



Full wwPDB EM Validation Report ⓘ

May 10, 2026 – 12:26 AM JST

PDB ID : 9W2S / pdb_00009w2s
EMDB ID : EMD-65578
Title : Cryo-EM structure of FoF1-ATPase monomer state 3 on the bovine heart submitochondrial particles (FoF1-2)
Authors : Nakano, A.; Masuya, T.; Akisada, S.; Ishikawa-Fukuda, M.; Mitsuoka, K.; Miyoshi, H.; Murai, M.; Yokoyama, K.
Deposited on : 2025-07-28
Resolution : 4.00 Å (reported)
Based on initial model : 6ZPO

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

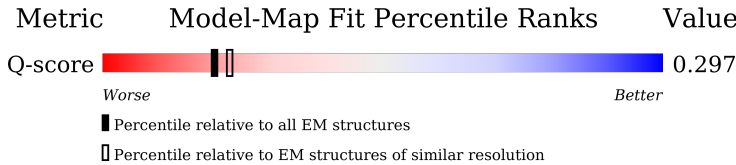
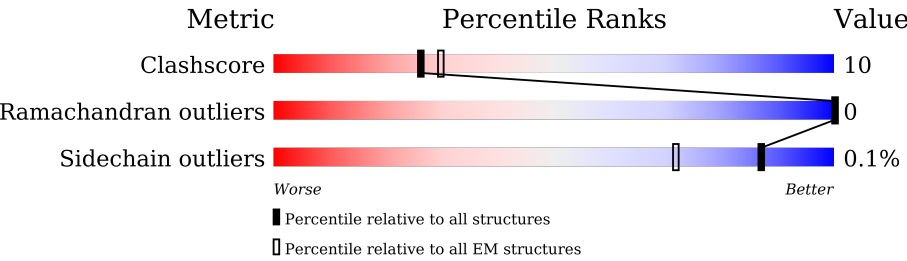
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.00 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.



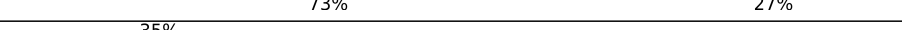
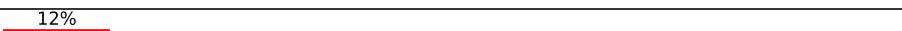
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	8	66	33% 29% 26% 45%
2	A	510	77% 21% .
2	B	510	82% 18%
2	C	510	78% 17% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	482	
3	E	482	
3	F	482	
4	G	273	
5	H	146	
6	I	50	
7	J	60	
8	K	75	
8	L	75	
8	M	75	
8	N	75	
8	O	75	
8	P	75	
8	Q	75	
8	R	75	
9	S	190	
10	a	226	
11	b	214	
12	d	160	
13	e	70	
14	f	87	
15	g	102	
16	h	76	
17	j	60	
18	k	57	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 39116 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 ATP synthase F(0) complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	36	Total	C	N	O	S	0	0
			294	199	43	49	3		

- Molecule 2 is a protein called ATP synthase F(1) complex subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	486	Total	C	N	O	S	0	0
			3710	2339	655	704	12		
2	A	501	Total	C	N	O	S	0	0
			3820	2406	673	729	12		
2	B	508	Total	C	N	O	S	0	0
			3870	2435	681	742	12		

- Molecule 3 is a protein called ATP synthase F(1) complex catalytic subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	467	Total	C	N	O	S	0	0
			3539	2243	601	684	11		
3	D	469	Total	C	N	O	S	0	0
			3558	2254	605	688	11		
3	E	467	Total	C	N	O	S	0	0
			3539	2243	601	684	11		

- Molecule 4 is a protein called ATP synthase F(1) complex subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2115	1330	368	409	8		

- Molecule 5 is a protein called ATP synthase F(1) complex subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	131	Total	C	N	O	S	0	0
			971	609	163	197	2		

- Molecule 6 is a protein called ATP synthase F(1) complex subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	47	Total	C	N	O	S	0	0
			369	237	66	64	2		

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	47	Total	C	N	O	S	0	0
			370	224	76	70			

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	74	Total	C	N	O	S	0	0
			529	351	82	93	3		
8	L	74	Total	C	N	O	S	0	0
			523	346	82	93	2		
8	M	75	Total	C	N	O	S	0	0
			538	356	83	95	4		
8	N	74	Total	C	N	O	S	0	0
			529	351	82	93	3		
8	O	75	Total	C	N	O	S	0	0
			538	356	83	95	4		
8	P	74	Total	C	N	O	S	0	0
			520	342	82	93	3		
8	Q	75	Total	C	N	O	S	0	0
			529	347	83	95	4		
8	R	75	Total	C	N	O	S	0	0
			538	356	83	95	4		

- Molecule 9 is a protein called ATP synthase peripheral stalk subunit OSCP, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	187	Total	C	N	O	S	0	0
			1438	915	248	266	9		

- Molecule 10 is a protein called ATP synthase F(0) complex subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	223	Total	C	N	O	S	0	0
			1690	1117	272	290	11		

- Molecule 11 is a protein called ATP synthase peripheral stalk subunit b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	b	205	Total	C	N	O	S	0	0
			1603	1014	282	301	6		

- Molecule 12 is a protein called ATP synthase peripheral stalk subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	155	Total	C	N	O	S	0	0
			1249	804	203	239	3		

- Molecule 13 is a protein called ATP synthase F(0) complex subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	55	Total	C	N	O	0	0
			410	252	81	77		

- Molecule 14 is a protein called ATP synthase F(0) complex subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	81	Total	C	N	O	S	0	0
			632	413	109	109	1		

- Molecule 15 is a protein called ATP synthase F(0) complex subunit g, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	g	79	Total	C	N	O	0	0
			551	361	95	95		

- Molecule 16 is a protein called ATP synthase peripheral stalk subunit F6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	62	Total	C	N	O	S	0	0
			514	326	87	99	2		

- Molecule 17 is a protein called ATP synthase F(0) complex subunit j, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	46	Total	C	N	O	S	0	0
			378	252	63	61	2		

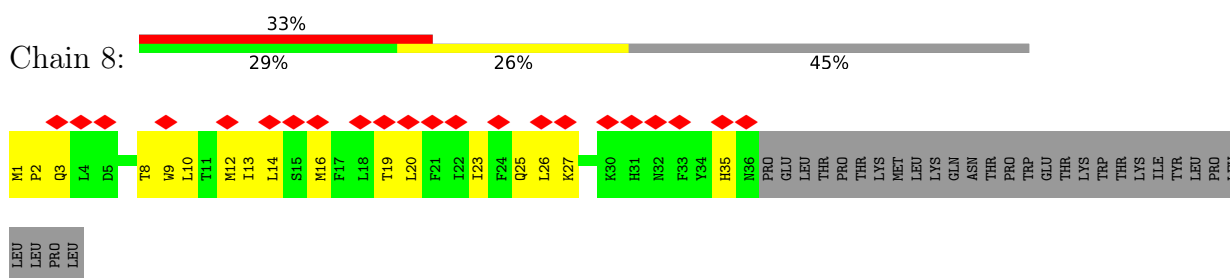
- Molecule 18 is a protein called ATP synthase F(0) complex subunit k, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	35	Total	C	N	O	S	0	0
			252	163	43	44	2		

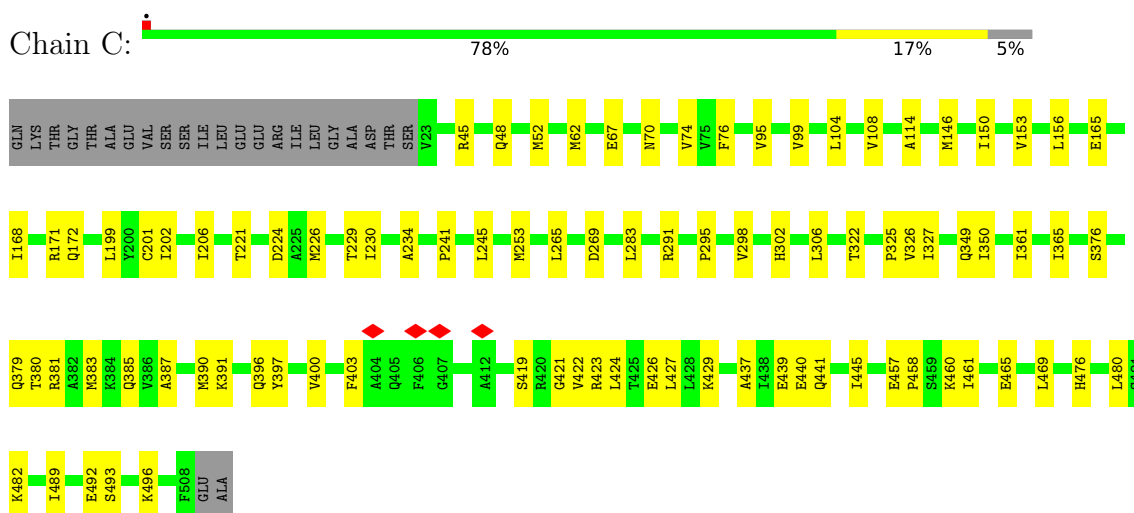
3 Residue-property plots

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.

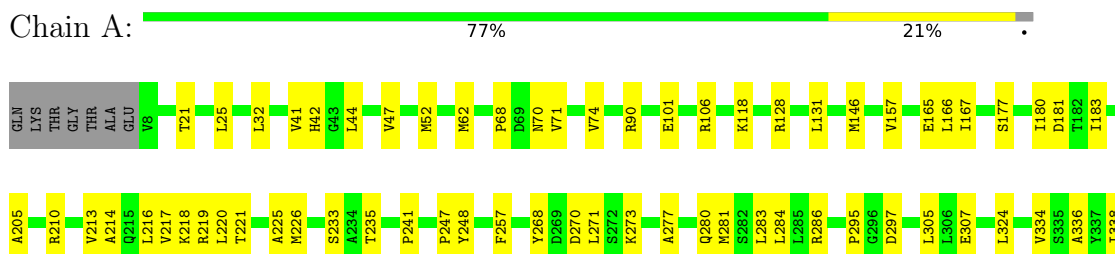
- Molecule 1: ATP synthase F(0) complex subunit 8

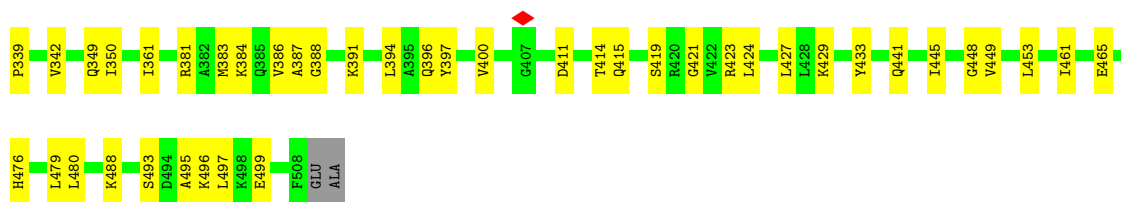


- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial

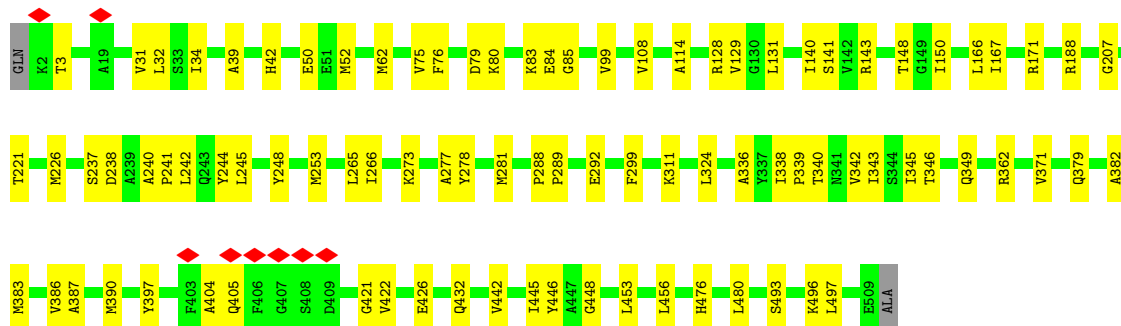
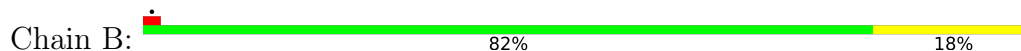


- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial

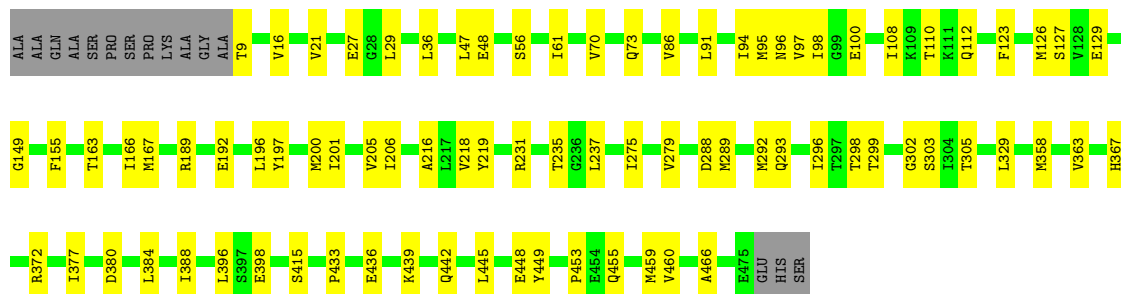
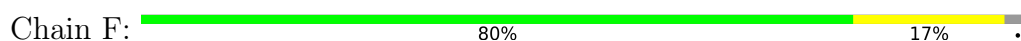




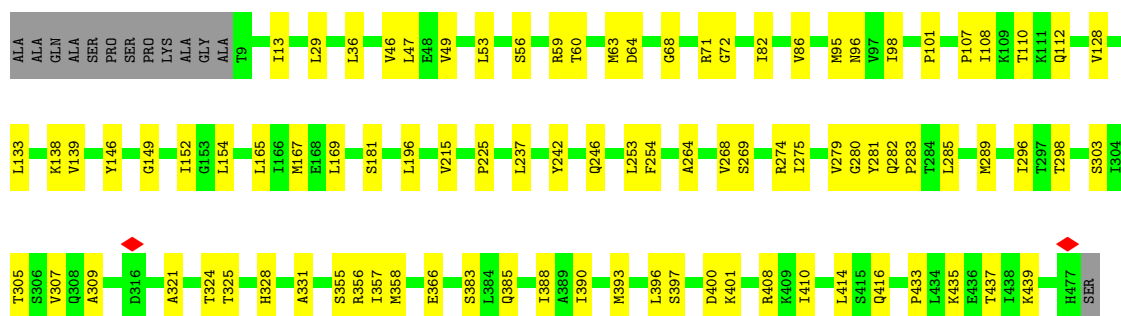
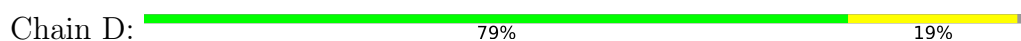
- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial



- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

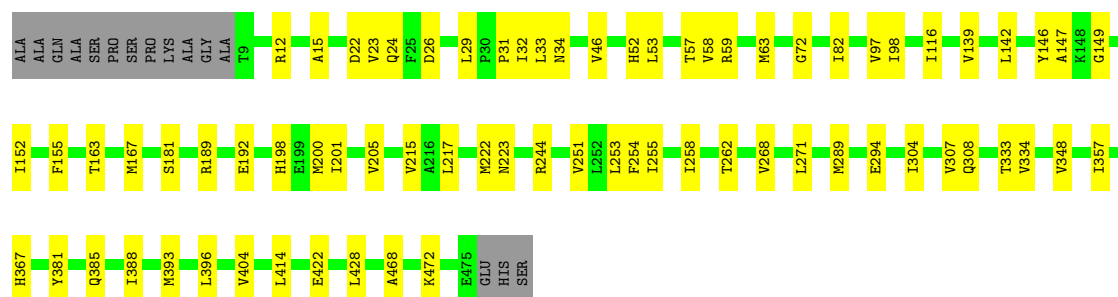


- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial



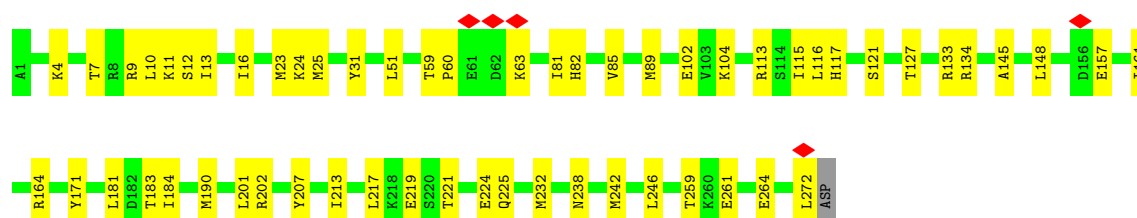
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain E:  82% 15% .



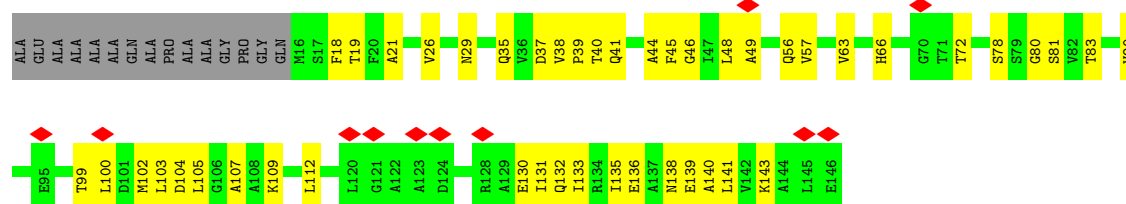
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial

Chain G:  79% 21%



- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

Chain H:  8% 58% 32% 10%



- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial

Chain I:  10% 56% 38% 6%

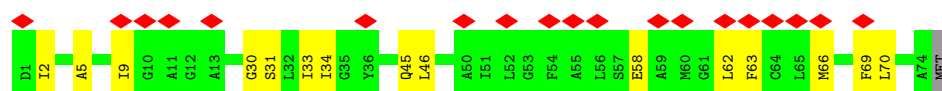
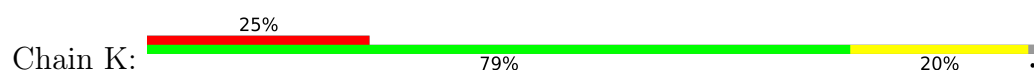


- Molecule 7: ATPase inhibitor, mitochondrial

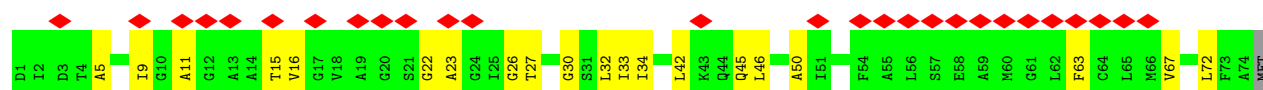
Chain J:  68% 10% 22%



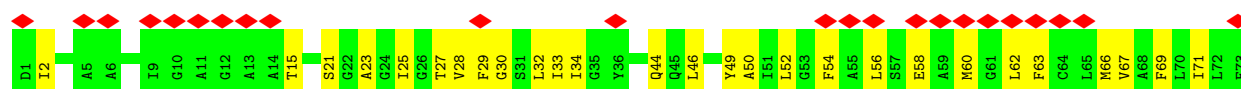
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



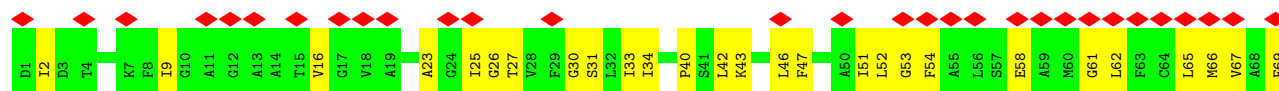
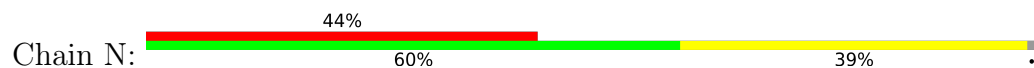
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



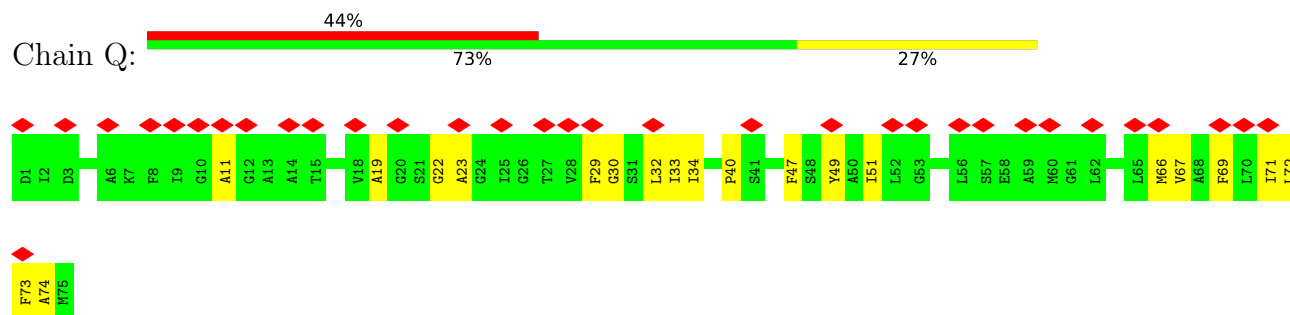
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



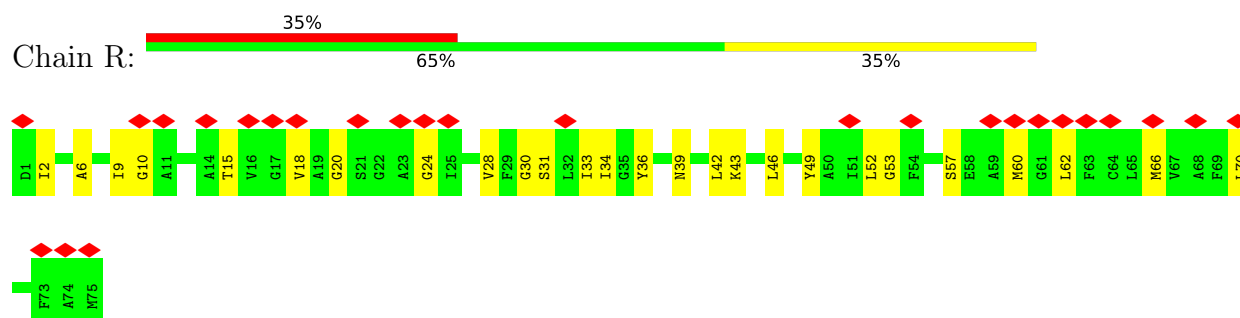
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



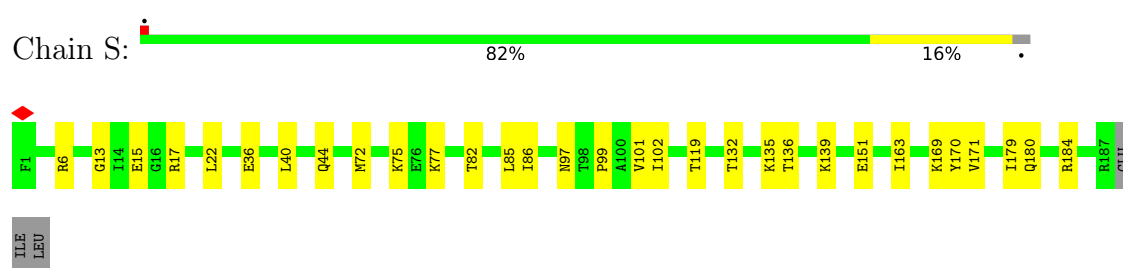
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



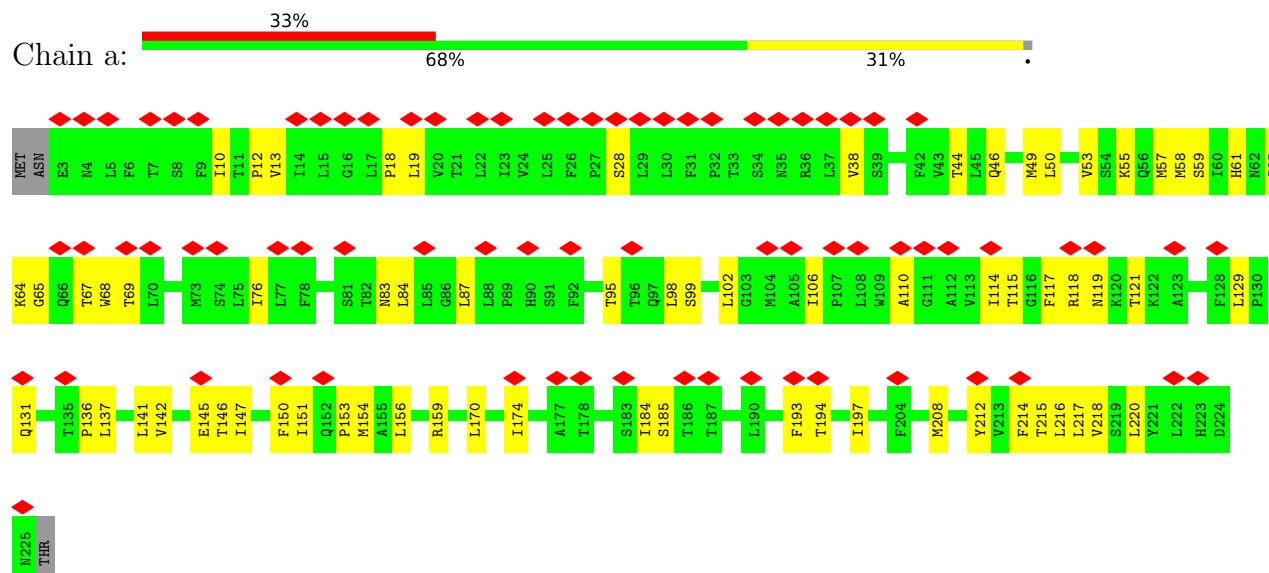
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

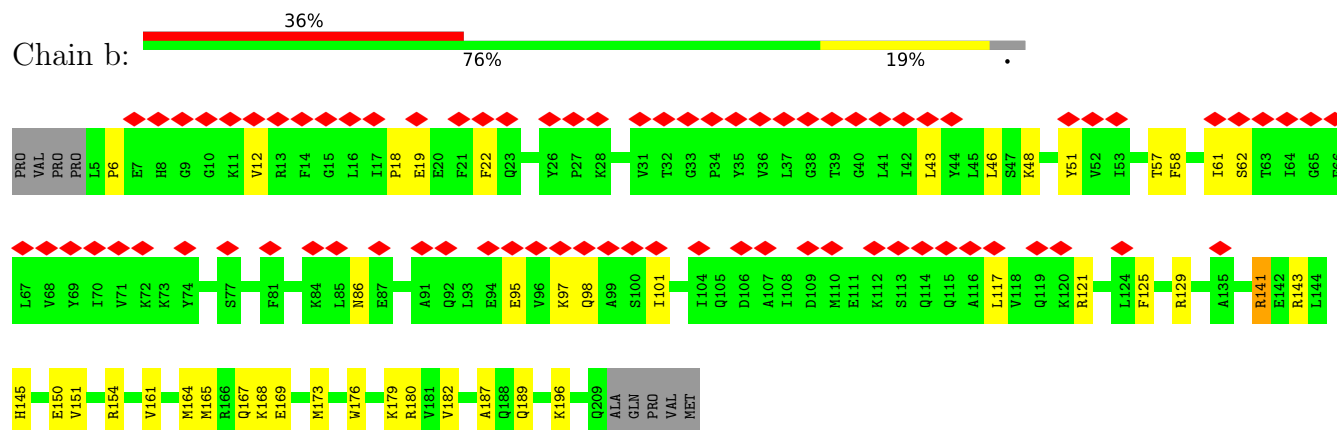


- Molecule 10: ATP synthase F(0) complex subunit a



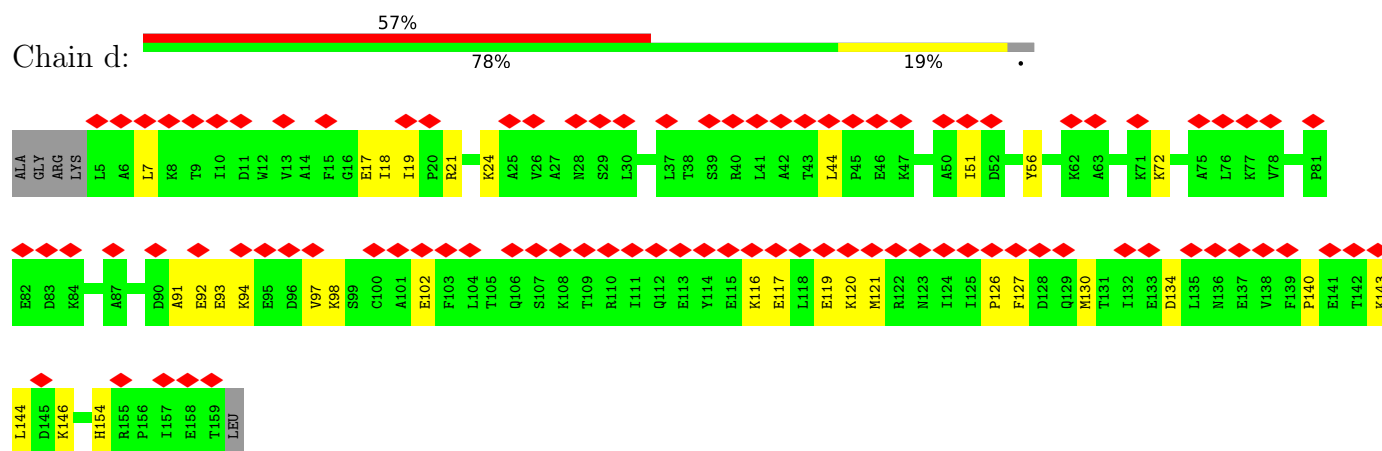
- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

Chain b:



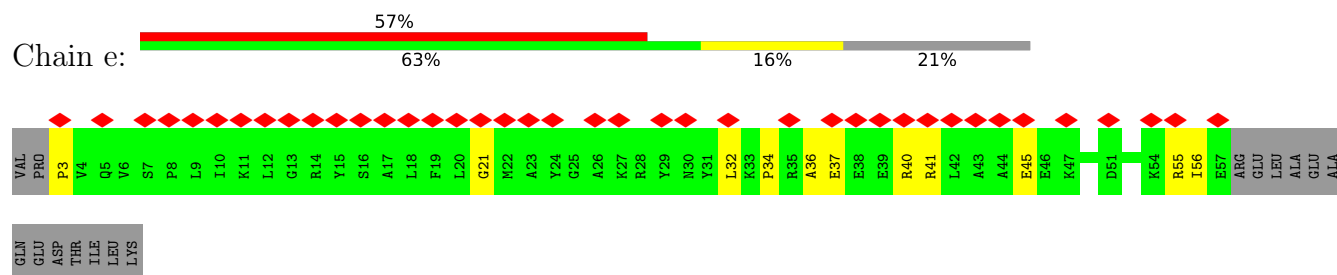
- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

Chain d:



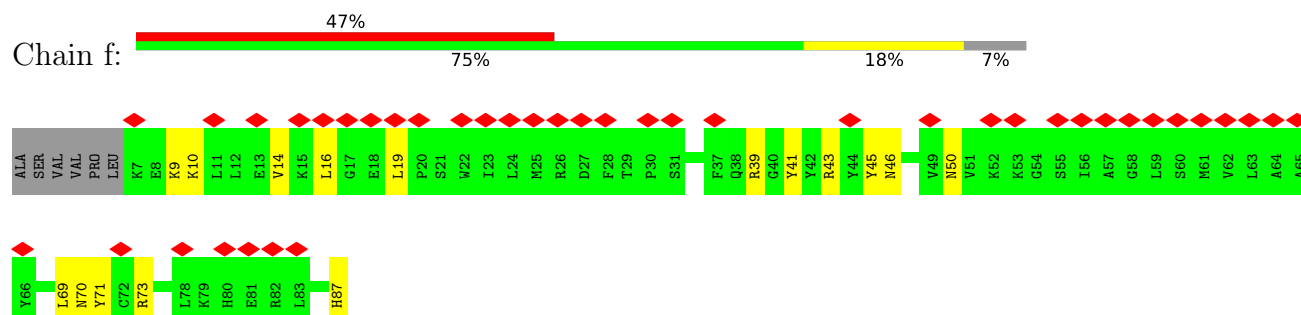
- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

Chain e:

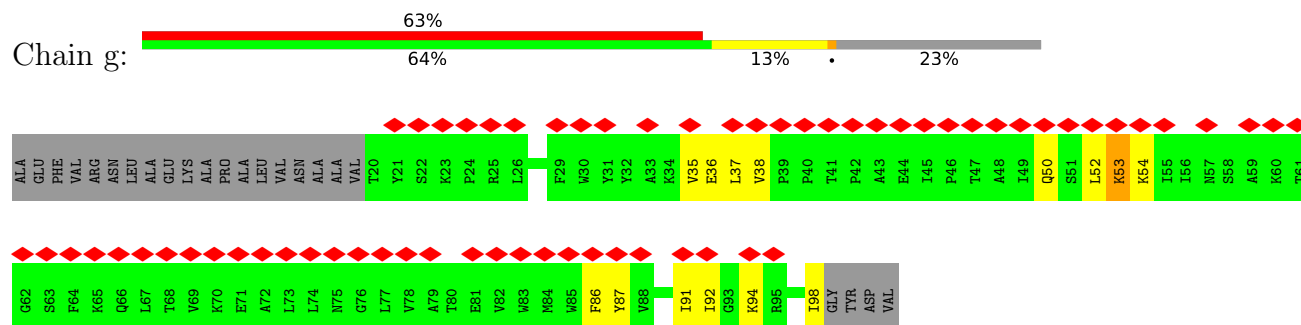


- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

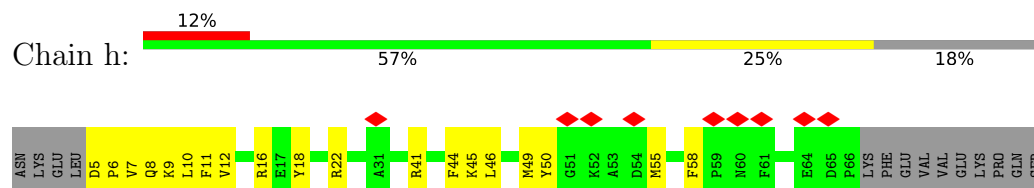
Chain f:



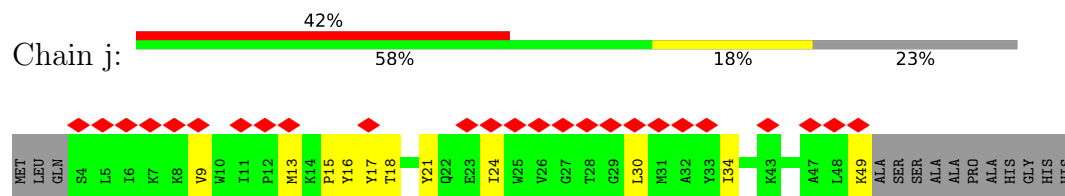
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial



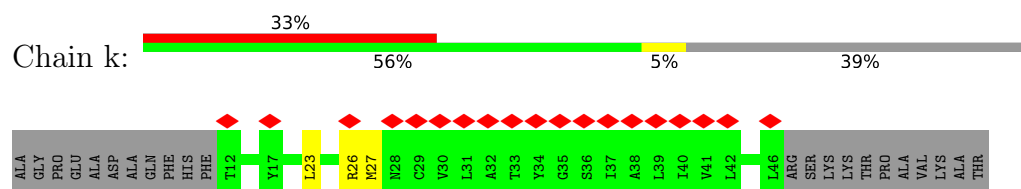
- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial



- Molecule 17: ATP synthase F(0) complex subunit j, mitochondrial



- Molecule 18: ATP synthase F(0) complex subunit k, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	328822	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)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.751	Depositor
Minimum map value	-0.269	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	654.0, 654.0, 654.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4533334, 1.4533334, 1.4533334	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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	8	0.16	0/302	0.48	0/410
2	A	0.15	0/3871	0.47	0/5223
2	B	0.29	0/3921	0.64	1/5290 (0.0%)
2	C	0.22	0/3761	0.52	2/5074 (0.0%)
3	D	0.27	0/3616	0.56	0/4906
3	E	0.14	0/3596	0.41	0/4879
3	F	0.22	0/3596	0.50	0/4879
4	G	0.14	0/2141	0.43	0/2876
5	H	0.12	0/983	0.43	0/1337
6	I	0.16	0/374	0.56	0/501
7	J	0.41	0/374	0.97	0/495
8	K	0.38	0/526	0.85	0/711
8	L	0.37	0/520	0.82	0/704
8	M	0.17	0/535	0.51	0/721
8	N	0.17	0/526	0.49	0/711
8	O	0.18	0/535	0.52	0/721
8	P	0.32	0/516	0.82	0/698
8	Q	0.50	0/525	0.92	0/708
8	R	0.31	0/535	0.65	0/721
9	S	0.18	0/1455	0.48	0/1957
10	a	0.34	0/1726	0.70	0/2363
11	b	0.36	0/1627	0.69	1/2190 (0.0%)
12	d	0.36	0/1279	0.70	0/1736
13	e	0.14	0/415	0.49	0/556
14	f	0.11	0/648	0.38	0/871
15	g	0.54	0/561	0.64	0/763
16	h	0.46	0/526	0.85	1/707 (0.1%)
17	j	0.16	0/388	0.49	0/522
18	k	0.09	0/256	0.30	0/344
All	All	0.26	0/39634	0.57	5/53574 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	b	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	172	GLN	CA-C-N	6.68	129.53	120.38
2	C	172	GLN	C-N-CA	6.68	129.53	120.38
16	h	16	ARG	NE-CZ-NH2	5.62	124.26	119.20
11	b	143	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	B	188	ARG	NE-CZ-NH2	5.25	123.93	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	b	141	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	294	0	294	16	0
2	A	3820	0	3927	79	0
2	B	3870	0	3974	64	0
2	C	3710	0	3815	62	0
3	D	3558	0	3606	63	0
3	E	3539	0	3593	52	0
3	F	3539	0	3593	63	0
4	G	2115	0	2185	39	0
5	H	971	0	970	42	0
6	I	369	0	395	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	370	0	361	7	0
8	K	529	0	550	12	0
8	L	523	0	534	17	0
8	M	538	0	559	34	0
8	N	529	0	550	26	0
8	O	538	0	559	23	0
8	P	520	0	534	26	0
8	Q	529	0	543	20	0
8	R	538	0	559	24	0
9	S	1438	0	1551	24	0
10	a	1690	0	1784	62	0
11	b	1603	0	1578	45	0
12	d	1249	0	1233	34	0
13	e	410	0	375	8	0
14	f	632	0	604	13	0
15	g	551	0	516	9	0
16	h	514	0	495	23	0
17	j	378	0	395	10	0
18	k	252	0	229	4	0
All	All	39116	0	39861	794	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 10.

All (794) 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)
5:H:40:THR:HG23	5:H:57:VAL:O	1.21	1.28
11:b:145:HIS:CD2	12:d:44:LEU:HD13	1.70	1.25
9:S:179:ILE:HB	16:h:10:LEU:HD13	1.17	1.13
2:B:362:ARG:NH1	2:B:432:GLN:HE22	1.49	1.10
2:B:362:ARG:CZ	2:B:432:GLN:NE2	2.13	1.09
2:B:362:ARG:CZ	2:B:432:GLN:HE22	1.66	1.05
8:P:32:LEU:HD12	8:P:50:ALA:CB	1.87	1.04
3:F:358:MET:HE1	3:F:372:ARG:NH1	1.71	1.03
8:M:32:LEU:HD12	8:M:50:ALA:HB2	1.39	1.03
8:M:32:LEU:HD12	8:M:50:ALA:CB	1.89	1.01
8:P:32:LEU:HD12	8:P:50:ALA:HB2	1.43	1.00
5:H:40:THR:CG2	5:H:57:VAL:O	2.11	0.97
9:S:179:ILE:HB	16:h:10:LEU:CD1	1.94	0.97
8:L:33:ILE:HD11	8:M:46:LEU:HG	1.45	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:16:VAL:HG22	8:P:13:ALA:O	1.66	0.95
8:M:32:LEU:CD1	8:M:50:ALA:CB	2.46	0.93
2:B:362:ARG:NE	2:B:432:GLN:NE2	2.16	0.92
11:b:196:LYS:HE2	16:h:7:VAL:HA	1.50	0.92
2:B:362:ARG:NH1	2:B:432:GLN:NE2	2.16	0.88
1:8:27:LYS:HE3	10:a:28:SER:O	1.73	0.87
5:H:40:THR:HG21	5:H:56:GLN:OE1	1.75	0.87
3:F:358:MET:CE	3:F:372:ARG:NH1	2.39	0.85
5:H:104:ASP:CG	5:H:107:ALA:HB3	2.01	0.85
8:M:32:LEU:CD1	8:M:50:ALA:HB2	2.07	0.84
10:a:106:ILE:HG22	10:a:153:PRO:HB2	1.61	0.83
2:A:165:GLU:OE2	2:A:350:ILE:HG12	1.78	0.82
5:H:104:ASP:OD2	5:H:107:ALA:HB3	1.80	0.81
2:C:67:GLU:OE1	2:C:70:ASN:ND2	2.13	0.81
3:F:126:MET:HE3	3:F:126:MET:H	1.45	0.81
10:a:76:ILE:HB	10:a:215:THR:HG21	1.61	0.81
9:S:179:ILE:CB	16:h:10:LEU:HD13	2.07	0.81
12:d:117:GLU:HG3	12:d:121:MET:HE1	1.64	0.80
11:b:145:HIS:HD2	12:d:44:LEU:HD13	1.39	0.79
3:F:358:MET:HE1	3:F:372:ARG:HH11	1.48	0.78
2:B:362:ARG:NE	2:B:432:GLN:HE21	1.80	0.77
3:E:24:GLN:HG3	3:E:57:THR:OG1	1.84	0.76
13:e:55:ARG:NH2	13:e:56:ILE:HG13	1.99	0.76
13:e:55:ARG:HH22	13:e:56:ILE:HG13	1.51	0.75
8:P:63:PHE:HA	8:P:66:MET:HG3	1.68	0.75
2:B:422:VAL:HG13	2:B:426:GLU:OE2	1.87	0.74
5:H:104:ASP:OD2	5:H:107:ALA:CB	2.36	0.74
3:D:152:ILE:HB	3:D:307:VAL:HG12	1.70	0.73
8:P:60:MET:HA	8:P:63:PHE:CE2	2.23	0.73
8:M:32:LEU:CD1	8:M:50:ALA:HB1	2.19	0.73
11:b:187:ALA:HB3	11:b:189:GLN:HE22	1.55	0.72
8:R:66:MET:HE3	8:R:70:LEU:HB2	1.70	0.72
8:K:45:GLN:HG3	8:R:36:TYR:HE2	1.55	0.72
2:C:390:MET:HE2	2:C:390:MET:HA	1.71	0.71
3:F:149:GLY:H	3:F:305:THR:HG22	1.55	0.71
3:F:155:PHE:HZ	3:F:329:LEU:HD11	1.55	0.71
2:B:362:ARG:HE	2:B:432:GLN:HE21	1.36	0.71
2:A:283:LEU:HD11	3:D:275:ILE:HB	1.72	0.70
4:G:115:ILE:HG23	4:G:116:LEU:HD22	1.74	0.69
2:A:62:MET:HE2	2:A:62:MET:HA	1.72	0.69
5:H:99:THR:H	5:H:102:MET:HE1	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:23:VAL:O	3:E:57:THR:HG23	1.92	0.69
3:F:358:MET:HE1	3:F:372:ARG:CZ	2.23	0.68
2:C:302:HIS:O	2:C:306:LEU:HD13	1.92	0.68
8:P:32:LEU:HD12	8:P:50:ALA:HB1	1.74	0.68
1:8:16:MET:O	1:8:20:LEU:HD12	1.94	0.68
3:E:24:GLN:CG	3:E:57:THR:OG1	2.42	0.67
8:M:32:LEU:HD12	8:M:50:ALA:HB1	1.72	0.67
2:C:265:LEU:HD23	2:C:322:THR:HB	1.76	0.67
8:P:32:LEU:CD1	8:P:50:ALA:CB	2.69	0.67
2:A:157:VAL:HG11	2:A:350:ILE:HD11	1.76	0.67
2:A:283:LEU:HD23	3:D:283:PRO:HB3	1.75	0.67
8:N:30:GLY:HA2	8:N:33:ILE:HD12	1.76	0.67
2:C:201:CYS:HB2	2:C:229:THR:HG23	1.76	0.66
8:O:19:ALA:HB2	8:P:17:GLY:HA2	1.77	0.66
8:R:30:GLY:O	8:R:34:ILE:HG12	1.94	0.65
3:D:139:VAL:HG12	3:D:414:LEU:HD12	1.77	0.65
3:F:16:VAL:HG22	3:F:21:VAL:HG13	1.79	0.65
3:F:96:ASN:HD21	3:F:100:GLU:HB2	1.62	0.64
5:H:18:PHE:HA	5:H:90:VAL:HB	1.79	0.64
11:b:196:LYS:HE2	16:h:7:VAL:CA	2.25	0.64
10:a:141:LEU:O	10:a:145:GLU:HG3	1.97	0.64
2:A:277:ALA:O	2:A:281:MET:HG2	1.97	0.64
3:D:95:MET:HE2	3:D:95:MET:HA	1.80	0.64
2:C:390:MET:HE1	2:C:424:LEU:HD13	1.80	0.63
2:A:180:ILE:HG22	2:A:183:ILE:HD11	1.80	0.63
8:O:54:PHE:CE1	8:P:56:LEU:HD11	2.33	0.63
2:C:376:SER:HA	2:C:379:GLN:HG2	1.80	0.63
10:a:156:LEU:HD21	10:a:217:LEU:HD22	1.81	0.63
3:D:275:ILE:HD12	3:D:275:ILE:H	1.63	0.63
3:E:52:HIS:HA	3:E:58:VAL:HG12	1.79	0.63
2:B:167:ILE:HD11	2:B:324:LEU:HD12	1.80	0.63
8:K:5:ALA:O	8:K:9:ILE:HG12	1.99	0.63
11:b:196:LYS:CE	16:h:7:VAL:HA	2.27	0.63
5:H:40:THR:HG22	5:H:41:GLN:N	2.14	0.62
2:B:422:VAL:CG1	2:B:426:GLU:OE2	2.47	0.62
2:A:381:ARG:HH11	2:A:488:LYS:HG2	1.63	0.62
10:a:208:MET:HE3	10:a:212:TYR:HB2	1.80	0.62
1:8:9:TRP:CZ3	10:a:102:LEU:HD22	2.35	0.62
8:K:30:GLY:HA2	8:K:33:ILE:HD12	1.80	0.62
10:a:55:LYS:O	10:a:59:SER:HB3	1.99	0.62
2:C:156:LEU:HD13	2:C:391:LYS:HE3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:167:MET:HE1	3:D:196:LEU:HD13	1.80	0.62
17:j:13:MET:HE2	17:j:17:TYR:CE1	2.35	0.62
2:B:80:LYS:HA	3:E:32:ILE:HD12	1.82	0.62
8:L:33:ILE:CD1	8:M:46:LEU:HG	2.24	0.61
8:M:30:GLY:O	8:M:33:ILE:HG13	2.00	0.61
8:M:32:LEU:HD11	8:M:50:ALA:CB	2.29	0.61
3:F:126:MET:HA	3:F:299:THR:HA	1.82	0.61
10:a:46:GLN:O	10:a:50:LEU:HG	2.00	0.61
8:M:71:ILE:HA	8:M:75:MET:HG2	1.83	0.61
8:P:24:GLY:O	8:P:28:VAL:HG23	2.00	0.61
2:A:44:LEU:HD12	2:A:47:VAL:HB	1.82	0.61
2:B:493:SER:HA	2:B:496:LYS:HD2	1.83	0.61
3:D:321:ALA:O	3:D:325:THR:HG23	2.00	0.61
2:A:44:LEU:HD11	2:A:90:ARG:HB3	1.82	0.60
2:B:453:LEU:HA	2:B:456:LEU:HD13	1.81	0.60
3:E:46:VAL:HG11	3:E:82:ILE:HD11	1.82	0.60
8:Q:66:MET:HG2	10:a:170:LEU:HD13	1.82	0.60
5:H:45:PHE:HZ	5:H:56:GLN:HG3	1.66	0.60
8:N:47:PHE:O	8:N:51:ILE:HG12	2.01	0.60
8:P:47:PHE:O	8:P:51:ILE:HG12	2.02	0.60
12:d:126:PRO:O	12:d:130:MET:HB2	2.02	0.59
5:H:19:THR:HG23	5:H:29:ASN:HA	1.83	0.59
8:L:33:ILE:HD11	8:M:46:LEU:CG	2.25	0.59
8:M:30:GLY:O	8:M:34:ILE:HG12	2.01	0.59
8:O:32:LEU:HD12	8:O:50:ALA:HB2	1.84	0.59
3:D:154:LEU:HB2	3:D:309:ALA:HA	1.84	0.59
2:A:411:ASP:HB2	2:A:414:THR:HG23	1.85	0.59
10:a:117:PHE:HB3	10:a:121:THR:HG22	1.83	0.59
3:F:384:LEU:HD23	3:F:396:LEU:HD23	1.83	0.59
8:K:9:ILE:HB	8:R:9:ILE:HG22	1.83	0.59
2:A:180:ILE:HA	2:A:183:ILE:HG12	1.85	0.59
2:A:387:ALA:O	2:A:391:LYS:HG3	2.03	0.59
2:A:453:LEU:HD23	2:A:453:LEU:H	1.68	0.59
6:I:36:LYS:HG2	6:I:37:THR:HG23	1.85	0.59
10:a:19:LEU:HD21	14:f:69:LEU:HD22	1.85	0.59
3:D:64:ASP:HA	3:D:225:PRO:HG3	1.85	0.58
2:C:156:LEU:HD22	2:C:391:LYS:HZ1	1.68	0.58
3:D:29:LEU:HD11	3:D:56:SER:HA	1.85	0.58
8:O:47:PHE:O	8:O:51:ILE:HD12	2.02	0.58
17:j:13:MET:HG3	17:j:16:TYR:HB3	1.84	0.58
2:C:361:ILE:HG13	2:C:429:LYS:HE3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLN:HE22	2:B:371:VAL:HG22	1.68	0.58
8:M:33:ILE:HD11	8:N:31:SER:C	2.29	0.58
8:N:23:ALA:O	8:N:27:THR:HG23	2.04	0.58
12:d:130:MET:HE2	12:d:130:MET:HA	1.85	0.58
3:F:97:VAL:HG13	3:F:98:ILE:HG23	1.84	0.58
8:L:23:ALA:O	8:L:27:THR:HG23	2.04	0.58
15:g:50:GLN:HA	15:g:53:LYS:HD3	1.86	0.58
2:A:220:LEU:HG	2:A:226:MET:HE1	1.86	0.57
3:E:97:VAL:HG13	3:E:98:ILE:HG23	1.86	0.57
8:L:5:ALA:O	8:L:9:ILE:HG12	2.04	0.57
12:d:140:PRO:HA	12:d:143:LYS:HG3	1.87	0.57
2:A:270:ASP:HB2	2:A:273:LYS:HG3	1.85	0.57
8:Q:69:PHE:HA	8:Q:72:LEU:HD12	1.87	0.57
3:F:197:TYR:CZ	3:F:201:ILE:HD11	2.39	0.57
3:F:298:THR:HG23	3:F:303:SER:HA	1.87	0.56
10:a:12:PRO:HB3	14:f:73:ARG:NH2	2.21	0.56
10:a:197:ILE:HG12	11:b:62:SER:HB2	1.88	0.56
11:b:121:ARG:HD2	12:d:18:ILE:HG13	1.86	0.56
10:a:147:ILE:O	10:a:151:ILE:HG12	2.05	0.56
2:C:291:ARG:HG3	3:D:280:GLY:HA3	1.87	0.56
3:F:155:PHE:HZ	3:F:329:LEU:CD1	2.17	0.55
5:H:66:HIS:HA	5:H:72:THR:HG22	1.86	0.55
11:b:187:ALA:CB	11:b:189:GLN:HE22	2.17	0.55
3:E:24:GLN:CB	3:E:57:THR:OG1	2.54	0.55
5:H:131:ILE:O	5:H:135:ILE:HG12	2.05	0.55
3:F:237:LEU:HD22	3:F:296:ILE:HG23	1.88	0.55
8:Q:22:GLY:HA3	8:R:60:MET:HE1	1.88	0.55
8:Q:30:GLY:O	8:Q:34:ILE:HG12	2.06	0.55
3:D:36:LEU:HB2	3:D:47:LEU:HB2	1.87	0.55
12:d:127:PHE:HA	12:d:130:MET:HB3	1.89	0.55
8:N:52:LEU:HD12	8:N:53:GLY:N	2.21	0.55
11:b:19:GLU:HG3	11:b:22:PHE:HD2	1.71	0.55
1:8:1:MET:HE3	1:8:3:GLN:HB2	1.89	0.55
2:A:247:PRO:HB2	2:A:305:LEU:HD11	1.89	0.55
3:E:200:MET:HE3	3:E:217:LEU:HD11	1.89	0.55
8:M:23:ALA:O	8:M:27:THR:HG23	2.06	0.55
16:h:9:LYS:HA	16:h:12:VAL:HG12	1.88	0.55
2:B:84:GLU:HB3	3:E:29:LEU:HD13	1.88	0.55
9:S:82:THR:O	9:S:86:ILE:HG22	2.07	0.55
10:a:38:VAL:HG13	10:a:38:VAL:O	2.07	0.55
1:8:9:TRP:CZ3	10:a:99:SER:HA	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:27:LYS:HB2	6:I:30:PHE:HD2	1.71	0.55
4:G:25:MET:N	4:G:25:MET:HE2	2.22	0.54
5:H:100:LEU:HA	5:H:103:LEU:HD12	1.89	0.54
10:a:170:LEU:HD21	10:a:174:ILE:CD1	2.38	0.54
2:B:387:ALA:HA	2:B:390:MET:HB3	1.88	0.54
3:E:189:ARG:HB2	3:E:192:GLU:HG3	1.89	0.54
7:J:31:GLU:O	7:J:35:ARG:HG2	2.07	0.54
2:C:99:VAL:HG12	2:C:253:MET:HE1	1.88	0.54
9:S:119:THR:HG23	9:S:151:GLU:HB2	1.90	0.54
3:D:237:LEU:HD13	3:D:296:ILE:HG22	1.89	0.54
4:G:133:ARG:HG2	4:G:134:ARG:HH22	1.72	0.54
2:C:52:MET:HB2	2:C:95:VAL:HG22	1.90	0.54
2:B:445:ILE:HD12	2:B:446:TYR:N	2.23	0.54
11:b:125:PHE:O	11:b:129:ARG:HG2	2.08	0.54
10:a:46:GLN:HA	10:a:49:MET:SD	2.47	0.54
11:b:154:ARG:CZ	16:h:55:MET:HG3	2.37	0.54
1:8:26:LEU:HD13	17:j:9:VAL:HG22	1.90	0.54
3:D:358:MET:N	3:D:358:MET:HE2	2.23	0.54
1:8:10:LEU:O	1:8:13:ILE:HG12	2.08	0.54
2:B:34:ILE:HD13	2:B:39:ALA:HB2	1.90	0.54
3:F:48:GLU:HB3	3:F:61:ILE:HG22	1.90	0.53
5:H:48:LEU:HD12	5:H:49:ALA:H	1.73	0.53
2:C:291:ARG:HD2	3:D:279:VAL:HG12	1.90	0.53
3:D:269:SER:HB3	3:D:274:ARG:HH11	1.72	0.53
3:E:63:MET:HE3	3:E:63:MET:HA	1.91	0.53
2:C:441:GLN:O	2:C:445:ILE:HG12	2.08	0.53
8:P:33:ILE:HG21	8:Q:32:LEU:HD23	1.89	0.53
15:g:87:TYR:O	15:g:91:ILE:HG12	2.08	0.53
2:B:379:GLN:CG	2:B:383:MET:HE1	2.38	0.53
3:F:237:LEU:HD22	3:F:296:ILE:CG2	2.39	0.53
8:Q:47:PHE:O	8:Q:51:ILE:HG12	2.08	0.53
12:d:116:LYS:O	12:d:119:GLU:HG2	2.08	0.53
11:b:145:HIS:CD2	12:d:44:LEU:CD1	2.66	0.53
3:E:244:ARG:HD3	3:E:304:ILE:HG13	1.91	0.53
16:h:5:ASP:N	16:h:8:GLN:OE1	2.41	0.53
3:E:422:GLU:HG2	3:E:428:LEU:HA	1.91	0.53
2:C:265:LEU:CD2	2:C:322:THR:HB	2.39	0.53
2:B:383:MET:HB3	2:B:442:VAL:HG12	1.90	0.53
8:M:63:PHE:HA	8:M:66:MET:HG3	1.91	0.53
3:E:152:ILE:HB	3:E:307:VAL:HG22	1.91	0.52
10:a:215:THR:HA	10:a:218:VAL:HG22	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:j:30:LEU:O	17:j:34:ILE:HG12	2.09	0.52
3:D:181:SER:HB3	3:D:215:VAL:HG22	1.92	0.52
8:L:33:ILE:HD13	8:M:32:LEU:HA	1.91	0.52
10:a:53:VAL:O	10:a:57:MET:HG2	2.09	0.52
16:h:18:TYR:O	16:h:22:ARG:HG2	2.10	0.52
3:E:163:THR:O	3:E:167:MET:HG2	2.09	0.52
2:C:199:LEU:HD21	2:C:265:LEU:HG	1.92	0.52
3:D:289:MET:HE1	3:D:328:HIS:CE1	2.45	0.52
10:a:142:VAL:O	10:a:146:THR:HG23	2.09	0.52
8:N:9:ILE:HD11	8:O:6:ALA:HA	1.92	0.52
10:a:13:VAL:HG22	10:a:18:PRO:HB3	1.92	0.52
2:A:41:VAL:HB	2:A:71:VAL:HG13	1.92	0.52
3:F:442:GLN:HA	3:F:445:LEU:HD12	1.92	0.52
3:D:253:LEU:HD12	3:D:254:PHE:N	2.25	0.52
3:E:155:PHE:HB2	3:E:334:VAL:HG22	1.92	0.52
8:L:30:GLY:O	8:L:34:ILE:HG12	2.10	0.52
8:R:24:GLY:O	8:R:28:VAL:HG13	2.10	0.52
8:M:44:GLN:CD	8:M:44:GLN:H	2.18	0.52
12:d:91:ALA:HA	12:d:94:LYS:HG2	1.92	0.52
12:d:98:LYS:HA	12:d:102:GLU:HB3	1.92	0.52
8:M:2:ILE:HA	8:N:2:ILE:HD11	1.92	0.51
8:O:28:VAL:HG23	8:O:29:PHE:HD1	1.74	0.51
3:E:12:ARG:HB3	3:E:72:GLY:HA2	1.91	0.51
11:b:145:HIS:NE2	12:d:44:LEU:HD13	2.21	0.51
2:C:422:VAL:HG12	2:C:426:GLU:OE2	2.10	0.51
3:F:155:PHE:CZ	3:F:329:LEU:HD11	2.41	0.51
8:L:32:LEU:HD12	8:L:50:ALA:HB2	1.92	0.51
2:B:493:SER:O	2:B:497:LEU:HG	2.11	0.51
9:S:180:GLN:O	9:S:184:ARG:HG2	2.10	0.51
2:C:241:PRO:O	2:C:245:LEU:HG	2.10	0.51
2:A:62:MET:HB3	2:A:74:VAL:HG22	1.92	0.51
2:A:210:ARG:HG3	2:A:235:THR:HG21	1.91	0.51
2:A:338:ILE:O	2:A:342:VAL:HG12	2.10	0.51
2:A:493:SER:O	2:A:497:LEU:HG	2.11	0.51
4:G:23:MET:HE1	4:G:232:MET:HG3	1.92	0.51
8:L:26:GLY:HA2	8:M:28:VAL:HG23	1.93	0.51
16:h:46:LEU:HA	16:h:49:MET:SD	2.51	0.51
2:B:140:ILE:HD11	2:B:311:LYS:HE3	1.93	0.51
8:M:58:GLU:O	8:M:62:LEU:HG	2.11	0.51
8:N:40:PRO:HB3	8:O:42:LEU:HD21	1.92	0.51
3:F:384:LEU:HD23	3:F:396:LEU:CD2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:96:ASN:HD22	3:D:98:ILE:HG12	1.76	0.51
3:E:198:HIS:HA	3:E:201:ILE:HD12	1.93	0.51
12:d:116:LYS:HG2	12:d:120:LYS:HE3	1.93	0.51
2:C:108:VAL:HG12	2:C:114:ALA:HA	1.92	0.50
3:E:381:TYR:O	3:E:385:GLN:HG2	2.11	0.50
8:Q:30:GLY:HA2	8:R:31:SER:HB3	1.92	0.50
14:f:9:LYS:HZ3	14:f:14:VAL:HA	1.76	0.50
3:E:251:VAL:HB	3:E:304:ILE:HG23	1.92	0.50
2:A:397:TYR:CG	2:A:421:GLY:HA3	2.47	0.50
3:F:289:MET:O	3:F:293:GLN:HB2	2.12	0.50
3:D:366:GLU:CD	3:D:366:GLU:H	2.19	0.50
5:H:138:ASN:O	5:H:141:LEU:HD12	2.11	0.50
8:O:15:THR:HG21	8:P:67:VAL:HG11	1.93	0.50
2:C:403:PHE:CZ	7:J:32:ARG:HB2	2.45	0.50
2:A:386:VAL:HB	2:A:445:ILE:HD12	1.92	0.50
8:R:57:SER:O	8:R:60:MET:HG2	2.12	0.50
2:B:62:MET:HA	2:B:62:MET:HE2	1.92	0.50
2:B:148:THR:HG22	2:B:150:ILE:HG12	1.93	0.50
5:H:35:GLN:HE22	8:Q:40:PRO:HG2	1.75	0.50
8:N:69:PHE:HA	8:N:72:LEU:HB2	1.92	0.50
2:A:448:GLY:HA2	2:A:453:LEU:HD21	1.93	0.50
3:D:46:VAL:HG11	3:D:82:ILE:HD11	1.94	0.50
3:D:388:ILE:CD1	7:J:26:GLU:OE2	2.59	0.50
12:d:72:LYS:HD3	16:h:58:PHE:HB2	1.94	0.50
2:A:21:THR:HG21	16:h:8:GLN:HG2	1.94	0.50
11:b:97:LYS:O	11:b:101:ILE:HG23	2.12	0.50
2:B:448:GLY:HA2	2:B:453:LEU:HD13	1.93	0.50
5:H:40:THR:CG2	5:H:41:GLN:N	2.75	0.50
1:8:8:THR:HG22	1:8:12:MET:HG2	1.94	0.50
1:8:27:LYS:CE	10:a:28:SER:O	2.55	0.50
2:C:380:THR:HG22	2:C:383:MET:HG2	1.92	0.50
3:D:356:ARG:HH11	3:D:357:ILE:HG22	1.77	0.50
8:Q:29:PHE:HA	8:Q:32:LEU:HG	1.94	0.50
12:d:21:ARG:HH11	12:d:98:LYS:HD3	1.76	0.50
2:A:241:PRO:HA	2:A:281:MET:HE1	1.93	0.49
2:B:382:ALA:O	2:B:386:VAL:HG23	2.11	0.49
3:F:9:THR:HA	3:F:27:GLU:HG3	1.94	0.49
5:H:104:ASP:OD1	5:H:104:ASP:O	2.30	0.49
10:a:184:ILE:HG22	10:a:185:SER:H	1.76	0.49
3:D:331:ALA:HA	3:D:355:SER:HA	1.93	0.49
5:H:102:MET:HA	6:I:27:LYS:HD2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:15:THR:HG21	8:N:67:VAL:HG21	1.95	0.49
8:N:70:LEU:HD12	8:N:70:LEU:H	1.77	0.49
3:F:155:PHE:CZ	3:F:329:LEU:CD1	2.95	0.49
8:K:66:MET:O	8:K:70:LEU:HG	2.12	0.49
16:h:46:LEU:O	16:h:50:TYR:HB2	2.13	0.49
3:E:26:ASP:HB3	9:S:6:ARG:HH11	1.75	0.49
8:O:28:VAL:HG23	8:O:29:PHE:CD1	2.47	0.49
3:D:149:GLY:N	3:D:305:THR:OG1	2.42	0.49
3:E:149:GLY:HA2	3:E:304:ILE:O	2.12	0.49
8:M:63:PHE:O	8:M:67:VAL:HG22	2.12	0.49
3:E:468:ALA:O	3:E:472:LYS:HG2	2.12	0.49
8:P:15:THR:OG1	8:Q:67:VAL:HG21	2.13	0.49
2:A:166:LEU:HD22	2:A:342:VAL:HG22	1.95	0.49
3:F:377:ILE:HA	3:F:380:ASP:OD1	2.12	0.49
4:G:272:LEU:HD23	4:G:272:LEU:H	1.78	0.49
9:S:22:LEU:HD13	9:S:85:LEU:HD22	1.95	0.49
2:C:224:ASP:HA	2:C:226:MET:HE1	1.94	0.49
9:S:15:GLU:HB2	9:S:101:VAL:HG22	1.95	0.49
8:K:46:LEU:HD22	8:R:33:ILE:CD1	2.44	0.48
2:A:213:VAL:O	2:A:216:LEU:HD12	2.13	0.48
8:L:42:LEU:O	8:L:46:LEU:HG	2.13	0.48
8:O:30:GLY:O	8:O:34:ILE:HG12	2.13	0.48
8:P:47:PHE:CE1	8:P:51:ILE:HD11	2.48	0.48
11:b:154:ARG:HD2	16:h:55:MET:HE3	1.94	0.48
2:A:424:LEU:HD23	2:A:427:LEU:HD21	1.95	0.48
3:D:410:ILE:O	3:D:414:LEU:HD22	2.12	0.48
6:I:9:LEU:HD12	6:I:9:LEU:H	1.78	0.48
2:A:307:GLU:HG3	3:E:223:ASN:HB3	1.95	0.48
2:A:128:ARG:HB2	2:A:131:LEU:HD21	1.94	0.48
2:A:226:MET:N	2:A:226:MET:HE2	2.29	0.48
2:B:108:VAL:HG12	2:B:114:ALA:HA	1.95	0.48
2:A:479:LEU:HD22	2:A:496:LYS:HE3	1.94	0.48
4:G:261:GLU:O	4:G:264:GLU:HG3	2.14	0.48
8:K:66:MET:HA	8:K:69:PHE:CD2	2.47	0.48
8:L:32:LEU:HD12	8:L:50:ALA:CB	2.44	0.48
12:d:7:LEU:HD23	12:d:7:LEU:H	1.77	0.48
2:A:32:LEU:HD11	2:A:42:HIS:HB2	1.96	0.48
2:B:50:GLU:C	2:B:62:MET:HE1	2.38	0.48
3:F:94:ILE:HD11	3:F:197:TYR:CZ	2.47	0.48
8:L:42:LEU:HB3	8:L:45:GLN:OE1	2.14	0.48
8:O:25:ILE:HA	8:O:28:VAL:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:GLU:OE1	2:C:461:ILE:HG13	2.14	0.48
3:F:279:VAL:HG12	3:F:279:VAL:O	2.13	0.48
3:F:363:VAL:HG11	3:F:367:HIS:CD2	2.49	0.48
8:L:63:PHE:O	8:L:67:VAL:HG13	2.14	0.48
8:L:72:LEU:HD21	8:M:75:MET:HE2	1.96	0.48
8:Q:30:GLY:HA2	8:Q:33:ILE:HD12	1.95	0.48
10:a:57:MET:HB2	10:a:58:MET:SD	2.54	0.48
2:A:391:LYS:O	2:A:394:LEU:HD12	2.14	0.48
2:B:221:THR:HA	2:B:226:MET:SD	2.54	0.48
3:D:264:ALA:O	3:D:268:VAL:HG12	2.13	0.48
4:G:13:ILE:HD13	4:G:16:ILE:HD11	1.96	0.48
4:G:59:THR:HG22	4:G:183:THR:HG21	1.96	0.48
4:G:59:THR:HG21	4:G:157:GLU:HG3	1.96	0.48
4:G:232:MET:N	4:G:232:MET:HE2	2.28	0.48
5:H:130:GLU:HA	5:H:133:ILE:HD12	1.95	0.48
10:a:110:ALA:O	10:a:114:ILE:HG22	2.14	0.48
2:C:150:ILE:HG23	2:C:153:VAL:HB	1.95	0.48
3:F:200:MET:HE2	3:F:200:MET:HA	1.95	0.48
4:G:60:PRO:HB2	4:G:63:LYS:HG2	1.95	0.48
2:B:99:VAL:HG12	2:B:253:MET:HE1	1.95	0.47
3:F:91:LEU:HA	3:F:216:ALA:HB2	1.95	0.47
4:G:12:SER:O	4:G:16:ILE:HG12	2.14	0.47
4:G:31:TYR:HB2	4:G:225:GLN:HB3	1.95	0.47
4:G:213:ILE:O	4:G:217:LEU:HG	2.14	0.47
8:R:52:LEU:HD12	8:R:53:GLY:N	2.29	0.47
2:C:387:ALA:O	2:C:391:LYS:HD3	2.14	0.47
2:B:241:PRO:O	2:B:245:LEU:HG	2.14	0.47
3:F:196:LEU:HD12	3:F:197:TYR:N	2.29	0.47
3:E:24:GLN:HB2	3:E:57:THR:OG1	2.14	0.47
2:C:385:GLN:HE22	2:C:489:ILE:H	1.61	0.47
2:A:280:GLN:O	2:A:284:LEU:HD22	2.13	0.47
2:B:75:VAL:HG21	2:B:79:ASP:HB3	1.96	0.47
3:F:299:THR:HG23	3:F:302:GLY:H	1.79	0.47
4:G:89:MET:HE1	4:G:161:ILE:HB	1.95	0.47
9:S:13:GLY:O	9:S:17:ARG:HG2	2.13	0.47
5:H:132:GLN:O	5:H:136:GLU:HG3	2.14	0.47
8:K:30:GLY:O	8:K:34:ILE:HG12	2.14	0.47
8:M:21:SER:O	8:M:25:ILE:HG12	2.14	0.47
8:N:61:GLY:O	8:N:65:LEU:HG	2.14	0.47
1:8:10:LEU:O	1:8:14:LEU:HG	2.14	0.47
2:A:180:ILE:HD12	2:A:181:ASP:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:200:MET:SD	3:F:205:VAL:HB	2.54	0.47
8:P:49:TYR:O	8:P:52:LEU:HD12	2.15	0.47
2:C:439:GLU:HG2	2:C:440:GLU:OE1	2.14	0.47
2:B:207:GLY:HA3	2:B:273:LYS:HD3	1.95	0.47
3:E:189:ARG:HA	3:E:222:MET:HE1	1.97	0.47
5:H:48:LEU:HB3	8:R:39:ASN:HD21	1.80	0.47
11:b:164:MET:HA	11:b:167:GLN:HG3	1.97	0.47
3:D:298:THR:HG23	3:D:303:SER:HA	1.97	0.47
3:E:388:ILE:HG12	3:E:396:LEU:HD11	1.96	0.47
8:L:11:ALA:O	8:L:15:THR:HG23	2.15	0.47
8:N:30:GLY:N	8:O:28:VAL:HG12	2.29	0.47
10:a:44:THR:HG21	11:b:86:ASN:HB2	1.97	0.47
12:d:19:ILE:HG12	12:d:24:LYS:HA	1.97	0.47
2:A:441:GLN:O	2:A:445:ILE:HG12	2.14	0.47
5:H:40:THR:CG2	5:H:56:GLN:OE1	2.55	0.47
8:R:15:THR:O	8:R:18:VAL:HG12	2.14	0.47
2:C:457:GLU:H	2:C:460:LYS:HE2	1.79	0.47
2:C:269:ASP:HA	2:C:326:VAL:HB	1.96	0.47
3:F:439:LYS:O	3:F:442:GLN:HG2	2.15	0.47
3:D:101:PRO:HG3	3:D:107:PRO:HA	1.96	0.47
3:D:397:SER:O	3:D:401:LYS:HG3	2.14	0.47
5:H:102:MET:HB3	6:I:30:PHE:CD2	2.50	0.47
6:I:23:ARG:HA	6:I:26:LEU:HD23	1.96	0.47
8:R:49:TYR:HA	8:R:52:LEU:HG	1.96	0.47
11:b:12:VAL:HA	11:b:18:PRO:HA	1.97	0.47
2:B:338:ILE:O	2:B:342:VAL:HG12	2.15	0.46
3:F:95:MET:HE2	3:F:95:MET:HA	1.96	0.46
3:F:460:VAL:HG21	3:F:466:ALA:HB2	1.97	0.46
3:D:282:GLN:HG2	3:D:285:LEU:HD22	1.97	0.46
5:H:136:GLU:O	5:H:139:GLU:HG2	2.16	0.46
8:O:51:ILE:HD12	8:O:51:ILE:H	1.80	0.46
10:a:212:TYR:CE2	10:a:216:LEU:HD11	2.51	0.46
12:d:51:ILE:HG23	12:d:56:TYR:HE2	1.80	0.46
2:C:381:ARG:O	2:C:385:GLN:HG3	2.16	0.46
2:B:265:LEU:HD12	2:B:266:ILE:N	2.31	0.46
8:N:58:GLU:O	8:N:62:LEU:HG	2.14	0.46
2:B:80:LYS:HD2	3:E:33:LEU:HD12	1.96	0.46
8:K:58:GLU:O	8:K:62:LEU:HD22	2.16	0.46
11:b:164:MET:HE1	11:b:168:LYS:HD3	1.97	0.46
3:D:63:MET:HE3	3:D:63:MET:HA	1.95	0.46
6:I:31:LYS:O	6:I:35:MET:SD	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:a:83:ASN:HA	10:a:95:THR:HG21	1.98	0.46
11:b:150:GLU:O	11:b:154:ARG:HG2	2.15	0.46
13:e:36:ALA:HB1	13:e:40:ARG:HE	1.79	0.46
2:A:25:LEU:HD12	9:S:171:VAL:HB	1.96	0.46
5:H:140:ALA:HA	5:H:143:LYS:HZ2	1.80	0.46
10:a:131:GLN:HE22	18:k:26:ARG:CZ	2.29	0.46
10:a:156:LEU:HD23	10:a:159:ARG:HH11	1.80	0.46
10:a:170:LEU:HD21	10:a:174:ILE:HD12	1.97	0.46
17:j:15:PRO:HA	17:j:18:THR:OG1	2.15	0.46
2:C:48:GLN:HB3	3:D:68:GLY:HA2	1.96	0.46
2:B:237:SER:HB3	3:E:294:GLU:HG3	1.96	0.46
4:G:7:THR:O	4:G:11:LYS:HG3	2.16	0.46
8:O:22:GLY:HA2	8:O:25:ILE:HG22	1.98	0.46
2:A:177:SER:O	2:A:180:ILE:HD12	2.16	0.46
2:B:244:TYR:CD2	2:B:245:LEU:HD23	2.51	0.46
2:B:299:PHE:CE1	2:B:345:ILE:HD11	2.51	0.46
3:D:393:MET:HA	3:D:396:LEU:HG	1.98	0.46
6:I:13:ARG:HH12	6:I:17:ILE:HD11	1.81	0.46
5:H:133:ILE:HA	5:H:136:GLU:OE2	2.16	0.46
8:L:16:VAL:HG12	8:L:16:VAL:O	2.16	0.46
10:a:61:HIS:HB3	10:a:65:GLY:HA3	1.98	0.46
10:a:102:LEU:O	10:a:106:ILE:HG12	2.16	0.46
12:d:51:ILE:HG23	12:d:56:TYR:CE2	2.51	0.46
2:C:419:SER:O	2:C:423:ARG:HG2	2.16	0.46
2:A:361:ILE:HG12	2:A:429:LYS:HE2	1.97	0.46
2:B:238:ASP:HB3	2:B:242:LEU:HD12	1.97	0.46
2:B:336:ALA:HB3	2:B:339:PRO:HG2	1.96	0.46
3:F:415:SER:HB3	3:F:459:MET:H	1.81	0.46
2:C:283:LEU:HD12	3:F:275:ILE:HB	1.98	0.46
16:h:18:TYR:CZ	16:h:22:ARG:HD3	2.51	0.46
2:C:45:ARG:HA	3:D:71:ARG:HH11	1.80	0.45
10:a:64:LYS:O	10:a:68:TRP:HD1	1.99	0.45
1:8:1:MET:HA	1:8:2:PRO:HD3	1.81	0.45
1:8:13:ILE:O	1:8:16:MET:HE3	2.17	0.45
2:A:205:ALA:HB3	2:A:233:SER:HB2	1.98	0.45
2:A:248:TYR:CZ	2:A:305:LEU:HD12	2.51	0.45
2:B:141:SER:HB3	2:B:143:ARG:HH22	1.81	0.45
4:G:51:LEU:HD21	5:H:83:THR:HG21	1.98	0.45
8:O:65:LEU:HD12	8:O:65:LEU:H	1.81	0.45
3:D:86:VAL:HG23	3:D:112:GLN:HB2	1.97	0.45
5:H:38:VAL:HG12	5:H:63:VAL:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:41:ARG:HA	16:h:44:PHE:CD2	2.52	0.45
2:C:476:HIS:O	2:C:480:LEU:HG	2.16	0.45
2:A:476:HIS:O	2:A:480:LEU:HG	2.17	0.45
2:B:476:HIS:O	2:B:480:LEU:HG	2.16	0.45
3:E:22:ASP:OD1	3:E:57:THR:HG22	2.16	0.45
8:M:67:VAL:O	8:M:71:ILE:HG22	2.16	0.45
8:N:43:M3L:O	8:N:46:LEU:HD12	2.17	0.45
8:N:66:MET:HG2	8:N:69:PHE:CZ	2.52	0.45
2:C:165:GLU:O	2:C:325:PRO:HD2	2.16	0.45
2:A:386:VAL:HG13	2:A:449:VAL:HG21	1.97	0.45
8:P:23:ALA:O	8:P:27:THR:HG23	2.16	0.45
10:a:84:LEU:HA	10:a:87:LEU:HD23	1.97	0.45
2:C:437:ALA:HB3	2:C:440:GLU:OE1	2.16	0.45
2:A:180:ILE:HD13	2:A:433:TYR:HE1	1.82	0.45
3:F:123:PHE:O	3:F:126:MET:HE1	2.16	0.45
3:F:398:GLU:H	3:F:398:GLU:CD	2.25	0.45
4:G:207:TYR:CZ	5:H:80:GLY:HA2	2.51	0.45
2:B:31:VAL:HB	2:B:85:GLY:H	1.81	0.45
3:F:231:ARG:O	3:F:235:THR:HG23	2.17	0.45
3:D:165:LEU:O	3:D:169:LEU:HG	2.16	0.45
3:D:281:TYR:HB3	3:D:285:LEU:HD21	1.98	0.45
12:d:146:LYS:HD3	12:d:154:HIS:CE1	2.52	0.45
1:8:25:GLN:HG3	17:j:13:MET:HE1	1.99	0.45
2:B:383:MET:C	2:B:383:MET:HE2	2.41	0.45
3:D:138:LYS:HE2	3:D:416:GLN:HB2	1.98	0.45
11:b:125:PHE:HB2	12:d:92:GLU:HG3	1.99	0.45
2:A:218:LYS:HD3	3:D:128:VAL:HG21	1.99	0.45
3:F:433:PRO:HB2	3:F:436:GLU:OE1	2.16	0.45
4:G:81:ILE:HG22	4:G:171:TYR:CE2	2.52	0.45
5:H:112:LEU:HB2	5:H:138:ASN:HB3	1.99	0.45
12:d:93:GLU:O	12:d:97:VAL:HG23	2.17	0.45
2:C:171:ARG:HA	2:C:171:ARG:HD3	1.77	0.45
2:C:396:GLN:O	2:C:400:VAL:HG22	2.16	0.45
3:F:363:VAL:HG12	3:F:367:HIS:CG	2.51	0.45
4:G:145:ALA:O	4:G:148:LEU:HD12	2.17	0.45
11:b:161:VAL:O	11:b:165:MET:HG3	2.17	0.45
3:E:253:LEU:HD12	3:E:254:PHE:N	2.32	0.44
4:G:10:LEU:HD21	4:G:246:LEU:HB3	2.00	0.44
9:S:97:ASN:O	9:S:101:VAL:HG23	2.17	0.44
3:D:385:GLN:O	3:D:388:ILE:HG13	2.17	0.44
3:E:200:MET:HB3	3:E:205:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:22:GLY:N	8:M:60:MET:HE1	2.32	0.44
8:M:33:ILE:HD11	8:N:31:SER:HB3	1.99	0.44
8:N:42:LEU:O	8:N:46:LEU:HG	2.16	0.44
17:j:17:TYR:HA	17:j:21:TYR:HD1	1.83	0.44
3:E:255:ILE:HB	3:E:308:GLN:HG3	2.00	0.44
4:G:85:VAL:O	4:G:89:MET:HG2	2.16	0.44
5:H:141:LEU:HD23	6:I:22:VAL:HG22	1.98	0.44
8:Q:33:ILE:HG23	8:R:46:LEU:HD22	1.98	0.44
2:C:295:PRO:O	2:C:298:VAL:HG13	2.18	0.44
2:A:146:MET:HE3	2:A:146:MET:HB3	1.78	0.44
11:b:179:LYS:O	11:b:182:VAL:HG12	2.18	0.44
2:B:52:MET:HA	2:B:52:MET:HE2	2.00	0.44
3:F:363:VAL:CG1	3:F:367:HIS:CD2	3.00	0.44
3:E:23:VAL:C	3:E:57:THR:HG23	2.43	0.44
8:O:32:LEU:CD1	8:O:50:ALA:HB2	2.46	0.44
10:a:212:TYR:O	10:a:216:LEU:HG	2.18	0.44
18:k:23:LEU:HD21	18:k:27:MET:HE3	1.99	0.44
2:A:167:ILE:HD11	2:A:324:LEU:HD12	1.99	0.44
3:D:49:VAL:HA	3:D:60:THR:HG22	1.98	0.44
4:G:181:LEU:HA	4:G:184:ILE:HG12	2.00	0.44
11:b:51:TYR:HA	14:f:71:TYR:OH	2.18	0.44
17:j:13:MET:HG3	17:j:16:TYR:CB	2.46	0.44
2:A:157:VAL:HG11	2:A:350:ILE:CD1	2.46	0.44
4:G:117:HIS:HA	4:G:121:SER:HB3	1.99	0.44
8:P:71:ILE:HD13	8:P:71:ILE:HA	1.90	0.44
2:A:268:TYR:HB3	2:A:271:LEU:HD21	1.99	0.44
2:A:336:ALA:HB3	2:A:339:PRO:HG2	2.00	0.44
2:B:52:MET:HE1	2:B:76:PHE:HE2	1.83	0.44
3:D:53:LEU:HD11	3:D:59:ARG:HB2	2.00	0.44
8:Q:66:MET:HA	10:a:170:LEU:CD1	2.48	0.44
10:a:129:LEU:HB3	18:k:26:ARG:HD2	2.00	0.44
14:f:16:LEU:HD22	14:f:19:LEU:HD11	1.99	0.44
16:h:9:LYS:O	16:h:10:LEU:C	2.58	0.44
2:A:214:ALA:HA	2:A:217:VAL:HG22	1.99	0.44
2:A:388:GLY:HA2	2:A:391:LYS:NZ	2.33	0.44
5:H:78:SER:HB3	6:I:22:VAL:HG21	1.98	0.44
12:d:117:GLU:O	12:d:120:LYS:HB2	2.18	0.44
2:C:465:GLU:O	2:C:469:LEU:HG	2.18	0.43
4:G:4:LYS:H	4:G:4:LYS:HZ2	1.66	0.43
8:O:63:PHE:O	8:O:66:MET:HE3	2.18	0.43
2:A:106:ARG:NH1	2:A:118:LYS:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:381:ARG:HB2	2:A:488:LYS:HB3	2.00	0.43
3:F:108:ILE:HG22	3:F:110:THR:HG23	1.99	0.43
8:O:25:ILE:HG21	8:P:60:MET:HG2	2.00	0.43
13:e:41:ARG:O	13:e:45:GLU:HG2	2.18	0.43
15:g:53:LYS:HB2	15:g:54:LYS:NZ	2.33	0.43
3:F:127:SER:OG	3:F:129:GLU:HG2	2.19	0.43
3:D:13:ILE:HB	3:D:72:GLY:H	1.83	0.43
5:H:39:PRO:HA	5:H:44:ALA:HA	2.01	0.43
9:S:132:THR:O	9:S:136:THR:HG23	2.18	0.43
4:G:184:ILE:HD12	4:G:201:LEU:HD22	2.00	0.43
8:K:63:PHE:HA	8:K:66:MET:HG3	2.01	0.43
2:C:350:ILE:HG23	2:C:365:ILE:HG23	1.99	0.43
2:A:165:GLU:OE2	2:A:350:ILE:CG1	2.57	0.43
4:G:238:ASN:O	4:G:242:MET:SD	2.76	0.43
5:H:57:VAL:HA	5:H:81:SER:HA	2.00	0.43
5:H:105:LEU:O	5:H:109:LYS:HG2	2.19	0.43
8:M:54:PHE:O	8:M:58:GLU:HG2	2.19	0.43
8:R:42:LEU:O	8:R:46:LEU:HG	2.19	0.43
11:b:48:LYS:HA	11:b:48:LYS:HD2	1.71	0.43
11:b:161:VAL:HA	11:b:164:MET:HG3	2.00	0.43
2:A:383:MET:HA	2:A:383:MET:HE2	2.01	0.43
2:B:140:ILE:HG13	2:B:311:LYS:HG3	2.00	0.43
2:B:288:PRO:HA	2:B:289:PRO:HD3	1.86	0.43
3:F:86:VAL:HG23	3:F:112:GLN:HB2	2.00	0.43
3:F:167:MET:HA	3:F:167:MET:HE3	2.01	0.43
3:E:289:MET:HE2	3:E:289:MET:HA	2.00	0.43
8:M:56:LEU:C	8:M:56:LEU:HD23	2.44	0.43
10:a:217:LEU:O	10:a:220:LEU:HG	2.19	0.43
11:b:95:GLU:CD	11:b:95:GLU:H	2.26	0.43
3:E:146:TYR:CZ	3:E:152:ILE:HG21	2.54	0.43
4:G:190:MET:H	4:G:190:MET:HG2	1.57	0.43
5:H:37:ASP:HA	5:H:46:GLY:HA2	2.00	0.43
10:a:184:ILE:HG22	10:a:185:SER:N	2.34	0.43
2:A:218:LYS:NZ	2:A:219:ARG:HG2	2.34	0.43
2:A:286:ARG:HE	3:D:275:ILE:HD11	1.83	0.43
2:A:334:VAL:HG12	2:A:334:VAL:O	2.18	0.43
2:B:128:ARG:HB2	2:B:131:LEU:HD21	2.01	0.43
8:M:49:TYR:O	8:M:52:LEU:HD12	2.17	0.43
3:E:258:ILE:O	3:E:262:THR:HG23	2.18	0.43
9:S:163:ILE:HG23	9:S:170:TYR:HE1	1.83	0.43
11:b:176:TRP:CZ3	11:b:180:ARG:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:19:THR:HA	1:8:23:ILE:HB	2.01	0.43
10:a:170:LEU:HD21	10:a:174:ILE:HD11	2.01	0.43
14:f:45:TYR:CE1	14:f:50:ASN:HB2	2.53	0.43
2:A:52:MET:HE2	2:A:52:MET:HA	2.00	0.42
2:B:32:LEU:HD21	2:B:42:HIS:HB3	2.00	0.42
3:F:95:MET:HB3	3:F:218:VAL:HG22	2.01	0.42
3:D:383:SER:HA	7:J:12:ALA:HB1	2.01	0.42
3:D:435:LYS:O	3:D:439:LYS:HG2	2.19	0.42
8:O:29:PHE:HD2	8:P:53:GLY:HA2	1.84	0.42
8:P:63:PHE:O	8:P:67:VAL:HG23	2.19	0.42
8:R:9:ILE:HG13	8:R:10:GLY:N	2.34	0.42
12:d:130:MET:HE1	12:d:134:ASP:HB3	2.00	0.42
13:e:34:PRO:HA	13:e:37:GLU:HG3	2.01	0.42
16:h:41:ARG:O	16:h:45:LYS:HG2	2.18	0.42
2:C:221:THR:HA	2:C:226:MET:SD	2.59	0.42
2:A:225:ALA:H	2:A:226:MET:HE2	1.83	0.42
2:A:495:ALA:O	2:A:499:GLU:HG3	2.18	0.42
3:D:167:MET:HE1	3:D:196:LEU:CD1	2.48	0.42
10:a:58:MET:HE3	10:a:69:THR:HG23	2.01	0.42
10:a:170:LEU:C	10:a:170:LEU:HD23	2.44	0.42
14:f:10:LYS:HE3	14:f:43:ARG:HD3	2.01	0.42
2:A:68:PRO:HD3	3:E:15:ALA:HB2	2.02	0.42
3:F:200:MET:HG3	3:F:206:ILE:CD1	2.49	0.42
4:G:202:ARG:NH1	6:I:5:ARG:HD2	2.35	0.42
2:C:146:MET:HE2	2:C:146:MET:HA	2.01	0.42
2:B:83:LYS:HD3	3:E:31:PRO:HG3	2.02	0.42
2:B:141:SER:HB3	2:B:143:ARG:NH2	2.35	0.42
2:B:166:LEU:HB2	2:B:346:THR:HG21	2.01	0.42
3:F:388:ILE:HG22	3:F:396:LEU:HD11	2.01	0.42
4:G:102:GLU:OE1	4:G:104:LYS:HG2	2.20	0.42
8:Q:73:PHE:O	8:Q:74:ALA:C	2.62	0.42
9:S:77:LYS:HE2	9:S:77:LYS:HB2	1.89	0.42
10:a:193:PHE:O	10:a:197:ILE:HG13	2.20	0.42
2:B:171:ARG:HA	2:B:171:ARG:CZ	2.50	0.42
2:B:240:ALA:HB1	2:B:277:ALA:HB1	2.01	0.42
3:F:453:PRO:HB2	3:F:455:GLN:OE1	2.19	0.42
3:D:146:TYR:CZ	3:D:152:ILE:HG21	2.54	0.42
8:Q:19:ALA:HA	8:R:60:MET:HE3	2.01	0.42
11:b:169:GLU:O	11:b:173:MET:HG2	2.19	0.42
2:C:349:GLN:N	2:C:349:GLN:OE1	2.52	0.42
2:B:281:MET:HE2	2:B:281:MET:HB3	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:388:ILE:HD12	7:J:26:GLU:OE2	2.20	0.42
3:E:393:MET:HE2	3:E:393:MET:HA	2.02	0.42
6:I:5:ARG:NH1	6:I:11:TYR:H	2.17	0.42
8:N:66:MET:HG2	8:N:69:PHE:HZ	1.82	0.42
10:a:136:PRO:C	10:a:137:LEU:HD23	2.45	0.42
10:a:214:PHE:O	10:a:218:VAL:HG13	2.19	0.42
14:f:39:ARG:NH2	14:f:43:ARG:HH12	2.18	0.42
14:f:70:ASN:HA	14:f:73:ARG:NH2	2.34	0.42
2:C:253:MET:HA	2:C:253:MET:HE3	2.00	0.42
4:G:9:ARG:O	4:G:13:ILE:HG12	2.20	0.42
5:H:35:GLN:HG3	5:H:48:LEU:HD13	2.02	0.42
8:N:26:GLY:HA3	8:O:24:GLY:CA	2.50	0.42
8:Q:19:ALA:HB1	8:R:20:GLY:HA3	2.01	0.42
9:S:163:ILE:HD13	9:S:163:ILE:HA	1.92	0.42
10:a:170:LEU:CD2	10:a:174:ILE:HD12	2.49	0.42
11:b:43:LEU:O	11:b:46:LEU:HG	2.19	0.42
2:C:492:GLU:O	2:C:496:LYS:HG3	2.20	0.42
2:B:397:TYR:CG	2:B:421:GLY:HA3	2.54	0.42
3:F:70:VAL:H	3:F:73:GLN:CD	2.28	0.42
3:F:163:THR:HA	3:F:166:ILE:HG22	2.02	0.42
3:F:196:LEU:HD11	3:F:219:TYR:OH	2.20	0.42
3:D:165:LEU:H	3:D:165:LEU:HD22	1.85	0.42
3:D:433:PRO:O	3:D:437:THR:HG23	2.19	0.42
3:E:381:TYR:HE1	3:E:404:VAL:HG13	1.84	0.42
4:G:221:THR:O	4:G:224:GLU:HG3	2.20	0.42
8:R:6:ALA:HA	8:R:9:ILE:HG12	2.02	0.42
1:8:35:HIS:NE2	12:d:144:LEU:HA	2.35	0.42
2:B:292:GLU:HA	4:G:259:THR:HG21	2.02	0.42
3:D:397:SER:HB3	3:D:400:ASP:OD1	2.19	0.42
3:E:181:SER:HB2	3:E:215:VAL:HG22	2.01	0.42
8:O:62:LEU:HD22	8:O:62:LEU:H	1.85	0.42
9:S:72:MET:HE3	9:S:72:MET:HB3	1.90	0.42
11:b:57:THR:O	11:b:61:ILE:HG22	2.19	0.42
11:b:117:LEU:HD22	12:d:17:GLU:HB3	2.02	0.42
2:A:221:THR:HA	2:A:226:MET:HE3	2.02	0.42
8:N:25:ILE:HG12	8:N:54:PHE:CE2	2.55	0.42
8:Q:23:ALA:HA	8:R:24:GLY:HA2	2.01	0.42
9:S:40:LEU:O	9:S:44:GLN:HG2	2.19	0.42
10:a:193:PHE:CZ	10:a:197:ILE:HD11	2.55	0.42
11:b:117:LEU:HB3	11:b:121:ARG:HH21	1.84	0.42
2:C:423:ARG:HA	2:C:426:GLU:CD	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:86:VAL:HB	3:D:242:TYR:CD2	2.54	0.41
3:E:31:PRO:HD2	3:E:34:ASN:ND2	2.34	0.41
3:E:139:VAL:HB	3:E:414:LEU:HD22	2.02	0.41
3:E:142:LEU:HD12	3:E:367:HIS:HE1	1.85	0.41
3:E:147:ALA:HB2	3:E:357:ILE:HG21	2.02	0.41
8:P:67:VAL:O	8:P:71:ILE:HG12	2.19	0.41
10:a:63:SER:O	10:a:67:THR:HG23	2.20	0.41
10:a:131:GLN:HE22	18:k:26:ARG:NE	2.17	0.41
10:a:150:PHE:O	10:a:154:MET:HE1	2.19	0.41
11:b:101:ILE:HG22	12:d:121:MET:HG3	2.02	0.41
15:g:92:ILE:HD12	15:g:92:ILE:HA	1.91	0.41
2:A:180:ILE:HD12	2:A:181:ASP:H	1.86	0.41
2:A:411:ASP:O	2:A:415:GLN:HG3	2.20	0.41
3:F:29:LEU:HD11	3:F:56:SER:HA	2.02	0.41
3:D:289:MET:HE2	3:D:324:THR:HG22	2.01	0.41
4:G:104:LYS:HA	4:G:104:LYS:HD2	1.91	0.41
5:H:21:ALA:HB2	5:H:26:VAL:HG23	2.02	0.41
8:P:32:LEU:CD1	8:P:50:ALA:HB1	2.43	0.41
11:b:141:ARG:HG2	12:d:44:LEU:HD12	2.02	0.41
2:A:453:LEU:H	2:A:453:LEU:CD2	2.31	0.41
8:K:2:ILE:HD11	8:R:2:ILE:HD12	2.02	0.41
8:R:43:M3L:HM22	8:R:43:M3L:HD3	1.80	0.41
9:S:75:LYS:HB3	9:S:75:LYS:HE2	1.72	0.41
14:f:87:HIS:HA	15:g:98:ILE:HD12	2.02	0.41
2:A:25:LEU:HD11	9:S:169:LYS:HB3	2.01	0.41
4:G:127:THR:HB	6:I:45:VAL:HG22	2.03	0.41
8:Q:66:MET:HA	10:a:170:LEU:HD11	2.01	0.41
12:d:126:PRO:O	12:d:130:MET:CB	2.67	0.41
2:C:361:ILE:H	2:C:361:ILE:HD12	1.85	0.41
3:F:36:LEU:HB2	3:F:47:LEU:HB2	2.02	0.41
4:G:113:ARG:HH21	4:G:113:ARG:HB3	1.85	0.41
4:G:164:ARG:HA	4:G:219:GLU:HB3	2.03	0.41
8:K:31:SER:HB3	8:R:34:ILE:HD11	2.03	0.41
8:N:30:GLY:O	8:N:34:ILE:HG12	2.21	0.41
13:e:3:PRO:HB2	15:g:35:VAL:HG23	2.02	0.41
2:C:104:LEU:HA	2:C:230:ILE:HG13	2.03	0.41
2:C:206:ILE:HA	2:C:234:ALA:HB3	2.02	0.41
2:C:397:TYR:CD1	2:C:421:GLY:HA3	2.56	0.41
8:N:9:ILE:H	8:N:9:ILE:HG12	1.74	0.41
8:R:62:LEU:HD12	8:R:62:LEU:O	2.20	0.41
17:j:21:TYR:HB3	17:j:24:ILE:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:GLU:HG3	2:A:257:PHE:CZ	2.56	0.41
2:A:384:LYS:HE2	2:A:384:LYS:HB2	1.88	0.41
2:B:3:THR:HG21	9:S:17:ARG:HH22	1.85	0.41
10:a:98:LEU:HD23	10:a:98:LEU:HA	1.85	0.41
2:C:482:LYS:HD2	2:C:482:LYS:C	2.45	0.41
4:G:81:ILE:HG13	4:G:82:HIS:N	2.35	0.41
10:a:194:THR:HA	10:a:197:ILE:HD12	2.03	0.41
11:b:165:MET:O	11:b:168:LYS:HG2	2.21	0.41
14:f:41:TYR:O	14:f:45:TYR:HB2	2.21	0.41
2:C:426:GLU:OE2	2:C:458:PRO:HB3	2.21	0.41
2:A:70:ASN:OD1	2:A:70:ASN:C	2.64	0.41
2:A:349:GLN:O	2:A:350:ILE:HD13	2.21	0.41
3:F:288:ASP:O	3:F:292:MET:HG3	2.21	0.41
3:D:388:ILE:HD11	7:J:26:GLU:OE2	2.21	0.41
3:D:408:ARG:HD2	7:J:30:GLU:OE2	2.21	0.41
3:E:22:ASP:OD1	3:E:57:THR:CG2	2.69	0.41
3:E:53:LEU:HD11	3:E:59:ARG:HB2	2.03	0.41
3:E:268:VAL:HA	3:E:271:LEU:HD12	2.03	0.41
3:E:333:THR:HG23	3:E:348:VAL:HG21	2.03	0.41
4:G:24:LYS:HB3	4:G:25:MET:HE2	2.03	0.41
6:I:34:ALA:O	6:I:38:SER:HB3	2.21	0.41
8:M:66:MET:HA	8:M:69:PHE:CD2	2.54	0.41
11:b:19:GLU:HG3	11:b:22:PHE:CD2	2.54	0.41
14:f:69:LEU:HD12	14:f:70:ASN:N	2.36	0.41
15:g:53:LYS:HB2	15:g:53:LYS:HE2	1.76	0.41
1:8:2:PRO:HB3	10:a:10:ILE:HA	2.02	0.41
3:F:363:VAL:CG1	3:F:367:HIS:CG	3.04	0.41
8:P:36:TYR:CZ	8:Q:49:TYR:HE2	2.39	0.41
10:a:193:PHE:HD1	11:b:58:PHE:HB3	1.86	0.41
12:d:117:GLU:HA	12:d:120:LYS:HD2	2.02	0.41
13:e:21:GLY:HA2	15:g:86:PHE:HA	2.02	0.41
2:C:62:MET:HB3	2:C:74:VAL:HG22	2.03	0.40
2:C:426:GLU:HA	2:C:429:LYS:HD3	2.02	0.40
3:D:108:ILE:HG22	3:D:110:THR:HG23	2.02	0.40
3:D:133:LEU:HD12	3:D:133:LEU:HA	1.89	0.40
3:E:82:ILE:O	3:E:116:ILE:HG12	2.21	0.40
8:N:54:PHE:O	8:N:58:GLU:HG2	2.21	0.40
8:P:43:M3L:HE3	8:P:43:M3L:HB2	1.90	0.40
9:S:135:LYS:O	9:S:139:LYS:HG2	2.21	0.40
10:a:84:LEU:HA	10:a:84:LEU:HD13	1.96	0.40
13:e:32:LEU:HD22	15:g:94:LYS:NZ	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ILE:HD12	2:C:327:ILE:O	2.21	0.40
2:C:202:ILE:HD13	2:C:202:ILE:HA	1.89	0.40
2:A:419:SER:O	2:A:423:ARG:HG2	2.21	0.40
2:A:461:ILE:O	2:A:465:GLU:HG3	2.21	0.40
2:B:340:THR:HA	2:B:343:ILE:HG22	2.01	0.40
2:B:404:ALA:O	2:B:405:GLN:HG3	2.20	0.40
3:D:390:ILE:HD13	3:D:390:ILE:HA	1.86	0.40
8:M:27:THR:HG22	8:N:27:THR:HG21	2.04	0.40
8:P:31:SER:HA	8:P:34:ILE:HG22	2.02	0.40
9:S:99:PRO:HA	9:S:102:ILE:HG12	2.02	0.40
10:a:115:THR:HG23	10:a:118:ARG:HG3	2.03	0.40
11:b:6:PRO:HG2	14:f:46:ASN:O	2.21	0.40
11:b:121:ARG:HH12	12:d:21:ARG:HH12	1.69	0.40
11:b:189:GLN:HG2	16:h:9:LYS:CD	2.52	0.40
2:C:424:LEU:O	2:C:427:LEU:HD12	2.22	0.40
5:H:39:PRO:HD2	5:H:63:VAL:HG22	2.02	0.40
6:I:16:GLN:O	6:I:20:LYS:HG2	2.21	0.40
8:Q:11:ALA:HB2	8:Q:71:ILE:HB	2.03	0.40
10:a:83:ASN:OD1	10:a:83:ASN:C	2.65	0.40
12:d:117:GLU:O	12:d:121:MET:SD	2.80	0.40
16:h:5:ASP:HB3	16:h:6:PRO:HD3	2.03	0.40
2:C:492:GLU:HG2	2:C:493:SER:N	2.36	0.40
2:A:295:PRO:HB2	2:A:297:ASP:OD1	2.22	0.40
2:B:129:VAL:HB	2:B:248:TYR:HB3	2.02	0.40
3:F:123:PHE:C	3:F:126:MET:HE1	2.46	0.40
8:M:29:PHE:N	8:M:29:PHE:CD1	2.90	0.40
9:S:36:GLU:O	9:S:40:LEU:HG	2.21	0.40
10:a:64:LYS:HE2	10:a:119:ASN:HD22	1.86	0.40
11:b:145:HIS:HD2	12:d:44:LEU:CD1	2.19	0.40
11:b:151:VAL:HA	11:b:154:ARG:HG2	2.02	0.40
16:h:9:LYS:C	16:h:11:PHE:N	2.79	0.40
17:j:49:LYS:HA	17:j:49:LYS:HD3	1.90	0.40
2:C:62:MET:HB2	2:C:76:PHE:CZ	2.56	0.40
2:A:396:GLN:O	2:A:400:VAL:HG22	2.22	0.40
2:B:278:TYR:HA	2:B:281:MET:HG2	2.04	0.40
3:F:189:ARG:HD2	3:F:192:GLU:OE2	2.21	0.40
3:F:396:LEU:H	3:F:396:LEU:HD12	1.87	0.40
3:F:448:GLU:HB3	3:F:449:TYR:CE2	2.57	0.40
3:D:246:GLN:HA	16:h:41:ARG:HH22	1.86	0.40
5:H:136:GLU:HA	5:H:139:GLU:CD	2.47	0.40
8:N:16:VAL:CG2	8:O:16:VAL:HB	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:98:GLN:HA	11:b:101:ILE:HG12	2.03	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	8	34/66 (52%)	33 (97%)	1 (3%)	0	100	100
2	A	499/510 (98%)	492 (99%)	7 (1%)	0	100	100
2	B	506/510 (99%)	484 (96%)	22 (4%)	0	100	100
2	C	484/510 (95%)	469 (97%)	15 (3%)	0	100	100
3	D	467/482 (97%)	449 (96%)	18 (4%)	0	100	100
3	E	465/482 (96%)	451 (97%)	14 (3%)	0	100	100
3	F	465/482 (96%)	453 (97%)	12 (3%)	0	100	100
4	G	270/273 (99%)	269 (100%)	1 (0%)	0	100	100
5	H	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
6	I	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
7	J	45/60 (75%)	45 (100%)	0	0	100	100
8	K	71/75 (95%)	71 (100%)	0	0	100	100
8	L	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
8	M	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
8	N	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
8	O	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
8	P	71/75 (95%)	71 (100%)	0	0	100	100
8	Q	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
8	R	72/75 (96%)	71 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	S	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
10	a	221/226 (98%)	211 (96%)	10 (4%)	0	100	100
11	b	203/214 (95%)	200 (98%)	3 (2%)	0	100	100
12	d	153/160 (96%)	142 (93%)	11 (7%)	0	100	100
13	e	53/70 (76%)	52 (98%)	1 (2%)	0	100	100
14	f	79/87 (91%)	73 (92%)	6 (8%)	0	100	100
15	g	77/102 (76%)	72 (94%)	5 (6%)	0	100	100
16	h	60/76 (79%)	55 (92%)	5 (8%)	0	100	100
17	j	44/60 (73%)	42 (96%)	2 (4%)	0	100	100
18	k	33/57 (58%)	32 (97%)	1 (3%)	0	100	100
All	All	5089/5413 (94%)	4930 (97%)	159 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	8	33/66 (50%)	33 (100%)	0	100	100
2	A	407/413 (98%)	407 (100%)	0	100	100
2	B	412/413 (100%)	412 (100%)	0	100	100
2	C	394/413 (95%)	394 (100%)	0	100	100
3	D	379/386 (98%)	379 (100%)	0	100	100
3	E	377/386 (98%)	377 (100%)	0	100	100
3	F	377/386 (98%)	377 (100%)	0	100	100
4	G	230/231 (100%)	230 (100%)	0	100	100
5	H	104/109 (95%)	104 (100%)	0	100	100
6	I	38/41 (93%)	38 (100%)	0	100	100
7	J	34/44 (77%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	49/50 (98%)	49 (100%)	0	100	100
8	L	47/50 (94%)	47 (100%)	0	100	100
8	M	50/50 (100%)	50 (100%)	0	100	100
8	N	49/50 (98%)	49 (100%)	0	100	100
8	O	50/50 (100%)	50 (100%)	0	100	100
8	P	47/50 (94%)	47 (100%)	0	100	100
8	Q	48/50 (96%)	48 (100%)	0	100	100
8	R	50/50 (100%)	50 (100%)	0	100	100
9	S	162/165 (98%)	162 (100%)	0	100	100
10	a	188/200 (94%)	188 (100%)	0	100	100
11	b	164/190 (86%)	164 (100%)	0	100	100
12	d	133/142 (94%)	133 (100%)	0	100	100
13	e	33/59 (56%)	33 (100%)	0	100	100
14	f	58/75 (77%)	58 (100%)	0	100	100
15	g	44/83 (53%)	39 (89%)	5 (11%)	5	22
16	h	56/70 (80%)	56 (100%)	0	100	100
17	j	38/49 (78%)	38 (100%)	0	100	100
18	k	21/46 (46%)	21 (100%)	0	100	100
All	All	4072/4367 (93%)	4067 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	g	36	GLU
15	g	37	LEU
15	g	38	VAL
15	g	52	LEU
15	g	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	8	36	ASN
2	C	190	ASN
2	C	263	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	366	ASN
2	C	379	GLN
2	C	466	ASN
2	A	215	GLN
2	A	263	HIS
2	A	471	HIS
2	A	476	HIS
2	A	503	ASN
2	B	147	GLN
2	B	341	ASN
2	B	349	GLN
2	B	379	GLN
2	B	432	GLN
3	F	39	GLN
3	D	24	GLN
3	D	51	GLN
3	D	117	HIS
3	E	117	HIS
3	E	249	GLN
5	H	91	GLN
7	J	41	GLN
8	K	44	GLN
8	O	44	GLN
8	P	44	GLN
9	S	29	GLN
10	a	47	GLN
10	a	101	ASN
10	a	131	GLN
11	b	175	ASN
11	b	189	GLN
11	b	209	GLN
12	d	28	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
8	M3L	O	43	8	10,11,12	0.37	0	9,14,16	0.40	0
8	M3L	M	43	8	10,11,12	0.33	0	9,14,16	0.26	0
8	M3L	R	43	8	10,11,12	0.36	0	9,14,16	0.32	0
8	M3L	Q	43	8	10,11,12	0.34	0	9,14,16	0.30	0
8	M3L	L	43	8	10,11,12	0.36	0	9,14,16	0.27	0
8	M3L	P	43	8	10,11,12	0.32	0	9,14,16	0.28	0
8	M3L	K	43	8	10,11,12	0.33	0	9,14,16	0.33	0
8	M3L	N	43	8	10,11,12	0.36	0	9,14,16	0.28	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
8	M3L	O	43	8	-	0/9/10/12	-
8	M3L	M	43	8	-	0/9/10/12	-
8	M3L	R	43	8	-	2/9/10/12	-
8	M3L	Q	43	8	-	0/9/10/12	-
8	M3L	L	43	8	-	0/9/10/12	-
8	M3L	P	43	8	-	0/9/10/12	-
8	M3L	K	43	8	-	1/9/10/12	-
8	M3L	N	43	8	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	K	43	M3L	C-CA-CB-CG
8	R	43	M3L	CA-CB-CG-CD
8	R	43	M3L	CG-CD-CE-NZ
8	N	43	M3L	CE-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	43	M3L	1	0
8	P	43	M3L	1	0
8	N	43	M3L	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

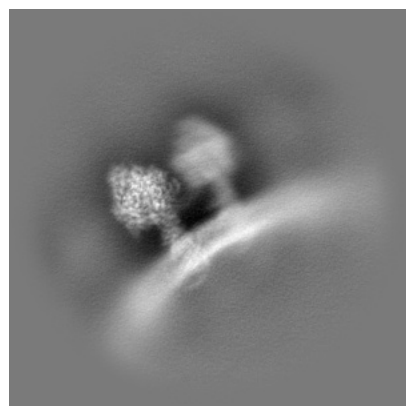
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65578. These allow visual inspection of the internal detail of the map and identification of artifacts.

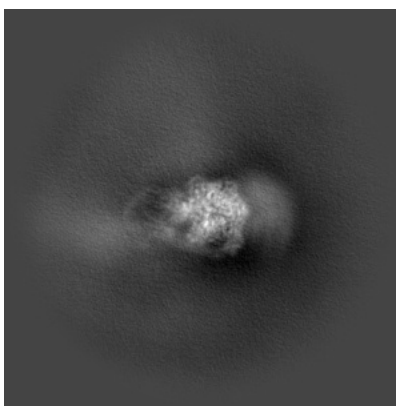
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

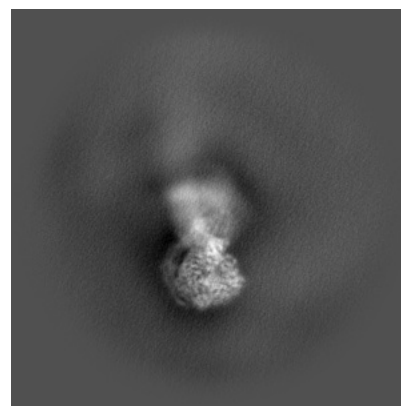
6.1.1 Primary map



X

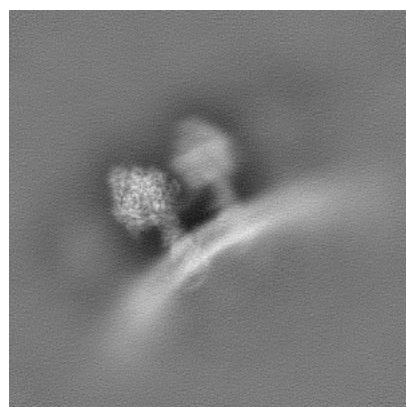


Y

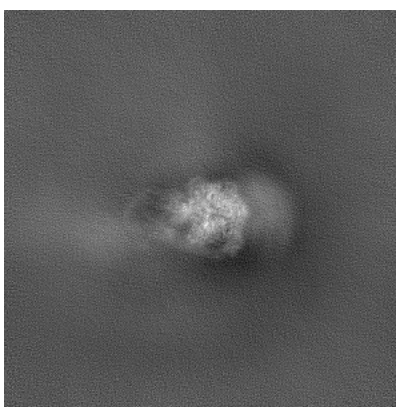


Z

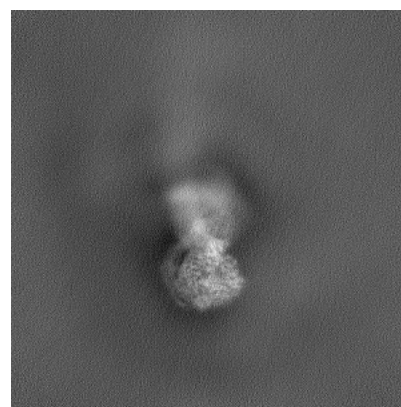
6.1.2 Raw map



X



Y

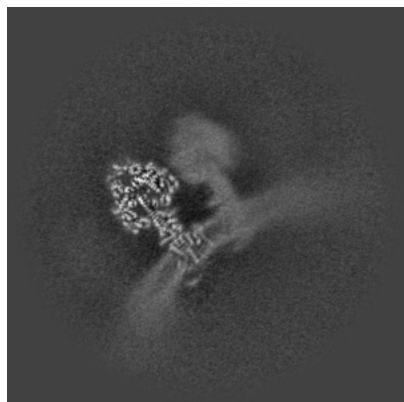


Z

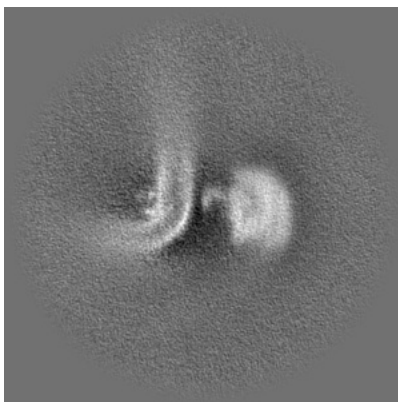
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

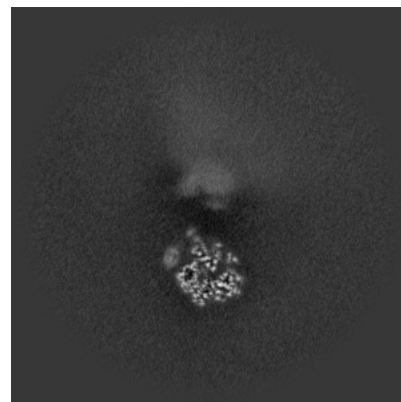
6.2.1 Primary map



X Index: 225



Y Index: 225

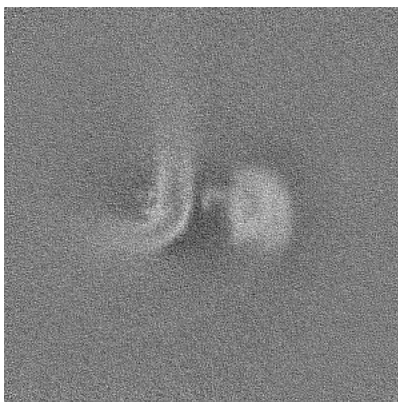


Z Index: 225

6.2.2 Raw map



X Index: 225



Y Index: 225

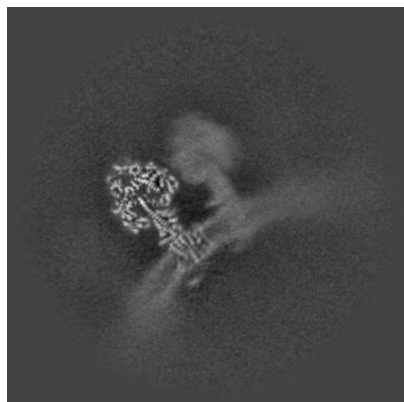


Z Index: 225

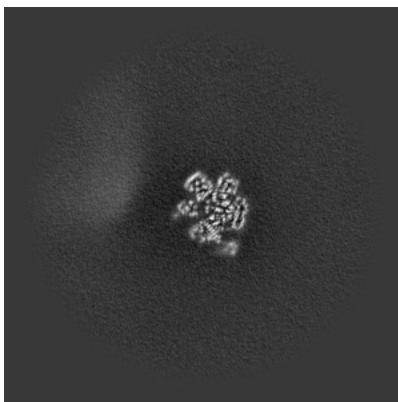
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

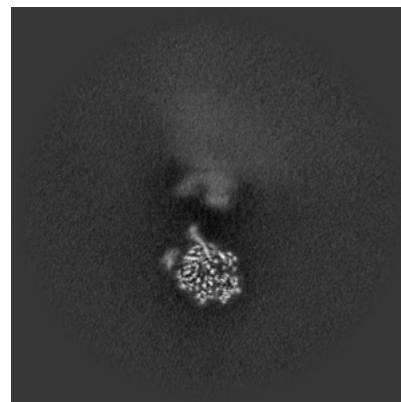
6.3.1 Primary map



X Index: 226

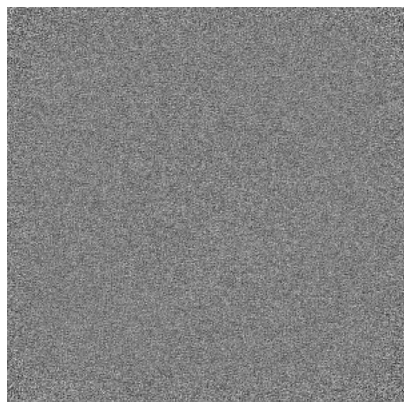


Y Index: 145

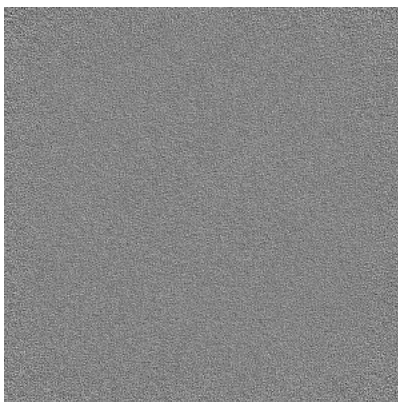


Z Index: 229

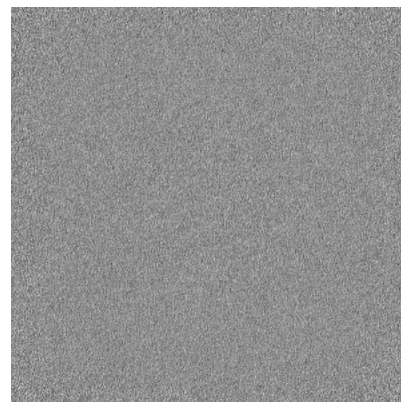
6.3.2 Raw map



X Index: 0



Y Index: 0

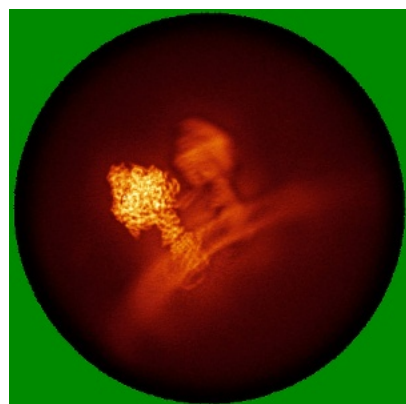


Z Index: 0

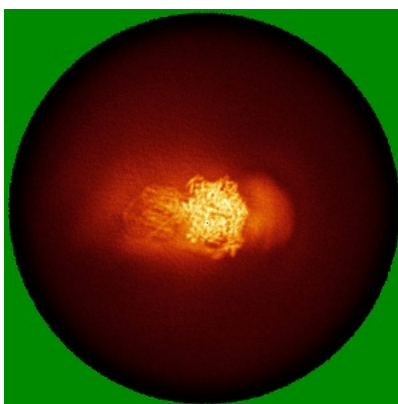
The images above show the largest variance slices of the map in three orthogonal directions.

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

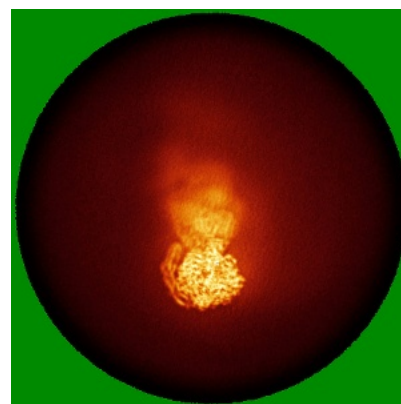
6.4.1 Primary map



X

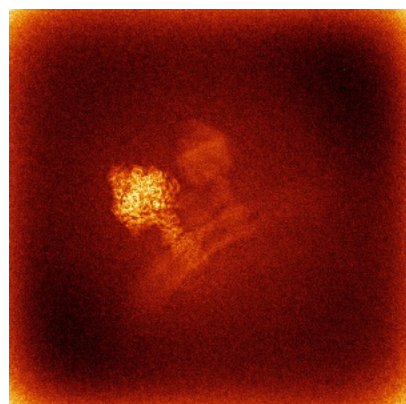


Y

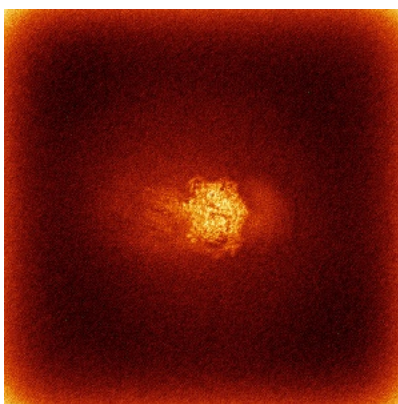


Z

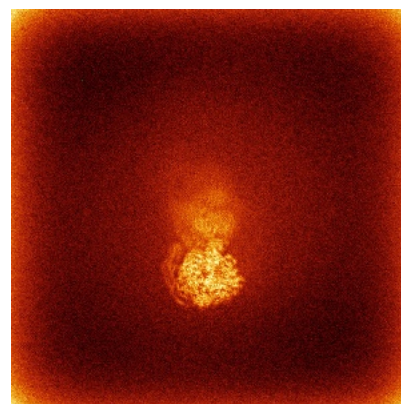
6.4.2 Raw map



X



Y



Z

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

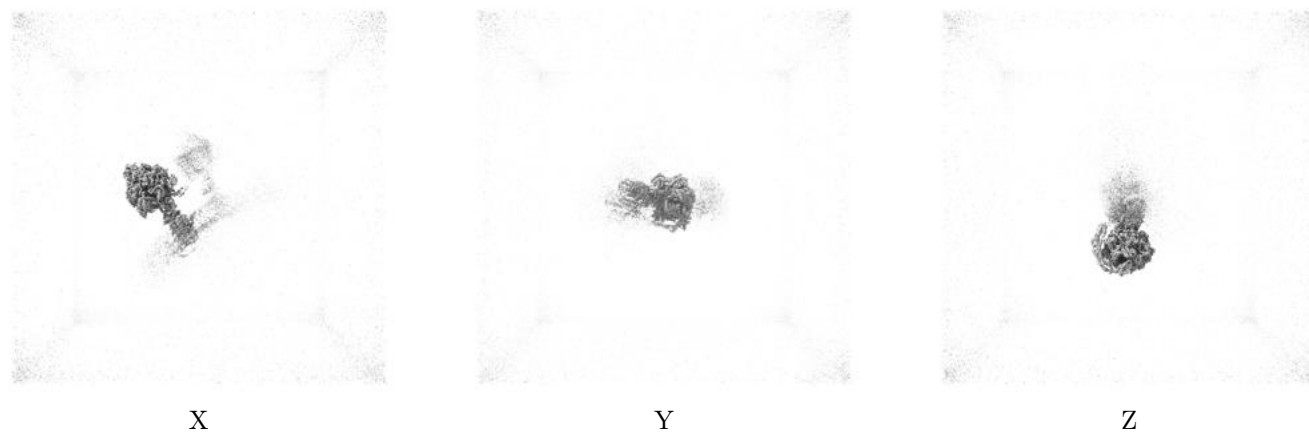
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

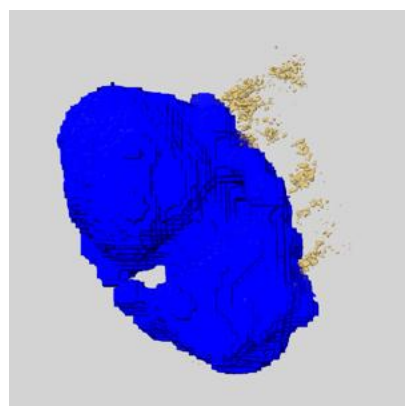
6.6 Mask visualisation [i](#)

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

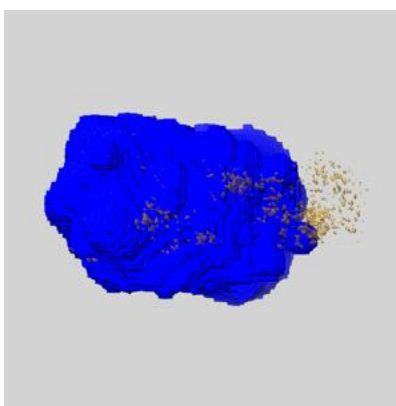
A mask typically either:

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

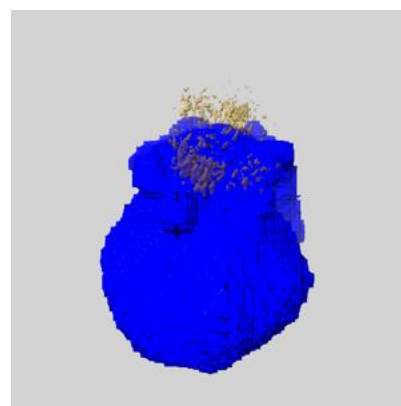
6.6.1 emd_65578_msk_1.map [i](#)



X



Y

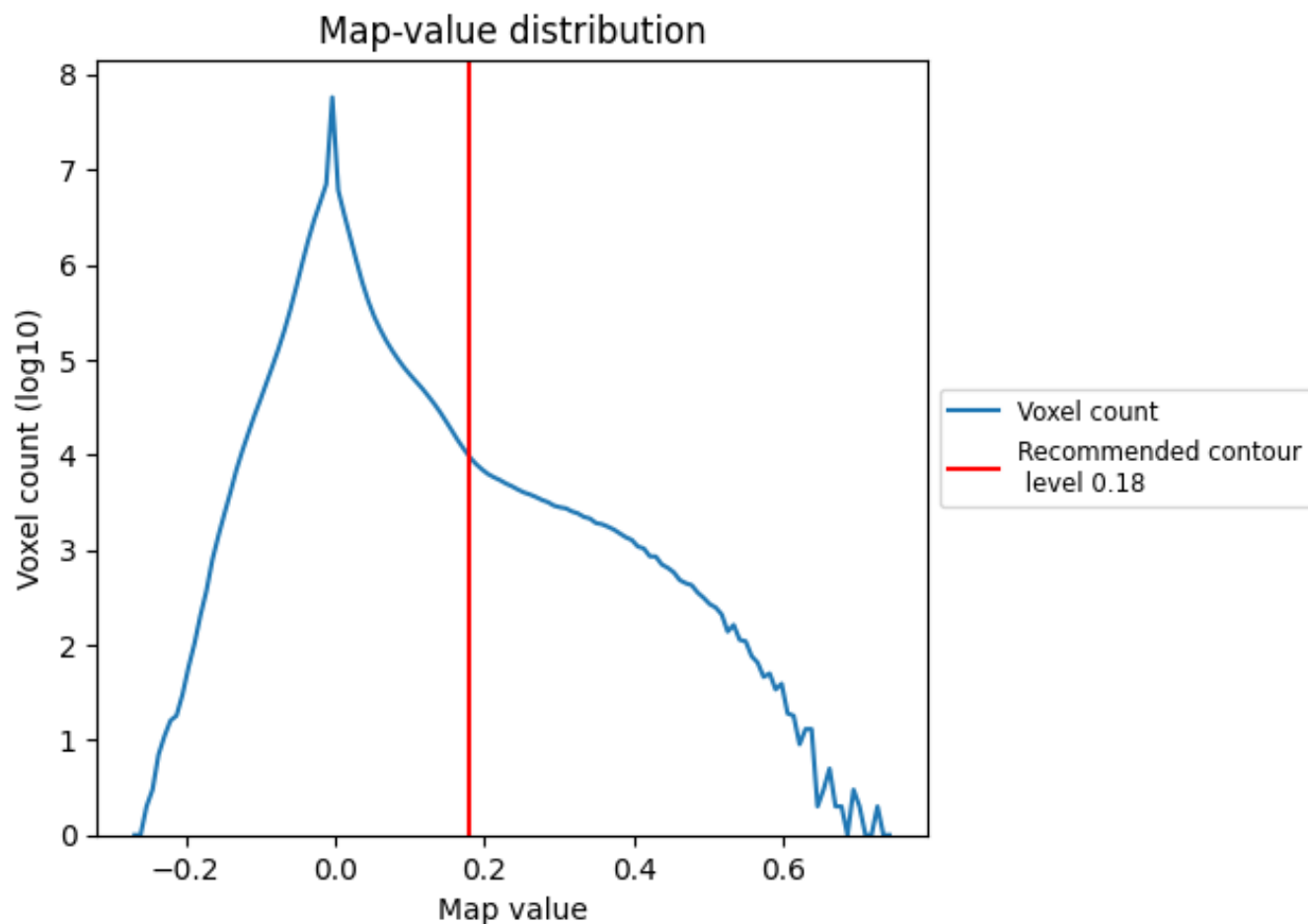


Z

7 Map analysis [i](#)

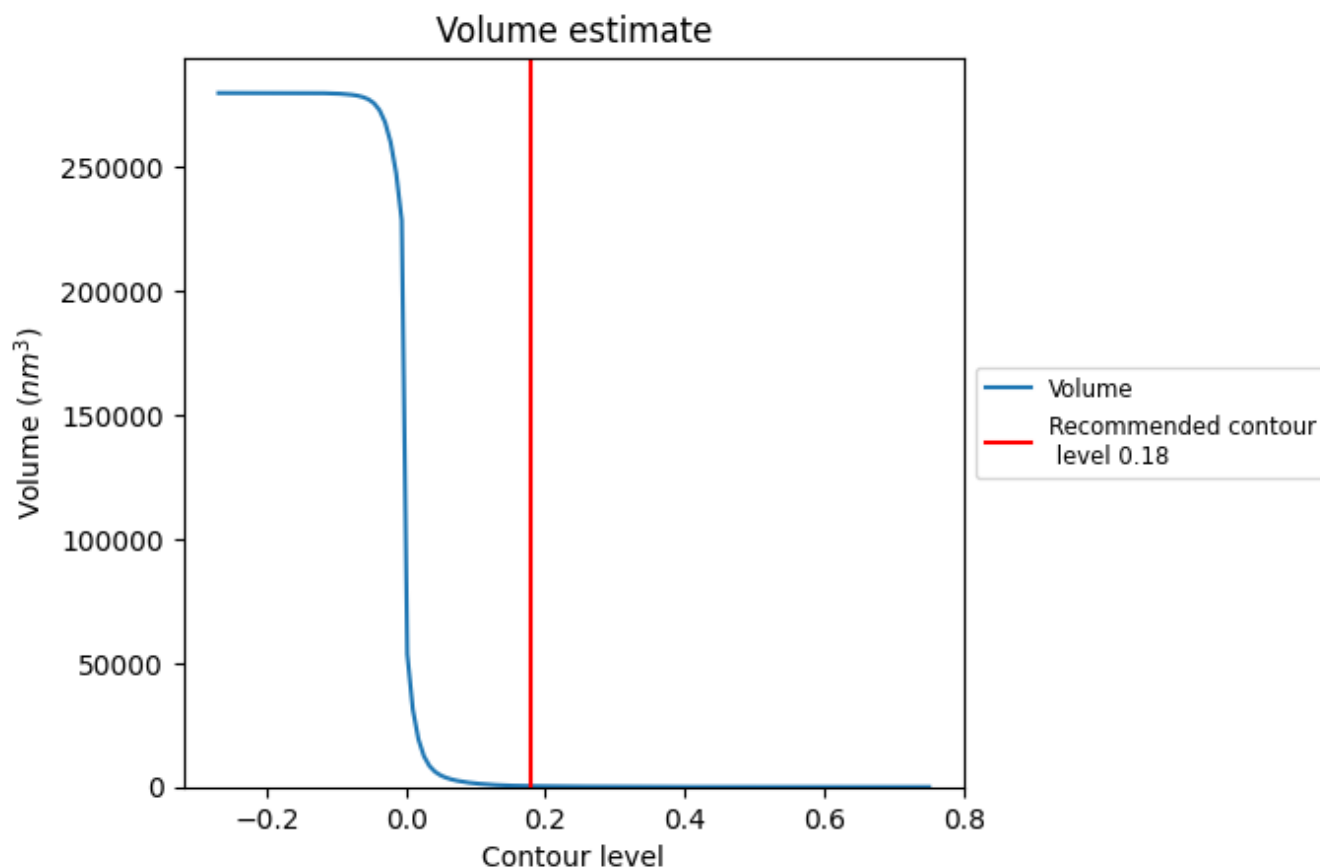
This section contains the results of statistical analysis of the map.

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.

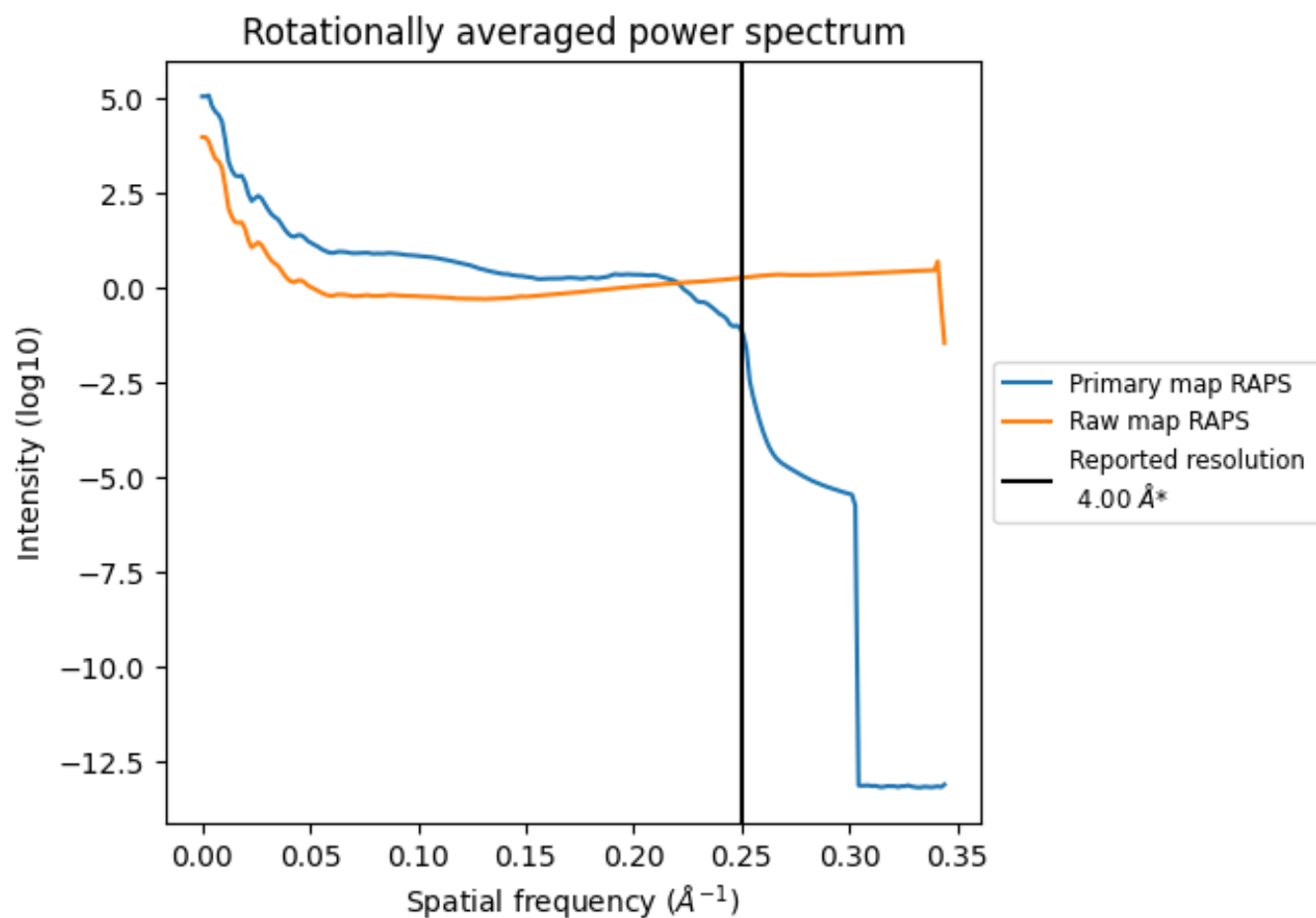
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm³; this corresponds to an approximate mass of 314 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 ⓘ

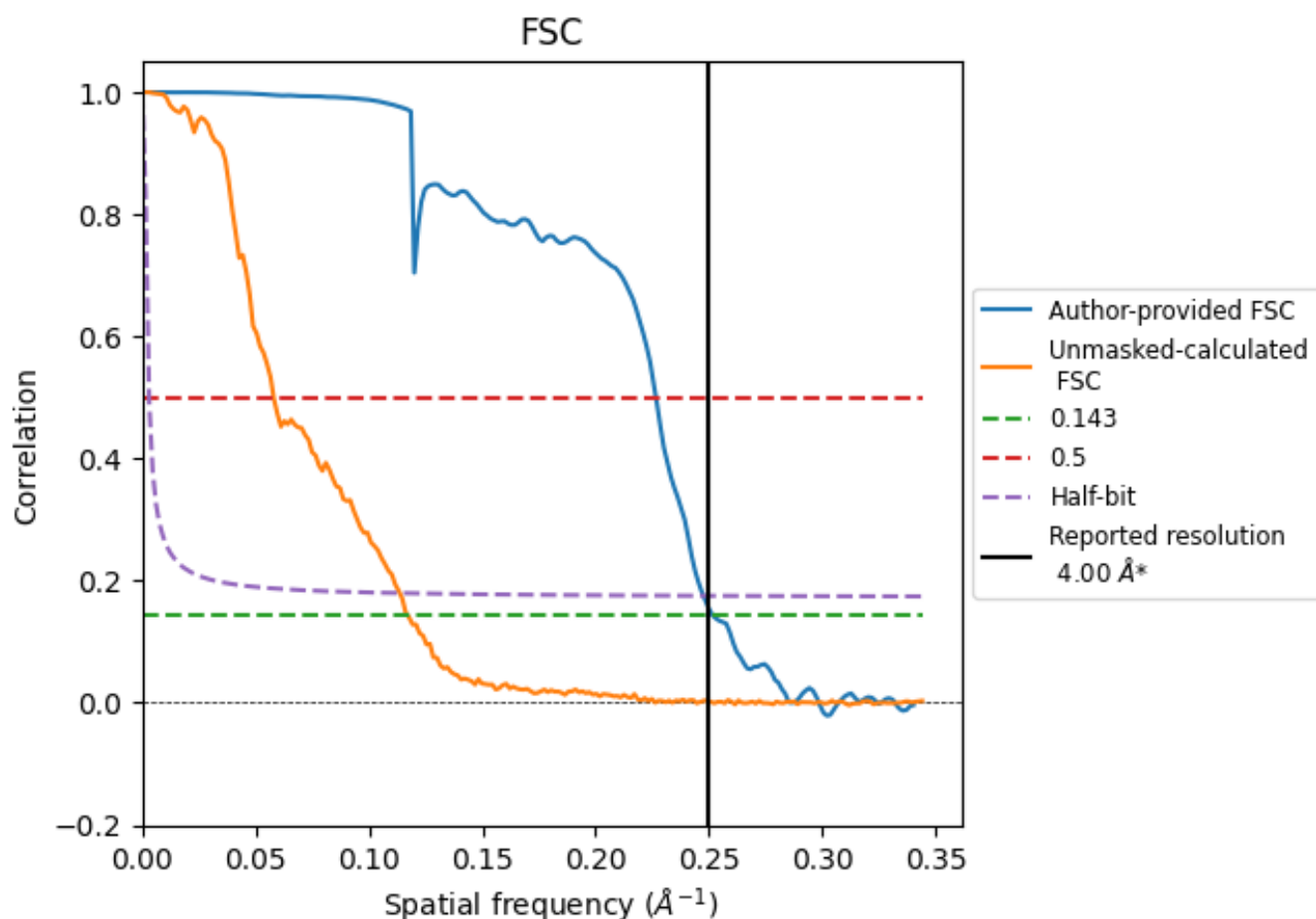


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

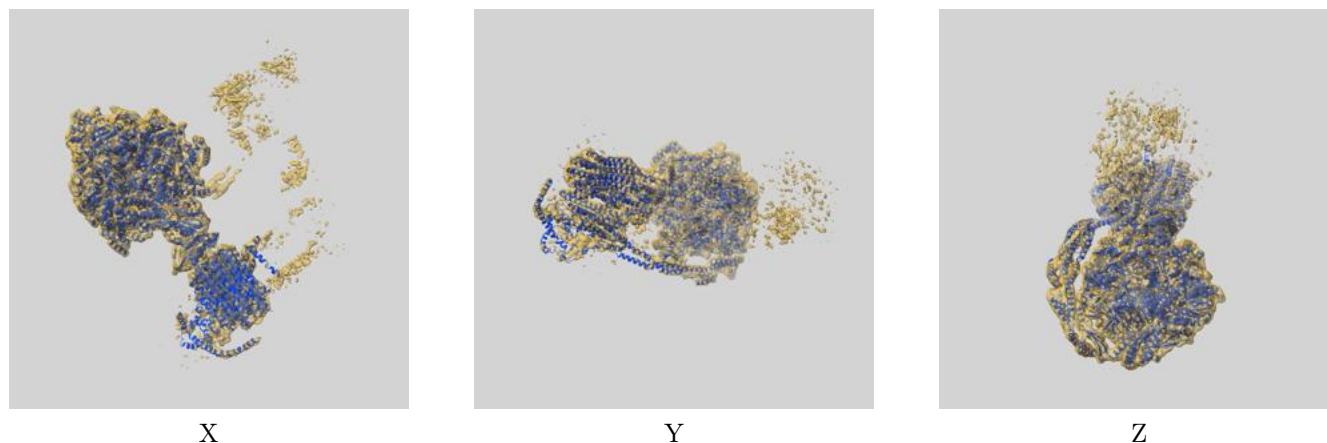
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.41	4.04
Unmasked-calculated*	8.54	17.24	8.80

*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 8.54 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

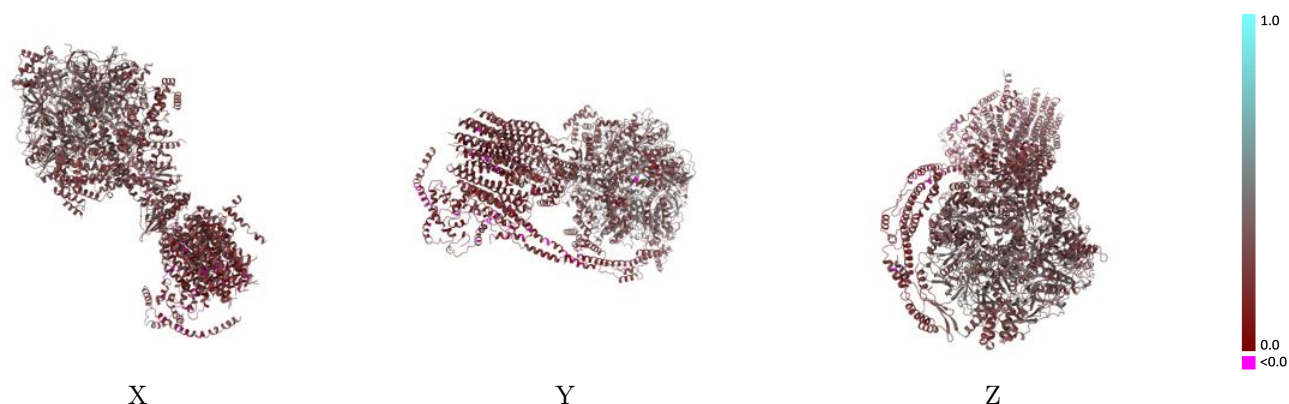
This section contains information regarding the fit between EMDB map EMD-65578 and PDB model 9W2S. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



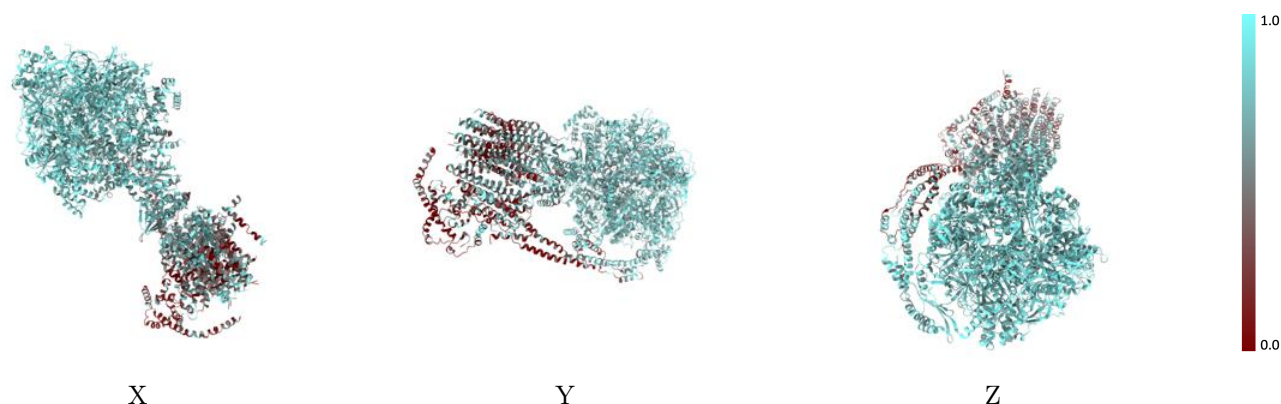
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



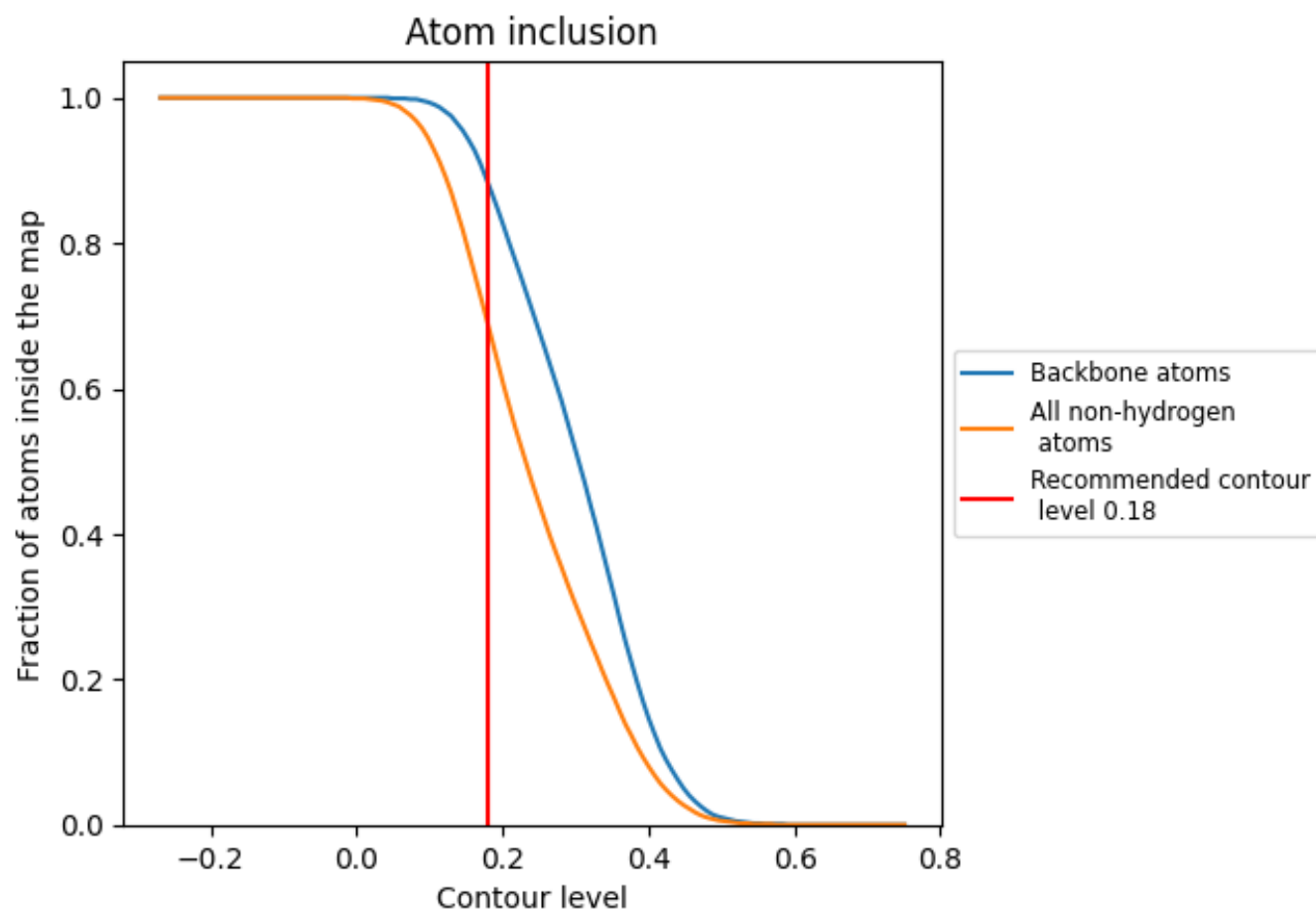
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 69% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.2970
8	 0.3700	 0.1760
A	 0.7860	 0.3390
B	 0.8090	 0.3380
C	 0.7850	 0.3330
D	 0.7830	 0.3520
E	 0.8000	 0.3490
F	 0.8060	 0.3480
G	 0.7380	 0.3070
H	 0.7020	 0.2910
I	 0.6960	 0.2690
J	 0.7510	 0.3160
K	 0.5540	 0.2620
L	 0.4970	 0.2500
M	 0.5090	 0.2380
N	 0.4610	 0.2610
O	 0.5210	 0.2410
P	 0.4880	 0.1860
Q	 0.4760	 0.1590
R	 0.5170	 0.2360
S	 0.7840	 0.2980
a	 0.4870	 0.2020
b	 0.5300	 0.1880
d	 0.3700	 0.1910
e	 0.2710	 0.1870
f	 0.4510	 0.2150
g	 0.2030	 0.2140
h	 0.6580	 0.2120
j	 0.4200	 0.1720
k	 0.4130	 0.2630

