



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 04:49 PM JST

PDB ID : 9VPB / pdb_00009vpb
EMDB ID : EMD-65237
Title : Cryo-EM structure of the IF1 bound bovine F-ATP synthase planar dimer
Authors : Nakano, A.; Jiko, C.; Yamashita, E.; Yokoyama, K.; Gerle, C.
Deposited on : 2025-07-03
Resolution : 5.00 Å (reported)
Based on initial models : 6ZIU, 6Z1U

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

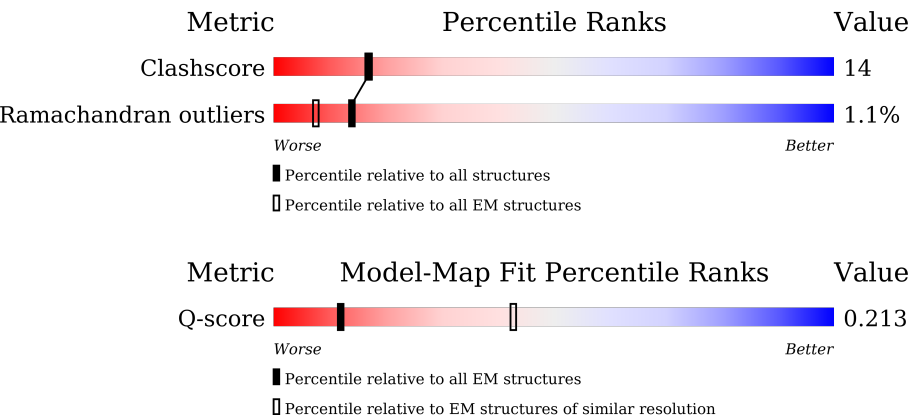
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.00 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.



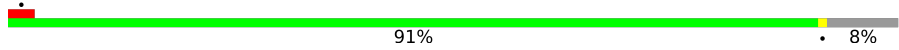





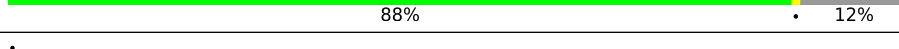
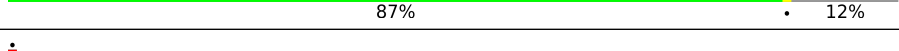
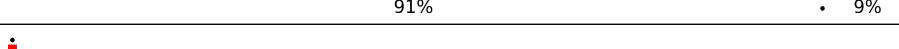
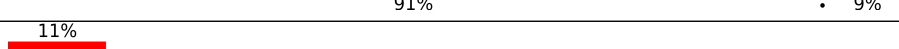
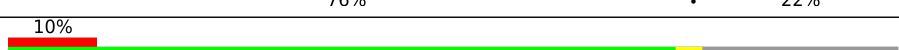

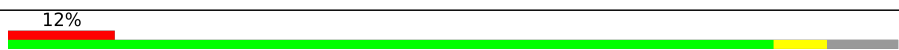
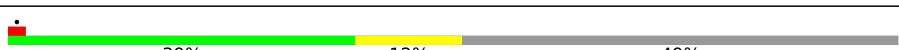
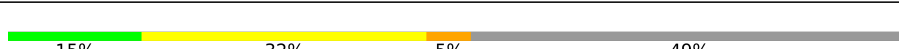







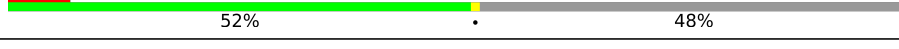


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	1057 (4.50 - 5.50)

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	<div><div>6%</div><div><div></div><div>58%</div><div>5%</div><div>38%</div></div></div>
1	A8	66	<div><div>17%</div><div><div></div><div>58%</div><div>5%</div><div>38%</div></div></div>
2	A	553	<div><div></div><div><div></div><div>89%</div><div>•</div><div>9%</div></div></div>
2	AA	553	<div><div></div><div><div></div><div>89%</div><div>•</div><div>9%</div></div></div>
2	AB	553	<div><div></div><div><div></div><div>91%</div><div>•</div><div>8%</div></div></div>
2	AC	553	<div><div></div><div><div></div><div>86%</div><div>•</div><div>12%</div></div></div>




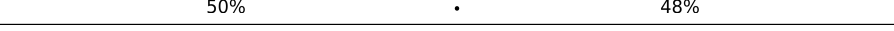
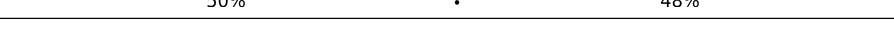
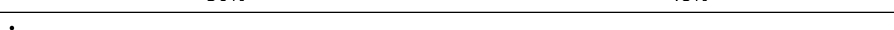
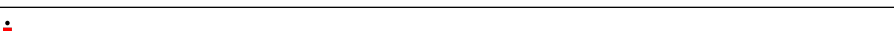
















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Mol	Chain	Length	Quality of chain
2	B	553	
2	C	553	
3	AD	528	
3	AE	528	
3	AF	528	
3	D	528	
3	E	528	
3	F	528	
4	AG	298	
4	G	298	
5	AH	168	
5	H	168	
6	AI	51	
6	I	51	
7	AJ	109	
7	J	109	
8	AK	143	
8	AL	143	
8	AM	143	
8	AN	143	
8	AO	143	
8	AP	143	
8	AQ	143	
8	AR	143	
8	K	143	

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Mol	Chain	Length	Quality of chain
8	L	143	
8	M	143	
8	N	143	
8	O	143	
8	P	143	
8	Q	143	
8	R	143	
9	AS	213	
9	S	213	
10	Aa	226	
10	a	226	
11	Ab	256	
11	b	256	
12	Ad	161	
12	d	161	
13	Ae	71	
13	e	71	
14	Af	88	
14	f	88	
15	Ag	103	
15	g	103	
16	Ah	108	
16	h	108	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49792 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	41	Total	C	N	O	0	0
			205	123	41	41		
1	A8	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	501	Total	C	N	O	0	0
			2457	1455	501	501		
2	AA	501	Total	C	N	O	0	0
			2457	1455	501	501		
2	AB	507	Total	C	N	O	0	0
			2486	1472	507	507		
2	AC	486	Total	C	N	O	0	0
			2383	1411	486	486		
2	B	507	Total	C	N	O	0	0
			2486	1472	507	507		
2	C	486	Total	C	N	O	0	0
			2383	1411	486	486		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	AD	469	Total	C	N	O	0	0
			2300	1362	469	469		
3	AE	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	AF	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	D	469	Total	C	N	O	0	0
			2300	1362	469	469		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	467	Total	C	N	O	0	0
			2290	1356	467	467		
3	F	467	Total	C	N	O	0	0
			2290	1356	467	467		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AG	272	Total	C	N	O	0	0
			1347	803	272	272		
4	G	272	Total	C	N	O	0	0
			1347	803	272	272		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AH	131	Total	C	N	O	0	0
			648	386	131	131		
5	H	131	Total	C	N	O	0	0
			648	386	131	131		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	AI	47	Total	C	N	O	0	0
			233	139	47	47		
6	I	47	Total	C	N	O	0	0
			233	139	47	47		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AJ	56	Total	C	N	O	0	0
			279	167	56	56		
7	J	56	Total	C	N	O	0	0
			279	167	56	56		

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AK	74	Total	C	N	O	0	0
			359	211	74	74		
8	AL	74	Total	C	N	O	0	0
			359	211	74	74		
8	AM	75	Total	C	N	O	0	0
			364	214	75	75		
8	AN	75	Total	C	N	O	0	0
			364	214	75	75		
8	AO	75	Total	C	N	O	0	0
			364	214	75	75		
8	AP	74	Total	C	N	O	0	0
			359	211	74	74		
8	AQ	75	Total	C	N	O	0	0
			364	214	75	75		
8	AR	75	Total	C	N	O	0	0
			364	214	75	75		
8	K	74	Total	C	N	O	0	0
			359	211	74	74		
8	L	74	Total	C	N	O	0	0
			359	211	74	74		
8	M	75	Total	C	N	O	0	0
			364	214	75	75		
8	N	75	Total	C	N	O	0	0
			364	214	75	75		
8	O	75	Total	C	N	O	0	0
			364	214	75	75		
8	P	74	Total	C	N	O	0	0
			359	211	74	74		
8	Q	75	Total	C	N	O	0	0
			364	214	75	75		
8	R	75	Total	C	N	O	0	0
			364	214	75	75		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AS	187	Total	C	N	O	0	0
			926	552	187	187		
9	S	187	Total	C	N	O	0	0
			926	552	187	187		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Aa	226	Total	C	N	O	0	0
			1119	667	226	226		
10	a	226	Total	C	N	O	0	0
			1119	667	226	226		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Ab	209	Total	C	N	O	0	0
			1035	617	209	209		
11	b	209	Total	C	N	O	0	0
			1035	617	209	209		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Ad	155	Total	C	N	O	0	0
			773	463	155	155		
12	d	155	Total	C	N	O	0	0
			773	463	155	155		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Ae	41	Total	C	N	O	0	0
			202	120	41	41		
13	e	41	Total	C	N	O	0	0
			202	120	41	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Af	83	Total	C	N	O	0	0
			409	243	83	83		
14	f	83	Total	C	N	O	0	0
			409	243	83	83		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Ag	79	Total	C	N	O	0	0
			390	232	79	79		

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Mol	Chain	Residues	Atoms				AltConf	Trace
15	g	79	Total 390	C 232	N 79	O 79	0	0

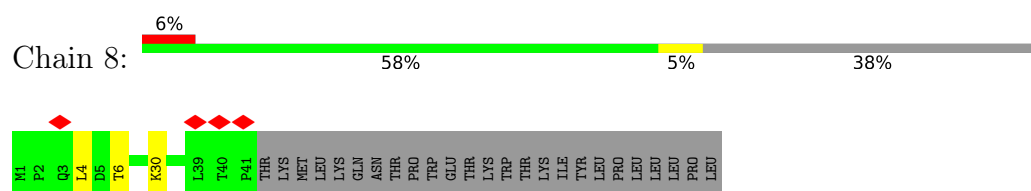
- Molecule 16 is a protein called ATP synthase peripheral stalk subunit F6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Ah	46	Total 227	C 135	N 46	O 46	0	0
16	h	46	Total 227	C 135	N 46	O 46	0	0

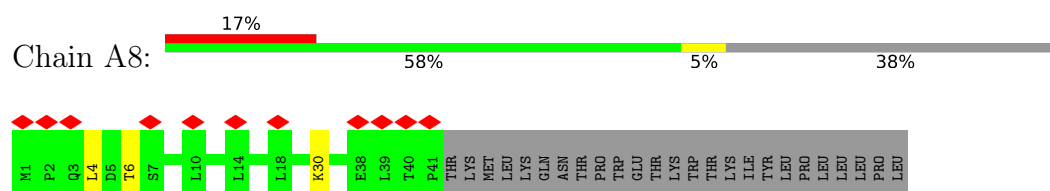
3 Residue-property plots [i](#)

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.

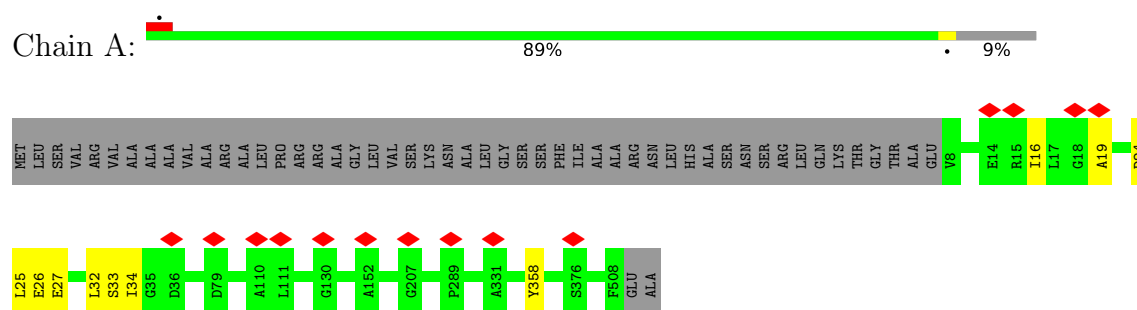
- Molecule 1: ATP synthase F(0) complex subunit 8



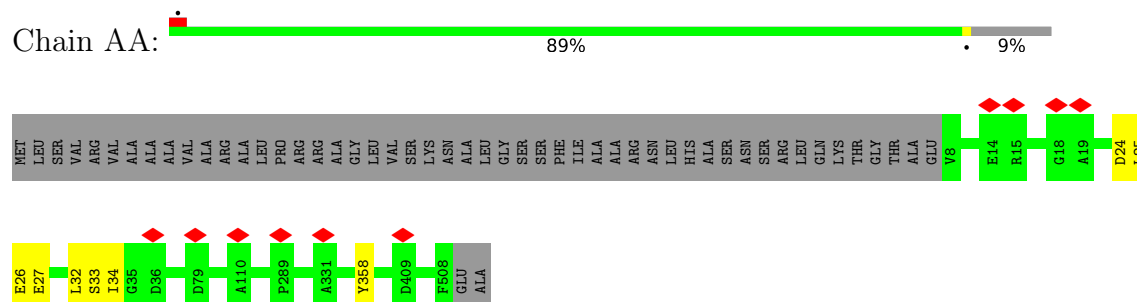
- Molecule 1: ATP synthase F(0) complex subunit 8



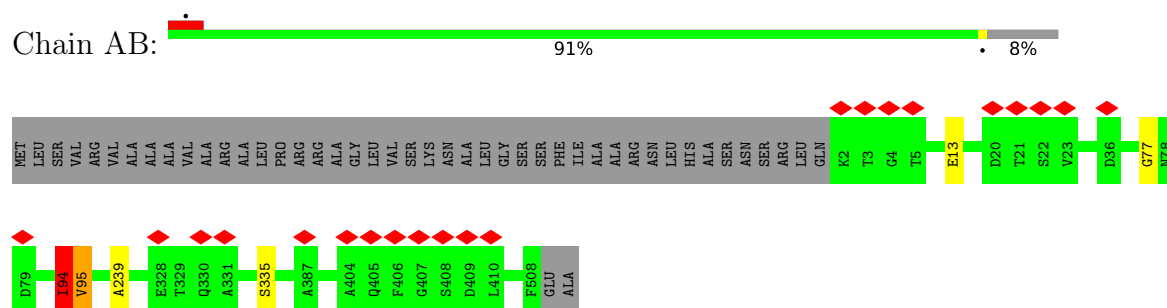
- Molecule 2: ATP synthase subunit alpha



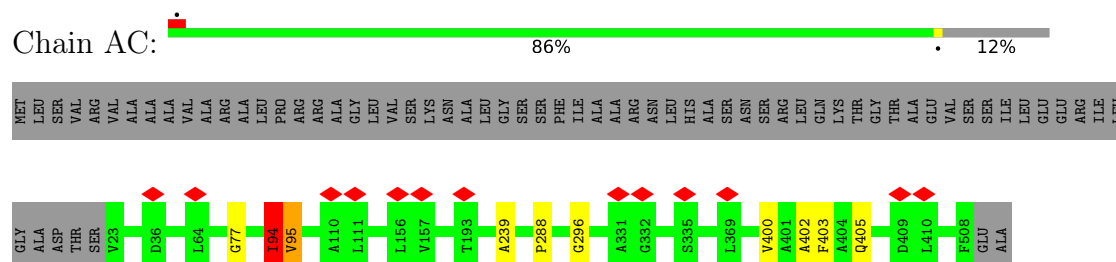
- Molecule 2: ATP synthase subunit alpha



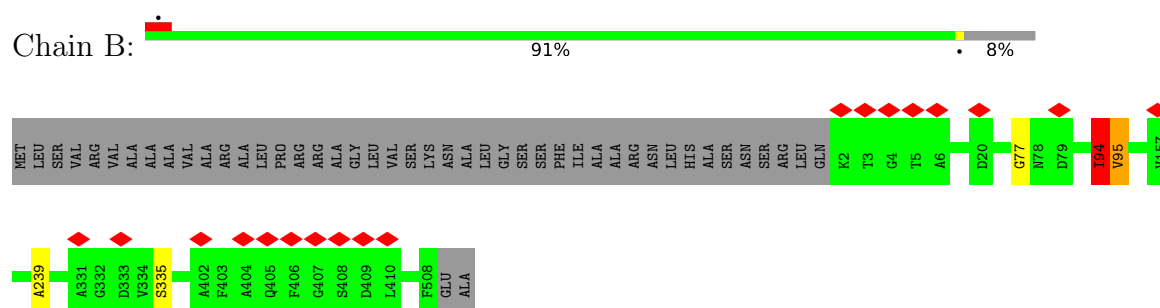
- Molecule 2: ATP synthase subunit alpha



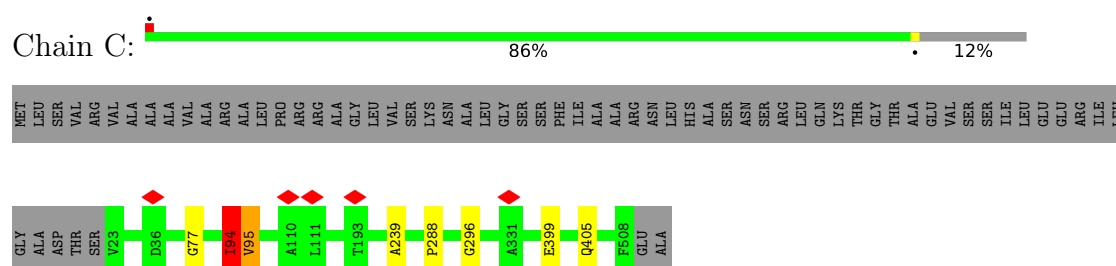
- Molecule 2: ATP synthase subunit alpha



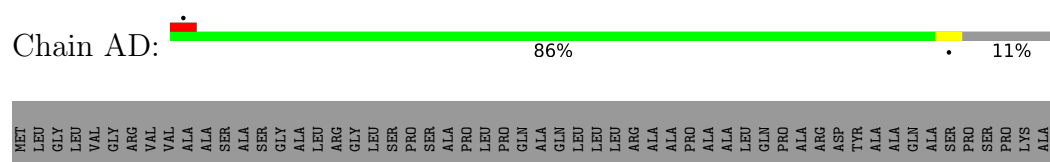
- Molecule 2: ATP synthase subunit alpha



- Molecule 2: ATP synthase subunit alpha



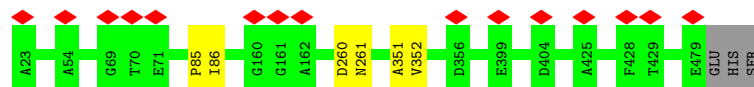
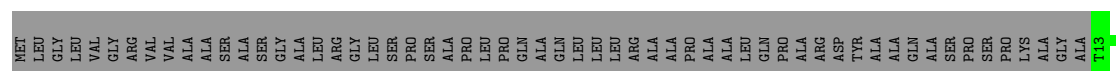
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial





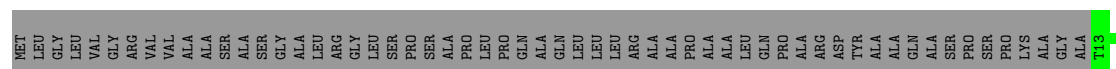
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain AE: 87% 12%



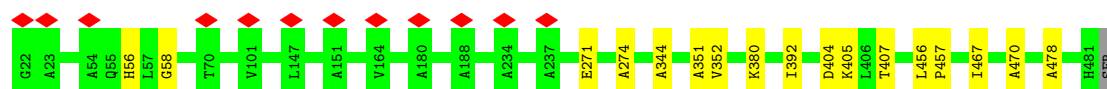
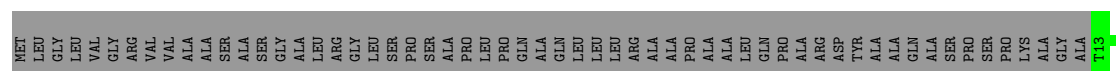
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain AF: 87% 12%



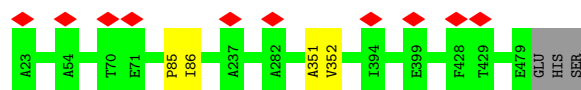
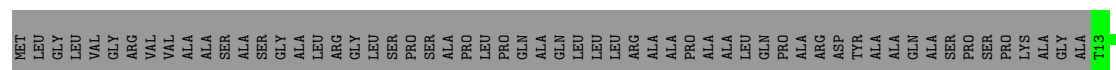
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain D: 86% 11%



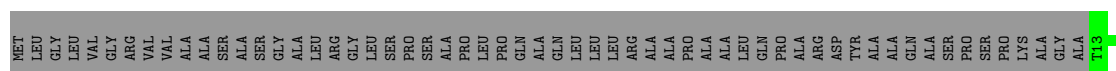
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain E: 88% 12%



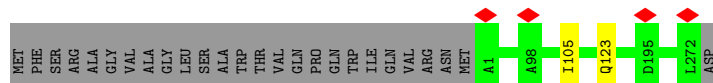
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain F: 87% 12%



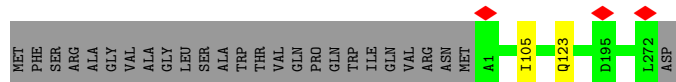
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial

Chain AG: 91% 9%



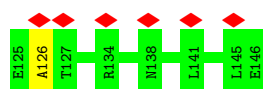
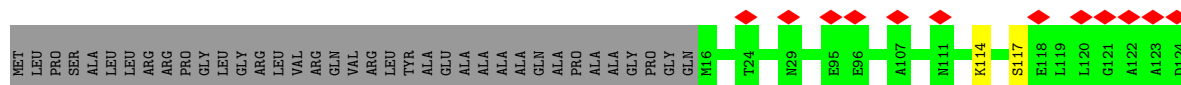
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial

Chain G: 91% 9%



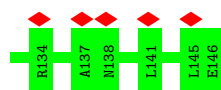
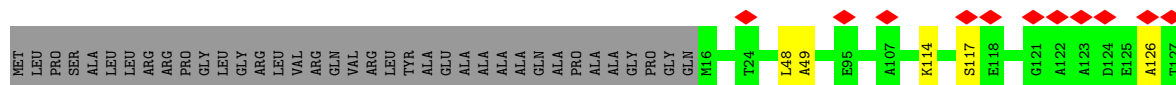
- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

Chain AH: 11% 76% 22%



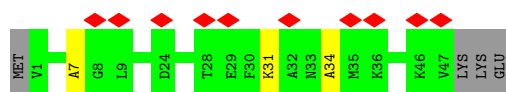
- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

Chain H: 10% 75% 22%

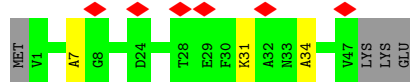
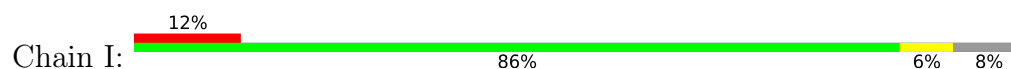


- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial

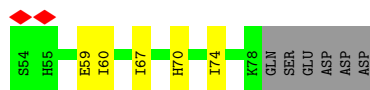
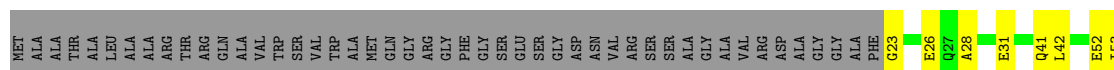
Chain AI: 20% 86% 6% 8%



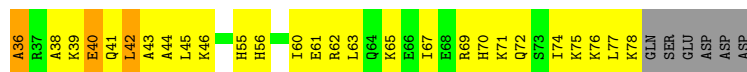
- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial



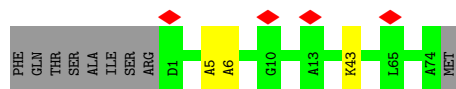
- Molecule 7: ATPase inhibitor, mitochondrial



- Molecule 7: ATPase inhibitor, mitochondrial

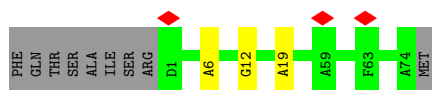


- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

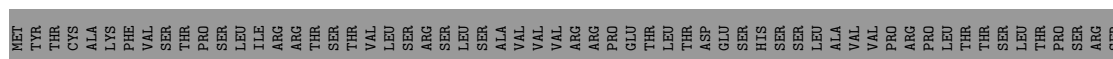




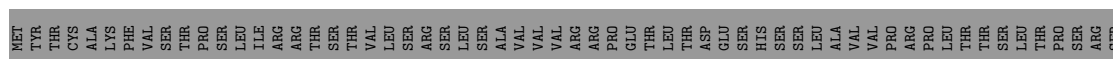
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



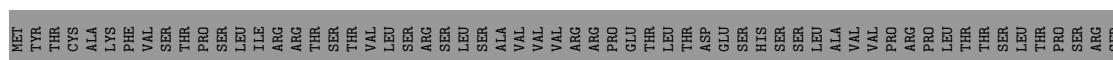
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



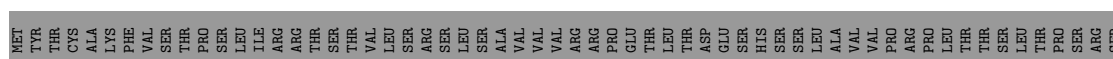
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

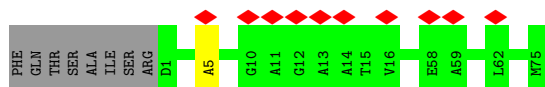


- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

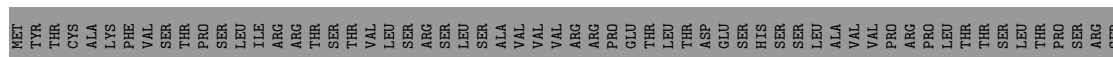




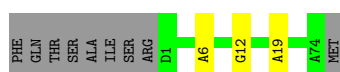
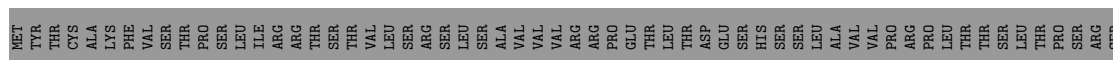
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



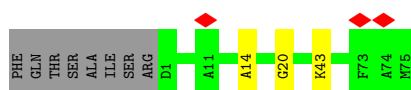
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



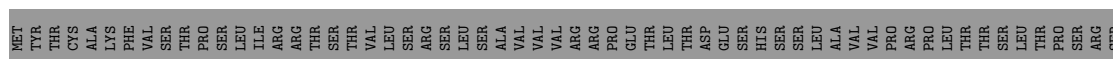
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

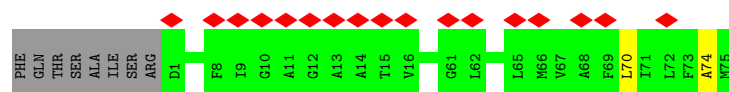


- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

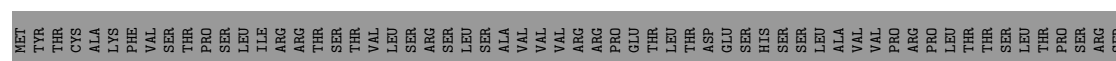




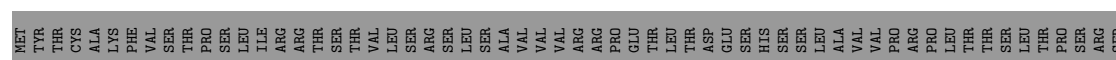
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



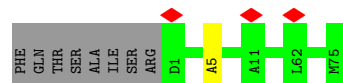
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



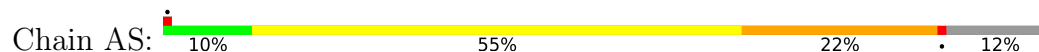
- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial

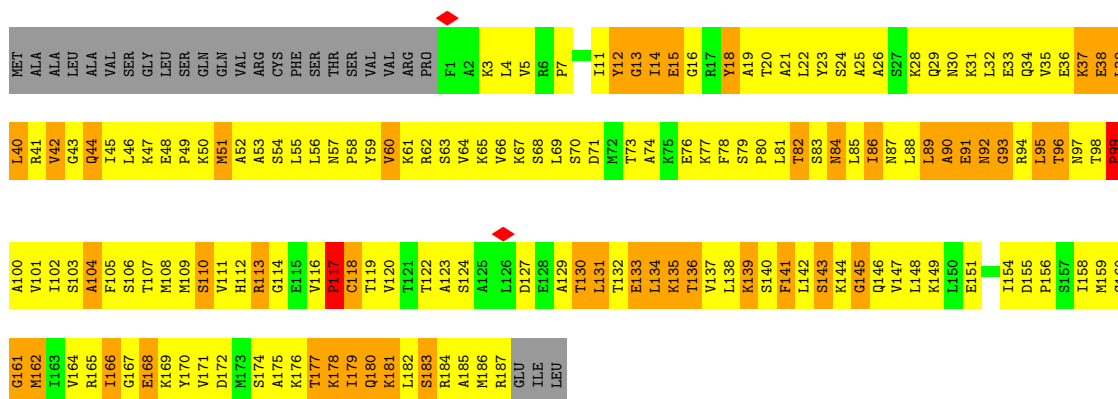


- Molecule 8: ATP synthase F(0) complex subunit C2, mitochondrial



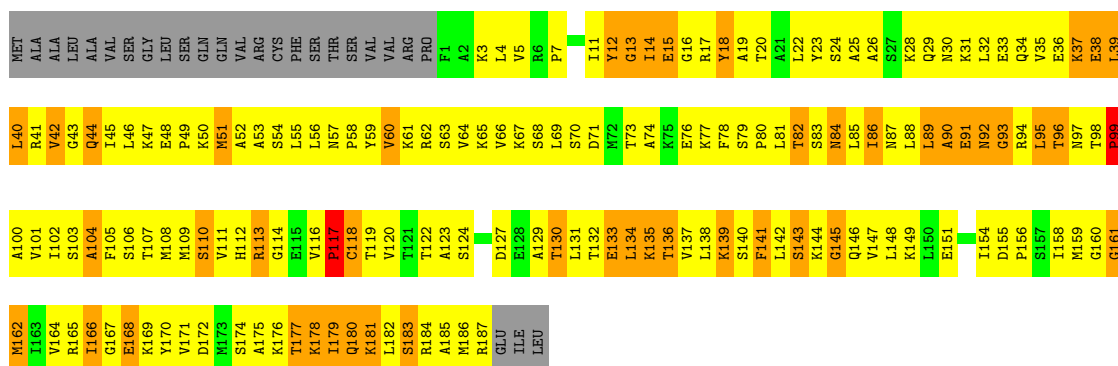
- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial





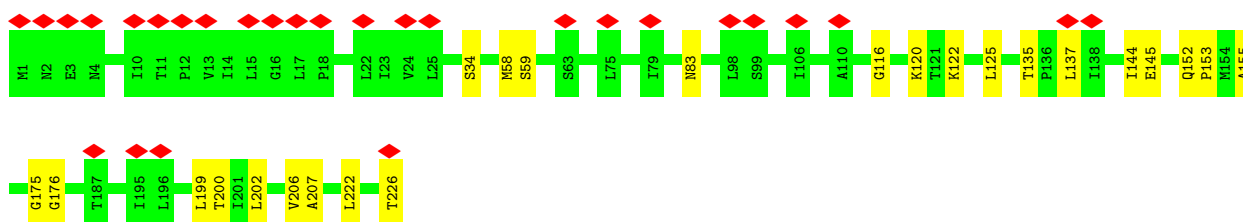
• Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

Chain S: 10% 55% 22% 12%



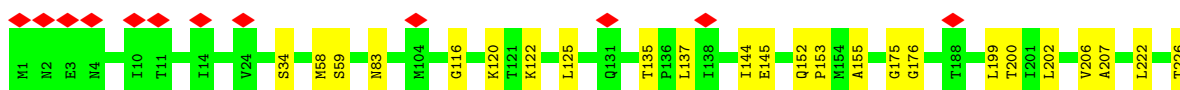
• Molecule 10: ATP synthase F(0) complex subunit a

Chain Aa: 12% 89% 11%



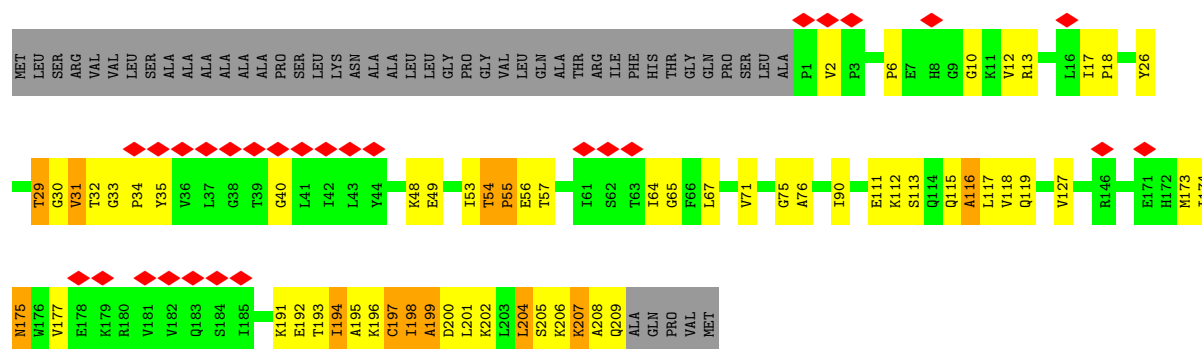
• Molecule 10: ATP synthase F(0) complex subunit a

Chain a: 5% 89% 11%

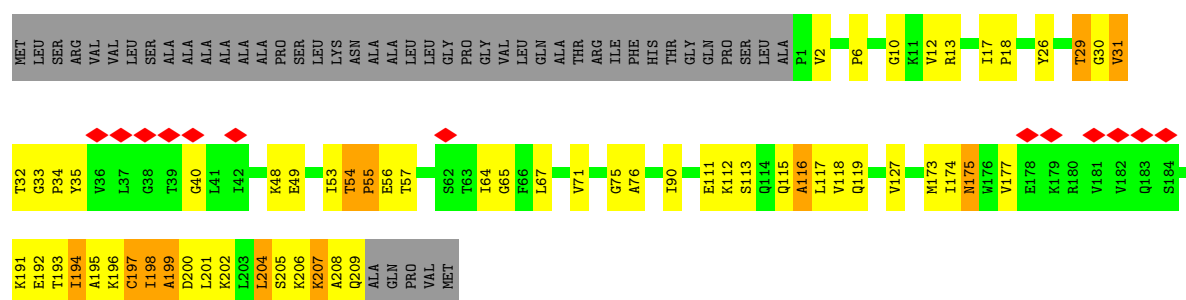


• Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

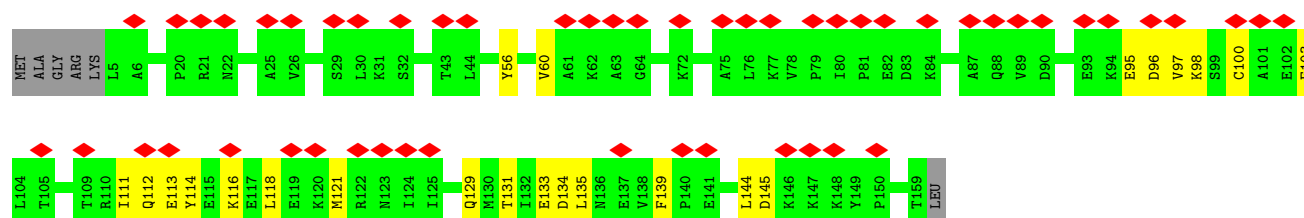
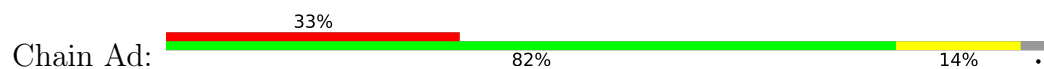
Chain Ab: 11% 58% 19% 5% 18%



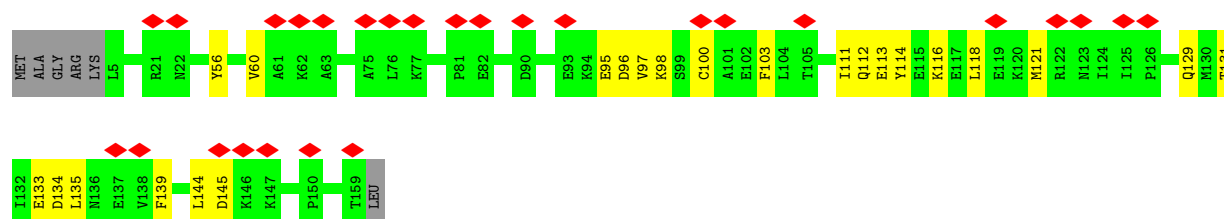
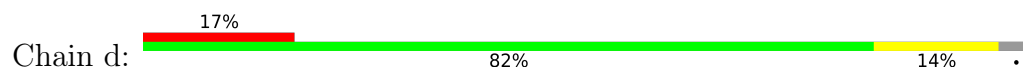
- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial



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

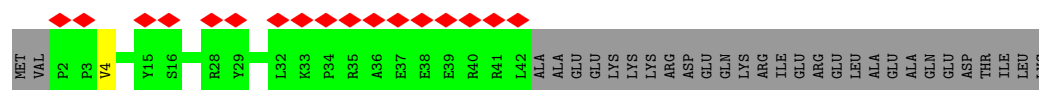


- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

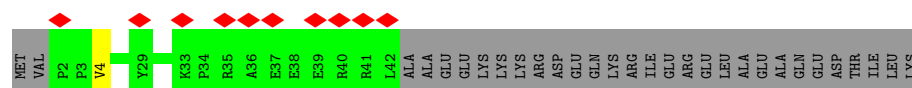


- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

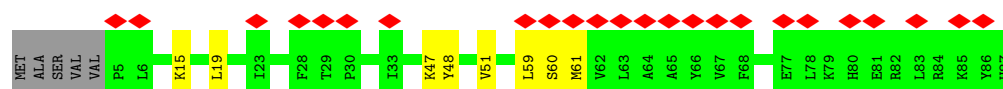
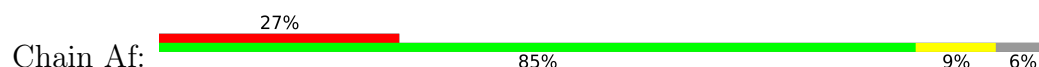




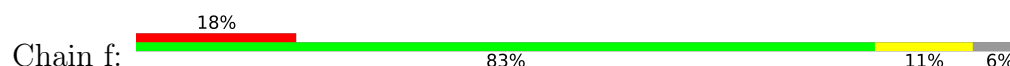
- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial



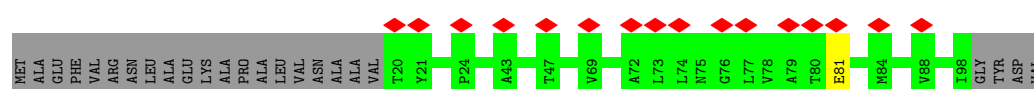
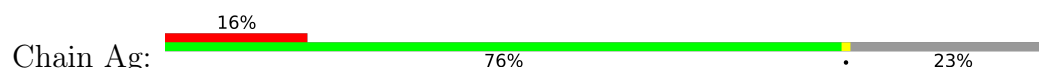
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial



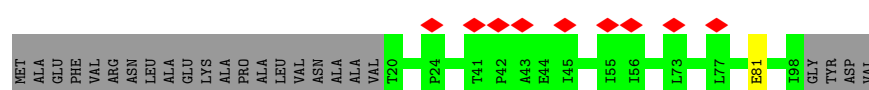
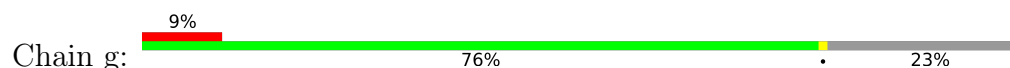
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial



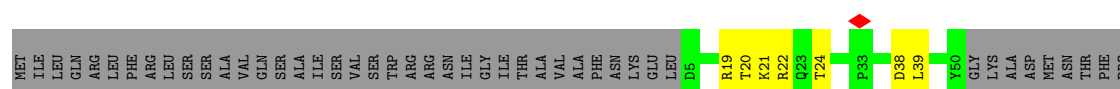
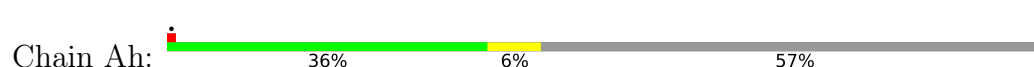
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial



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

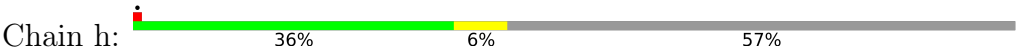


- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial



ASN
PHE
THR
PHE
GLU
ASP
PRO
LYS
PHE
GLU
VAL
VAL
GLU
LYS
PRO
GLN
SER

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



MET
ILE
LEU
GLN
ARG
LEU
PHE
ARG
LEU
SER
SER
ALA
VAL
GLN
SER
ALA
ILE
SER
VAL
SER
TRP
ARG
ARG
ASN
ILE
GLY
ILE
THR
ALA
VAL
ALA
PHE
ASN
LYS
GLU
LEU
D5
R19
T20
K21
R22
Q23
T24
D38
L39
Y50
GLY
LYS
ALA
ASP
MET
ASN
THR
PHE
PRO
ASN
PHE

THR
PHE
GLU
ASP
PRO
LYS
PHE
GLU
VAL
VAL
GLU
LYS
PRO
GLN
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22478	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)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.180	Depositor
Minimum map value	-0.588	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.555	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.184, 2.184, 2.184	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.25	0/204	0.49	0/284
1	A8	0.26	0/204	0.49	0/284
2	A	0.20	0/2456	0.44	0/3408
2	AA	0.20	0/2456	0.44	0/3408
2	AB	0.23	0/2485	0.49	1/3448 (0.0%)
2	AC	0.27	1/2382 (0.0%)	0.57	3/3305 (0.1%)
2	B	0.23	0/2485	0.49	1/3448 (0.0%)
2	C	0.27	1/2382 (0.0%)	0.57	3/3305 (0.1%)
3	AD	0.33	0/2299	0.42	0/3190
3	AE	0.32	0/2289	0.41	0/3176
3	AF	0.33	0/2289	0.44	0/3176
3	D	0.33	0/2299	0.42	0/3190
3	E	0.32	0/2289	0.41	0/3176
3	F	0.33	0/2289	0.44	0/3176
4	AG	0.27	0/1346	0.41	0/1875
4	G	0.27	0/1346	0.41	0/1875
5	AH	0.22	0/647	0.39	0/900
5	H	0.22	0/647	0.39	0/900
6	AI	0.22	0/232	0.32	0/322
6	I	0.22	0/232	0.32	0/322
7	AJ	1.09	0/278	1.49	0/387
7	J	1.00	0/278	1.72	4/387 (1.0%)
8	AK	0.24	0/358	0.42	0/493
8	AL	0.25	0/358	0.47	0/493
8	AM	0.25	0/363	0.57	1/500 (0.2%)
8	AN	0.23	0/363	0.38	0/500
8	AO	0.22	0/363	0.45	0/500
8	AP	0.26	0/358	0.47	0/493
8	AQ	0.23	0/363	0.45	0/500
8	AR	0.25	0/363	0.41	0/500
8	K	0.24	0/358	0.42	0/493
8	L	0.24	0/358	0.47	0/493
8	M	0.25	0/363	0.57	1/500 (0.2%)
8	N	0.23	0/363	0.38	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	O	0.22	0/363	0.44	0/500
8	P	0.25	0/358	0.47	0/493
8	Q	0.23	0/363	0.45	0/500
8	R	0.24	0/363	0.41	0/500
9	AS	0.98	0/925	1.85	24/1288 (1.9%)
9	S	0.98	0/925	1.85	23/1288 (1.8%)
10	Aa	0.26	0/1118	0.51	0/1557
10	a	0.26	0/1118	0.51	0/1557
11	Ab	1.16	0/1034	1.48	4/1440 (0.3%)
11	b	1.16	0/1034	1.48	4/1440 (0.3%)
12	Ad	0.23	0/772	0.50	0/1078
12	d	0.22	0/772	0.49	0/1078
13	Ae	0.23	0/201	0.42	0/278
13	e	0.23	0/201	0.42	0/278
14	Af	0.24	0/408	0.50	0/566
14	f	0.23	0/408	0.50	0/566
15	Ag	0.21	0/389	0.46	0/540
15	g	0.21	0/389	0.46	0/540
16	Ah	0.21	0/226	0.65	0/313
16	h	0.21	0/226	0.65	0/313
All	All	0.41	2/49738 (0.0%)	0.66	69/69020 (0.1%)

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
2	AB	0	1
2	AC	0	1
2	B	0	1
2	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AC	94	ILE	C-N	-6.60	1.24	1.33
2	C	94	ILE	C-N	-6.57	1.24	1.33

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	94	ILE	O-C-N	-18.25	99.75	122.57
2	C	94	ILE	O-C-N	-18.23	99.78	122.57
2	AB	94	ILE	O-C-N	-13.59	105.58	122.57
2	B	94	ILE	O-C-N	-13.54	105.64	122.57
7	J	25	ARG	N-CA-C	-9.20	101.16	112.38
9	AS	99	PRO	N-CA-CB	-9.12	93.68	103.25
9	S	99	PRO	N-CA-CB	-9.12	93.68	103.25
11	b	174	ILE	N-CA-C	-8.41	102.04	110.62
11	Ab	174	ILE	N-CA-C	-8.38	102.07	110.62
9	AS	113	ARG	N-CA-C	-7.73	103.96	113.15
9	S	113	ARG	N-CA-C	-7.71	103.97	113.15
7	J	36	ALA	N-CA-C	-7.17	103.40	111.07
9	S	15	GLU	N-CA-C	-6.92	104.56	112.87
9	AS	15	GLU	N-CA-C	-6.91	104.58	112.87
9	S	133	GLU	N-CA-C	-6.91	103.83	111.36
9	AS	133	GLU	N-CA-C	-6.89	103.85	111.36
2	AC	94	ILE	CA-C-N	6.89	134.37	121.97
2	AC	94	ILE	C-N-CA	6.89	134.37	121.97
2	C	94	ILE	CA-C-N	6.87	134.33	121.97
2	C	94	ILE	C-N-CA	6.87	134.33	121.97
9	S	91	GLU	N-CA-C	-6.72	103.95	111.28
9	AS	91	GLU	N-CA-C	-6.72	103.96	111.28
9	AS	51	MET	N-CA-C	-6.68	103.25	111.33
9	S	51	MET	N-CA-C	-6.65	103.28	111.33
9	S	117	PRO	N-CA-CB	-6.58	96.34	103.25
9	AS	117	PRO	N-CA-CB	-6.54	96.39	103.25
9	AS	130	THR	N-CA-C	-6.47	104.23	111.28
9	S	130	THR	N-CA-C	-6.46	104.24	111.28
11	b	174	ILE	CB-CA-C	-6.42	103.48	112.14
11	Ab	174	ILE	CB-CA-C	-6.41	103.49	112.14
9	AS	183	SER	N-CA-C	-6.31	105.30	112.87
9	S	44	GLN	N-CA-C	-6.29	103.34	111.02
9	S	110	SER	N-CA-C	-6.29	103.72	111.33
9	S	141	PHE	N-CA-C	-6.29	104.71	112.38
9	S	183	SER	N-CA-C	-6.28	105.33	112.87
9	AS	110	SER	N-CA-C	-6.28	103.73	111.33
9	AS	44	GLN	N-CA-C	-6.28	103.36	111.02
9	AS	141	PHE	N-CA-C	-6.27	104.73	112.38
9	AS	89	LEU	N-CA-C	-6.20	104.98	112.54
9	S	89	LEU	N-CA-C	-6.20	104.98	112.54
8	M	43	LYS	N-CA-C	6.00	117.48	111.07
8	AM	43	LYS	N-CA-C	5.96	117.45	111.07
9	S	180	GLN	N-CA-C	-5.86	105.98	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AS	180	GLN	N-CA-C	-5.82	106.02	113.01
11	Ab	174	ILE	N-CA-CB	5.82	118.46	110.54
11	b	174	ILE	N-CA-CB	5.76	118.38	110.54
7	J	27	GLN	N-CA-C	-5.69	104.94	112.34
9	AS	139	LYS	N-CA-C	-5.68	106.06	112.87
9	S	139	LYS	N-CA-C	-5.66	106.08	112.87
9	S	90	ALA	N-CA-C	-5.61	105.24	111.36
9	AS	90	ALA	N-CA-C	-5.58	105.28	111.36
9	AS	162	MET	CB-CA-C	-5.58	109.15	115.79
9	S	162	MET	CB-CA-C	-5.56	109.17	115.79
9	AS	12	TYR	N-CA-C	-5.56	106.58	113.19
9	S	12	TYR	N-CA-C	-5.54	106.60	113.19
9	S	134	LEU	N-CA-C	-5.50	105.38	111.71
9	S	135	LYS	N-CA-C	-5.50	105.20	111.14
9	AS	135	LYS	N-CA-C	-5.49	105.21	111.14
9	AS	134	LEU	N-CA-C	-5.47	105.42	111.71
9	S	92	ASN	N-CA-C	-5.36	106.00	112.54
9	AS	92	ASN	N-CA-C	-5.34	106.03	112.54
9	AS	136	THR	N-CA-C	-5.26	104.97	111.33
9	S	136	THR	N-CA-C	-5.25	104.97	111.33
9	S	7	PRO	N-CA-C	-5.23	104.32	110.70
9	AS	7	PRO	N-CA-C	-5.21	104.35	110.70
11	Ab	204	LEU	N-CA-C	-5.13	105.59	111.14
11	b	204	LEU	N-CA-C	-5.13	105.60	111.14
7	J	35	ARG	N-CA-C	-5.07	105.84	111.36
9	AS	131	LEU	N-CA-C	-5.03	105.80	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	94	ILE	Mainchain
2	AC	94	ILE	Mainchain
2	B	94	ILE	Mainchain
2	C	94	ILE	Mainchain

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	8	205	0	81	2	0
1	A8	205	0	81	2	0
2	A	2457	0	1173	20	0
2	AA	2457	0	1173	19	0
2	AB	2486	0	1189	12	0
2	AC	2383	0	1139	24	0
2	B	2486	0	1189	11	0
2	C	2383	0	1139	8	0
3	AD	2300	0	1094	19	0
3	AE	2290	0	1090	3	0
3	AF	2290	0	1090	6	0
3	D	2300	0	1094	23	0
3	E	2290	0	1090	2	0
3	F	2290	0	1090	5	0
4	AG	1347	0	641	1	0
4	G	1347	0	641	1	0
5	AH	648	0	324	2	0
5	H	648	0	324	3	0
6	AI	233	0	119	2	0
6	I	233	0	119	2	0
7	AJ	279	0	130	48	0
7	J	279	0	130	71	0
8	AK	359	0	199	2	0
8	AL	359	0	199	3	0
8	AM	364	0	201	2	0
8	AN	364	0	201	1	0
8	AO	364	0	201	4	0
8	AP	359	0	199	4	0
8	AQ	364	0	201	2	0
8	AR	364	0	201	1	0
8	K	359	0	199	3	0
8	L	359	0	199	3	0
8	M	364	0	201	2	0
8	N	364	0	201	1	0
8	O	364	0	201	4	0
8	P	359	0	199	4	0
8	Q	364	0	201	2	0
8	R	364	0	201	1	0
9	AS	926	0	425	311	0
9	S	926	0	425	308	0
10	Aa	1119	0	498	28	0
10	a	1119	0	498	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Ab	1035	0	459	69	0
11	b	1035	0	459	70	0
12	Ad	773	0	342	15	0
12	d	773	0	342	15	0
13	Ae	202	0	93	1	0
13	e	202	0	93	1	0
14	Af	409	0	184	7	0
14	f	409	0	184	7	0
15	Ag	390	0	178	1	0
15	g	390	0	178	1	0
16	Ah	227	0	94	6	0
16	h	227	0	94	6	0
All	All	49792	0	23890	1025	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1025) 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)
9:AS:141:PHE:CB	11:Ab:205:SER:CB	1.88	1.50
9:S:141:PHE:CB	11:b:205:SER:CB	1.88	1.49
10:a:175:GLY:HA3	11:b:56:GLU:CB	1.44	1.46
10:Aa:175:GLY:HA3	11:Ab:56:GLU:CB	1.44	1.45
10:a:176:GLY:CA	11:b:55:PRO:O	1.68	1.41
7:AJ:60:ILE:CB	7:J:74:ILE:C	1.91	1.40
9:AS:124:SER:HA	9:AS:156:PRO:CA	1.52	1.38
10:Aa:176:GLY:CA	11:Ab:55:PRO:O	1.68	1.38
9:AS:139:LYS:CB	9:AS:146:GLN:CB	2.03	1.37
9:S:139:LYS:CB	9:S:146:GLN:CB	2.03	1.37
2:AC:402:ALA:CB	7:AJ:28:ALA:HB2	1.56	1.36
9:S:124:SER:HA	9:S:156:PRO:CA	1.52	1.35
2:AA:27:GLU:HA	9:AS:168:GLU:CB	1.59	1.33
2:A:25:LEU:CA	9:S:171:VAL:CB	2.08	1.31
2:A:27:GLU:HA	9:S:168:GLU:CB	1.59	1.31
2:AA:25:LEU:CA	9:AS:171:VAL:CB	2.07	1.29
9:AS:161:GLY:CA	9:AS:174:SER:HA	1.69	1.23
9:S:161:GLY:CA	9:S:174:SER:HA	1.69	1.22
10:Aa:175:GLY:CA	11:Ab:56:GLU:CB	2.19	1.21
2:B:77:GLY:O	2:B:239:ALA:HB2	1.40	1.20
10:a:175:GLY:CA	11:b:56:GLU:CB	2.19	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:77:GLY:O	2:AB:239:ALA:HB2	1.40	1.19
2:AC:402:ALA:C	7:AJ:28:ALA:HB2	1.66	1.19
7:AJ:74:ILE:CB	7:J:60:ILE:CB	2.21	1.19
2:AA:25:LEU:N	9:AS:171:VAL:CB	2.08	1.16
2:A:25:LEU:N	9:S:171:VAL:CB	2.08	1.16
11:b:12:VAL:HA	11:b:18:PRO:CA	1.77	1.15
10:Aa:176:GLY:HA2	11:Ab:55:PRO:O	0.97	1.15
9:S:124:SER:CA	9:S:156:PRO:HA	1.78	1.14
10:a:176:GLY:HA2	11:b:55:PRO:O	0.97	1.13
9:AS:124:SER:CA	9:AS:156:PRO:HA	1.78	1.13
11:Ab:12:VAL:HA	11:Ab:18:PRO:CA	1.77	1.13
9:AS:161:GLY:HA3	9:AS:174:SER:CA	1.78	1.12
9:S:161:GLY:HA3	9:S:174:SER:CA	1.78	1.12
2:AC:402:ALA:C	7:AJ:28:ALA:CB	2.23	1.11
11:Ab:12:VAL:CA	11:Ab:18:PRO:HA	1.80	1.11
11:b:12:VAL:CA	11:b:18:PRO:HA	1.80	1.11
2:A:25:LEU:HA	9:S:171:VAL:CB	1.77	1.11
2:AA:25:LEU:HA	9:AS:171:VAL:CB	1.77	1.11
2:B:77:GLY:O	2:B:239:ALA:CB	1.99	1.11
3:D:478:ALA:HB1	7:J:46:LYS:HA	1.11	1.10
2:AB:77:GLY:O	2:AB:239:ALA:CB	1.99	1.10
2:AC:402:ALA:CA	7:AJ:28:ALA:HB2	1.84	1.07
2:AA:25:LEU:HA	9:AS:171:VAL:CA	1.85	1.06
9:S:118:CYS:HA	9:S:166:ILE:HA	1.09	1.06
3:AD:393:ALA:HB2	7:AJ:23:GLY:HA3	1.34	1.06
9:AS:117:PRO:HA	9:AS:148:LEU:HA	1.38	1.05
9:AS:118:CYS:HA	9:AS:166:ILE:HA	1.10	1.05
2:A:25:LEU:HA	9:S:171:VAL:CA	1.85	1.05
7:AJ:67:ILE:HA	7:J:67:ILE:CB	1.87	1.04
2:AC:402:ALA:HB3	7:AJ:28:ALA:HB2	1.34	1.03
2:AC:402:ALA:HB3	7:AJ:28:ALA:CB	1.91	1.01
9:S:117:PRO:HA	9:S:148:LEU:HA	1.38	1.01
9:S:33:GLU:HA	9:S:36:GLU:CB	1.93	0.99
9:AS:33:GLU:HA	9:AS:36:GLU:CB	1.93	0.99
2:AC:403:PHE:N	7:AJ:28:ALA:HB1	1.77	0.99
9:S:87:ASN:HA	9:S:90:ALA:HB3	1.43	0.98
2:C:288:PRO:CB	3:D:274:ALA:HB1	1.92	0.98
2:AC:288:PRO:CB	3:AD:274:ALA:HB1	1.94	0.98
9:AS:87:ASN:HA	9:AS:90:ALA:HB3	1.43	0.98
2:AC:402:ALA:CB	7:AJ:28:ALA:CB	2.42	0.97
7:AJ:60:ILE:CB	7:J:75:LYS:N	2.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AJ:67:ILE:HA	7:J:67:ILE:HA	1.48	0.96
2:B:77:GLY:C	2:B:239:ALA:HB2	1.90	0.96
3:D:392:ILE:O	7:J:23:GLY:N	1.98	0.95
3:D:457:PRO:N	7:J:41:GLN:CB	2.29	0.94
2:AA:25:LEU:CB	9:AS:171:VAL:CB	2.45	0.94
2:A:25:LEU:CB	9:S:171:VAL:CB	2.45	0.94
2:AB:77:GLY:C	2:AB:239:ALA:HB2	1.91	0.94
2:AA:25:LEU:HA	9:AS:171:VAL:N	1.83	0.94
10:a:176:GLY:N	11:b:55:PRO:O	2.01	0.93
2:AC:402:ALA:HB3	7:AJ:28:ALA:CA	1.96	0.93
2:A:26:GLU:O	9:S:168:GLU:O	1.86	0.93
9:S:117:PRO:CA	9:S:148:LEU:HA	1.99	0.93
2:AA:26:GLU:O	9:AS:168:GLU:O	1.86	0.93
2:A:25:LEU:HA	9:S:171:VAL:N	1.83	0.92
10:Aa:176:GLY:N	11:Ab:55:PRO:O	2.01	0.92
3:D:478:ALA:HB1	7:J:46:LYS:CA	1.98	0.92
3:D:478:ALA:CB	7:J:46:LYS:HA	1.99	0.92
9:AS:117:PRO:CA	9:AS:148:LEU:HA	1.99	0.91
9:AS:161:GLY:HA3	9:AS:174:SER:HA	0.93	0.91
7:AJ:67:ILE:HA	7:J:67:ILE:CA	2.01	0.91
11:Ab:71:VAL:HA	11:Ab:75:GLY:HA3	1.52	0.91
9:S:117:PRO:HA	9:S:148:LEU:CA	2.01	0.90
10:Aa:175:GLY:O	11:Ab:56:GLU:HA	1.71	0.90
10:a:175:GLY:O	11:b:56:GLU:HA	1.71	0.90
9:S:124:SER:HA	9:S:156:PRO:HA	0.90	0.90
9:S:161:GLY:HA3	9:S:174:SER:HA	0.93	0.90
9:AS:124:SER:HA	9:AS:156:PRO:HA	0.90	0.89
9:AS:117:PRO:HA	9:AS:148:LEU:CA	2.01	0.89
11:b:71:VAL:HA	11:b:75:GLY:HA3	1.51	0.89
9:S:111:VAL:HA	9:S:114:GLY:HA2	1.55	0.88
7:AJ:60:ILE:CB	7:J:74:ILE:O	2.22	0.88
9:AS:41:ARG:O	9:AS:42:VAL:C	2.17	0.88
9:AS:111:VAL:HA	9:AS:114:GLY:HA2	1.55	0.87
2:A:27:GLU:CA	9:S:168:GLU:CB	2.52	0.86
9:AS:118:CYS:CA	9:AS:166:ILE:HA	2.03	0.86
2:AA:27:GLU:CA	9:AS:168:GLU:CB	2.52	0.86
10:Aa:175:GLY:C	11:Ab:56:GLU:HA	2.01	0.85
9:S:35:VAL:O	9:S:36:GLU:C	2.19	0.85
10:a:175:GLY:C	11:b:56:GLU:HA	2.01	0.84
7:AJ:67:ILE:CA	7:J:67:ILE:CB	2.55	0.84
9:AS:35:VAL:O	9:AS:36:GLU:C	2.19	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:38:GLU:O	9:AS:39:LEU:C	2.20	0.84
9:S:38:GLU:O	9:S:39:LEU:C	2.20	0.83
7:AJ:70:HIS:CB	7:J:63:LEU:C	2.52	0.83
9:S:41:ARG:O	9:S:42:VAL:C	2.17	0.83
9:S:124:SER:CA	9:S:156:PRO:CA	2.48	0.83
7:AJ:70:HIS:CB	7:J:63:LEU:O	2.27	0.83
2:AC:296:GLY:O	3:AD:271:GLU:HA	1.79	0.82
9:S:41:ARG:O	9:S:45:ILE:N	2.12	0.82
2:B:94:ILE:O	2:B:95:VAL:C	2.20	0.82
9:AS:41:ARG:O	9:AS:45:ILE:N	2.13	0.82
12:d:96:ASP:O	12:d:100:CYS:N	2.13	0.81
2:AC:403:PHE:N	7:AJ:28:ALA:CB	2.42	0.81
9:AS:111:VAL:C	9:AS:114:GLY:H	1.89	0.81
2:AA:34:ILE:O	3:AD:56:HIS:N	2.14	0.81
2:AB:94:ILE:O	2:AB:95:VAL:C	2.20	0.80
9:S:111:VAL:C	9:S:114:GLY:H	1.88	0.80
11:b:10:GLY:H	14:f:48:TYR:HA	1.46	0.80
9:AS:124:SER:CA	9:AS:156:PRO:CA	2.48	0.80
11:Ab:10:GLY:H	14:Af:48:TYR:HA	1.46	0.80
2:A:34:ILE:O	3:D:56:HIS:N	2.14	0.79
16:Ah:21:LYS:O	16:Ah:24:THR:N	2.15	0.79
9:S:46:LEU:O	9:S:47:LYS:C	2.24	0.79
16:h:21:LYS:O	16:h:24:THR:N	2.15	0.79
2:AC:402:ALA:HB3	7:AJ:28:ALA:N	1.98	0.79
9:AS:43:GLY:HA2	9:AS:46:LEU:CB	2.13	0.78
9:S:43:GLY:HA2	9:S:46:LEU:CB	2.13	0.78
9:S:118:CYS:CA	9:S:166:ILE:HA	2.03	0.78
9:AS:46:LEU:O	9:AS:47:LYS:C	2.24	0.78
9:AS:167:GLY:C	9:AS:169:LYS:H	1.92	0.77
7:AJ:74:ILE:CB	7:J:60:ILE:CA	2.62	0.77
9:S:41:ARG:HA	9:S:45:ILE:H	1.50	0.77
9:S:167:GLY:C	9:S:169:LYS:H	1.92	0.76
9:AS:41:ARG:HA	9:AS:45:ILE:H	1.50	0.76
7:AJ:74:ILE:CB	7:J:60:ILE:HA	2.16	0.76
12:Ad:96:ASP:O	12:Ad:100:CYS:N	2.13	0.76
7:AJ:52:GLU:CB	7:AJ:53:ILE:HA	2.16	0.76
9:AS:109:MET:HA	9:AS:112:HIS:CB	2.16	0.74
9:S:109:MET:HA	9:S:112:HIS:CB	2.16	0.74
9:S:47:LYS:O	9:S:48:GLU:C	2.30	0.74
9:AS:87:ASN:CA	9:AS:90:ALA:HB3	2.18	0.73
9:AS:35:VAL:O	9:AS:39:LEU:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:47:LYS:O	9:AS:48:GLU:C	2.30	0.73
9:S:161:GLY:C	9:S:174:SER:HA	2.14	0.73
9:S:35:VAL:O	9:S:39:LEU:N	2.21	0.73
11:b:206:LYS:O	11:b:207:LYS:C	2.32	0.73
9:AS:60:VAL:O	9:AS:61:LYS:C	2.31	0.73
9:S:118:CYS:HA	9:S:166:ILE:CA	2.05	0.73
9:S:38:GLU:O	9:S:42:VAL:N	2.22	0.72
9:AS:29:GLN:C	9:AS:31:LYS:H	1.97	0.72
11:Ab:206:LYS:O	11:Ab:207:LYS:C	2.32	0.72
9:S:144:LYS:O	9:S:145:GLY:C	2.32	0.72
2:AC:403:PHE:CA	7:AJ:28:ALA:HB1	2.20	0.72
9:AS:104:ALA:O	9:AS:105:PHE:C	2.33	0.72
11:Ab:196:LYS:O	11:Ab:199:ALA:HB3	1.89	0.72
9:AS:43:GLY:O	9:AS:47:LYS:N	2.22	0.72
9:AS:119:THR:O	9:AS:164:VAL:HA	1.90	0.72
9:S:119:THR:O	9:S:164:VAL:HA	1.90	0.72
9:S:89:LEU:O	9:S:93:GLY:N	2.23	0.72
9:S:43:GLY:O	9:S:47:LYS:N	2.22	0.71
9:S:41:ARG:CA	9:S:45:ILE:H	2.03	0.71
9:AS:89:LEU:O	9:AS:93:GLY:N	2.23	0.71
9:AS:38:GLU:O	9:AS:42:VAL:N	2.22	0.71
9:S:60:VAL:O	9:S:61:LYS:C	2.31	0.71
11:b:196:LYS:O	11:b:199:ALA:HB3	1.89	0.71
2:A:24:ASP:O	9:S:171:VAL:HA	1.91	0.71
9:AS:41:ARG:O	9:AS:43:GLY:N	2.24	0.70
9:S:29:GLN:C	9:S:31:LYS:H	1.97	0.70
9:AS:161:GLY:C	9:AS:174:SER:HA	2.14	0.70
9:AS:33:GLU:O	9:AS:34:GLN:C	2.33	0.70
7:AJ:67:ILE:CB	7:J:67:ILE:CB	2.69	0.70
9:AS:144:LYS:O	9:AS:145:GLY:C	2.32	0.70
9:S:100:ALA:O	9:S:101:VAL:C	2.34	0.70
9:AS:41:ARG:CA	9:AS:45:ILE:H	2.03	0.70
9:S:87:ASN:CA	9:S:90:ALA:HB3	2.18	0.70
11:b:12:VAL:HA	11:b:18:PRO:HA	0.84	0.70
7:AJ:67:ILE:CA	7:J:67:ILE:HA	2.19	0.70
9:AS:177:THR:O	9:AS:178:LYS:C	2.34	0.70
10:Aa:175:GLY:C	11:Ab:56:GLU:CA	2.64	0.70
7:J:71:LYS:O	7:J:72:GLN:C	2.34	0.70
9:AS:161:GLY:N	9:AS:175:ALA:H	1.89	0.70
9:S:33:GLU:O	9:S:34:GLN:C	2.33	0.70
9:S:160:GLY:C	9:S:162:MET:H	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:161:GLY:N	9:S:175:ALA:H	1.89	0.70
9:S:177:THR:O	9:S:178:LYS:C	2.34	0.70
2:AA:24:ASP:O	9:AS:171:VAL:HA	1.91	0.69
9:AS:73:THR:HA	9:AS:76:GLU:CB	2.22	0.69
9:S:73:THR:HA	9:S:76:GLU:CB	2.22	0.69
10:a:175:GLY:C	11:b:56:GLU:CA	2.64	0.69
8:AK:5:ALA:HB1	8:AL:6:ALA:HB2	1.74	0.69
9:AS:105:PHE:O	9:AS:109:MET:N	2.20	0.69
11:Ab:197:CYS:O	11:Ab:198:ILE:C	2.36	0.69
9:AS:19:ALA:HA	9:AS:22:LEU:CB	2.23	0.69
9:S:41:ARG:O	9:S:43:GLY:N	2.24	0.69
9:S:104:ALA:O	9:S:105:PHE:C	2.33	0.69
11:b:13:ARG:H	11:b:17:ILE:C	2.00	0.69
9:AS:139:LYS:HA	9:AS:142:LEU:CB	2.23	0.69
8:K:5:ALA:HB1	8:L:6:ALA:HB2	1.74	0.69
11:Ab:195:ALA:O	11:Ab:199:ALA:N	2.22	0.69
11:b:197:CYS:O	11:b:198:ILE:C	2.36	0.69
9:AS:100:ALA:O	9:AS:101:VAL:C	2.34	0.69
9:S:139:LYS:HA	9:S:142:LEU:CB	2.23	0.69
11:b:195:ALA:O	11:b:196:LYS:C	2.36	0.68
9:S:180:GLN:HA	9:S:183:SER:CB	2.23	0.68
9:AS:160:GLY:C	9:AS:162:MET:H	2.00	0.68
3:F:235:ARG:O	3:F:238:LEU:N	2.27	0.68
11:Ab:13:ARG:H	11:Ab:17:ILE:C	2.00	0.68
9:S:101:VAL:O	9:S:104:ALA:HB3	1.94	0.68
9:AS:101:VAL:O	9:AS:104:ALA:HB3	1.93	0.68
10:Aa:199:LEU:O	10:Aa:202:LEU:N	2.27	0.68
10:a:199:LEU:O	10:a:202:LEU:N	2.27	0.68
9:S:87:ASN:HA	9:S:90:ALA:CB	2.23	0.68
9:S:19:ALA:HA	9:S:22:LEU:CB	2.22	0.68
9:S:124:SER:HA	9:S:156:PRO:N	2.08	0.68
7:AJ:70:HIS:CB	7:J:63:LEU:CA	2.72	0.67
9:AS:40:LEU:O	9:AS:44:GLN:N	2.19	0.67
9:AS:124:SER:HA	9:AS:156:PRO:N	2.08	0.67
9:S:40:LEU:O	9:S:44:GLN:N	2.19	0.67
9:AS:180:GLN:HA	9:AS:183:SER:CB	2.23	0.67
2:C:296:GLY:O	3:D:271:GLU:HA	1.93	0.67
2:AC:296:GLY:O	3:AD:271:GLU:CA	2.43	0.67
3:AF:235:ARG:O	3:AF:238:LEU:N	2.27	0.67
9:AS:117:PRO:HA	9:AS:148:LEU:C	2.19	0.67
11:Ab:202:LYS:O	11:Ab:206:LYS:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:117:PRO:HA	9:S:148:LEU:C	2.19	0.67
7:AJ:70:HIS:O	7:J:63:LEU:CB	2.43	0.66
2:A:25:LEU:HA	9:S:171:VAL:H	1.60	0.66
9:S:131:LEU:O	9:S:135:LYS:N	2.27	0.66
9:AS:118:CYS:HA	9:AS:166:ILE:CA	2.05	0.66
9:AS:131:LEU:O	9:AS:135:LYS:N	2.27	0.66
11:b:195:ALA:O	11:b:199:ALA:N	2.22	0.66
9:S:165:ARG:O	9:S:167:GLY:N	2.28	0.66
9:AS:108:MET:O	9:AS:112:HIS:N	2.28	0.66
11:b:30:GLY:O	11:b:31:VAL:C	2.39	0.66
11:b:202:LYS:O	11:b:206:LYS:N	2.28	0.66
9:S:65:LYS:O	9:S:69:LEU:N	2.27	0.66
9:AS:41:ARG:HA	9:AS:44:GLN:CB	2.26	0.65
10:a:175:GLY:C	11:b:55:PRO:O	2.39	0.65
9:AS:160:GLY:CA	9:AS:175:ALA:HB3	2.26	0.65
11:Ab:195:ALA:O	11:Ab:196:LYS:C	2.36	0.65
3:AD:393:ALA:HA	7:AJ:26:GLU:CB	2.27	0.65
9:S:160:GLY:C	9:S:175:ALA:H	2.04	0.65
9:AS:95:LEU:C	9:AS:97:ASN:N	2.53	0.65
9:AS:165:ARG:O	9:AS:167:GLY:N	2.28	0.65
9:S:41:ARG:HA	9:S:44:GLN:CB	2.26	0.65
2:A:24:ASP:C	9:S:171:VAL:HA	2.22	0.65
2:AA:25:LEU:HA	9:AS:171:VAL:H	1.60	0.65
9:S:117:PRO:C	9:S:148:LEU:HA	2.22	0.65
9:S:160:GLY:CA	9:S:175:ALA:HB3	2.26	0.65
2:AA:24:ASP:C	9:AS:171:VAL:HA	2.22	0.65
9:S:108:MET:O	9:S:112:HIS:N	2.28	0.65
9:AS:160:GLY:C	9:AS:175:ALA:H	2.03	0.65
9:AS:117:PRO:HA	9:AS:149:LYS:N	2.12	0.64
9:S:105:PHE:O	9:S:109:MET:N	2.21	0.64
2:AC:296:GLY:O	3:AD:271:GLU:CB	2.45	0.64
11:Ab:30:GLY:O	11:Ab:31:VAL:C	2.39	0.64
10:Aa:175:GLY:C	11:Ab:55:PRO:O	2.39	0.64
9:AS:90:ALA:C	9:AS:93:GLY:H	2.06	0.64
9:S:117:PRO:HA	9:S:149:LYS:N	2.12	0.64
9:S:160:GLY:N	9:S:175:ALA:HB3	2.13	0.64
3:AD:457:PRO:CB	7:AJ:41:GLN:CB	2.76	0.63
9:AS:117:PRO:C	9:AS:148:LEU:HA	2.22	0.63
9:AS:123:ALA:HB2	9:AS:162:MET:CA	2.29	0.63
9:AS:137:VAL:HA	9:AS:140:SER:CB	2.28	0.63
7:J:35:ARG:HA	7:J:38:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:87:ASN:HA	9:AS:90:ALA:CB	2.23	0.63
9:S:137:VAL:HA	9:S:140:SER:CB	2.28	0.63
9:S:90:ALA:C	9:S:93:GLY:H	2.06	0.63
11:b:191:LYS:O	11:b:194:ILE:N	2.32	0.63
9:S:95:LEU:O	9:S:97:ASN:N	2.31	0.63
9:AS:29:GLN:C	9:AS:31:LYS:N	2.54	0.63
9:AS:95:LEU:O	9:AS:97:ASN:N	2.31	0.63
7:J:40:GLU:O	7:J:41:GLN:C	2.42	0.63
11:b:197:CYS:O	11:b:201:LEU:N	2.28	0.63
9:AS:167:GLY:C	9:AS:169:LYS:N	2.55	0.63
11:Ab:191:LYS:O	11:Ab:194:ILE:N	2.32	0.62
12:d:98:LYS:O	12:d:103:PHE:N	2.32	0.62
2:AC:402:ALA:HB1	7:AJ:28:ALA:HB2	1.70	0.62
9:AS:65:LYS:O	9:AS:69:LEU:N	2.27	0.62
9:AS:160:GLY:N	9:AS:175:ALA:HB3	2.12	0.62
7:J:34:PHE:O	7:J:38:ALA:N	2.33	0.62
9:S:94:ARG:C	9:S:96:THR:H	2.07	0.62
9:S:80:PRO:O	9:S:81:LEU:C	2.41	0.62
9:S:123:ALA:HB2	9:S:162:MET:CA	2.29	0.62
12:Ad:98:LYS:O	12:Ad:103:PHE:N	2.32	0.62
9:AS:80:PRO:O	9:AS:81:LEU:C	2.41	0.62
9:AS:129:ALA:O	9:AS:133:GLU:N	2.33	0.62
9:S:49:PRO:O	9:S:53:ALA:N	2.33	0.62
9:S:129:ALA:O	9:S:133:GLU:N	2.33	0.62
9:S:177:THR:O	9:S:179:ILE:N	2.33	0.62
9:AS:61:LYS:O	9:AS:64:VAL:N	2.32	0.62
9:S:167:GLY:C	9:S:169:LYS:N	2.55	0.62
2:AA:24:ASP:C	9:AS:171:VAL:CB	2.73	0.61
7:AJ:67:ILE:CA	7:J:67:ILE:CA	2.75	0.61
9:S:61:LYS:O	9:S:64:VAL:N	2.32	0.61
9:AS:105:PHE:O	9:AS:106:SER:C	2.43	0.61
2:A:24:ASP:C	9:S:171:VAL:CB	2.73	0.61
2:C:296:GLY:O	3:D:271:GLU:CB	2.49	0.61
7:J:33:TYR:O	7:J:36:ALA:HB3	2.01	0.61
9:S:95:LEU:C	9:S:97:ASN:N	2.53	0.61
9:AS:177:THR:O	9:AS:179:ILE:N	2.33	0.61
9:AS:94:ARG:C	9:AS:96:THR:H	2.07	0.61
11:b:13:ARG:O	11:b:17:ILE:N	2.34	0.61
9:AS:116:VAL:O	9:AS:148:LEU:N	2.34	0.60
2:AC:400:VAL:HA	7:AJ:31:GLU:CB	2.30	0.60
11:Ab:12:VAL:HA	11:Ab:18:PRO:HA	0.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:105:PHE:O	9:S:106:SER:C	2.43	0.60
9:AS:49:PRO:O	9:AS:53:ALA:N	2.33	0.60
3:D:456:LEU:C	7:J:41:GLN:CB	2.74	0.60
9:S:116:VAL:O	9:S:148:LEU:N	2.34	0.60
7:AJ:67:ILE:CB	7:J:67:ILE:CA	2.79	0.60
7:J:35:ARG:O	7:J:38:ALA:HB3	2.02	0.60
9:AS:87:ASN:O	9:AS:91:GLU:N	2.34	0.60
9:S:87:ASN:O	9:S:91:GLU:N	2.34	0.60
3:AD:393:ALA:HB2	7:AJ:23:GLY:CA	2.23	0.60
9:AS:41:ARG:C	9:AS:43:GLY:N	2.59	0.60
11:Ab:13:ARG:O	11:Ab:17:ILE:N	2.34	0.60
9:S:13:GLY:HA3	9:S:16:GLY:HA3	1.84	0.60
9:S:92:ASN:C	9:S:94:ARG:H	2.10	0.60
11:b:115:GLN:O	11:b:116:ALA:C	2.45	0.60
9:AS:58:PRO:O	9:AS:59:TYR:C	2.44	0.60
9:S:58:PRO:O	9:S:59:TYR:C	2.44	0.60
11:Ab:115:GLN:O	11:Ab:116:ALA:C	2.45	0.60
9:S:73:THR:O	9:S:77:LYS:N	2.35	0.59
9:S:100:ALA:O	9:S:104:ALA:N	2.28	0.59
9:S:107:THR:O	9:S:110:SER:N	2.35	0.59
7:AJ:67:ILE:CB	7:J:67:ILE:O	2.50	0.59
9:AS:71:ASP:O	9:AS:74:ALA:HB3	2.02	0.59
9:S:56:LEU:O	9:S:57:ASN:C	2.45	0.59
11:Ab:197:CYS:O	11:Ab:201:LEU:N	2.28	0.59
9:AS:35:VAL:O	9:AS:38:GLU:N	2.36	0.59
9:AS:73:THR:O	9:AS:77:LYS:N	2.35	0.59
9:S:35:VAL:O	9:S:38:GLU:N	2.36	0.59
9:AS:56:LEU:O	9:AS:57:ASN:C	2.45	0.59
9:AS:92:ASN:C	9:AS:94:ARG:H	2.10	0.59
9:AS:98:THR:O	9:AS:99:PRO:C	2.46	0.59
9:AS:107:THR:O	9:AS:110:SER:N	2.35	0.59
2:B:77:GLY:O	2:B:239:ALA:HB1	2.00	0.59
9:S:71:ASP:O	9:S:74:ALA:HB3	2.02	0.59
9:S:98:THR:O	9:S:99:PRO:C	2.45	0.59
7:AJ:67:ILE:CB	7:J:67:ILE:C	2.75	0.59
9:AS:44:GLN:O	9:AS:47:LYS:N	2.35	0.59
9:S:44:GLN:O	9:S:47:LYS:N	2.35	0.59
9:S:102:ILE:O	9:S:106:SER:N	2.32	0.59
11:Ab:175:ASN:C	11:Ab:177:VAL:H	2.11	0.59
9:AS:38:GLU:C	9:AS:42:VAL:H	2.11	0.58
10:a:222:LEU:O	10:a:226:THR:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Aa:222:LEU:O	10:Aa:226:THR:N	2.36	0.58
9:AS:63:SER:O	9:AS:64:VAL:C	2.46	0.58
9:S:165:ARG:C	9:S:167:GLY:N	2.61	0.58
2:AC:402:ALA:C	7:AJ:28:ALA:HB1	2.09	0.58
9:AS:12:TYR:O	9:AS:13:GLY:C	2.47	0.58
9:AS:56:LEU:O	9:AS:58:PRO:N	2.37	0.58
9:AS:13:GLY:HA3	9:AS:16:GLY:HA3	1.84	0.58
9:AS:82:THR:O	9:AS:83:SER:C	2.47	0.58
12:Ad:135:LEU:O	12:Ad:139:PHE:N	2.34	0.58
2:A:358:TYR:O	3:D:380:LYS:HA	2.04	0.58
9:S:41:ARG:C	9:S:43:GLY:N	2.59	0.58
9:AS:39:LEU:O	9:AS:40:LEU:C	2.46	0.58
7:J:24:LYS:C	7:J:26:GLU:N	2.53	0.58
2:AA:358:TYR:O	3:AD:380:LYS:HA	2.04	0.58
10:Aa:176:GLY:CA	11:Ab:55:PRO:C	2.70	0.58
9:S:38:GLU:C	9:S:42:VAL:H	2.11	0.58
9:S:82:THR:O	9:S:83:SER:C	2.47	0.58
9:AS:165:ARG:C	9:AS:167:GLY:N	2.61	0.57
9:S:12:TYR:O	9:S:13:GLY:C	2.47	0.57
9:S:39:LEU:O	9:S:40:LEU:C	2.46	0.57
9:S:141:PHE:CB	11:b:205:SER:CA	2.78	0.57
7:J:35:ARG:HA	7:J:38:ALA:CB	2.34	0.57
9:S:159:MET:C	9:S:175:ALA:HB3	2.29	0.57
9:S:19:ALA:O	9:S:23:TYR:N	2.32	0.57
9:S:133:GLU:O	9:S:137:VAL:N	2.35	0.57
5:AH:126:ALA:HA	6:AI:7:ALA:HB1	1.87	0.57
9:S:29:GLN:C	9:S:31:LYS:N	2.54	0.57
11:b:175:ASN:C	11:b:177:VAL:H	2.11	0.57
9:AS:19:ALA:O	9:AS:23:TYR:N	2.32	0.57
9:S:107:THR:O	9:S:108:MET:C	2.48	0.57
9:AS:102:ILE:O	9:AS:103:SER:C	2.47	0.57
10:Aa:175:GLY:C	11:Ab:56:GLU:CB	2.78	0.57
9:S:56:LEU:O	9:S:58:PRO:N	2.37	0.57
9:S:65:LYS:O	9:S:66:VAL:C	2.48	0.57
9:S:102:ILE:O	9:S:103:SER:C	2.47	0.57
9:AS:65:LYS:O	9:AS:66:VAL:C	2.48	0.57
9:AS:94:ARG:C	9:AS:96:THR:N	2.62	0.57
9:AS:159:MET:C	9:AS:175:ALA:HB3	2.29	0.57
9:AS:167:GLY:O	9:AS:169:LYS:N	2.35	0.57
11:Ab:197:CYS:O	11:Ab:200:ASP:N	2.38	0.57
3:AD:481:HIS:CB	7:AJ:42:LEU:CB	2.83	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:28:LYS:O	9:AS:30:ASN:N	2.36	0.57
9:S:182:LEU:C	9:S:184:ARG:N	2.61	0.57
9:AS:182:LEU:C	9:AS:184:ARG:N	2.61	0.56
11:Ab:54:THR:C	11:Ab:56:GLU:H	2.13	0.56
11:Ab:116:ALA:O	11:Ab:117:LEU:C	2.47	0.56
9:S:167:GLY:O	9:S:169:LYS:N	2.35	0.56
9:AS:123:ALA:HB2	9:AS:162:MET:HA	1.87	0.56
9:S:63:SER:O	9:S:64:VAL:C	2.46	0.56
10:a:175:GLY:C	11:b:56:GLU:CB	2.78	0.56
11:b:116:ALA:O	11:b:117:LEU:C	2.47	0.56
2:AB:77:GLY:O	2:AB:239:ALA:HB1	2.00	0.56
9:AS:100:ALA:HA	9:AS:103:SER:CB	2.35	0.56
7:J:29:GLU:O	7:J:30:GLU:C	2.48	0.56
9:S:123:ALA:HB2	9:S:162:MET:HA	1.87	0.56
11:b:54:THR:C	11:b:56:GLU:H	2.13	0.56
2:AC:77:GLY:O	2:AC:239:ALA:HB2	2.05	0.56
5:H:126:ALA:HA	6:I:7:ALA:HB1	1.87	0.56
9:AS:28:LYS:C	9:AS:30:ASN:H	2.13	0.56
9:AS:99:PRO:O	9:AS:101:VAL:N	2.39	0.56
9:AS:122:THR:C	9:AS:124:SER:H	2.13	0.56
9:S:99:PRO:O	9:S:101:VAL:N	2.39	0.56
9:AS:82:THR:O	9:AS:86:ILE:N	2.30	0.56
9:AS:102:ILE:O	9:AS:106:SER:N	2.32	0.56
9:S:122:THR:C	9:S:124:SER:H	2.13	0.56
10:a:206:VAL:O	10:a:207:ALA:C	2.48	0.56
9:AS:100:ALA:O	9:AS:103:SER:N	2.39	0.56
9:S:100:ALA:O	9:S:103:SER:N	2.39	0.56
9:S:160:GLY:C	9:S:175:ALA:N	2.64	0.56
11:b:193:THR:O	11:b:194:ILE:C	2.49	0.56
11:b:197:CYS:O	11:b:200:ASP:N	2.38	0.56
12:Ad:111:ILE:O	12:Ad:114:TYR:N	2.39	0.56
2:AB:77:GLY:N	2:AB:239:ALA:HB3	2.21	0.55
2:B:77:GLY:N	2:B:239:ALA:HB3	2.21	0.55
2:C:77:GLY:O	2:C:239:ALA:HB2	2.05	0.55
2:C:296:GLY:O	3:D:271:GLU:CA	2.54	0.55
9:S:28:LYS:O	9:S:30:ASN:N	2.36	0.55
9:S:28:LYS:C	9:S:30:ASN:H	2.13	0.55
9:S:63:SER:HA	9:S:66:VAL:CB	2.37	0.55
12:d:111:ILE:O	12:d:114:TYR:N	2.39	0.55
9:AS:45:ILE:O	9:AS:46:LEU:C	2.49	0.55
9:AS:63:SER:HA	9:AS:66:VAL:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:ILE:O	2:C:95:VAL:C	2.48	0.55
9:S:38:GLU:O	9:S:40:LEU:N	2.39	0.55
9:AS:38:GLU:O	9:AS:40:LEU:N	2.40	0.55
2:C:405:GLN:O	3:F:401:SER:CB	2.55	0.55
9:S:94:ARG:C	9:S:96:THR:N	2.62	0.55
9:S:100:ALA:HA	9:S:103:SER:CB	2.35	0.55
9:AS:110:SER:O	9:AS:114:GLY:N	2.40	0.55
10:Aa:206:VAL:O	10:Aa:207:ALA:C	2.48	0.55
9:AS:73:THR:C	9:AS:76:GLU:H	2.15	0.55
9:AS:104:ALA:O	9:AS:107:THR:N	2.40	0.55
9:AS:107:THR:O	9:AS:108:MET:C	2.48	0.55
9:S:14:ILE:C	9:S:16:GLY:N	2.64	0.55
9:S:136:THR:O	9:S:140:SER:N	2.40	0.55
9:S:174:SER:O	9:S:175:ALA:C	2.50	0.55
7:AJ:60:ILE:CB	7:J:75:LYS:CA	2.84	0.55
9:AS:160:GLY:C	9:AS:175:ALA:N	2.64	0.55
9:S:45:ILE:O	9:S:46:LEU:C	2.49	0.55
9:S:104:ALA:O	9:S:107:THR:N	2.40	0.55
9:AS:31:LYS:O	9:AS:32:LEU:C	2.50	0.55
9:AS:144:LYS:O	9:AS:146:GLN:N	2.40	0.55
9:S:138:LEU:C	9:S:140:SER:N	2.64	0.55
11:b:208:ALA:O	11:b:209:GLN:C	2.50	0.55
9:AS:124:SER:O	9:AS:155:ASP:N	2.40	0.54
9:S:160:GLY:C	9:S:162:MET:N	2.65	0.54
2:A:33:SER:CB	3:D:56:HIS:O	2.55	0.54
9:AS:13:GLY:C	9:AS:16:GLY:H	2.16	0.54
9:S:31:LYS:O	9:S:32:LEU:C	2.50	0.54
2:AA:33:SER:CB	3:AD:56:HIS:O	2.55	0.54
9:S:67:LYS:O	9:S:71:ASP:N	2.34	0.54
9:S:110:SER:O	9:S:114:GLY:N	2.40	0.54
9:AS:15:GLU:O	9:AS:16:GLY:C	2.50	0.54
9:AS:141:PHE:CB	11:Ab:205:SER:CA	2.78	0.54
9:AS:145:GLY:O	9:AS:147:VAL:N	2.37	0.54
9:S:113:ARG:O	9:S:114:GLY:C	2.50	0.54
9:AS:136:THR:O	9:AS:140:SER:N	2.40	0.54
9:AS:98:THR:O	9:AS:101:VAL:N	2.36	0.54
11:Ab:208:ALA:O	11:Ab:209:GLN:C	2.50	0.54
12:d:118:LEU:O	12:d:121:MET:N	2.35	0.54
9:AS:100:ALA:O	9:AS:104:ALA:N	2.28	0.54
9:S:98:THR:O	9:S:101:VAL:N	2.36	0.54
7:J:40:GLU:HA	7:J:44:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:30:ASN:O	9:S:31:LYS:C	2.51	0.54
9:S:124:SER:O	9:S:155:ASP:N	2.40	0.54
9:AS:30:ASN:O	9:AS:31:LYS:C	2.51	0.54
9:AS:113:ARG:O	9:AS:114:GLY:C	2.50	0.54
11:Ab:33:GLY:C	11:Ab:35:TYR:H	2.16	0.54
9:S:13:GLY:C	9:S:16:GLY:H	2.16	0.54
9:S:59:TYR:O	9:S:60:VAL:C	2.51	0.54
2:AB:77:GLY:C	2:AB:239:ALA:CB	2.66	0.53
2:AB:335:SER:O	3:AF:318:ALA:HB1	2.08	0.53
7:J:26:GLU:C	7:J:28:ALA:N	2.62	0.53
9:S:42:VAL:O	9:S:46:LEU:CB	2.57	0.53
11:Ab:193:THR:O	11:Ab:194:ILE:C	2.49	0.53
9:S:15:GLU:O	9:S:16:GLY:C	2.50	0.53
9:S:144:LYS:O	9:S:146:GLN:N	2.40	0.53
11:b:191:LYS:O	11:b:192:GLU:C	2.49	0.53
3:D:457:PRO:CA	7:J:41:GLN:CB	2.86	0.53
9:S:145:GLY:O	9:S:147:VAL:N	2.37	0.53
9:AS:67:LYS:O	9:AS:71:ASP:N	2.34	0.53
9:AS:95:LEU:O	9:AS:96:THR:C	2.52	0.53
10:Aa:152:GLN:O	10:Aa:155:ALA:N	2.42	0.53
11:Ab:198:ILE:O	11:Ab:202:LYS:N	2.32	0.53
11:Ab:204:LEU:O	11:Ab:205:SER:C	2.52	0.53
3:D:404:ASP:O	3:D:407:THR:N	2.42	0.53
9:S:73:THR:C	9:S:76:GLU:H	2.15	0.53
3:AD:404:ASP:O	3:AD:407:THR:N	2.42	0.53
9:S:134:LEU:HA	9:S:137:VAL:CB	2.38	0.53
11:Ab:191:LYS:O	11:Ab:192:GLU:C	2.49	0.53
9:S:122:THR:CB	9:S:154:ILE:HA	2.39	0.53
9:AS:83:SER:O	9:AS:87:ASN:N	2.37	0.53
7:J:76:LYS:O	7:J:77:LEU:C	2.52	0.53
9:S:47:LYS:O	9:S:52:ALA:HB2	2.09	0.53
9:S:94:ARG:O	9:S:96:THR:N	2.42	0.53
9:S:166:ILE:N	9:S:169:LYS:CB	2.72	0.53
9:AS:70:SER:O	9:AS:74:ALA:N	2.35	0.53
11:Ab:64:ILE:HA	11:Ab:67:LEU:CB	2.39	0.53
9:S:158:ILE:O	9:S:159:MET:C	2.52	0.53
2:B:77:GLY:C	2:B:239:ALA:CB	2.66	0.53
1:8:30:LYS:O	10:a:34:SER:O	2.27	0.52
9:AS:42:VAL:O	9:AS:46:LEU:CB	2.57	0.52
9:AS:94:ARG:O	9:AS:96:THR:N	2.42	0.52
12:d:135:LEU:O	12:d:139:PHE:N	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:38:GLU:O	9:AS:41:ARG:N	2.43	0.52
7:J:42:LEU:O	7:J:43:ALA:C	2.51	0.52
2:AC:94:ILE:O	2:AC:95:VAL:C	2.49	0.52
9:AS:44:GLN:O	9:AS:45:ILE:C	2.52	0.52
9:AS:58:PRO:C	9:AS:60:VAL:N	2.65	0.52
9:S:116:VAL:O	9:S:149:LYS:N	2.37	0.52
10:a:152:GLN:O	10:a:155:ALA:N	2.42	0.52
11:b:33:GLY:C	11:b:35:TYR:H	2.16	0.52
9:S:37:LYS:O	9:S:38:GLU:C	2.52	0.52
9:S:67:LYS:O	9:S:70:SER:N	2.43	0.52
9:S:95:LEU:O	9:S:96:THR:C	2.52	0.52
9:AS:14:ILE:C	9:AS:16:GLY:N	2.64	0.52
9:AS:90:ALA:O	9:AS:93:GLY:N	2.42	0.52
9:AS:133:GLU:O	9:AS:137:VAL:N	2.35	0.52
9:AS:158:ILE:O	9:AS:159:MET:C	2.52	0.52
9:AS:166:ILE:N	9:AS:169:LYS:CB	2.72	0.52
7:J:32:ARG:O	7:J:36:ALA:N	2.42	0.52
7:J:38:ALA:O	7:J:39:LYS:C	2.52	0.52
9:S:90:ALA:O	9:S:93:GLY:N	2.42	0.52
2:A:25:LEU:CA	9:S:171:VAL:CA	2.65	0.52
9:AS:67:LYS:O	9:AS:70:SER:N	2.43	0.52
9:AS:122:THR:CB	9:AS:154:ILE:HA	2.39	0.52
9:S:58:PRO:C	9:S:60:VAL:N	2.64	0.52
9:S:160:GLY:O	9:S:162:MET:N	2.39	0.52
2:AB:335:SER:O	3:AF:318:ALA:CB	2.58	0.52
9:AS:134:LEU:HA	9:AS:137:VAL:CB	2.38	0.52
1:A8:30:LYS:O	10:Aa:34:SER:O	2.27	0.52
9:AS:37:LYS:O	9:AS:38:GLU:C	2.52	0.52
9:AS:67:LYS:O	9:AS:68:SER:C	2.53	0.52
9:AS:174:SER:O	9:AS:178:LYS:N	2.43	0.52
9:S:44:GLN:O	9:S:45:ILE:C	2.52	0.52
9:S:159:MET:CB	9:S:176:LYS:HA	2.40	0.52
10:a:176:GLY:N	11:b:55:PRO:C	2.67	0.52
9:AS:174:SER:O	9:AS:175:ALA:C	2.50	0.52
11:b:64:ILE:HA	11:b:67:LEU:CB	2.39	0.52
9:AS:86:ILE:C	9:AS:88:LEU:H	2.18	0.51
9:AS:159:MET:CB	9:AS:176:LYS:HA	2.40	0.51
12:Ad:118:LEU:O	12:Ad:121:MET:N	2.35	0.51
9:S:38:GLU:O	9:S:41:ARG:N	2.43	0.51
9:AS:59:TYR:O	9:AS:60:VAL:C	2.51	0.51
9:S:83:SER:HA	9:S:86:ILE:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:47:LYS:O	9:AS:52:ALA:HB2	2.09	0.51
9:AS:160:GLY:C	9:AS:162:MET:N	2.65	0.51
9:S:82:THR:O	9:S:86:ILE:N	2.30	0.51
2:AC:405:GLN:O	3:AF:401:SER:CB	2.59	0.51
9:S:174:SER:O	9:S:178:LYS:N	2.43	0.51
2:B:335:SER:O	3:F:318:ALA:CB	2.58	0.51
11:b:204:LEU:O	11:b:205:SER:C	2.52	0.51
9:S:99:PRO:C	9:S:101:VAL:N	2.68	0.51
7:J:31:GLU:O	7:J:32:ARG:C	2.52	0.51
9:S:65:LYS:O	9:S:68:SER:N	2.44	0.51
9:S:102:ILE:C	9:S:104:ALA:N	2.68	0.51
9:AS:41:ARG:C	9:AS:45:ILE:H	2.18	0.51
9:AS:116:VAL:O	9:AS:149:LYS:N	2.37	0.51
9:S:5:VAL:N	9:S:24:SER:CB	2.74	0.51
9:AS:83:SER:HA	9:AS:86:ILE:CB	2.41	0.51
9:S:116:VAL:H	9:S:147:VAL:CB	2.24	0.51
9:S:70:SER:O	9:S:74:ALA:N	2.35	0.51
10:a:176:GLY:HA2	11:b:55:PRO:C	2.08	0.51
7:AJ:74:ILE:CA	7:J:60:ILE:CB	2.89	0.50
9:AS:99:PRO:C	9:AS:101:VAL:N	2.68	0.50
9:AS:111:VAL:CA	9:AS:114:GLY:HA2	2.36	0.50
9:S:92:ASN:C	9:S:94:ARG:N	2.69	0.50
9:S:35:VAL:O	9:S:37:LYS:N	2.44	0.50
9:S:41:ARG:C	9:S:45:ILE:H	2.18	0.50
9:AS:65:LYS:O	9:AS:68:SER:N	2.44	0.50
9:AS:111:VAL:O	9:AS:114:GLY:N	2.45	0.50
9:S:124:SER:HA	9:S:156:PRO:CB	2.34	0.50
9:AS:5:VAL:N	9:AS:24:SER:CB	2.74	0.50
9:AS:95:LEU:C	9:AS:97:ASN:H	2.19	0.50
9:AS:116:VAL:H	9:AS:147:VAL:CB	2.24	0.50
10:Aa:176:GLY:N	11:Ab:55:PRO:C	2.67	0.50
9:S:95:LEU:C	9:S:97:ASN:H	2.19	0.50
9:AS:102:ILE:C	9:AS:104:ALA:N	2.68	0.50
9:AS:138:LEU:C	9:AS:140:SER:N	2.64	0.50
9:AS:160:GLY:O	9:AS:162:MET:N	2.39	0.50
9:S:170:TYR:O	9:S:171:VAL:C	2.53	0.50
9:S:185:ALA:O	9:S:186:MET:C	2.55	0.50
9:S:86:ILE:C	9:S:88:LEU:H	2.18	0.50
9:S:111:VAL:O	9:S:114:GLY:N	2.45	0.50
9:AS:124:SER:HA	9:AS:156:PRO:CB	2.34	0.50
9:AS:185:ALA:O	9:AS:186:MET:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:31:GLU:O	7:J:35:ARG:N	2.29	0.50
9:S:67:LYS:O	9:S:68:SER:C	2.53	0.50
9:AS:123:ALA:H	9:AS:162:MET:CB	2.25	0.50
11:Ab:54:THR:O	11:Ab:56:GLU:N	2.45	0.50
9:S:147:VAL:O	9:S:148:LEU:C	2.54	0.50
9:AS:33:GLU:O	9:AS:37:LYS:N	2.38	0.50
10:Aa:176:GLY:HA2	11:Ab:55:PRO:C	2.08	0.50
9:AS:92:ASN:C	9:AS:94:ARG:N	2.69	0.49
14:Af:59:LEU:O	14:Af:60:SER:C	2.55	0.49
7:J:40:GLU:HA	7:J:44:ALA:CB	2.42	0.49
9:AS:13:GLY:CA	9:AS:16:GLY:HA3	2.42	0.49
9:AS:49:PRO:HA	9:AS:52:ALA:HB3	1.93	0.49
12:Ad:111:ILE:O	12:Ad:112:GLN:C	2.55	0.49
9:S:65:LYS:HA	9:S:68:SER:CB	2.42	0.49
12:d:111:ILE:O	12:d:112:GLN:C	2.55	0.49
9:AS:147:VAL:O	9:AS:148:LEU:C	2.54	0.49
9:S:83:SER:O	9:S:87:ASN:N	2.37	0.49
9:S:123:ALA:H	9:S:162:MET:CB	2.25	0.49
8:AK:6:ALA:HB2	8:AR:5:ALA:HB1	1.94	0.49
9:AS:35:VAL:O	9:AS:37:LYS:N	2.44	0.49
8:K:6:ALA:HB2	8:R:5:ALA:HB1	1.94	0.49
2:AA:32:LEU:O	3:AD:58:GLY:HA2	2.13	0.49
9:AS:80:PRO:C	9:AS:82:THR:N	2.70	0.49
9:S:165:ARG:HA	9:S:169:LYS:C	2.37	0.49
11:b:54:THR:O	11:b:56:GLU:N	2.45	0.49
9:AS:65:LYS:HA	9:AS:68:SER:CB	2.41	0.49
7:J:28:ALA:O	7:J:29:GLU:C	2.54	0.49
9:S:49:PRO:HA	9:S:52:ALA:HB3	1.93	0.49
9:S:159:MET:CB	9:S:176:LYS:CA	2.91	0.49
9:AS:165:ARG:HA	9:AS:169:LYS:C	2.37	0.49
7:J:24:LYS:C	7:J:26:GLU:H	2.20	0.49
9:AS:35:VAL:O	9:AS:37:LYS:C	2.56	0.49
4:G:105:ILE:N	4:G:123:GLN:O	2.37	0.49
2:A:32:LEU:O	3:D:58:GLY:HA2	2.13	0.49
4:AG:105:ILE:N	4:AG:123:GLN:O	2.37	0.49
9:AS:161:GLY:CA	9:AS:175:ALA:H	2.26	0.49
11:Ab:197:CYS:O	11:Ab:199:ALA:N	2.46	0.49
9:S:35:VAL:O	9:S:37:LYS:C	2.56	0.49
7:AJ:59:GLU:O	7:J:74:ILE:CB	2.53	0.48
9:AS:159:MET:CB	9:AS:176:LYS:CA	2.91	0.48
9:AS:99:PRO:O	9:AS:100:ALA:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:13:GLY:CA	9:S:16:GLY:HA3	2.42	0.48
9:AS:104:ALA:O	9:AS:108:MET:N	2.37	0.48
9:AS:15:GLU:O	9:AS:18:TYR:N	2.47	0.48
9:AS:61:LYS:O	9:AS:62:ARG:C	2.56	0.48
9:AS:123:ALA:HA	9:AS:158:ILE:CB	2.43	0.48
7:J:38:ALA:O	7:J:40:GLU:N	2.47	0.48
9:S:33:GLU:O	9:S:37:LYS:N	2.38	0.48
9:S:161:GLY:CA	9:S:175:ALA:H	2.26	0.48
2:AB:13:GLU:CB	9:AS:21:ALA:HB1	2.43	0.48
9:AS:80:PRO:O	9:AS:83:SER:N	2.47	0.48
10:a:135:THR:O	10:a:137:LEU:N	2.47	0.48
8:AO:5:ALA:HB1	8:AP:6:ALA:HB2	1.95	0.48
9:AS:161:GLY:HA3	9:AS:174:SER:C	2.36	0.48
14:f:59:LEU:O	14:f:60:SER:C	2.55	0.48
9:AS:86:ILE:C	9:AS:88:LEU:N	2.70	0.48
9:S:15:GLU:O	9:S:18:TYR:N	2.47	0.48
9:S:80:PRO:O	9:S:83:SER:N	2.47	0.48
9:AS:28:LYS:C	9:AS:30:ASN:N	2.72	0.48
9:AS:161:GLY:HA3	9:AS:175:ALA:N	2.29	0.48
7:J:29:GLU:O	7:J:32:ARG:N	2.47	0.48
7:J:30:GLU:O	7:J:31:GLU:C	2.56	0.48
11:b:6:PRO:O	14:f:51:VAL:HA	2.14	0.48
9:AS:78:PHE:O	9:AS:79:SER:C	2.55	0.48
9:AS:111:VAL:C	9:AS:114:GLY:N	2.66	0.48
11:Ab:30:GLY:HA2	13:Ae:4:VAL:C	2.39	0.48
9:S:32:LEU:C	9:S:34:GLN:N	2.70	0.48
12:d:97:VAL:O	12:d:98:LYS:C	2.57	0.48
9:AS:78:PHE:O	9:AS:80:PRO:N	2.47	0.47
9:AS:109:MET:C	9:AS:112:HIS:H	2.22	0.47
7:J:40:GLU:CA	7:J:44:ALA:HB3	2.44	0.47
8:O:5:ALA:HB1	8:P:6:ALA:HB2	1.95	0.47
9:S:86:ILE:C	9:S:88:LEU:N	2.70	0.47
10:a:175:GLY:CA	11:b:56:GLU:CA	2.90	0.47
11:b:111:GLU:O	11:b:112:LYS:C	2.57	0.47
11:b:197:CYS:O	11:b:199:ALA:N	2.46	0.47
11:Ab:6:PRO:O	14:Af:51:VAL:HA	2.14	0.47
9:S:78:PHE:O	9:S:80:PRO:N	2.47	0.47
9:S:112:HIS:C	9:S:114:GLY:H	2.21	0.47
9:S:123:ALA:HA	9:S:158:ILE:CB	2.43	0.47
7:J:40:GLU:C	7:J:44:ALA:HB3	2.39	0.47
7:J:62:ARG:O	7:J:63:LEU:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:17:ILE:O	11:b:18:PRO:C	2.56	0.47
9:AS:32:LEU:O	9:AS:34:GLN:N	2.47	0.47
9:AS:39:LEU:O	9:AS:40:LEU:O	2.32	0.47
9:AS:102:ILE:O	9:AS:104:ALA:N	2.48	0.47
9:AS:170:TYR:O	9:AS:171:VAL:C	2.53	0.47
9:S:32:LEU:O	9:S:34:GLN:N	2.48	0.47
9:S:111:VAL:CA	9:S:114:GLY:HA2	2.36	0.47
7:AJ:70:HIS:CB	7:J:63:LEU:HA	2.43	0.47
9:AS:132:THR:HA	9:AS:135:LYS:CB	2.44	0.47
2:B:94:ILE:O	2:B:95:VAL:O	2.32	0.47
11:b:30:GLY:HA2	13:e:4:VAL:C	2.39	0.47
9:S:3:LYS:O	9:S:4:LEU:C	2.56	0.47
9:S:28:LYS:C	9:S:30:ASN:N	2.72	0.47
9:S:39:LEU:O	9:S:40:LEU:O	2.32	0.47
9:S:78:PHE:O	9:S:79:SER:C	2.55	0.47
9:AS:112:HIS:C	9:AS:114:GLY:H	2.21	0.47
9:AS:182:LEU:C	9:AS:184:ARG:H	2.22	0.47
10:Aa:122:LYS:O	10:Aa:125:LEU:N	2.45	0.47
10:Aa:135:THR:O	10:Aa:137:LEU:N	2.47	0.47
11:Ab:17:ILE:O	11:Ab:18:PRO:C	2.56	0.47
9:S:104:ALA:O	9:S:108:MET:N	2.37	0.47
9:S:132:THR:HA	9:S:135:LYS:CB	2.44	0.47
9:S:138:LEU:O	9:S:142:LEU:N	2.43	0.47
9:S:161:GLY:HA3	9:S:175:ALA:N	2.29	0.47
9:AS:32:LEU:O	9:AS:33:GLU:C	2.58	0.47
9:AS:48:GLU:O	9:AS:52:ALA:N	2.26	0.47
11:Ab:29:THR:O	11:Ab:30:GLY:C	2.57	0.47
7:J:40:GLU:O	7:J:44:ALA:HB3	2.14	0.47
9:S:61:LYS:O	9:S:62:ARG:C	2.56	0.47
10:a:144:ILE:O	10:a:145:GLU:C	2.58	0.47
11:b:53:ILE:H	11:b:57:THR:HA	1.80	0.47
16:h:38:ASP:O	16:h:39:LEU:C	2.56	0.47
9:AS:3:LYS:O	9:AS:4:LEU:C	2.56	0.47
9:AS:46:LEU:O	9:AS:48:GLU:N	2.48	0.47
9:AS:168:GLU:C	9:AS:170:TYR:H	2.23	0.47
11:Ab:111:GLU:O	11:Ab:112:LYS:C	2.57	0.47
7:J:35:ARG:C	7:J:38:ALA:H	2.22	0.47
9:S:99:PRO:O	9:S:100:ALA:C	2.57	0.47
9:S:168:GLU:C	9:S:170:TYR:H	2.23	0.47
9:S:177:THR:C	9:S:179:ILE:N	2.73	0.47
16:Ah:38:ASP:O	16:Ah:39:LEU:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:114:LYS:O	5:H:117:SER:N	2.48	0.47
9:S:32:LEU:O	9:S:33:GLU:C	2.58	0.47
9:S:105:PHE:HA	9:S:108:MET:CB	2.45	0.47
9:S:109:MET:C	9:S:112:HIS:H	2.22	0.47
6:AI:31:LYS:HA	6:AI:34:ALA:HB3	1.97	0.46
10:Aa:144:ILE:O	10:Aa:145:GLU:C	2.58	0.46
9:S:130:THR:O	9:S:134:LEU:N	2.42	0.46
9:AS:145:GLY:C	9:AS:147:VAL:H	2.22	0.46
11:b:29:THR:O	11:b:30:GLY:C	2.57	0.46
9:AS:138:LEU:C	9:AS:140:SER:H	2.23	0.46
10:a:122:LYS:O	10:a:125:LEU:N	2.45	0.46
12:d:56:TYR:O	12:d:60:VAL:N	2.30	0.46
9:AS:80:PRO:O	9:AS:84:ASN:N	2.38	0.46
9:AS:135:LYS:O	9:AS:138:LEU:N	2.49	0.46
9:S:138:LEU:C	9:S:140:SER:H	2.23	0.46
5:AH:114:LYS:O	5:AH:117:SER:N	2.48	0.46
9:AS:26:ALA:O	9:AS:30:ASN:HA	2.15	0.46
9:AS:105:PHE:HA	9:AS:108:MET:CB	2.45	0.46
9:AS:31:LYS:O	9:AS:34:GLN:N	2.36	0.46
9:AS:130:THR:O	9:AS:134:LEU:N	2.42	0.46
11:Ab:53:ILE:H	11:Ab:57:THR:HA	1.80	0.46
2:AB:94:ILE:O	2:AB:95:VAL:O	2.32	0.46
12:Ad:97:VAL:O	12:Ad:98:LYS:C	2.57	0.46
2:B:335:SER:O	3:F:318:ALA:HB1	2.15	0.46
9:S:37:LYS:O	9:S:38:GLU:O	2.34	0.46
9:S:100:ALA:C	9:S:102:ILE:N	2.71	0.46
9:S:102:ILE:O	9:S:104:ALA:N	2.48	0.46
1:8:4:LEU:O	1:8:6:THR:N	2.49	0.46
2:AA:25:LEU:CA	9:AS:171:VAL:CA	2.65	0.46
9:AS:33:GLU:O	9:AS:36:GLU:N	2.49	0.46
16:Ah:19:ARG:O	16:Ah:22:ARG:N	2.49	0.46
7:J:77:LEU:O	7:J:78:LYS:C	2.58	0.46
9:S:26:ALA:O	9:S:30:ASN:HA	2.15	0.46
9:S:33:GLU:O	9:S:36:GLU:N	2.49	0.46
9:AS:37:LYS:O	9:AS:38:GLU:O	2.34	0.46
9:AS:119:THR:CB	9:AS:165:ARG:N	2.79	0.46
9:S:11:ILE:C	9:S:13:GLY:H	2.24	0.46
9:S:182:LEU:C	9:S:184:ARG:H	2.22	0.46
11:b:13:ARG:N	11:b:17:ILE:O	2.48	0.46
2:AB:77:GLY:H	2:AB:239:ALA:HB3	1.80	0.46
9:S:80:PRO:C	9:S:82:THR:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:135:LYS:O	9:S:138:LEU:N	2.48	0.46
9:S:139:LYS:O	9:S:143:SER:HA	2.16	0.46
14:f:60:SER:O	14:f:61:MET:C	2.59	0.46
2:B:77:GLY:H	2:B:239:ALA:HB3	1.80	0.45
9:S:14:ILE:C	9:S:16:GLY:H	2.23	0.45
9:S:111:VAL:C	9:S:114:GLY:N	2.66	0.45
10:a:152:GLN:O	10:a:153:PRO:C	2.58	0.45
16:h:21:LYS:O	16:h:22:ARG:C	2.59	0.45
9:AS:15:GLU:O	9:AS:19:ALA:N	2.45	0.45
9:AS:109:MET:O	9:AS:110:SER:C	2.59	0.45
14:Af:60:SER:O	14:Af:61:MET:C	2.59	0.45
3:D:344:ALA:HB2	3:D:351:ALA:HB2	1.98	0.45
9:S:161:GLY:HA3	9:S:174:SER:C	2.36	0.45
3:AD:344:ALA:HB2	3:AD:351:ALA:HB2	1.98	0.45
9:AS:23:TYR:O	9:AS:24:SER:C	2.60	0.45
9:AS:100:ALA:C	9:AS:102:ILE:N	2.71	0.45
9:AS:11:ILE:C	9:AS:13:GLY:H	2.24	0.45
11:Ab:71:VAL:HA	11:Ab:75:GLY:CA	2.36	0.45
9:S:46:LEU:O	9:S:48:GLU:N	2.48	0.45
1:A8:4:LEU:O	1:A8:6:THR:N	2.49	0.45
9:AS:32:LEU:C	9:AS:34:GLN:N	2.70	0.45
9:AS:139:LYS:O	9:AS:142:LEU:C	2.60	0.45
6:I:31:LYS:HA	6:I:34:ALA:HB3	1.98	0.45
7:J:69:ARG:O	7:J:70:HIS:C	2.59	0.45
9:S:109:MET:O	9:S:110:SER:C	2.59	0.45
10:Aa:152:GLN:O	10:Aa:153:PRO:C	2.58	0.45
9:S:119:THR:CB	9:S:165:ARG:N	2.79	0.45
9:S:123:ALA:C	9:S:155:ASP:O	2.60	0.45
11:b:30:GLY:O	11:b:32:THR:N	2.50	0.45
7:AJ:60:ILE:CB	7:J:75:LYS:HA	2.47	0.45
16:h:19:ARG:O	16:h:22:ARG:N	2.49	0.45
9:AS:123:ALA:C	9:AS:155:ASP:O	2.60	0.45
9:AS:139:LYS:O	9:AS:143:SER:HA	2.16	0.45
9:S:16:GLY:O	9:S:20:THR:N	2.41	0.45
9:S:23:TYR:O	9:S:24:SER:C	2.60	0.45
10:a:116:GLY:O	10:a:120:LYS:N	2.46	0.45
9:AS:44:GLN:O	9:AS:47:LYS:CB	2.65	0.45
16:Ah:21:LYS:O	16:Ah:22:ARG:C	2.59	0.45
7:J:39:LYS:O	7:J:43:ALA:N	2.50	0.45
10:a:176:GLY:CA	11:b:55:PRO:C	2.70	0.45
2:AC:403:PHE:CB	7:AJ:28:ALA:HB1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AS:146:GLN:O	9:AS:147:VAL:C	2.60	0.45
3:D:351:ALA:O	3:D:352:VAL:C	2.60	0.45
11:Ab:10:GLY:N	14:Af:47:LYS:O	2.50	0.44
7:J:71:LYS:O	7:J:75:LYS:N	2.32	0.44
11:b:71:VAL:HA	11:b:75:GLY:CA	2.35	0.44
9:AS:145:GLY:C	9:AS:147:VAL:N	2.76	0.44
11:Ab:202:LYS:HA	11:Ab:205:SER:CB	2.48	0.44
3:D:478:ALA:HB1	7:J:46:LYS:CB	2.47	0.44
7:J:55:HIS:O	7:J:56:HIS:C	2.60	0.44
9:S:15:GLU:O	9:S:19:ALA:N	2.45	0.44
9:S:129:ALA:O	9:S:132:THR:N	2.51	0.44
9:S:139:LYS:O	9:S:142:LEU:C	2.60	0.44
11:b:10:GLY:N	14:f:47:LYS:O	2.50	0.44
9:AS:177:THR:C	9:AS:179:ILE:N	2.73	0.44
11:Ab:33:GLY:C	11:Ab:35:TYR:N	2.76	0.44
12:Ad:113:GLU:O	12:Ad:116:LYS:N	2.50	0.44
9:S:44:GLN:O	9:S:47:LYS:CB	2.65	0.44
9:AS:129:ALA:O	9:AS:132:THR:N	2.51	0.44
11:Ab:30:GLY:O	11:Ab:32:THR:N	2.50	0.44
9:S:48:GLU:O	9:S:52:ALA:N	2.26	0.44
12:d:113:GLU:O	12:d:116:LYS:N	2.50	0.44
9:AS:122:THR:C	9:AS:124:SER:N	2.76	0.44
9:AS:138:LEU:O	9:AS:142:LEU:N	2.43	0.44
9:S:87:ASN:C	9:S:90:ALA:HB3	2.43	0.44
10:a:83:ASN:CB	10:a:207:ALA:HB1	2.47	0.44
11:b:202:LYS:HA	11:b:205:SER:CB	2.48	0.44
10:Aa:175:GLY:CA	11:Ab:56:GLU:CA	2.90	0.44
3:F:351:ALA:O	3:F:352:VAL:C	2.59	0.44
11:b:198:ILE:O	11:b:202:LYS:N	2.32	0.44
11:b:33:GLY:C	11:b:35:TYR:N	2.76	0.44
9:AS:69:LEU:O	9:AS:70:SER:C	2.61	0.44
10:Aa:83:ASN:CB	10:Aa:207:ALA:HB1	2.47	0.44
11:Ab:2:VAL:O	12:Ad:129:GLN:HA	2.17	0.44
3:D:467:ILE:O	3:D:470:ALA:HB3	2.17	0.44
8:O:19:ALA:O	8:P:20:GLY:HA3	2.18	0.44
9:S:31:LYS:O	9:S:34:GLN:N	2.36	0.44
9:AS:14:ILE:C	9:AS:16:GLY:H	2.23	0.44
9:AS:183:SER:C	9:AS:185:ALA:N	2.76	0.44
9:S:117:PRO:O	9:S:148:LEU:HA	2.18	0.44
9:S:145:GLY:C	9:S:147:VAL:N	2.76	0.44
11:b:2:VAL:O	12:d:129:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:133:GLU:O	12:d:134:ASP:C	2.61	0.44
9:AS:132:THR:C	9:AS:135:LYS:H	2.26	0.43
11:Ab:13:ARG:N	11:Ab:17:ILE:O	2.48	0.43
11:Ab:64:ILE:O	11:Ab:65:GLY:C	2.61	0.43
12:Ad:56:TYR:O	12:Ad:60:VAL:N	2.30	0.43
9:S:185:ALA:C	9:S:187:ARG:N	2.76	0.43
11:b:54:THR:C	11:b:56:GLU:N	2.76	0.43
9:AS:46:LEU:C	9:AS:48:GLU:N	2.75	0.43
11:Ab:118:VAL:O	11:Ab:119:GLN:C	2.61	0.43
2:C:399:GLU:O	7:J:28:ALA:HB1	2.18	0.43
8:Q:14:ALA:HB3	8:Q:68:ALA:HB2	2.00	0.43
9:S:132:THR:C	9:S:135:LYS:H	2.26	0.43
3:AD:467:ILE:O	3:AD:470:ALA:HB3	2.17	0.43
8:AQ:14:ALA:HB3	8:AQ:68:ALA:HB2	2.00	0.43
9:AS:52:ALA:C	9:AS:54:SER:N	2.76	0.43
9:AS:87:ASN:C	9:AS:90:ALA:HB3	2.43	0.43
11:Ab:175:ASN:C	11:Ab:177:VAL:N	2.77	0.43
9:S:67:LYS:C	9:S:69:LEU:N	2.76	0.43
9:S:69:LEU:O	9:S:70:SER:C	2.61	0.43
9:S:80:PRO:O	9:S:84:ASN:N	2.38	0.43
3:D:344:ALA:HB2	3:D:351:ALA:CB	2.48	0.43
9:S:146:GLN:O	9:S:147:VAL:C	2.60	0.43
11:b:64:ILE:O	11:b:65:GLY:C	2.61	0.43
3:AD:351:ALA:O	3:AD:352:VAL:C	2.60	0.43
9:AS:122:THR:O	9:AS:155:ASP:N	2.52	0.43
9:S:92:ASN:O	9:S:94:ARG:N	2.51	0.43
9:S:177:THR:O	9:S:181:LYS:N	2.39	0.43
11:b:118:VAL:O	11:b:119:GLN:C	2.61	0.43
9:AS:41:ARG:O	9:AS:43:GLY:C	2.62	0.43
9:AS:61:LYS:C	9:AS:63:SER:N	2.74	0.43
11:Ab:48:LYS:O	11:Ab:49:GLU:C	2.61	0.43
9:S:41:ARG:O	9:S:43:GLY:C	2.62	0.43
9:S:46:LEU:C	9:S:48:GLU:N	2.75	0.43
9:S:156:PRO:C	9:S:158:ILE:N	2.76	0.43
3:AF:351:ALA:O	3:AF:352:VAL:C	2.59	0.43
8:AL:19:ALA:O	8:AM:20:GLY:HA3	2.19	0.43
8:AO:19:ALA:O	8:AP:20:GLY:HA3	2.18	0.43
9:AS:92:ASN:O	9:AS:94:ARG:N	2.51	0.43
9:AS:117:PRO:O	9:AS:148:LEU:HA	2.18	0.43
9:AS:156:PRO:C	9:AS:158:ILE:N	2.76	0.43
12:Ad:133:GLU:O	12:Ad:134:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:40:GLU:C	7:J:42:LEU:N	2.76	0.43
16:Ah:19:ARG:O	16:Ah:20:THR:C	2.62	0.43
9:S:129:ALA:C	9:S:132:THR:H	2.27	0.43
9:AS:47:LYS:O	9:AS:49:PRO:N	2.52	0.43
7:J:41:GLN:HA	7:J:45:LEU:CB	2.48	0.43
8:L:19:ALA:O	8:M:20:GLY:HA3	2.19	0.43
11:b:40:GLY:HA3	15:g:81:GLU:HA	2.01	0.43
11:b:175:ASN:C	11:b:177:VAL:N	2.77	0.43
16:h:21:LYS:O	16:h:24:THR:CA	2.67	0.43
8:AN:70:LEU:O	8:AN:74:ALA:O	2.37	0.42
9:S:48:GLU:O	9:S:51:MET:N	2.52	0.42
9:S:122:THR:O	9:S:155:ASP:N	2.52	0.42
9:S:175:ALA:O	9:S:176:LYS:C	2.62	0.42
3:AD:344:ALA:HB2	3:AD:351:ALA:CB	2.48	0.42
9:AS:82:THR:O	9:AS:84:ASN:N	2.52	0.42
10:Aa:58:MET:O	10:Aa:59:SER:C	2.63	0.42
11:Ab:200:ASP:O	11:Ab:201:LEU:C	2.62	0.42
8:O:30:GLY:HA2	8:P:31:SER:CB	2.49	0.42
9:S:63:SER:O	9:S:66:VAL:N	2.53	0.42
9:S:82:THR:O	9:S:84:ASN:N	2.52	0.42
9:S:178:LYS:O	9:S:179:ILE:O	2.37	0.42
3:AE:85:PRO:O	3:AE:86:ILE:C	2.62	0.42
9:S:134:LEU:O	9:S:138:LEU:N	2.52	0.42
11:b:48:LYS:O	11:b:49:GLU:C	2.61	0.42
12:d:95:GLU:O	12:d:96:ASP:C	2.61	0.42
9:AS:16:GLY:O	9:AS:20:THR:N	2.41	0.42
11:Ab:111:GLU:O	11:Ab:113:SER:N	2.53	0.42
9:S:123:ALA:CB	9:S:160:GLY:HA2	2.50	0.42
8:AO:30:GLY:HA2	8:AP:31:SER:CB	2.49	0.42
8:AQ:56:LEU:O	8:AQ:59:ALA:HB3	2.20	0.42
9:AS:25:ALA:O	9:AS:28:LYS:N	2.53	0.42
10:Aa:199:LEU:O	10:Aa:200:THR:C	2.61	0.42
16:Ah:21:LYS:O	16:Ah:24:THR:CA	2.67	0.42
9:S:48:GLU:O	9:S:49:PRO:C	2.62	0.42
9:S:61:LYS:C	9:S:63:SER:N	2.74	0.42
9:S:160:GLY:HA3	9:S:175:ALA:HB3	2.00	0.42
11:b:111:GLU:O	11:b:113:SER:N	2.53	0.42
2:A:24:ASP:C	9:S:171:VAL:CA	2.92	0.42
3:AF:260:ASP:HA	3:AF:261:ASN:HA	1.89	0.42
9:AS:48:GLU:O	9:AS:49:PRO:C	2.62	0.42
9:AS:48:GLU:O	9:AS:51:MET:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Ad:96:ASP:O	12:Ad:97:VAL:C	2.62	0.42
3:E:85:PRO:O	3:E:86:ILE:C	2.62	0.42
7:J:60:ILE:O	7:J:61:GLU:C	2.62	0.42
9:AS:63:SER:O	9:AS:66:VAL:N	2.53	0.42
9:S:79:SER:C	9:S:81:LEU:N	2.75	0.42
9:S:142:LEU:O	9:S:143:SER:CB	2.67	0.42
12:d:131:THR:O	12:d:134:ASP:N	2.52	0.42
9:AS:134:LEU:O	9:AS:138:LEU:N	2.52	0.42
9:S:13:GLY:C	9:S:16:GLY:N	2.78	0.42
9:AS:13:GLY:C	9:AS:16:GLY:N	2.78	0.42
12:d:144:LEU:O	12:d:145:ASP:C	2.63	0.42
3:AE:260:ASP:HA	3:AE:261:ASN:HA	1.81	0.42
9:AS:4:LEU:O	9:AS:5:VAL:C	2.62	0.42
9:AS:67:LYS:C	9:AS:69:LEU:N	2.76	0.42
9:S:43:GLY:O	9:S:44:GLN:C	2.63	0.42
12:d:96:ASP:O	12:d:97:VAL:C	2.62	0.42
9:AS:41:ARG:O	9:AS:44:GLN:N	2.53	0.41
8:K:69:PHE:O	8:K:73:PHE:N	2.51	0.41
9:S:4:LEU:O	9:S:5:VAL:C	2.62	0.41
9:S:41:ARG:O	9:S:44:GLN:N	2.53	0.41
9:S:47:LYS:O	9:S:49:PRO:N	2.52	0.41
9:S:180:GLN:O	9:S:181:LYS:C	2.63	0.41
9:AS:123:ALA:CB	9:AS:160:GLY:HA2	2.49	0.41
9:AS:185:ALA:O	9:AS:187:ARG:N	2.53	0.41
7:J:38:ALA:C	7:J:40:GLU:N	2.76	0.41
9:AS:50:LYS:HA	9:AS:53:ALA:CB	2.50	0.41
9:AS:129:ALA:C	9:AS:132:THR:H	2.27	0.41
11:Ab:40:GLY:HA3	15:Ag:81:GLU:HA	2.01	0.41
11:Ab:54:THR:C	11:Ab:56:GLU:N	2.76	0.41
12:Ad:131:THR:O	12:Ad:134:ASP:N	2.52	0.41
12:Ad:144:LEU:O	12:Ad:145:ASP:C	2.63	0.41
8:L:12:GLY:HA2	8:M:14:ALA:HB2	2.01	0.41
11:b:200:ASP:O	11:b:201:LEU:C	2.62	0.41
3:AE:351:ALA:O	3:AE:352:VAL:C	2.63	0.41
9:AS:59:TYR:O	9:AS:61:LYS:N	2.52	0.41
9:AS:112:HIS:C	9:AS:114:GLY:N	2.78	0.41
9:AS:175:ALA:O	9:AS:176:LYS:C	2.62	0.41
9:S:52:ALA:O	9:S:53:ALA:C	2.63	0.41
9:S:59:TYR:O	9:S:61:LYS:N	2.52	0.41
9:S:158:ILE:C	9:S:160:GLY:N	2.77	0.41
10:a:199:LEU:O	10:a:200:THR:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:204:LEU:C	11:b:206:LYS:N	2.77	0.41
14:f:15:LYS:O	14:f:19:LEU:N	2.54	0.41
9:AS:52:ALA:O	9:AS:53:ALA:C	2.63	0.41
9:AS:178:LYS:O	9:AS:179:ILE:O	2.37	0.41
10:Aa:116:GLY:O	10:Aa:120:LYS:O	2.39	0.41
12:Ad:95:GLU:O	12:Ad:96:ASP:C	2.61	0.41
8:N:70:LEU:O	8:N:74:ALA:O	2.37	0.41
8:Q:56:LEU:O	8:Q:59:ALA:HB3	2.20	0.41
9:S:17:ARG:O	9:S:18:TYR:C	2.63	0.41
9:S:25:ALA:O	9:S:28:LYS:N	2.53	0.41
9:S:124:SER:CA	9:S:156:PRO:N	2.77	0.41
9:S:145:GLY:C	9:S:147:VAL:H	2.22	0.41
10:a:175:GLY:HA2	11:b:56:GLU:CB	2.35	0.41
9:AS:185:ALA:C	9:AS:187:ARG:N	2.76	0.41
11:Ab:71:VAL:O	11:Ab:76:ALA:N	2.54	0.41
3:D:404:ASP:O	3:D:405:LYS:C	2.63	0.41
10:a:58:MET:O	10:a:59:SER:C	2.63	0.41
11:b:71:VAL:O	11:b:76:ALA:N	2.54	0.41
2:AC:402:ALA:CB	7:AJ:28:ALA:N	2.78	0.41
9:S:84:ASN:O	9:S:85:LEU:C	2.62	0.41
2:AA:24:ASP:C	9:AS:171:VAL:CA	2.92	0.41
9:AS:35:VAL:HA	9:AS:38:GLU:CB	2.51	0.41
9:AS:79:SER:C	9:AS:81:LEU:N	2.75	0.41
9:AS:84:ASN:O	9:AS:85:LEU:C	2.62	0.41
9:S:35:VAL:HA	9:S:38:GLU:CB	2.51	0.41
8:AL:12:GLY:HA2	8:AM:14:ALA:HB2	2.01	0.41
9:AS:30:ASN:C	9:AS:32:LEU:N	2.76	0.41
9:AS:139:LYS:O	9:AS:143:SER:N	2.54	0.41
11:Ab:10:GLY:N	14:Af:48:TYR:HA	2.26	0.41
9:S:185:ALA:O	9:S:187:ARG:N	2.53	0.41
14:f:66:TYR:O	14:f:67:VAL:C	2.64	0.41
16:h:19:ARG:O	16:h:20:THR:C	2.62	0.41
9:AS:29:GLN:O	9:AS:31:LYS:N	2.54	0.41
9:AS:62:ARG:O	9:AS:65:LYS:N	2.54	0.41
9:AS:123:ALA:O	9:AS:156:PRO:HA	2.21	0.41
9:AS:180:GLN:O	9:AS:181:LYS:C	2.63	0.41
9:S:50:LYS:HA	9:S:53:ALA:CB	2.50	0.41
9:S:52:ALA:C	9:S:54:SER:N	2.76	0.41
9:AS:13:GLY:O	9:AS:14:ILE:C	2.64	0.40
14:Af:15:LYS:O	14:Af:19:LEU:N	2.54	0.40
3:D:467:ILE:O	3:D:470:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:5:ALA:HB1	8:P:6:ALA:CB	2.51	0.40
9:S:139:LYS:O	9:S:143:SER:N	2.54	0.40
2:A:16:ILE:HA	2:A:19:ALA:HB3	2.03	0.40
8:AO:5:ALA:HB1	8:AP:6:ALA:CB	2.51	0.40
3:E:351:ALA:O	3:E:352:VAL:C	2.63	0.40
9:S:48:GLU:CB	9:S:51:MET:CB	2.99	0.40
3:AD:404:ASP:O	3:AD:405:LYS:C	2.63	0.40
9:AS:124:SER:CA	9:AS:156:PRO:N	2.77	0.40
9:S:62:ARG:O	9:S:65:LYS:N	2.54	0.40
9:S:164:VAL:O	9:S:170:TYR:HA	2.22	0.40
10:a:116:GLY:O	10:a:120:LYS:O	2.39	0.40
9:AS:48:GLU:CB	9:AS:51:MET:CB	2.99	0.40
9:AS:109:MET:O	9:AS:112:HIS:N	2.54	0.40
9:AS:142:LEU:O	9:AS:143:SER:CB	2.67	0.40
10:Aa:116:GLY:O	10:Aa:120:LYS:N	2.46	0.40
9:S:112:HIS:C	9:S:114:GLY:N	2.78	0.40
9:S:183:SER:C	9:S:185:ALA:N	2.76	0.40
9:AS:160:GLY:HA3	9:AS:175:ALA:HB3	2.00	0.40
9:AS:161:GLY:HA3	9:AS:175:ALA:H	1.87	0.40
5:H:48:LEU:O	5:H:49:ALA:C	2.64	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	39/66 (59%)	28 (72%)	11 (28%)	0	100	100
1	A8	39/66 (59%)	28 (72%)	11 (28%)	0	100	100
2	A	499/553 (90%)	493 (99%)	6 (1%)	0	100	100
2	AA	499/553 (90%)	493 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	505/553 (91%)	491 (97%)	13 (3%)	1 (0%)	43	77
2	AC	484/553 (88%)	469 (97%)	14 (3%)	1 (0%)	43	77
2	B	505/553 (91%)	491 (97%)	13 (3%)	1 (0%)	43	77
2	C	484/553 (88%)	469 (97%)	14 (3%)	1 (0%)	43	77
3	AD	467/528 (88%)	417 (89%)	50 (11%)	0	100	100
3	AE	465/528 (88%)	415 (89%)	50 (11%)	0	100	100
3	AF	465/528 (88%)	415 (89%)	50 (11%)	0	100	100
3	D	467/528 (88%)	418 (90%)	49 (10%)	0	100	100
3	E	465/528 (88%)	414 (89%)	51 (11%)	0	100	100
3	F	465/528 (88%)	415 (89%)	50 (11%)	0	100	100
4	AG	270/298 (91%)	255 (94%)	15 (6%)	0	100	100
4	G	270/298 (91%)	256 (95%)	14 (5%)	0	100	100
5	AH	129/168 (77%)	118 (92%)	11 (8%)	0	100	100
5	H	129/168 (77%)	118 (92%)	11 (8%)	0	100	100
6	AI	45/51 (88%)	42 (93%)	3 (7%)	0	100	100
6	I	45/51 (88%)	42 (93%)	3 (7%)	0	100	100
7	AJ	54/109 (50%)	54 (100%)	0	0	100	100
7	J	54/109 (50%)	38 (70%)	12 (22%)	4 (7%)	1	10
8	AK	72/143 (50%)	67 (93%)	4 (6%)	1 (1%)	9	38
8	AL	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
8	AM	73/143 (51%)	71 (97%)	2 (3%)	0	100	100
8	AN	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	AO	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	AP	72/143 (50%)	66 (92%)	6 (8%)	0	100	100
8	AQ	73/143 (51%)	73 (100%)	0	0	100	100
8	AR	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	K	72/143 (50%)	67 (93%)	4 (6%)	1 (1%)	9	38
8	L	72/143 (50%)	69 (96%)	3 (4%)	0	100	100
8	M	73/143 (51%)	71 (97%)	2 (3%)	0	100	100
8	N	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
8	O	73/143 (51%)	69 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	P	72/143 (50%)	66 (92%)	6 (8%)	0	100	100
8	Q	73/143 (51%)	73 (100%)	0	0	100	100
8	R	73/143 (51%)	69 (94%)	4 (6%)	0	100	100
9	AS	185/213 (87%)	93 (50%)	59 (32%)	33 (18%)	0	2
9	S	185/213 (87%)	93 (50%)	59 (32%)	33 (18%)	0	2
10	Aa	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
10	a	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
11	Ab	207/256 (81%)	167 (81%)	24 (12%)	16 (8%)	1	9
11	b	207/256 (81%)	167 (81%)	24 (12%)	16 (8%)	1	9
12	Ad	153/161 (95%)	129 (84%)	24 (16%)	0	100	100
12	d	153/161 (95%)	129 (84%)	24 (16%)	0	100	100
13	Ae	39/71 (55%)	36 (92%)	3 (8%)	0	100	100
13	e	39/71 (55%)	36 (92%)	3 (8%)	0	100	100
14	Af	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
14	f	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
15	Ag	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
15	g	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
16	Ah	44/108 (41%)	35 (80%)	9 (20%)	0	100	100
16	h	44/108 (41%)	35 (80%)	9 (20%)	0	100	100
All	All	10026/12610 (80%)	9101 (91%)	817 (8%)	108 (1%)	14	45

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	95	VAL
2	AC	95	VAL
9	AS	14	ILE
9	AS	39	LEU
9	AS	40	LEU
9	AS	55	LEU
9	AS	84	ASN
9	AS	99	PRO
9	AS	117	PRO
9	AS	143	SER
9	AS	151	GLU

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Mol	Chain	Res	Type
9	AS	179	ILE
11	Ab	31	VAL
11	Ab	116	ALA
11	Ab	173	MET
11	Ab	207	LYS
2	B	95	VAL
2	C	95	VAL
7	J	24	LYS
7	J	40	GLU
7	J	42	LEU
9	S	14	ILE
9	S	39	LEU
9	S	40	LEU
9	S	55	LEU
9	S	84	ASN
9	S	99	PRO
9	S	117	PRO
9	S	143	SER
9	S	151	GLU
9	S	179	ILE
11	b	31	VAL
11	b	116	ALA
11	b	173	MET
11	b	207	LYS
9	AS	38	GLU
9	AS	60	VAL
9	AS	96	THR
9	AS	104	ALA
9	AS	118	CYS
9	AS	120	VAL
9	AS	145	GLY
9	AS	166	ILE
9	AS	178	LYS
11	Ab	175	ASN
11	Ab	198	ILE
7	J	65	LYS
9	S	38	GLU
9	S	60	VAL
9	S	96	THR
9	S	104	ALA
9	S	118	CYS
9	S	120	VAL

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Mol	Chain	Res	Type
9	S	145	GLY
9	S	166	ILE
9	S	178	LYS
11	b	175	ASN
11	b	198	ILE
9	AS	13	GLY
9	AS	82	THR
9	AS	95	LEU
11	Ab	55	PRO
11	Ab	197	CYS
11	Ab	199	ALA
9	S	13	GLY
9	S	82	THR
9	S	95	LEU
11	b	55	PRO
11	b	197	CYS
11	b	199	ALA
8	AK	43	LYS
9	AS	37	LYS
9	AS	93	GLY
9	AS	168	GLU
9	AS	177	THR
11	Ab	29	THR
8	K	43	LYS
9	S	37	LYS
9	S	93	GLY
9	S	168	GLU
9	S	177	THR
11	b	29	THR
9	AS	18	TYR
9	AS	86	ILE
9	AS	172	ASP
9	AS	181	LYS
11	Ab	54	THR
11	Ab	90	ILE
9	S	18	TYR
9	S	86	ILE
9	S	172	ASP
9	S	181	LYS
11	b	54	THR
11	b	90	ILE
9	AS	42	VAL

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Mol	Chain	Res	Type
9	AS	127	ASP
9	AS	161	GLY
11	Ab	26	TYR
11	Ab	34	PRO
9	S	42	VAL
9	S	127	ASP
9	S	161	GLY
11	b	26	TYR
11	b	34	PRO
11	Ab	127	VAL
11	b	127	VAL
11	Ab	194	ILE
11	b	194	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

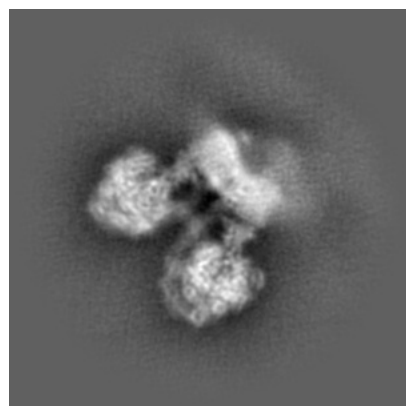
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65237. These allow visual inspection of the internal detail of the map and identification of artifacts.

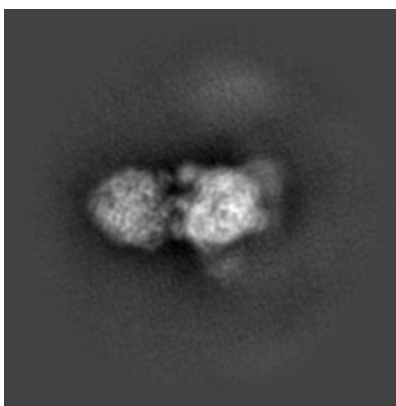
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

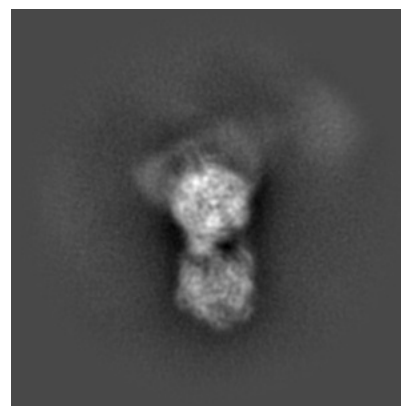
6.1.1 Primary map



X

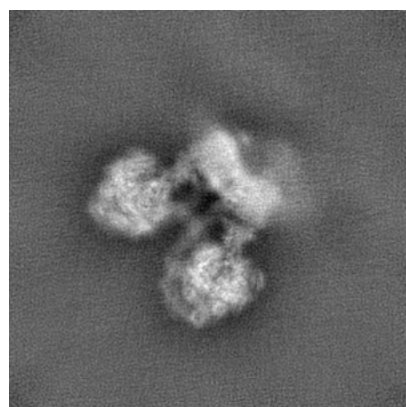


Y

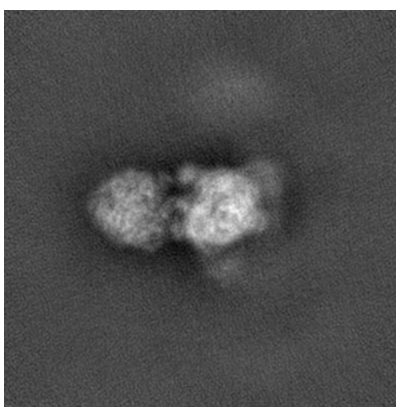


Z

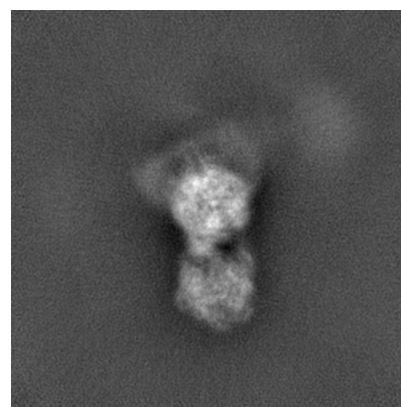
6.1.2 Raw map



X



Y

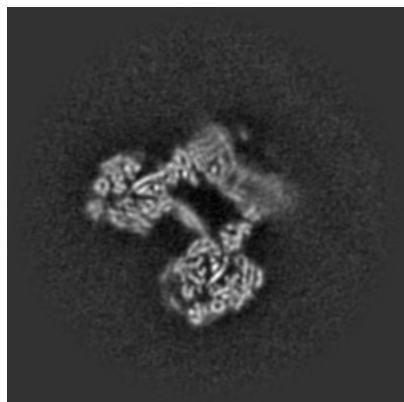


Z

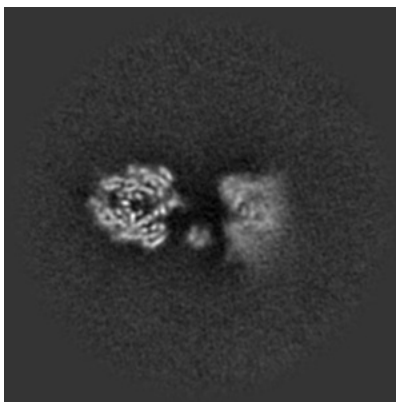
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

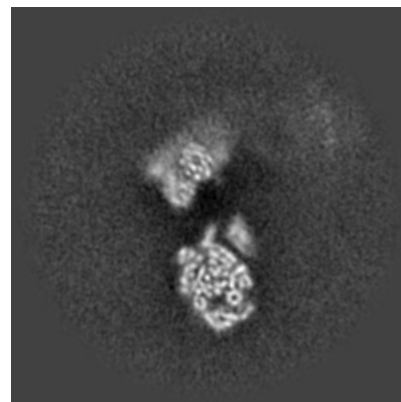
6.2.1 Primary map



X Index: 125

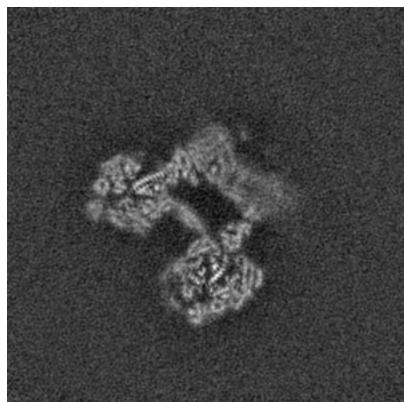


Y Index: 125

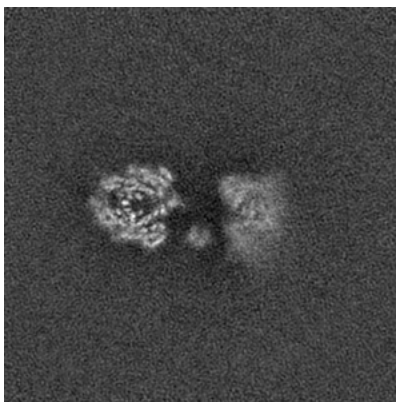


Z Index: 125

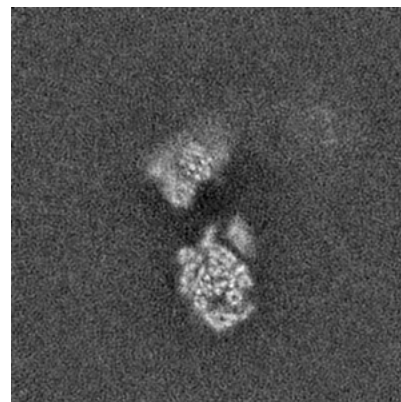
6.2.2 Raw map



X Index: 125



Y Index: 125

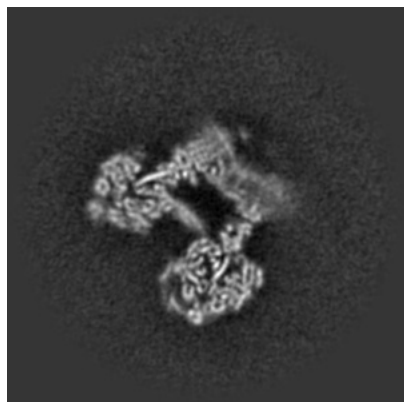


Z Index: 125

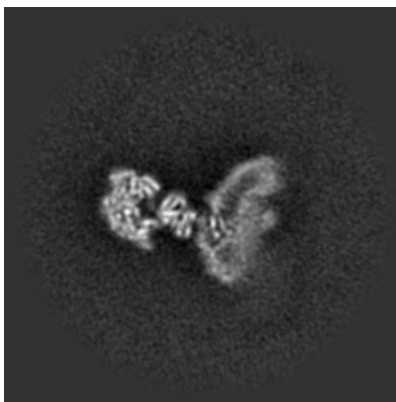
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

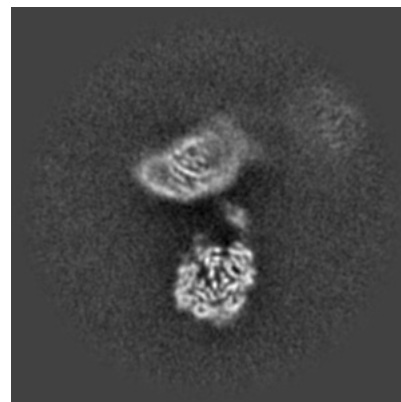
6.3.1 Primary map



X Index: 124

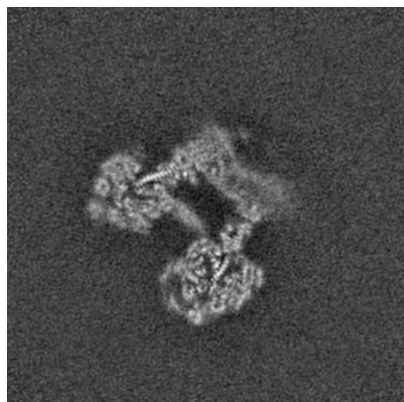


Y Index: 141

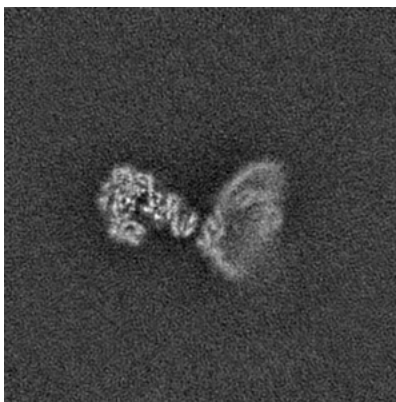


Z Index: 134

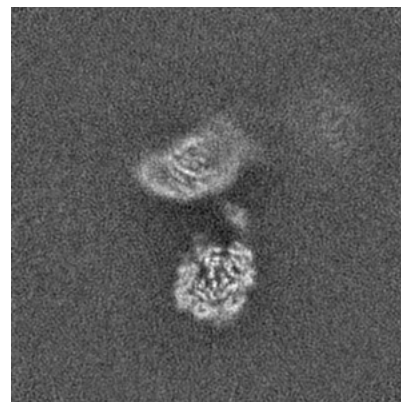
6.3.2 Raw map



X Index: 124



Y Index: 136

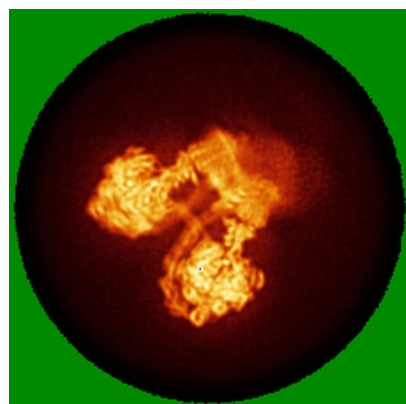


Z Index: 134

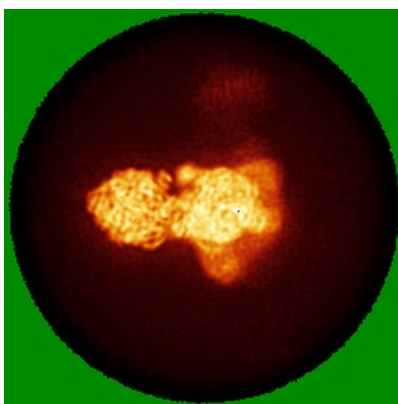
The images above show the largest variance slices of the map in three orthogonal directions.

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

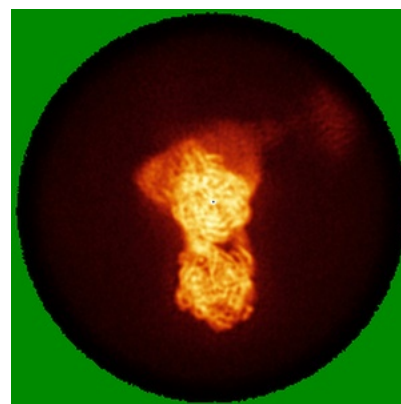
6.4.1 Primary map



X

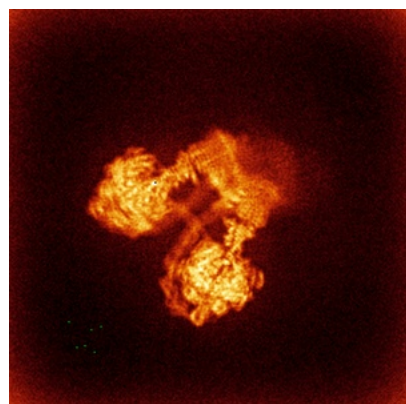


Y

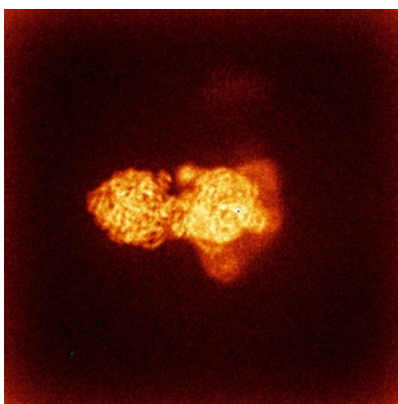


Z

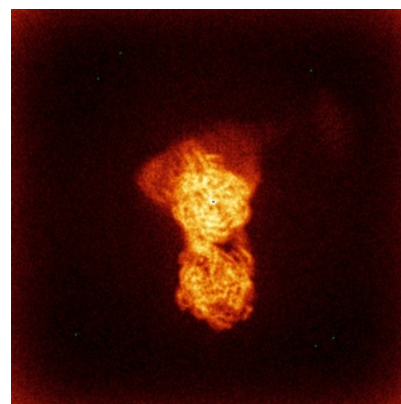
6.4.2 Raw map



X



Y

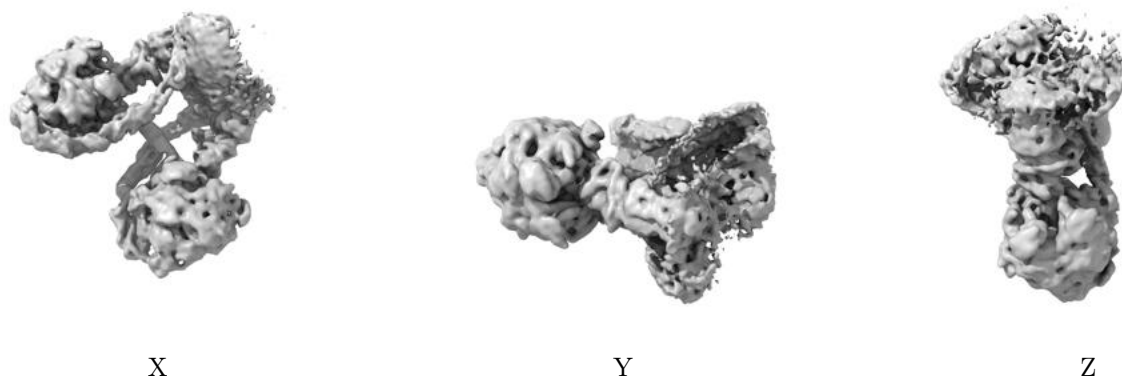


Z

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.

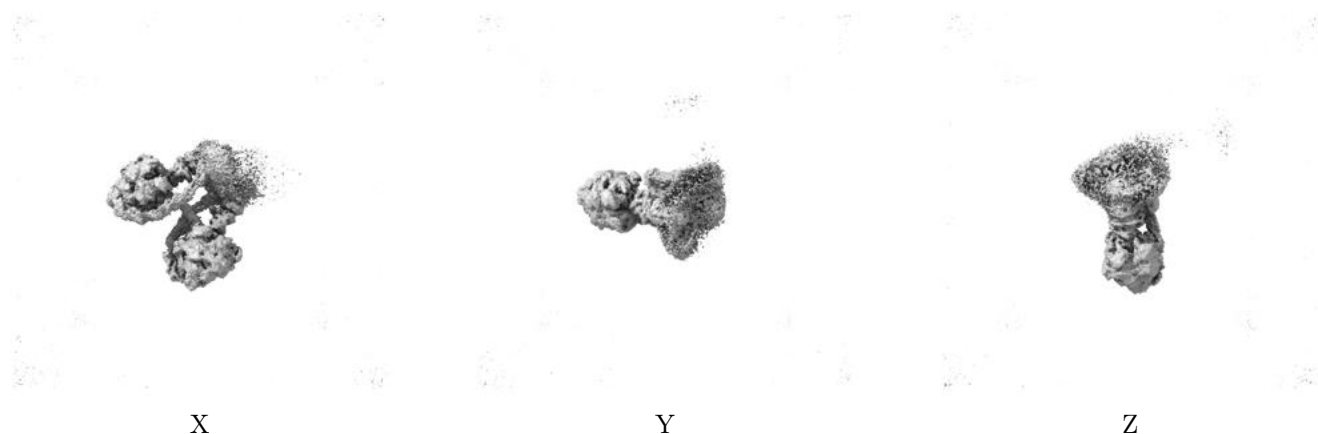
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.555. 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.

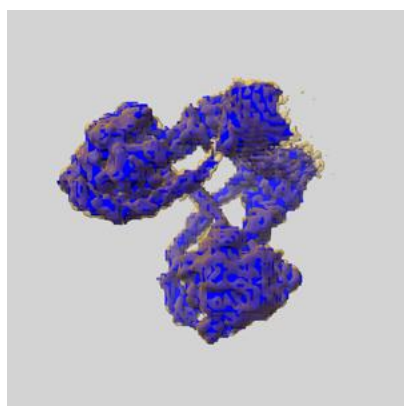
6.6 Mask visualisation [i](#)

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

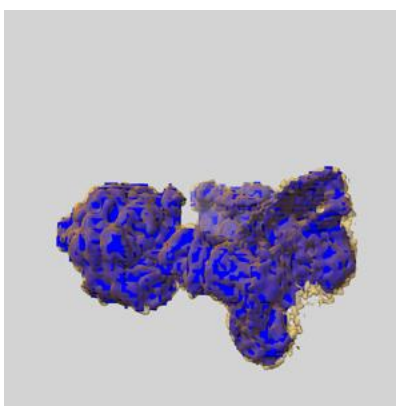
A mask typically either:

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

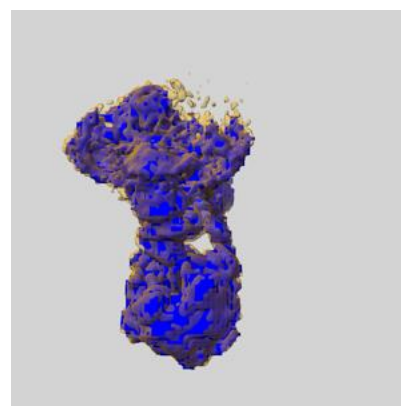
6.6.1 emd_65237_msk_1.map [i](#)



X



Y

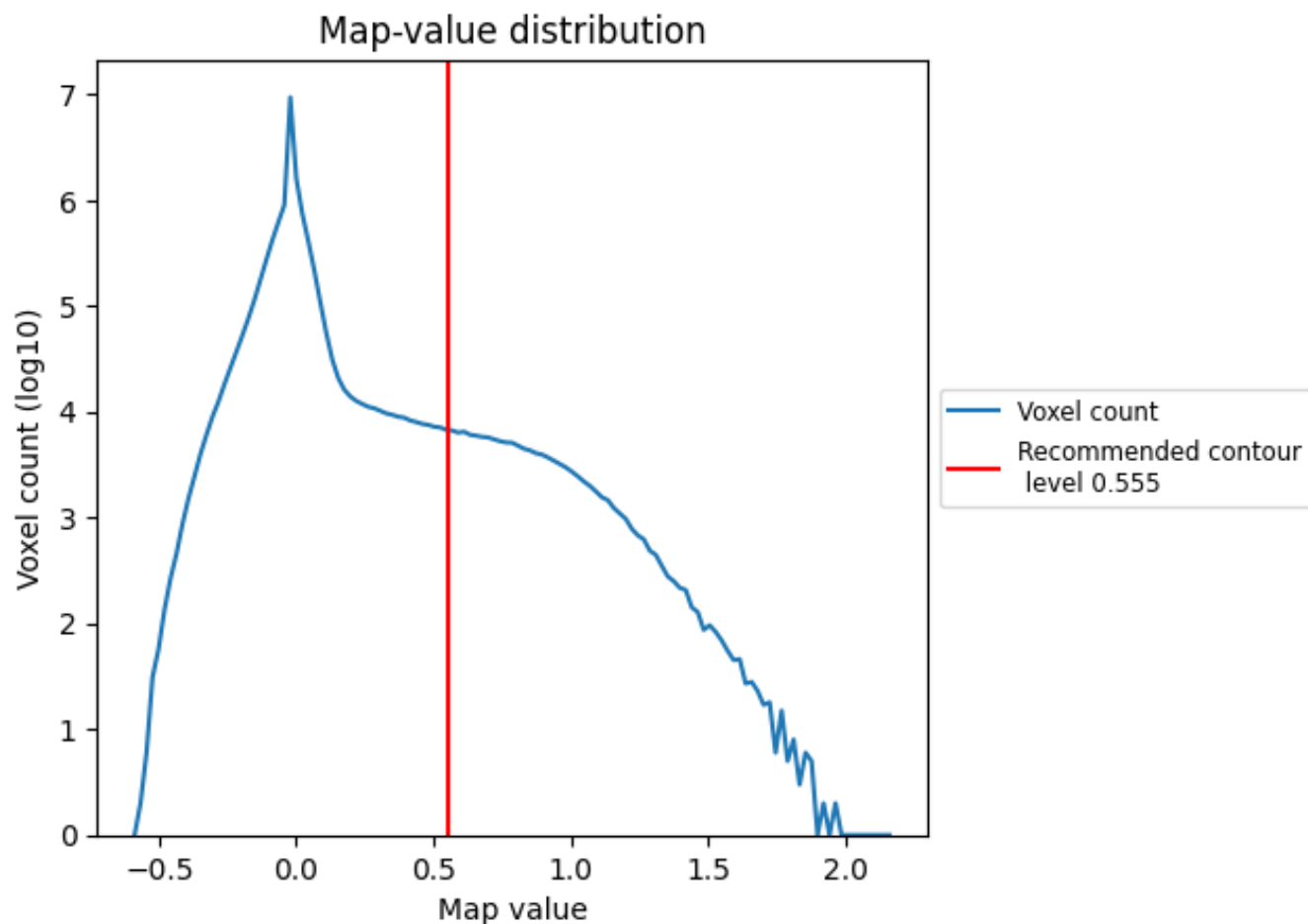


Z

7 Map analysis [i](#)

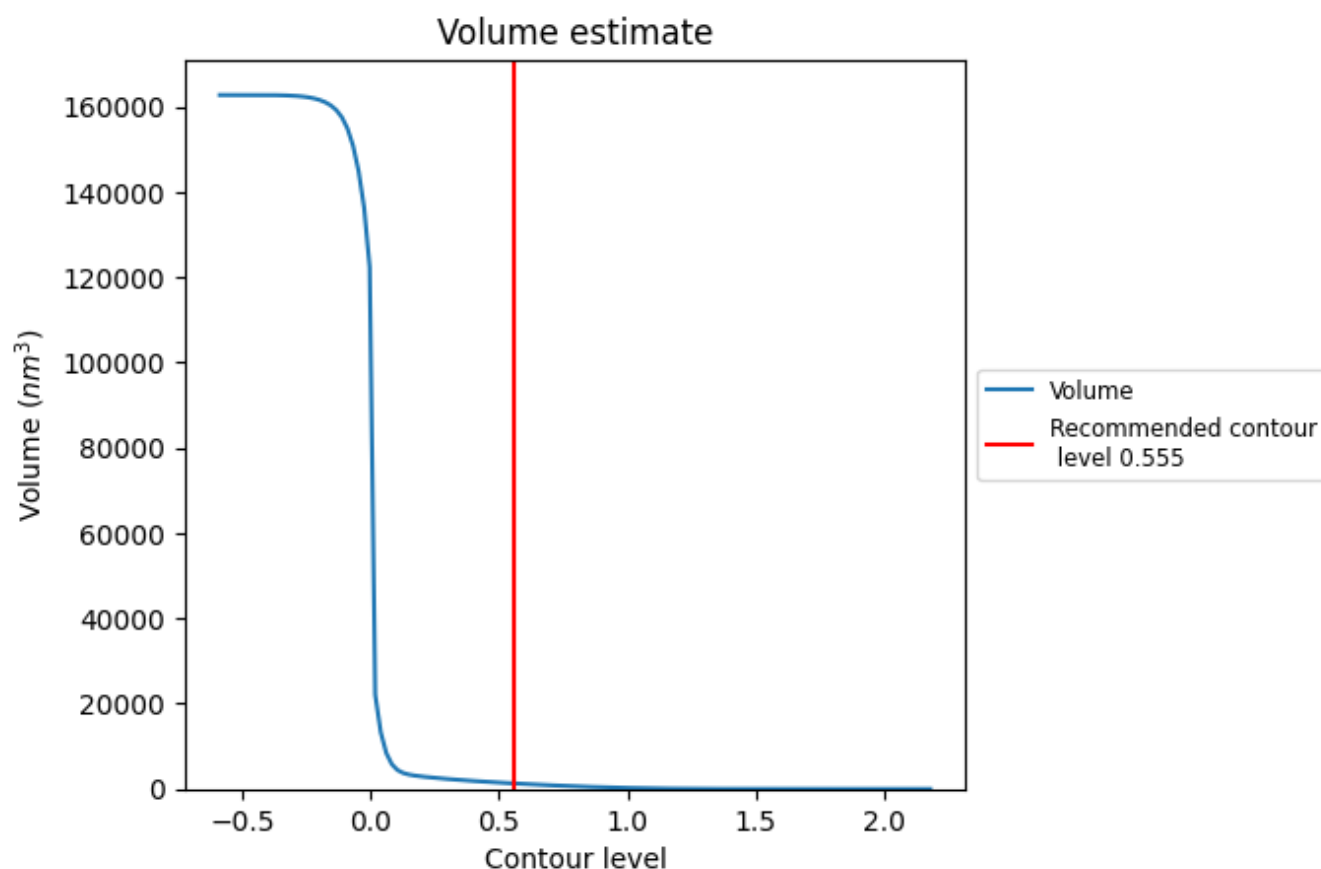
This section contains the results of statistical analysis of the map.

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.

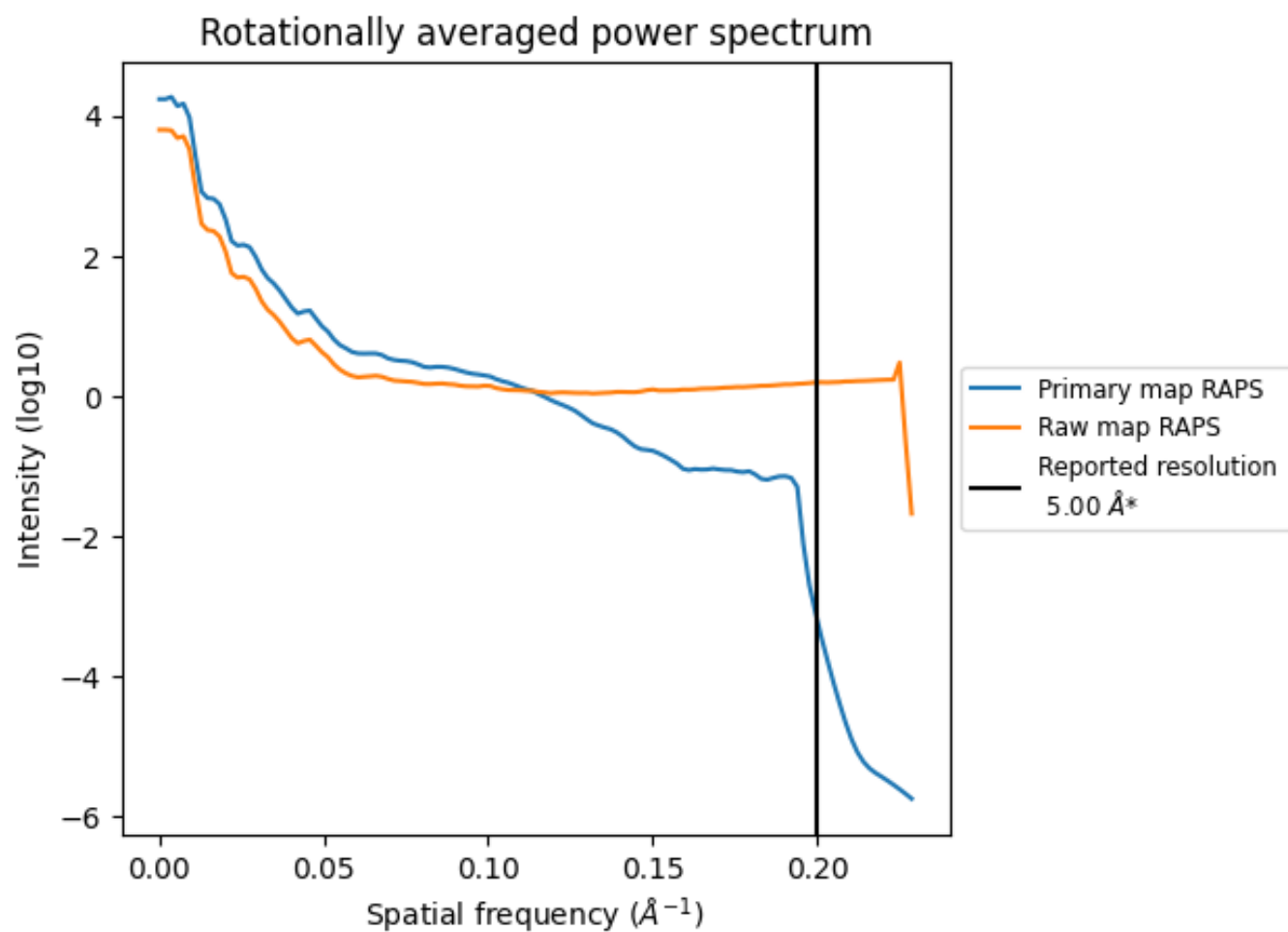
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1306 nm^3 ; this corresponds to an approximate mass of 1180 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 ⓘ

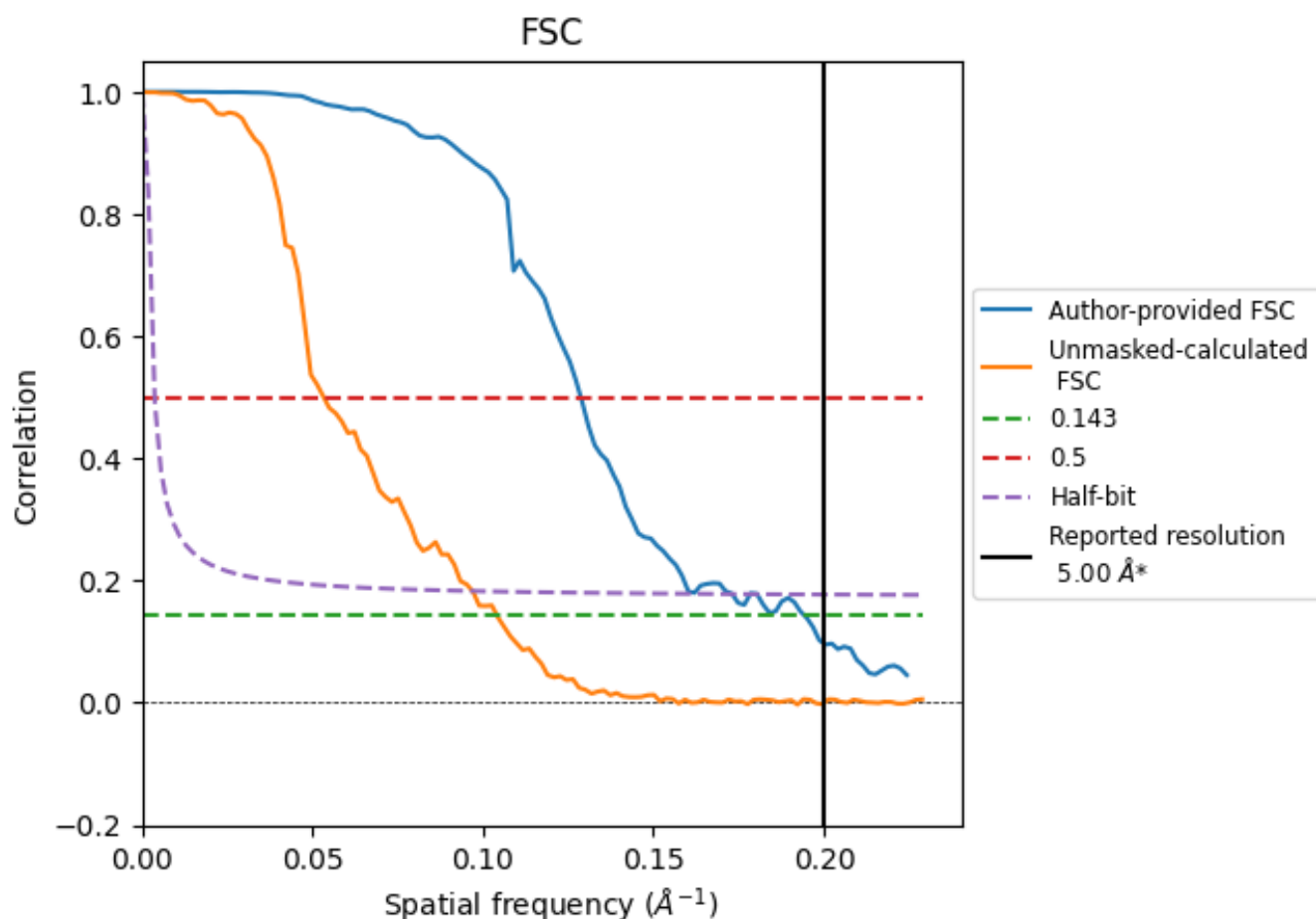


*Reported resolution corresponds to spatial frequency of 0.200 \AA^{-1}

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 0.200 \AA^{-1}

8.2 Resolution estimates [i](#)

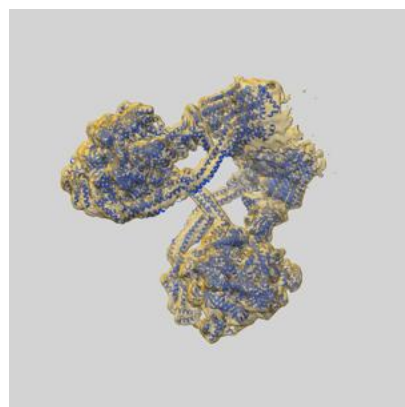
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	5.15	7.77	5.78
Unmasked-calculated*	9.61	18.76	10.32

*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 9.61 differs from the reported value 5.0 by more than 10 %

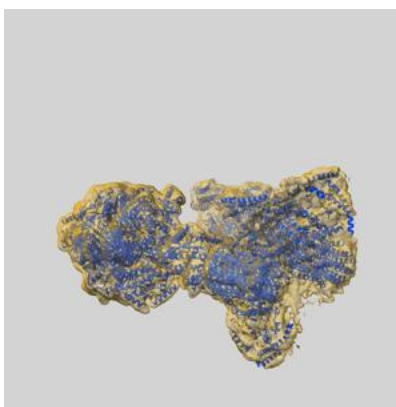
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65237 and PDB model 9VPB. Per-residue inclusion information can be found in section 3 on page 10.

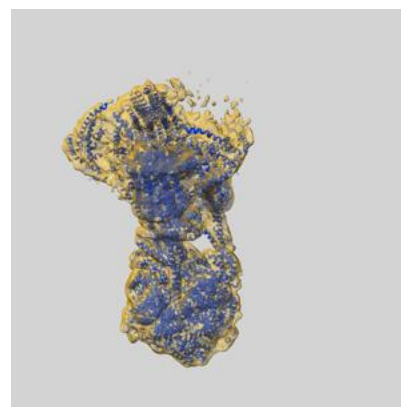
9.1 Map-model overlay [i](#)



X



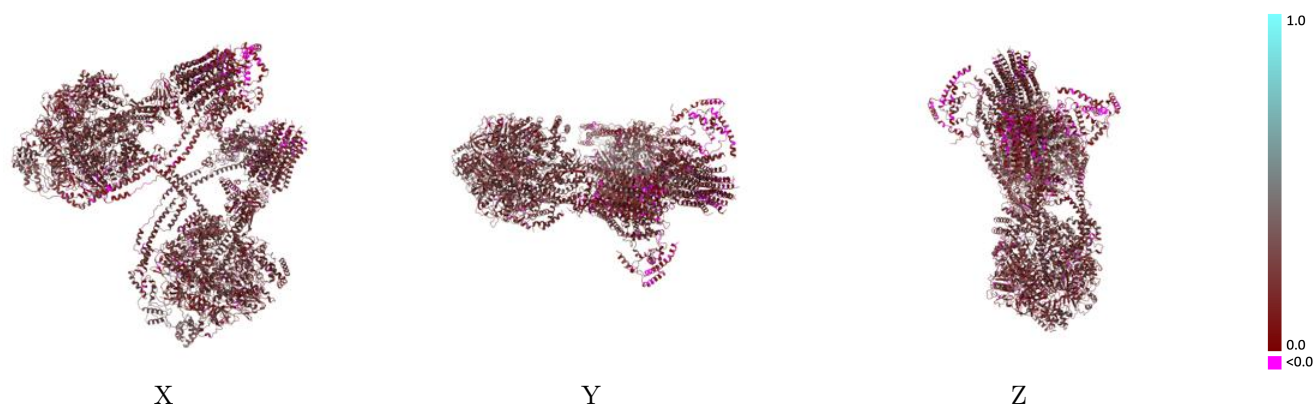
Y



Z

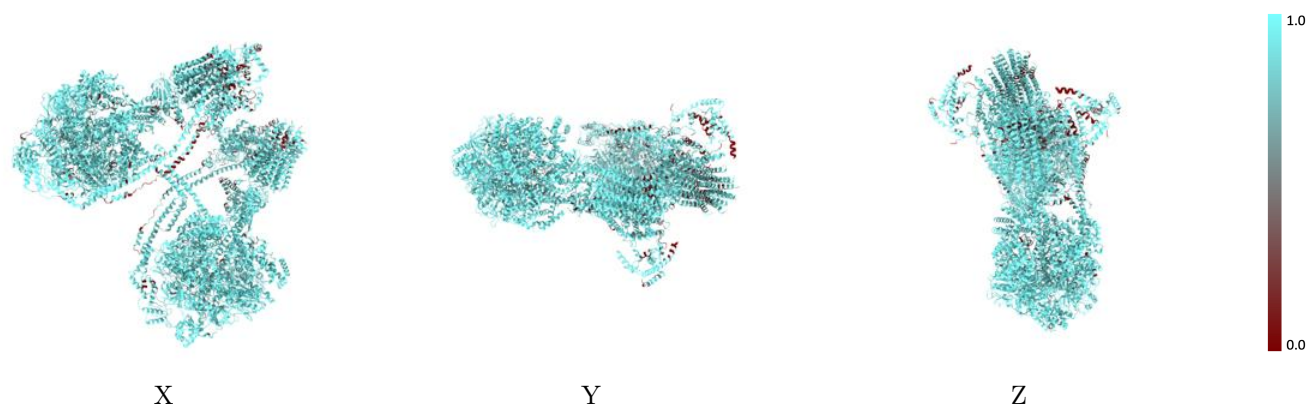
The images above show the 3D surface view of the map at the recommended contour level 0.555 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



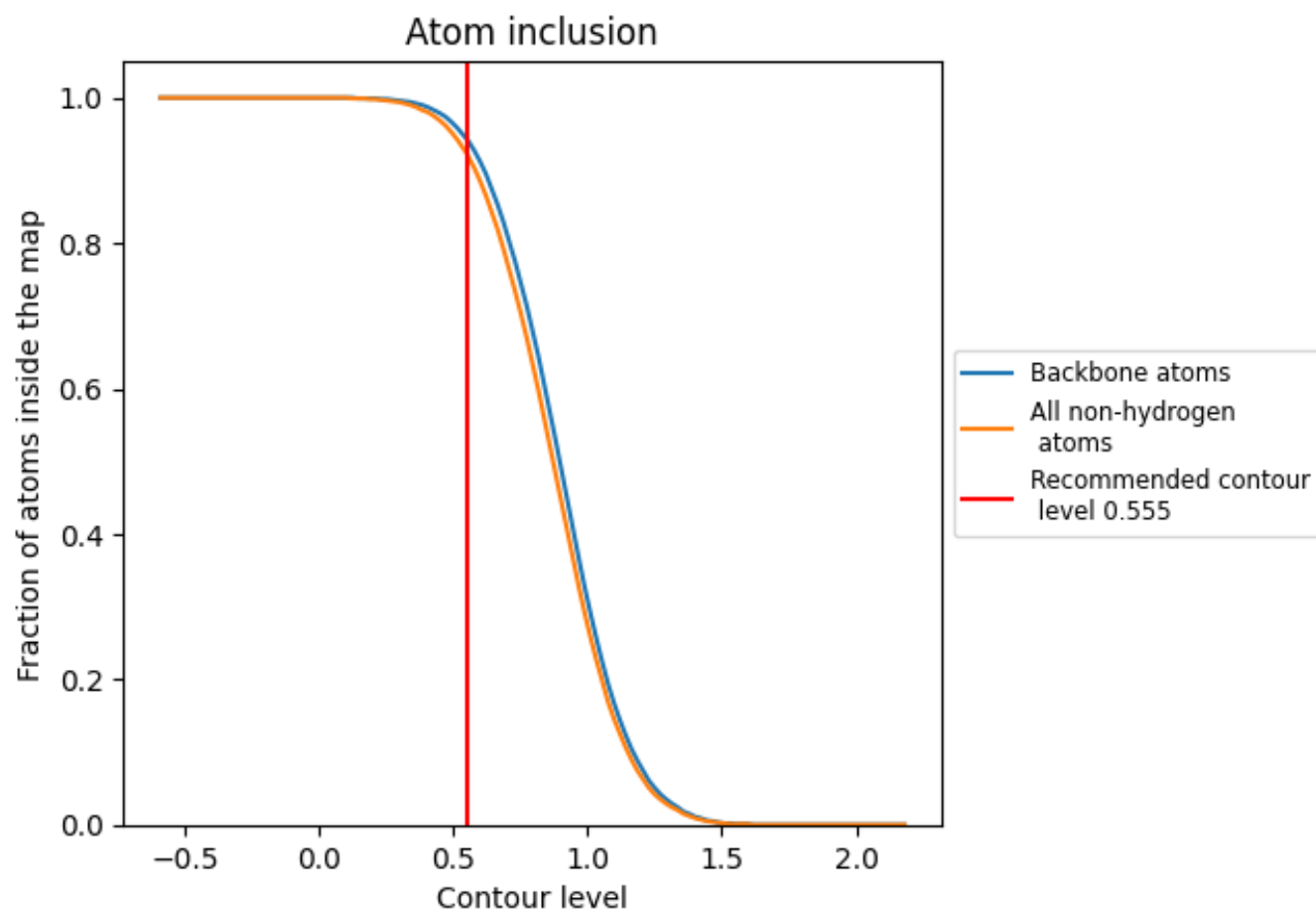
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.555).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.555) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9210	 0.2130
8	 0.8630	 0.2190
A	 0.9480	 0.2290
A8	 0.7370	 0.1810
AA	 0.9540	 0.2390
AB	 0.9330	 0.2100
AC	 0.9500	 0.2090
AD	 0.9330	 0.2060
AE	 0.9430	 0.2040
AF	 0.9660	 0.2100
AG	 0.9640	 0.2440
AH	 0.8600	 0.1470
AI	 0.7900	 0.1580
AJ	 0.9530	 0.2260
AK	 0.9360	 0.1550
AL	 0.9500	 0.1570
AM	 0.9290	 0.1330
AN	 0.8020	 0.1430
AO	 0.7660	 0.1850
AP	 0.8660	 0.2020
AQ	 0.8540	 0.1700
AR	 0.8600	 0.1710
AS	 0.9900	 0.3070
Aa	 0.8400	 0.2020
Ab	 0.8560	 0.1900
Ad	 0.6400	 0.1410
Ae	 0.5740	 0.0460
Af	 0.6970	 0.1310
Ag	 0.7950	 0.1090
Ah	 0.9560	 0.2340
B	 0.9440	 0.2300
C	 0.9710	 0.2260
D	 0.9420	 0.2190
E	 0.9600	 0.2360
F	 0.9640	 0.2300



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Chain	Atom inclusion	Q-score
G	 0.9680	 0.2390
H	 0.8660	 0.1350
I	 0.8370	 0.1750
J	 1.0000	 0.3290
K	 0.9780	 0.2030
L	 0.9780	 0.2230
M	 0.9040	 0.1950
N	 0.7640	 0.1550
O	 0.8350	 0.1880
P	 0.8970	 0.1940
Q	 0.9040	 0.1770
R	 0.9090	 0.1850
S	 1.0000	 0.3650
a	 0.9220	 0.2540
b	 0.9290	 0.2500
d	 0.8010	 0.1790
e	 0.7480	 0.0470
f	 0.8040	 0.1520
g	 0.8790	 0.1190
h	 0.9600	 0.2530