



Full wwPDB EM Validation Report ⓘ

Aug 13, 2025 – 06:17 PM EDT

PDB ID : 9ML1 / pdb_00009ml1
EMDB ID : EMD-48344
Title : D24.1M01 Fab bound to HPV16 L1 pentamer
Authors : Hurlburt, N.K.; Singh, S.; Rodarte, J.V.; Pancera, M.
Deposited on : 2024-12-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

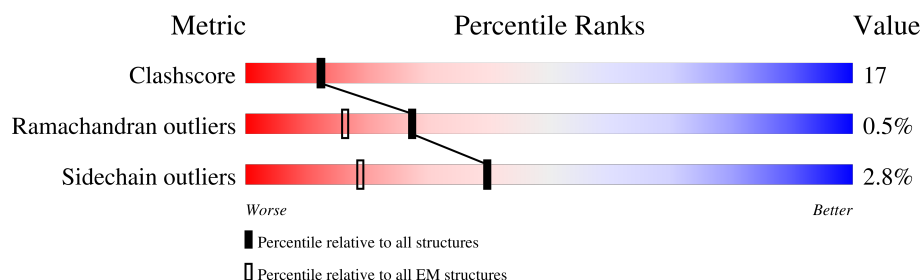
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.





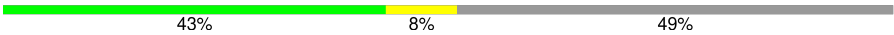
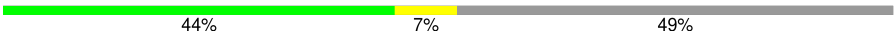
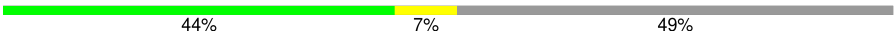
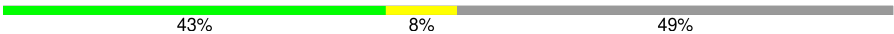
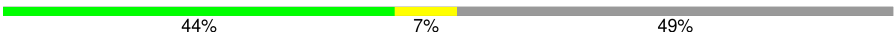
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	426	
1	B	426	
1	C	426	
1	D	426	
1	E	426	
2	H	235	
2	M	235	
2	O	235	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Q	235	 35% 17% 48%
2	S	235	 34% 17% 48%
3	L	217	 43% 8% 49%
3	N	217	 44% 7% 49%
3	P	217	 44% 7% 49%
3	R	217	 43% 8% 49%
3	T	217	 44% 7% 49%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49909 atoms, of which 24609 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	0
			6497	2098	3202	553	624	20		
1	B	418	Total	C	H	N	O	S	0	0
			6496	2098	3201	553	624	20		
1	C	418	Total	C	H	N	O	S	0	0
			6496	2098	3201	553	624	20		
1	D	418	Total	C	H	N	O	S	0	0
			6490	2098	3195	553	624	20		
1	E	418	Total	C	H	N	O	S	0	0
			6490	2098	3195	553	624	20		

There are 170 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	expression tag	UNP A0A161GYK1
A	280	THR	ALA	conflict	UNP A0A161GYK1
A	?	-	PHE	deletion	UNP A0A161GYK1
A	?	-	GLY	deletion	UNP A0A161GYK1
A	?	-	LEU	deletion	UNP A0A161GYK1
A	?	-	GLN	deletion	UNP A0A161GYK1
A	?	-	PRO	deletion	UNP A0A161GYK1
A	?	-	PRO	deletion	UNP A0A161GYK1
A	?	-	PRO	deletion	UNP A0A161GYK1
A	448	SER	THR	conflict	UNP A0A161GYK1
A	?	-	LEU	deletion	UNP A0A161GYK1
A	?	-	GLU	deletion	UNP A0A161GYK1
A	?	-	ASP	deletion	UNP A0A161GYK1
A	?	-	THR	deletion	UNP A0A161GYK1
A	?	-	TYR	deletion	UNP A0A161GYK1
A	?	-	ARG	deletion	UNP A0A161GYK1
A	?	-	PHE	deletion	UNP A0A161GYK1
A	?	-	VAL	deletion	UNP A0A161GYK1
A	?	-	THR	deletion	UNP A0A161GYK1
A	?	-	SER	deletion	UNP A0A161GYK1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP A0A161GYK1
A	?	-	ALA	deletion	UNP A0A161GYK1
A	?	-	ILE	deletion	UNP A0A161GYK1
A	?	-	ALA	deletion	UNP A0A161GYK1
A	?	-	CYS	deletion	UNP A0A161GYK1
A	?	-	GLN	deletion	UNP A0A161GYK1
A	?	-	LYS	deletion	UNP A0A161GYK1
A	?	-	HIS	deletion	UNP A0A161GYK1
A	?	-	THR	deletion	UNP A0A161GYK1
A	?	-	PRO	deletion	UNP A0A161GYK1
A	?	-	PRO	deletion	UNP A0A161GYK1
A	?	-	VAL	deletion	UNP A0A161GYK1
A	449	GLY	PRO	conflict	UNP A0A161GYK1
A	450	ALA	LYS	conflict	UNP A0A161GYK1
B	34	ALA	-	expression tag	UNP A0A161GYK1
B	280	THR	ALA	conflict	UNP A0A161GYK1
B	?	-	PHE	deletion	UNP A0A161GYK1
B	?	-	GLY	deletion	UNP A0A161GYK1
B	?	-	LEU	deletion	UNP A0A161GYK1
B	?	-	GLN	deletion	UNP A0A161GYK1
B	?	-	PRO	deletion	UNP A0A161GYK1
B	?	-	PRO	deletion	UNP A0A161GYK1
B	?	-	PRO	deletion	UNP A0A161GYK1
B	448	SER	THR	conflict	UNP A0A161GYK1
B	?	-	LEU	deletion	UNP A0A161GYK1
B	?	-	GLU	deletion	UNP A0A161GYK1
B	?	-	ASP	deletion	UNP A0A161GYK1
B	?	-	THR	deletion	UNP A0A161GYK1
B	?	-	TYR	deletion	UNP A0A161GYK1
B	?	-	ARG	deletion	UNP A0A161GYK1
B	?	-	PHE	deletion	UNP A0A161GYK1
B	?	-	VAL	deletion	UNP A0A161GYK1
B	?	-	THR	deletion	UNP A0A161GYK1
B	?	-	SER	deletion	UNP A0A161GYK1
B	?	-	GLN	deletion	UNP A0A161GYK1
B	?	-	ALA	deletion	UNP A0A161GYK1
B	?	-	ILE	deletion	UNP A0A161GYK1
B	?	-	ALA	deletion	UNP A0A161GYK1
B	?	-	CYS	deletion	UNP A0A161GYK1
B	?	-	GLN	deletion	UNP A0A161GYK1
B	?	-	LYS	deletion	UNP A0A161GYK1
B	?	-	HIS	deletion	UNP A0A161GYK1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP A0A161GYK1
B	?	-	PRO	deletion	UNP A0A161GYK1
B	?	-	PRO	deletion	UNP A0A161GYK1
B	?	-	VAL	deletion	UNP A0A161GYK1
B	449	GLY	PRO	conflict	UNP A0A161GYK1
B	450	ALA	LYS	conflict	UNP A0A161GYK1
C	34	ALA	-	expression tag	UNP A0A161GYK1
C	280	THR	ALA	conflict	UNP A0A161GYK1
C	?	-	PHE	deletion	UNP A0A161GYK1
C	?	-	GLY	deletion	UNP A0A161GYK1
C	?	-	LEU	deletion	UNP A0A161GYK1
C	?	-	GLN	deletion	UNP A0A161GYK1
C	?	-	PRO	deletion	UNP A0A161GYK1
C	?	-	PRO	deletion	UNP A0A161GYK1
C	?	-	PRO	deletion	UNP A0A161GYK1
C	448	SER	THR	conflict	UNP A0A161GYK1
C	?	-	LEU	deletion	UNP A0A161GYK1
C	?	-	GLU	deletion	UNP A0A161GYK1
C	?	-	ASP	deletion	UNP A0A161GYK1
C	?	-	THR	deletion	UNP A0A161GYK1
C	?	-	TYR	deletion	UNP A0A161GYK1
C	?	-	ARG	deletion	UNP A0A161GYK1
C	?	-	PHE	deletion	UNP A0A161GYK1
C	?	-	VAL	deletion	UNP A0A161GYK1
C	?	-	THR	deletion	UNP A0A161GYK1
C	?	-	SER	deletion	UNP A0A161GYK1
C	?	-	GLN	deletion	UNP A0A161GYK1
C	?	-	ALA	deletion	UNP A0A161GYK1
C	?	-	ILE	deletion	UNP A0A161GYK1
C	?	-	ALA	deletion	UNP A0A161GYK1
C	?	-	CYS	deletion	UNP A0A161GYK1
C	?	-	GLN	deletion	UNP A0A161GYK1
C	?	-	LYS	deletion	UNP A0A161GYK1
C	?	-	HIS	deletion	UNP A0A161GYK1
C	?	-	THR	deletion	UNP A0A161GYK1
C	?	-	PRO	deletion	UNP A0A161GYK1
C	?	-	PRO	deletion	UNP A0A161GYK1
C	?	-	VAL	deletion	UNP A0A161GYK1
C	449	GLY	PRO	conflict	UNP A0A161GYK1
C	450	ALA	LYS	conflict	UNP A0A161GYK1
D	34	ALA	-	expression tag	UNP A0A161GYK1
D	280	THR	ALA	conflict	UNP A0A161GYK1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PHE	deletion	UNP A0A161GYK1
D	?	-	GLY	deletion	UNP A0A161GYK1
D	?	-	LEU	deletion	UNP A0A161GYK1
D	?	-	GLN	deletion	UNP A0A161GYK1
D	?	-	PRO	deletion	UNP A0A161GYK1
D	?	-	PRO	deletion	UNP A0A161GYK1
D	?	-	PRO	deletion	UNP A0A161GYK1
D	448	SER	THR	conflict	UNP A0A161GYK1
D	?	-	LEU	deletion	UNP A0A161GYK1
D	?	-	GLU	deletion	UNP A0A161GYK1
D	?	-	ASP	deletion	UNP A0A161GYK1
D	?	-	THR	deletion	UNP A0A161GYK1
D	?	-	TYR	deletion	UNP A0A161GYK1
D	?	-	ARG	deletion	UNP A0A161GYK1
D	?	-	PHE	deletion	UNP A0A161GYK1
D	?	-	VAL	deletion	UNP A0A161GYK1
D	?	-	THR	deletion	UNP A0A161GYK1
D	?	-	SER	deletion	UNP A0A161GYK1
D	?	-	GLN	deletion	UNP A0A161GYK1
D	?	-	ALA	deletion	UNP A0A161GYK1
D	?	-	ILE	deletion	UNP A0A161GYK1
D	?	-	ALA	deletion	UNP A0A161GYK1
D	?	-	CYS	deletion	UNP A0A161GYK1
D	?	-	GLN	deletion	UNP A0A161GYK1
D	?	-	LYS	deletion	UNP A0A161GYK1
D	?	-	HIS	deletion	UNP A0A161GYK1
D	?	-	THR	deletion	UNP A0A161GYK1
D	?	-	PRO	deletion	UNP A0A161GYK1
D	?	-	PRO	deletion	UNP A0A161GYK1
D	?	-	VAL	deletion	UNP A0A161GYK1
D	449	GLY	PRO	conflict	UNP A0A161GYK1
D	450	ALA	LYS	conflict	UNP A0A161GYK1
E	34	ALA	-	expression tag	UNP A0A161GYK1
E	280	THR	ALA	conflict	UNP A0A161GYK1
E	?	-	PHE	deletion	UNP A0A161GYK1
E	?	-	GLY	deletion	UNP A0A161GYK1
E	?	-	LEU	deletion	UNP A0A161GYK1
E	?	-	GLN	deletion	UNP A0A161GYK1
E	?	-	PRO	deletion	UNP A0A161GYK1
E	?	-	PRO	deletion	UNP A0A161GYK1
E	?	-	PRO	deletion	UNP A0A161GYK1
E	448	SER	THR	conflict	UNP A0A161GYK1

Continued on next page...

Continued from previous page...

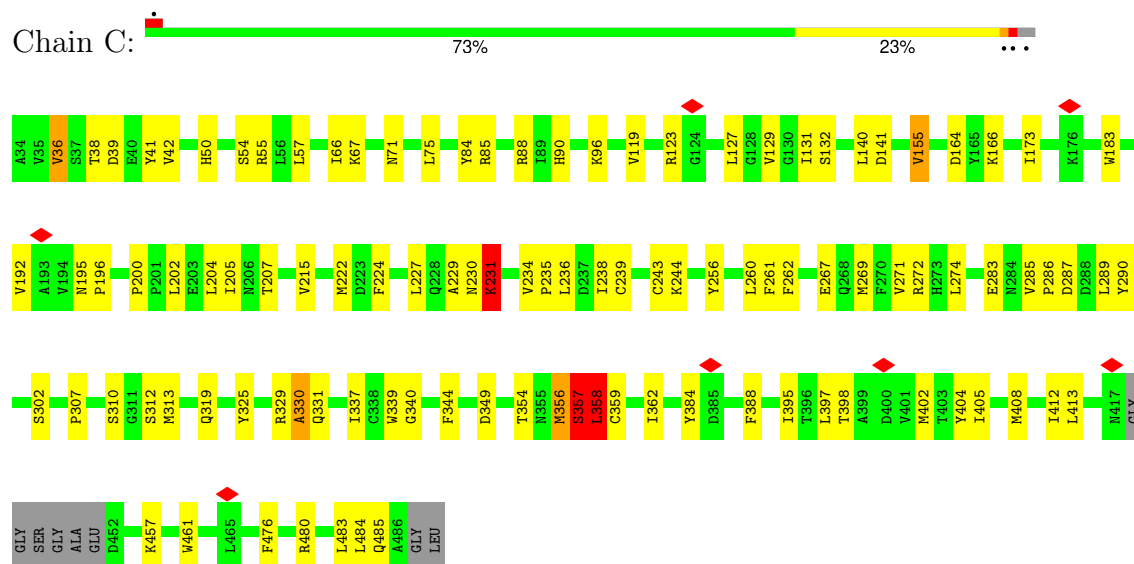
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP A0A161GYK1
E	?	-	GLU	deletion	UNP A0A161GYK1
E	?	-	ASP	deletion	UNP A0A161GYK1
E	?	-	THR	deletion	UNP A0A161GYK1
E	?	-	TYR	deletion	UNP A0A161GYK1
E	?	-	ARG	deletion	UNP A0A161GYK1
E	?	-	PHE	deletion	UNP A0A161GYK1
E	?	-	VAL	deletion	UNP A0A161GYK1
E	?	-	THR	deletion	UNP A0A161GYK1
E	?	-	SER	deletion	UNP A0A161GYK1
E	?	-	GLN	deletion	UNP A0A161GYK1
E	?	-	ALA	deletion	UNP A0A161GYK1
E	?	-	ILE	deletion	UNP A0A161GYK1
E	?	-	ALA	deletion	UNP A0A161GYK1
E	?	-	CYS	deletion	UNP A0A161GYK1
E	?	-	GLN	deletion	UNP A0A161GYK1
E	?	-	LYS	deletion	UNP A0A161GYK1
E	?	-	HIS	deletion	UNP A0A161GYK1
E	?	-	THR	deletion	UNP A0A161GYK1
E	?	-	PRO	deletion	UNP A0A161GYK1
E	?	-	PRO	deletion	UNP A0A161GYK1
E	?	-	VAL	deletion	UNP A0A161GYK1
E	449	GLY	PRO	conflict	UNP A0A161GYK1
E	450	ALA	LYS	conflict	UNP A0A161GYK1

- Molecule 2 is a protein called D24.1M01 Heavy Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	122	Total	C	H	N	O	S	0	0
			1903	604	947	162	184	6		
2	M	122	Total	C	H	N	O	S	0	0
			1903	604	947	162	184	6		
2	O	122	Total	C	H	N	O	S	0	0
			1903	604	947	162	184	6		
2	Q	122	Total	C	H	N	O	S	0	0
			1903	604	947	162	184	6		
2	S	122	Total	C	H	N	O	S	0	0
			1903	604	947	162	184	6		

- Molecule 3 is a protein called D24.1M01 Light Chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	111	Total	C	H	N	O	S	0	0
			1585	507	776	138	162	2		
3	N	111	Total	C	H	N	O	S	0	0
			1585	507	776	138	162	2		
3	P	111	Total	C	H	N	O	S	0	0
			1585	507	776	138	162	2		
3	R	111	Total	C	H	N	O	S	0	0
			1585	507	776	138	162	2		
3	T	111	Total	C	H	N	O	S	0	0
			1585	507	776	138	162	2		



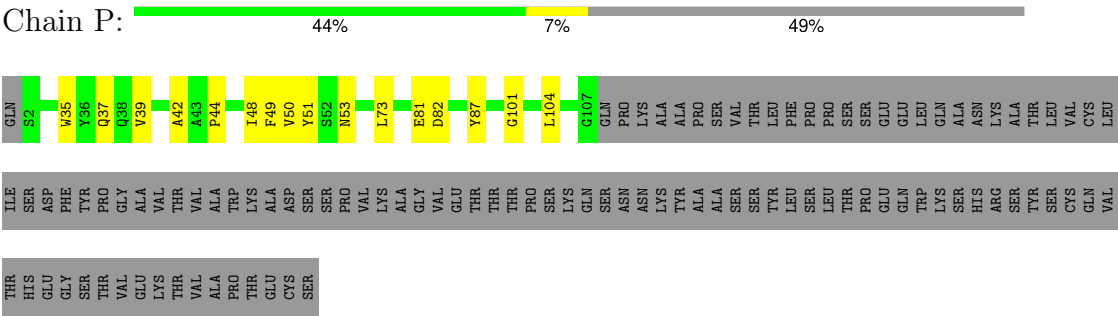
• Molecule 1: Major capsid protein L1



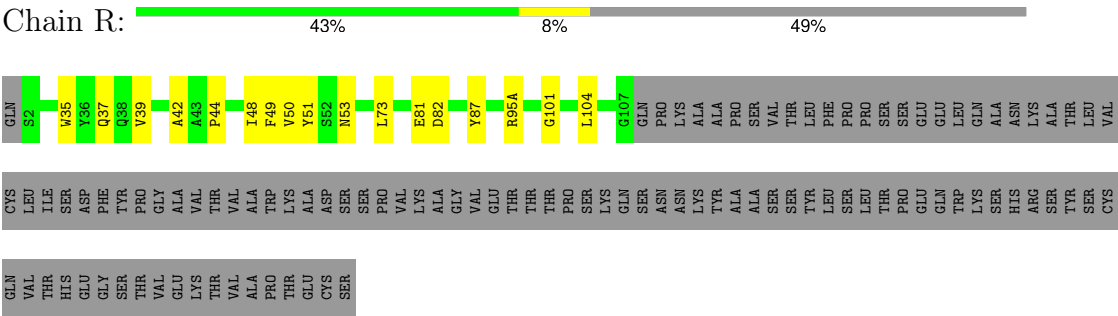
• Molecule 1: Major capsid protein L1



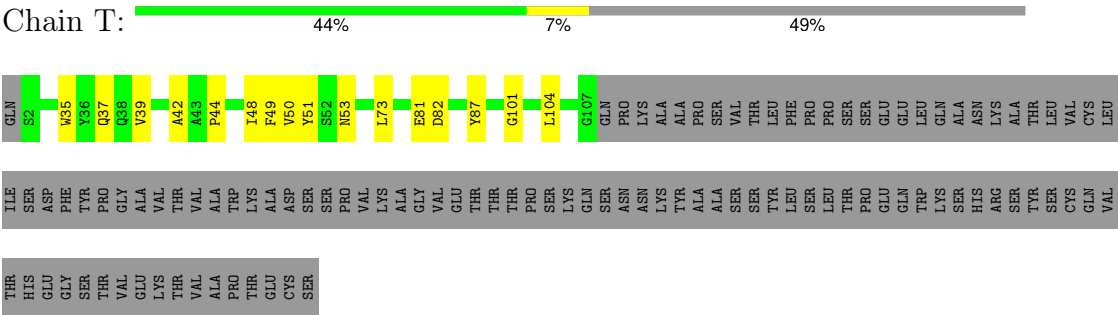
• Molecule 3: D24.1M01 Light Chain



• Molecule 3: D24.1M01 Light Chain



• Molecule 3: D24.1M01 Light Chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188743	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)	2200	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.070	Depositor
Minimum map value	-3.816	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.172	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	231.88, 231.88, 231.88	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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	A	0.29	0/3380	0.48	3/4598 (0.1%)
1	B	0.29	0/3380	0.49	2/4598 (0.0%)
1	C	0.28	0/3380	0.49	4/4598 (0.1%)
1	D	0.29	0/3380	0.50	3/4598 (0.1%)
1	E	0.28	0/3380	0.48	4/4598 (0.1%)
2	H	0.21	0/977	0.32	0/1335
2	M	0.21	0/977	0.32	0/1335
2	O	0.21	0/977	0.32	0/1335
2	Q	0.21	0/977	0.32	0/1335
2	S	0.21	0/977	0.32	0/1335
3	L	0.13	0/828	0.30	0/1129
3	N	0.13	0/828	0.30	0/1129
3	P	0.14	0/828	0.30	0/1129
3	R	0.14	0/828	0.30	0/1129
3	T	0.13	0/828	0.30	0/1129
All	All	0.25	0/25925	0.43	16/35310 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	356	MET	O-C-N	-8.34	113.43	123.19
1	C	356	MET	O-C-N	-8.13	113.67	123.19
1	C	231	LYS	N-CA-C	-5.97	105.58	112.86
1	A	231	LYS	N-CA-C	-5.86	106.08	113.23
1	D	231	LYS	N-CA-C	-5.72	104.91	112.24
1	E	231	LYS	N-CA-C	-5.71	105.89	112.86
1	D	330	ALA	CA-C-N	-5.07	113.75	120.79
1	D	330	ALA	C-N-CA	-5.07	113.75	120.79
1	C	330	ALA	CA-C-N	-5.06	113.76	120.79
1	C	330	ALA	C-N-CA	-5.06	113.76	120.79
1	B	330	ALA	CA-C-N	-5.05	113.76	120.79
1	B	330	ALA	C-N-CA	-5.05	113.76	120.79
1	A	330	ALA	CA-C-N	-5.05	113.77	120.79
1	A	330	ALA	C-N-CA	-5.05	113.77	120.79
1	E	330	ALA	CA-C-N	-5.02	113.81	120.79
1	E	330	ALA	C-N-CA	-5.02	113.81	120.79

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	ARG	Sidechain
1	B	480	ARG	Sidechain
1	C	480	ARG	Sidechain
1	D	480	ARG	Sidechain
1	E	480	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3295	3202	3197	119	0
1	B	3295	3201	3197	112	0
1	C	3295	3201	3197	113	0
1	D	3295	3195	3197	109	0
1	E	3295	3195	3197	118	0
2	H	956	947	947	58	0
2	M	956	947	947	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	956	947	947	58	0
2	Q	956	947	947	60	0
2	S	956	947	947	60	0
3	L	809	776	775	29	0
3	N	809	776	775	25	0
3	P	809	776	775	27	0
3	R	809	776	775	27	0
3	T	809	776	775	24	0
All	All	25300	24609	24595	832	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 17.

All (832) 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)
2:H:103:TRP:CZ3	3:L:44:PRO:HG2	1.86	1.11
2:Q:103:TRP:CZ3	3:R:44:PRO:HG2	1.88	1.08
2:S:103:TRP:CZ3	3:T:44:PRO:HG2	1.88	1.08
2:O:103:TRP:CZ3	3:P:44:PRO:HG2	1.89	1.07
2:M:103:TRP:CZ3	3:N:44:PRO:HG2	1.92	1.04
1:D:397:LEU:C	1:D:402:MET:HE2	1.94	0.93
1:C:397:LEU:C	1:C:402:MET:HE2	1.94	0.93
1:E:397:LEU:C	1:E:402:MET:HE2	1.94	0.93
1:A:397:LEU:C	1:A:402:MET:HE2	1.94	0.93
1:B:397:LEU:C	1:B:402:MET:HE2	1.94	0.92
1:A:398:THR:O	1:A:402:MET:HE3	1.74	0.88
1:E:398:THR:O	1:E:402:MET:HE3	1.74	0.87
1:C:398:THR:O	1:C:402:MET:HE3	1.74	0.87
1:B:398:THR:O	1:B:402:MET:HE3	1.74	0.86
2:H:103:TRP:CE3	3:L:44:PRO:HD2	2.10	0.86
3:T:48:ILE:HD11	3:T:73:LEU:HD13	1.58	0.86
3:R:48:ILE:HD11	3:R:73:LEU:HD13	1.58	0.85
1:D:398:THR:O	1:D:402:MET:HE3	1.74	0.85
3:L:48:ILE:HD11	3:L:73:LEU:HD13	1.58	0.84
2:H:18:LEU:CD1	2:H:20:LEU:HD22	2.07	0.84
2:S:18:LEU:CD1	2:S:20:LEU:HD22	2.07	0.84
3:N:48:ILE:HD11	3:N:73:LEU:HD13	1.58	0.84
2:M:18:LEU:CD1	2:M:20:LEU:HD22	2.07	0.84
2:O:18:LEU:CD1	2:O:20:LEU:HD22	2.07	0.84
3:P:48:ILE:HD11	3:P:73:LEU:HD13	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:18:LEU:CD1	2:Q:20:LEU:HD22	2.07	0.83
2:Q:103:TRP:CE3	3:R:44:PRO:HD2	2.15	0.82
1:A:222:MET:HE1	1:A:228:GLN:HG3	1.62	0.80
1:B:222:MET:HE1	1:B:228:GLN:HG3	1.62	0.80
2:S:103:TRP:CE3	3:T:44:PRO:HD2	2.16	0.80
2:O:103:TRP:CE3	3:P:44:PRO:HD2	2.17	0.79
2:M:103:TRP:CE3	3:N:44:PRO:HD2	2.18	0.78
1:A:397:LEU:O	1:A:402:MET:CE	2.34	0.75
1:B:397:LEU:O	1:B:402:MET:CE	2.34	0.75
1:C:397:LEU:O	1:C:402:MET:CE	2.34	0.75
1:E:140:LEU:HG	1:E:141:ASP:OD1	1.87	0.75
1:E:397:LEU:O	1:E:402:MET:CE	2.34	0.75
1:C:140:LEU:HG	1:C:141:ASP:OD1	1.87	0.74
1:A:140:LEU:HG	1:A:141:ASP:OD1	1.87	0.74
1:D:140:LEU:HG	1:D:141:ASP:OD1	1.87	0.74
1:D:397:LEU:O	1:D:402:MET:CE	2.34	0.74
1:B:140:LEU:HG	1:B:141:ASP:OD1	1.87	0.74
1:E:38:THR:CB	1:E:337:ILE:HD13	2.18	0.73
1:A:155:VAL:HG13	1:A:155:VAL:O	1.88	0.73
1:D:38:THR:CB	1:D:337:ILE:HD13	2.19	0.73
1:D:155:VAL:O	1:D:155:VAL:HG13	1.88	0.72
1:B:155:VAL:HG13	1:B:155:VAL:O	1.88	0.72
1:E:397:LEU:HB3	1:E:402:MET:HE2	1.72	0.72
1:C:155:VAL:HG13	1:C:155:VAL:O	1.88	0.72
1:B:397:LEU:HB3	1:B:402:MET:HE2	1.72	0.71
1:D:397:LEU:O	1:D:402:MET:HE2	1.90	0.71
1:D:397:LEU:HB3	1:D:402:MET:HE2	1.72	0.71
1:A:398:THR:C	1:A:402:MET:HE3	2.15	0.71
1:E:398:THR:C	1:E:402:MET:HE3	2.15	0.71
1:C:397:LEU:HB3	1:C:402:MET:HE2	1.72	0.71
1:E:155:VAL:O	1:E:155:VAL:HG13	1.88	0.71
1:D:398:THR:C	1:D:402:MET:HE3	2.15	0.71
1:B:398:THR:C	1:B:402:MET:HE3	2.15	0.70
1:A:397:LEU:HB3	1:A:402:MET:HE2	1.72	0.70
1:B:397:LEU:O	1:B:402:MET:HE2	1.91	0.70
1:C:398:THR:C	1:C:402:MET:HE3	2.15	0.70
1:A:397:LEU:O	1:A:402:MET:HE2	1.90	0.70
2:S:100(E):PHE:HB2	2:S:103:TRP:HE1	1.57	0.69
1:C:397:LEU:O	1:C:402:MET:HE2	1.90	0.69
2:H:100(E):PHE:HB2	2:H:103:TRP:HE1	1.57	0.69
2:M:100(E):PHE:HB2	2:M:103:TRP:HE1	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:100(E):PHE:HB2	2:O:103:TRP:HE1	1.57	0.69
2:O:18:LEU:HD12	2:O:20:LEU:HD22	1.75	0.69
1:A:200:PRO:HG2	1:E:358:LEU:HD23	1.75	0.68
2:Q:18:LEU:HD12	2:Q:20:LEU:HD22	1.75	0.68
2:Q:100(E):PHE:HB2	2:Q:103:TRP:HE1	1.57	0.68
1:C:397:LEU:C	1:C:402:MET:CE	2.67	0.68
1:E:397:LEU:O	1:E:402:MET:HE2	1.90	0.68
1:D:397:LEU:C	1:D:402:MET:CE	2.67	0.67
1:E:397:LEU:C	1:E:402:MET:CE	2.67	0.67
2:H:18:LEU:HD12	2:H:20:LEU:HD22	1.75	0.67
2:S:18:LEU:HD12	2:S:20:LEU:HD22	1.75	0.67
2:O:35(B):SER:OG	2:O:50:LEU:HD23	1.95	0.66
2:H:103:TRP:CZ3	3:L:44:PRO:CG	2.72	0.66
1:A:358:LEU:HD23	1:B:200:PRO:HG2	1.78	0.66
2:H:35(B):SER:OG	2:H:50:LEU:HD23	1.95	0.66
2:M:18:LEU:HD12	2:M:20:LEU:HD22	1.75	0.66
1:A:397:LEU:C	1:A:402:MET:CE	2.67	0.66
2:Q:35(B):SER:OG	2:Q:50:LEU:HD23	1.95	0.66
2:M:35(B):SER:OG	2:M:50:LEU:HD23	1.95	0.66
2:Q:103:TRP:CZ3	3:R:44:PRO:CG	2.76	0.65
1:B:397:LEU:C	1:B:402:MET:CE	2.67	0.65
2:S:103:TRP:CZ3	3:T:44:PRO:CG	2.75	0.65
2:H:103:TRP:HE3	3:L:44:PRO:HD2	1.61	0.65
2:S:35(B):SER:OG	2:S:50:LEU:HD23	1.95	0.65
1:D:38:THR:HA	1:D:41:TYR:CE1	2.32	0.64
1:B:358:LEU:HD23	1:C:200:PRO:HG2	1.77	0.64
1:D:358:LEU:CD2	1:E:202:LEU:HD21	2.28	0.64
1:D:358:LEU:HD21	1:E:202:LEU:CD2	2.27	0.64
1:E:155:VAL:O	1:E:155:VAL:CG1	2.46	0.64
1:B:155:VAL:O	1:B:155:VAL:CG1	2.46	0.64
1:D:155:VAL:O	1:D:155:VAL:CG1	2.46	0.63
1:C:155:VAL:O	1:C:155:VAL:CG1	2.46	0.63
1:B:358:LEU:CD2	1:C:202:LEU:HD21	2.29	0.63
1:B:38:THR:HB	1:B:337:ILE:HD13	1.81	0.63
1:C:38:THR:CB	1:C:337:ILE:HD13	2.29	0.63
2:M:67:LEU:HD11	2:M:80:LEU:HD11	1.81	0.63
1:E:123:ARG:HH21	1:E:349:ASP:HB3	1.64	0.63
2:H:67:LEU:HD11	2:H:80:LEU:HD11	1.81	0.63
1:D:38:THR:HB	1:D:337:ILE:HD13	1.80	0.63
2:S:67:LEU:HD11	2:S:80:LEU:HD11	1.81	0.63
1:B:38:THR:CB	1:B:337:ILE:HD13	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:MET:CE	1:B:228:GLN:HG3	2.28	0.63
1:A:155:VAL:O	1:A:155:VAL:CG1	2.46	0.62
1:C:57:LEU:HD21	1:D:183:TRP:HH2	1.64	0.62
2:O:67:LEU:HD11	2:O:80:LEU:HD11	1.81	0.62
1:A:222:MET:CE	1:A:228:GLN:HG3	2.28	0.62
2:M:103:TRP:CZ3	3:N:44:PRO:CG	2.78	0.62
2:H:6:GLU:HB2	2:H:107:THR:HG23	1.82	0.62
1:A:358:LEU:CD2	1:B:202:LEU:HD21	2.29	0.62
1:C:123:ARG:HH21	1:C:349:ASP:HB3	1.64	0.62
2:Q:103:TRP:HE3	3:R:44:PRO:HD2	1.65	0.62
1:A:123:ARG:HH21	1:A:349:ASP:HB3	1.64	0.62
1:D:123:ARG:HH21	1:D:349:ASP:HB3	1.64	0.62
2:M:15:THR:HG22	2:M:15:THR:O	2.00	0.62
2:M:12:VAL:HG21	2:M:18:LEU:HD23	1.81	0.61
2:Q:67:LEU:HD11	2:Q:80:LEU:HD11	1.81	0.61
2:S:12:VAL:HG21	2:S:18:LEU:HD23	1.81	0.61
2:M:6:GLU:HB2	2:M:107:THR:HG23	1.81	0.61
2:S:6:GLU:HB2	2:S:107:THR:HG23	1.81	0.61
2:H:15:THR:HG22	2:H:15:THR:O	2.00	0.61
2:O:103:TRP:CZ3	3:P:44:PRO:CG	2.76	0.61
2:S:15:THR:HG22	2:S:15:THR:O	2.00	0.61
2:Q:66:ARG:HH21	2:Q:82:MET:HE3	1.66	0.61
1:A:57:LEU:HD21	1:B:183:TRP:HH2	1.65	0.61
2:O:15:THR:O	2:O:15:THR:HG22	2.00	0.61
2:O:66:ARG:HH21	2:O:82:MET:HE3	1.66	0.61
1:B:123:ARG:HH21	1:B:349:ASP:HB3	1.64	0.61
2:Q:12:VAL:HG21	2:Q:18:LEU:HD23	1.82	0.61
2:H:12:VAL:HG21	2:H:18:LEU:HD23	1.81	0.61
2:O:12:VAL:HG21	2:O:18:LEU:HD23	1.81	0.61
2:Q:15:THR:O	2:Q:15:THR:HG22	2.00	0.61
1:C:38:THR:HB	1:C:337:ILE:HD13	1.82	0.60
3:L:35:TRP:CD1	3:L:48:ILE:HD12	2.37	0.60
2:S:66:ARG:HH21	2:S:82:MET:HE3	1.66	0.60
3:R:35:TRP:CD1	3:R:48:ILE:HD12	2.36	0.60
1:A:38:THR:CB	1:A:337:ILE:HD13	2.31	0.60
2:M:66:ARG:HH21	2:M:82:MET:HE3	1.66	0.60
2:Q:6:GLU:HB2	2:Q:107:THR:HG23	1.81	0.60
1:D:260:LEU:HD12	1:D:260:LEU:O	2.02	0.60
2:O:6:GLU:HB2	2:O:107:THR:HG23	1.82	0.60
1:A:358:LEU:HD21	1:B:202:LEU:CD2	2.32	0.60
3:N:35:TRP:CD1	3:N:48:ILE:HD12	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:35:TRP:CD1	3:P:48:ILE:HD12	2.37	0.60
2:H:66:ARG:HH21	2:H:82:MET:HE3	1.66	0.60
1:B:57:LEU:HD21	1:C:183:TRP:HH2	1.67	0.60
1:E:260:LEU:HD12	1:E:260:LEU:O	2.02	0.60
1:C:260:LEU:HD12	1:C:260:LEU:O	2.02	0.60
1:E:38:THR:HB	1:E:337:ILE:HD13	1.83	0.60
2:O:103:TRP:HE3	3:P:44:PRO:HD2	1.66	0.60
3:T:35:TRP:CD1	3:T:48:ILE:HD12	2.37	0.60
1:A:260:LEU:O	1:A:260:LEU:HD12	2.02	0.59
1:A:38:THR:HB	1:A:337:ILE:HD13	1.83	0.59
1:B:71:ASN:ND2	2:H:56:ASP:OD2	2.35	0.59
1:B:260:LEU:HD12	1:B:260:LEU:O	2.02	0.59
1:A:358:LEU:HD21	1:B:202:LEU:HD21	1.85	0.59
1:A:202:LEU:HD21	1:E:358:LEU:CD2	2.33	0.59
1:D:207:THR:CG2	1:D:244:LYS:HD3	2.33	0.59
1:A:192:VAL:HG22	1:A:192:VAL:O	2.04	0.58
1:C:207:THR:CG2	1:C:244:LYS:HD3	2.33	0.58
2:Q:66:ARG:NH2	2:Q:82:MET:HE3	2.19	0.58
1:D:358:LEU:HD21	1:E:202:LEU:HD21	1.85	0.58
2:M:18:LEU:HD11	2:M:20:LEU:HD22	1.85	0.58
2:S:18:LEU:HD11	2:S:20:LEU:HD22	1.85	0.58
1:A:183:TRP:HH2	1:E:57:LEU:HD21	1.68	0.58
1:E:207:THR:CG2	1:E:244:LYS:HD3	2.33	0.58
1:B:192:VAL:HG22	1:B:192:VAL:O	2.04	0.58
1:D:57:LEU:HD21	1:E:183:TRP:HH2	1.69	0.58
1:E:88:ARG:HG3	1:E:344:PHE:CE1	2.39	0.58
1:C:192:VAL:O	1:C:192:VAL:HG22	2.04	0.58
1:D:192:VAL:HG22	1:D:192:VAL:O	2.04	0.58
1:D:358:LEU:HD23	1:E:200:PRO:HG2	1.84	0.58
1:B:358:LEU:HD21	1:C:202:LEU:HD21	1.86	0.58
2:O:18:LEU:HD11	2:O:20:LEU:HD22	1.85	0.58
1:D:358:LEU:CD2	1:E:200:PRO:HG2	2.34	0.57
2:O:66:ARG:NH2	2:O:82:MET:HE3	2.19	0.57
1:A:88:ARG:HG3	1:A:344:PHE:CE1	2.39	0.57
1:D:88:ARG:HG3	1:D:344:PHE:CE1	2.39	0.57
2:S:103:TRP:HE3	3:T:44:PRO:HD2	1.65	0.57
1:E:192:VAL:HG22	1:E:192:VAL:O	2.04	0.57
2:M:66:ARG:NH2	2:M:82:MET:HE3	2.19	0.57
1:A:207:THR:CG2	1:A:244:LYS:HD3	2.33	0.57
2:Q:18:LEU:HD11	2:Q:20:LEU:HD22	1.85	0.57
1:B:358:LEU:HD21	1:C:202:LEU:CD2	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ARG:HG3	1:C:344:PHE:CE1	2.39	0.57
1:E:38:THR:HA	1:E:41:TYR:CE1	2.39	0.57
1:B:88:ARG:HG3	1:B:344:PHE:CE1	2.39	0.57
1:B:207:THR:CG2	1:B:244:LYS:HD3	2.33	0.57
1:A:358:LEU:CD2	1:B:200:PRO:HG2	2.33	0.57
2:H:66:ARG:NH2	2:H:82:MET:HE3	2.19	0.57
1:B:358:LEU:CD2	1:C:200:PRO:HG2	2.35	0.57
1:A:71:ASN:ND2	2:S:56:ASP:OD2	2.38	0.56
1:E:71:ASN:ND2	2:Q:56:ASP:OD2	2.38	0.56
2:S:66:ARG:NH2	2:S:82:MET:HE3	2.19	0.56
1:E:397:LEU:CB	1:E:402:MET:HE2	2.36	0.56
1:A:356:MET:HE1	1:B:183:TRP:CG	2.41	0.56
2:M:103:TRP:HE3	3:N:44:PRO:HD2	1.70	0.56
1:A:397:LEU:CB	1:A:402:MET:HE2	2.36	0.56
1:D:397:LEU:CB	1:D:402:MET:HE2	2.36	0.56
1:A:229:ALA:HB3	1:E:359:CYS:SG	2.46	0.56
1:C:57:LEU:HD11	1:D:204:LEU:HD22	1.88	0.56
1:D:236:LEU:HD21	1:E:285:VAL:HG13	1.88	0.56
1:D:85:ARG:HD2	1:D:461:TRP:CZ3	2.41	0.56
2:Q:18:LEU:CD1	2:Q:20:LEU:CD2	2.82	0.56
1:A:85:ARG:HD2	1:A:461:TRP:CZ3	2.41	0.56
1:A:222:MET:HE3	1:A:227:LEU:HB3	1.88	0.56
1:E:38:THR:CB	1:E:337:ILE:CD1	2.85	0.55
1:E:85:ARG:HD2	1:E:461:TRP:CZ3	2.41	0.55
1:B:57:LEU:HD11	1:C:204:LEU:CD2	2.37	0.55
1:C:85:ARG:HD2	1:C:461:TRP:CZ3	2.41	0.55
1:A:361:ALA:HB2	1:B:229:ALA:HB1	1.88	0.55
1:B:222:MET:HE3	1:B:227:LEU:HB3	1.88	0.55
1:B:397:LEU:CB	1:B:402:MET:HE2	2.36	0.55
1:E:397:LEU:CA	1:E:402:MET:HE2	2.37	0.55
2:H:18:LEU:HD11	2:H:20:LEU:HD22	1.85	0.55
2:S:18:LEU:CD1	2:S:20:LEU:CD2	2.82	0.55
1:D:397:LEU:CA	1:D:402:MET:HE2	2.37	0.55
3:N:49:PHE:CD1	3:N:50:VAL:HG23	2.42	0.55
1:B:85:ARG:HD2	1:B:461:TRP:CZ3	2.41	0.55
1:C:397:LEU:CB	1:C:402:MET:HE2	2.36	0.55
1:E:362:ILE:HD13	3:R:50:VAL:HG21	1.88	0.55
3:P:49:PHE:CD1	3:P:50:VAL:HG23	2.42	0.55
2:S:100(E):PHE:CB	2:S:103:TRP:HE1	2.20	0.55
1:C:397:LEU:CA	1:C:402:MET:HE2	2.37	0.55
2:O:18:LEU:CD1	2:O:20:LEU:CD2	2.82	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:CD2	1:E:57:LEU:HD11	2.37	0.55
2:H:18:LEU:CD1	2:H:20:LEU:CD2	2.82	0.55
3:L:49:PHE:CD1	3:L:50:VAL:HG23	2.42	0.55
2:M:18:LEU:CD1	2:M:20:LEU:CD2	2.82	0.55
2:Q:100(E):PHE:CB	2:Q:103:TRP:HE1	2.20	0.55
1:A:397:LEU:CA	1:A:402:MET:HE2	2.37	0.55
1:C:131:ILE:HD12	1:D:274:LEU:HD23	1.89	0.55
2:H:103:TRP:CE3	3:L:44:PRO:CD	2.86	0.55
1:A:329:ARG:CZ	1:E:484:LEU:HD11	2.37	0.55
1:D:71:ASN:ND2	2:O:56:ASP:OD2	2.39	0.55
1:E:222:MET:HE3	1:E:227:LEU:HB3	1.88	0.55
1:B:57:LEU:HD11	1:C:204:LEU:HD22	1.88	0.55
3:T:49:PHE:CD1	3:T:50:VAL:HG23	2.42	0.55
1:C:358:LEU:CD2	1:D:200:PRO:HG2	2.37	0.54
1:D:57:LEU:HD11	1:E:204:LEU:HD22	1.90	0.54
2:M:18:LEU:HD13	2:M:19:THR:N	2.23	0.54
2:Q:18:LEU:HD13	2:Q:19:THR:N	2.22	0.54
2:Q:67:LEU:CD1	2:Q:82:MET:HG2	2.37	0.54
2:S:18:LEU:HD13	2:S:19:THR:N	2.23	0.54
2:S:67:LEU:CD1	2:S:82:MET:HG2	2.37	0.54
1:B:236:LEU:HD21	1:C:285:VAL:HG13	1.89	0.54
1:C:222:MET:HE3	1:C:227:LEU:HB3	1.88	0.54
2:M:67:LEU:CD1	2:M:82:MET:HG2	2.38	0.54
2:M:100(E):PHE:CB	2:M:103:TRP:HE1	2.19	0.54
3:R:49:PHE:CD1	3:R:50:VAL:HG23	2.42	0.54
1:D:57:LEU:HD11	1:E:204:LEU:CD2	2.37	0.54
1:A:356:MET:HG2	1:A:379:ARG:O	2.08	0.54
1:B:397:LEU:CA	1:B:402:MET:HE2	2.37	0.54
2:O:18:LEU:HD13	2:O:19:THR:N	2.23	0.54
1:A:131:ILE:HD12	1:B:274:LEU:HD23	1.90	0.54
2:O:100(E):PHE:CB	2:O:103:TRP:HE1	2.19	0.54
1:A:204:LEU:HD22	1:E:57:LEU:HD11	1.89	0.54
2:H:67:LEU:CD1	2:H:82:MET:HG2	2.37	0.54
1:A:57:LEU:HD11	1:B:204:LEU:HD22	1.89	0.53
1:D:222:MET:HE3	1:D:227:LEU:HB3	1.88	0.53
2:O:67:LEU:CD1	2:O:82:MET:HG2	2.37	0.53
2:S:15:THR:O	2:S:15:THR:CG2	2.57	0.53
2:H:15:THR:O	2:H:15:THR:CG2	2.57	0.53
2:M:15:THR:O	2:M:15:THR:CG2	2.57	0.53
1:C:57:LEU:HD11	1:D:204:LEU:CD2	2.38	0.53
2:H:18:LEU:HD13	2:H:19:THR:N	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:98:THR:CG2	2:M:100(D):TYR:HE1	2.22	0.53
1:B:484:LEU:HD11	1:C:329:ARG:CZ	2.39	0.53
1:C:71:ASN:ND2	2:M:56:ASP:OD2	2.40	0.53
2:H:100(E):PHE:CB	2:H:103:TRP:HE1	2.20	0.53
2:Q:18:LEU:HD12	2:Q:20:LEU:CD2	2.39	0.53
2:M:100(D):TYR:CZ	3:N:49:PHE:HE2	2.26	0.53
1:C:38:THR:HA	1:C:41:TYR:CE1	2.44	0.53
1:E:38:THR:HG21	1:E:337:ILE:HD13	1.90	0.53
2:M:21:THR:HG22	2:M:77:GLN:OE1	2.09	0.53
2:O:98:THR:CG2	2:O:100(D):TYR:HE1	2.22	0.53
1:A:67:LYS:O	2:S:100(A):TRP:CH2	2.61	0.52
2:H:21:THR:HG22	2:H:77:GLN:OE1	2.09	0.52
2:O:12:VAL:HG21	2:O:18:LEU:CD2	2.39	0.52
2:Q:103:TRP:CE3	3:R:44:PRO:CD	2.90	0.52
1:C:67:LYS:O	2:M:100(A):TRP:CH2	2.62	0.52
2:H:98:THR:CG2	2:H:100(D):TYR:HE1	2.22	0.52
2:O:15:THR:O	2:O:15:THR:CG2	2.57	0.52
2:Q:15:THR:O	2:Q:15:THR:CG2	2.57	0.52
2:S:18:LEU:HD12	2:S:20:LEU:CD2	2.39	0.52
1:C:119:VAL:HG13	1:C:388:PHE:CE1	2.45	0.52
1:A:57:LEU:HD11	1:B:204:LEU:CD2	2.38	0.52
2:Q:21:THR:HG22	2:Q:77:GLN:OE1	2.09	0.52
2:S:21:THR:HG22	2:S:77:GLN:OE1	2.09	0.52
2:Q:12:VAL:HG21	2:Q:18:LEU:CD2	2.39	0.52
1:A:362:ILE:HD13	3:T:50:VAL:HG21	1.91	0.52
2:O:45:LEU:HD22	2:O:103:TRP:HH2	1.75	0.52
1:A:119:VAL:HG13	1:A:388:PHE:CE1	2.45	0.52
2:H:18:LEU:HD12	2:H:20:LEU:CD2	2.39	0.52
1:A:397:LEU:O	1:A:402:MET:HE1	2.10	0.52
1:B:397:LEU:O	1:B:402:MET:HE1	2.10	0.52
2:H:45:LEU:HD22	2:H:103:TRP:HH2	1.75	0.52
2:M:12:VAL:HG21	2:M:18:LEU:CD2	2.39	0.52
2:Q:98:THR:CG2	2:Q:100(D):TYR:HE1	2.22	0.52
2:H:12:VAL:HG21	2:H:18:LEU:CD2	2.39	0.52
1:D:339:TRP:HB3	1:D:412:ILE:HD11	1.92	0.52
2:S:45:LEU:HD22	2:S:103:TRP:HH2	1.75	0.52
1:A:285:VAL:HG13	1:E:236:LEU:HD21	1.92	0.51
1:C:339:TRP:HB3	1:C:412:ILE:HD11	1.92	0.51
2:H:96:ARG:HG3	2:H:101:ASP:HB2	1.93	0.51
2:M:18:LEU:HD12	2:M:20:LEU:CD2	2.39	0.51
2:S:98:THR:CG2	2:S:100(D):TYR:HE1	2.22	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:VAL:HG13	1:B:388:PHE:CE1	2.45	0.51
1:B:339:TRP:HB3	1:B:412:ILE:HD11	1.92	0.51
2:Q:24:ILE:HD13	2:Q:29:LEU:HD21	1.92	0.51
2:S:12:VAL:HG21	2:S:18:LEU:CD2	2.39	0.51
1:A:274:LEU:HD23	1:E:131:ILE:HD12	1.91	0.51
1:D:207:THR:HG23	1:D:244:LYS:HD3	1.93	0.51
2:M:96:ARG:HG3	2:M:101:ASP:HB2	1.93	0.51
2:O:21:THR:HG22	2:O:77:GLN:OE1	2.09	0.51
1:A:202:LEU:HD21	1:E:358:LEU:HD21	1.91	0.51
1:C:397:LEU:O	1:C:402:MET:HE1	2.10	0.51
1:D:38:THR:OG1	1:D:337:ILE:CD1	2.59	0.51
1:D:119:VAL:HG13	1:D:388:PHE:CE1	2.45	0.51
1:E:119:VAL:HG13	1:E:388:PHE:CE1	2.44	0.51
2:S:103:TRP:CE3	3:T:44:PRO:CD	2.91	0.51
2:O:103:TRP:CE3	3:P:44:PRO:CD	2.92	0.51
1:D:67:LYS:O	2:O:100(A):TRP:CH2	2.63	0.51
1:E:38:THR:OG1	1:E:337:ILE:CD1	2.59	0.51
1:E:397:LEU:O	1:E:402:MET:HE1	2.10	0.51
2:O:100(D):TYR:CZ	3:P:49:PHE:HE2	2.29	0.51
1:A:339:TRP:HB3	1:A:412:ILE:HD11	1.92	0.51
1:B:38:THR:HA	1:B:41:TYR:CE1	2.45	0.51
1:C:484:LEU:HD11	1:D:329:ARG:CZ	2.41	0.51
1:D:484:LEU:HD11	1:E:329:ARG:CZ	2.41	0.51
1:E:67:LYS:O	2:Q:100(A):TRP:CH2	2.64	0.51
1:E:339:TRP:HB3	1:E:412:ILE:HD11	1.92	0.51
1:B:362:ILE:HG23	3:L:49:PHE:CE1	2.46	0.51
1:E:96:LYS:N	1:E:96:LYS:CD	2.74	0.51
1:E:207:THR:HG23	1:E:244:LYS:HD3	1.93	0.51
1:D:238:ILE:HD12	1:D:243:CYS:SG	2.51	0.50
2:M:45:LEU:HD22	2:M:103:TRP:HH2	1.75	0.50
2:O:24:ILE:HD13	2:O:29:LEU:HD21	1.92	0.50
2:O:96:ARG:HG3	2:O:101:ASP:HB2	1.93	0.50
2:Q:45:LEU:HD22	2:Q:103:TRP:HH2	1.75	0.50
2:S:96:ARG:HG3	2:S:101:ASP:HB2	1.93	0.50
1:C:236:LEU:HD21	1:D:285:VAL:HG13	1.93	0.50
2:H:24:ILE:HD13	2:H:29:LEU:HD21	1.92	0.50
1:C:207:THR:HG23	1:C:244:LYS:HD3	1.93	0.50
1:E:238:ILE:HD12	1:E:243:CYS:SG	2.51	0.50
2:M:24:ILE:HD13	2:M:29:LEU:HD21	1.92	0.50
2:O:18:LEU:HD12	2:O:20:LEU:CD2	2.39	0.50
2:S:24:ILE:HD13	2:S:29:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HD21	1:B:285:VAL:HG13	1.92	0.50
1:D:96:LYS:CD	1:D:96:LYS:N	2.75	0.50
1:A:96:LYS:CD	1:A:96:LYS:N	2.74	0.50
1:A:261:PHE:HB2	1:A:330:ALA:HB1	1.94	0.50
1:B:96:LYS:N	1:B:96:LYS:CD	2.74	0.50
1:B:207:THR:HG23	1:B:244:LYS:HD3	1.93	0.50
1:D:229:ALA:O	1:D:230:ASN:C	2.54	0.50
1:B:356:MET:HE1	1:C:183:TRP:CG	2.47	0.50
1:D:289:LEU:O	1:D:290:TYR:HB3	2.12	0.50
1:A:238:ILE:HD12	1:A:243:CYS:SG	2.51	0.50
1:B:289:LEU:O	1:B:290:TYR:HB3	2.12	0.50
1:C:96:LYS:N	1:C:96:LYS:CD	2.74	0.50
1:C:229:ALA:O	1:C:230:ASN:C	2.55	0.50
1:C:238:ILE:HD12	1:C:243:CYS:SG	2.51	0.50
1:E:261:PHE:HB2	1:E:330:ALA:HB1	1.94	0.50
1:E:457:LYS:CD	1:E:457:LYS:N	2.75	0.50
1:C:358:LEU:CD2	1:D:202:LEU:HD21	2.42	0.49
1:D:131:ILE:HD12	1:E:274:LEU:HD23	1.94	0.49
3:P:50:VAL:HG12	3:P:51:TYR:N	2.27	0.49
1:D:457:LYS:N	1:D:457:LYS:CD	2.75	0.49
1:E:38:THR:CG2	1:E:337:ILE:HD13	2.42	0.49
1:E:289:LEU:O	1:E:290:TYR:HB3	2.12	0.49
1:B:131:ILE:HD12	1:C:274:LEU:HD23	1.93	0.49
1:C:289:LEU:O	1:C:290:TYR:HB3	2.12	0.49
3:L:50:VAL:HG12	3:L:51:TYR:N	2.28	0.49
1:A:289:LEU:O	1:A:290:TYR:HB3	2.12	0.49
1:D:38:THR:CB	1:D:337:ILE:CD1	2.89	0.49
3:T:50:VAL:HG12	3:T:51:TYR:N	2.27	0.49
1:A:457:LYS:N	1:A:457:LYS:CD	2.75	0.49
1:B:238:ILE:HD12	1:B:243:CYS:SG	2.51	0.49
2:Q:96:ARG:HG3	2:Q:101:ASP:HB2	1.93	0.49
1:A:207:THR:HG23	1:A:244:LYS:HD3	1.93	0.49
1:C:457:LYS:CD	1:C:457:LYS:N	2.75	0.49
1:D:397:LEU:O	1:D:402:MET:HE1	2.10	0.49
3:T:82:ASP:O	3:T:104:LEU:HD23	2.13	0.49
1:C:50:HIS:CG	1:C:476:PHE:CD2	3.01	0.49
1:C:261:PHE:HB2	1:C:330:ALA:HB1	1.94	0.49
1:D:356:MET:HE3	1:E:202:LEU:HD11	1.94	0.49
2:H:103:TRP:CE3	3:L:44:PRO:HG2	2.44	0.49
3:N:50:VAL:HG12	3:N:51:TYR:N	2.28	0.49
2:S:100(D):TYR:CZ	3:T:49:PHE:HE2	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:HG2	1:E:358:LEU:CD2	2.41	0.48
1:A:484:LEU:HD11	1:B:329:ARG:CZ	2.43	0.48
2:Q:73:ILE:HD12	2:Q:74:SER:N	2.29	0.48
1:A:50:HIS:CG	1:A:476:PHE:CD2	3.01	0.48
1:D:50:HIS:CG	1:D:476:PHE:CD2	3.01	0.48
1:E:229:ALA:O	1:E:230:ASN:C	2.55	0.48
3:R:82:ASP:O	3:R:104:LEU:HD23	2.13	0.48
2:S:73:ILE:HD12	2:S:74:SER:N	2.28	0.48
1:C:362:ILE:HD13	3:N:50:VAL:HG21	1.94	0.48
3:P:82:ASP:O	3:P:104:LEU:HD23	2.13	0.48
1:B:50:HIS:CG	1:B:476:PHE:CD2	3.01	0.48
1:B:261:PHE:HB2	1:B:330:ALA:HB1	1.94	0.48
1:E:50:HIS:CG	1:E:476:PHE:CD2	3.01	0.48
1:A:38:THR:HA	1:A:41:TYR:CE1	2.47	0.48
1:B:457:LYS:N	1:B:457:LYS:CD	2.76	0.48
1:C:66:ILE:CG1	1:D:283:GLU:HG2	2.44	0.48
2:H:73:ILE:HD12	2:H:74:SER:N	2.29	0.48
3:R:50:VAL:HG12	3:R:51:TYR:N	2.27	0.48
1:D:261:PHE:HB2	1:D:330:ALA:HB1	1.94	0.48
3:L:82:ASP:O	3:L:104:LEU:HD23	2.13	0.48
3:N:82:ASP:O	3:N:104:LEU:HD23	2.13	0.48
3:R:48:ILE:HG23	3:R:53:ASN:O	2.14	0.48
2:O:73:ILE:HD12	2:O:74:SER:N	2.29	0.48
3:T:39:VAL:HG23	3:T:42:ALA:HB3	1.96	0.48
3:L:48:ILE:HG23	3:L:53:ASN:O	2.14	0.48
3:T:48:ILE:HG23	3:T:53:ASN:O	2.14	0.48
1:A:229:ALA:HB1	1:E:361:ALA:HB2	1.95	0.47
1:A:267:GLU:CG	1:E:127:LEU:HD12	2.44	0.47
2:M:73:ILE:HD12	2:M:74:SER:N	2.29	0.47
1:C:271:VAL:HG22	1:C:307:PRO:HB2	1.96	0.47
1:D:356:MET:HE1	1:E:183:TRP:CG	2.50	0.47
1:E:271:VAL:HG22	1:E:307:PRO:HB2	1.96	0.47
3:L:39:VAL:HG23	3:L:42:ALA:HB3	1.96	0.47
3:P:48:ILE:HG23	3:P:53:ASN:O	2.14	0.47
1:A:229:ALA:O	1:A:230:ASN:C	2.58	0.47
1:C:57:LEU:HD21	1:D:183:TRP:CH2	2.45	0.47
1:B:271:VAL:HG22	1:B:307:PRO:HB2	1.96	0.47
1:D:271:VAL:HG22	1:D:307:PRO:HB2	1.96	0.47
3:N:48:ILE:HG23	3:N:53:ASN:O	2.14	0.47
3:R:39:VAL:HG23	3:R:42:ALA:HB3	1.96	0.47
3:T:35:TRP:CG	3:T:48:ILE:HD12	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD21	1:B:183:TRP:CH2	2.47	0.47
1:C:54:SER:O	1:C:55:ARG:HG3	2.15	0.47
2:H:103:TRP:CE3	3:L:44:PRO:CG	2.97	0.47
2:Q:103:TRP:CE3	3:R:44:PRO:HG2	2.44	0.47
3:R:35:TRP:CG	3:R:48:ILE:HD12	2.50	0.47
2:S:18:LEU:HB2	2:S:82(C):MET:SD	2.55	0.47
1:A:54:SER:O	1:A:55:ARG:HG3	2.15	0.47
1:A:140:LEU:CG	1:A:141:ASP:OD1	2.62	0.47
3:L:35:TRP:CG	3:L:48:ILE:HD12	2.50	0.47
2:M:18:LEU:HB2	2:M:82(C):MET:SD	2.54	0.47
3:N:39:VAL:HG23	3:N:42:ALA:HB3	1.96	0.47
2:O:18:LEU:HB2	2:O:82(C):MET:SD	2.54	0.47
2:Q:18:LEU:HB2	2:Q:82(C):MET:SD	2.55	0.47
1:B:127:LEU:HD12	1:C:267:GLU:CG	2.45	0.47
1:D:54:SER:O	1:D:55:ARG:HG3	2.15	0.47
2:H:18:LEU:HB2	2:H:82(C):MET:SD	2.55	0.47
3:P:39:VAL:HG23	3:P:42:ALA:HB3	1.96	0.47
1:A:66:ILE:CG1	1:B:283:GLU:HG2	2.45	0.46
3:P:35:TRP:CG	3:P:48:ILE:HD12	2.50	0.46
1:D:358:LEU:HB3	1:D:377:TYR:HB2	1.97	0.46
3:N:35:TRP:CG	3:N:48:ILE:HD12	2.50	0.46
2:S:96:ARG:HB2	2:S:100(D):TYR:CE1	2.50	0.46
1:A:202:LEU:CD2	1:E:358:LEU:HD21	2.45	0.46
1:B:54:SER:O	1:B:55:ARG:HG3	2.15	0.46
1:B:67:LYS:O	2:H:100(A):TRP:CH2	2.68	0.46
3:R:50:VAL:CG1	3:R:51:TYR:N	2.79	0.46
1:A:271:VAL:HG22	1:A:307:PRO:HB2	1.96	0.46
1:C:222:MET:HE2	1:C:224:PHE:CD1	2.51	0.46
2:O:11:LEU:C	2:O:11:LEU:HD13	2.41	0.46
1:B:358:LEU:HD22	1:C:202:LEU:HD21	1.96	0.46
1:D:66:ILE:CG1	1:E:283:GLU:HG2	2.46	0.46
2:H:96:ARG:HB2	2:H:100(D):TYR:CE1	2.50	0.46
2:Q:96:ARG:HD3	2:Q:100(D):TYR:OH	2.16	0.46
1:E:54:SER:O	1:E:55:ARG:HG3	2.15	0.46
2:H:18:LEU:HD11	2:H:20:LEU:CD2	2.45	0.46
2:H:98:THR:CG2	2:H:100(D):TYR:CE1	2.99	0.46
2:S:96:ARG:HD3	2:S:100(D):TYR:OH	2.16	0.46
1:B:222:MET:HE2	1:B:224:PHE:CD1	2.51	0.46
1:C:192:VAL:HG23	2:H:34:VAL:CG2	2.45	0.46
1:C:457:LYS:H	1:C:457:LYS:HD3	1.81	0.46
1:D:222:MET:HE2	1:D:224:PHE:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:LYS:H	1:E:457:LYS:HD3	1.81	0.46
2:H:11:LEU:C	2:H:11:LEU:HD13	2.41	0.46
2:Q:96:ARG:HB2	2:Q:100(D):TYR:CE1	2.50	0.46
2:Q:103:TRP:CE3	3:R:44:PRO:CG	2.99	0.46
1:C:127:LEU:HD12	1:D:267:GLU:CG	2.46	0.46
1:D:256:TYR:CZ	1:D:408:MET:HG3	2.51	0.46
1:E:256:TYR:CZ	1:E:408:MET:HG3	2.51	0.46
2:H:103:TRP:CH2	3:L:44:PRO:HG2	2.44	0.46
2:M:18:LEU:HD11	2:M:20:LEU:CD2	2.45	0.46
2:O:96:ARG:HB2	2:O:100(D):TYR:CE1	2.50	0.46
2:S:11:LEU:HD13	2:S:11:LEU:C	2.41	0.46
2:S:103:TRP:CE3	3:T:44:PRO:CG	2.99	0.46
1:A:256:TYR:CZ	1:A:408:MET:HG3	2.51	0.46
1:A:457:LYS:H	1:A:457:LYS:HD3	1.81	0.46
1:B:457:LYS:HD3	1:B:457:LYS:H	1.81	0.46
2:O:27:LEU:HD21	2:O:34:VAL:CG2	2.46	0.46
2:M:11:LEU:C	2:M:11:LEU:HD13	2.41	0.45
2:M:96:ARG:HB2	2:M:100(D):TYR:CE1	2.50	0.45
2:O:98:THR:CG2	2:O:100(D):TYR:CE1	2.99	0.45
2:Q:98:THR:CG2	2:Q:100(D):TYR:CE1	2.99	0.45
2:M:66:ARG:HH21	2:M:82:MET:CE	2.29	0.45
2:M:98:THR:CG2	2:M:100(D):TYR:CE1	2.99	0.45
3:P:50:VAL:CG1	3:P:51:TYR:N	2.79	0.45
2:S:66:ARG:NH2	2:S:82:MET:CE	2.79	0.45
1:A:127:LEU:HD12	1:B:267:GLU:CG	2.47	0.45
1:C:256:TYR:CZ	1:C:408:MET:HG3	2.51	0.45
2:M:27:LEU:HD21	2:M:34:VAL:CG2	2.46	0.45
2:O:66:ARG:NH2	2:O:82:MET:CE	2.79	0.45
2:Q:11:LEU:C	2:Q:11:LEU:HD13	2.41	0.45
2:Q:66:ARG:NH2	2:Q:82:MET:CE	2.79	0.45
1:B:140:LEU:CG	1:B:141:ASP:OD1	2.62	0.45
2:M:66:ARG:NH2	2:M:82:MET:CE	2.79	0.45
2:O:66:ARG:HH21	2:O:82:MET:CE	2.29	0.45
2:Q:66:ARG:HH21	2:Q:82:MET:CE	2.29	0.45
2:S:98:THR:CG2	2:S:100(D):TYR:CE1	2.99	0.45
3:T:50:VAL:CG1	3:T:51:TYR:N	2.79	0.45
1:B:57:LEU:HD21	1:C:183:TRP:CH2	2.47	0.45
1:C:229:ALA:C	1:C:231:LYS:N	2.74	0.45
2:H:27:LEU:HD21	2:H:34:VAL:CG2	2.46	0.45
2:M:99:SER:O	2:M:100(A):TRP:CZ3	2.70	0.45
2:O:99:SER:O	2:O:100(A):TRP:CZ3	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:18:LEU:HD11	2:S:20:LEU:CD2	2.45	0.45
2:S:66:ARG:HH21	2:S:82:MET:CE	2.29	0.45
3:T:49:PHE:CE1	3:T:50:VAL:HG23	2.51	0.45
1:A:196:PRO:HB2	1:E:362:ILE:O	2.16	0.45
1:E:38:THR:HB	1:E:337:ILE:CD1	2.46	0.45
1:E:222:MET:HE2	1:E:224:PHE:CD1	2.51	0.45
2:H:66:ARG:HH21	2:H:82:MET:CE	2.29	0.45
3:L:50:VAL:CG1	3:L:51:TYR:N	2.79	0.45
3:N:50:VAL:CG1	3:N:51:TYR:N	2.79	0.45
3:P:49:PHE:CE1	3:P:50:VAL:HG23	2.51	0.45
3:R:49:PHE:CE1	3:R:50:VAL:HG23	2.51	0.45
1:A:222:MET:HE2	1:A:224:PHE:CD1	2.51	0.45
1:B:256:TYR:CZ	1:B:408:MET:HG3	2.51	0.45
1:D:457:LYS:H	1:D:457:LYS:HD3	1.81	0.45
2:H:66:ARG:NH2	2:H:82:MET:CE	2.79	0.45
2:O:18:LEU:HD11	2:O:20:LEU:CD2	2.45	0.45
1:A:183:TRP:CH2	1:E:57:LEU:HD21	2.49	0.45
1:D:119:VAL:HG22	1:D:388:PHE:HD1	1.82	0.45
1:D:362:ILE:HG23	3:P:49:PHE:CE1	2.51	0.45
1:B:141:ASP:OD1	1:B:141:ASP:N	2.50	0.45
1:E:119:VAL:HG22	1:E:388:PHE:HD1	1.82	0.45
1:E:192:VAL:HG23	2:O:34:VAL:CG2	2.47	0.45
2:O:96:ARG:HD3	2:O:100(D):TYR:OH	2.16	0.45
2:Q:27:LEU:HD21	2:Q:34:VAL:CG2	2.46	0.45
2:S:27:LEU:HD21	2:S:34:VAL:CG2	2.46	0.45
1:C:330:ALA:O	1:C:331:GLN:C	2.60	0.45
1:E:140:LEU:CG	1:E:141:ASP:OD1	2.62	0.45
2:H:96:ARG:HD3	2:H:100(D):TYR:OH	2.16	0.45
2:M:96:ARG:HD3	2:M:100(D):TYR:OH	2.16	0.45
1:B:192:VAL:HG23	2:S:34:VAL:CG2	2.47	0.44
1:E:141:ASP:OD1	1:E:141:ASP:N	2.50	0.44
2:H:100(D):TYR:CZ	3:L:49:PHE:HE2	2.34	0.44
1:C:207:THR:HG21	1:C:244:LYS:HD3	1.98	0.44
1:E:330:ALA:O	1:E:331:GLN:C	2.59	0.44
2:Q:18:LEU:HD11	2:Q:20:LEU:CD2	2.45	0.44
1:E:207:THR:HG21	1:E:244:LYS:HD3	1.98	0.44
2:Q:99:SER:O	2:Q:100(A):TRP:CZ3	2.70	0.44
3:N:49:PHE:CE1	3:N:50:VAL:HG23	2.51	0.44
1:C:119:VAL:HG22	1:C:388:PHE:HD1	1.82	0.44
2:H:99:SER:O	2:H:100(A):TRP:CZ3	2.70	0.44
1:A:127:LEU:HD22	1:A:319:GLN:NE2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD21	1:E:358:LEU:HD22	1.98	0.44
1:B:66:ILE:CG1	1:C:283:GLU:HG2	2.46	0.44
1:D:57:LEU:HD21	1:E:183:TRP:CH2	2.49	0.44
1:D:207:THR:HG21	1:D:244:LYS:HD3	1.98	0.44
1:A:67:LYS:O	2:S:100(A):TRP:HH2	2.00	0.44
1:D:141:ASP:OD1	1:D:141:ASP:N	2.50	0.44
1:D:192:VAL:HG23	2:M:34:VAL:CG2	2.48	0.44
1:E:127:LEU:HD22	1:E:319:GLN:NE2	2.33	0.44
2:Q:100(D):TYR:CZ	3:R:49:PHE:HE2	2.35	0.44
3:T:82:ASP:HB3	3:T:104:LEU:HD21	1.99	0.44
1:A:183:TRP:CG	1:E:356:MET:HE1	2.53	0.44
1:E:66:ILE:HG22	1:E:75:LEU:HB2	2.00	0.44
1:E:234:VAL:HG13	1:E:239:CYS:HA	2.00	0.44
2:S:103:TRP:CE3	3:T:44:PRO:HG2	2.44	0.44
1:A:164:ASP:OD1	1:A:310:SER:HA	2.18	0.44
1:B:57:LEU:CD1	1:C:204:LEU:HD23	2.47	0.44
1:C:140:LEU:CG	1:C:141:ASP:OD1	2.62	0.44
1:C:141:ASP:OD1	1:C:141:ASP:N	2.50	0.44
3:L:49:PHE:CE1	3:L:50:VAL:HG23	2.51	0.44
1:A:207:THR:HG21	1:A:244:LYS:HD3	1.98	0.43
1:B:119:VAL:HG22	1:B:388:PHE:HD1	1.82	0.43
1:C:127:LEU:HD22	1:C:319:GLN:NE2	2.33	0.43
1:D:57:LEU:CD1	1:E:204:LEU:HD23	2.48	0.43
3:P:82:ASP:HB3	3:P:104:LEU:HD21	1.99	0.43
1:A:119:VAL:HG22	1:A:388:PHE:HD1	1.82	0.43
1:B:127:LEU:CD2	1:B:319:GLN:NE2	2.82	0.43
1:B:207:THR:HG21	1:B:244:LYS:HD3	1.98	0.43
1:B:260:LEU:HD12	1:B:260:LEU:C	2.43	0.43
3:R:82:ASP:HB3	3:R:104:LEU:HD21	1.99	0.43
2:S:99:SER:O	2:S:100(A):TRP:CZ3	2.70	0.43
1:B:36:VAL:HG13	1:B:404:TYR:CE1	2.52	0.43
1:B:70:ASN:HD21	3:L:95(A):ARG:HB3	1.83	0.43
1:D:260:LEU:HD12	1:D:260:LEU:C	2.43	0.43
1:E:164:ASP:OD1	1:E:310:SER:HA	2.18	0.43
2:H:100(A):TRP:HA	2:H:100(A):TRP:HE3	1.83	0.43
2:O:6:GLU:OE1	2:O:92:CYS:SG	2.77	0.43
2:O:103:TRP:CE3	3:P:44:PRO:CG	3.01	0.43
1:C:66:ILE:HG22	1:C:75:LEU:HB2	2.00	0.43
1:C:234:VAL:HG13	1:C:239:CYS:HA	2.00	0.43
1:C:260:LEU:HD12	1:C:260:LEU:C	2.43	0.43
1:D:127:LEU:HD12	1:E:267:GLU:CG	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:82:ASP:HB3	3:L:104:LEU:HD21	1.99	0.43
2:M:100(A):TRP:HA	2:M:100(A):TRP:HE3	1.83	0.43
2:O:12:VAL:CG1	2:O:13:LYS:N	2.81	0.43
1:A:234:VAL:HG13	1:A:239:CYS:HA	2.00	0.43
1:C:196:PRO:HG2	3:L:49:PHE:CZ	2.54	0.43
1:D:127:LEU:HD22	1:D:319:GLN:NE2	2.33	0.43
1:D:164:ASP:OD1	1:D:310:SER:HA	2.18	0.43
3:N:82:ASP:HB3	3:N:104:LEU:HD21	2.00	0.43
2:Q:6:GLU:HB2	2:Q:107:THR:CG2	2.48	0.43
2:Q:6:GLU:OE1	2:Q:92:CYS:SG	2.77	0.43
1:B:66:ILE:HG22	1:B:75:LEU:HB2	2.00	0.43
1:B:164:ASP:OD1	1:B:310:SER:HA	2.18	0.43
1:B:330:ALA:O	1:B:331:GLN:C	2.59	0.43
1:D:140:LEU:CG	1:D:141:ASP:OD1	2.62	0.43
2:S:6:GLU:OE1	2:S:92:CYS:SG	2.77	0.43
2:S:12:VAL:CG1	2:S:13:LYS:N	2.81	0.43
1:A:141:ASP:OD1	1:A:141:ASP:N	2.50	0.43
1:A:283:GLU:HG2	1:E:66:ILE:CG1	2.49	0.43
1:B:38:THR:OG1	1:B:337:ILE:CD1	2.67	0.43
1:E:42:VAL:HG12	1:E:395:ILE:HD12	2.01	0.43
1:E:222:MET:HE2	1:E:224:PHE:HD1	1.84	0.43
2:M:103:TRP:CE3	3:N:44:PRO:CD	2.94	0.43
1:A:42:VAL:HG12	1:A:395:ILE:HD12	2.01	0.43
1:A:204:LEU:HD23	1:E:57:LEU:CD1	2.48	0.43
1:A:222:MET:HE2	1:A:224:PHE:HD1	1.84	0.43
1:A:312:SER:O	1:A:313:MET:C	2.62	0.43
1:A:405:ILE:HG22	1:A:413:LEU:HG	2.01	0.43
1:B:127:LEU:HD22	1:B:319:GLN:NE2	2.33	0.43
1:C:50:HIS:ND1	1:C:476:PHE:CD2	2.87	0.43
1:C:67:LYS:O	2:M:100(A):TRP:HH2	2.02	0.43
1:C:164:ASP:OD1	1:C:310:SER:HA	2.18	0.43
1:D:127:LEU:CD2	1:D:319:GLN:NE2	2.82	0.43
1:D:222:MET:HE2	1:D:224:PHE:HD1	1.84	0.43
1:B:50:HIS:ND1	1:B:476:PHE:CD2	2.87	0.43
1:C:357:SER:O	1:C:358:LEU:HB2	2.18	0.43
1:D:38:THR:O	1:D:42:VAL:HG13	2.18	0.43
1:E:50:HIS:ND1	1:E:476:PHE:CD2	2.87	0.43
1:E:260:LEU:HD12	1:E:260:LEU:C	2.43	0.43
2:M:6:GLU:OE1	2:M:92:CYS:SG	2.77	0.43
2:M:12:VAL:CG1	2:M:13:LYS:N	2.81	0.43
2:Q:27:LEU:HD21	2:Q:34:VAL:HG21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:100(A):TRP:HE3	2:S:100(A):TRP:HA	1.83	0.43
1:A:66:ILE:HG22	1:A:75:LEU:HB2	2.00	0.43
1:B:222:MET:HE2	1:B:224:PHE:HD1	1.84	0.43
1:C:222:MET:HE2	1:C:224:PHE:HD1	1.84	0.43
1:D:50:HIS:ND1	1:D:476:PHE:CD2	2.87	0.43
1:D:234:VAL:HG13	1:D:239:CYS:HA	2.00	0.43
1:E:405:ILE:HG22	1:E:413:LEU:HG	2.01	0.43
2:M:103:TRP:CH2	3:N:44:PRO:HG2	2.51	0.43
2:Q:12:VAL:CG1	2:Q:13:LYS:N	2.81	0.43
1:A:38:THR:OG1	1:A:337:ILE:CD1	2.67	0.42
1:A:50:HIS:ND1	1:A:476:PHE:CD2	2.87	0.42
1:B:234:VAL:HG13	1:B:239:CYS:HA	2.00	0.42
1:C:57:LEU:CD1	1:D:204:LEU:HD23	2.50	0.42
1:C:66:ILE:HG12	1:D:283:GLU:HG2	1.99	0.42
1:D:66:ILE:HG22	1:D:75:LEU:HB2	2.00	0.42
1:E:229:ALA:C	1:E:231:LYS:N	2.76	0.42
1:E:234:VAL:HG23	1:E:235:PRO:HD2	2.01	0.42
2:H:6:GLU:OE1	2:H:92:CYS:SG	2.77	0.42
2:O:27:LEU:HD21	2:O:34:VAL:HG21	2.01	0.42
1:E:196:PRO:HG2	3:P:49:PHE:CZ	2.54	0.42
2:M:6:GLU:HB2	2:M:107:THR:CG2	2.48	0.42
2:Q:100(A):TRP:HE3	2:Q:100(A):TRP:HA	1.83	0.42
2:S:27:LEU:HD21	2:S:34:VAL:HG21	2.01	0.42
1:A:66:ILE:HG12	1:B:283:GLU:HG2	2.01	0.42
1:A:166:LYS:HB2	1:A:269:MET:HG2	2.01	0.42
1:C:127:LEU:CD2	1:C:319:GLN:NE2	2.82	0.42
1:A:127:LEU:CD2	1:A:319:GLN:NE2	2.82	0.42
1:A:329:ARG:NH1	1:E:484:LEU:HD11	2.34	0.42
1:B:312:SER:O	1:B:313:MET:C	2.62	0.42
1:B:405:ILE:HG22	1:B:413:LEU:HG	2.01	0.42
1:C:39:ASP:HA	1:C:42:VAL:HG22	2.02	0.42
1:C:312:SER:O	1:C:313:MET:C	2.62	0.42
1:A:85:ARG:HD2	1:A:461:TRP:HZ3	1.85	0.42
1:B:42:VAL:HG12	1:B:395:ILE:HD12	2.01	0.42
1:B:272:ARG:HB2	1:B:310:SER:HB2	2.02	0.42
1:C:38:THR:OG1	1:C:337:ILE:CD1	2.67	0.42
1:C:123:ARG:HD3	1:C:384:TYR:CD1	2.54	0.42
1:E:67:LYS:O	2:Q:100(A):TRP:HH2	2.02	0.42
1:E:127:LEU:CD2	1:E:319:GLN:NE2	2.82	0.42
1:E:166:LYS:HB2	1:E:269:MET:HG2	2.01	0.42
1:E:272:ARG:HB2	1:E:310:SER:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:39:VAL:CG2	3:L:42:ALA:HB3	2.50	0.42
3:P:50:VAL:O	3:P:51:TYR:C	2.63	0.42
1:A:358:LEU:HB3	1:A:377:TYR:HB2	2.02	0.42
1:D:123:ARG:HD3	1:D:384:TYR:CD1	2.54	0.42
1:E:85:ARG:HD2	1:E:461:TRP:HZ3	1.85	0.42
2:H:12:VAL:CG1	2:H:13:LYS:N	2.81	0.42
2:O:100(A):TRP:HE3	2:O:100(A):TRP:HA	1.84	0.42
3:R:39:VAL:CG2	3:R:42:ALA:HB3	2.50	0.42
1:A:260:LEU:HD12	1:A:260:LEU:C	2.43	0.42
1:A:272:ARG:HB2	1:A:310:SER:HB2	2.02	0.42
1:B:84:TYR:CE2	1:B:215:VAL:HA	2.55	0.42
1:C:234:VAL:HG23	1:C:235:PRO:HD2	2.01	0.42
1:E:312:SER:O	1:E:313:MET:C	2.62	0.42
3:N:50:VAL:O	3:N:51:TYR:C	2.63	0.42
1:D:272:ARG:HB2	1:D:310:SER:HB2	2.02	0.42
2:S:28:SER:O	2:S:31:THR:OG1	2.38	0.42
3:T:39:VAL:CG2	3:T:42:ALA:HB3	2.50	0.42
1:A:57:LEU:CD1	1:B:204:LEU:HD23	2.50	0.42
1:C:272:ARG:HB2	1:C:310:SER:HB2	2.02	0.42
1:D:234:VAL:HG23	1:D:235:PRO:HD2	2.01	0.42
1:D:256:TYR:CE2	1:D:408:MET:HA	2.55	0.42
1:D:312:SER:O	1:D:313:MET:C	2.62	0.42
1:E:84:TYR:CE2	1:E:215:VAL:HA	2.55	0.42
1:A:84:TYR:CE2	1:A:215:VAL:HA	2.55	0.42
1:C:84:TYR:CE2	1:C:215:VAL:HA	2.55	0.42
1:C:405:ILE:HG22	1:C:413:LEU:HG	2.01	0.42
1:D:84:TYR:CE2	1:D:215:VAL:HA	2.55	0.42
1:D:85:ARG:HD2	1:D:461:TRP:HZ3	1.85	0.42
1:D:405:ILE:HG22	1:D:413:LEU:HG	2.01	0.42
1:E:70:ASN:HD21	3:R:95(A):ARG:HB3	1.85	0.42
1:E:123:ARG:HD3	1:E:384:TYR:CD1	2.54	0.42
2:H:27:LEU:HD21	2:H:34:VAL:HG21	2.01	0.42
3:N:39:VAL:CG2	3:N:42:ALA:HB3	2.50	0.42
3:N:87:TYR:CD1	3:N:101:GLY:HA2	2.55	0.42
3:P:81:GLU:C	3:P:81:GLU:OE1	2.63	0.42
2:Q:28:SER:O	2:Q:31:THR:OG1	2.38	0.42
3:T:81:GLU:OE1	3:T:81:GLU:C	2.63	0.42
1:C:36:VAL:HG13	1:C:404:TYR:CE1	2.55	0.41
1:C:256:TYR:CE2	1:C:408:MET:HA	2.55	0.41
2:H:6:GLU:HB2	2:H:107:THR:CG2	2.49	0.41
3:L:87:TYR:CD1	3:L:101:GLY:HA2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:100(A):TRP:HA	2:M:100(A):TRP:CE3	2.55	0.41
2:M:100(D):TYR:CZ	3:N:49:PHE:CE2	3.07	0.41
3:P:39:VAL:CG2	3:P:42:ALA:HB3	2.50	0.41
2:Q:93:ALA:HB1	2:Q:103:TRP:CD1	2.55	0.41
2:S:67:LEU:HD12	2:S:67:LEU:HA	1.93	0.41
1:B:38:THR:CB	1:B:337:ILE:CD1	2.96	0.41
1:B:85:ARG:HD2	1:B:461:TRP:HZ3	1.85	0.41
1:B:123:ARG:HD3	1:B:384:TYR:CD1	2.54	0.41
1:C:42:VAL:HG12	1:C:395:ILE:HD12	2.01	0.41
1:C:483:LEU:HD13	1:C:483:LEU:C	2.45	0.41
1:D:42:VAL:HG12	1:D:395:ILE:HD12	2.01	0.41
2:H:28:SER:O	2:H:31:THR:OG1	2.38	0.41
3:N:81:GLU:C	3:N:81:GLU:OE1	2.63	0.41
1:B:483:LEU:C	1:B:483:LEU:HD13	2.45	0.41
1:D:166:LYS:HB2	1:D:269:MET:HG2	2.01	0.41
1:D:358:LEU:HD22	1:D:379:ARG:HG3	2.02	0.41
2:H:100(A):TRP:HA	2:H:100(A):TRP:CE3	2.55	0.41
2:M:27:LEU:HD21	2:M:34:VAL:HG21	2.01	0.41
3:P:87:TYR:CD1	3:P:101:GLY:HA2	2.55	0.41
2:S:100(A):TRP:HA	2:S:100(A):TRP:CE3	2.55	0.41
1:B:234:VAL:HG23	1:B:235:PRO:HD2	2.01	0.41
1:B:256:TYR:CE2	1:B:408:MET:HA	2.55	0.41
1:C:85:ARG:HD2	1:C:461:TRP:HZ3	1.85	0.41
1:D:67:LYS:O	2:O:100(A):TRP:HH2	2.02	0.41
2:O:6:GLU:HB2	2:O:107:THR:CG2	2.48	0.41
2:O:100(A):TRP:HA	2:O:100(A):TRP:CE3	2.55	0.41
2:Q:100(A):TRP:HA	2:Q:100(A):TRP:CE3	2.55	0.41
2:Q:103:TRP:CH2	3:R:44:PRO:HG2	2.49	0.41
3:R:49:PHE:CD1	3:R:49:PHE:C	2.99	0.41
1:A:358:LEU:HD22	1:B:202:LEU:HD21	2.01	0.41
1:B:166:LYS:HB2	1:B:269:MET:HG2	2.01	0.41
1:E:483:LEU:HD13	1:E:483:LEU:C	2.45	0.41
3:L:50:VAL:O	3:L:51:TYR:C	2.63	0.41
2:O:93:ALA:HB1	2:O:103:TRP:CD1	2.55	0.41
3:R:87:TYR:CD1	3:R:101:GLY:HA2	2.55	0.41
3:T:87:TYR:CD1	3:T:101:GLY:HA2	2.55	0.41
1:C:286:PRO:HD2	1:C:289:LEU:HD12	2.03	0.41
2:H:93:ALA:HB1	2:H:103:TRP:CD1	2.55	0.41
3:P:49:PHE:CD1	3:P:49:PHE:C	2.99	0.41
3:R:81:GLU:OE1	3:R:81:GLU:C	2.63	0.41
1:A:123:ARG:HD3	1:A:384:TYR:CD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:HE	1:C:85:ARG:HB2	1.73	0.41
1:C:166:LYS:HB2	1:C:269:MET:HG2	2.01	0.41
2:M:93:ALA:HB1	2:M:103:TRP:CD1	2.55	0.41
2:O:100(D):TYR:CZ	3:P:49:PHE:CE2	3.08	0.41
2:O:103:TRP:CE3	3:P:44:PRO:HG2	2.46	0.41
1:A:330:ALA:O	1:A:331:GLN:C	2.60	0.41
1:E:256:TYR:CE2	1:E:408:MET:HA	2.55	0.41
1:E:362:ILE:HG23	3:R:49:PHE:CE1	2.55	0.41
2:H:93:ALA:HB1	2:H:100(E):PHE:HB3	2.03	0.41
2:M:93:ALA:HB1	2:M:100(E):PHE:HB3	2.03	0.41
1:A:192:VAL:HG23	2:Q:34:VAL:CG2	2.51	0.41
1:A:234:VAL:HG23	1:A:235:PRO:HD2	2.01	0.41
1:C:38:THR:CB	1:C:337:ILE:CD1	2.96	0.41
1:C:173:ILE:CG1	1:C:262:PHE:CD2	3.04	0.41
1:D:286:PRO:HD2	1:D:289:LEU:HD12	2.03	0.41
1:D:340:GLY:N	1:D:412:ILE:HD11	2.36	0.41
2:M:31:THR:OG1	2:M:34:VAL:HG21	2.21	0.41
2:M:50:LEU:HD13	2:M:51:ILE:N	2.36	0.41
2:O:93:ALA:HB1	2:O:100(E):PHE:HB3	2.03	0.41
2:Q:11:LEU:HD13	2:Q:12:VAL:N	2.36	0.41
2:Q:50:LEU:HD13	2:Q:51:ILE:N	2.36	0.41
2:Q:93:ALA:HB1	2:Q:100(E):PHE:HB3	2.03	0.41
1:C:356:MET:O	1:C:357:SER:O	2.38	0.41
1:D:358:LEU:HD21	1:E:200:PRO:O	2.20	0.41
1:E:340:GLY:N	1:E:412:ILE:HD11	2.36	0.41
2:M:28:SER:O	2:M:31:THR:OG1	2.38	0.41
2:O:50:LEU:HD13	2:O:51:ILE:N	2.36	0.41
1:A:361:ALA:HB2	1:B:229:ALA:CB	2.49	0.40
1:A:483:LEU:HD13	1:A:483:LEU:C	2.45	0.40
1:C:38:THR:O	1:C:42:VAL:HG13	2.21	0.40
1:D:330:ALA:O	1:D:331:GLN:C	2.59	0.40
2:H:50:LEU:HD13	2:H:51:ILE:N	2.36	0.40
3:L:49:PHE:CD1	3:L:49:PHE:C	2.99	0.40
3:L:81:GLU:OE1	3:L:81:GLU:C	2.63	0.40
2:O:75:LYS:N	2:O:75:LYS:HD3	2.36	0.40
2:Q:31:THR:OG1	2:Q:34:VAL:HG21	2.21	0.40
2:S:11:LEU:HD13	2:S:12:VAL:N	2.36	0.40
2:S:93:ALA:HB1	2:S:103:TRP:CD1	2.55	0.40
2:S:93:ALA:HB1	2:S:100(E):PHE:HB3	2.03	0.40
3:T:49:PHE:CD1	3:T:49:PHE:C	2.99	0.40
1:A:38:THR:CB	1:A:337:ILE:CD1	2.98	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:TYR:CE2	1:A:408:MET:HA	2.55	0.40
1:C:340:GLY:N	1:C:412:ILE:HD11	2.36	0.40
1:D:229:ALA:C	1:D:231:LYS:N	2.78	0.40
2:H:5:ARG:HG2	2:H:105:ARG:NH1	2.37	0.40
2:S:5:ARG:HG2	2:S:105:ARG:NH1	2.37	0.40
2:S:6:GLU:HB2	2:S:107:THR:CG2	2.48	0.40
1:A:89:ILE:CD1	1:A:388:PHE:CZ	3.05	0.40
1:B:38:THR:O	1:B:42:VAL:HG13	2.22	0.40
1:B:89:ILE:CD1	1:B:388:PHE:CZ	3.05	0.40
1:B:484:LEU:HD11	1:C:329:ARG:NH1	2.37	0.40
1:C:358:LEU:HD22	1:D:202:LEU:HD21	2.02	0.40
1:D:173:ILE:CG1	1:D:262:PHE:CD2	3.04	0.40
1:E:173:ILE:CG1	1:E:262:PHE:CD2	3.04	0.40
1:E:286:PRO:HD2	1:E:289:LEU:HD12	2.03	0.40
2:S:50:LEU:HD13	2:S:51:ILE:N	2.36	0.40
1:A:173:ILE:CG1	1:A:262:PHE:CD2	3.04	0.40
1:A:329:ARG:O	1:A:330:ALA:C	2.64	0.40
1:A:340:GLY:N	1:A:412:ILE:HD11	2.36	0.40
1:B:340:GLY:N	1:B:412:ILE:HD11	2.36	0.40
1:C:287:ASP:CG	3:L:95(A):ARG:HH12	2.29	0.40
1:D:483:LEU:HD13	1:D:483:LEU:C	2.45	0.40
2:H:11:LEU:HD13	2:H:12:VAL:N	2.36	0.40
3:N:49:PHE:CD1	3:N:49:PHE:C	2.99	0.40
2:Q:75:LYS:N	2:Q:75:LYS:HD3	2.36	0.40
1:A:286:PRO:HD2	1:A:289:LEU:HD12	2.03	0.40
1:D:229:ALA:O	1:D:231:LYS:N	2.54	0.40
2:O:31:THR:OG1	2:O:34:VAL:HG21	2.21	0.40
2:S:75:LYS:HD3	2:S:75:LYS:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/426 (97%)	386 (93%)	25 (6%)	3 (1%)	19	54
1	B	414/426 (97%)	387 (94%)	24 (6%)	3 (1%)	19	54
1	C	414/426 (97%)	387 (94%)	24 (6%)	3 (1%)	19	54
1	D	414/426 (97%)	384 (93%)	27 (6%)	3 (1%)	19	54
1	E	414/426 (97%)	387 (94%)	24 (6%)	3 (1%)	19	54
2	H	120/235 (51%)	115 (96%)	5 (4%)	0	100	100
2	M	120/235 (51%)	114 (95%)	6 (5%)	0	100	100
2	O	120/235 (51%)	114 (95%)	6 (5%)	0	100	100
2	Q	120/235 (51%)	115 (96%)	5 (4%)	0	100	100
2	S	120/235 (51%)	115 (96%)	5 (4%)	0	100	100
3	L	109/217 (50%)	106 (97%)	3 (3%)	0	100	100
3	N	109/217 (50%)	106 (97%)	3 (3%)	0	100	100
3	P	109/217 (50%)	106 (97%)	3 (3%)	0	100	100
3	R	109/217 (50%)	106 (97%)	3 (3%)	0	100	100
3	T	109/217 (50%)	106 (97%)	3 (3%)	0	100	100
All	All	3215/4390 (73%)	3034 (94%)	166 (5%)	15 (0%)	27	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	358	LEU
1	B	155	VAL
1	B	358	LEU
1	C	155	VAL
1	C	358	LEU
1	D	155	VAL
1	D	358	LEU
1	E	155	VAL
1	E	358	LEU
1	C	357	SER
1	D	357	SER
1	E	357	SER
1	B	357	SER
1	A	357	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	352 (96%)	13 (4%)	30	64
1	B	365/368 (99%)	350 (96%)	15 (4%)	26	60
1	C	365/368 (99%)	351 (96%)	14 (4%)	28	62
1	D	365/368 (99%)	353 (97%)	12 (3%)	33	67
1	E	365/368 (99%)	352 (96%)	13 (4%)	30	64
2	H	109/209 (52%)	108 (99%)	1 (1%)	75	89
2	M	109/209 (52%)	108 (99%)	1 (1%)	75	89
2	O	109/209 (52%)	108 (99%)	1 (1%)	75	89
2	Q	109/209 (52%)	108 (99%)	1 (1%)	75	89
2	S	109/209 (52%)	108 (99%)	1 (1%)	75	89
3	L	86/179 (48%)	85 (99%)	1 (1%)	67	86
3	N	86/179 (48%)	85 (99%)	1 (1%)	67	86
3	P	86/179 (48%)	85 (99%)	1 (1%)	67	86
3	R	86/179 (48%)	85 (99%)	1 (1%)	67	86
3	T	86/179 (48%)	85 (99%)	1 (1%)	67	86
All	All	2800/3780 (74%)	2723 (97%)	77 (3%)	40	70

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	90	HIS
1	A	129	VAL
1	A	132	SER
1	A	195	ASN
1	A	205	ILE
1	A	231	LYS
1	A	302	SER
1	A	325	TYR
1	A	354	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	358	LEU
1	A	359	CYS
1	A	485	GLN
1	B	36	VAL
1	B	90	HIS
1	B	129	VAL
1	B	132	SER
1	B	182	HIS
1	B	195	ASN
1	B	205	ILE
1	B	231	LYS
1	B	302	SER
1	B	325	TYR
1	B	354	THR
1	B	356	MET
1	B	358	LEU
1	B	359	CYS
1	B	485	GLN
1	C	36	VAL
1	C	90	HIS
1	C	129	VAL
1	C	132	SER
1	C	195	ASN
1	C	205	ILE
1	C	231	LYS
1	C	302	SER
1	C	325	TYR
1	C	354	THR
1	C	357	SER
1	C	358	LEU
1	C	359	CYS
1	C	485	GLN
1	D	90	HIS
1	D	129	VAL
1	D	132	SER
1	D	195	ASN
1	D	205	ILE
1	D	231	LYS
1	D	302	SER
1	D	325	TYR
1	D	354	THR
1	D	358	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	359	CYS
1	D	485	GLN
1	E	90	HIS
1	E	129	VAL
1	E	132	SER
1	E	195	ASN
1	E	205	ILE
1	E	231	LYS
1	E	302	SER
1	E	325	TYR
1	E	354	THR
1	E	357	SER
1	E	358	LEU
1	E	359	CYS
1	E	485	GLN
2	H	27	LEU
3	L	37	GLN
2	M	27	LEU
3	N	37	GLN
2	O	27	LEU
3	P	37	GLN
2	Q	27	LEU
3	R	37	GLN
2	S	27	LEU
3	T	37	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	169	GLN
1	A	195	ASN
1	A	230	ASN
1	A	284	ASN
1	A	299	ASN
1	A	304	ASN
1	A	341	ASN
1	A	342	GLN
1	A	371	ASN
1	A	380	HIS
1	A	406	HIS
1	A	409	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	70	ASN
1	B	169	GLN
1	B	195	ASN
1	B	230	ASN
1	B	284	ASN
1	B	299	ASN
1	B	304	ASN
1	B	341	ASN
1	B	342	GLN
1	B	371	ASN
1	B	406	HIS
1	B	409	ASN
1	C	70	ASN
1	C	195	ASN
1	C	230	ASN
1	C	284	ASN
1	C	299	ASN
1	C	304	ASN
1	C	341	ASN
1	C	342	GLN
1	C	371	ASN
1	C	406	HIS
1	C	409	ASN
1	D	70	ASN
1	D	195	ASN
1	D	230	ASN
1	D	284	ASN
1	D	299	ASN
1	D	304	ASN
1	D	341	ASN
1	D	342	GLN
1	D	371	ASN
1	D	406	HIS
1	D	409	ASN
1	E	70	ASN
1	E	195	ASN
1	E	230	ASN
1	E	284	ASN
1	E	299	ASN
1	E	304	ASN
1	E	341	ASN
1	E	342	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	371	ASN
1	E	380	HIS
1	E	406	HIS
1	E	409	ASN
3	L	37	GLN
3	L	38	GLN
3	N	38	GLN
3	P	38	GLN
3	R	37	GLN
3	R	38	GLN
3	T	37	GLN
3	T	38	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

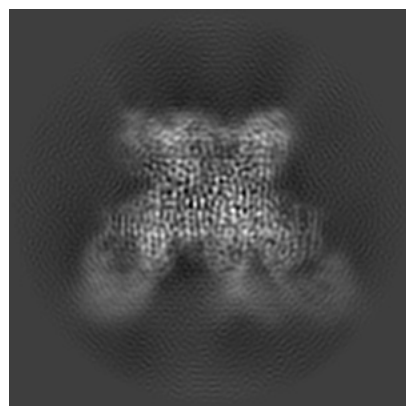
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48344. These allow visual inspection of the internal detail of the map and identification of artifacts.

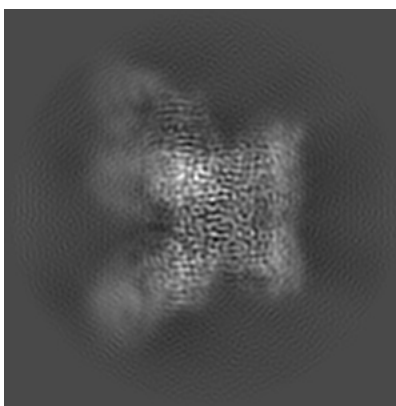
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

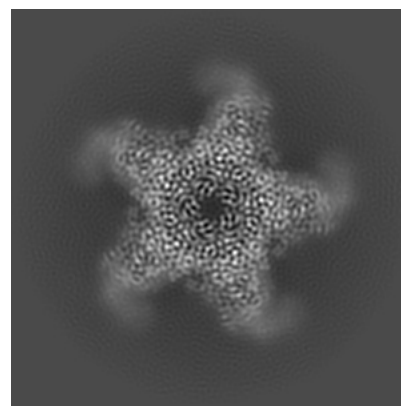
6.1.1 Primary map



X

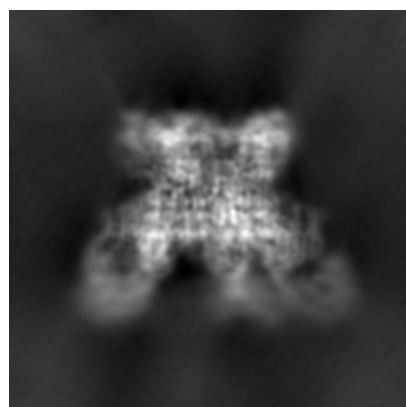


Y

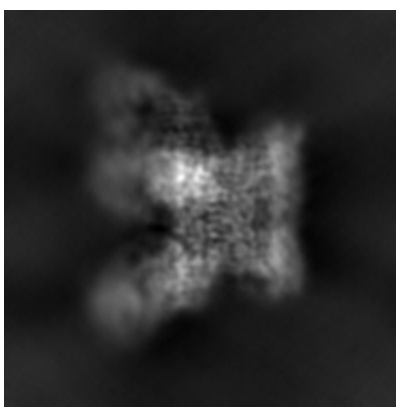


Z

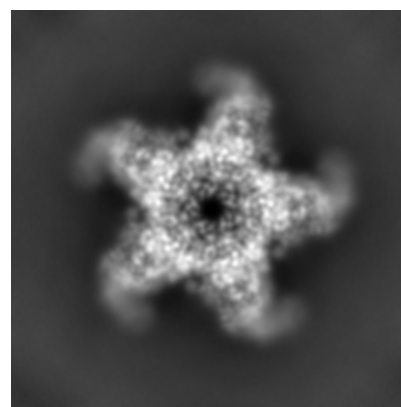
6.1.2 Raw map



X



Y

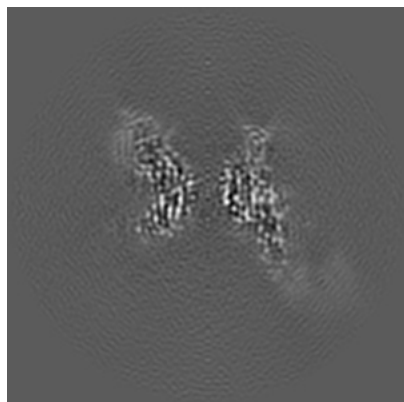


Z

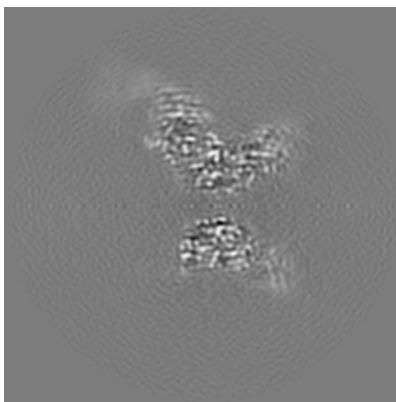
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

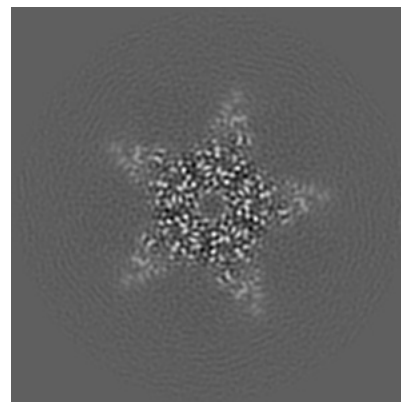
6.2.1 Primary map



X Index: 110

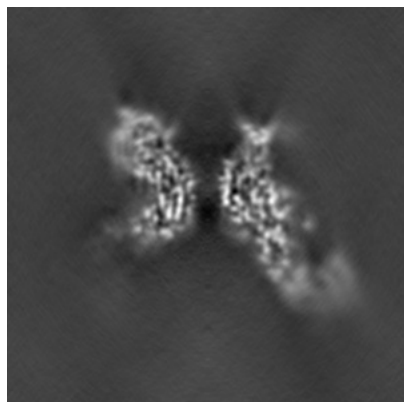


Y Index: 110

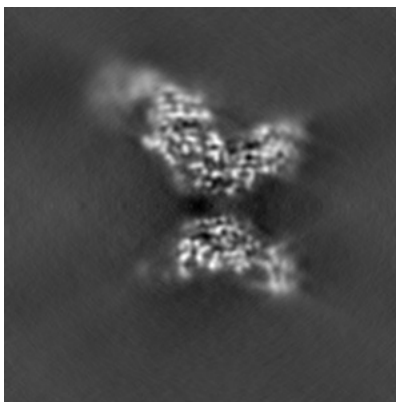


Z Index: 110

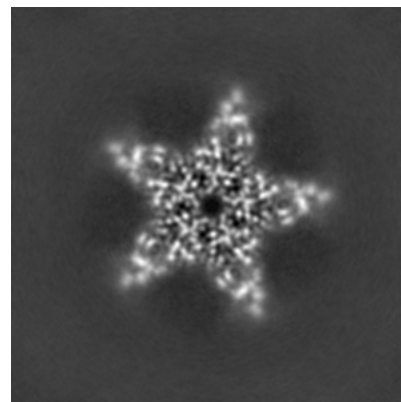
6.2.2 Raw map



X Index: 110



Y Index: 110

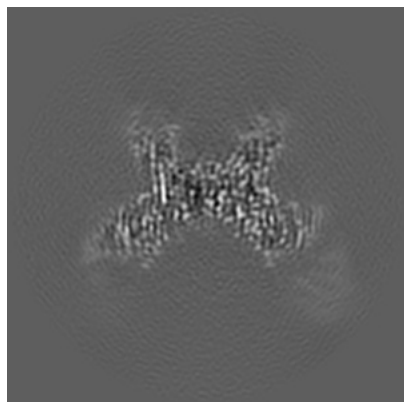


Z Index: 110

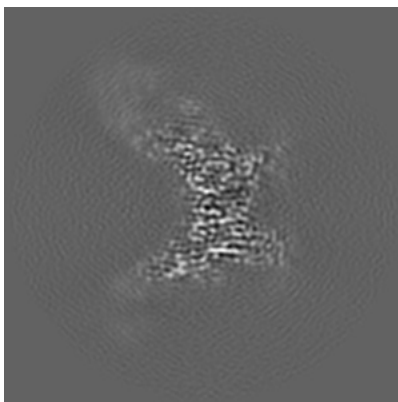
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

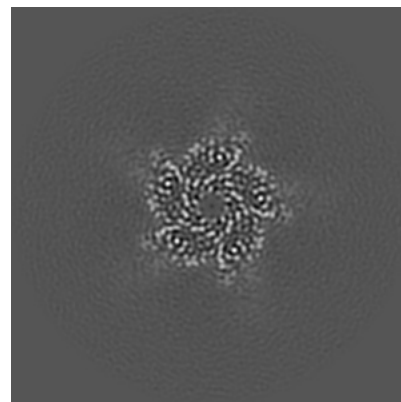
6.3.1 Primary map



X Index: 122

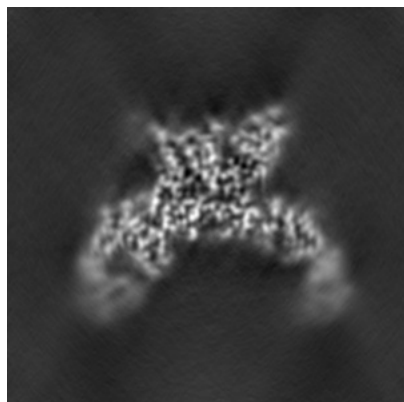


Y Index: 123

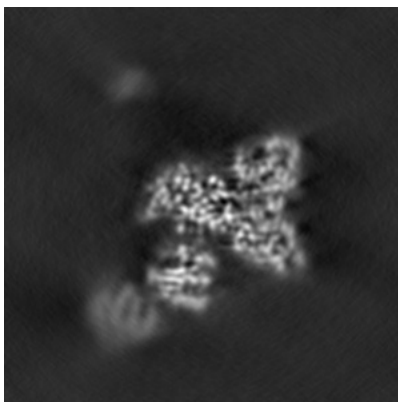


Z Index: 114

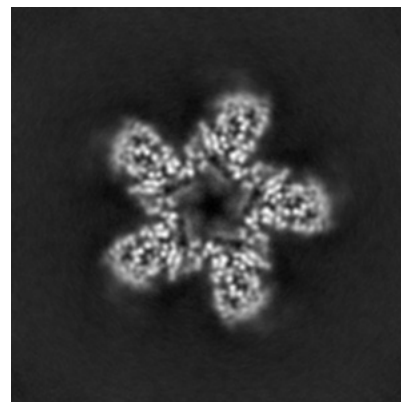
6.3.2 Raw map



X Index: 130



Y Index: 140

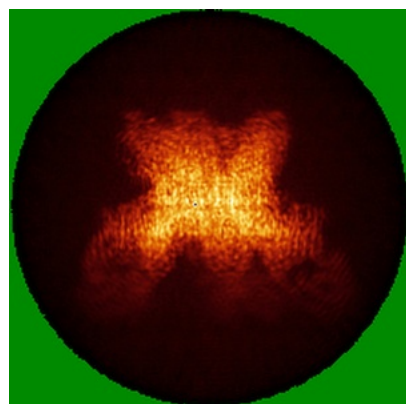


Z Index: 96

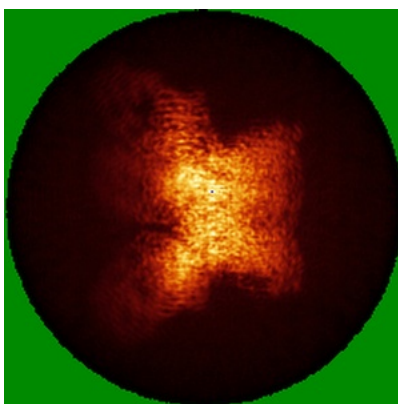
The images above show the largest variance slices of the map in three orthogonal directions.

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

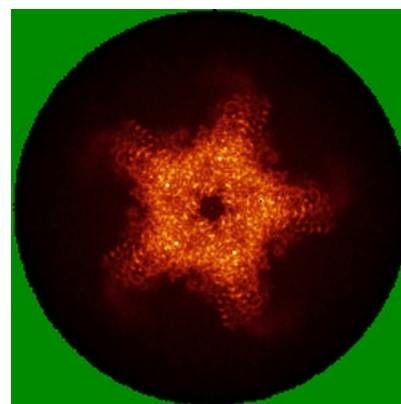
6.4.1 Primary map



X

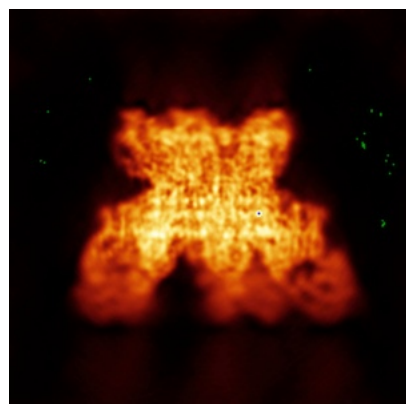


Y

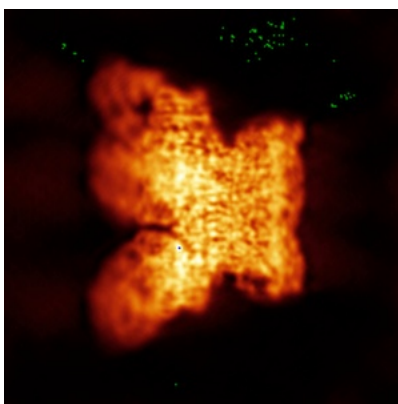


Z

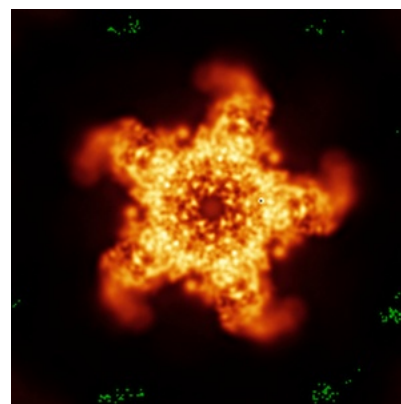
6.4.2 Raw map



X



Y

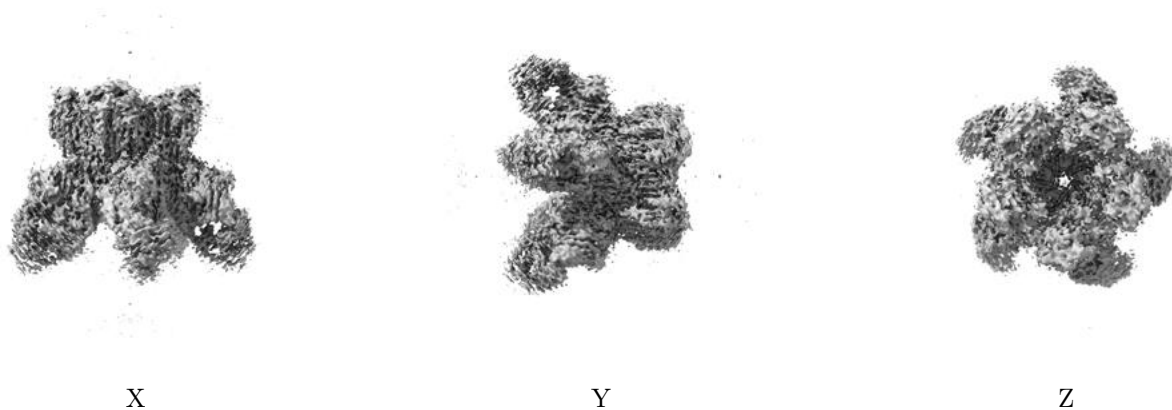


Z

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.

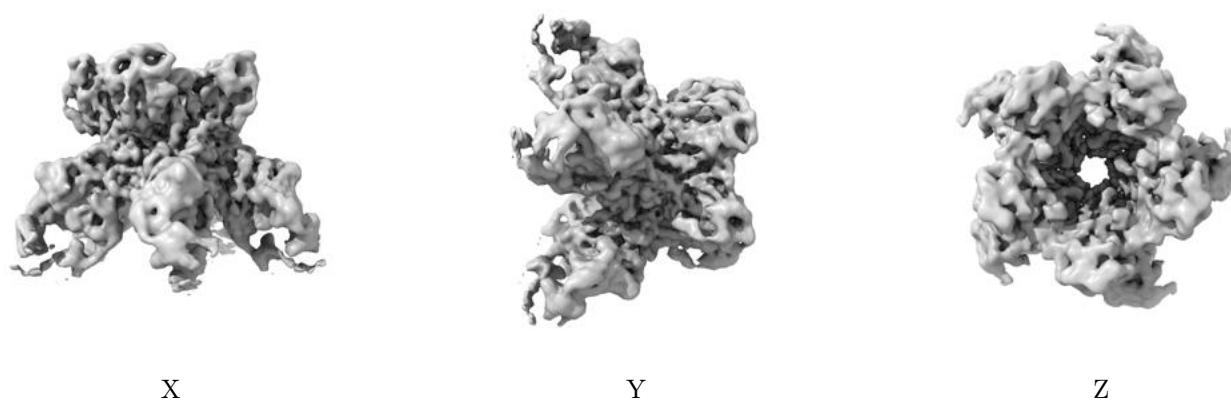
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

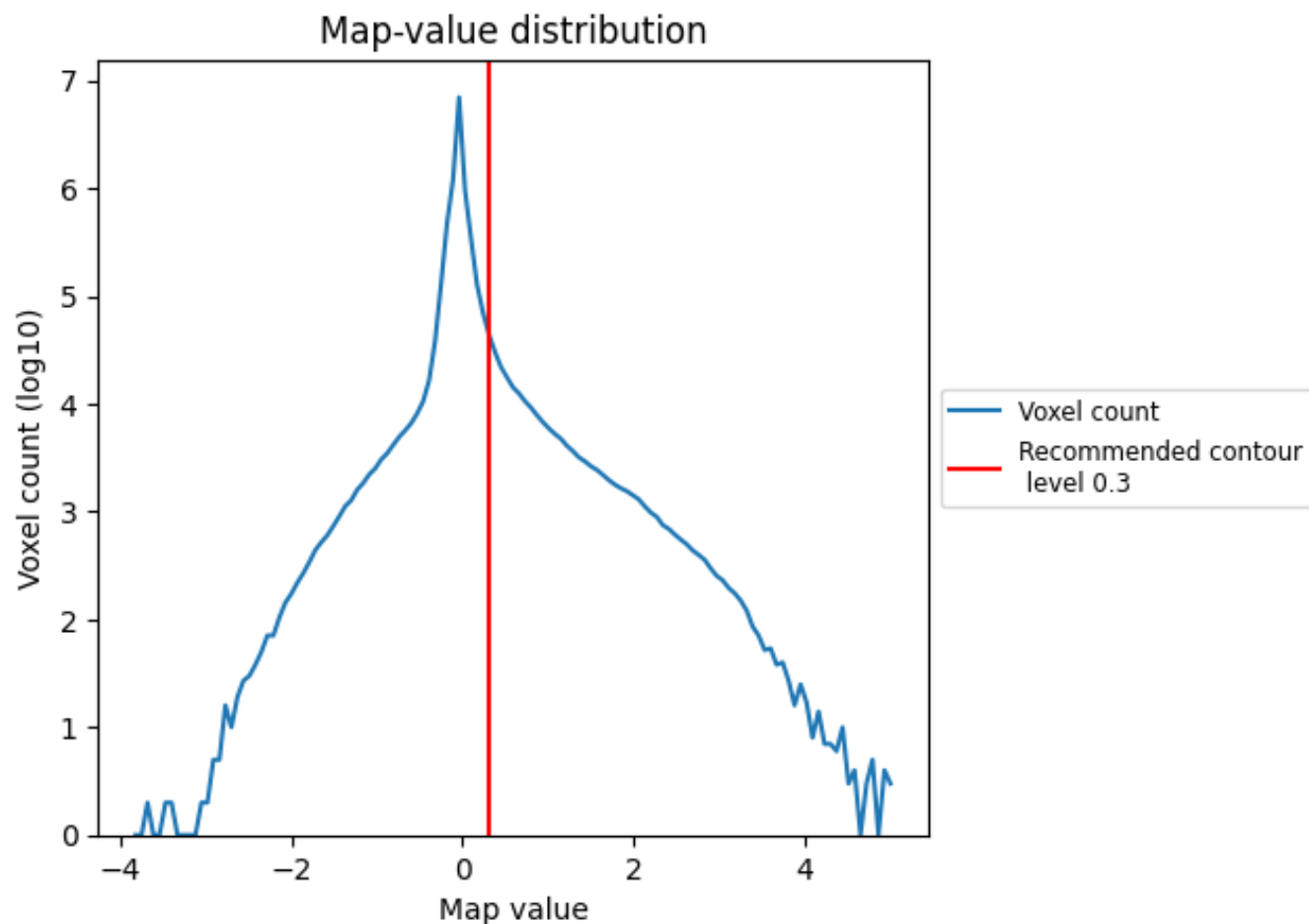
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

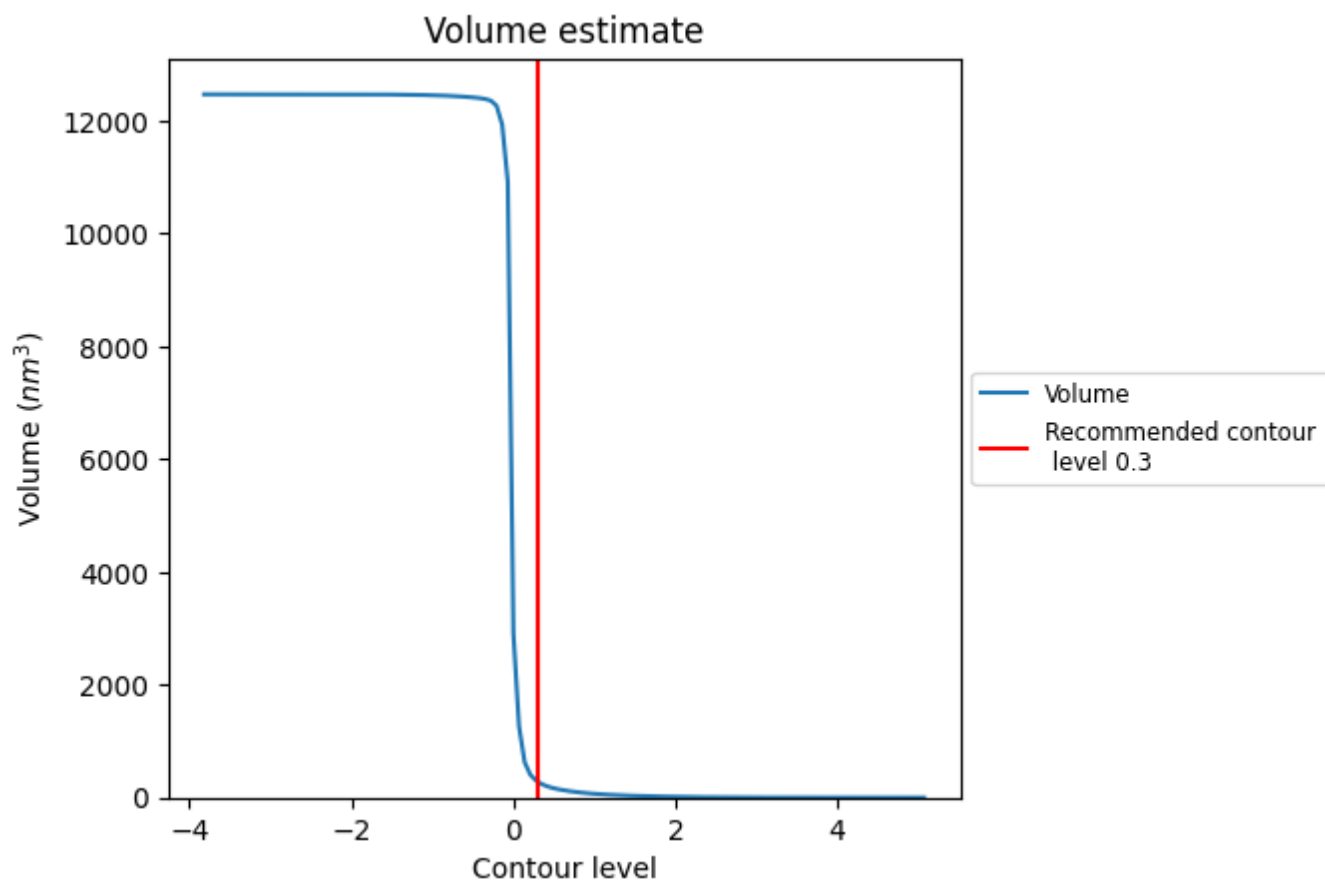
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

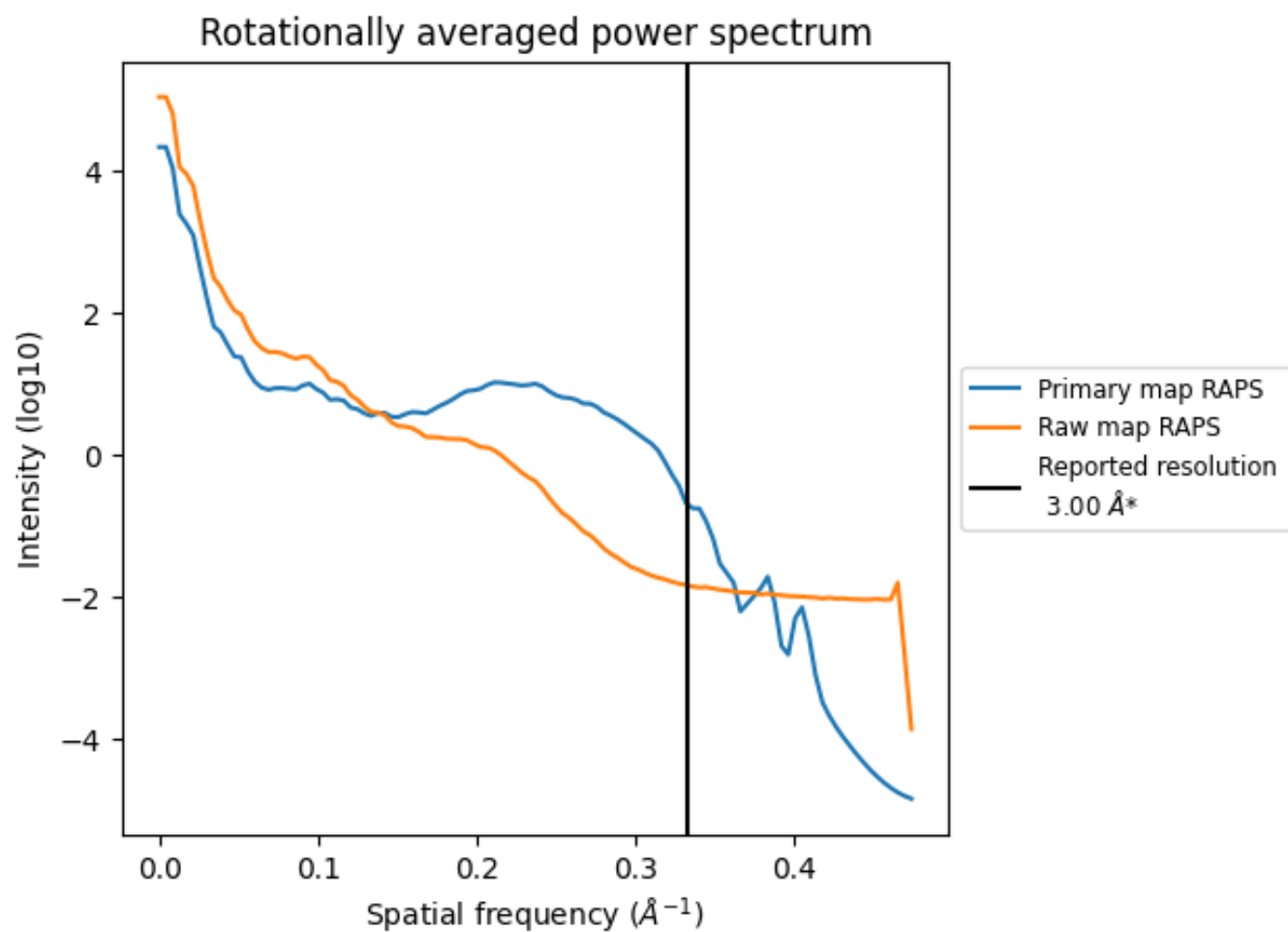
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 257 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 ⓘ

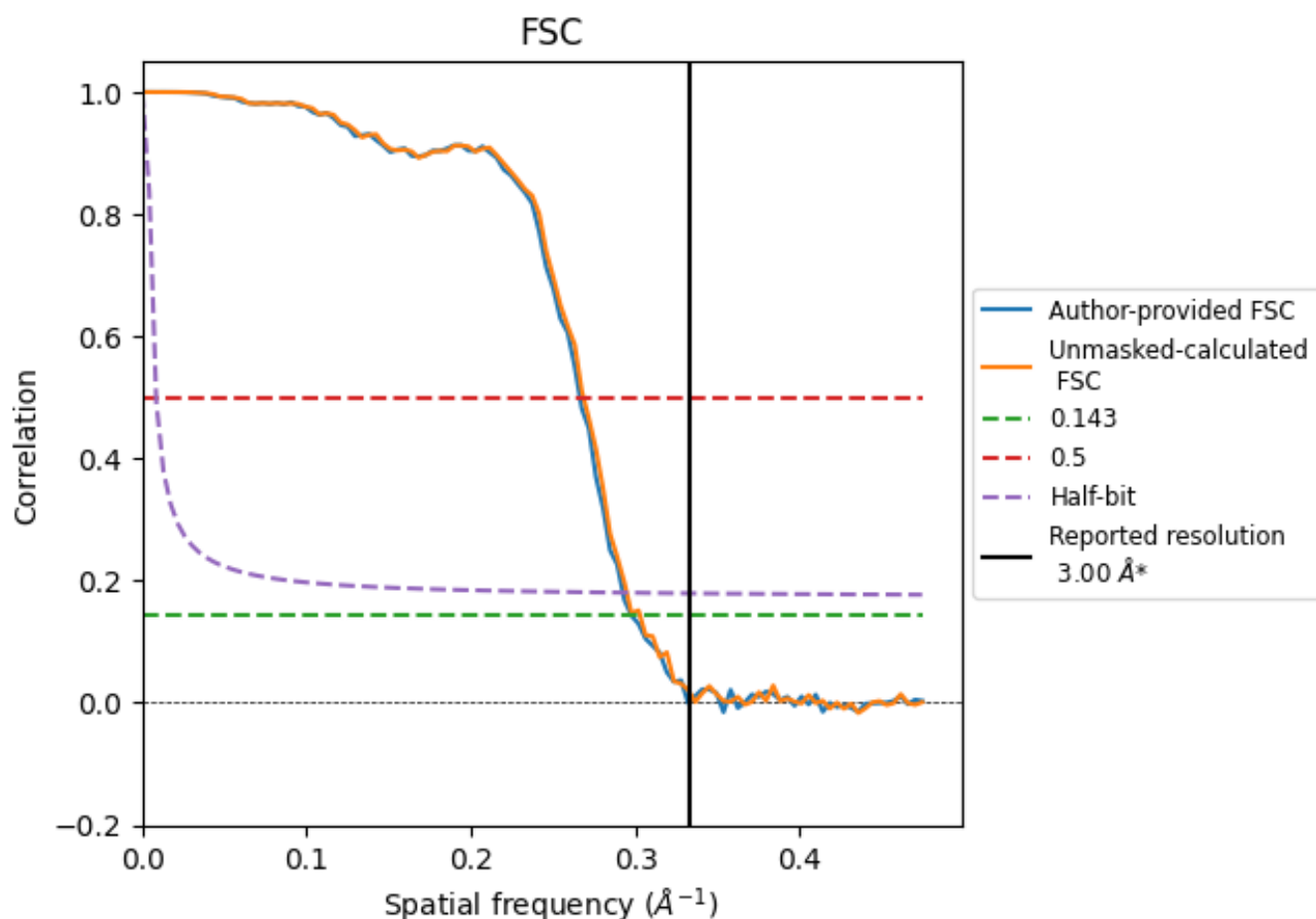


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

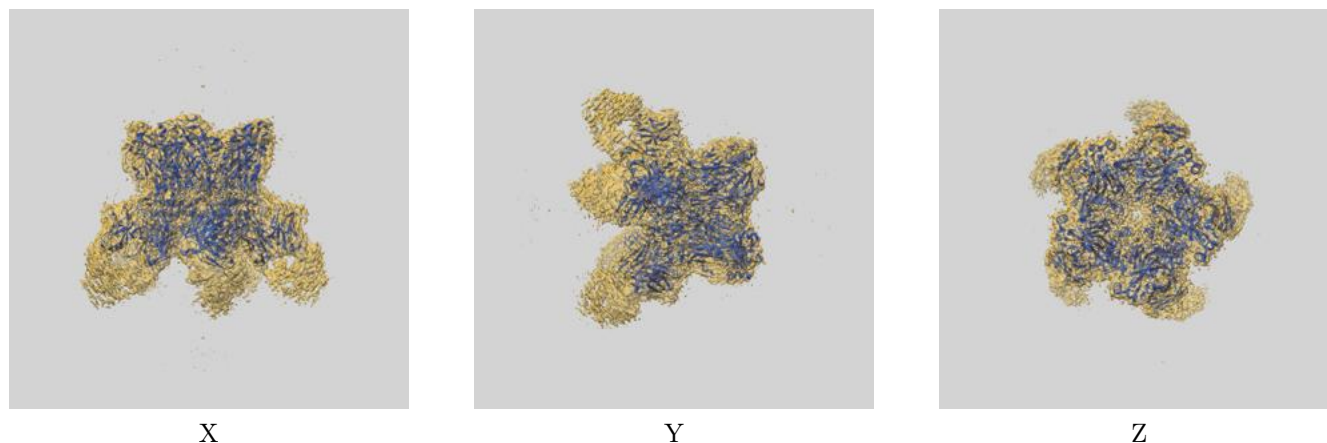
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.36	3.76	3.42
Unmasked-calculated*	3.30	3.73	3.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.36 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48344 and PDB model 9ML1. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



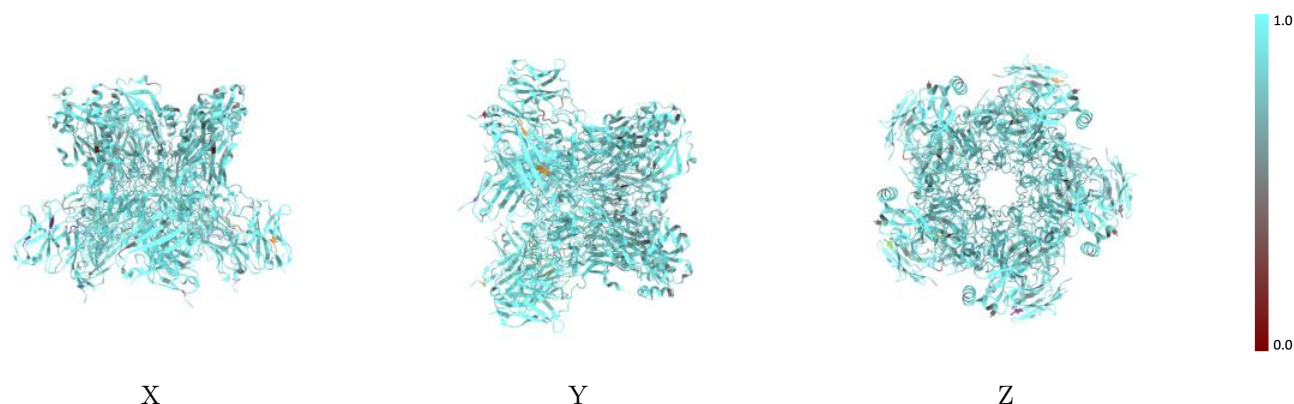
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



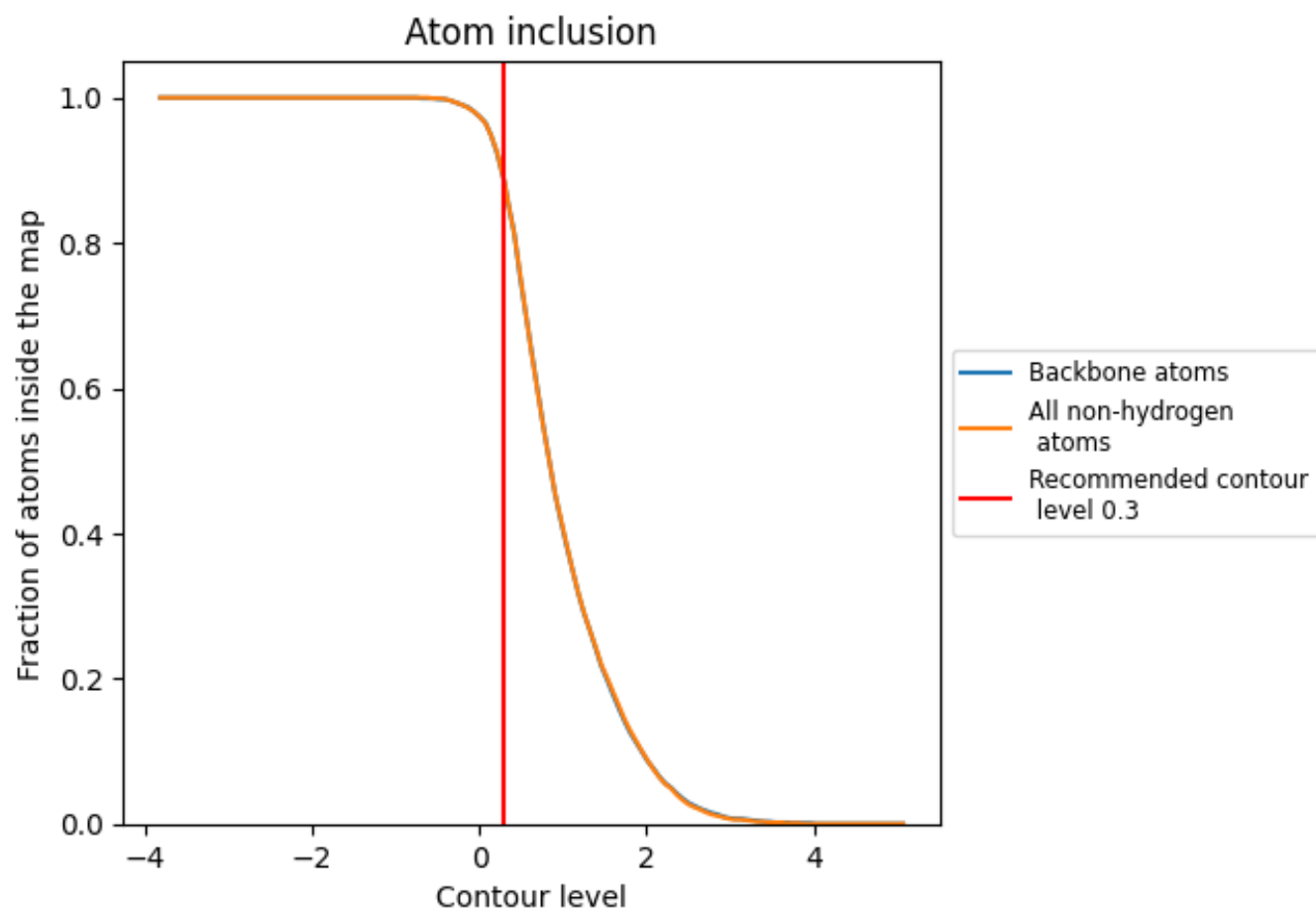
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8840	<div><div></div></div> 0.4510
A	<div><div></div></div> 0.8760	<div><div></div></div> 0.4470
B	<div><div></div></div> 0.8750	<div><div></div></div> 0.4480
C	<div><div></div></div> 0.8760	<div><div></div></div> 0.4480
D	<div><div></div></div> 0.8750	<div><div></div></div> 0.4480
E	<div><div></div></div> 0.8750	<div><div></div></div> 0.4450
H	<div><div></div></div> 0.9240	<div><div></div></div> 0.4500
L	<div><div></div></div> 0.9040	<div><div></div></div> 0.4650
M	<div><div></div></div> 0.9220	<div><div></div></div> 0.4520
N	<div><div></div></div> 0.9050	<div><div></div></div> 0.4630
O	<div><div></div></div> 0.9200	<div><div></div></div> 0.4500
P	<div><div></div></div> 0.9080	<div><div></div></div> 0.4660
Q	<div><div></div></div> 0.9270	<div><div></div></div> 0.4490
R	<div><div></div></div> 0.9040	<div><div></div></div> 0.4650
S	<div><div></div></div> 0.9230	<div><div></div></div> 0.4480
T	<div><div></div></div> 0.9090	<div><div></div></div> 0.4660

1.0

0.0

<0.0