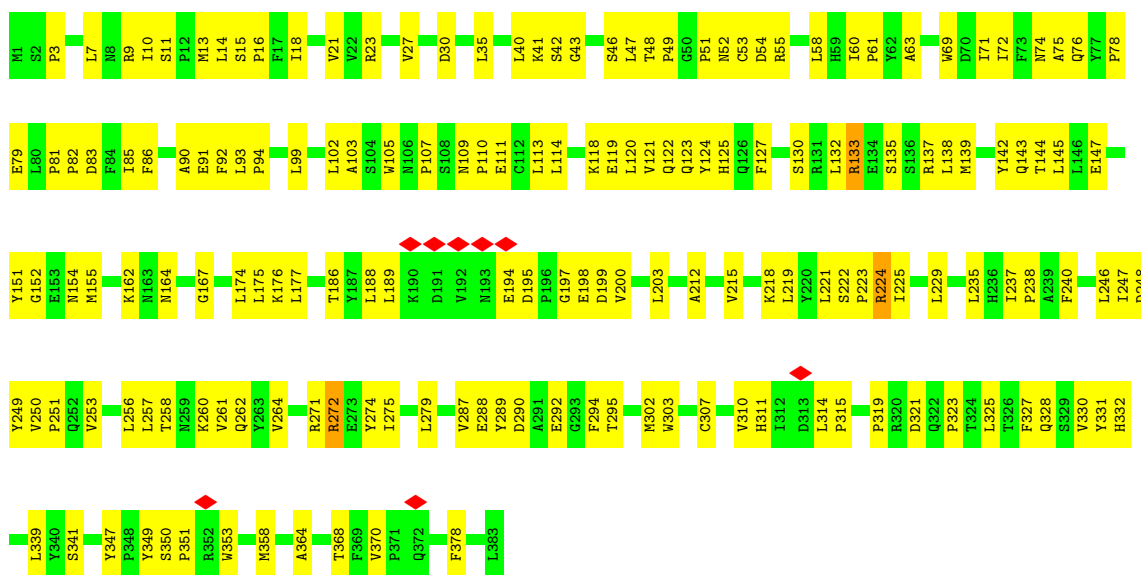
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	B	1	Total 1	Zn 1	0
9	G	1	Total 1	Zn 1	0



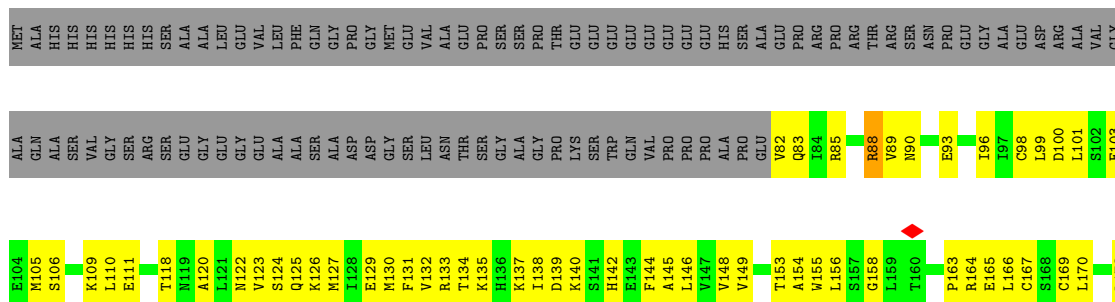
• Molecule 3: BRISC and BRCA1-A complex member 2

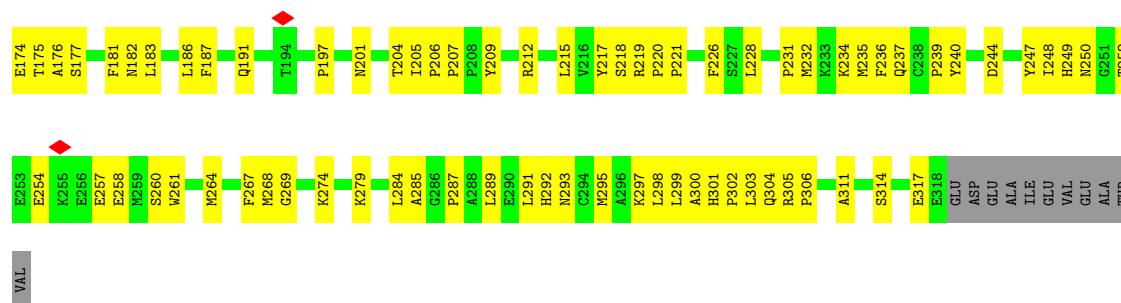
Chain H: 56% 44%



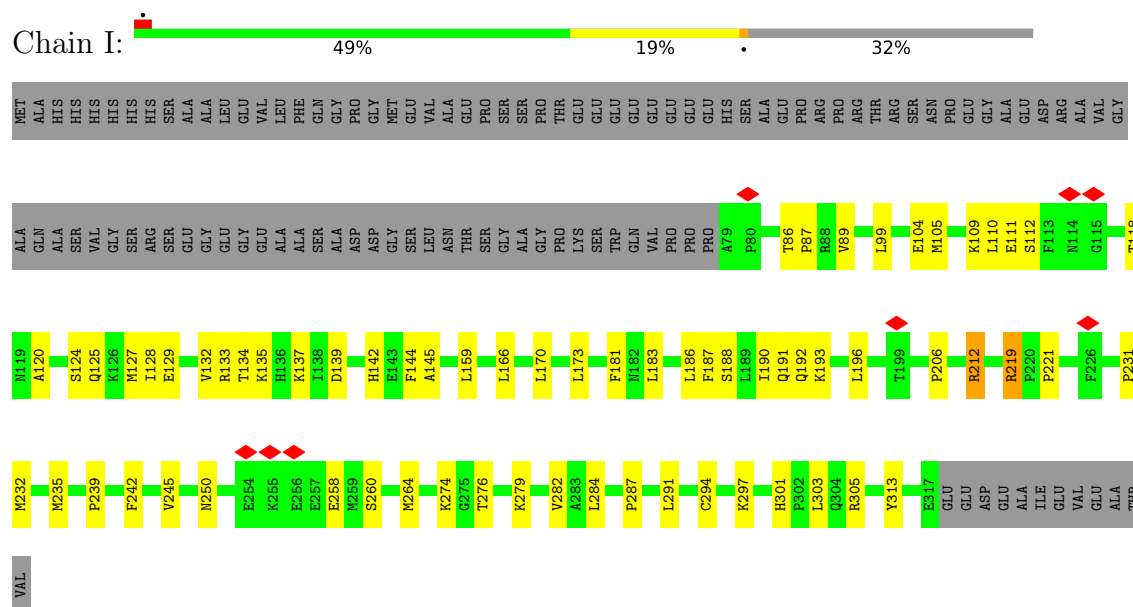
• Molecule 4: BRISC and BRCA1-A complex member 1

Chain D: 31% 36% 32%

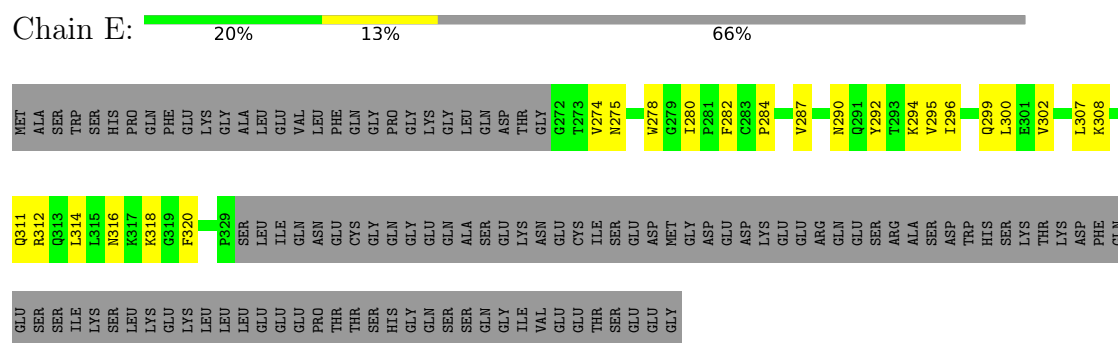




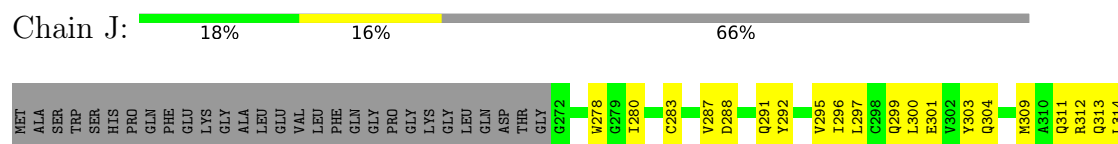
• Molecule 4: BRISC and BRCA1-A complex member 1

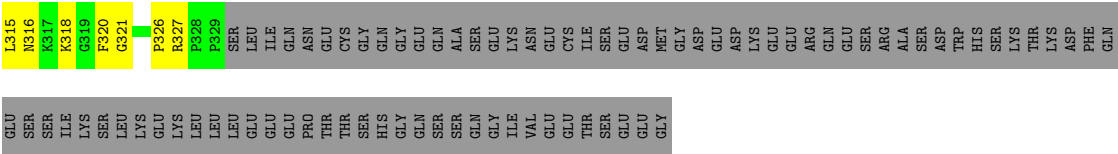


• Molecule 5: BRCA1-A complex subunit RAP80



• Molecule 5: BRCA1-A complex subunit RAP80





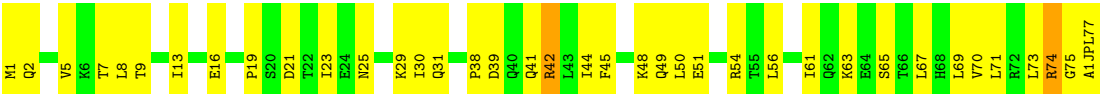
• Molecule 6: Ubiquitin



• Molecule 7: Polyubiquitin-C



• Molecule 8: Polyubiquitin-C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74906	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.694	Depositor
Minimum map value	-0.335	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	436.30078, 436.30078, 436.30078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1362, 1.1362, 1.1362	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: DAB, ZN, A1JPL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/2334	0.73	0/3133
1	F	0.60	0/2004	0.89	0/2691
2	B	0.63	0/2124	0.84	0/2869
2	G	0.54	0/2105	0.74	0/2845
3	C	0.38	0/3147	0.66	0/4283
3	H	0.32	0/3169	0.62	0/4310
4	D	0.19	0/1934	0.51	0/2623
4	I	0.15	0/1947	0.42	0/2642
5	E	0.27	0/480	0.57	0/652
5	J	0.23	0/480	0.55	0/652
6	L	0.31	0/603	0.58	0/811
7	M	0.28	0/570	0.61	0/767
8	N	0.46	0/603	0.77	0/811
All	All	0.43	0/21500	0.68	0/29089

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	F	0	1
2	B	0	2
3	C	0	2
3	H	0	4
4	D	0	2
4	I	0	2
8	N	0	2
All	All	0	17

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	A	193	ARG	Sidechain
2	B	137	ARG	Sidechain
2	B	211	ARG	Sidechain
3	C	271	ARG	Sidechain
3	C	272	ARG	Sidechain
4	D	85	ARG	Sidechain
4	D	88	ARG	Sidechain
1	F	113	ARG	Sidechain
3	H	133	ARG	Sidechain
3	H	224	ARG	Sidechain
3	H	272	ARG	Sidechain
3	H	9	ARG	Sidechain
4	I	212	ARG	Sidechain
4	I	219	ARG	Sidechain
8	N	42	ARG	Sidechain
8	N	74	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2293	0	2290	183	0
1	F	1970	0	1979	184	0
2	B	2088	0	2070	162	0
2	G	2069	0	2056	168	0
3	C	3056	0	2974	151	0
3	H	3078	0	3001	157	0
4	D	1889	0	1871	104	0
4	I	1901	0	1883	52	0
5	E	466	0	472	21	0
5	J	466	0	472	26	0
6	L	597	0	626	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	572	0	591	13	0
8	N	604	0	626	36	0
9	B	1	0	0	0	0
9	G	1	0	0	0	0
All	All	21051	0	20911	1115	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 27.

All (1115) 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:H:195:ASP:HB2	5:J:318:LYS:HB2	1.35	1.06
2:B:142:TYR:HE1	8:N:71:LEU:HB2	1.22	1.02
1:F:257:ARG:HH12	2:G:312:LEU:HG	1.27	0.96
1:F:104:ARG:HD2	1:F:137:PRO:HG2	1.51	0.92
2:B:172:CYS:HB2	2:B:216:ILE:HD12	1.52	0.91
1:A:203:PHE:HB3	1:A:209:LEU:HA	1.53	0.89
2:B:35:MET:HE3	2:B:92:ILE:HG13	1.56	0.88
1:F:77:SER:HB3	1:F:116:LEU:HD22	1.56	0.87
1:F:28:ASP:H	3:H:74:ASN:HD21	1.23	0.87
1:F:77:SER:H	1:F:113:ARG:HH21	1.20	0.85
2:G:276:MET:HA	2:G:280:SER:HB3	1.56	0.84
4:D:302:PRO:HA	4:D:305:ARG:HD3	1.60	0.83
1:A:76:SER:HA	1:A:113:ARG:HH22	1.43	0.82
3:H:238:PRO:HD2	3:H:253:VAL:HG22	1.61	0.82
2:B:142:TYR:CE1	8:N:71:LEU:HB2	2.13	0.82
2:G:80:LEU:HD22	2:G:96:GLN:HB3	1.62	0.82
1:A:214:LYS:HE3	1:F:201:LYS:HB3	1.61	0.81
2:B:116:ARG:HB2	8:N:9:THR:O	1.80	0.81
1:F:89:LEU:HD21	1:F:96:VAL:CG2	2.11	0.81
4:D:132:VAL:HG21	4:D:166:LEU:HD11	1.61	0.81
1:A:135:LEU:HG	1:A:151:HIS:HB3	1.63	0.80
4:D:204:THR:HA	5:E:278:TRP:HZ2	1.46	0.80
2:B:276:MET:O	2:B:281:GLY:HA3	1.82	0.80
8:N:7:THR:HA	8:N:69:LEU:HB3	1.61	0.80
2:G:122:HIS:CE1	2:G:153:ILE:HG12	2.17	0.79
1:F:88:ILE:HG13	1:F:89:LEU:HD12	1.63	0.79
2:B:153:ILE:HB	2:B:171:THR:O	1.82	0.79
2:B:153:ILE:HG21	2:B:171:THR:HG22	1.63	0.78
1:A:11:SER:HA	1:A:169:ALA:HB3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:MET:HE2	2:B:90:VAL:HG22	1.64	0.78
1:F:28:ASP:H	3:H:74:ASN:ND2	1.80	0.78
1:A:104:ARG:HD2	1:A:137:PRO:HG2	1.66	0.78
1:F:160:LEU:HD21	3:H:90:ALA:HB1	1.66	0.77
7:M:2:GLN:HG2	7:M:16:GLU:HG2	1.65	0.77
2:B:8:ALA:HB1	2:B:147:GLN:HB3	1.66	0.77
2:G:35:MET:HE3	2:G:90:VAL:HG13	1.64	0.77
3:C:287:VAL:HG13	4:D:300:ALA:HA	1.66	0.77
3:H:295:THR:HA	3:H:314:LEU:HD12	1.66	0.76
3:C:237:ILE:HD11	3:C:253:VAL:HG13	1.68	0.76
4:D:232:MET:HA	4:D:235:MET:HE2	1.68	0.76
1:A:26:ASP:HB2	3:C:76:GLN:HB2	1.67	0.76
4:I:89:VAL:HG11	4:I:206:PRO:HB3	1.68	0.75
1:F:85:LEU:HD12	1:F:89:LEU:HD13	1.69	0.75
3:C:315:PRO:HD3	3:C:323:PRO:HA	1.69	0.74
3:H:133:ARG:HA	3:H:139:MET:HG3	1.68	0.74
3:H:235:LEU:HD23	3:H:260:LYS:HD3	1.68	0.74
3:C:347:TYR:CZ	3:C:349:TYR:HB2	2.22	0.74
2:G:124:HIS:O	2:G:155:SER:HA	1.87	0.74
2:B:84:ASP:HB3	2:B:91:GLU:HB3	1.68	0.74
2:B:158:ILE:HG13	2:B:167:ARG:HG3	1.68	0.74
2:G:120:TRP:CH2	6:L:75:GLY:HA3	2.23	0.73
1:A:187:MET:HB2	2:G:285:GLN:HE21	1.53	0.73
8:N:2:GLN:HB3	8:N:16:GLU:HG2	1.71	0.73
3:C:274:TYR:HE2	3:C:358:MET:HG2	1.52	0.73
1:F:20:PHE:HB2	2:G:20:LEU:HD13	1.70	0.73
4:D:127:MET:HB3	4:D:295:MET:HG2	1.69	0.73
7:M:23:ILE:HB	7:M:52:ASP:HA	1.70	0.73
3:C:18:ILE:HD12	3:C:56:PHE:CE1	2.23	0.73
3:C:350:SER:HB3	3:C:353:TRP:CD2	2.23	0.73
2:B:29:THR:HG22	2:B:31:LYS:H	1.54	0.72
1:F:135:LEU:HD21	1:F:149:LEU:HD11	1.71	0.72
3:C:307:CYS:H	3:C:331:TYR:HE2	1.36	0.72
2:B:124:HIS:HE1	2:B:153:ILE:HG12	1.54	0.72
2:B:276:MET:HA	2:B:281:GLY:H	1.54	0.72
4:I:134:THR:HA	4:I:137:LYS:HD3	1.71	0.72
1:A:79:GLU:HA	1:A:120:ASN:HD22	1.53	0.72
4:D:105:MET:HA	4:D:120:ALA:HB3	1.70	0.72
8:N:23:ILE:HD12	8:N:54:ARG:O	1.90	0.72
3:H:86:PHE:HZ	3:H:120:LEU:HD22	1.55	0.72
1:F:105:HIS:CE1	1:F:139:ILE:H	2.07	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:149:VAL:HG22	4:D:186:LEU:HD11	1.73	0.71
1:A:104:ARG:HG2	3:C:43:GLY:HA2	1.73	0.71
2:B:301:LEU:O	2:B:305:LYS:HG2	1.91	0.70
1:F:156:PRO:HA	1:F:159:GLY:O	1.90	0.70
2:B:113:ARG:HB2	2:B:115:MET:HE2	1.73	0.70
1:F:103:ARG:HB2	1:F:136:THR:HG22	1.73	0.70
7:M:31:GLN:HB2	7:M:38:PRO:HG3	1.73	0.70
1:A:223:GLN:HA	1:A:226:LEU:HB2	1.72	0.70
1:F:36:GLU:HG3	1:F:38:LYS:NZ	2.07	0.70
2:G:246:ALA:O	2:G:250:ILE:HG12	1.91	0.70
2:B:124:HIS:ND1	2:B:153:ILE:HG23	2.07	0.69
2:G:34:VAL:HG22	2:G:123:SER:HB3	1.73	0.69
1:A:33:LEU:HD22	1:A:61:ILE:HG21	1.75	0.69
1:A:79:GLU:HA	1:A:120:ASN:ND2	2.08	0.69
1:F:77:SER:N	1:F:113:ARG:HH21	1.88	0.69
1:F:28:ASP:N	3:H:74:ASN:HD21	1.91	0.69
2:B:124:HIS:HE1	2:B:153:ILE:CG1	2.06	0.69
4:D:258:GLU:HA	4:D:261:TRP:CD1	2.27	0.69
2:B:41:GLU:HG2	2:B:75:HIS:HE1	1.56	0.69
8:N:8:LEU:HD22	8:N:70:VAL:HG13	1.73	0.69
2:B:101:SER:O	2:B:105:GLU:HG3	1.92	0.68
1:F:222:LEU:HD22	2:G:284:LEU:HD11	1.73	0.68
1:F:25:THR:HG22	1:F:27:SER:H	1.59	0.68
3:H:130:SER:HA	3:H:133:ARG:HH11	1.57	0.68
1:A:89:LEU:HD22	1:A:92:VAL:HG21	1.75	0.68
3:H:133:ARG:HA	3:H:139:MET:CG	2.22	0.68
3:H:133:ARG:HG2	3:H:139:MET:HE2	1.76	0.68
2:B:82:ARG:HE	2:B:85:LYS:HG2	1.58	0.68
4:I:181:PHE:HB3	4:I:221:PRO:HG3	1.75	0.68
3:C:155:MET:HE3	3:C:157:ILE:HD11	1.75	0.68
3:C:278:PHE:HE1	3:C:359:ALA:HA	1.58	0.68
1:F:110:MET:HE3	1:F:132:PHE:CD2	2.27	0.68
2:G:286:TRP:HE1	2:G:290:ARG:HH21	1.41	0.68
3:H:200:VAL:H	3:H:222:SER:HB2	1.58	0.67
1:A:303:ASN:HB3	1:A:305:HIS:HD2	1.59	0.67
1:F:59:ILE:HG23	1:F:97:VAL:HB	1.76	0.67
1:F:182:VAL:HG12	1:F:183:SER:N	2.08	0.67
2:B:267:VAL:HA	2:B:270:LYS:HE3	1.77	0.67
1:A:203:PHE:HA	1:A:210:LYS:N	2.10	0.67
2:B:124:HIS:CE1	2:B:153:ILE:HG23	2.30	0.67
2:B:155:SER:N	2:B:169:LEU:O	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:ASP:O	1:F:70:LEU:HD11	1.93	0.67
5:J:287:VAL:HB	5:J:291:GLN:HE21	1.58	0.67
4:D:82:VAL:HG21	4:D:274:LYS:HA	1.76	0.67
1:F:77:SER:H	1:F:113:ARG:NH2	1.91	0.67
2:B:25:HIS:CE1	2:B:34:VAL:HB	2.30	0.66
3:C:286:VAL:HA	3:C:299:LEU:HA	1.77	0.66
2:B:42:LEU:HD22	2:B:148:GLY:HA3	1.77	0.66
3:C:43:GLY:HA3	3:C:55:ARG:NH1	2.09	0.66
3:C:63:ALA:HA	3:C:174:LEU:HD11	1.77	0.66
1:A:5:SER:HB3	1:A:129:ASP:HB3	1.77	0.66
1:F:121:LEU:HB3	1:F:130:LEU:HD21	1.77	0.66
2:G:18:ALA:HB1	2:G:77:VAL:HG23	1.78	0.66
2:G:42:LEU:HD21	2:G:148:GLY:HA3	1.77	0.66
2:G:143:GLN:HG3	2:G:147:GLN:HA	1.77	0.66
3:H:229:LEU:HD23	3:H:264:VAL:HG21	1.77	0.66
3:H:137:ARG:HH21	3:H:212:ALA:HB3	1.60	0.66
4:I:187:PHE:HD2	4:I:232:MET:HE3	1.60	0.66
1:A:203:PHE:HA	1:A:210:LYS:H	1.61	0.66
1:F:257:ARG:NH1	2:G:312:LEU:HG	2.07	0.66
1:A:201:LYS:HG3	1:F:214:LYS:HE3	1.76	0.65
4:I:111:GLU:HB2	4:I:287:PRO:HA	1.76	0.65
1:F:105:HIS:HA	1:F:138:SER:HB3	1.78	0.65
3:H:55:ARG:HE	3:H:72:ILE:HG23	1.60	0.65
3:C:31:ALA:H	3:C:202:LEU:HD21	1.62	0.65
3:H:315:PRO:HD3	3:H:323:PRO:HA	1.79	0.65
2:B:103:GLU:O	2:B:107:LEU:HG	1.97	0.65
3:H:347:TYR:CZ	3:H:349:TYR:HB2	2.32	0.65
3:H:238:PRO:HG3	3:H:256:LEU:HD22	1.79	0.64
3:C:193:ASN:HA	5:E:314:LEU:HD11	1.79	0.64
3:H:350:SER:HB3	3:H:353:TRP:CD2	2.33	0.64
4:D:218:SER:HA	4:D:248:ILE:HB	1.79	0.64
2:G:15:GLU:HG2	2:G:74:ILE:O	1.97	0.64
6:L:8:LEU:HD12	6:L:70:VAL:HG12	1.79	0.64
3:H:223:PRO:HG2	5:J:321:GLY:H	1.62	0.64
3:C:238:PRO:HD3	3:C:256:LEU:HD13	1.79	0.64
2:B:35:MET:HE1	2:B:91:GLU:HA	1.80	0.64
1:F:244:VAL:HG11	2:G:222:VAL:HG11	1.78	0.64
2:G:291:LEU:HG	2:G:295:GLN:HE22	1.62	0.64
2:B:281:GLY:HA2	2:B:284:LEU:HD12	1.78	0.64
3:C:229:LEU:HD23	3:C:264:VAL:HG21	1.80	0.64
3:C:333:PHE:HA	3:C:340:TYR:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:44:ILE:HB	6:L:68:HIS:HB2	1.79	0.64
1:A:104:ARG:HA	1:A:137:PRO:HD2	1.80	0.63
2:B:42:LEU:HB3	2:B:116:ARG:HH21	1.63	0.63
4:D:88:ARG:HB3	4:D:304:GLN:HG2	1.79	0.63
2:G:86:ARG:HD2	2:G:89:ARG:HB2	1.79	0.63
4:D:204:THR:HA	5:E:278:TRP:CZ2	2.31	0.63
2:G:81:ARG:HG3	2:G:242:GLU:HG2	1.81	0.63
2:B:42:LEU:HB3	2:B:116:ARG:NH2	2.14	0.63
1:F:83:GLN:O	1:F:87:LYS:HG3	1.98	0.63
1:F:102:PHE:HA	1:F:135:LEU:O	1.99	0.63
1:F:221:SER:O	1:F:225:GLU:HG2	1.98	0.63
1:A:20:PHE:CG	2:B:20:LEU:HD12	2.33	0.63
1:A:171:LEU:HD21	1:A:176:GLN:NE2	2.14	0.63
2:B:276:MET:HA	2:B:281:GLY:N	2.13	0.63
1:F:36:GLU:HG3	1:F:38:LYS:HZ2	1.62	0.63
1:F:79:GLU:H	1:F:120:ASN:HB2	1.64	0.63
1:A:185:SER:HB2	1:A:191:PHE:HE2	1.64	0.63
1:F:229:ILE:HG21	2:G:287:LEU:HB3	1.81	0.63
1:A:99:TRP:CZ3	1:A:117:LEU:HD23	2.33	0.63
1:A:199:SER:HA	1:A:202:PHE:CD2	2.34	0.63
2:B:158:ILE:O	2:B:167:ARG:HG2	1.99	0.63
1:F:240:VAL:HG13	2:G:301:LEU:HD11	1.81	0.63
2:G:142:TYR:HB3	2:G:149:PHE:CD1	2.34	0.63
3:C:189:LEU:HD13	5:E:318:LYS:HG2	1.79	0.62
3:C:319:PRO:HB2	3:C:351:PRO:O	1.98	0.62
1:F:230:CYS:HA	1:F:233:VAL:HG12	1.81	0.62
1:A:301:LEU:HD12	5:E:274:VAL:HB	1.80	0.62
4:D:153:THR:HB	4:D:186:LEU:HD12	1.81	0.62
1:F:243:LEU:HB3	2:G:301:LEU:HB3	1.81	0.62
4:D:148:VAL:HB	4:D:154:ALA:HB3	1.80	0.62
1:A:230:CYS:O	1:A:234:GLU:HG3	1.99	0.62
2:B:239:LEU:O	2:B:243:GLU:HG3	2.00	0.62
3:H:221:LEU:HD12	3:H:225:ILE:HD12	1.81	0.62
4:I:245:VAL:HB	4:I:279:LYS:HG3	1.81	0.62
3:C:274:TYR:CE2	3:C:358:MET:HG2	2.35	0.62
2:B:234:GLU:O	2:B:238:ILE:HG12	2.00	0.61
4:D:228:LEU:HD12	4:D:232:MET:HE2	1.82	0.61
1:A:9:VAL:CG1	1:A:169:ALA:HB2	2.29	0.61
3:C:27:VAL:HG21	3:C:60:ILE:HG12	1.81	0.61
4:D:101:LEU:HG	4:D:176:ALA:H	1.64	0.61
4:I:301:HIS:CE1	4:I:303:LEU:HB2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:PHE:CZ	3:C:94:PRO:HG3	2.36	0.61
3:C:266:GLN:HA	3:C:269:HIS:ND1	2.15	0.61
1:A:31:GLY:HA3	1:A:100:TYR:CE2	2.36	0.61
3:C:350:SER:HB3	3:C:353:TRP:CG	2.35	0.61
3:C:27:VAL:HB	3:C:60:ILE:HG23	1.82	0.61
2:G:240:CYS:O	2:G:244:GLN:HG3	2.01	0.61
3:C:330:VAL:HG22	4:D:130:MET:HB3	1.81	0.61
4:D:126:LYS:O	4:D:130:MET:HG2	2.01	0.61
1:A:243:LEU:HG	2:B:305:LYS:HE3	1.83	0.61
3:H:271:ARG:HH22	3:H:274:TYR:HD2	1.49	0.60
2:B:38:CYS:HB3	2:B:74:ILE:HG21	1.84	0.60
3:H:111:GLU:O	3:H:114:LEU:HG	2.01	0.60
3:H:188:LEU:HB2	3:H:292:GLU:HB2	1.83	0.60
2:G:84:ASP:OD2	2:G:89:ARG:HB3	2.01	0.60
1:A:277:ASN:HB3	1:A:280:LEU:HB3	1.82	0.60
2:G:158:ILE:O	2:G:167:ARG:HG2	2.00	0.60
1:A:34:LEU:HD13	1:A:92:VAL:HG13	1.83	0.60
1:A:139:ILE:HG22	1:A:147:HIS:CD2	2.36	0.60
4:D:133:ARG:HG2	4:D:163:PRO:HB2	1.83	0.60
4:D:182:ASN:O	4:D:186:LEU:HD13	2.02	0.60
3:H:319:PRO:HB2	3:H:351:PRO:O	2.02	0.60
1:F:227:LYS:HB3	1:F:231:LYS:HE3	1.84	0.60
2:G:103:GLU:O	2:G:107:LEU:HG	2.01	0.60
3:H:258:THR:O	3:H:262:GLN:HG2	2.02	0.60
7:M:26:VAL:O	7:M:30:ILE:HG13	2.02	0.60
8:N:42:ARG:HB2	8:N:49:GLN:OE1	2.02	0.60
1:F:233:VAL:O	1:F:237:GLU:HG2	2.02	0.59
3:C:339:LEU:HD21	4:D:133:ARG:HH11	1.67	0.59
1:A:27:SER:HB3	3:C:76:GLN:HB3	1.84	0.59
2:B:38:CYS:HB3	2:B:74:ILE:HD13	1.85	0.59
1:F:222:LEU:HD12	2:G:276:MET:HE2	1.84	0.59
2:B:142:TYR:HD2	2:B:149:PHE:CE2	2.20	0.59
2:G:19:PHE:CE1	2:G:154:PHE:HE2	2.21	0.59
8:N:2:GLN:HA	8:N:16:GLU:HA	1.84	0.59
1:A:15:LEU:HA	1:A:18:LEU:HD12	1.85	0.59
1:F:219:TYR:O	1:F:223:GLN:N	2.34	0.59
3:H:82:PRO:HD3	3:H:105:TRP:CZ3	2.38	0.59
4:I:297:LYS:HG2	4:I:313:TYR:HE2	1.68	0.59
1:A:223:GLN:HG2	1:A:227:LYS:HE3	1.83	0.59
4:D:106:SER:HB2	4:D:175:THR:HG21	1.84	0.59
2:G:36:GLY:HA3	2:G:121:TYR:CE2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:222:SER:HB3	3:H:225:ILE:HG12	1.85	0.59
1:F:20:PHE:CG	2:G:20:LEU:HD22	2.38	0.59
1:A:115:ARG:NH1	1:A:160:LEU:HD13	2.17	0.58
1:A:141:THR:HG22	1:A:143:SER:H	1.68	0.58
3:C:82:PRO:HD3	3:C:105:TRP:CE3	2.38	0.58
2:G:120:TRP:CD2	6:L:73:LEU:HD11	2.38	0.58
1:F:230:CYS:HB2	2:G:233:VAL:HG11	1.83	0.58
2:G:234:GLU:O	2:G:238:ILE:N	2.34	0.58
4:D:101:LEU:HB2	4:D:148:VAL:HG13	1.85	0.58
2:G:70:ARG:NH1	2:G:147:GLN:HB2	2.18	0.58
4:D:96:ILE:HG23	4:D:145:ALA:HB3	1.86	0.58
1:F:85:LEU:O	1:F:89:LEU:HD13	2.03	0.58
2:B:126:HIS:O	7:M:1:MET:HE2	2.04	0.58
2:B:311:GLU:O	2:B:315:LEU:HG	2.03	0.58
1:A:185:SER:HB2	1:A:191:PHE:CE2	2.39	0.58
3:C:339:LEU:HD21	4:D:133:ARG:HD3	1.86	0.58
3:H:71:ILE:HG12	3:H:113:LEU:HD11	1.85	0.58
3:H:195:ASP:CB	5:J:318:LYS:HB2	2.20	0.58
2:B:142:TYR:CD2	2:B:149:PHE:CE2	2.91	0.58
5:E:280:ILE:HG22	5:E:282:PHE:H	1.69	0.58
3:C:18:ILE:HD12	3:C:56:PHE:HE1	1.69	0.57
4:D:93:GLU:HB3	4:D:142:HIS:CE1	2.40	0.57
1:A:26:ASP:HB2	3:C:76:GLN:HE21	1.68	0.57
3:C:81:PRO:HG3	3:C:105:TRP:HB2	1.86	0.57
5:E:284:PRO:HD2	5:E:287:VAL:HG21	1.85	0.57
1:F:122:GLN:HB2	1:F:126:SER:HA	1.86	0.57
1:A:213:HIS:O	1:A:217:GLU:HG3	2.04	0.57
2:B:280:SER:O	2:B:284:LEU:HG	2.03	0.57
3:H:189:LEU:HD11	3:H:194:GLU:O	2.03	0.57
4:I:212:ARG:HD2	4:I:305:ARG:HH12	1.69	0.57
5:J:296:ILE:O	5:J:299:GLN:HG2	2.04	0.57
2:B:80:LEU:HD12	2:B:92:ILE:HD13	1.86	0.57
1:F:252:ARG:O	1:F:255:GLU:HG2	2.03	0.57
2:G:38:CYS:HB3	2:G:74:ILE:HD13	1.85	0.57
1:A:28:ASP:CG	3:C:74:ASN:HD21	2.11	0.57
4:I:170:LEU:HD23	4:I:173:LEU:HD21	1.86	0.57
8:N:38:PRO:HA	8:N:41:GLN:HE21	1.68	0.57
4:D:201:ASN:H	4:D:205:ILE:HD11	1.70	0.57
8:N:23:ILE:HD13	8:N:51:GLU:O	2.05	0.57
8:N:31:GLN:CD	8:N:38:PRO:HD3	2.30	0.57
1:A:105:HIS:CD2	1:A:138:SER:HA	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:125:GLN:HG2	4:I:170:LEU:HB3	1.87	0.57
2:G:116:ARG:HE	6:L:10:GLY:HA3	1.70	0.57
1:A:110:MET:HE1	1:A:156:PRO:HG3	1.87	0.56
3:C:35:LEU:HD23	3:C:61:PRO:HD3	1.86	0.56
4:D:123:VAL:HB	4:D:292:HIS:HE1	1.69	0.56
1:F:193:ARG:HH22	1:F:194:ALA:HB2	1.70	0.56
2:G:134:VAL:HG12	2:G:137:ARG:HE	1.70	0.56
1:A:11:SER:CA	1:A:169:ALA:HB3	2.35	0.56
1:A:118:HIS:CG	1:A:156:PRO:HG2	2.41	0.56
2:B:246:ALA:O	2:B:250:ILE:HG13	2.05	0.56
3:C:140:PHE:O	3:C:144:THR:HG23	2.04	0.56
2:G:174:GLN:HB2	2:G:214:ILE:HD11	1.87	0.56
2:G:174:GLN:HG3	2:G:214:ILE:HG13	1.87	0.56
3:C:25:GLY:C	3:C:35:LEU:HG	2.30	0.56
3:C:86:PHE:CZ	3:C:120:LEU:HD13	2.41	0.56
1:A:187:MET:HB3	2:G:285:GLN:HG2	1.88	0.56
2:B:275:GLN:O	2:B:280:SER:N	2.38	0.56
3:H:86:PHE:CZ	3:H:120:LEU:HD22	2.38	0.56
1:A:20:PHE:HA	1:A:23:LEU:HD12	1.87	0.56
4:D:254:GLU:HB2	4:D:257:GLU:HG2	1.87	0.56
2:G:234:GLU:O	2:G:238:ILE:HG12	2.05	0.56
2:G:277:SER:O	2:G:282:PRO:HD3	2.06	0.56
4:I:145:ALA:HB2	4:I:159:LEU:HD23	1.87	0.56
4:D:218:SER:HB2	4:D:248:ILE:HD12	1.86	0.56
2:G:224:ILE:HG13	2:G:228:CYS:HB2	1.87	0.56
1:A:76:SER:HA	1:A:113:ARG:NH2	2.17	0.56
1:F:117:LEU:O	1:F:118:HIS:C	2.49	0.56
4:I:231:PRO:O	4:I:235:MET:HG3	2.06	0.56
3:C:171:ALA:HB1	3:C:173:PHE:HE1	1.70	0.56
8:N:45:PHE:HD1	8:N:67:LEU:HB3	1.71	0.56
1:F:99:TRP:CZ2	1:F:117:LEU:HD23	2.40	0.56
1:A:250:LEU:O	1:A:253:GLU:HG3	2.06	0.55
1:F:182:VAL:HG12	1:F:183:SER:H	1.71	0.55
1:F:182:VAL:CG1	1:F:183:SER:N	2.68	0.55
1:A:203:PHE:CB	1:A:209:LEU:HA	2.32	0.55
1:F:10:LEU:O	1:F:169:ALA:N	2.40	0.55
3:C:133:ARG:HH12	3:C:143:GLN:HE21	1.55	0.55
5:E:296:ILE:O	5:E:300:LEU:HG	2.07	0.55
5:E:308:LYS:O	5:E:312:ARG:HG3	2.06	0.55
3:H:14:LEU:HD11	3:H:75:ALA:HA	1.89	0.55
8:N:44:ILE:HG23	8:N:48:LYS:H	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:VAL:O	2:B:236:PRO:HD2	2.06	0.55
4:D:166:LEU:HA	4:D:169:CYS:SG	2.46	0.55
2:G:178:ALA:HB2	2:G:210:GLU:HG2	1.88	0.55
2:G:235:LEU:HB3	2:G:236:PRO:HD3	1.88	0.55
3:C:181:PHE:HB3	3:C:199:ASP:HB3	1.88	0.55
4:D:93:GLU:HB2	4:D:301:HIS:CD2	2.42	0.55
2:G:15:GLU:CG	2:G:75:HIS:HA	2.36	0.55
3:H:328:GLN:HG2	3:H:341:SER:HA	1.87	0.55
3:C:29:LEU:HD11	3:C:176:LYS:HB2	1.87	0.55
4:D:135:LYS:HG2	4:D:299:LEU:HD23	1.89	0.55
3:H:186:THR:OG1	5:J:304:GLN:HG3	2.07	0.55
3:H:197:GLY:HA2	5:J:318:LYS:HG3	1.87	0.55
2:B:174:GLN:HB2	2:B:214:ILE:HD11	1.89	0.55
3:C:137:ARG:O	3:C:141:GLU:HG2	2.07	0.55
3:C:275:ILE:HG13	3:C:294:PHE:HB3	1.89	0.55
2:G:116:ARG:NE	6:L:10:GLY:HA3	2.22	0.55
3:H:91:GLU:HB2	3:H:127:PHE:HZ	1.72	0.55
8:N:44:ILE:HG23	8:N:48:LYS:N	2.22	0.55
1:A:115:ARG:NH2	3:C:93:LEU:HD22	2.22	0.55
3:C:149:PRO:HB2	3:C:150:GLN:HE21	1.70	0.55
6:L:26:VAL:O	6:L:30:ILE:HG13	2.07	0.55
3:C:86:PHE:HZ	3:C:120:LEU:HD22	1.72	0.55
2:G:9:VAL:HG21	2:G:148:GLY:HA2	1.89	0.55
2:G:120:TRP:CZ3	6:L:75:GLY:HA3	2.41	0.55
1:F:108:GLN:HG3	2:G:165:THR:HG21	1.89	0.54
1:F:245:LYS:O	1:F:249:ARG:HG2	2.08	0.54
2:G:156:CYS:HB3	2:G:168:VAL:HG13	1.89	0.54
4:D:148:VAL:HG21	4:D:173:LEU:HD21	1.90	0.54
3:H:143:GLN:O	3:H:147:GLU:HG3	2.07	0.54
6:L:42:ARG:HB2	6:L:70:VAL:O	2.07	0.54
1:A:247:VAL:HG21	2:B:305:LYS:HD3	1.88	0.54
1:F:208:SER:HB3	1:F:213:HIS:CE1	2.41	0.54
6:L:36:ILE:HD12	6:L:69:LEU:HD21	1.90	0.54
4:D:163:PRO:O	4:D:166:LEU:HG	2.07	0.54
1:F:118:HIS:CD2	1:F:156:PRO:HG2	2.42	0.54
4:D:234:LYS:HA	4:D:237:GLN:HE21	1.72	0.54
1:F:182:VAL:CG1	1:F:183:SER:H	2.20	0.54
3:H:13:MET:SD	3:H:78:PRO:HG3	2.48	0.54
8:N:41:GLN:HA	8:N:71:LEU:HD23	1.90	0.54
1:A:20:PHE:CB	2:B:20:LEU:HD12	2.37	0.54
2:B:297:HIS:O	2:B:301:LEU:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:GLY:HA3	1:F:60:ASP:O	2.08	0.54
3:H:203:LEU:HD13	3:H:219:LEU:HD13	1.89	0.54
6:L:45:PHE:HB2	6:L:50:LEU:HD11	1.89	0.54
1:A:105:HIS:CE1	1:A:139:ILE:HG12	2.43	0.54
2:B:125:PRO:C	2:B:127:ILE:H	2.16	0.54
1:F:193:ARG:HA	1:F:196:GLN:HG2	1.89	0.54
1:A:76:SER:CA	1:A:113:ARG:HH22	2.16	0.54
2:B:250:ILE:HG22	2:B:254:THR:OG1	2.07	0.54
2:G:72:VAL:HG11	2:G:150:VAL:HG22	1.90	0.54
3:H:350:SER:HB3	3:H:353:TRP:CG	2.42	0.54
4:D:127:MET:HG2	4:D:292:HIS:CD2	2.43	0.53
2:G:133:HIS:CD2	2:G:134:VAL:HG13	2.43	0.53
3:C:35:LEU:O	3:C:36:ARG:HG3	2.08	0.53
3:C:228:ALA:HB1	3:C:264:VAL:HG11	1.89	0.53
2:G:25:HIS:O	2:G:34:VAL:HG11	2.08	0.53
1:A:102:PHE:CZ	1:A:135:LEU:HD22	2.43	0.53
1:A:141:THR:HG21	2:B:213:GLU:OE1	2.09	0.53
2:B:30:GLU:HB3	2:B:157:PHE:CD2	2.43	0.53
3:C:306:PHE:CE2	3:C:308:PHE:HB3	2.43	0.53
4:D:131:PHE:CD2	4:D:295:MET:HE3	2.43	0.53
1:F:133:LEU:HD13	1:F:166:LEU:HD13	1.90	0.53
2:G:15:GLU:HG3	2:G:75:HIS:HA	1.91	0.53
2:B:156:CYS:HA	2:B:168:VAL:HA	1.91	0.53
2:G:236:PRO:HG3	2:G:283:LEU:HD13	1.89	0.53
3:H:339:LEU:HD21	4:I:133:ARG:HB3	1.91	0.53
4:D:83:GLN:OE1	5:E:275:ASN:HB3	2.09	0.53
4:D:155:TRP:HE1	4:D:158:GLY:HA2	1.73	0.53
1:F:255:GLU:O	1:F:258:ARG:HG2	2.07	0.53
6:L:72:ARG:HD3	6:L:74:ARG:NE	2.23	0.53
2:B:22:CYS:SG	2:B:77:VAL:HG11	2.49	0.53
2:B:278:ALA:C	2:B:282:PRO:HG2	2.34	0.53
1:F:89:LEU:HD22	1:F:125:PHE:HE2	1.73	0.53
1:F:188:SER:HB3	1:F:191:PHE:HB3	1.90	0.53
2:G:121:TYR:HB2	2:G:154:PHE:HE1	1.74	0.53
2:B:142:TYR:HB3	2:B:149:PHE:CD2	2.44	0.53
3:C:241:PRO:HD2	3:C:249:TYR:CD1	2.44	0.53
4:D:221:PRO:HG3	4:D:264:MET:HB2	1.89	0.53
1:F:225:GLU:O	1:F:229:ILE:HG12	2.09	0.53
1:F:112:PHE:HD2	1:F:116:LEU:HD13	1.74	0.52
3:H:11:SER:HA	3:H:51:PRO:O	2.10	0.52
3:H:222:SER:H	3:H:225:ILE:HD11	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:282:VAL:HG21	4:I:291:LEU:HD13	1.91	0.52
3:C:314:LEU:HD23	3:C:323:PRO:HB3	1.91	0.52
1:F:137:PRO:HA	1:F:149:LEU:HA	1.90	0.52
2:B:38:CYS:HB3	2:B:74:ILE:CG2	2.39	0.52
3:C:282:PHE:HZ	3:C:366:PHE:HE2	1.55	0.52
2:G:217:HIS:CB	3:H:47:LEU:HD22	2.39	0.52
3:H:35:LEU:HD22	3:H:58:LEU:HD22	1.91	0.52
1:A:28:ASP:H	3:C:74:ASN:ND2	2.06	0.52
1:A:137:PRO:HA	1:A:148:ARG:O	2.10	0.52
2:B:300:GLU:HG3	2:B:301:LEU:N	2.25	0.52
1:F:64:TYR:O	1:F:65:ILE:C	2.52	0.52
3:H:16:PRO:HB3	3:H:110:PRO:HB3	1.91	0.52
3:C:54:ASP:HB2	3:C:73:PHE:HB2	1.91	0.52
3:C:133:ARG:HA	3:C:139:MET:HG3	1.90	0.52
1:F:89:LEU:HD21	1:F:96:VAL:HG21	1.88	0.52
1:F:172:GLY:HA3	2:G:30:GLU:HG2	1.92	0.52
2:G:141:MET:O	2:G:144:MET:HG2	2.10	0.52
3:C:86:PHE:CZ	3:C:120:LEU:HD22	2.44	0.52
3:C:181:PHE:HZ	3:C:201:ALA:HB2	1.74	0.52
2:G:13:HIS:CD2	3:H:47:LEU:HD11	2.45	0.52
3:C:128:GLN:OE1	3:C:131:ARG:HD3	2.10	0.52
2:G:94:PRO:HA	2:G:97:LEU:HG	1.92	0.52
2:G:120:TRP:CE3	6:L:73:LEU:HD11	2.44	0.52
1:F:77:SER:HB3	1:F:116:LEU:CD2	2.35	0.52
1:F:170:ASN:H	1:F:173:MET:HB3	1.73	0.52
2:G:134:VAL:HA	2:G:137:ARG:HG2	1.92	0.52
1:A:112:PHE:CZ	1:A:116:LEU:HD11	2.45	0.52
2:B:127:ILE:HG21	7:M:63(A):DAB:HG2	1.92	0.52
5:E:314:LEU:HD23	5:E:316:ASN:H	1.74	0.52
1:F:103:ARG:HH22	1:F:134:LEU:HD21	1.75	0.52
1:A:160:LEU:HD21	3:C:90:ALA:HB1	1.93	0.51
1:A:215:ILE:HG21	2:B:269:THR:HG22	1.91	0.51
1:F:74:TYR:CD2	1:F:117:LEU:HD22	2.45	0.51
1:F:145:SER:HB2	2:G:213:GLU:HB3	1.93	0.51
4:I:86:THR:HG21	4:I:303:LEU:HD22	1.90	0.51
4:I:99:LEU:HD11	4:I:105:MET:HE2	1.92	0.51
4:I:128:ILE:O	4:I:132:VAL:HG23	2.11	0.51
1:A:103:ARG:HD2	1:A:106:SER:HB2	1.91	0.51
3:C:82:PRO:HD3	3:C:105:TRP:CZ3	2.45	0.51
1:F:85:LEU:HD12	1:F:89:LEU:CD1	2.36	0.51
4:I:187:PHE:CD2	4:I:232:MET:HE3	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:GLN:HE21	1:F:150:GLU:HB3	1.76	0.51
1:A:36:GLU:HB3	1:A:38:LYS:NZ	2.26	0.51
2:B:155:SER:HB3	2:B:169:LEU:HB2	1.93	0.51
1:F:23:LEU:HD11	2:G:19:PHE:CD2	2.46	0.51
1:F:247:VAL:HG12	2:G:305:LYS:HA	1.91	0.51
2:B:82:ARG:HD2	2:B:90:VAL:HG23	1.92	0.51
3:C:269:HIS:HA	3:C:272:ARG:HE	1.76	0.51
1:F:93:LYS:O	1:F:94:LYS:HD2	2.11	0.51
3:H:3:PRO:HG3	5:J:316:ASN:HA	1.92	0.51
3:H:272:ARG:HH22	5:J:300:LEU:HD13	1.75	0.51
1:A:11:SER:HB3	1:A:14:VAL:HG22	1.91	0.51
1:A:35:GLY:O	1:A:95:ASN:HB2	2.11	0.51
2:B:95:GLU:CD	2:B:95:GLU:H	2.19	0.51
4:D:123:VAL:O	4:D:127:MET:HG3	2.11	0.51
4:D:187:PHE:CD2	4:D:232:MET:HE3	2.46	0.51
4:I:129:GLU:HG3	4:I:170:LEU:HD12	1.92	0.51
1:A:210:LYS:O	1:A:214:LYS:HG3	2.10	0.51
3:C:145:LEU:HD11	3:C:246:LEU:HD23	1.93	0.51
4:D:123:VAL:HB	4:D:292:HIS:CE1	2.45	0.51
4:D:89:VAL:HG21	4:D:206:PRO:HB3	1.93	0.51
5:E:314:LEU:HD23	5:E:316:ASN:N	2.25	0.51
1:F:104:ARG:CD	1:F:137:PRO:HG2	2.33	0.51
1:A:92:VAL:O	1:A:93:LYS:HG2	2.11	0.51
4:D:100:ASP:HB3	4:D:217:TYR:HA	1.93	0.51
1:F:135:LEU:HA	1:F:150:GLU:O	2.10	0.51
2:G:35:MET:HG2	2:G:92:ILE:CD1	2.40	0.51
2:G:306:GLU:O	2:G:310:GLN:HG2	2.11	0.51
4:I:132:VAL:HG21	4:I:166:LEU:HG	1.93	0.51
4:I:221:PRO:HD2	4:I:264:MET:HE2	1.92	0.51
3:C:10:ILE:HG13	3:C:53:CYS:O	2.10	0.50
1:A:36:GLU:HB3	1:A:38:LYS:HZ2	1.76	0.50
2:G:143:GLN:HA	2:G:146:ASP:O	2.11	0.50
3:H:215:VAL:HG21	3:H:240:PHE:CE1	2.46	0.50
1:F:103:ARG:NH2	1:F:134:LEU:HD21	2.25	0.50
3:C:177:LEU:HD11	3:C:203:LEU:HB2	1.94	0.50
3:C:339:LEU:HD12	4:D:137:LYS:HE3	1.93	0.50
1:F:29:THR:H	1:F:102:PHE:HB2	1.77	0.50
3:H:48:THR:CG2	3:H:49:PRO:HD2	2.41	0.50
1:A:33:LEU:HB3	1:A:61:ILE:HG23	1.94	0.50
5:E:295:VAL:O	5:E:299:GLN:HG3	2.12	0.50
1:A:153:LEU:HB3	1:A:164:VAL:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:GLN:O	2:B:300:GLU:HG2	2.11	0.50
3:C:42:SER:HB2	3:C:53:CYS:HA	1.93	0.50
3:C:207:PHE:HZ	3:C:246:LEU:HD13	1.77	0.50
1:F:97:VAL:HG12	1:F:127:ASN:ND2	2.26	0.50
2:G:271:ASN:O	2:G:275:GLN:HG3	2.12	0.50
1:F:99:TRP:CH2	1:F:117:LEU:HD23	2.46	0.50
3:H:48:THR:HG23	3:H:49:PRO:HD2	1.93	0.50
4:D:127:MET:SD	4:D:291:LEU:HG	2.52	0.50
1:F:102:PHE:CZ	1:F:135:LEU:HD22	2.47	0.50
1:F:212:VAL:HA	1:F:215:ILE:HG22	1.94	0.50
3:H:69:TRP:CD1	3:H:86:PHE:HA	2.47	0.50
4:I:109:LYS:HB2	4:I:284:LEU:HG	1.94	0.50
8:N:23:ILE:HG12	8:N:50:LEU:HB3	1.94	0.50
1:A:220:ALA:O	1:A:224:GLU:HG3	2.12	0.50
2:B:32:GLU:CD	2:B:85:LYS:HD3	2.37	0.50
2:B:138:THR:HG21	8:N:73:LEU:HD23	1.93	0.50
1:F:233:VAL:HG23	2:G:294:ASN:HD21	1.77	0.50
1:A:133:LEU:HG	1:A:135:LEU:CD1	2.42	0.49
3:C:105:TRP:CD1	3:C:107:PRO:HB3	2.47	0.49
3:H:81:PRO:HB3	3:H:105:TRP:CG	2.46	0.49
3:H:311:HIS:CE1	4:I:137:LYS:HE3	2.48	0.49
1:A:13:PHE:HE1	2:B:279:VAL:HA	1.77	0.49
2:B:82:ARG:HE	2:B:85:LYS:CG	2.24	0.49
2:B:124:HIS:CE1	2:B:153:ILE:HG12	2.42	0.49
1:F:64:TYR:O	1:F:64:TYR:CD2	2.65	0.49
1:F:233:VAL:HG13	2:G:229:LEU:HD13	1.93	0.49
1:A:168:VAL:HG21	2:B:157:PHE:HE1	1.77	0.49
1:A:215:ILE:HD11	2:B:276:MET:HE1	1.94	0.49
3:H:94:PRO:HB2	3:H:99:LEU:HD11	1.93	0.49
4:I:212:ARG:HG3	4:I:242:PHE:HB2	1.93	0.49
6:L:8:LEU:HD12	6:L:70:VAL:CG1	2.42	0.49
1:F:104:ARG:HB2	3:H:55:ARG:NH1	2.27	0.49
4:D:109:LYS:HE2	4:D:285:ALA:HB2	1.93	0.49
2:G:224:ILE:HG12	2:G:229:LEU:HG	1.94	0.49
2:B:117:VAL:HG21	8:N:8:LEU:HD11	1.94	0.49
2:B:216:ILE:HG12	2:B:216:ILE:O	2.12	0.49
3:C:278:PHE:O	3:C:282:PHE:HB3	2.13	0.49
4:D:133:ARG:HG2	4:D:163:PRO:CB	2.42	0.49
1:F:28:ASP:HB2	1:F:70:LEU:HD21	1.94	0.49
3:H:237:ILE:HG12	5:J:327:ARG:HG2	1.94	0.49
6:L:27:LYS:HA	6:L:41:GLN:OE1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD11	2:B:19:PHE:CE1	2.47	0.49
2:B:36:GLY:HA3	2:B:121:TYR:CE2	2.48	0.49
3:C:181:PHE:CZ	3:C:201:ALA:HB2	2.48	0.49
2:G:86:ARG:HB2	2:G:89:ARG:HB2	1.94	0.49
4:D:221:PRO:HG2	4:D:260:SER:HB2	1.93	0.49
3:H:250:VAL:HB	3:H:251:PRO:HD3	1.95	0.49
3:C:10:ILE:HD13	3:C:15:SER:HA	1.95	0.49
3:C:311:HIS:NE2	4:D:138:ILE:HG12	2.28	0.49
2:G:230:GLU:O	2:G:234:GLU:HG3	2.12	0.49
3:H:42:SER:HA	3:H:53:CYS:HA	1.94	0.49
5:J:283:CYS:HA	5:J:292:TYR:CD2	2.48	0.49
1:A:170:ASN:ND2	1:A:172:GLY:H	2.11	0.49
1:A:185:SER:HB2	2:B:259:VAL:HB	1.94	0.49
1:A:254:ILE:HG13	2:B:312:LEU:HG	1.95	0.49
2:B:35:MET:HE1	2:B:91:GLU:CA	2.42	0.49
2:B:134:VAL:HG13	2:B:137:ARG:NH2	2.27	0.49
2:B:231:SER:O	2:B:234:GLU:HB2	2.13	0.49
3:C:18:ILE:HD12	3:C:56:PHE:CZ	2.48	0.49
3:C:269:HIS:NE2	3:C:270:LYS:HG3	2.27	0.49
4:D:101:LEU:HD11	4:D:174:GLU:O	2.12	0.49
1:F:32:PHE:HZ	1:F:73:PHE:CD1	2.31	0.49
3:H:275:ILE:O	3:H:279:LEU:HG	2.12	0.49
1:A:113:ARG:HG2	3:C:83:ASP:OD1	2.13	0.48
3:C:322:GLN:HG2	3:C:349:TYR:HD2	1.78	0.48
3:C:340:TYR:HE2	3:C:373:PHE:HE1	1.61	0.48
4:D:181:PHE:HA	4:D:219:ARG:HH21	1.78	0.48
3:C:349:TYR:CZ	3:C:351:PRO:HA	2.47	0.48
1:F:110:MET:HE1	1:F:156:PRO:HG3	1.95	0.48
2:G:139:GLN:HG2	2:G:174:GLN:HA	1.95	0.48
1:A:103:ARG:O	1:A:136:THR:HA	2.13	0.48
1:A:190:GLY:C	1:A:192:SER:H	2.22	0.48
1:A:251:LYS:HG3	1:A:252:ARG:N	2.28	0.48
2:B:33:GLU:HG3	2:B:87:LYS:O	2.14	0.48
3:C:71:ILE:HD13	3:C:113:LEU:HD11	1.95	0.48
4:D:146:LEU:HB3	4:D:156:LEU:HB2	1.95	0.48
1:F:33:LEU:HD13	1:F:61:ILE:CD1	2.43	0.48
2:G:217:HIS:HB3	3:H:47:LEU:HD22	1.95	0.48
3:H:349:TYR:CZ	3:H:351:PRO:HA	2.48	0.48
2:B:35:MET:HB2	2:B:90:VAL:HG11	1.94	0.48
3:H:30:ASP:HB3	3:H:61:PRO:O	2.13	0.48
1:A:147:HIS:HB2	2:B:170:TYR:CZ	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:ALA:O	2:B:70:ARG:HD3	2.14	0.48
4:D:129:GLU:HG2	4:D:167:CYS:SG	2.53	0.48
2:G:25:HIS:CE1	2:G:34:VAL:HB	2.49	0.48
4:I:297:LYS:HG2	4:I:313:TYR:CE2	2.48	0.48
4:D:124:SER:HA	4:D:127:MET:HE2	1.95	0.48
1:F:33:LEU:HD13	1:F:61:ILE:HD11	1.96	0.48
2:G:38:CYS:HB3	2:G:74:ILE:HG21	1.94	0.48
3:H:81:PRO:HB3	3:H:105:TRP:HB2	1.96	0.48
3:H:199:ASP:HA	3:H:222:SER:CB	2.44	0.48
1:A:26:ASP:OD2	3:C:44:CYS:HB2	2.14	0.48
1:A:103:ARG:HD2	1:A:106:SER:CB	2.43	0.48
1:A:198:HIS:HB2	1:A:202:PHE:CZ	2.49	0.48
1:A:201:LYS:O	1:A:210:LYS:HE2	2.14	0.48
2:G:35:MET:CE	2:G:90:VAL:HG13	2.40	0.48
1:A:278:ILE:O	1:A:282:GLN:HG2	2.13	0.48
4:D:103:GLU:HB3	4:D:177:SER:HA	1.95	0.48
4:D:170:LEU:HD12	4:D:173:LEU:HD12	1.95	0.48
2:G:38:CYS:HB3	2:G:74:ILE:CG2	2.44	0.48
2:G:126:HIS:HA	2:G:158:ILE:HG12	1.96	0.48
2:G:212:ILE:HG23	2:G:214:ILE:HD11	1.95	0.48
2:G:217:HIS:ND1	3:H:46:SER:HB3	2.28	0.48
4:I:112:SER:HB3	4:I:118:THR:CG2	2.43	0.48
1:A:104:ARG:HH12	3:C:45:THR:HA	1.78	0.48
4:D:212:ARG:HH12	4:D:298:LEU:HB3	1.79	0.48
3:C:94:PRO:HB2	3:C:99:LEU:HD11	1.95	0.47
3:C:196:PRO:HD2	3:C:224:ARG:HH21	1.80	0.47
1:A:170:ASN:C	1:A:172:GLY:N	2.71	0.47
1:F:237:GLU:HG3	2:G:229:LEU:HD11	1.95	0.47
5:J:291:GLN:O	5:J:295:VAL:HG23	2.15	0.47
3:C:202:LEU:O	3:C:219:LEU:HD12	2.14	0.47
3:C:278:PHE:CE1	3:C:359:ALA:HA	2.43	0.47
4:D:181:PHE:CE2	4:D:183:LEU:HB3	2.49	0.47
1:F:33:LEU:HB3	1:F:61:ILE:HG12	1.96	0.47
1:F:112:PHE:HZ	3:H:102:LEU:CD2	2.28	0.47
2:G:91:GLU:CD	6:L:74:ARG:HG2	2.38	0.47
2:G:128:THR:HG1	2:G:130:TRP:CD1	2.31	0.47
3:H:152:GLY:HA2	3:H:155:MET:SD	2.53	0.47
1:A:78:GLY:O	1:A:117:LEU:HA	2.14	0.47
1:F:191:PHE:CE2	2:G:259:VAL:HG21	2.49	0.47
4:I:301:HIS:HE1	4:I:303:LEU:HB2	1.78	0.47
4:D:232:MET:O	4:D:236:PHE:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:PHE:HB2	1:F:65:ILE:HG23	1.95	0.47
3:H:58:LEU:HB3	3:H:60:ILE:HD11	1.95	0.47
1:A:280:LEU:HA	5:E:302:VAL:HG21	1.96	0.47
2:B:276:MET:HB3	1:F:191:PHE:CZ	2.50	0.47
3:C:69:TRP:CD1	3:C:86:PHE:HA	2.50	0.47
3:C:323:PRO:O	3:C:325:LEU:HD12	2.15	0.47
3:H:155:MET:HG2	3:H:175:LEU:HD22	1.97	0.47
6:L:8:LEU:HB2	6:L:70:VAL:HG12	1.95	0.47
1:A:26:ASP:HB3	3:C:44:CYS:HA	1.97	0.47
1:A:31:GLY:HA3	1:A:100:TYR:CZ	2.49	0.47
1:A:76:SER:HA	1:A:113:ARG:HH12	1.79	0.47
1:A:99:TRP:CE2	1:A:132:PHE:CD1	3.03	0.47
1:A:119:LYS:O	1:A:122:GLN:HG2	2.14	0.47
2:B:245:ASP:O	2:B:249:ARG:HG2	2.14	0.47
3:C:306:PHE:HE2	3:C:308:PHE:HB3	1.78	0.47
4:D:111:GLU:HB2	4:D:287:PRO:HA	1.97	0.47
5:E:290:ASN:O	5:E:294:LYS:HG3	2.14	0.47
1:F:20:PHE:CD1	2:G:20:LEU:HB2	2.49	0.47
2:G:35:MET:HG2	2:G:92:ILE:HD11	1.96	0.47
2:G:292:GLU:HA	2:G:295:GLN:OE1	2.14	0.47
3:H:7:LEU:HD12	5:J:315:LEU:HD13	1.96	0.47
3:H:198:GLU:HB3	5:J:320:PHE:HE1	1.79	0.47
3:H:315:PRO:HD3	3:H:323:PRO:CA	2.45	0.47
4:I:105:MET:HA	4:I:120:ALA:HB3	1.95	0.47
7:M:4:PHE:O	7:M:66:THR:HA	2.15	0.47
8:N:5:VAL:HG13	8:N:67:LEU:HD11	1.97	0.47
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.71	0.47
2:B:304:GLU:HG2	2:B:308:LEU:HD23	1.96	0.47
1:F:241:ASP:HA	2:G:223:THR:HG21	1.97	0.47
1:A:33:LEU:HD13	1:A:61:ILE:CD1	2.45	0.47
1:A:105:HIS:ND1	3:C:41:LYS:HB3	2.30	0.47
2:B:270:LYS:HE3	2:B:270:LYS:HB3	1.60	0.47
3:C:11:SER:HB3	3:C:14:LEU:HD23	1.97	0.47
1:F:122:GLN:HG3	1:F:122:GLN:O	2.15	0.47
2:G:97:LEU:O	2:G:100:ALA:HB3	2.15	0.47
1:A:140:ILE:HG12	1:A:146:THR:HB	1.96	0.47
1:F:20:PHE:HA	1:F:23:LEU:HD12	1.97	0.47
2:G:38:CYS:CB	2:G:74:ILE:HD13	2.45	0.47
3:H:303:TRP:HB2	3:H:370:VAL:HG11	1.97	0.47
3:H:332:HIS:CE1	3:H:378:PHE:HA	2.50	0.47
5:J:280:ILE:HD12	5:J:280:ILE:H	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:GLU:HB2	2:B:86:ARG:O	2.14	0.46
2:B:135:ASP:HB3	2:B:173:PHE:CZ	2.50	0.46
5:E:280:ILE:HB	5:E:292:TYR:OH	2.15	0.46
2:G:138:THR:HG21	6:L:73:LEU:HD12	1.96	0.46
3:H:287:VAL:HG12	3:H:288:GLU:HG2	1.96	0.46
1:A:210:LYS:HG2	1:A:214:LYS:HD2	1.98	0.46
3:H:257:LEU:O	3:H:261:VAL:HG13	2.15	0.46
3:H:271:ARG:NH2	3:H:274:TYR:HD2	2.14	0.46
1:A:9:VAL:HG13	1:A:169:ALA:HB2	1.97	0.46
1:A:104:ARG:HG3	1:A:105:HIS:N	2.29	0.46
4:D:226:PHE:HB3	4:D:267:PHE:CZ	2.50	0.46
2:G:33:GLU:HG3	2:G:87:LYS:O	2.16	0.46
3:H:302:MET:HG2	3:H:307:CYS:SG	2.56	0.46
4:D:129:GLU:O	4:D:133:ARG:HG3	2.15	0.46
5:J:299:GLN:HG3	5:J:303:TYR:CE2	2.51	0.46
8:N:21:ASP:HB3	8:N:25:ASN:HD22	1.81	0.46
1:A:187:MET:HE3	2:G:285:GLN:NE2	2.31	0.46
1:A:221:SER:O	1:A:224:GLU:HB2	2.16	0.46
2:B:174:GLN:HB2	2:B:214:ILE:CD1	2.45	0.46
2:B:235:LEU:HB3	2:B:236:PRO:HD3	1.96	0.46
4:D:306:PRO:HG2	4:D:311:ALA:HB2	1.98	0.46
4:I:173:LEU:HD12	4:I:173:LEU:O	2.15	0.46
1:A:26:ASP:CB	3:C:76:GLN:HE21	2.28	0.46
2:B:160:ASP:HB2	2:B:167:ARG:CZ	2.46	0.46
2:B:219:VAL:HG22	3:C:47:LEU:HD11	1.97	0.46
3:C:266:GLN:O	3:C:270:LYS:HD2	2.16	0.46
3:C:303:TRP:HB2	3:C:370:VAL:HG11	1.98	0.46
1:F:28:ASP:OD1	1:F:102:PHE:O	2.34	0.46
3:H:199:ASP:OD2	3:H:224:ARG:HD2	2.15	0.46
8:N:5:VAL:HG13	8:N:67:LEU:CD1	2.46	0.46
8:N:56:LEU:HB3	8:N:61:ILE:HB	1.97	0.46
1:A:170:ASN:C	1:A:172:GLY:H	2.24	0.46
2:B:13:HIS:CE1	3:C:47:LEU:HD21	2.51	0.46
2:B:106:ARG:O	2:B:110:LEU:HG	2.15	0.46
2:B:131:PRO:HG3	2:B:153:ILE:HD12	1.98	0.46
4:D:239:PRO:HA	4:D:274:LYS:HE2	1.98	0.46
3:H:307:CYS:HB2	3:H:330:VAL:HG11	1.97	0.46
1:A:116:LEU:HD13	3:C:96:PRO:HG3	1.98	0.46
1:A:151:HIS:CE1	2:B:166:GLY:HA3	2.51	0.46
1:F:137:PRO:HB3	1:F:149:LEU:CD1	2.46	0.46
3:C:11:SER:HB2	3:C:52:ASN:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:109:ASN:HB3	3:H:111:GLU:OE1	2.16	0.46
8:N:63:LYS:HE2	8:N:63:LYS:HB3	1.80	0.46
1:A:244:VAL:HA	2:B:305:LYS:NZ	2.31	0.46
4:D:247:TYR:CE2	4:D:261:TRP:HB2	2.51	0.46
3:H:63:ALA:HA	3:H:174:LEU:HB2	1.97	0.46
3:H:219:LEU:HG	3:H:221:LEU:HD22	1.97	0.46
3:H:323:PRO:O	3:H:325:LEU:HD12	2.15	0.46
1:A:292:GLU:HG2	1:A:295:HIS:CE1	2.51	0.45
1:F:222:LEU:HD22	2:G:284:LEU:CD1	2.45	0.45
3:H:58:LEU:HA	3:H:58:LEU:HD23	1.58	0.45
4:I:258:GLU:C	4:I:260:SER:H	2.24	0.45
1:A:222:LEU:HD22	2:B:284:LEU:HD13	1.98	0.45
1:A:247:VAL:HG11	2:B:304:GLU:OE2	2.15	0.45
1:A:280:LEU:HB2	5:E:302:VAL:HG11	1.98	0.45
1:F:13:PHE:HZ	2:G:279:VAL:HG13	1.81	0.45
2:G:155:SER:O	2:G:169:LEU:N	2.45	0.45
3:H:81:PRO:HA	3:H:105:TRP:CD2	2.51	0.45
3:H:315:PRO:HB2	3:H:321:ASP:HB2	1.97	0.45
4:I:183:LEU:HG	4:I:187:PHE:CE2	2.51	0.45
8:N:45:PHE:CD1	8:N:67:LEU:HB3	2.50	0.45
3:C:86:PHE:HZ	3:C:120:LEU:HD13	1.81	0.45
1:F:254:ILE:HG23	2:G:315:LEU:HD12	1.98	0.45
2:G:15:GLU:HG2	2:G:75:HIS:HA	1.99	0.45
2:G:115:MET:C	2:G:116:ARG:HG3	2.41	0.45
6:L:46:ALA:HB3	6:L:48:LYS:NZ	2.31	0.45
1:A:227:LYS:HB3	1:A:231:LYS:NZ	2.31	0.45
1:A:241:ASP:O	1:A:245:LYS:HG2	2.17	0.45
3:C:37:ILE:HG23	3:C:56:PHE:CD2	2.52	0.45
4:D:110:LEU:HD11	4:D:118:THR:HG22	1.98	0.45
1:F:102:PHE:CE2	1:F:135:LEU:HD22	2.51	0.45
1:A:248:ASN:O	1:A:252:ARG:HG3	2.16	0.45
3:C:266:GLN:HA	3:C:269:HIS:CE1	2.51	0.45
1:F:105:HIS:HA	1:F:138:SER:CB	2.46	0.45
1:F:214:LYS:O	1:F:218:MET:HG3	2.17	0.45
2:G:73:HIS:CD2	2:G:74:ILE:N	2.85	0.45
6:L:7:THR:HA	6:L:69:LEU:HB3	1.99	0.45
2:B:81:ARG:HG3	2:B:242:GLU:HG3	1.97	0.45
4:D:101:LEU:HG	4:D:176:ALA:N	2.29	0.45
1:F:104:ARG:HA	1:F:137:PRO:O	2.15	0.45
2:G:155:SER:N	2:G:169:LEU:O	2.47	0.45
3:H:54:ASP:HB3	3:H:75:ALA:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:102:LEU:HD12	3:H:102:LEU:HA	1.73	0.45
1:A:149:LEU:O	2:B:167:ARG:HA	2.16	0.45
1:A:172:GLY:HA3	2:B:30:GLU:HG2	1.99	0.45
2:B:86:ARG:HH22	2:B:89:ARG:HB2	1.81	0.45
2:B:124:HIS:O	2:B:155:SER:HA	2.17	0.45
3:C:262:GLN:HB3	3:C:266:GLN:HE22	1.82	0.45
4:D:293:ASN:O	4:D:297:LYS:HG3	2.16	0.45
1:F:37:VAL:HG12	1:F:59:ILE:HD13	1.98	0.45
1:F:161:PHE:HE1	1:F:163:ARG:NH2	2.15	0.45
2:G:80:LEU:HD23	2:G:80:LEU:HA	1.76	0.45
3:H:10:ILE:HD11	3:H:40:LEU:HD11	1.98	0.45
3:H:132:LEU:HD21	3:H:142:TYR:CB	2.47	0.45
1:A:103:ARG:HH22	1:A:114:GLU:CD	2.25	0.45
1:F:234:GLU:HG3	1:F:235:ASP:N	2.32	0.45
8:N:39:ASP:OD1	8:N:39:ASP:N	2.50	0.45
1:A:110:MET:SD	1:A:156:PRO:HG3	2.57	0.45
2:B:153:ILE:HD12	2:B:171:THR:CG2	2.47	0.45
4:D:164:ARG:HG3	4:D:165:GLU:N	2.32	0.45
1:F:79:GLU:O	1:F:117:LEU:HD13	2.17	0.45
2:G:120:TRP:HB2	6:L:73:LEU:HD21	1.98	0.45
2:G:244:GLN:O	2:G:248:ARG:HG3	2.17	0.45
3:H:218:LYS:HD3	5:J:326:PRO:HD3	1.99	0.45
3:C:215:VAL:HG21	3:C:240:PHE:CE2	2.52	0.45
2:G:33:GLU:OE2	2:G:88:ASP:HA	2.16	0.45
2:G:293:GLN:O	2:G:297:HIS:HB2	2.17	0.45
5:J:288:ASP:O	5:J:291:GLN:HG3	2.17	0.45
1:A:298:VAL:HG23	1:A:307:SER:HB2	1.97	0.44
3:C:207:PHE:CZ	3:C:246:LEU:HD13	2.52	0.44
3:C:322:GLN:HG2	3:C:349:TYR:CD2	2.52	0.44
2:G:102:THR:O	2:G:106:ARG:HG3	2.16	0.44
3:H:79:GLU:HA	3:H:107:PRO:HG3	1.99	0.44
1:A:11:SER:HA	1:A:169:ALA:CB	2.43	0.44
3:C:113:LEU:HD12	3:C:113:LEU:HA	1.77	0.44
3:C:269:HIS:HA	3:C:272:ARG:NE	2.32	0.44
5:E:284:PRO:HD3	5:E:292:TYR:CE1	2.52	0.44
1:F:192:SER:HA	1:F:195:VAL:HG22	1.99	0.44
2:G:172:CYS:CB	2:G:216:ILE:HB	2.47	0.44
3:H:43:GLY:CA	3:H:55:ARG:HH12	2.29	0.44
3:H:55:ARG:NE	3:H:72:ILE:HG23	2.29	0.44
6:L:23:ILE:HG12	6:L:54:ARG:O	2.17	0.44
1:A:214:LYS:CE	1:F:201:LYS:HB3	2.40	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:ARG:O	3:C:275:ILE:HG12	2.17	0.44
3:C:328:GLN:C	3:C:373:PHE:HZ	2.25	0.44
1:F:14:VAL:HG13	1:F:64:TYR:HB3	1.99	0.44
1:F:76:SER:CB	3:H:103:ALA:HA	2.48	0.44
3:H:92:PHE:CD2	3:H:124:TYR:HD1	2.34	0.44
3:H:154:ASN:HD22	3:H:176:LYS:NZ	2.15	0.44
3:H:246:LEU:HG	3:H:250:VAL:HG23	1.99	0.44
1:A:30:GLU:OE2	1:A:70:LEU:HD12	2.16	0.44
4:D:181:PHE:HE2	4:D:183:LEU:HB3	1.83	0.44
1:F:109:ILE:HA	1:F:154:TYR:OH	2.17	0.44
2:G:8:ALA:O	2:G:70:ARG:HB2	2.17	0.44
4:I:196:LEU:HD11	4:I:235:MET:HA	1.98	0.44
1:A:104:ARG:H	3:C:55:ARG:NH2	2.14	0.44
2:B:131:PRO:HG3	2:B:153:ILE:CD1	2.48	0.44
3:C:92:PHE:CE1	3:C:94:PRO:HG3	2.53	0.44
3:C:333:PHE:CE2	4:D:133:ARG:HD2	2.52	0.44
1:F:219:TYR:HE1	1:F:223:GLN:OE1	2.01	0.44
1:F:250:LEU:CB	2:G:308:LEU:HB3	2.47	0.44
2:G:278:ALA:O	2:G:282:PRO:HG2	2.17	0.44
2:G:289:ASP:O	2:G:293:GLN:HG3	2.17	0.44
1:A:110:MET:HB3	1:A:110:MET:HE2	1.71	0.44
3:C:32:THR:O	3:C:32:THR:HG22	2.17	0.44
1:F:219:TYR:O	1:F:223:GLN:HG2	2.17	0.44
3:H:43:GLY:HA3	3:H:55:ARG:HH12	1.83	0.44
4:D:134:THR:O	4:D:138:ILE:HG13	2.18	0.44
1:F:244:VAL:O	1:F:247:VAL:HG22	2.18	0.44
1:A:204:GLU:OE2	1:A:213:HIS:HD2	2.01	0.44
1:A:245:LYS:HA	1:A:245:LYS:HD3	1.68	0.44
2:B:35:MET:HG3	2:B:122:HIS:HB3	2.00	0.44
3:H:15:SER:OG	3:H:16:PRO:HD3	2.17	0.44
3:H:246:LEU:HD12	3:H:249:TYR:HB3	2.00	0.44
3:H:307:CYS:H	3:H:331:TYR:HE2	1.65	0.44
1:A:112:PHE:CE1	1:A:116:LEU:HD11	2.53	0.44
1:A:254:ILE:HG13	2:B:312:LEU:CG	2.48	0.44
4:D:252:THR:HG21	4:D:285:ALA:HB3	1.98	0.44
1:F:64:TYR:O	1:F:64:TYR:CG	2.71	0.44
1:F:215:ILE:HD12	1:F:218:MET:SD	2.58	0.44
2:G:30:GLU:HB3	2:G:157:PHE:CD2	2.52	0.44
3:H:290:ASP:O	3:H:294:PHE:HA	2.18	0.44
1:A:163:ARG:HG3	2:B:163:THR:HA	2.00	0.43
2:B:177:GLN:HB3	2:B:207:GLU:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:GLN:O	2:B:307:GLU:HG2	2.18	0.43
3:C:282:PHE:CE1	3:C:299:LEU:HD22	2.53	0.43
3:C:360:LYS:HA	3:C:360:LYS:HD2	1.88	0.43
2:G:70:ARG:HH12	2:G:147:GLN:HB2	1.80	0.43
2:G:152:LEU:HD11	2:G:216:ILE:HD12	1.99	0.43
8:N:69:LEU:HA	8:N:69:LEU:HD12	1.65	0.43
1:A:10:LEU:C	1:A:169:ALA:H	2.27	0.43
1:A:59:ILE:HG23	1:A:97:VAL:HB	1.99	0.43
2:B:302:GLN:HA	2:B:305:LYS:HG2	2.00	0.43
3:C:286:VAL:HG13	3:C:298:THR:O	2.18	0.43
1:A:13:PHE:CE1	2:B:279:VAL:HA	2.54	0.43
3:C:199:ASP:OD1	3:C:224:ARG:HD2	2.18	0.43
2:G:172:CYS:HB2	2:G:216:ILE:HD12	1.99	0.43
3:H:118:LYS:O	3:H:121:VAL:HG12	2.18	0.43
1:A:11:SER:O	1:A:14:VAL:HG22	2.19	0.43
1:A:254:ILE:CG2	1:A:257:ARG:HH21	2.31	0.43
3:H:197:GLY:CA	5:J:318:LYS:HG3	2.47	0.43
4:I:301:HIS:O	4:I:305:ARG:HG3	2.18	0.43
3:C:358:MET:HE2	3:C:358:MET:HB2	1.78	0.43
4:D:139:ASP:HB3	4:D:142:HIS:CD2	2.53	0.43
4:D:258:GLU:HA	4:D:261:TRP:HD1	1.76	0.43
1:F:193:ARG:NH2	1:F:194:ALA:HB2	2.32	0.43
2:G:160:ASP:HB3	2:G:163:THR:HG22	1.99	0.43
3:H:145:LEU:HD22	3:H:151:TYR:CE2	2.53	0.43
3:H:199:ASP:OD1	3:H:224:ARG:HB3	2.18	0.43
4:I:193:LYS:HA	4:I:193:LYS:HD3	1.82	0.43
3:C:80:LEU:C	3:C:105:TRP:CD1	2.97	0.43
3:C:152:GLY:HA2	3:C:155:MET:SD	2.58	0.43
3:C:339:LEU:CD2	4:D:133:ARG:HD3	2.48	0.43
4:D:217:TYR:CZ	4:D:247:TYR:HB2	2.54	0.43
1:F:180:LYS:HA	1:F:180:LYS:HD3	1.75	0.43
2:G:129:VAL:CG2	2:G:171:THR:HG23	2.48	0.43
2:G:251:HIS:O	2:G:252:SER:HB3	2.19	0.43
6:L:15:LEU:HB3	6:L:17:VAL:HG23	2.00	0.43
1:A:9:VAL:HG12	1:A:169:ALA:HB2	1.99	0.43
1:A:11:SER:HA	1:A:169:ALA:O	2.19	0.43
1:A:33:LEU:HD13	1:A:61:ILE:HD13	2.00	0.43
3:C:262:GLN:O	3:C:266:GLN:NE2	2.51	0.43
4:D:93:GLU:HB3	4:D:142:HIS:ND1	2.34	0.43
2:G:40:GLY:HA2	2:G:115:MET:SD	2.59	0.43
3:H:144:THR:HA	3:H:147:GLU:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:63:LYS:HG2	6:L:64:GLU:HG3	1.99	0.43
8:N:5:VAL:HG21	8:N:30:ILE:HD11	2.00	0.43
1:A:74:TYR:CD2	1:A:117:LEU:HD22	2.54	0.43
1:A:168:VAL:HG21	2:B:157:PHE:CE1	2.53	0.43
1:A:171:LEU:HD11	1:A:176:GLN:CD	2.44	0.43
3:C:270:LYS:HD3	3:C:319:PRO:HD3	2.01	0.43
1:F:155:LYS:C	1:F:157:GLN:H	2.26	0.43
3:H:79:GLU:HA	3:H:107:PRO:CB	2.48	0.43
3:H:246:LEU:HD12	3:H:246:LEU:HA	1.78	0.43
4:I:110:LEU:HD12	4:I:120:ALA:HA	2.00	0.43
1:A:209:LEU:HD21	2:B:262:ILE:HA	2.00	0.43
3:C:240:PHE:HA	3:C:249:TYR:CE1	2.54	0.43
3:C:349:TYR:OH	3:C:351:PRO:HA	2.18	0.43
4:D:191:GLN:HE22	4:D:231:PRO:HB3	1.82	0.43
4:D:249:HIS:HB2	4:D:261:TRP:CG	2.54	0.43
1:F:11:SER:HA	1:F:169:ALA:HB3	2.01	0.43
1:F:136:THR:O	1:F:150:GLU:HB2	2.18	0.43
3:H:177:LEU:HD11	3:H:203:LEU:HD22	2.00	0.43
7:M:56:LEU:HD23	7:M:56:LEU:HA	1.82	0.43
1:A:32:PHE:CE2	1:A:73:PHE:CD2	3.07	0.43
1:A:75:ASN:O	1:A:113:ARG:NH2	2.52	0.43
1:A:108:GLN:OE1	1:A:134:LEU:HD23	2.19	0.43
2:B:145:MET:HE1	8:N:8:LEU:HB3	2.01	0.43
2:B:271:ASN:O	2:B:275:GLN:HG3	2.19	0.43
3:C:278:PHE:HE1	3:C:359:ALA:CA	2.29	0.43
1:F:105:HIS:CG	3:H:41:LYS:HB3	2.54	0.43
2:G:263:HIS:O	2:G:267:VAL:HG23	2.19	0.43
2:G:291:LEU:O	2:G:294:ASN:HB2	2.18	0.43
3:H:139:MET:O	3:H:143:GLN:HG3	2.19	0.43
4:I:294:CYS:HA	4:I:297:LYS:HD2	2.01	0.43
2:B:140:ALA:HB2	2:B:175:SER:OG	2.19	0.42
3:C:47:LEU:HD23	3:C:47:LEU:HA	1.74	0.42
1:F:34:LEU:HD13	1:F:92:VAL:CG1	2.50	0.42
2:G:21:VAL:CG1	2:G:79:ILE:HD11	2.49	0.42
2:G:152:LEU:HD11	2:G:216:ILE:CD1	2.49	0.42
3:H:271:ARG:NH2	3:H:314:LEU:HD11	2.34	0.42
6:L:27:LYS:HB3	6:L:38:PRO:HB3	2.00	0.42
1:A:103:ARG:HD3	3:C:72:ILE:HD13	2.01	0.42
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.83	0.42
1:A:108:GLN:HG3	1:A:108:GLN:O	2.19	0.42
1:A:122:GLN:HG3	1:A:128:GLN:HE22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:MET:O	2:B:35:MET:HG2	2.19	0.42
3:C:54:ASP:OD1	3:C:54:ASP:N	2.51	0.42
4:D:99:LEU:HD11	4:D:105:MET:HE1	2.01	0.42
5:E:292:TYR:O	5:E:296:ILE:HG12	2.19	0.42
1:F:42:LYS:HD2	1:F:56:VAL:HG21	2.00	0.42
3:H:119:GLU:O	3:H:123:GLN:HG2	2.18	0.42
1:F:28:ASP:HA	1:F:102:PHE:O	2.19	0.42
1:F:78:GLY:HA2	1:F:117:LEU:HA	2.02	0.42
2:G:117:VAL:HB	6:L:8:LEU:O	2.19	0.42
3:H:133:ARG:HG2	3:H:139:MET:CE	2.47	0.42
3:H:162:LYS:HB2	3:H:167:GLY:O	2.19	0.42
4:I:104:GLU:HG2	4:I:250:ASN:HD22	1.84	0.42
6:L:31:GLN:O	6:L:35:GLY:HA2	2.19	0.42
1:A:59:ILE:HD11	1:A:129:ASP:O	2.18	0.42
1:A:112:PHE:HE2	3:C:102:LEU:HD13	1.84	0.42
2:B:17:ASP:O	2:B:21:VAL:HG23	2.19	0.42
2:B:31:LYS:HE2	2:B:31:LYS:HB3	1.69	0.42
2:B:35:MET:HB2	2:B:90:VAL:CG1	2.49	0.42
2:B:85:LYS:HB3	2:B:85:LYS:HE3	1.65	0.42
4:D:183:LEU:HD22	4:D:268:MET:HE1	2.01	0.42
4:D:314:SER:O	4:D:317:GLU:HB2	2.19	0.42
1:F:70:LEU:N	1:F:70:LEU:HD12	2.34	0.42
1:F:153:LEU:HA	1:F:153:LEU:HD12	1.82	0.42
2:G:12:VAL:CG2	2:G:150:VAL:HG11	2.49	0.42
2:G:231:SER:O	2:G:234:GLU:HB2	2.19	0.42
4:I:191:GLN:HE22	4:I:231:PRO:HB3	1.84	0.42
7:M:5:VAL:HG22	7:M:67:LEU:HB2	2.01	0.42
1:A:211:GLU:HA	1:A:214:LYS:HD3	2.02	0.42
1:A:221:SER:O	1:A:225:GLU:HG2	2.19	0.42
1:A:243:LEU:HG	2:B:305:LYS:HG3	2.00	0.42
3:C:308:PHE:CE1	3:C:370:VAL:HG11	2.54	0.42
1:F:20:PHE:CB	2:G:20:LEU:HD13	2.43	0.42
1:F:109:ILE:HB	3:H:85:ILE:HG21	2.00	0.42
2:G:21:VAL:HG12	2:G:79:ILE:HD11	2.00	0.42
3:H:200:VAL:HG22	5:J:320:PHE:CZ	2.54	0.42
5:J:297:LEU:O	5:J:301:GLU:HG2	2.20	0.42
6:L:45:PHE:HB3	6:L:50:LEU:HD21	2.02	0.42
1:F:110:MET:HE3	1:F:132:PHE:CG	2.54	0.42
1:F:253:GLU:HA	1:F:256:LYS:NZ	2.35	0.42
3:H:18:ILE:O	3:H:21:VAL:HG12	2.20	0.42
4:I:87:PRO:HA	5:J:278:TRP:NE1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASP:OD1	1:A:108:GLN:N	2.52	0.42
1:A:187:MET:CB	2:G:285:GLN:HG2	2.49	0.42
1:A:222:LEU:HD22	2:B:284:LEU:CD1	2.50	0.42
2:B:20:LEU:HD23	2:B:20:LEU:C	2.44	0.42
1:A:64:TYR:HE2	1:A:66:PRO:HB3	1.85	0.42
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.82	0.42
1:A:303:ASN:HB3	1:A:305:HIS:CD2	2.47	0.42
2:B:153:ILE:CG2	2:B:171:THR:HG22	2.43	0.42
2:B:283:LEU:HD12	2:B:286:TRP:HE3	1.85	0.42
2:B:301:LEU:HB3	2:B:305:LYS:HE2	2.01	0.42
3:C:3:PRO:HB2	3:C:4:GLU:OE2	2.19	0.42
4:D:140:LYS:C	4:D:142:HIS:H	2.27	0.42
2:G:9:VAL:HA	2:G:70:ARG:HB2	2.01	0.42
4:I:139:ASP:HB3	4:I:142:HIS:CD2	2.54	0.42
7:M:18:GLU:O	7:M:56:LEU:HD12	2.20	0.42
7:M:37:PRO:O	7:M:41:GLN:HG3	2.20	0.42
3:C:15:SER:OG	3:C:16:PRO:HD3	2.20	0.42
4:D:207:PRO:HG2	4:D:303:LEU:HD11	2.01	0.42
1:F:7:SER:O	1:F:58:THR:HA	2.20	0.42
1:F:13:PHE:CE1	2:G:279:VAL:HA	2.55	0.42
1:F:160:LEU:HG	1:F:161:PHE:N	2.35	0.42
2:G:234:GLU:O	2:G:235:LEU:C	2.60	0.42
2:B:81:ARG:HH21	2:B:96:GLN:HE22	1.68	0.42
4:D:197:PRO:HG2	4:D:240:TYR:CD2	2.55	0.42
5:E:307:LEU:HG	5:E:311:GLN:NE2	2.34	0.42
1:F:36:GLU:HG3	1:F:38:LYS:HZ1	1.85	0.42
1:F:76:SER:HB2	3:H:103:ALA:HA	2.01	0.42
1:F:111:THR:HG21	3:H:83:ASP:HB3	2.02	0.42
1:F:243:LEU:O	1:F:247:VAL:HG13	2.20	0.42
3:H:290:ASP:HB3	3:H:295:THR:N	2.34	0.42
4:I:129:GLU:HG3	4:I:170:LEU:CD1	2.50	0.42
6:L:61:ILE:HG23	6:L:65:SER:CB	2.50	0.42
7:M:42:ARG:HB3	7:M:70:VAL:HG23	2.01	0.42
1:A:153:LEU:HD23	1:A:164:VAL:HB	2.01	0.41
1:A:171:LEU:HB3	2:B:28:SER:O	2.20	0.41
1:A:201:LYS:O	1:A:201:LYS:HD3	2.20	0.41
1:A:201:LYS:CG	1:F:214:LYS:HE3	2.48	0.41
2:B:177:GLN:HG2	2:B:209:TYR:CE2	2.54	0.41
3:C:151:TYR:O	3:C:155:MET:HG3	2.19	0.41
1:F:196:GLN:HA	1:F:199:SER:HB3	2.02	0.41
2:G:278:ALA:C	2:G:282:PRO:HG2	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:25:ASN:O	8:N:29:LYS:HG2	2.19	0.41
1:A:160:LEU:H	1:A:160:LEU:HD23	1.85	0.41
2:B:98:SER:O	2:B:102:THR:HG23	2.20	0.41
2:B:128:THR:HG23	7:M:1:MET:HE1	2.03	0.41
2:B:263:HIS:O	2:B:266:SER:HB3	2.20	0.41
3:C:275:ILE:HG13	3:C:294:PHE:CD1	2.55	0.41
3:C:363:LYS:HE2	3:C:363:LYS:HB2	1.93	0.41
4:D:220:PRO:HA	4:D:247:TYR:OH	2.20	0.41
1:F:213:HIS:O	1:F:217:GLU:HG2	2.20	0.41
3:H:11:SER:HB2	3:H:52:ASN:HA	2.02	0.41
3:H:18:ILE:HA	3:H:21:VAL:HG12	2.02	0.41
4:D:125:GLN:HA	4:D:170:LEU:HD21	2.02	0.41
4:D:148:VAL:O	4:D:154:ALA:N	2.54	0.41
1:F:33:LEU:HD22	1:F:61:ILE:HG21	2.01	0.41
2:G:272:LEU:HD12	2:G:272:LEU:HA	1.82	0.41
4:I:242:PHE:HD2	4:I:276:THR:O	2.03	0.41
1:A:14:VAL:HB	1:A:64:TYR:CD1	2.55	0.41
1:A:20:PHE:HB2	2:B:20:LEU:HD12	2.02	0.41
1:A:115:ARG:CZ	3:C:93:LEU:HD22	2.51	0.41
4:D:212:ARG:HD2	4:D:244:ASP:OD2	2.20	0.41
1:F:115:ARG:HH21	3:H:93:LEU:HG	1.86	0.41
2:G:12:VAL:HG22	2:G:150:VAL:HG11	2.03	0.41
3:H:91:GLU:HB2	3:H:127:PHE:CZ	2.53	0.41
3:H:247:ILE:HG23	3:H:248:ASP:OD1	2.21	0.41
5:J:309:MET:O	5:J:313:GLN:HG2	2.21	0.41
1:A:254:ILE:HG23	1:A:257:ARG:HH21	1.85	0.41
4:D:132:VAL:HG12	4:D:144:PHE:CD1	2.54	0.41
2:G:275:GLN:O	2:G:280:SER:N	2.51	0.41
3:H:76:GLN:O	3:H:76:GLN:HG2	2.20	0.41
3:H:279:LEU:HD21	3:H:289:TYR:CE1	2.56	0.41
3:H:302:MET:HA	3:H:307:CYS:HA	2.02	0.41
3:H:310:VAL:HG22	3:H:327:PHE:CD2	2.55	0.41
1:A:248:ASN:HA	1:A:251:LYS:HG2	2.03	0.41
2:B:130:TRP:HA	2:B:130:TRP:CE3	2.56	0.41
2:B:239:LEU:HD23	2:B:239:LEU:HA	1.79	0.41
3:C:32:THR:HG23	5:E:320:PHE:CB	2.51	0.41
3:C:133:ARG:HD3	3:C:139:MET:HG2	2.03	0.41
4:D:100:ASP:CB	4:D:217:TYR:HA	2.51	0.41
4:D:289:LEU:HD12	4:D:289:LEU:H	1.85	0.41
1:F:104:ARG:HG3	3:H:43:GLY:O	2.21	0.41
1:F:115:ARG:HG3	1:F:156:PRO:CB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:PHE:CZ	2:G:259:VAL:HG21	2.55	0.41
2:G:108:ALA:HA	2:G:113:ARG:O	2.20	0.41
1:A:218:MET:HA	1:F:198:HIS:HD2	1.86	0.41
2:B:123:SER:HA	2:B:154:PHE:HB2	2.03	0.41
2:B:138:THR:HA	2:B:141:MET:HE2	2.01	0.41
2:B:276:MET:HB3	1:F:191:PHE:HZ	1.85	0.41
3:C:40:LEU:HD12	3:C:56:PHE:HB3	2.02	0.41
3:C:205:VAL:HG11	3:C:246:LEU:HD11	2.03	0.41
1:F:104:ARG:HB2	3:H:43:GLY:HA2	2.03	0.41
1:F:108:GLN:HG3	2:G:165:THR:CG2	2.51	0.41
1:F:150:GLU:HA	2:G:166:GLY:O	2.19	0.41
2:G:72:VAL:HG21	2:G:150:VAL:HG13	2.03	0.41
6:L:23:ILE:HG22	6:L:27:LYS:HE2	2.03	0.41
1:A:150:GLU:HA	2:B:166:GLY:O	2.21	0.41
1:A:222:LEU:O	1:A:225:GLU:HB2	2.21	0.41
2:B:25:HIS:O	2:B:34:VAL:HG11	2.21	0.41
2:G:116:ARG:HD2	6:L:10:GLY:CA	2.51	0.41
2:G:159:GLU:HG3	2:G:165:THR:C	2.45	0.41
4:I:188:SER:O	4:I:192:GLN:HG3	2.21	0.41
6:L:17:VAL:HG11	6:L:26:VAL:HG22	2.02	0.41
2:B:37:LEU:HD21	2:B:117:VAL:HG13	2.01	0.41
2:B:124:HIS:CD2	8:N:77:A1JPL:S1	3.14	0.41
2:B:176:ILE:HG22	2:B:210:GLU:O	2.21	0.41
2:B:230:GLU:O	2:B:234:GLU:HG3	2.21	0.41
2:B:235:LEU:O	2:B:239:LEU:HG	2.20	0.41
3:C:7:LEU:O	3:C:10:ILE:HG22	2.21	0.41
3:C:288:GLU:HB2	4:D:90:ASN:CB	2.50	0.41
4:D:98:CYS:O	4:D:215:LEU:HD12	2.21	0.41
1:F:27:SER:CA	3:H:74:ASN:HD21	2.34	0.41
1:F:78:GLY:HA3	1:F:120:ASN:HD22	1.85	0.41
1:F:104:ARG:HB2	3:H:55:ARG:HH12	1.86	0.41
2:G:114:PRO:HB2	2:G:116:ARG:NH1	2.35	0.41
2:G:142:TYR:HB3	2:G:149:PHE:CG	2.55	0.41
3:H:40:LEU:HA	3:H:40:LEU:HD12	1.71	0.41
3:H:81:PRO:HB3	3:H:105:TRP:CB	2.50	0.41
3:H:145:LEU:HD11	3:H:246:LEU:HD23	2.02	0.41
3:H:162:LYS:HE3	3:H:164:ASN:O	2.20	0.41
4:I:125:GLN:HA	4:I:170:LEU:HD13	2.02	0.41
4:I:132:VAL:HG13	4:I:144:PHE:CG	2.55	0.41
8:N:45:PHE:HZ	8:N:65:SER:HB3	1.85	0.41
1:A:104:ARG:HG3	1:A:105:HIS:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:GLY:O	2:B:269:THR:HG23	2.20	0.41
1:F:151:HIS:NE2	2:G:166:GLY:HA3	2.36	0.41
1:F:155:LYS:HD2	1:F:158:LYS:HG2	2.03	0.41
1:F:170:ASN:HB2	2:G:28:SER:O	2.21	0.41
3:H:122:GLN:O	3:H:125:HIS:HB3	2.21	0.41
1:A:276:GLU:HG2	1:A:297:CYS:HB2	2.02	0.40
3:C:30:ASP:HB2	3:C:156:GLU:OE1	2.21	0.40
3:C:235:LEU:HD22	3:C:260:LYS:NZ	2.36	0.40
4:D:197:PRO:HB3	4:D:209:TYR:CZ	2.56	0.40
1:F:89:LEU:HD22	1:F:125:PHE:CE2	2.54	0.40
1:F:136:THR:N	1:F:150:GLU:O	2.52	0.40
1:F:140:ILE:HD11	1:F:146:THR:HG21	2.03	0.40
2:G:291:LEU:O	2:G:295:GLN:OE1	2.38	0.40
3:H:135:SER:OG	3:H:138:LEU:HG	2.21	0.40
3:H:176:LYS:HE2	3:H:177:LEU:O	2.20	0.40
3:H:364:ALA:O	3:H:368:THR:HG23	2.21	0.40
4:I:135:LYS:HB3	4:I:144:PHE:HZ	1.85	0.40
8:N:1:MET:HE3	8:N:19:PRO:HD3	2.03	0.40
2:B:177:GLN:HG2	2:B:209:TYR:HE2	1.87	0.40
1:F:146:THR:HA	2:G:171:THR:HG22	2.03	0.40
2:G:33:GLU:HG2	2:G:123:SER:O	2.20	0.40
2:G:239:LEU:HD12	2:G:279:VAL:HG11	2.02	0.40
3:H:23:ARG:HB3	5:J:312:ARG:O	2.20	0.40
3:H:257:LEU:HD13	3:H:257:LEU:HA	1.91	0.40
3:H:290:ASP:HB3	3:H:295:THR:H	1.86	0.40
4:I:181:PHE:HB2	4:I:219:ARG:HH11	1.86	0.40
8:N:41:GLN:H	8:N:41:GLN:HG2	1.67	0.40
1:A:215:ILE:HD12	1:A:215:ILE:HA	1.83	0.40
2:B:287:LEU:HD23	2:B:287:LEU:HA	1.89	0.40
1:F:19:ALA:O	1:F:23:LEU:HG	2.21	0.40
1:F:64:TYR:O	1:F:66:PRO:N	2.54	0.40
2:G:104:ALA:HB1	2:G:115:MET:O	2.21	0.40
2:G:153:ILE:O	2:G:170:TYR:HA	2.21	0.40
4:I:112:SER:HB3	4:I:118:THR:HG21	2.03	0.40
1:A:241:ASP:HA	2:B:223:THR:HG21	2.03	0.40
2:B:26:ALA:HA	2:B:34:VAL:HG21	2.03	0.40
3:C:237:ILE:HD12	3:C:237:ILE:HA	1.93	0.40
3:C:330:VAL:CG2	4:D:130:MET:HB3	2.48	0.40
4:D:122:ASN:O	4:D:126:LYS:HG2	2.22	0.40
1:F:88:ILE:HG13	1:F:89:LEU:CD1	2.42	0.40
2:G:231:SER:HA	2:G:234:GLU:OE1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:286:TRP:NE1	2:G:290:ARG:HH21	2.13	0.40
2:G:303:GLN:O	2:G:307:GLU:HG2	2.21	0.40
3:H:27:VAL:HG21	3:H:60:ILE:HD12	2.02	0.40
3:H:35:LEU:HA	3:H:35:LEU:HD23	1.81	0.40
3:H:350:SER:HB3	3:H:353:TRP:CE2	2.56	0.40
4:I:124:SER:HA	4:I:127:MET:HE2	2.03	0.40
4:I:186:LEU:O	4:I:190:ILE:HG13	2.21	0.40
2:B:99:ALA:O	2:B:103:GLU:HG2	2.22	0.40
2:B:142:TYR:HD1	8:N:71:LEU:HD12	1.86	0.40
4:D:250:ASN:ND2	4:D:284:LEU:HD23	2.36	0.40
4:D:269:GLY:HA3	4:D:279:LYS:NZ	2.36	0.40
1:F:103:ARG:NH1	1:F:111:THR:HG23	2.37	0.40
1:F:243:LEU:HD23	2:G:301:LEU:HB3	2.03	0.40
2:G:235:LEU:O	2:G:239:LEU:HG	2.21	0.40
3:H:358:MET:HE2	3:H:358:MET:HB2	1.81	0.40
4:I:239:PRO:HA	4:I:274:LYS:HE3	2.03	0.40
5:J:311:GLN:HA	5:J:314:LEU:HD12	2.02	0.40
5:J:311:GLN:O	5:J:314:LEU:HB2	2.22	0.40
6:L:37:PRO:HA	6:L:38:PRO:HD3	1.97	0.40
8:N:5:VAL:HB	8:N:13:ILE:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/409 (68%)	262 (94%)	17 (6%)	0	100	100
1	F	241/409 (59%)	215 (89%)	26 (11%)	0	100	100
2	B	254/316 (80%)	244 (96%)	10 (4%)	0	100	100
2	G	252/316 (80%)	237 (94%)	15 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	378/383 (99%)	353 (93%)	25 (7%)	0	100	100
3	H	381/383 (100%)	347 (91%)	34 (9%)	0	100	100
4	D	235/349 (67%)	212 (90%)	23 (10%)	0	100	100
4	I	237/349 (68%)	226 (95%)	11 (5%)	0	100	100
5	E	56/171 (33%)	52 (93%)	4 (7%)	0	100	100
5	J	56/171 (33%)	54 (96%)	2 (4%)	0	100	100
6	L	73/76 (96%)	67 (92%)	6 (8%)	0	100	100
7	M	69/76 (91%)	65 (94%)	4 (6%)	0	100	100
8	N	74/76 (97%)	68 (92%)	5 (7%)	1 (1%)	9	31
All	All	2585/3484 (74%)	2402 (93%)	182 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	N	75	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/373 (70%)	261 (100%)	0	100	100
1	F	223/373 (60%)	222 (100%)	1 (0%)	84	83
2	B	236/286 (82%)	234 (99%)	2 (1%)	73	77
2	G	234/286 (82%)	233 (100%)	1 (0%)	84	83
3	C	335/337 (99%)	335 (100%)	0	100	100
3	H	337/337 (100%)	337 (100%)	0	100	100
4	D	219/305 (72%)	219 (100%)	0	100	100
4	I	220/305 (72%)	220 (100%)	0	100	100
5	E	52/150 (35%)	52 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	52/150 (35%)	52 (100%)	0	100	100
6	L	68/68 (100%)	68 (100%)	0	100	100
7	M	65/67 (97%)	64 (98%)	1 (2%)	57	69
8	N	68/68 (100%)	67 (98%)	1 (2%)	57	69
All	All	2370/3105 (76%)	2364 (100%)	6 (0%)	84	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	153	ILE
2	B	174	GLN
1	F	74	TYR
2	G	222	VAL
7	M	62	GLN
8	N	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	95	ASN
1	A	120	ASN
1	A	127	ASN
1	A	128	GLN
1	A	147	HIS
1	A	170	ASN
1	A	176	GLN
1	A	198	HIS
1	A	305	HIS
2	B	13	HIS
2	B	73	HIS
2	B	124	HIS
2	B	244	GLN
2	B	263	HIS
2	B	293	GLN
2	B	296	GLN
3	C	74	ASN
3	C	76	GLN
3	C	101	ASN
3	C	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	143	GLN
3	C	150	GLN
3	C	266	GLN
3	C	342	GLN
3	C	344	GLN
3	C	380	ASN
4	D	191	GLN
4	D	237	GLN
4	D	249	HIS
4	D	292	HIS
4	D	293	ASN
4	D	310	HIS
5	E	313	GLN
1	F	21	GLN
1	F	95	ASN
1	F	105	HIS
1	F	118	HIS
1	F	120	ASN
1	F	122	GLN
1	F	162	HIS
1	F	216	ASN
1	F	238	GLN
2	G	13	HIS
2	G	43	ASN
2	G	73	HIS
2	G	75	HIS
2	G	96	GLN
2	G	139	GLN
2	G	285	GLN
2	G	294	ASN
2	G	297	HIS
2	G	303	GLN
3	H	33	ASN
3	H	59	HIS
3	H	74	ASN
3	H	100	GLN
3	H	154	ASN
3	H	214	GLN
3	H	227	HIS
3	H	269	HIS
3	H	281	HIS
3	H	338	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	372	GLN
4	I	90	ASN
4	I	119	ASN
4	I	122	ASN
4	I	125	GLN
4	I	192	GLN
4	I	201	ASN
4	I	203	GLN
4	I	225	GLN
4	I	250	ASN
5	J	290	ASN
5	J	291	GLN
6	L	62	GLN
6	L	68	HIS
7	M	2	GLN
8	N	40	GLN
8	N	62	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	DAB	M	63(A)	7,8	5,6,7	0.87	0	1,6,8	0.89	0
8	A1JPL	N	77	7,9,8	5,6,7	1.36	0	1,6,8	1.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	DAB	M	63(A)	7,8	-	1/4/5/7	-
8	A1JPL	N	77	7,9,8	-	1/2/5/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	63(A)	DAB	CA-CB-CG-ND
8	N	77	A1JPL	C-C2-C3-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	63(A)	DAB	1	0
8	N	77	A1JPL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

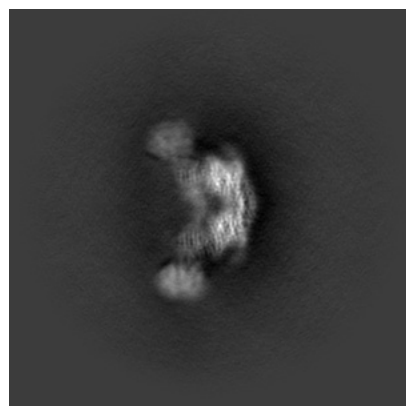
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55053. These allow visual inspection of the internal detail of the map and identification of artifacts.

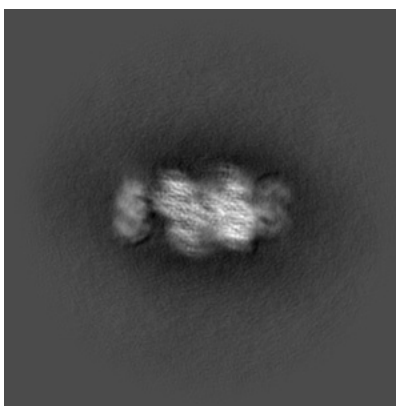
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

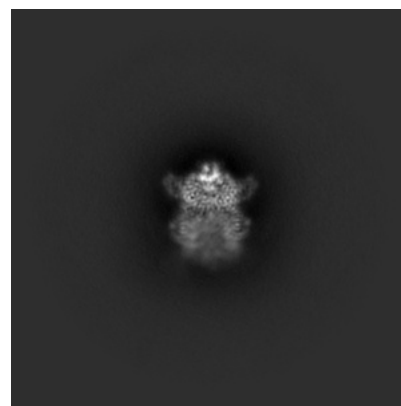
6.1.1 Primary map



X

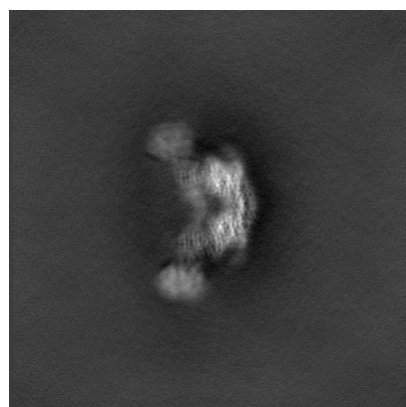


Y

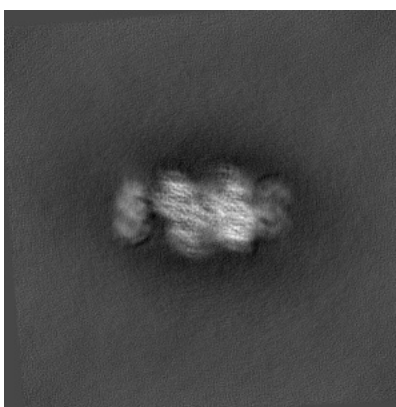


Z

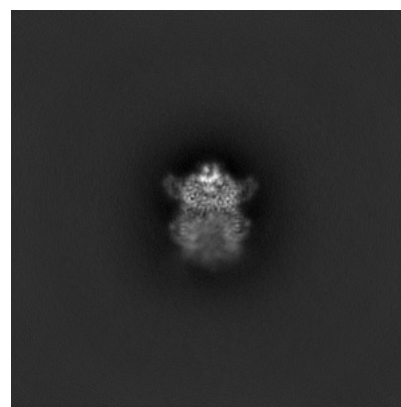
6.1.2 Raw map



X



Y

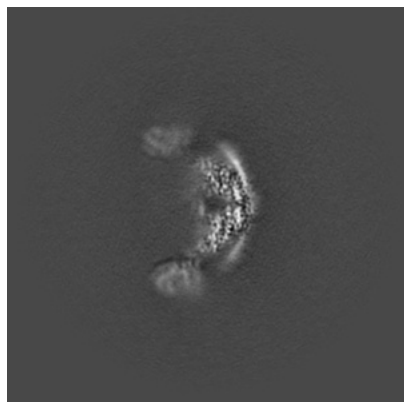


Z

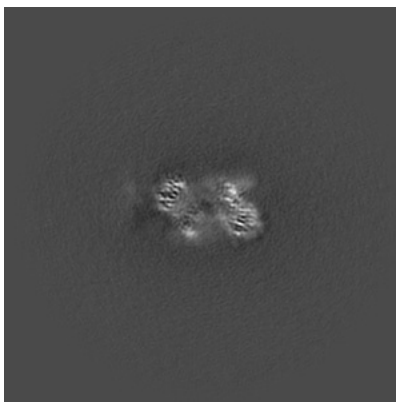
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

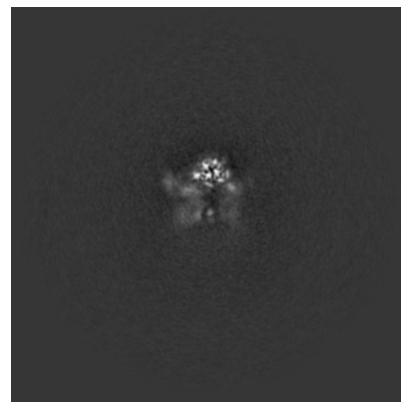
6.2.1 Primary map



X Index: 192

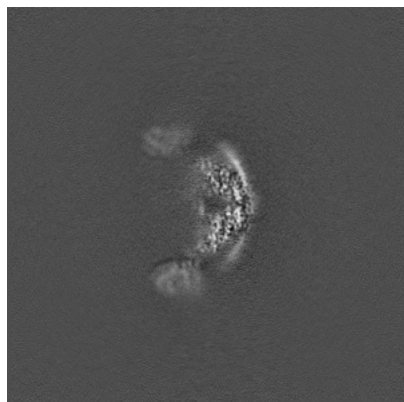


Y Index: 192

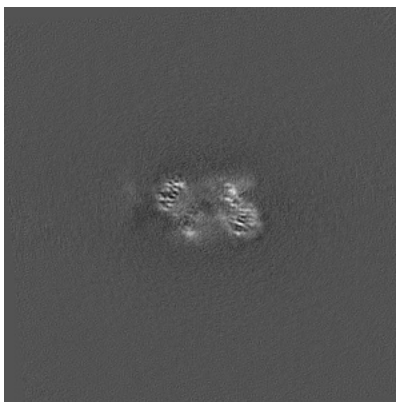


Z Index: 192

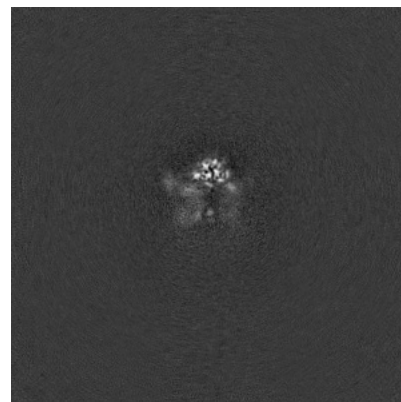
6.2.2 Raw map



X Index: 192



Y Index: 192

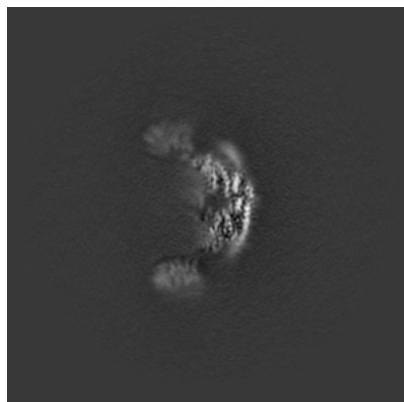


Z Index: 192

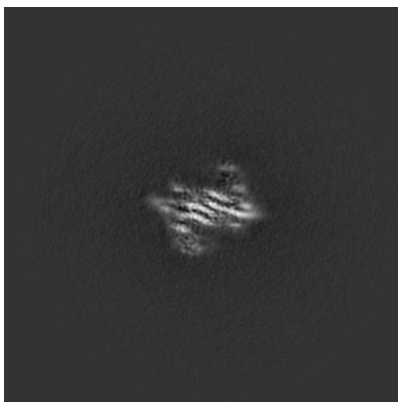
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

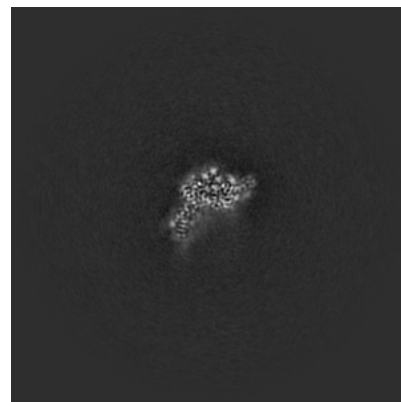
6.3.1 Primary map



X Index: 188

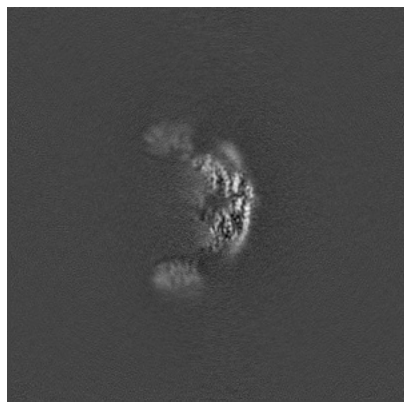


Y Index: 221

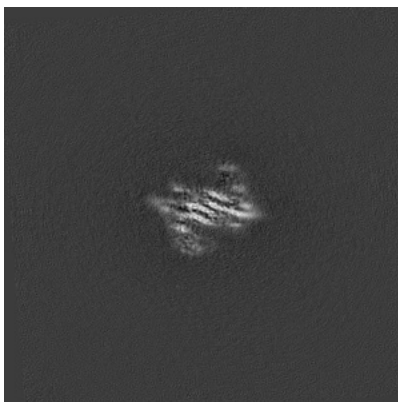


Z Index: 221

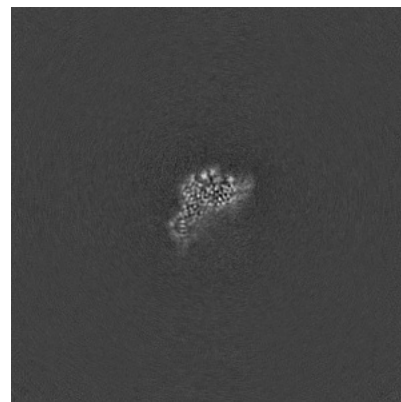
6.3.2 Raw map



X Index: 188



Y Index: 221

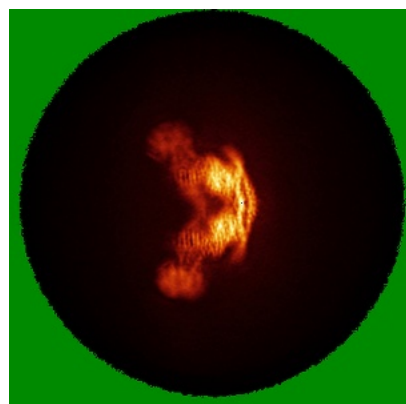


Z Index: 224

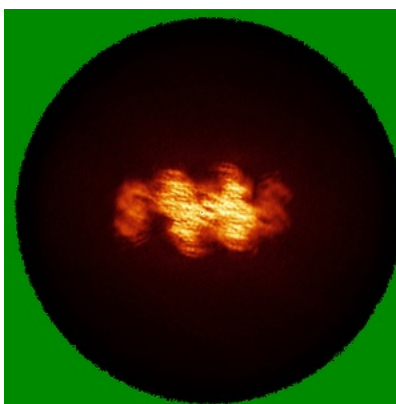
The images above show the largest variance slices of the map in three orthogonal directions.

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

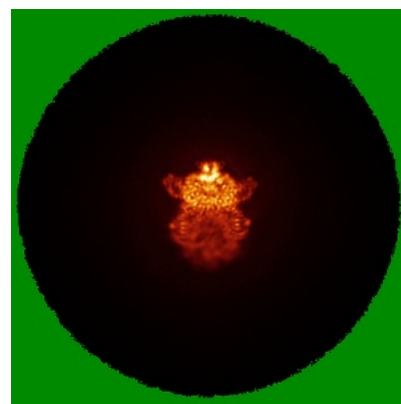
6.4.1 Primary map



X

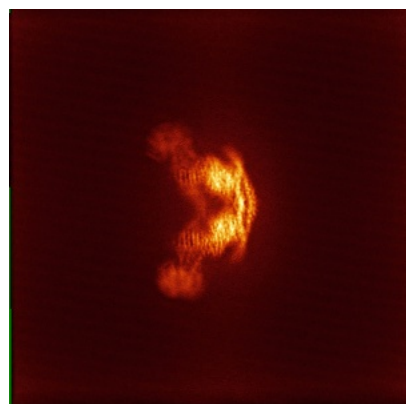


Y

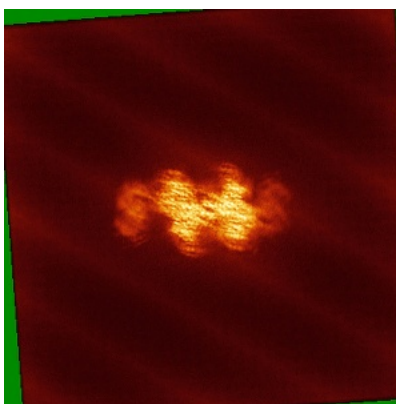


Z

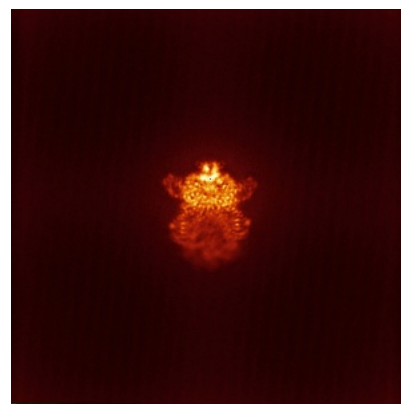
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

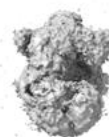
6.5.1 Primary map



X



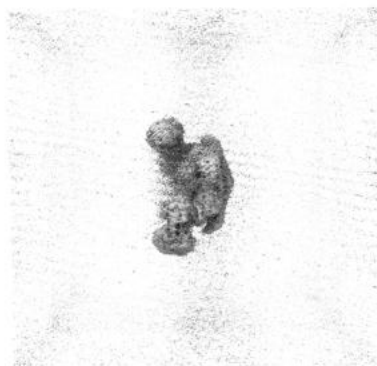
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

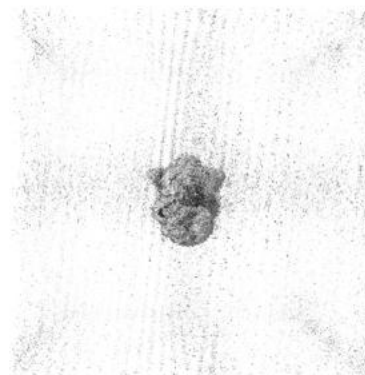
6.5.2 Raw map



X



Y



Z

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

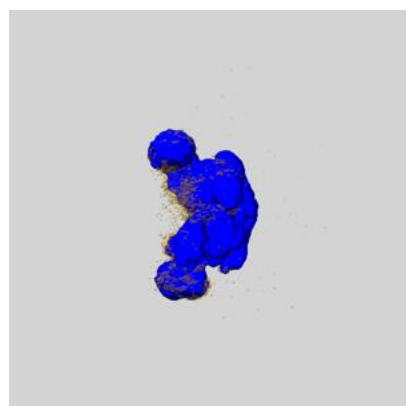
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

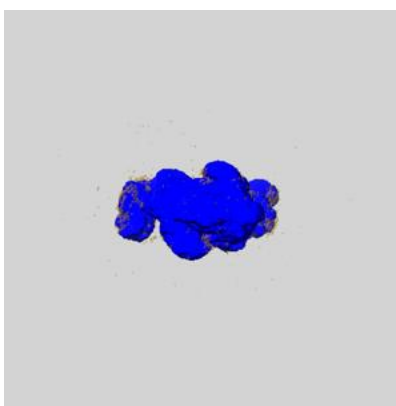
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

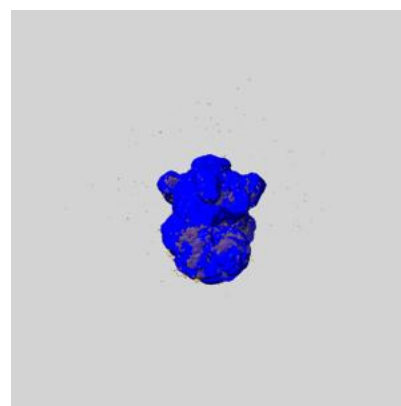
6.6.1 emd_55053_msk_1.map [i](#)



X



Y

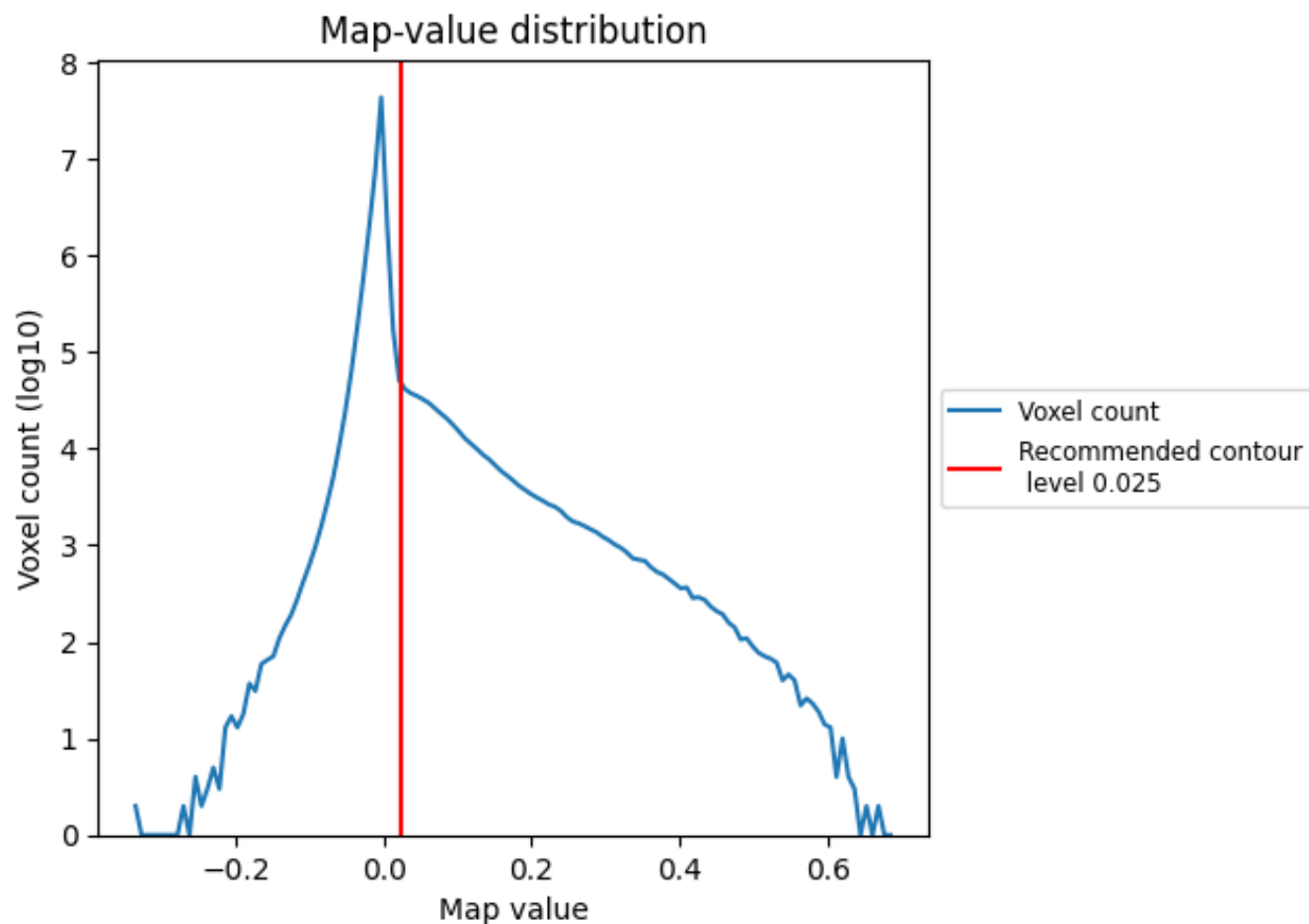


Z

7 Map analysis [i](#)

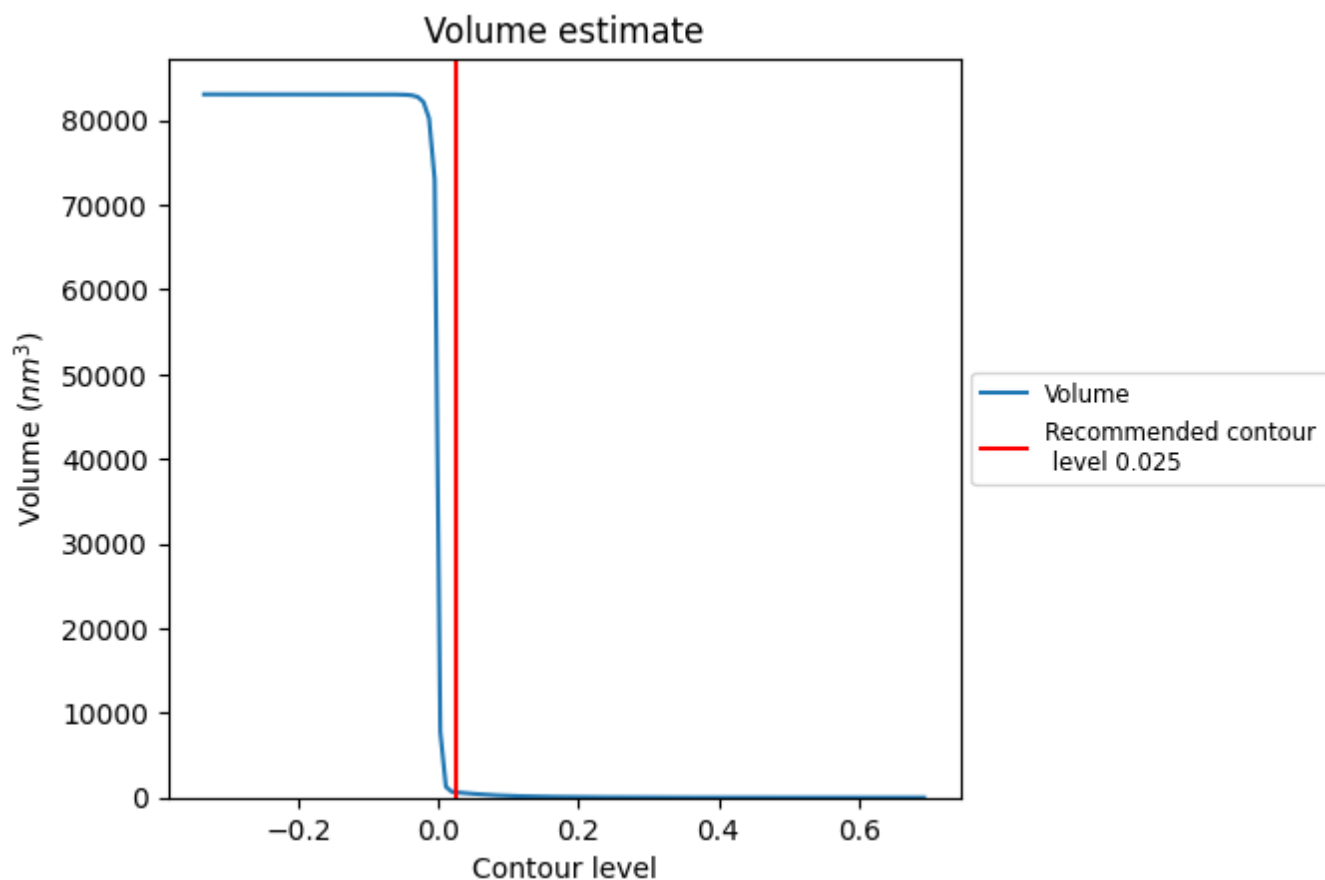
This section contains the results of statistical analysis of the map.

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.

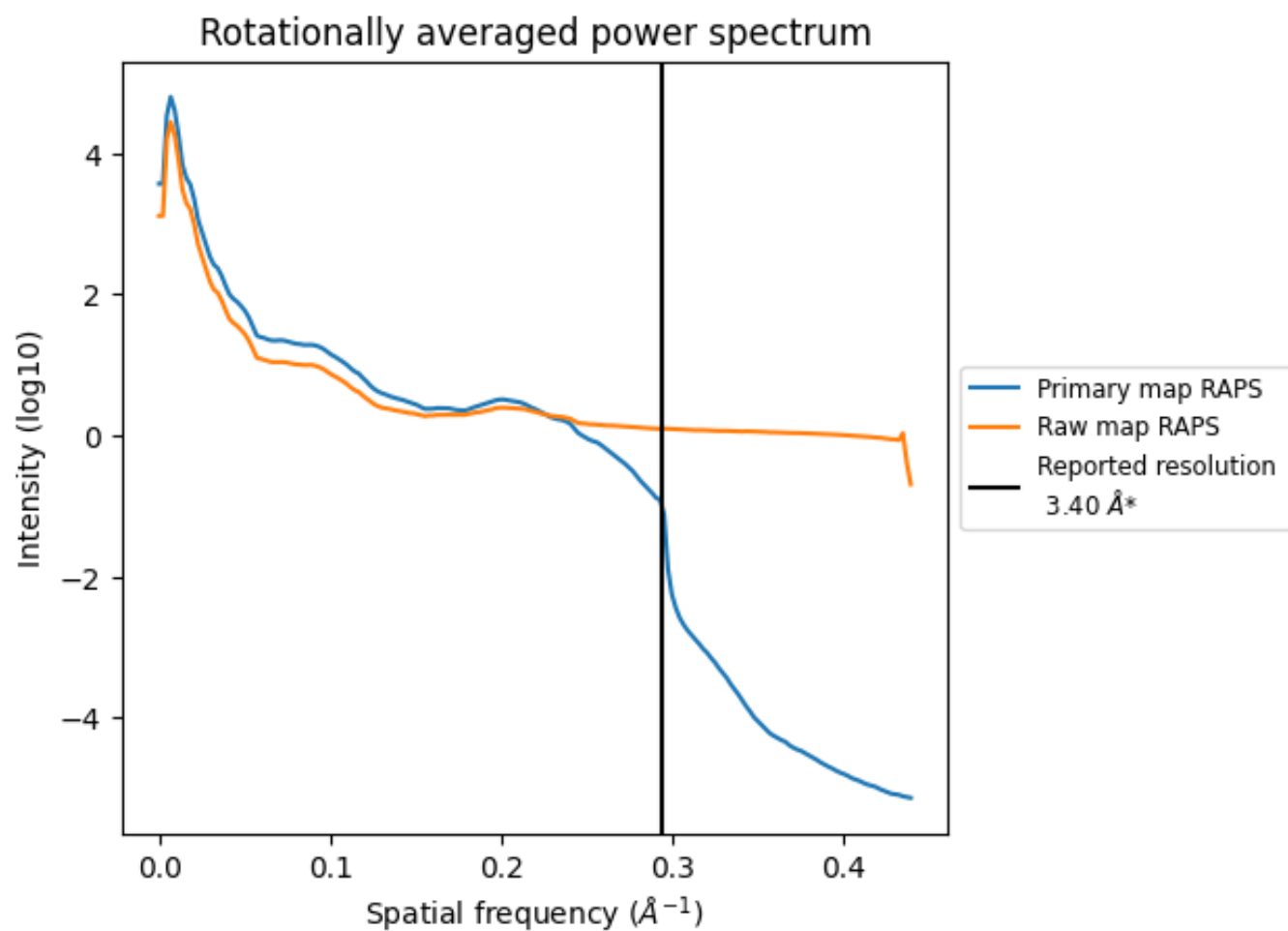
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 627 nm^3 ; this corresponds to an approximate mass of 566 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 ⓘ

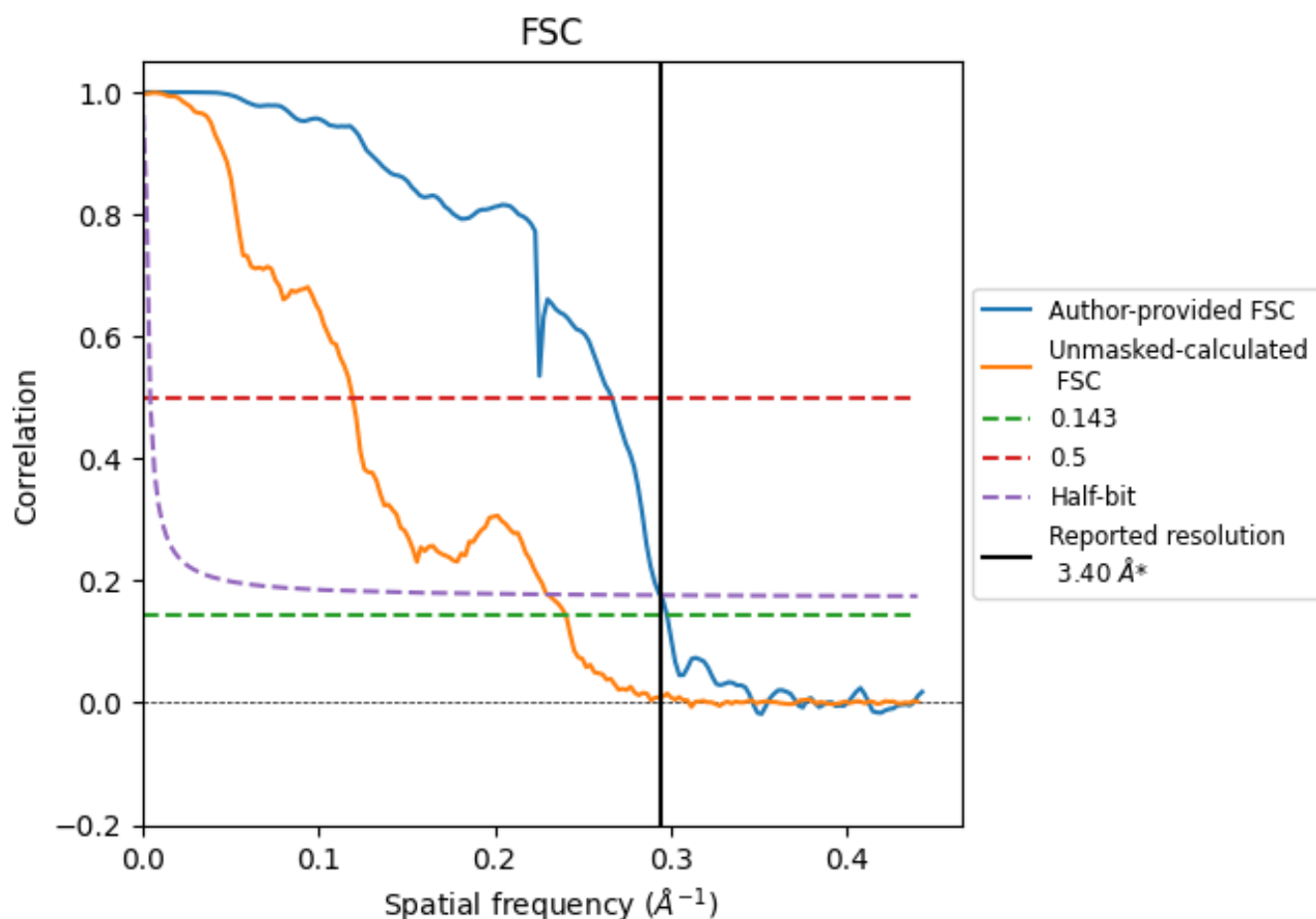


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

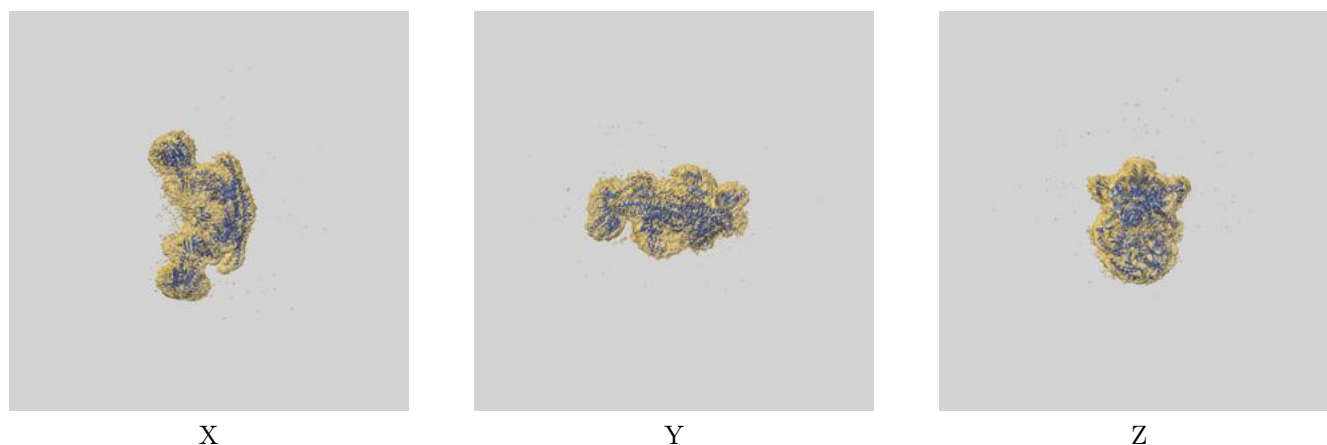
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.75	3.40
Unmasked-calculated*	4.16	8.38	4.35

*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 4.16 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

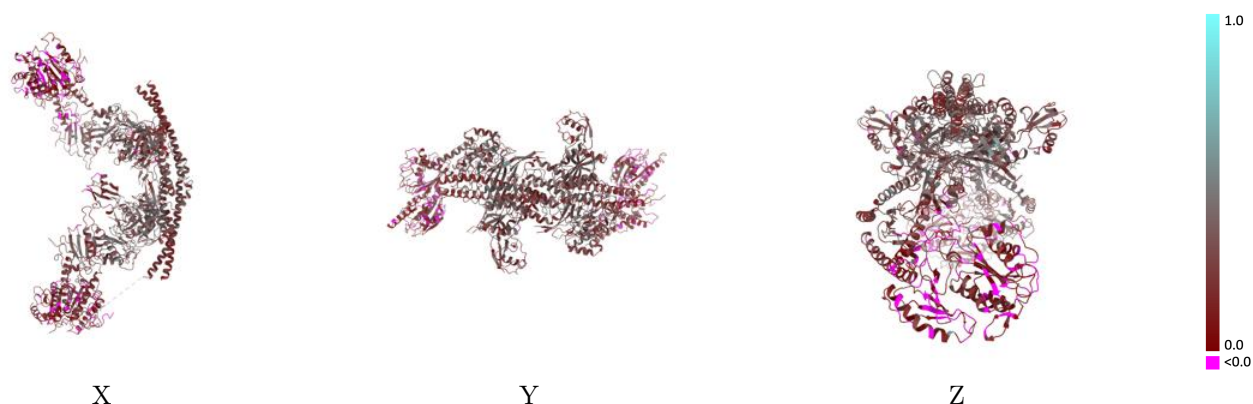
This section contains information regarding the fit between EMDB map EMD-55053 and PDB model 9SO9. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



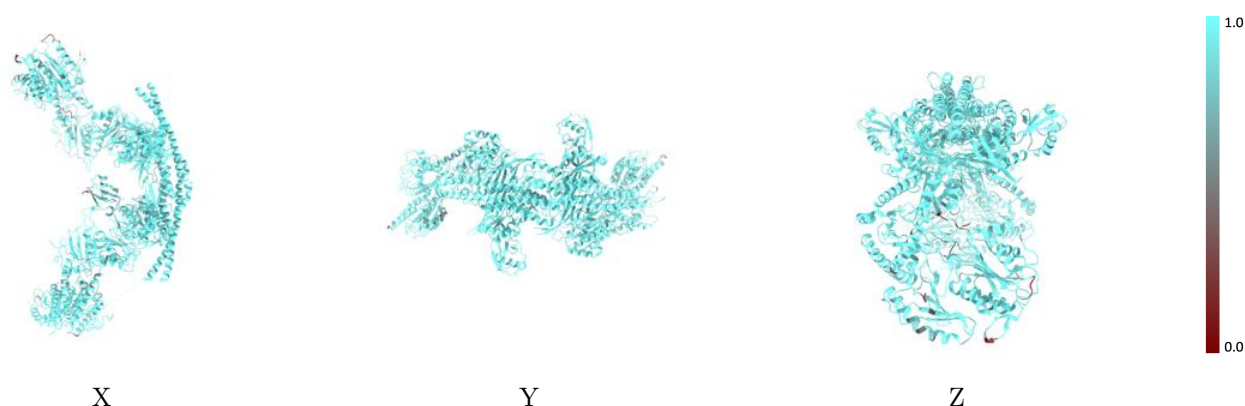
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



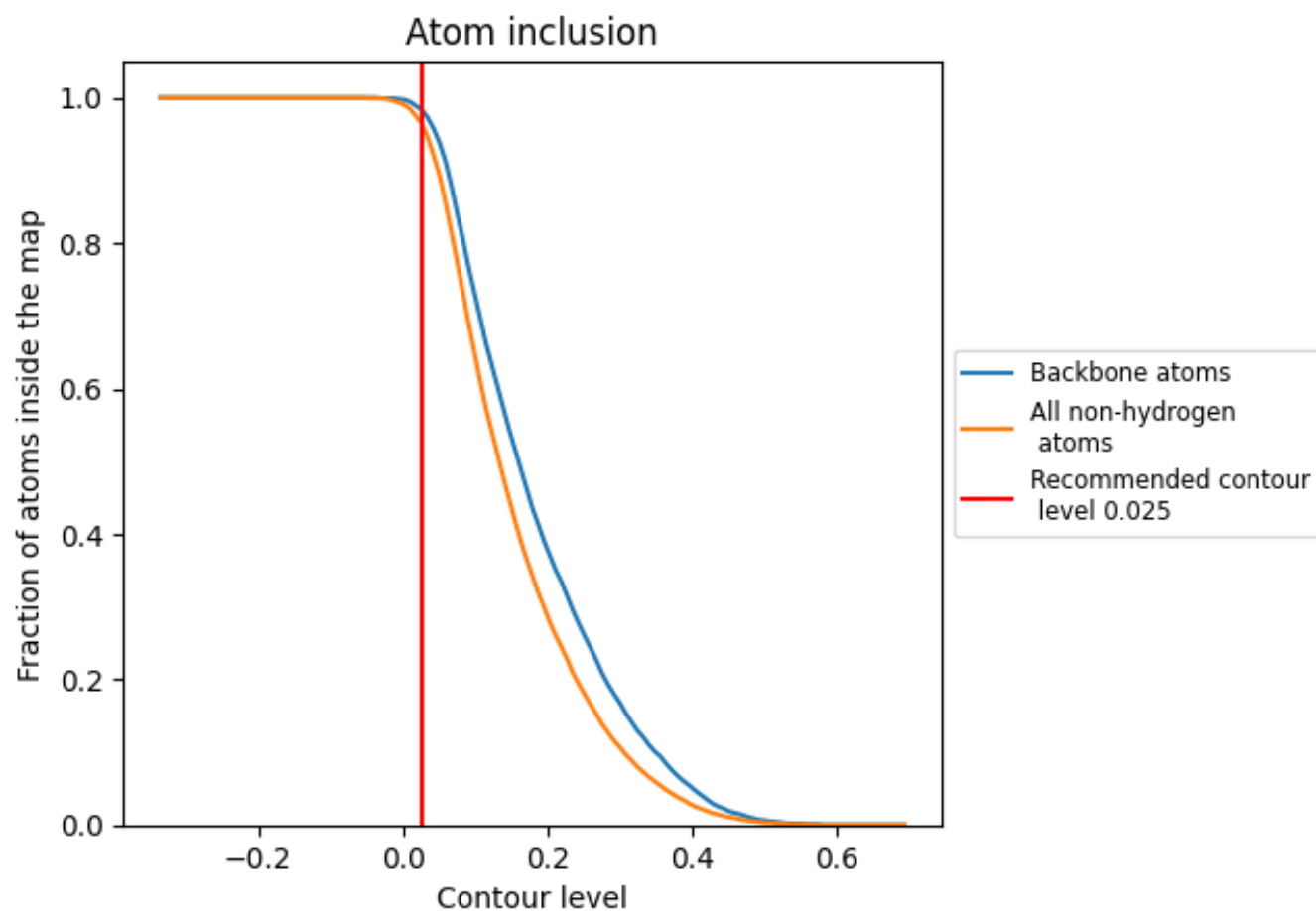
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9660	0.2530
A	0.9870	0.3200
B	0.9880	0.3230
C	0.9700	0.2810
D	0.9420	0.1340
E	0.9760	0.2380
F	0.9960	0.3230
G	0.9950	0.3220
H	0.9540	0.2160
I	0.9270	0.1230
J	0.9650	0.1670
L	0.9460	0.2530
M	0.8320	0.1830
N	0.9770	0.2730

1.0

0.0

<0.0