



## Full wwPDB EM Validation Report ⓘ

Aug 18, 2025 – 02:17 PM JST

PDB ID : 8YAE / pdb\_00008yae  
EMDB ID : EMD-39097  
Title : Cryo-ET structure of huntingtin actin complex  
Authors : Kim, J.; Kim, H.; Fassler, F.; Hansen, J.M.; Schur, F.K.M.; Song, J.J.  
Deposited on : 2024-02-09  
Resolution : 10.08 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](mailto: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

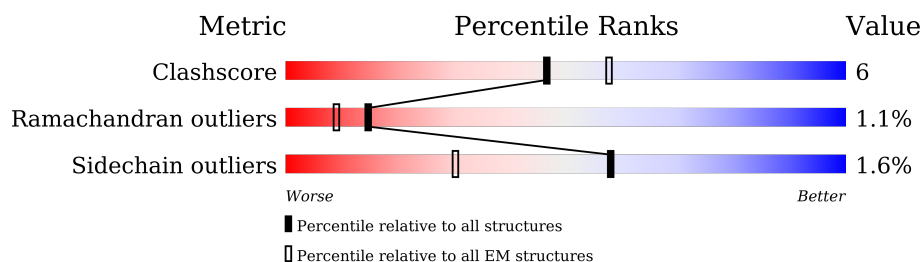
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.08 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  $\geq 3$ , 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	3144	
2	B	375	
2	C	375	
2	D	375	
2	E	375	
2	F	375	
2	G	375	
2	H	375	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	375	<div><div></div><div>85%</div><div>13%</div><div></div></div>
2	J	375	<div><div>9%</div><div>84%</div><div>14%</div><div></div></div>
2	K	375	<div><div>5%</div><div>84%</div><div>14%</div><div></div></div>
2	L	375	<div><div>46%</div><div>85%</div><div>13%</div><div></div></div>
2	M	375	<div><div>37%</div><div>84%</div><div>14%</div><div></div></div>
2	N	375	<div><div></div><div>89%</div><div>9%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 49440 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 Huntingtin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1451	Total	C	N	O	S	0	0
			11415	7311	1968	2061	75		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42858
A	0	ALA	-	expression tag	UNP P42858
A	1238	ARG	LYS	conflict	UNP P42858

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	B	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	C	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	D	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	E	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	F	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	G	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	H	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	I	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	J	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		

*Continued on next page...*

*Continued from previous page...*


Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	L	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		
2	M	374	Total	C	N	O	S	0	0
			2925	1850	492	562	21		

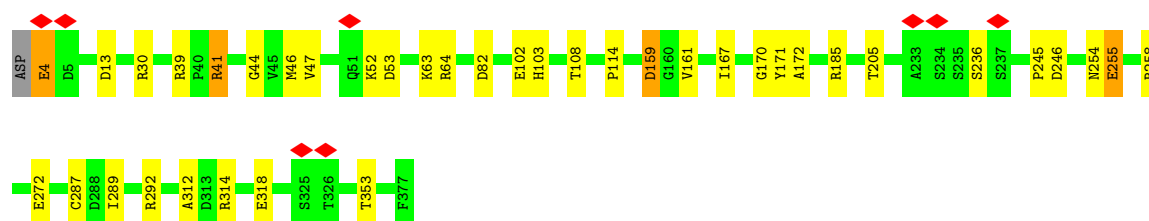




- Molecule 2: Actin, alpha skeletal muscle

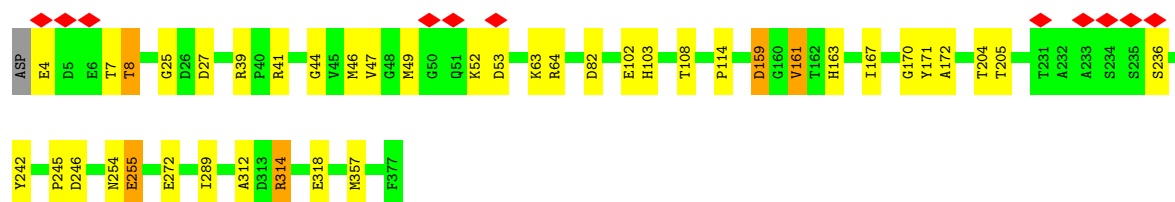


Chain N:  89% 9% .




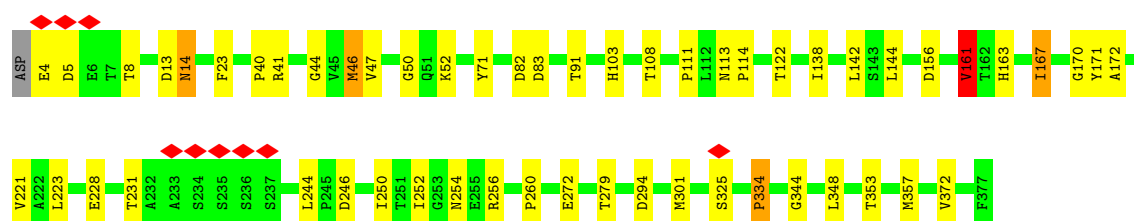
• Molecule 2: Actin, alpha skeletal muscle

Chain B:  89% 10% .




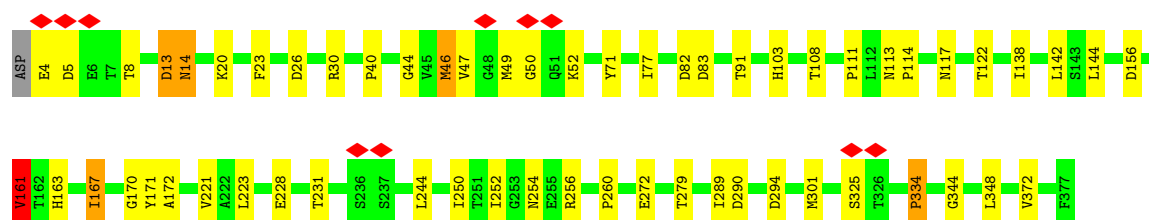
• Molecule 2: Actin, alpha skeletal muscle

Chain C:  85% 13% .




• Molecule 2: Actin, alpha skeletal muscle

Chain D:  84% 14% .



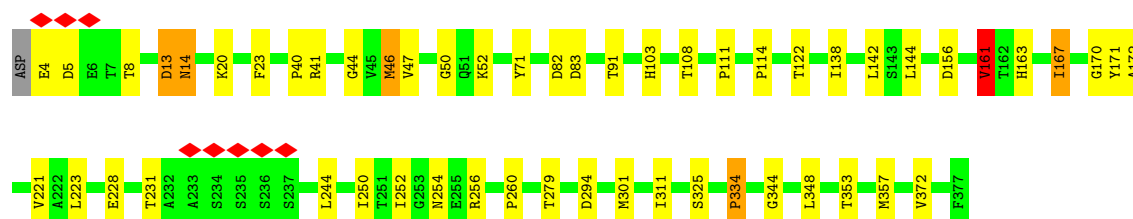
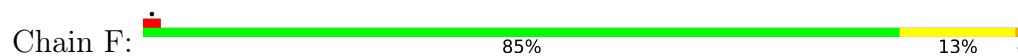
• Molecule 2: Actin, alpha skeletal muscle

Chain E:  85% 13% .

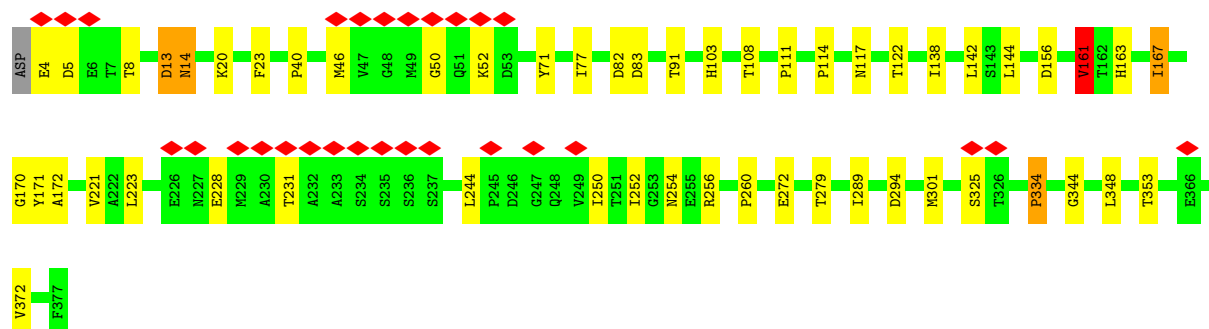
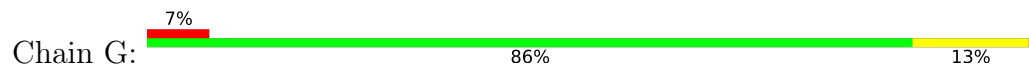




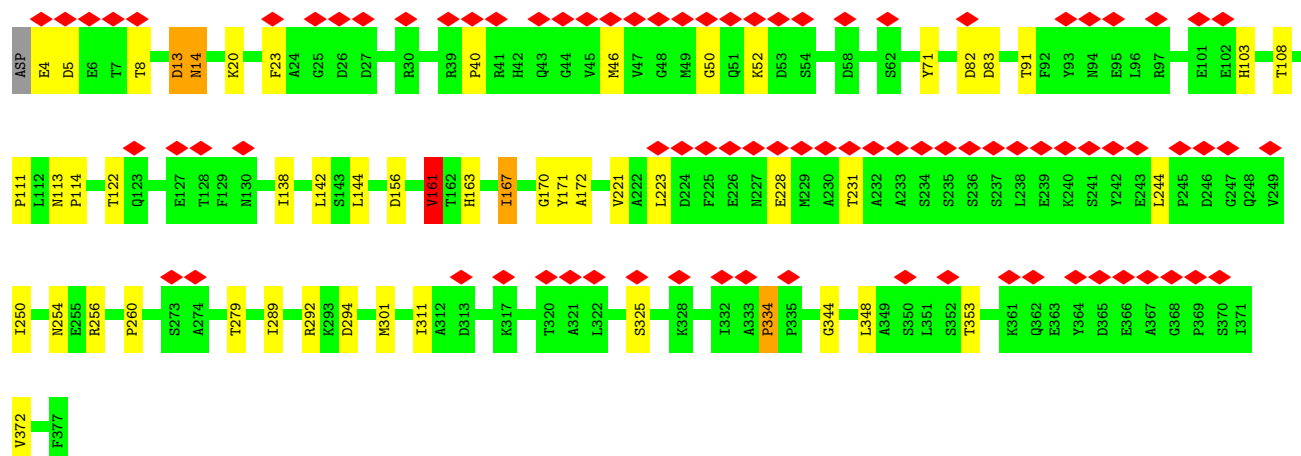
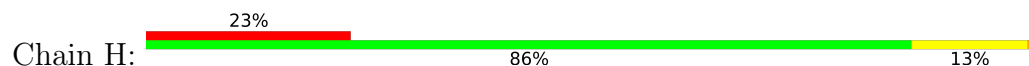
- Molecule 2: Actin, alpha skeletal muscle



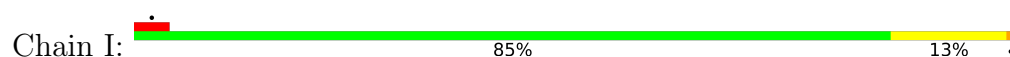
- Molecule 2: Actin, alpha skeletal muscle

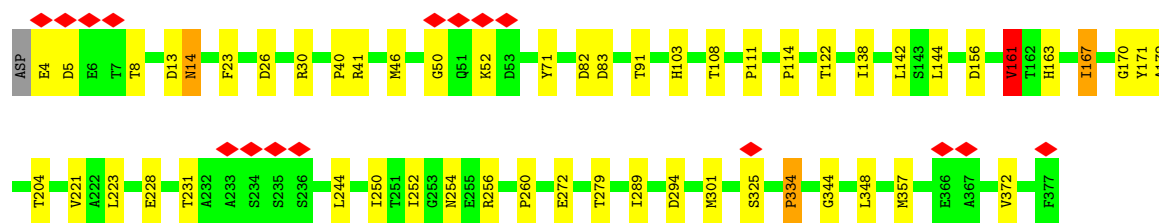


- Molecule 2: Actin, alpha skeletal muscle

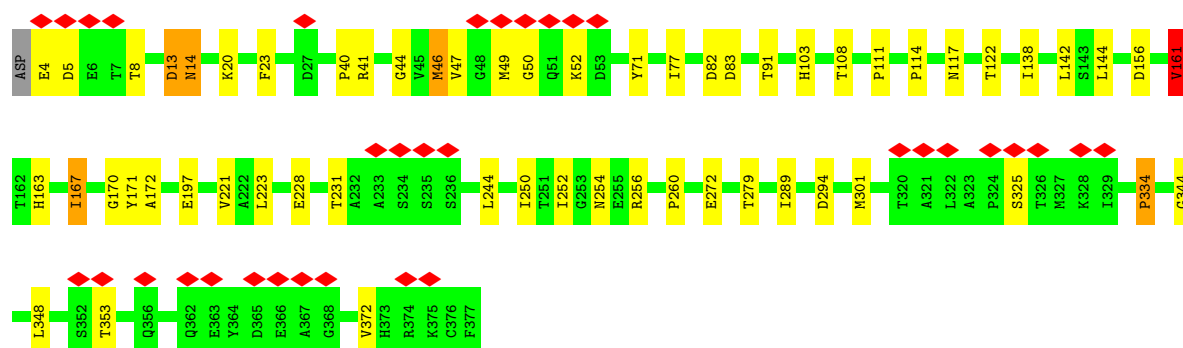
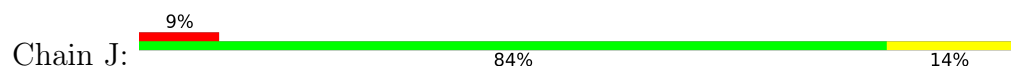


- Molecule 2: Actin, alpha skeletal muscle

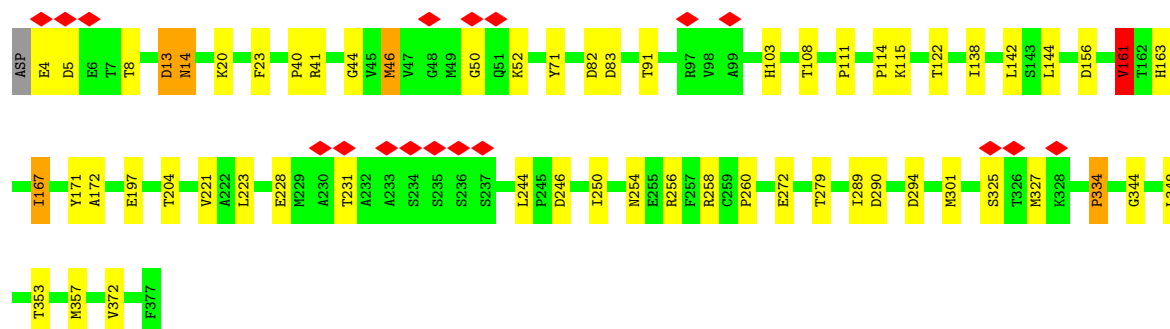
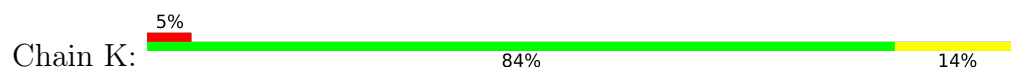




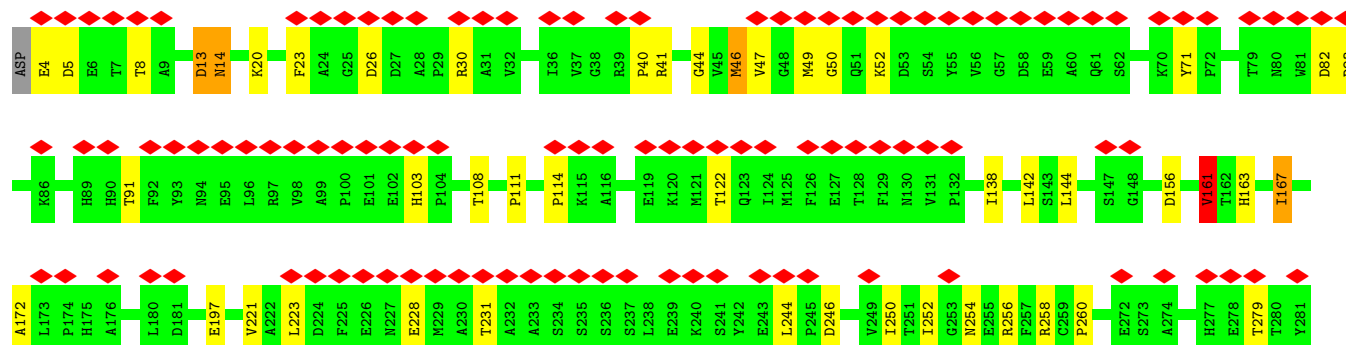
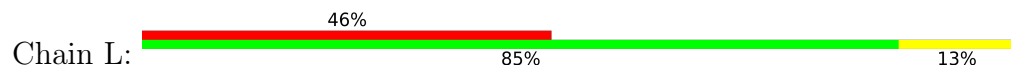
- Molecule 2: Actin, alpha skeletal muscle



- Molecule 2: Actin, alpha skeletal muscle

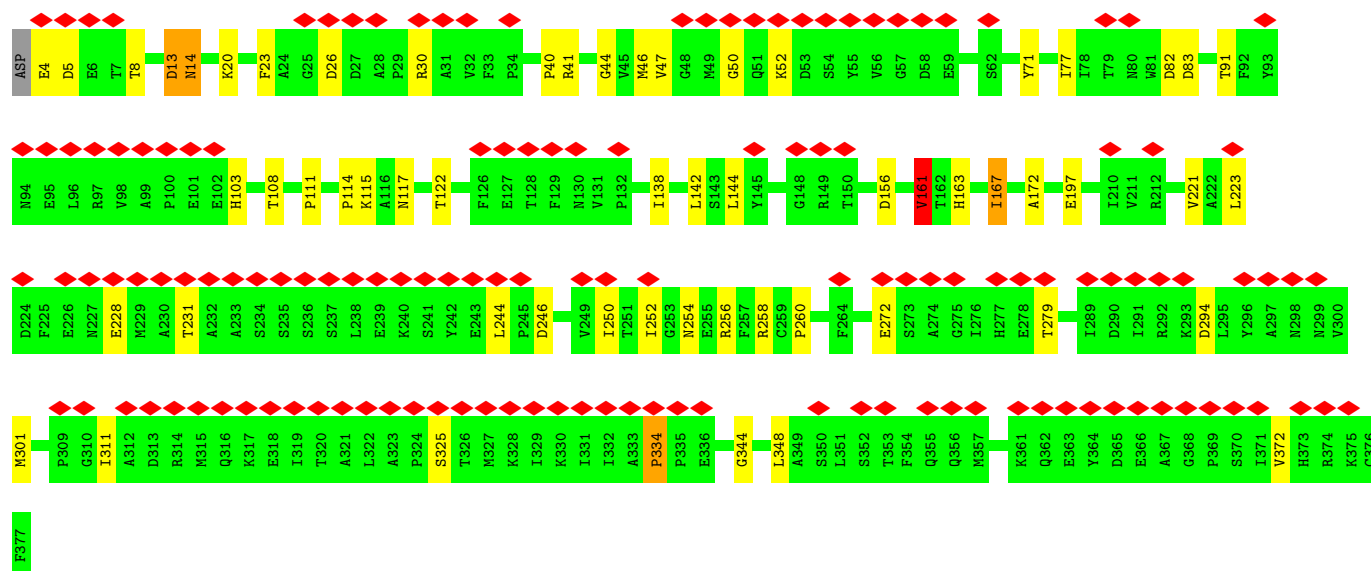
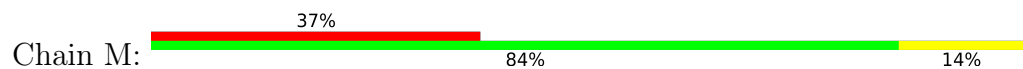


- Molecule 2: Actin, alpha skeletal muscle





• Molecule 2: Actin, alpha skeletal muscle



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	22664	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 ( $e^-/\text{\AA}^2$ )	2.79	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.907	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	441.92, 441.92, 441.92	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.762, 2.762, 2.762	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.33	0/11619	0.78	3/15765 (0.0%)
2	B	0.88	0/2988	1.54	13/4047 (0.3%)
2	C	1.01	0/2988	1.64	25/4047 (0.6%)
2	D	1.01	0/2988	1.64	26/4047 (0.6%)
2	E	1.01	0/2988	1.64	24/4047 (0.6%)
2	F	1.01	0/2988	1.64	24/4047 (0.6%)
2	G	1.01	0/2988	1.64	24/4047 (0.6%)
2	H	1.01	0/2988	1.64	25/4047 (0.6%)
2	I	1.01	0/2988	1.64	26/4047 (0.6%)
2	J	1.01	0/2988	1.64	24/4047 (0.6%)
2	K	1.01	0/2988	1.64	25/4047 (0.6%)
2	L	1.01	0/2988	1.64	24/4047 (0.6%)
2	M	1.01	0/2988	1.64	24/4047 (0.6%)
2	N	0.87	0/2988	1.53	17/4047 (0.4%)
All	All	0.88	0/50463	1.47	304/68376 (0.4%)

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	4
2	B	0	5
2	C	0	5
2	D	0	5
2	E	0	5
2	F	0	5
2	G	0	5
2	H	0	5
2	I	0	5
2	J	0	5
2	K	0	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	5
2	M	0	5
2	N	0	6
All	All	0	70

There are no bond length outliers.

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	THR	N-CA-CB	7.89	123.82	110.49
2	D	334	PRO	O-C-N	-7.64	117.56	121.15
2	H	334	PRO	O-C-N	-7.59	117.58	121.15
2	G	334	PRO	O-C-N	-7.50	117.62	121.15
2	M	334	PRO	O-C-N	-7.49	117.63	121.15
2	C	334	PRO	O-C-N	-7.47	117.64	121.15
2	K	334	PRO	O-C-N	-7.47	117.64	121.15
2	E	334	PRO	O-C-N	-7.46	117.65	121.15
2	F	334	PRO	O-C-N	-7.41	117.67	121.15
2	L	334	PRO	O-C-N	-7.36	117.69	121.15
2	I	334	PRO	O-C-N	-7.33	117.70	121.15
1	A	1649	VAL	N-CA-C	-7.32	105.40	111.91
2	J	334	PRO	O-C-N	-7.27	117.73	121.15
2	J	254	ASN	CA-C-N	7.22	130.27	120.38
2	J	254	ASN	C-N-CA	7.22	130.27	120.38
2	G	254	ASN	CA-C-N	7.22	130.27	120.38
2	G	254	ASN	C-N-CA	7.22	130.27	120.38
2	L	254	ASN	CA-C-N	7.20	130.24	120.38
2	L	254	ASN	C-N-CA	7.20	130.24	120.38
2	F	254	ASN	CA-C-N	7.20	130.24	120.38
2	F	254	ASN	C-N-CA	7.20	130.24	120.38
2	H	254	ASN	CA-C-N	7.19	130.23	120.38
2	H	254	ASN	C-N-CA	7.19	130.23	120.38
2	D	254	ASN	CA-C-N	7.17	130.21	120.38
2	D	254	ASN	C-N-CA	7.17	130.21	120.38
2	C	254	ASN	CA-C-N	7.15	130.18	120.38
2	C	254	ASN	C-N-CA	7.15	130.18	120.38
2	I	254	ASN	CA-C-N	7.14	130.16	120.38
2	I	254	ASN	C-N-CA	7.14	130.16	120.38
2	M	254	ASN	CA-C-N	7.13	130.15	120.38
2	M	254	ASN	C-N-CA	7.13	130.15	120.38
2	E	254	ASN	CA-C-N	7.12	130.14	120.38
2	E	254	ASN	C-N-CA	7.12	130.14	120.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	254	ASN	CA-C-N	7.11	130.12	120.38
2	K	254	ASN	C-N-CA	7.11	130.12	120.38
2	N	255	GLU	N-CA-CB	-7.04	98.60	110.49
1	A	674	THR	N-CA-C	-7.00	105.93	114.75
2	N	312	ALA	CA-C-N	6.91	129.42	120.44
2	N	312	ALA	C-N-CA	6.91	129.42	120.44
2	B	255	GLU	N-CA-CB	-6.78	99.03	110.49
2	D	13	ASP	CA-CB-CG	6.52	119.12	112.60
2	B	312	ALA	CA-C-N	6.52	128.91	120.44
2	B	312	ALA	C-N-CA	6.52	128.91	120.44
2	E	13	ASP	CA-CB-CG	6.51	119.11	112.60
2	F	13	ASP	CA-CB-CG	6.51	119.11	112.60
2	I	13	ASP	CA-CB-CG	6.51	119.11	112.60
2	L	13	ASP	CA-CB-CG	6.51	119.11	112.60
2	M	13	ASP	CA-CB-CG	6.51	119.11	112.60
2	G	13	ASP	CA-CB-CG	6.51	119.11	112.60
2	K	13	ASP	CA-CB-CG	6.50	119.10	112.60
2	J	13	ASP	CA-CB-CG	6.47	119.07	112.60
2	H	13	ASP	CA-CB-CG	6.45	119.05	112.60
2	C	13	ASP	CA-CB-CG	6.45	119.05	112.60
2	G	83	ASP	CA-CB-CG	6.21	118.81	112.60
2	J	83	ASP	CA-CB-CG	6.20	118.80	112.60
2	N	245	PRO	CA-C-N	6.20	128.58	120.28
2	N	245	PRO	C-N-CA	6.20	128.58	120.28
2	L	83	ASP	CA-CB-CG	6.19	118.79	112.60
2	K	83	ASP	CA-CB-CG	6.17	118.77	112.60
2	I	83	ASP	CA-CB-CG	6.16	118.76	112.60
2	C	83	ASP	CA-CB-CG	6.15	118.75	112.60
2	M	83	ASP	CA-CB-CG	6.13	118.73	112.60
2	B	159	ASP	N-CA-C	-6.10	106.10	112.93
2	F	83	ASP	CA-CB-CG	6.09	118.69	112.60
2	H	83	ASP	CA-CB-CG	6.08	118.69	112.60
2	I	279	THR	N-CA-CB	6.08	119.06	110.12
2	D	83	ASP	CA-CB-CG	6.08	118.68	112.60
2	D	279	THR	N-CA-CB	6.07	119.05	110.12
2	E	83	ASP	CA-CB-CG	6.07	118.67	112.60
2	E	279	THR	N-CA-CB	6.07	119.05	110.12
2	F	279	THR	N-CA-CB	6.07	119.04	110.12
2	G	279	THR	N-CA-CB	6.07	119.04	110.12
2	K	279	THR	N-CA-CB	6.05	119.01	110.12
2	M	279	THR	N-CA-CB	6.05	119.01	110.12
2	C	279	THR	N-CA-CB	6.03	118.98	110.12

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	279	THR	N-CA-CB	6.03	118.98	110.12
2	H	279	THR	N-CA-CB	6.02	118.97	110.12
2	L	279	THR	N-CA-CB	5.95	118.87	110.12
2	F	325	SER	CA-C-N	5.94	128.84	120.28
2	F	325	SER	C-N-CA	5.94	128.84	120.28
2	M	325	SER	CA-C-N	5.91	128.79	120.28
2	M	325	SER	C-N-CA	5.91	128.79	120.28
2	B	245	PRO	CA-C-N	5.91	128.68	120.29
2	B	245	PRO	C-N-CA	5.91	128.68	120.29
2	E	325	SER	CA-C-N	5.91	128.79	120.28
2	E	325	SER	C-N-CA	5.91	128.79	120.28
2	L	91	THR	N-CA-CB	5.90	118.56	110.01
2	J	91	THR	N-CA-CB	5.88	118.54	110.01
2	H	91	THR	N-CA-CB	5.87	118.52	110.01
2	G	325	SER	CA-C-N	5.87	128.73	120.28
2	G	325	SER	C-N-CA	5.87	128.73	120.28
2	H	325	SER	CA-C-N	5.87	128.72	120.28
2	H	325	SER	C-N-CA	5.87	128.72	120.28
2	N	64	ARG	N-CA-C	5.86	117.67	111.28
2	C	325	SER	CA-C-N	5.86	128.72	120.28
2	C	325	SER	C-N-CA	5.86	128.72	120.28
2	K	91	THR	N-CA-CB	5.86	118.51	110.01
2	J	294	ASP	CA-CB-CG	5.86	118.46	112.60
2	K	325	SER	CA-C-N	5.85	128.71	120.28
2	K	325	SER	C-N-CA	5.85	128.71	120.28
2	D	91	THR	N-CA-CB	5.85	118.49	110.01
2	M	91	THR	N-CA-CB	5.85	118.49	110.01
2	G	156	ASP	CA-CB-CG	5.84	118.44	112.60
2	I	91	THR	N-CA-CB	5.84	118.48	110.01
2	K	156	ASP	CA-CB-CG	5.84	118.44	112.60
2	D	156	ASP	CA-CB-CG	5.83	118.44	112.60
2	E	91	THR	N-CA-CB	5.83	118.47	110.01
2	F	91	THR	N-CA-CB	5.83	118.47	110.01
2	J	325	SER	CA-C-N	5.83	128.68	120.28
2	J	325	SER	C-N-CA	5.83	128.68	120.28
2	G	91	THR	N-CA-CB	5.83	118.46	110.01
2	C	91	THR	N-CA-CB	5.82	118.45	110.01
2	E	294	ASP	CA-CB-CG	5.82	118.42	112.60
2	H	294	ASP	CA-CB-CG	5.82	118.42	112.60
2	I	325	SER	CA-C-N	5.81	128.65	120.28
2	I	325	SER	C-N-CA	5.81	128.65	120.28
2	C	156	ASP	CA-CB-CG	5.81	118.41	112.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	156	ASP	CA-CB-CG	5.80	118.40	112.60
2	H	156	ASP	CA-CB-CG	5.80	118.40	112.60
2	L	325	SER	CA-C-N	5.79	128.62	120.28
2	L	325	SER	C-N-CA	5.79	128.62	120.28
2	M	156	ASP	CA-CB-CG	5.79	118.39	112.60
2	I	294	ASP	CA-CB-CG	5.79	118.39	112.60
2	F	294	ASP	CA-CB-CG	5.78	118.38	112.60
2	E	156	ASP	CA-CB-CG	5.78	118.38	112.60
2	C	294	ASP	CA-CB-CG	5.78	118.38	112.60
2	L	294	ASP	CA-CB-CG	5.78	118.38	112.60
2	D	325	SER	CA-C-N	5.77	128.59	120.28
2	D	325	SER	C-N-CA	5.77	128.59	120.28
2	K	294	ASP	CA-CB-CG	5.76	118.36	112.60
2	L	103	HIS	CB-CG-ND1	-5.76	114.06	122.70
2	M	294	ASP	CA-CB-CG	5.76	118.36	112.60
2	G	294	ASP	CA-CB-CG	5.75	118.35	112.60
2	I	156	ASP	CA-CB-CG	5.75	118.35	112.60
2	E	103	HIS	CB-CG-ND1	-5.74	114.09	122.70
2	D	294	ASP	CA-CB-CG	5.74	118.34	112.60
2	N	318	GLU	CB-CG-CD	5.73	122.34	112.60
2	N	159	ASP	N-CA-C	-5.71	106.53	112.93
2	J	156	ASP	CA-CB-CG	5.71	118.31	112.60
2	C	103	HIS	CB-CG-ND1	-5.71	114.14	122.70
2	L	156	ASP	CA-CB-CG	5.71	118.31	112.60
2	J	103	HIS	CB-CG-ND1	-5.71	114.14	122.70
2	B	64	ARG	N-CA-C	5.70	117.49	111.28
2	D	103	HIS	CB-CG-ND1	-5.68	114.18	122.70
2	G	103	HIS	CB-CG-ND1	-5.68	114.19	122.70
2	M	103	HIS	CB-CG-ND1	-5.68	114.19	122.70
2	K	103	HIS	CB-CG-ND1	-5.67	114.19	122.70
2	F	103	HIS	CB-CG-ND1	-5.67	114.19	122.70
2	H	103	HIS	CB-CG-ND1	-5.67	114.20	122.70
2	I	103	HIS	CB-CG-ND1	-5.65	114.22	122.70
2	F	301	MET	CG-SD-CE	-5.64	88.50	100.90
2	H	301	MET	CG-SD-CE	-5.63	88.52	100.90
2	D	301	MET	CG-SD-CE	-5.62	88.54	100.90
2	C	301	MET	CG-SD-CE	-5.61	88.55	100.90
1	A	1263	PHE	N-CA-C	-5.61	106.36	113.43
2	J	301	MET	CG-SD-CE	-5.61	88.56	100.90
2	M	301	MET	CG-SD-CE	-5.61	88.56	100.90
2	G	301	MET	CG-SD-CE	-5.60	88.58	100.90
2	L	301	MET	CG-SD-CE	-5.59	88.59	100.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	MET	CG-SD-CE	-5.59	88.60	100.90
2	I	301	MET	CG-SD-CE	-5.59	88.60	100.90
2	C	46	MET	N-CA-C	-5.59	100.86	108.24
2	K	301	MET	CG-SD-CE	-5.58	88.63	100.90
2	N	13	ASP	CA-CB-CG	5.57	118.17	112.60
2	I	46	MET	N-CA-C	-5.57	100.89	108.24
2	G	46	MET	N-CA-C	-5.55	100.91	108.24
2	L	46	MET	N-CA-C	-5.53	100.94	108.24
2	H	91	THR	CB-CA-C	-5.53	102.20	110.88
2	H	46	MET	N-CA-C	-5.52	100.95	108.24
2	M	46	MET	N-CA-C	-5.52	100.95	108.24
2	J	46	MET	N-CA-C	-5.52	100.95	108.24
2	D	46	MET	N-CA-C	-5.52	100.96	108.24
2	E	46	MET	N-CA-C	-5.51	100.97	108.24
2	F	91	THR	CB-CA-C	-5.50	102.24	110.88
2	L	91	THR	CB-CA-C	-5.50	102.24	110.88
2	J	91	THR	CB-CA-C	-5.50	102.25	110.88
2	M	91	THR	CB-CA-C	-5.50	102.25	110.88
2	K	46	MET	N-CA-C	-5.49	100.99	108.24
2	F	46	MET	N-CA-C	-5.49	101.00	108.24
2	K	91	THR	CB-CA-C	-5.49	102.27	110.88
2	I	91	THR	CB-CA-C	-5.48	102.28	110.88
2	D	91	THR	CB-CA-C	-5.47	102.29	110.88
2	E	91	THR	CB-CA-C	-5.43	102.35	110.88
2	G	91	THR	CB-CA-C	-5.42	102.37	110.88
2	C	91	THR	CB-CA-C	-5.41	102.38	110.88
2	F	91	THR	CA-CB-OG1	5.39	117.69	109.60
2	D	91	THR	CA-CB-OG1	5.38	117.67	109.60
2	L	91	THR	CA-CB-OG1	5.38	117.67	109.60
2	J	91	THR	CA-CB-OG1	5.38	117.66	109.60
2	H	161	VAL	CA-C-N	5.36	129.74	122.19
2	H	161	VAL	C-N-CA	5.36	129.74	122.19
2	E	91	THR	CA-CB-OG1	5.34	117.61	109.60
2	C	91	THR	CA-CB-OG1	5.34	117.61	109.60
2	H	91	THR	CA-CB-OG1	5.34	117.60	109.60
2	G	91	THR	CA-CB-OG1	5.33	117.60	109.60
2	M	161	VAL	CA-C-N	5.33	129.70	122.19
2	M	161	VAL	C-N-CA	5.33	129.70	122.19
2	K	91	THR	CA-CB-OG1	5.32	117.57	109.60
2	H	14	ASN	CA-CB-CG	-5.31	107.29	112.60
2	E	161	VAL	CA-C-N	5.30	129.66	122.19
2	E	161	VAL	C-N-CA	5.30	129.66	122.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	91	THR	CA-CB-OG1	5.29	117.54	109.60
2	I	161	VAL	CA-C-N	5.29	129.64	122.19
2	I	161	VAL	C-N-CA	5.29	129.64	122.19
2	L	14	ASN	CA-CB-CG	-5.28	107.32	112.60
2	C	82	ASP	CA-CB-CG	5.28	117.88	112.60
2	F	161	VAL	CA-C-N	5.27	129.62	122.19
2	F	161	VAL	C-N-CA	5.27	129.62	122.19
2	C	161	VAL	CA-C-N	5.27	129.62	122.19
2	C	161	VAL	C-N-CA	5.27	129.62	122.19
2	C	14	ASN	CA-CB-CG	-5.27	107.33	112.60
2	D	14	ASN	CA-CB-CG	-5.27	107.33	112.60
2	I	91	THR	CA-CB-OG1	5.27	117.50	109.60
2	D	161	VAL	CA-C-N	5.26	129.61	122.19
2	D	161	VAL	C-N-CA	5.26	129.61	122.19
2	J	161	VAL	CA-C-N	5.26	129.61	122.19
2	J	161	VAL	C-N-CA	5.26	129.61	122.19
2	F	5	ASP	CA-CB-CG	-5.25	107.35	112.60
2	G	161	VAL	CA-C-N	5.25	129.59	122.19
2	G	161	VAL	C-N-CA	5.25	129.59	122.19
2	J	14	ASN	CA-CB-CG	-5.23	107.37	112.60
2	E	8	THR	N-CA-CB	5.23	119.33	110.49
2	K	14	ASN	CA-CB-CG	-5.22	107.38	112.60
2	L	161	VAL	CA-C-N	5.22	129.56	122.19
2	L	161	VAL	C-N-CA	5.22	129.56	122.19
2	E	14	ASN	CA-CB-CG	-5.21	107.39	112.60
2	M	14	ASN	CA-CB-CG	-5.21	107.39	112.60
2	C	8	THR	N-CA-CB	5.21	119.29	110.49
2	G	14	ASN	CA-CB-CG	-5.21	107.39	112.60
2	K	5	ASP	CA-CB-CG	-5.21	107.39	112.60
2	N	254	ASN	CA-C-N	5.20	131.47	121.54
2	N	254	ASN	C-N-CA	5.20	131.47	121.54
2	K	82	ASP	CA-CB-CG	5.20	117.80	112.60
2	F	14	ASN	CA-CB-CG	-5.20	107.41	112.60
2	D	8	THR	N-CA-CB	5.19	119.27	110.49
2	N	63	LYS	CA-C-N	5.19	127.23	120.28
2	N	63	LYS	C-N-CA	5.19	127.23	120.28
2	G	8	THR	N-CA-CB	5.17	119.23	110.49
2	L	5	ASP	CA-CB-CG	-5.17	107.43	112.60
2	M	5	ASP	CA-CB-CG	-5.17	107.43	112.60
2	H	8	THR	N-CA-CB	5.17	119.23	110.49
2	I	8	THR	N-CA-CB	5.17	119.23	110.49
2	B	63	LYS	CA-C-N	5.17	127.21	120.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	LYS	C-N-CA	5.17	127.21	120.28
2	D	5	ASP	CA-CB-CG	-5.16	107.44	112.60
2	F	8	THR	N-CA-CB	5.16	119.22	110.49
2	E	82	ASP	CA-CB-CG	5.16	117.76	112.60
2	L	82	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	254	ASN	CA-C-N	5.15	131.37	121.54
2	B	254	ASN	C-N-CA	5.15	131.37	121.54
2	J	82	ASP	CA-CB-CG	5.15	117.75	112.60
2	K	8	THR	N-CA-CB	5.15	119.19	110.49
2	G	5	ASP	CA-CB-CG	-5.14	107.46	112.60
2	M	82	ASP	CA-CB-CG	5.14	117.74	112.60
2	C	5	ASP	CA-CB-CG	-5.14	107.46	112.60
2	J	8	THR	N-CA-CB	5.14	119.17	110.49
2	I	14	ASN	CA-CB-CG	-5.13	107.47	112.60
2	N	287	CYS	CA-C-N	5.12	128.95	121.31
2	N	287	CYS	C-N-CA	5.12	128.95	121.31
2	G	82	ASP	CA-CB-CG	5.12	117.72	112.60
2	M	8	THR	N-CA-CB	5.12	119.14	110.49
2	L	8	THR	N-CA-CB	5.12	119.14	110.49
2	J	5	ASP	CA-CB-CG	-5.11	107.49	112.60
2	F	23	PHE	CA-CB-CG	-5.11	108.69	113.80
2	H	82	ASP	CA-CB-CG	5.11	117.71	112.60
2	E	23	PHE	CA-CB-CG	-5.11	108.69	113.80
2	H	111	PRO	N-CA-C	5.10	119.32	111.21
2	I	5	ASP	CA-CB-CG	-5.09	107.51	112.60
2	I	23	PHE	CA-CB-CG	-5.09	108.71	113.80
2	F	82	ASP	CA-CB-CG	5.09	117.69	112.60
2	H	5	ASP	CA-CB-CG	-5.09	107.51	112.60
2	M	23	PHE	CA-CB-CG	-5.09	108.71	113.80
2	C	23	PHE	CA-CB-CG	-5.09	108.71	113.80
2	I	111	PRO	N-CA-C	5.08	119.29	111.21
2	K	161	VAL	CA-C-N	5.08	129.61	122.09
2	K	161	VAL	C-N-CA	5.08	129.61	122.09
2	L	23	PHE	CA-CB-CG	-5.08	108.72	113.80
2	K	23	PHE	CA-CB-CG	-5.08	108.72	113.80
2	C	111	PRO	N-CA-C	5.07	119.27	111.21
2	H	113	ASN	CB-CA-C	5.07	116.02	108.87
2	J	23	PHE	CA-CB-CG	-5.07	108.73	113.80
2	D	111	PRO	N-CA-C	5.06	119.26	111.21
2	I	82	ASP	CA-CB-CG	5.06	117.66	112.60
2	D	82	ASP	CA-CB-CG	5.06	117.66	112.60
2	G	111	PRO	N-CA-C	5.05	119.25	111.21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	23	PHE	CA-CB-CG	-5.05	108.75	113.80
2	D	23	PHE	CA-CB-CG	-5.05	108.75	113.80
2	D	290	ASP	CA-CB-CG	-5.05	107.55	112.60
2	E	111	PRO	N-CA-C	5.05	119.23	111.21
2	B	7	THR	N-CA-CB	5.03	118.99	110.49
2	D	113	ASN	CB-CA-C	5.03	115.96	108.87
2	F	111	PRO	N-CA-C	5.02	119.20	111.21
2	K	290	ASP	CA-CB-CG	-5.02	107.58	112.60
2	N	255	GLU	CA-C-N	5.02	127.01	120.28
2	N	255	GLU	C-N-CA	5.02	127.01	120.28
2	E	5	ASP	CA-CB-CG	-5.02	107.58	112.60
2	L	111	PRO	N-CA-C	5.01	119.18	111.21
2	K	111	PRO	N-CA-C	5.01	119.18	111.21
2	M	111	PRO	N-CA-C	5.01	119.17	111.21
2	G	23	PHE	CA-CB-CG	-5.00	108.80	113.80
2	J	111	PRO	N-CA-C	5.00	119.17	111.21
2	I	289	ILE	CA-C-N	5.00	126.94	120.44
2	I	289	ILE	C-N-CA	5.00	126.94	120.44
2	C	113	ASN	CB-CA-C	5.00	115.92	108.87

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1049	VAL	Peptide
1	A	1318	THR	Peptide
1	A	1842	LEU	Peptide
1	A	300	VAL	Peptide
2	B	242	TYR	Sidechain
2	B	25	GLY	Peptide
2	B	314	ARG	Sidechain
2	B	39	ARG	Sidechain
2	B	41	ARG	Sidechain
2	C	14	ASN	Peptide
2	C	223	LEU	Peptide
2	C	256	ARG	Sidechain
2	C	334	PRO	Peptide
2	C	71	TYR	Sidechain
2	D	14	ASN	Peptide
2	D	223	LEU	Peptide
2	D	256	ARG	Sidechain
2	D	334	PRO	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	D	71	TYR	Sidechain
2	E	14	ASN	Peptide
2	E	223	LEU	Peptide
2	E	256	ARG	Sidechain
2	E	334	PRO	Peptide
2	E	71	TYR	Sidechain
2	F	14	ASN	Peptide
2	F	223	LEU	Peptide
2	F	256	ARG	Sidechain
2	F	334	PRO	Peptide
2	F	71	TYR	Sidechain
2	G	14	ASN	Peptide
2	G	223	LEU	Peptide
2	G	256	ARG	Sidechain
2	G	334	PRO	Peptide
2	G	71	TYR	Sidechain
2	H	14	ASN	Peptide
2	H	223	LEU	Peptide
2	H	256	ARG	Sidechain
2	H	334	PRO	Peptide
2	H	71	TYR	Sidechain
2	I	14	ASN	Peptide
2	I	223	LEU	Peptide
2	I	256	ARG	Sidechain
2	I	334	PRO	Peptide
2	I	71	TYR	Sidechain
2	J	14	ASN	Peptide
2	J	223	LEU	Peptide
2	J	256	ARG	Sidechain
2	J	334	PRO	Peptide
2	J	71	TYR	Sidechain
2	K	14	ASN	Peptide
2	K	223	LEU	Peptide
2	K	256	ARG	Sidechain
2	K	334	PRO	Peptide
2	K	71	TYR	Sidechain
2	L	14	ASN	Peptide
2	L	223	LEU	Peptide
2	L	256	ARG	Sidechain
2	L	334	PRO	Peptide
2	L	71	TYR	Sidechain
2	M	14	ASN	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	M	223	LEU	Peptide
2	M	256	ARG	Sidechain
2	M	334	PRO	Peptide
2	M	71	TYR	Sidechain
2	N	185	ARG	Sidechain
2	N	258	ARG	Sidechain
2	N	30	ARG	Sidechain
2	N	314	ARG	Sidechain
2	N	39	ARG	Sidechain
2	N	41	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	11415	0	11748	141	0
2	B	2925	0	2885	70	0
2	C	2925	0	2887	68	0
2	D	2925	0	2885	71	0
2	E	2925	0	2887	56	0
2	F	2925	0	2887	62	0
2	G	2925	0	2887	44	0
2	H	2925	0	2887	37	0
2	I	2925	0	2887	46	0
2	J	2925	0	2887	71	0
2	K	2925	0	2887	89	0
2	L	2925	0	2887	52	0
2	M	2925	0	2887	66	0
2	N	2925	0	2887	50	0
All	All	49440	0	49275	578	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 6.

All (578) 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:K:353:THR:CG2	2:M:47:VAL:HG11	1.27	1.62
2:K:353:THR:HG21	2:M:47:VAL:CG1	1.14	1.60
2:D:289:ILE:CG2	2:K:246:ASP:CB	1.74	1.59
2:B:246:ASP:HB2	2:H:289:ILE:CG2	1.25	1.59
2:D:289:ILE:CG2	2:K:246:ASP:HB2	1.14	1.58
2:N:246:ASP:HB2	2:B:289:ILE:CG2	1.34	1.56
2:N:246:ASP:CG	2:B:289:ILE:HG23	1.30	1.55
2:C:246:ASP:CG	2:G:289:ILE:HG23	1.14	1.55
2:C:246:ASP:HB2	2:G:289:ILE:CG2	1.39	1.53
2:K:353:THR:CG2	2:M:47:VAL:CG1	1.83	1.51
2:D:289:ILE:HG23	2:K:246:ASP:CG	1.03	1.46
2:N:47:VAL:HG21	2:B:357:MET:SD	1.56	1.46
2:L:197:GLU:HB2	2:M:115:LYS:CG	1.47	1.46
2:B:246:ASP:CB	2:H:289:ILE:HG23	1.45	1.45
2:J:41:ARG:HH11	2:K:272:GLU:CG	1.33	1.41
2:D:289:ILE:CG2	2:K:246:ASP:CG	1.90	1.41
2:C:246:ASP:CB	2:G:289:ILE:CG2	1.95	1.40
2:D:170:GLY:HA2	2:K:46:MET:SD	1.64	1.37
2:N:246:ASP:CB	2:B:289:ILE:CG2	2.00	1.37
2:C:246:ASP:CG	2:G:289:ILE:CG2	2.00	1.34
2:C:357:MET:SD	2:F:47:VAL:HG21	1.66	1.34
1:A:2002:ARG:CB	2:E:27:ASP:OD2	1.75	1.31
2:I:357:MET:SD	2:J:47:VAL:HG21	1.69	1.30
2:N:47:VAL:CG2	2:B:357:MET:SD	2.19	1.30
1:A:2003:VAL:HG11	2:E:26:ASP:C	1.58	1.29
1:A:2006:ARG:HH21	2:E:347:ILE:CD1	1.46	1.29
2:N:246:ASP:OD1	2:B:289:ILE:HG23	1.13	1.28
2:K:353:THR:CB	2:M:47:VAL:HG11	1.63	1.28
1:A:2006:ARG:NH2	2:E:347:ILE:HD13	1.47	1.27
2:J:170:GLY:CA	2:L:46:MET:SD	2.22	1.27
2:I:170:GLY:CA	2:J:46:MET:HE2	1.64	1.26
2:B:204:THR:HG23	2:G:272:GLU:OE1	1.33	1.24
1:A:2006:ARG:CZ	2:E:347:ILE:HD12	1.67	1.23
1:A:2006:ARG:NH2	2:E:347:ILE:CD1	1.98	1.23
2:C:46:MET:SD	2:G:170:GLY:HA2	1.79	1.22
2:L:197:GLU:CB	2:M:115:LYS:HG3	1.70	1.21
1:A:2006:ARG:NE	2:E:347:ILE:HD12	1.54	1.20
2:K:289:ILE:HG23	2:M:246:ASP:OD2	1.39	1.19
2:B:272:GLU:OE2	2:C:41:ARG:NH1	1.75	1.18
2:J:170:GLY:HA3	2:L:46:MET:SD	1.82	1.18
2:K:289:ILE:HG22	2:M:246:ASP:HB2	1.25	1.17
2:D:170:GLY:CA	2:K:46:MET:SD	2.33	1.17

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLY:HA3	2:H:171:TYR:CE1	1.80	1.17
2:I:170:GLY:CA	2:J:46:MET:CE	2.23	1.17
2:N:246:ASP:CG	2:B:289:ILE:CG2	2.13	1.16
2:C:357:MET:SD	2:F:47:VAL:CG2	2.33	1.16
2:J:41:ARG:NH1	2:K:272:GLU:CG	2.09	1.15
2:B:44:GLY:HA3	2:H:171:TYR:HE1	1.04	1.14
1:A:2003:VAL:HG13	2:E:27:ASP:N	1.63	1.14
2:J:170:GLY:HA2	2:L:46:MET:SD	1.83	1.13
2:I:171:TYR:CE1	2:J:49:MET:SD	2.43	1.11
2:J:41:ARG:NH1	2:K:272:GLU:HG3	1.63	1.10
2:C:44:GLY:HA2	2:G:171:TYR:CD1	1.87	1.10
2:D:289:ILE:HG21	2:K:246:ASP:HB2	1.26	1.10
2:D:289:ILE:HG21	2:K:246:ASP:CB	1.78	1.08
1:A:2003:VAL:CG1	2:E:27:ASP:N	2.17	1.08
2:I:171:TYR:CZ	2:J:49:MET:SD	2.46	1.08
2:J:41:ARG:HH11	2:K:272:GLU:HG3	0.99	1.08
2:I:170:GLY:HA2	2:J:46:MET:CE	1.82	1.07
2:I:170:GLY:HA3	2:J:46:MET:CE	1.83	1.07
2:N:246:ASP:OD1	2:B:289:ILE:CG2	2.03	1.06
2:B:47:VAL:HG11	2:H:353:THR:HG21	1.35	1.06
2:D:289:ILE:HG23	2:K:246:ASP:OD1	1.55	1.06
2:K:289:ILE:HG23	2:M:246:ASP:CG	1.80	1.05
2:D:171:TYR:CD1	2:K:44:GLY:HA2	1.91	1.04
2:D:170:GLY:HA3	2:K:46:MET:CG	1.88	1.03
2:I:170:GLY:HA3	2:J:46:MET:HE2	1.05	1.03
1:A:2003:VAL:CG1	2:E:26:ASP:C	2.31	1.03
2:D:289:ILE:HG23	2:K:246:ASP:CB	1.60	1.02
1:A:2002:ARG:HB2	2:E:27:ASP:OD2	0.84	1.02
2:N:41:ARG:NH1	2:C:272:GLU:OE2	1.94	1.00
2:K:289:ILE:HG22	2:M:246:ASP:CB	1.90	1.00
2:K:353:THR:HG21	2:M:47:VAL:HG13	1.04	1.00
2:D:272:GLU:OE1	2:I:204:THR:HG23	1.60	1.00
1:A:2003:VAL:HG11	2:E:26:ASP:CA	1.92	0.99
2:D:47:VAL:HG21	2:F:357:MET:SD	2.02	0.99
2:D:170:GLY:HA3	2:K:46:MET:HG3	1.44	0.98
2:K:353:THR:HG21	2:M:47:VAL:HG12	1.45	0.98
2:N:246:ASP:CB	2:B:289:ILE:HG22	1.76	0.98
2:L:197:GLU:HB2	2:M:115:LYS:CD	1.93	0.98
2:C:46:MET:SD	2:G:170:GLY:CA	2.52	0.98
1:A:2002:ARG:HB2	2:E:27:ASP:CG	1.87	0.98
2:N:272:GLU:OE2	2:F:41:ARG:NH1	1.96	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44:GLY:CA	2:G:171:TYR:CE1	2.47	0.98
2:I:272:GLU:OE2	2:K:41:ARG:NH1	1.96	0.97
2:D:171:TYR:CE1	2:K:44:GLY:HA3	1.99	0.97
2:L:197:GLU:CG	2:M:115:LYS:HD2	1.94	0.97
2:K:353:THR:HG22	2:M:47:VAL:HG11	1.46	0.96
2:B:246:ASP:CB	2:H:289:ILE:CG2	2.21	0.96
2:J:41:ARG:CD	2:K:272:GLU:HG2	1.96	0.96
1:A:2006:ARG:HH21	2:E:347:ILE:HD13	0.79	0.96
2:C:246:ASP:CB	2:G:289:ILE:HG23	1.78	0.96
1:A:2003:VAL:HG21	2:E:26:ASP:HA	1.48	0.95
2:C:44:GLY:HA3	2:G:171:TYR:CE1	2.02	0.95
2:K:353:THR:HB	2:M:47:VAL:HG11	1.48	0.94
2:L:41:ARG:HH11	2:M:272:GLU:HG3	1.32	0.94
2:D:46:MET:SD	2:F:170:GLY:CA	2.54	0.94
2:B:44:GLY:CA	2:H:171:TYR:CE1	2.51	0.94
2:J:41:ARG:HH11	2:K:272:GLU:HG2	1.33	0.93
2:D:171:TYR:CE1	2:K:44:GLY:CA	2.52	0.93
1:A:2006:ARG:CZ	2:E:347:ILE:CD1	2.42	0.93
2:N:246:ASP:CB	2:B:289:ILE:HG23	1.83	0.92
2:C:46:MET:CG	2:G:170:GLY:HA3	1.99	0.92
2:N:246:ASP:HB2	2:B:289:ILE:HG22	0.94	0.92
2:D:272:GLU:OE2	2:I:41:ARG:NH1	2.03	0.92
2:N:246:ASP:HB2	2:B:289:ILE:HG21	1.52	0.91
2:C:246:ASP:OD2	2:G:289:ILE:HG23	1.71	0.91
2:C:46:MET:HG3	2:G:170:GLY:HA3	1.52	0.91
2:L:197:GLU:HB2	2:M:115:LYS:HG3	0.93	0.91
2:K:289:ILE:CG2	2:M:246:ASP:CB	2.49	0.90
2:C:246:ASP:CB	2:G:289:ILE:HG22	1.75	0.90
2:N:47:VAL:HG22	2:B:357:MET:SD	2.08	0.90
2:B:246:ASP:CG	2:H:289:ILE:HG23	1.96	0.89
2:D:289:ILE:HG22	2:K:246:ASP:CB	1.68	0.89
2:C:44:GLY:HA2	2:G:171:TYR:HD1	1.37	0.89
2:L:197:GLU:CB	2:M:115:LYS:CG	2.41	0.89
2:B:204:THR:HG23	2:G:272:GLU:CD	1.98	0.88
2:L:41:ARG:HH11	2:M:272:GLU:CG	1.76	0.88
2:K:289:ILE:O	2:M:246:ASP:OD1	1.92	0.87
2:D:171:TYR:HD1	2:K:44:GLY:HA2	1.33	0.87
2:C:246:ASP:HB2	2:G:289:ILE:HG22	0.88	0.87
1:A:2006:ARG:NE	2:E:347:ILE:CD1	2.37	0.87
2:L:197:GLU:CD	2:M:115:LYS:HD2	1.99	0.87
2:J:272:GLU:OE2	2:M:41:ARG:HD3	1.74	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:MET:SD	2:F:170:GLY:HA3	2.13	0.86
2:C:246:ASP:OD1	2:G:289:ILE:HG23	1.74	0.86
2:D:47:VAL:CG1	2:F:353:THR:HG21	2.04	0.86
1:A:2006:ARG:HE	2:E:347:ILE:HD12	1.37	0.85
2:B:44:GLY:CA	2:H:171:TYR:HE1	1.86	0.85
2:J:41:ARG:CZ	2:K:272:GLU:OE2	2.24	0.85
2:K:289:ILE:CG2	2:M:246:ASP:CG	2.49	0.85
2:B:246:ASP:OD1	2:H:292:ARG:NH1	2.10	0.85
2:I:357:MET:SD	2:J:47:VAL:CG2	2.61	0.84
2:D:289:ILE:HG22	2:K:246:ASP:HB2	0.86	0.84
2:B:246:ASP:HB2	2:H:289:ILE:HG22	1.55	0.84
2:J:41:ARG:NH1	2:K:272:GLU:OE2	2.10	0.84
2:I:170:GLY:CA	2:J:46:MET:SD	2.65	0.84
2:B:44:GLY:HA2	2:H:171:TYR:CD1	2.12	0.83
2:D:46:MET:SD	2:F:170:GLY:HA2	2.17	0.83
2:B:47:VAL:CG1	2:H:353:THR:HG21	2.09	0.83
2:K:327:MET:HE1	2:M:246:ASP:O	1.78	0.83
2:D:171:TYR:HE1	2:K:44:GLY:HA3	1.41	0.82
2:J:41:ARG:HD2	2:K:272:GLU:HG2	1.61	0.82
2:D:47:VAL:HG11	2:F:353:THR:CG2	2.09	0.82
2:J:353:THR:HG21	2:L:47:VAL:CG1	2.09	0.82
2:C:246:ASP:CB	2:G:289:ILE:HG21	2.09	0.81
2:B:272:GLU:CG	2:C:41:ARG:HH11	1.93	0.81
2:D:47:VAL:HG11	2:F:353:THR:HG21	1.62	0.81
2:D:44:GLY:HA3	2:F:171:TYR:HE1	1.45	0.81
2:N:46:MET:HE2	2:B:170:GLY:HA2	1.61	0.81
2:D:171:TYR:CD1	2:K:44:GLY:CA	2.65	0.80
2:C:44:GLY:CA	2:G:171:TYR:CD1	2.64	0.80
2:B:272:GLU:HG2	2:C:41:ARG:HH11	1.45	0.79
2:B:204:THR:CG2	2:G:272:GLU:CD	2.55	0.79
2:B:204:THR:CG2	2:G:272:GLU:OE1	2.24	0.79
1:A:2006:ARG:HE	2:E:347:ILE:CD1	1.93	0.78
2:B:47:VAL:HG11	2:H:353:THR:CG2	2.12	0.78
2:N:41:ARG:HH11	2:C:272:GLU:HG2	1.49	0.78
2:N:170:GLY:HA3	2:E:46:MET:HE2	1.64	0.77
2:K:353:THR:CB	2:M:47:VAL:CG1	2.43	0.77
2:J:170:GLY:HA3	2:L:46:MET:CG	2.14	0.77
2:I:272:GLU:OE1	2:K:204:THR:HG23	1.84	0.77
2:C:246:ASP:HB2	2:G:289:ILE:HG21	1.63	0.77
2:B:44:GLY:HA2	2:H:171:TYR:HD1	1.48	0.76
2:I:272:GLU:CG	2:K:41:ARG:HH11	1.98	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:197:GLU:CA	2:M:115:LYS:HG3	2.16	0.76
2:N:46:MET:HG3	2:B:170:GLY:HA3	1.66	0.76
2:N:41:ARG:HH11	2:C:272:GLU:CG	1.99	0.76
2:D:47:VAL:CG2	2:F:357:MET:SD	2.74	0.76
2:J:41:ARG:NH1	2:K:272:GLU:CD	2.43	0.76
2:C:44:GLY:CA	2:G:171:TYR:HE1	1.97	0.75
2:B:49:MET:SD	2:H:171:TYR:CZ	2.79	0.75
2:N:47:VAL:CG2	2:B:357:MET:CE	2.64	0.75
2:B:46:MET:HG3	2:H:170:GLY:HA3	1.67	0.75
2:C:44:GLY:HA3	2:G:171:TYR:HE1	1.51	0.75
2:L:197:GLU:CB	2:M:115:LYS:CD	2.64	0.74
2:D:289:ILE:HG23	2:K:246:ASP:OD2	1.85	0.74
2:B:272:GLU:CD	2:C:41:ARG:NH1	2.46	0.73
2:K:289:ILE:CG2	2:M:246:ASP:HB2	2.11	0.73
2:L:197:GLU:CB	2:M:115:LYS:HD2	2.19	0.72
2:D:171:TYR:HE1	2:K:44:GLY:CA	1.99	0.72
1:A:2054:ARG:HE	2:E:148:GLY:C	1.99	0.71
2:B:246:ASP:HB2	2:H:289:ILE:HG23	0.72	0.71
2:B:44:GLY:CA	2:H:171:TYR:CD1	2.72	0.71
1:A:2003:VAL:HG13	2:E:27:ASP:CA	2.19	0.71
2:D:272:GLU:CD	2:I:204:THR:HG23	2.16	0.70
2:L:197:GLU:CG	2:M:115:LYS:CD	2.68	0.70
2:C:46:MET:CG	2:G:170:GLY:CA	2.70	0.70
2:B:272:GLU:CG	2:C:41:ARG:NH1	2.54	0.70
2:C:357:MET:SD	2:F:47:VAL:HG22	2.29	0.70
2:I:170:GLY:HA2	2:J:46:MET:SD	2.30	0.70
2:C:170:GLY:HA2	2:F:46:MET:SD	2.32	0.69
2:J:41:ARG:HD3	2:K:272:GLU:HG2	1.71	0.69
1:A:2003:VAL:CG2	2:E:26:ASP:HA	2.22	0.69
2:B:204:THR:HG21	2:G:272:GLU:OE2	1.93	0.69
1:A:2002:ARG:CA	2:E:27:ASP:OD2	2.41	0.68
1:A:1080:PRO:HB2	1:A:1239:LEU:HD21	1.74	0.68
2:D:44:GLY:CA	2:F:171:TYR:HE1	2.06	0.68
2:J:171:TYR:HE1	2:L:44:GLY:HA3	1.57	0.68
2:J:171:TYR:CD1	2:L:44:GLY:HA2	2.29	0.68
1:A:2054:ARG:NE	2:E:148:GLY:O	2.26	0.68
2:C:353:THR:HG21	2:F:47:VAL:CG1	2.24	0.68
2:N:44:GLY:HA2	2:B:171:TYR:HD1	1.57	0.68
2:K:357:MET:SD	2:M:47:VAL:CG2	2.81	0.68
2:N:47:VAL:CG2	2:B:357:MET:HE1	2.24	0.68
2:N:292:ARG:HD2	2:E:246:ASP:OD1	1.94	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:353:THR:HG21	2:L:47:VAL:HG11	1.75	0.67
2:L:41:ARG:NH1	2:M:272:GLU:HG3	2.09	0.67
1:A:2002:ARG:O	2:E:27:ASP:HB3	1.94	0.67
2:N:46:MET:HG3	2:B:170:GLY:CA	2.24	0.67
2:I:170:GLY:HA2	2:J:46:MET:HE1	1.73	0.67
2:J:353:THR:CG2	2:L:47:VAL:HG11	2.24	0.67
2:D:44:GLY:CA	2:F:171:TYR:CE1	2.79	0.66
2:D:44:GLY:HA3	2:F:171:TYR:CE1	2.29	0.66
2:B:46:MET:CG	2:H:170:GLY:HA3	2.25	0.66
2:J:171:TYR:CE1	2:L:44:GLY:CA	2.80	0.65
2:D:170:GLY:HA2	2:K:46:MET:CE	2.27	0.64
2:D:170:GLY:CA	2:K:46:MET:CG	2.63	0.64
2:J:171:TYR:CE1	2:L:44:GLY:HA3	2.33	0.64
2:B:246:ASP:HB2	2:H:289:ILE:HG21	1.62	0.64
2:N:289:ILE:O	2:E:246:ASP:HA	1.96	0.64
2:C:170:GLY:CA	2:F:46:MET:SD	2.86	0.63
2:D:44:GLY:HA2	2:F:171:TYR:CD1	2.33	0.63
2:K:289:ILE:O	2:M:246:ASP:CG	2.40	0.63
1:A:2002:ARG:C	2:E:27:ASP:HB3	2.23	0.63
1:A:2003:VAL:HG13	2:E:27:ASP:H	1.62	0.63
2:D:46:MET:CE	2:F:170:GLY:HA3	2.29	0.62
1:A:312:LEU:HD21	1:A:372:VAL:HA	1.80	0.62
2:C:353:THR:CG2	2:F:47:VAL:CG1	2.78	0.62
2:D:49:MET:SD	2:F:171:TYR:CZ	2.92	0.62
2:I:357:MET:CE	2:J:47:VAL:HG21	2.29	0.62
2:K:353:THR:HG22	2:M:47:VAL:CG1	2.10	0.62
2:J:170:GLY:CA	2:L:46:MET:CE	2.78	0.61
2:D:46:MET:HE2	2:F:170:GLY:HA3	1.83	0.61
2:D:170:GLY:CA	2:K:46:MET:CE	2.79	0.61
2:J:171:TYR:HE1	2:L:44:GLY:CA	2.13	0.61
2:D:46:MET:CE	2:F:170:GLY:CA	2.78	0.61
2:N:272:GLU:HG2	2:F:41:ARG:HH11	1.66	0.61
2:B:46:MET:SD	2:H:170:GLY:CA	2.89	0.61
2:J:272:GLU:OE2	2:M:41:ARG:CD	2.47	0.61
2:N:44:GLY:CA	2:B:171:TYR:CD1	2.84	0.60
2:I:272:GLU:HG2	2:K:41:ARG:HH11	1.66	0.60
1:A:1670:GLN:HE21	1:A:1771:PHE:HD2	1.49	0.60
2:K:171:TYR:CE1	2:M:44:GLY:HA2	2.36	0.60
1:A:1373:ALA:O	1:A:1686:GLN:NE2	2.34	0.60
2:N:170:GLY:CA	2:E:46:MET:HE2	2.30	0.60
1:A:982:ARG:O	1:A:1317:LYS:NZ	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:GLY:HA3	2:K:46:MET:SD	2.24	0.59
1:A:177:ASN:OD1	1:A:219:ARG:NH2	2.36	0.59
1:A:865:ARG:NH1	1:A:918:ASP:OD1	2.36	0.59
2:K:353:THR:CG2	2:M:47:VAL:HG13	1.85	0.59
2:D:272:GLU:CD	2:I:204:THR:CG2	2.76	0.58
2:C:353:THR:CG2	2:F:47:VAL:HG11	2.33	0.58
2:N:171:TYR:CE1	2:E:49:MET:SD	2.96	0.58
2:D:272:GLU:CG	2:I:41:ARG:HH11	2.15	0.58
1:A:932:ILE:HD11	1:A:1031:LEU:HB3	1.84	0.58
2:N:44:GLY:HA3	2:B:171:TYR:CE1	2.39	0.58
2:B:46:MET:SD	2:H:170:GLY:HA2	2.43	0.58
1:A:1493:ILE:HG12	1:A:1497:ILE:HG13	1.86	0.58
2:C:171:TYR:HE1	2:F:44:GLY:HA3	1.68	0.58
2:N:47:VAL:HG22	2:B:357:MET:CE	2.33	0.57
2:N:46:MET:HE2	2:B:170:GLY:CA	2.32	0.57
1:A:924:ARG:HD2	1:A:1024:GLY:HA3	1.86	0.57
1:A:2054:ARG:NE	2:E:148:GLY:C	2.63	0.57
2:I:357:MET:CE	2:J:47:VAL:CG2	2.82	0.57
1:A:2003:VAL:HG11	2:E:26:ASP:HA	1.84	0.57
2:C:170:GLY:CA	2:F:46:MET:HE2	2.35	0.57
2:D:44:GLY:HA2	2:F:171:TYR:CE1	2.40	0.57
1:A:203:ARG:NH2	1:A:242:PHE:O	2.38	0.56
2:J:171:TYR:CE1	2:L:44:GLY:HA2	2.40	0.56
1:A:693:LEU:HB2	1:A:756:TYR:HE2	1.71	0.56
2:J:170:GLY:HA3	2:L:46:MET:CE	2.35	0.56
1:A:861:TYR:HD2	1:A:864:VAL:HG23	1.71	0.56
2:N:46:MET:CE	2:B:170:GLY:HA2	2.33	0.56
2:D:272:GLU:HG2	2:I:41:ARG:HH11	1.70	0.56
2:N:44:GLY:HA3	2:B:171:TYR:CD1	2.41	0.55
1:A:358:TYR:OH	1:A:684:CYS:SG	2.65	0.55
1:A:1978:GLU:O	1:A:2015:ARG:NH1	2.39	0.55
2:K:289:ILE:CG2	2:M:246:ASP:OD2	2.33	0.55
2:I:171:TYR:H	2:J:46:MET:CG	2.19	0.55
1:A:1787:PHE:HB3	1:A:1842:LEU:HD22	1.87	0.55
1:A:1737:GLU:HG2	1:A:1794:ARG:HB3	1.89	0.54
1:A:2003:VAL:HG13	2:E:27:ASP:CB	2.37	0.54
2:L:197:GLU:HB2	2:M:115:LYS:HD2	1.74	0.54
2:B:204:THR:CG2	2:G:272:GLU:OE2	2.55	0.54
1:A:1904:ASP:HB2	1:A:1935:PRO:HB3	1.89	0.54
2:L:197:GLU:HG3	2:M:115:LYS:CD	2.38	0.54
1:A:1708:CYS:O	1:A:1712:ASN:ND2	2.40	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:44:GLY:HA2	2:B:171:TYR:CD1	2.39	0.54
1:A:2001:PHE:HB2	1:A:2004:LEU:HB2	1.90	0.53
2:N:246:ASP:CB	2:B:289:ILE:HG21	2.17	0.53
2:C:170:GLY:HA2	2:F:46:MET:CE	2.38	0.53
1:A:360:LEU:O	1:A:364:HIS:ND1	2.39	0.53
2:N:272:GLU:CG	2:F:41:ARG:HH11	2.21	0.53
2:C:171:TYR:CE1	2:F:44:GLY:HA3	2.44	0.53
1:A:690:ALA:HB2	1:A:734:LEU:HD11	1.90	0.53
1:A:938:LEU:HD12	1:A:1001:ASN:HB3	1.90	0.53
2:B:46:MET:SD	2:H:170:GLY:HA3	2.49	0.53
2:B:204:THR:HG21	2:G:272:GLU:CD	2.33	0.53
2:N:41:ARG:NH1	2:C:272:GLU:CD	2.65	0.53
2:N:41:ARG:NH1	2:C:272:GLU:CG	2.70	0.53
1:A:1279:GLU:OE2	1:A:1314:GLN:NE2	2.42	0.52
2:J:272:GLU:CD	2:M:41:ARG:HD3	2.34	0.52
2:K:357:MET:SD	2:M:47:VAL:HG21	2.48	0.52
2:K:171:TYR:CE1	2:M:44:GLY:CA	2.93	0.52
1:A:297:GLY:HA2	1:A:300:VAL:HB	1.90	0.52
1:A:1979:GLY:HA2	1:A:2015:ARG:HH12	1.75	0.52
1:A:1081:LEU:HD21	1:A:1238:ARG:HB3	1.92	0.52
1:A:209:LEU:O	1:A:213:LEU:N	2.43	0.52
2:D:170:GLY:CA	2:K:46:MET:HE2	2.39	0.51
2:I:272:GLU:CG	2:K:41:ARG:NH1	2.71	0.51
2:C:171:TYR:CD1	2:F:44:GLY:HA2	2.45	0.51
1:A:2009:ASP:OD2	1:A:2052:HIS:ND1	2.44	0.51
1:A:1803:PHE:HD2	1:A:1843:VAL:HG11	1.75	0.51
2:I:170:GLY:C	2:J:46:MET:SD	2.93	0.51
1:A:1753:GLU:O	1:A:1757:THR:OG1	2.28	0.51
2:C:170:GLY:HA3	2:F:46:MET:HE2	1.93	0.50
2:J:41:ARG:HD3	2:K:272:GLU:CG	2.41	0.50
2:L:197:GLU:OE1	2:M:115:LYS:HD2	2.11	0.50
2:K:353:THR:HB	2:M:47:VAL:CG1	2.26	0.50
2:D:289:ILE:CG2	2:K:246:ASP:OD2	2.52	0.50
1:A:1087:GLN:HB3	1:A:1266:PHE:HD1	1.77	0.50
2:J:272:GLU:OE2	2:M:41:ARG:NH1	2.45	0.50
1:A:1614:ILE:HG13	1:A:1623:MET:HE3	1.94	0.50
1:A:2003:VAL:CG1	2:E:26:ASP:CA	2.79	0.50
1:A:1082:ASP:OD1	1:A:1082:ASP:N	2.44	0.49
2:G:122:THR:HG21	2:G:372:VAL:HG22	1.94	0.49
1:A:399:GLY:HA3	1:A:403:GLN:HE22	1.76	0.49
2:I:122:THR:HG21	2:I:372:VAL:HG22	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:171:TYR:CZ	2:L:49:MET:SD	3.06	0.49
2:M:122:THR:HG21	2:M:372:VAL:HG22	1.95	0.49
2:N:170:GLY:CA	2:E:46:MET:CE	2.90	0.49
2:D:122:THR:HG21	2:D:372:VAL:HG22	1.95	0.49
2:K:122:THR:HG21	2:K:372:VAL:HG22	1.94	0.49
2:F:122:THR:HG21	2:F:372:VAL:HG22	1.94	0.49
2:J:197:GLU:HB2	2:K:115:LYS:HG3	1.95	0.49
1:A:295:LEU:HB3	1:A:314:VAL:HG13	1.94	0.49
1:A:1593:GLN:HE21	1:A:1640:ILE:HD13	1.78	0.49
1:A:1910:LEU:HD12	1:A:1946:ASN:HD21	1.76	0.49
1:A:1693:LEU:HB3	1:A:1736:PRO:HB2	1.94	0.49
2:D:47:VAL:HG11	2:F:353:THR:HG22	1.92	0.49
1:A:948:ASP:HB2	1:A:951:VAL:HG23	1.94	0.48
2:C:170:GLY:CA	2:F:46:MET:CE	2.91	0.48
1:A:149:GLU:HB3	1:A:1252:VAL:HG13	1.95	0.48
2:J:122:THR:HG21	2:J:372:VAL:HG22	1.94	0.48
1:A:1932:HIS:HB3	2:E:5:ASP:OD2	2.14	0.48
2:H:122:THR:HG21	2:H:372:VAL:HG22	1.95	0.48
2:C:122:THR:HG21	2:C:372:VAL:HG22	1.94	0.48
1:A:171:TYR:CZ	1:A:208:ASN:HB3	2.49	0.48
1:A:300:VAL:HG22	1:A:301:PRO:HD3	1.96	0.48
1:A:1425:PHE:O	1:A:1429:VAL:N	2.43	0.48
2:C:171:TYR:CE1	2:F:44:GLY:CA	2.97	0.48
1:A:279:GLN:HE21	1:A:324:LEU:HD21	1.79	0.48
2:B:246:ASP:OD1	2:H:289:ILE:HG23	2.14	0.48
2:E:122:THR:HG21	2:E:372:VAL:HG22	1.94	0.48
1:A:2043:LEU:HB3	1:A:2049:ALA:HB2	1.95	0.48
2:N:289:ILE:O	2:E:246:ASP:OD1	2.31	0.48
2:D:46:MET:HE2	2:F:170:GLY:CA	2.41	0.48
2:L:122:THR:HG21	2:L:372:VAL:HG22	1.94	0.47
1:A:1535:VAL:HA	1:A:1539:ILE:HD12	1.95	0.47
2:I:272:GLU:CD	2:K:41:ARG:NH1	2.69	0.47
2:C:353:THR:HG22	2:F:47:VAL:HG11	1.95	0.47
2:I:357:MET:HE1	2:J:47:VAL:CG2	2.44	0.47
1:A:198:ARG:NH2	1:A:200:GLN:OE1	2.48	0.47
1:A:256:ILE:HA	1:A:259:LEU:HD23	1.97	0.47
1:A:679:ALA:HB3	1:A:682:VAL:HG23	1.97	0.47
1:A:1046:HIS:HB2	1:A:1063:THR:HG21	1.96	0.47
2:N:102:GLU:HB2	2:N:103:HIS:CD2	2.50	0.47
2:K:171:TYR:HE1	2:M:44:GLY:CA	2.28	0.47
1:A:354:LEU:HB3	1:A:391:LEU:HD12	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:GLU:CD	2:N:4:GLU:N	2.73	0.47
2:D:161:VAL:HG12	2:D:163:HIS:CE1	2.50	0.47
2:B:102:GLU:HB2	2:B:103:HIS:CD2	2.50	0.47
2:I:272:GLU:CD	2:K:204:THR:HG23	2.39	0.47
1:A:840:SER:OG	1:A:841:SER:N	2.49	0.46
1:A:1442:VAL:HG21	1:A:1489:GLU:HB2	1.98	0.46
2:L:161:VAL:HG12	2:L:163:HIS:CE1	2.51	0.46
1:A:170:LEU:HB3	1:A:190:PHE:CE1	2.50	0.46
2:N:41:ARG:HH11	2:C:272:GLU:CD	2.23	0.46
2:K:161:VAL:HG12	2:K:163:HIS:CE1	2.51	0.46
2:M:228:GLU:HA	2:M:231:THR:HG22	1.97	0.46
2:J:161:VAL:HG12	2:J:163:HIS:CE1	2.50	0.46
1:A:695:THR:O	1:A:748:GLN:NE2	2.48	0.46
2:N:353:THR:HG22	2:E:47:VAL:HG11	1.98	0.46
2:H:228:GLU:HA	2:H:231:THR:HG22	1.98	0.46
2:J:41:ARG:CD	2:K:272:GLU:CG	2.83	0.46
1:A:202:CYS:SG	1:A:203:ARG:N	2.89	0.46
1:A:1465:LEU:HD11	1:A:1471:PHE:HB3	1.98	0.46
2:F:161:VAL:HG12	2:F:163:HIS:CE1	2.51	0.46
2:G:161:VAL:HG12	2:G:163:HIS:CE1	2.51	0.46
2:H:161:VAL:HG12	2:H:163:HIS:CE1	2.50	0.46
2:M:161:VAL:HG12	2:M:163:HIS:CE1	2.51	0.46
1:A:1925:GLN:HG3	1:A:1960:ARG:HH11	1.79	0.46
1:A:1019:ARG:HG3	1:A:1078:TRP:HZ2	1.80	0.46
2:C:47:VAL:HG11	2:G:353:THR:HB	1.97	0.46
2:C:228:GLU:HA	2:C:231:THR:HG22	1.98	0.46
2:F:228:GLU:HA	2:F:231:THR:HG22	1.98	0.46
2:L:197:GLU:O	2:M:115:LYS:HB2	2.16	0.46
2:N:272:GLU:CG	2:F:41:ARG:NH1	2.79	0.46
2:J:171:TYR:HD1	2:L:44:GLY:HA2	1.75	0.46
2:J:353:THR:HG21	2:L:47:VAL:HG13	1.93	0.46
2:B:46:MET:HE2	2:H:170:GLY:CA	2.45	0.45
2:E:244:LEU:HD13	2:E:250:ILE:HG12	1.98	0.45
2:G:228:GLU:HA	2:G:231:THR:HG22	1.98	0.45
1:A:2001:PHE:HD2	1:A:2004:LEU:HD22	1.82	0.45
2:I:161:VAL:HG12	2:I:163:HIS:CE1	2.50	0.45
1:A:167:GLN:HE21	1:A:193:LEU:HB3	1.80	0.45
1:A:995:ASP:HB3	1:A:998:MET:HB3	1.97	0.45
1:A:1309:THR:O	1:A:1313:GLN:N	2.47	0.45
1:A:1892:GLU:OE1	1:A:1895:ARG:NH1	2.47	0.45
2:C:46:MET:CE	2:G:170:GLY:HA2	2.43	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:161:VAL:HG12	2:C:163:HIS:CE1	2.51	0.45
2:C:246:ASP:OD2	2:G:289:ILE:CG2	2.45	0.45
2:K:171:TYR:CD1	2:M:44:GLY:HA2	2.51	0.45
2:L:228:GLU:HA	2:L:231:THR:HG22	1.98	0.45
1:A:1452:LEU:HD23	1:A:1455:LEU:HD12	1.97	0.45
2:E:161:VAL:HG12	2:E:163:HIS:CE1	2.51	0.45
2:G:244:LEU:HD13	2:G:250:ILE:HG12	1.99	0.45
2:K:228:GLU:HA	2:K:231:THR:HG22	1.98	0.45
1:A:935:VAL:HG11	1:A:1002:LEU:HD23	1.97	0.45
1:A:1823:ARG:HD2	1:A:1853:GLU:HG2	1.98	0.45
2:I:228:GLU:HA	2:I:231:THR:HG22	1.98	0.45
2:D:46:MET:CG	2:F:170:GLY:HA3	2.46	0.45
1:A:1003:SER:HB2	1:A:1044:GLY:HA2	1.99	0.45
1:A:1599:ASN:N	1:A:1599:ASN:OD1	2.50	0.45
1:A:819:SER:HB2	1:A:822:THR:HG23	1.98	0.45
2:L:244:LEU:HD13	2:L:250:ILE:HG12	1.99	0.45
1:A:191:ALA:HB1	1:A:234:LYS:HB2	1.99	0.44
1:A:671:GLY:O	1:A:683:HIS:ND1	2.49	0.44
2:D:46:MET:CE	2:F:170:GLY:HA2	2.47	0.44
2:D:228:GLU:HA	2:D:231:THR:HG22	1.98	0.44
1:A:756:TYR:HB2	1:A:768:THR:HG21	1.99	0.44
1:A:1069:MET:O	1:A:1072:THR:OG1	2.32	0.44
1:A:2054:ARG:HG3	2:E:148:GLY:O	2.18	0.44
2:C:244:LEU:HD13	2:C:250:ILE:HG12	1.99	0.44
2:D:244:LEU:HD13	2:D:250:ILE:HG12	1.99	0.44
2:F:244:LEU:HD13	2:F:250:ILE:HG12	1.99	0.44
2:E:228:GLU:HA	2:E:231:THR:HG22	1.98	0.44
2:H:244:LEU:HD13	2:H:250:ILE:HG12	1.99	0.44
2:I:171:TYR:N	2:J:46:MET:CG	2.80	0.44
1:A:1895:ARG:NH2	1:A:1926:ASP:OD2	2.50	0.44
2:B:4:GLU:CD	2:B:4:GLU:N	2.76	0.44
1:A:1297:LEU:HA	1:A:1300:CYS:HB3	2.00	0.44
2:J:228:GLU:HA	2:J:231:THR:HG22	1.98	0.44
1:A:1263:PHE:O	1:A:1267:LEU:N	2.44	0.44
2:N:272:GLU:CD	2:F:41:ARG:NH1	2.71	0.44
2:D:142:LEU:O	2:D:344:GLY:HA3	2.18	0.44
2:F:142:LEU:O	2:F:344:GLY:HA3	2.18	0.44
2:I:272:GLU:CD	2:K:41:ARG:HH11	2.24	0.44
2:N:170:GLY:HA2	2:E:46:MET:CE	2.48	0.44
1:A:716:LEU:HD13	1:A:768:THR:HG23	2.00	0.44
2:M:244:LEU:HD13	2:M:250:ILE:HG12	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:MET:HB2	1:A:1669:VAL:HG22	1.99	0.43
2:I:142:LEU:O	2:I:344:GLY:HA3	2.18	0.43
2:J:170:GLY:HA3	2:L:46:MET:HG3	1.96	0.43
2:K:244:LEU:HD13	2:K:250:ILE:HG12	1.99	0.43
2:L:41:ARG:HD2	2:M:272:GLU:HG2	0.85	0.43
1:A:1689:GLU:HG3	1:A:1792:PHE:HA	1.99	0.43
2:C:171:TYR:HE1	2:F:44:GLY:CA	2.30	0.43
2:I:244:LEU:HD13	2:I:250:ILE:HG12	1.99	0.43
1:A:382:GLN:NE2	1:A:386:THR:OG1	2.50	0.43
2:C:142:LEU:O	2:C:344:GLY:HA3	2.18	0.43
2:E:142:LEU:O	2:E:344:GLY:HA3	2.18	0.43
2:G:142:LEU:O	2:G:344:GLY:HA3	2.18	0.43
2:B:46:MET:HE2	2:H:170:GLY:HA3	2.00	0.43
2:H:142:LEU:O	2:H:344:GLY:HA3	2.18	0.43
2:L:142:LEU:O	2:L:344:GLY:HA3	2.18	0.43
1:A:299:LEU:HD22	1:A:360:LEU:HD11	2.00	0.43
1:A:1787:PHE:HA	1:A:1796:THR:HG22	2.00	0.43
2:I:171:TYR:HE1	2:J:44:GLY:HA3	1.82	0.43
2:J:244:LEU:HD13	2:J:250:ILE:HG12	1.99	0.43
1:A:1854:VAL:HG13	1:A:1855:GLN:HG3	2.00	0.43
2:C:144:LEU:HD22	2:C:167:ILE:HG21	2.01	0.43
2:M:144:LEU:HD22	2:M:167:ILE:HG21	2.01	0.43
2:E:144:LEU:HD22	2:E:167:ILE:HG21	2.01	0.43
2:J:142:LEU:O	2:J:344:GLY:HA3	2.18	0.43
2:L:144:LEU:HD22	2:L:167:ILE:HG21	2.01	0.43
2:K:142:LEU:O	2:K:344:GLY:HA3	2.18	0.42
2:M:142:LEU:O	2:M:344:GLY:HA3	2.18	0.42
2:C:221:VAL:HG22	2:C:260:PRO:HB2	2.02	0.42
1:A:1315:LEU:HD12	1:A:1425:PHE:HZ	1.84	0.42
2:G:144:LEU:HD22	2:G:167:ILE:HG21	2.01	0.42
1:A:1642:ALA:HA	1:A:1643:PRO:HD3	1.91	0.42
2:D:144:LEU:HD22	2:D:167:ILE:HG21	2.01	0.42
2:I:170:GLY:HA3	2:J:46:MET:SD	2.45	0.42
1:A:111:VAL:HA	1:A:116:ARG:HH22	1.83	0.42
1:A:1528:MET:SD	1:A:1577:ARG:NH1	2.78	0.42
1:A:1834:LEU:HD21	1:A:1894:VAL:HA	2.01	0.42
2:D:221:VAL:HG22	2:D:260:PRO:HB2	2.02	0.42
2:I:144:LEU:HD22	2:I:167:ILE:HG21	2.01	0.42
2:K:144:LEU:HD22	2:K:167:ILE:HG21	2.01	0.42
2:M:221:VAL:HG22	2:M:260:PRO:HB2	2.02	0.42
1:A:1132:ARG:HE	1:A:1135:VAL:HG21	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1832:LEU:HD23	1:A:1832:LEU:HA	1.88	0.42
2:K:221:VAL:HG22	2:K:260:PRO:HB2	2.02	0.42
1:A:1528:MET:HB2	1:A:1528:MET:HE3	1.86	0.42
2:C:170:GLY:HA3	2:F:46:MET:HG3	2.01	0.42
2:F:4:GLU:N	2:F:4:GLU:OE1	2.53	0.42
2:J:144:LEU:HD22	2:J:167:ILE:HG21	2.01	0.42
2:K:4:GLU:N	2:K:4:GLU:OE1	2.53	0.42
2:C:4:GLU:N	2:C:4:GLU:OE1	2.53	0.42
2:E:221:VAL:HG22	2:E:260:PRO:HB2	2.02	0.42
2:G:221:VAL:HG22	2:G:260:PRO:HB2	2.02	0.42
1:A:395:LEU:HB3	1:A:681:LEU:HG	2.02	0.41
1:A:2003:VAL:CG1	2:E:27:ASP:CA	2.90	0.41
2:N:171:TYR:CZ	2:E:49:MET:SD	3.14	0.41
2:D:44:GLY:HA2	2:F:171:TYR:HD1	1.79	0.41
2:F:250:ILE:HG22	2:F:252:ILE:HG23	2.02	0.41
2:J:289:ILE:HD13	2:L:246:ASP:OD2	2.20	0.41
1:A:1684:ILE:HA	1:A:1792:PHE:HZ	1.85	0.41
2:F:221:VAL:HG22	2:F:260:PRO:HB2	2.02	0.41
2:L:13:ASP:OD2	2:L:20:LYS:HE3	2.21	0.41
2:L:221:VAL:HG22	2:L:260:PRO:HB2	2.02	0.41
1:A:156:LYS:HE2	1:A:156:LYS:HB2	1.86	0.41
1:A:884:GLU:O	1:A:891:HIS:NE2	2.46	0.41
2:B:314:ARG:HE	2:B:318:GLU:CD	2.28	0.41
2:C:250:ILE:HG22	2:C:252:ILE:HG23	2.03	0.41
2:F:144:LEU:HD22	2:F:167:ILE:HG21	2.01	0.41
2:G:4:GLU:N	2:G:4:GLU:OE1	2.53	0.41
2:M:4:GLU:N	2:M:4:GLU:OE1	2.53	0.41
1:A:1742:ARG:HH21	1:A:1802:LEU:HD13	1.84	0.41
1:A:1855:GLN:HA	1:A:1895:ARG:HG3	2.02	0.41
2:B:161:VAL:HG12	2:B:163:HIS:CE1	2.56	0.41
2:D:272:GLU:CG	2:I:41:ARG:NH1	2.82	0.41
2:G:13:ASP:OD2	2:G:20:LYS:HE3	2.20	0.41
2:H:144:LEU:HD22	2:H:167:ILE:HG21	2.01	0.41
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.85	0.41
1:A:783:SER:O	1:A:785:PHE:N	2.54	0.41
2:E:250:ILE:HG22	2:E:252:ILE:HG23	2.03	0.41
2:D:4:GLU:OE1	2:D:4:GLU:N	2.53	0.41
2:D:250:ILE:HG22	2:D:252:ILE:HG23	2.03	0.41
2:I:4:GLU:OE1	2:I:4:GLU:N	2.53	0.41
2:I:221:VAL:HG22	2:I:260:PRO:HB2	2.02	0.41
2:J:13:ASP:OD2	2:J:20:LYS:HE3	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:HD21	1:A:725:LEU:HD22	2.03	0.41
2:C:353:THR:HG21	2:F:47:VAL:HG12	2.00	0.41
2:F:13:ASP:OD2	2:F:20:LYS:HE3	2.20	0.41
2:H:13:ASP:OD2	2:H:20:LYS:HE3	2.21	0.41
2:M:13:ASP:OD2	2:M:20:LYS:HE3	2.20	0.41
1:A:1237:LEU:HD23	1:A:1237:LEU:HA	1.91	0.41
1:A:1800:THR:HG22	1:A:1843:VAL:HG23	2.01	0.41
2:C:170:GLY:HA3	2:F:46:MET:SD	2.61	0.41
2:D:13:ASP:OD2	2:D:20:LYS:HE3	2.21	0.41
2:D:77:ILE:HG23	2:D:117:ASN:HD21	1.86	0.41
2:E:13:ASP:OD2	2:E:20:LYS:HE3	2.21	0.41
2:H:4:GLU:N	2:H:4:GLU:OE1	2.53	0.41
2:I:250:ILE:HG22	2:I:252:ILE:HG23	2.03	0.41
2:J:4:GLU:N	2:J:4:GLU:OE1	2.53	0.41
2:J:221:VAL:HG22	2:J:260:PRO:HB2	2.02	0.41
2:J:250:ILE:HG22	2:J:252:ILE:HG23	2.03	0.41
2:J:289:ILE:CA	2:L:246:ASP:OD1	2.67	0.41
2:K:13:ASP:OD2	2:K:20:LYS:HE3	2.21	0.41
2:L:4:GLU:OE1	2:L:4:GLU:N	2.53	0.41
2:L:250:ILE:HG22	2:L:252:ILE:HG23	2.03	0.41
2:M:250:ILE:HG22	2:M:252:ILE:HG23	2.03	0.41
1:A:1425:PHE:HB3	1:A:1429:VAL:HG23	2.03	0.41
1:A:2003:VAL:HG13	2:E:27:ASP:HB3	2.02	0.41
2:D:47:VAL:HG12	2:F:353:THR:HG21	1.98	0.41
2:J:77:ILE:HG23	2:J:117:ASN:HD21	1.86	0.41
2:L:26:ASP:OD2	2:L:30:ARG:NH2	2.54	0.41
2:C:171:TYR:HD1	2:F:44:GLY:HA2	1.85	0.40
2:E:77:ILE:HG23	2:E:117:ASN:HD21	1.86	0.40
2:G:250:ILE:HG22	2:G:252:ILE:HG23	2.03	0.40
2:H:221:VAL:HG22	2:H:260:PRO:HB2	2.02	0.40
2:M:77:ILE:HG23	2:M:117:ASN:HD21	1.87	0.40
1:A:1830:PRO:HG3	1:A:1890:ASN:OD1	2.22	0.40
2:D:26:ASP:OD2	2:D:30:ARG:NH2	2.54	0.40
2:G:77:ILE:HG23	2:G:117:ASN:HD21	1.86	0.40
2:I:171:TYR:N	2:J:46:MET:SD	2.94	0.40
2:M:26:ASP:OD2	2:M:30:ARG:NH2	2.54	0.40
2:E:26:ASP:OD2	2:E:30:ARG:NH2	2.54	0.40
2:H:221:VAL:HG21	2:H:311:ILE:HG12	2.04	0.40
2:I:26:ASP:OD2	2:I:30:ARG:NH2	2.54	0.40
2:K:197:GLU:OE2	2:K:258:ARG:NH2	2.55	0.40
2:L:197:GLU:OE2	2:L:258:ARG:NH2	2.55	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:197:GLU:OE2	2:M:258:ARG:NH2	2.55	0.40
2:M:221:VAL:HG21	2:M:311:ILE:HG12	2.04	0.40
2:F:221:VAL:HG21	2:F:311:ILE:HG12	2.04	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	1425/3144 (45%)	1341 (94%)	82 (6%)	2 (0%)	48	83
2	B	372/375 (99%)	344 (92%)	23 (6%)	5 (1%)	10	43
2	C	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	D	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	E	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	F	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	G	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	H	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	I	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	J	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	K	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	L	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	M	372/375 (99%)	354 (95%)	13 (4%)	5 (1%)	10	43
2	N	372/375 (99%)	343 (92%)	25 (7%)	4 (1%)	12	47
All	All	6261/8019 (78%)	5922 (95%)	273 (4%)	66 (1%)	15	47

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	THR
2	C	50	GLY
2	C	172	ALA
2	D	50	GLY
2	D	172	ALA
2	E	50	GLY
2	E	172	ALA
2	F	50	GLY
2	F	172	ALA
2	G	50	GLY
2	G	172	ALA
2	H	50	GLY
2	H	172	ALA
2	I	50	GLY
2	I	172	ALA
2	J	50	GLY
2	J	172	ALA
2	K	50	GLY
2	K	172	ALA
2	L	50	GLY
2	L	172	ALA
2	M	50	GLY
2	M	172	ALA
2	N	172	ALA
2	N	236	SER
2	N	255	GLU
2	B	172	ALA
2	B	236	SER
2	B	255	GLU
2	C	52	LYS
2	D	52	LYS
2	E	52	LYS
2	F	52	LYS
2	G	52	LYS
2	H	52	LYS
2	I	52	LYS
2	J	52	LYS
2	K	52	LYS
2	L	52	LYS
2	M	52	LYS
1	A	281	SER
2	N	52	LYS
2	B	52	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	C	40	PRO
2	E	40	PRO
2	D	40	PRO
2	F	40	PRO
2	G	40	PRO
2	H	40	PRO
2	I	40	PRO
2	J	40	PRO
2	K	40	PRO
2	L	40	PRO
2	M	40	PRO
1	A	1050	PRO
2	C	114	PRO
2	D	114	PRO
2	E	114	PRO
2	F	114	PRO
2	G	114	PRO
2	H	114	PRO
2	I	114	PRO
2	J	114	PRO
2	K	114	PRO
2	L	114	PRO
2	M	114	PRO

### 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	1285/2767 (46%)	1273 (99%)	12 (1%)	75	83
2	B	317/318 (100%)	308 (97%)	9 (3%)	38	57
2	C	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	D	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	E	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	F	317/318 (100%)	312 (98%)	5 (2%)	58	73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	H	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	I	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	J	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	K	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	L	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	M	317/318 (100%)	312 (98%)	5 (2%)	58	73
2	N	317/318 (100%)	308 (97%)	9 (3%)	38	57
All	All	5406/6901 (78%)	5321 (98%)	85 (2%)	58	73

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LEU
1	A	187	LEU
1	A	244	ASN
1	A	259	LEU
1	A	392	LEU
1	A	709	VAL
1	A	993	ILE
1	A	1049	VAL
1	A	1267	LEU
1	A	1706	ILE
1	A	1747	LEU
1	A	1842	LEU
2	N	4	GLU
2	N	53	ASP
2	N	82	ASP
2	N	108	THR
2	N	114	PRO
2	N	159	ASP
2	N	161	VAL
2	N	167	ILE
2	N	205	THR
2	B	27	ASP
2	B	53	ASP
2	B	82	ASP
2	B	108	THR
2	B	114	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	159	ASP
2	B	161	VAL
2	B	167	ILE
2	B	205	THR
2	C	108	THR
2	C	138	ILE
2	C	161	VAL
2	C	167	ILE
2	C	348	LEU
2	D	108	THR
2	D	138	ILE
2	D	161	VAL
2	D	167	ILE
2	D	348	LEU
2	E	108	THR
2	E	138	ILE
2	E	161	VAL
2	E	167	ILE
2	E	348	LEU
2	F	108	THR
2	F	138	ILE
2	F	161	VAL
2	F	167	ILE
2	F	348	LEU
2	G	108	THR
2	G	138	ILE
2	G	161	VAL
2	G	167	ILE
2	G	348	LEU
2	H	108	THR
2	H	138	ILE
2	H	161	VAL
2	H	167	ILE
2	H	348	LEU
2	I	108	THR
2	I	138	ILE
2	I	161	VAL
2	I	167	ILE
2	I	348	LEU
2	J	108	THR
2	J	138	ILE
2	J	161	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	J	167	ILE
2	J	348	LEU
2	K	108	THR
2	K	138	ILE
2	K	161	VAL
2	K	167	ILE
2	K	348	LEU
2	L	108	THR
2	L	138	ILE
2	L	161	VAL
2	L	167	ILE
2	L	348	LEU
2	M	108	THR
2	M	138	ILE
2	M	161	VAL
2	M	167	ILE
2	M	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	208	ASN
1	A	244	ASN
1	A	285	GLN
1	A	381	GLN
1	A	382	GLN
1	A	403	GLN
1	A	726	HIS
1	A	848	GLN
1	A	957	GLN
1	A	1011	HIS
1	A	1095	ASN
1	A	1314	GLN
1	A	1368	GLN
1	A	1447	GLN
1	A	1567	GLN
1	A	1593	GLN
1	A	1609	GLN
1	A	1670	GLN
1	A	1686	GLN
1	A	1697	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1746	GLN
1	A	1946	ASN
1	A	2023	ASN
1	A	2044	GLN
2	N	42	HIS
2	N	103	HIS
2	N	163	HIS
2	B	42	HIS
2	B	103	HIS
2	B	163	HIS
2	C	61	GLN
2	C	90	HIS
2	C	94	ASN
2	C	117	ASN
2	C	123	GLN
2	C	139	GLN
2	C	298	ASN
2	D	90	HIS
2	D	94	ASN
2	D	117	ASN
2	D	139	GLN
2	D	298	ASN
2	D	373	HIS
2	E	90	HIS
2	E	94	ASN
2	E	117	ASN
2	E	298	ASN
2	F	90	HIS
2	F	94	ASN
2	F	117	ASN
2	F	123	GLN
2	F	298	ASN
2	G	90	HIS
2	G	117	ASN
2	G	298	ASN
2	H	117	ASN
2	H	123	GLN
2	H	139	GLN
2	H	298	ASN
2	I	90	HIS
2	I	117	ASN
2	I	139	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	I	298	ASN
2	I	373	HIS
2	J	61	GLN
2	J	117	ASN
2	J	123	GLN
2	J	139	GLN
2	J	298	ASN
2	K	61	GLN
2	K	117	ASN
2	K	123	GLN
2	K	139	GLN
2	K	298	ASN
2	L	90	HIS
2	L	94	ASN
2	L	117	ASN
2	L	123	GLN
2	L	139	GLN
2	L	298	ASN
2	L	373	HIS
2	M	117	ASN
2	M	123	GLN
2	M	139	GLN
2	M	298	ASN

### 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.

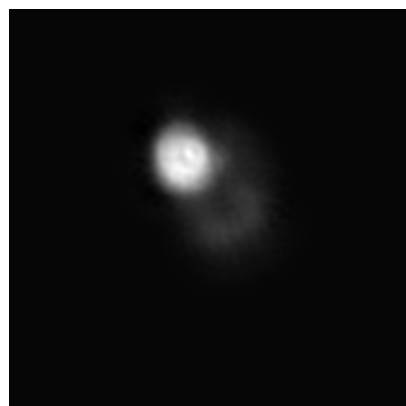
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39097. These allow visual inspection of the internal detail of the map and identification of artifacts.

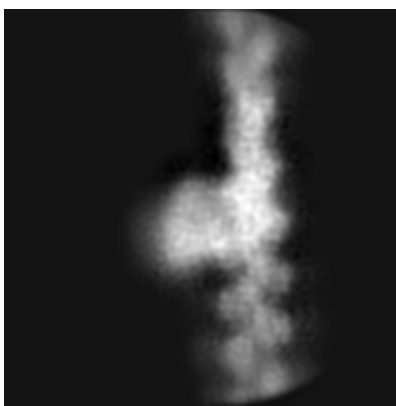
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

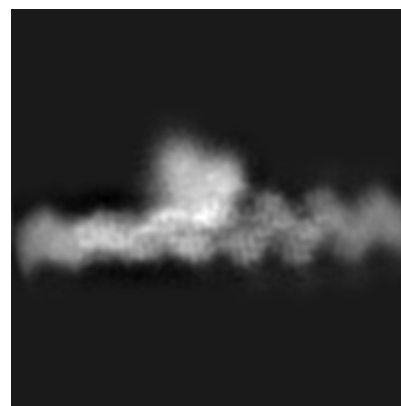
#### 6.1.1 Primary map



X

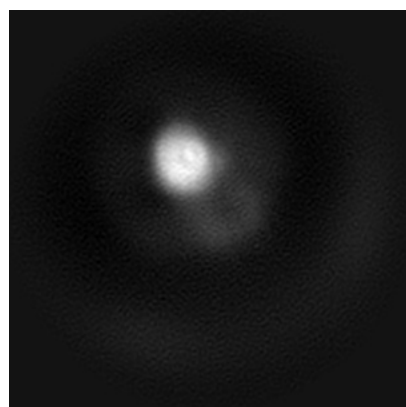


Y

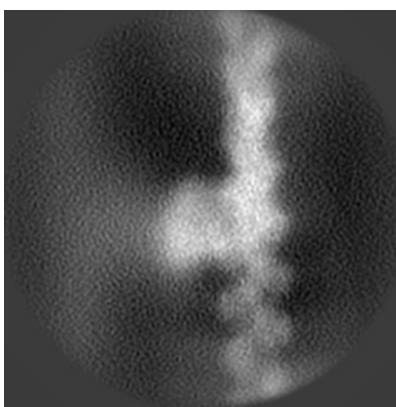


Z

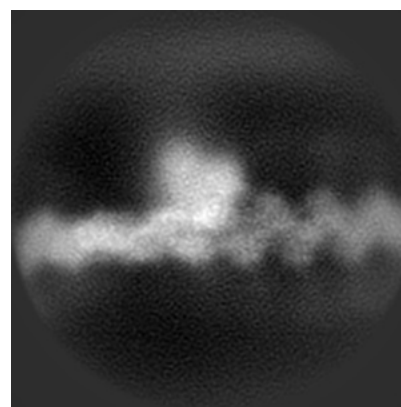
#### 6.1.2 Raw map



X



Y



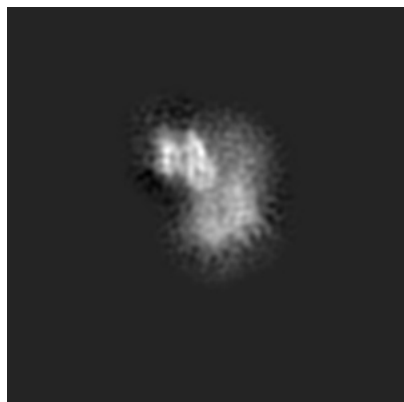
Z

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

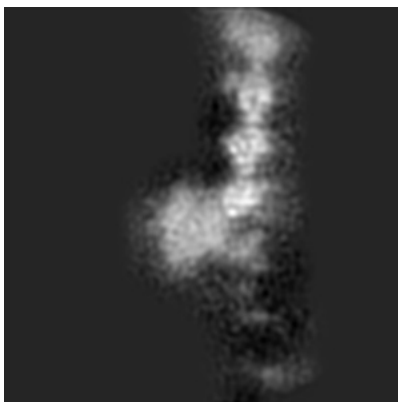


## 6.2 Central slices [i](#)

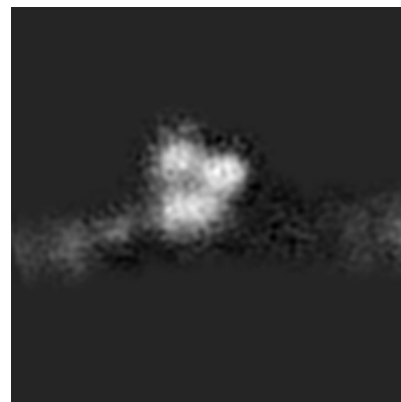
### 6.2.1 Primary map



X Index: 80

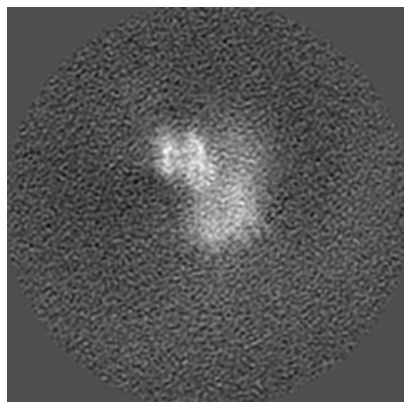


Y Index: 80

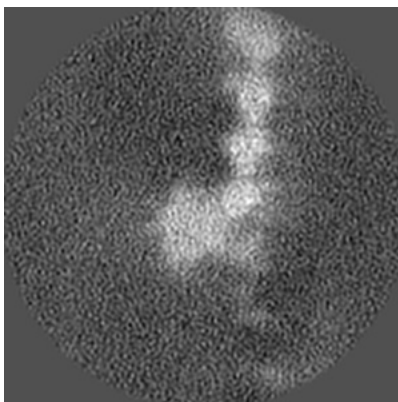


Z Index: 80

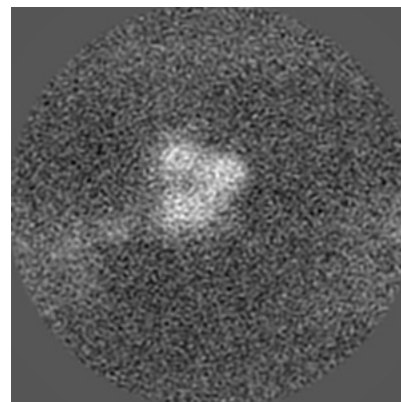
### 6.2.2 Raw map



X Index: 80



Y Index: 80

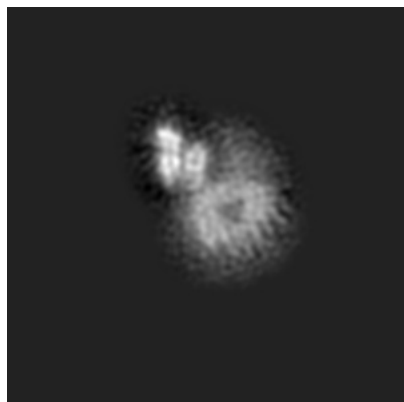


Z Index: 80

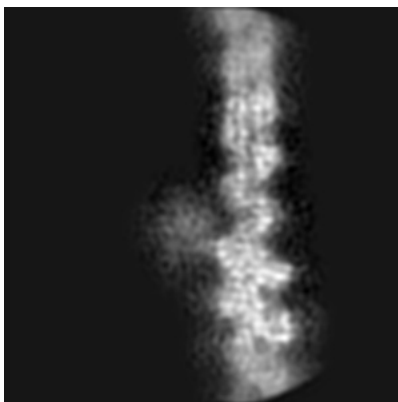
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

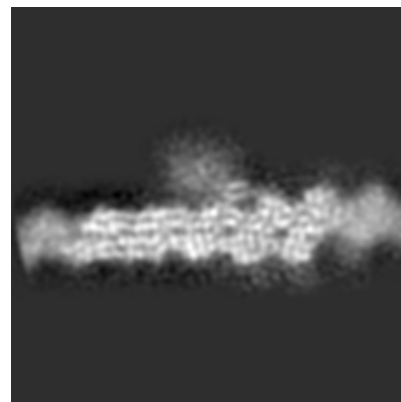
### 6.3.1 Primary map



X Index: 68

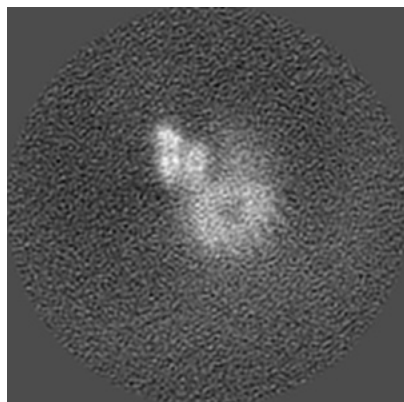


Y Index: 71

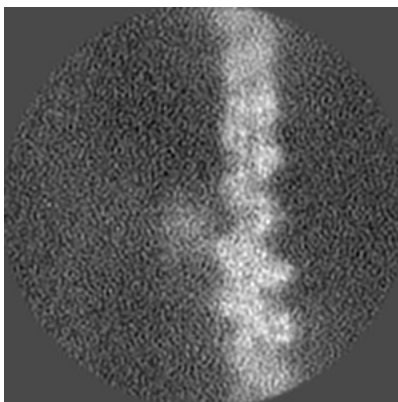


Z Index: 101

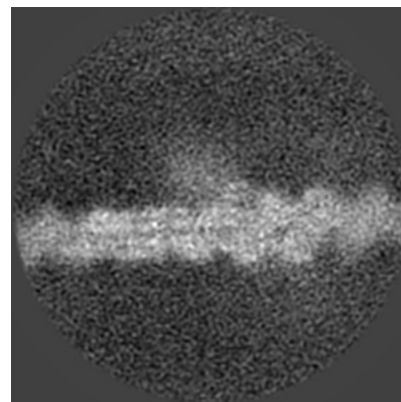
### 6.3.2 Raw map



X Index: 68



Y Index: 71



Z Index: 100

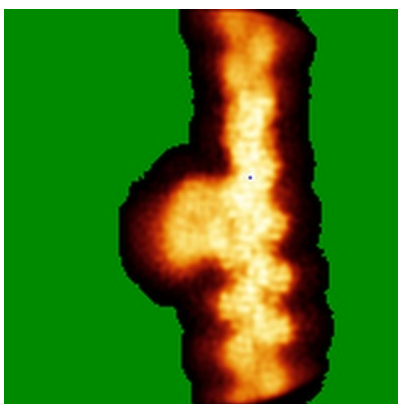
The images above show the largest variance slices of the map in three orthogonal directions.

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

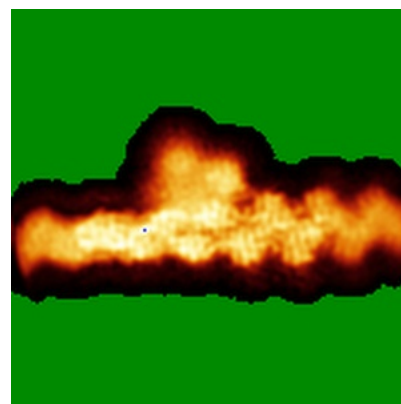
### 6.4.1 Primary map



X

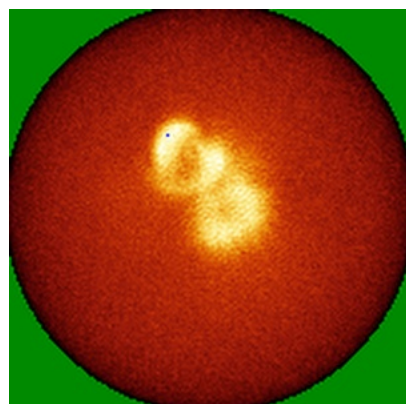


Y

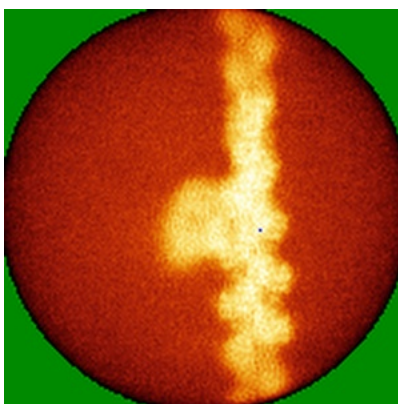


Z

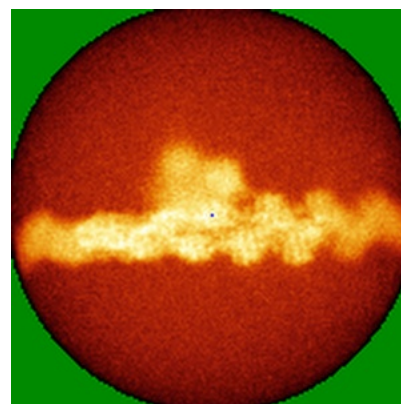
### 6.4.2 Raw map



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.

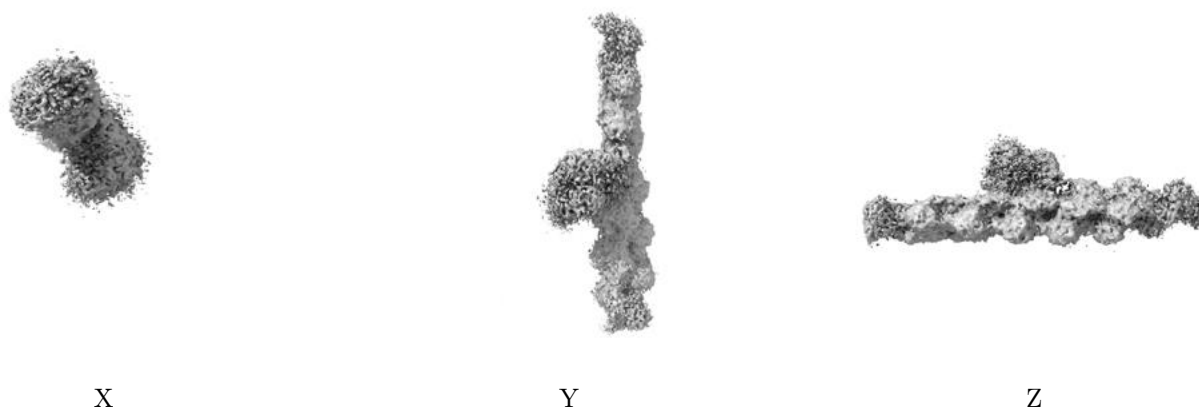
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

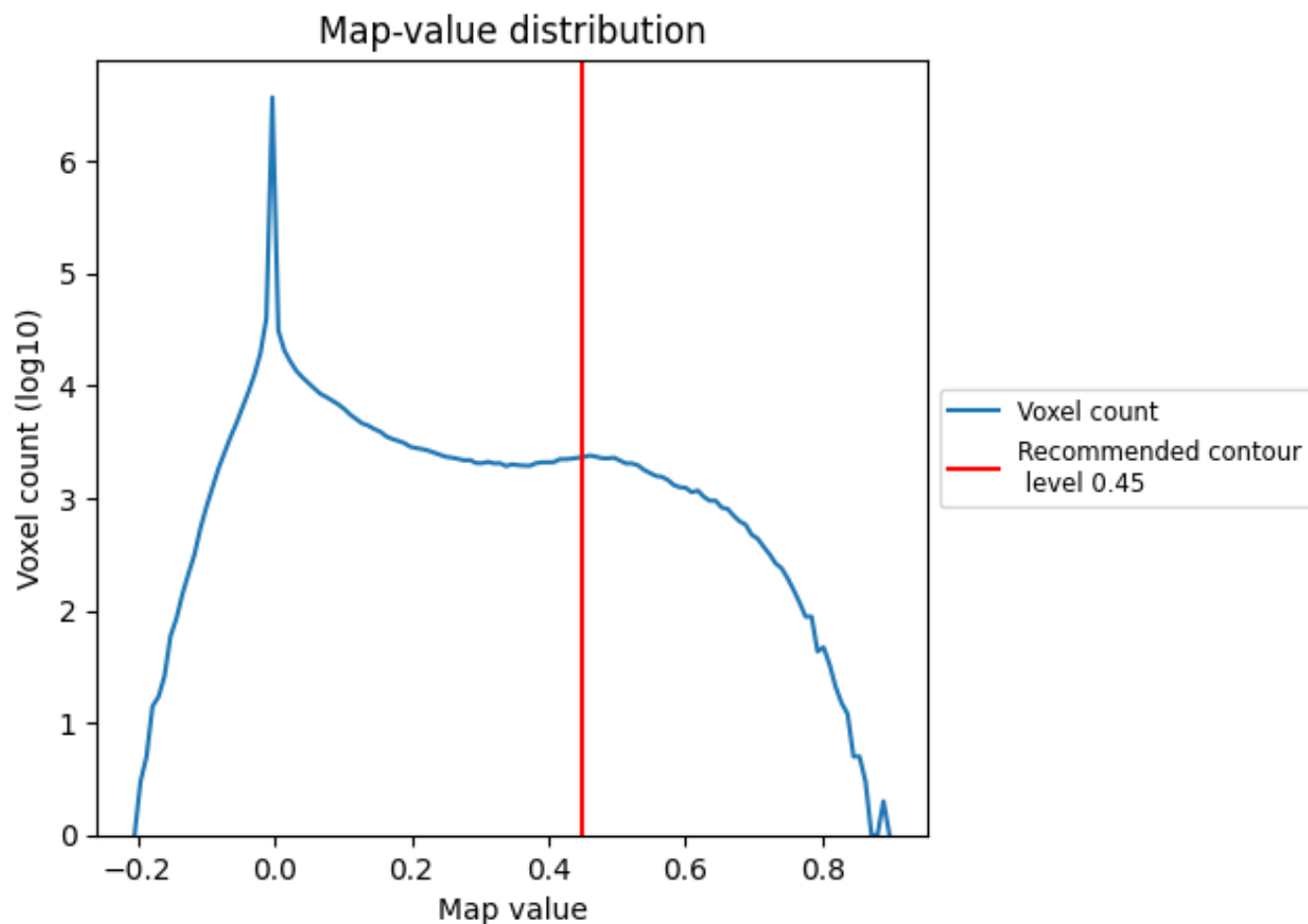
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

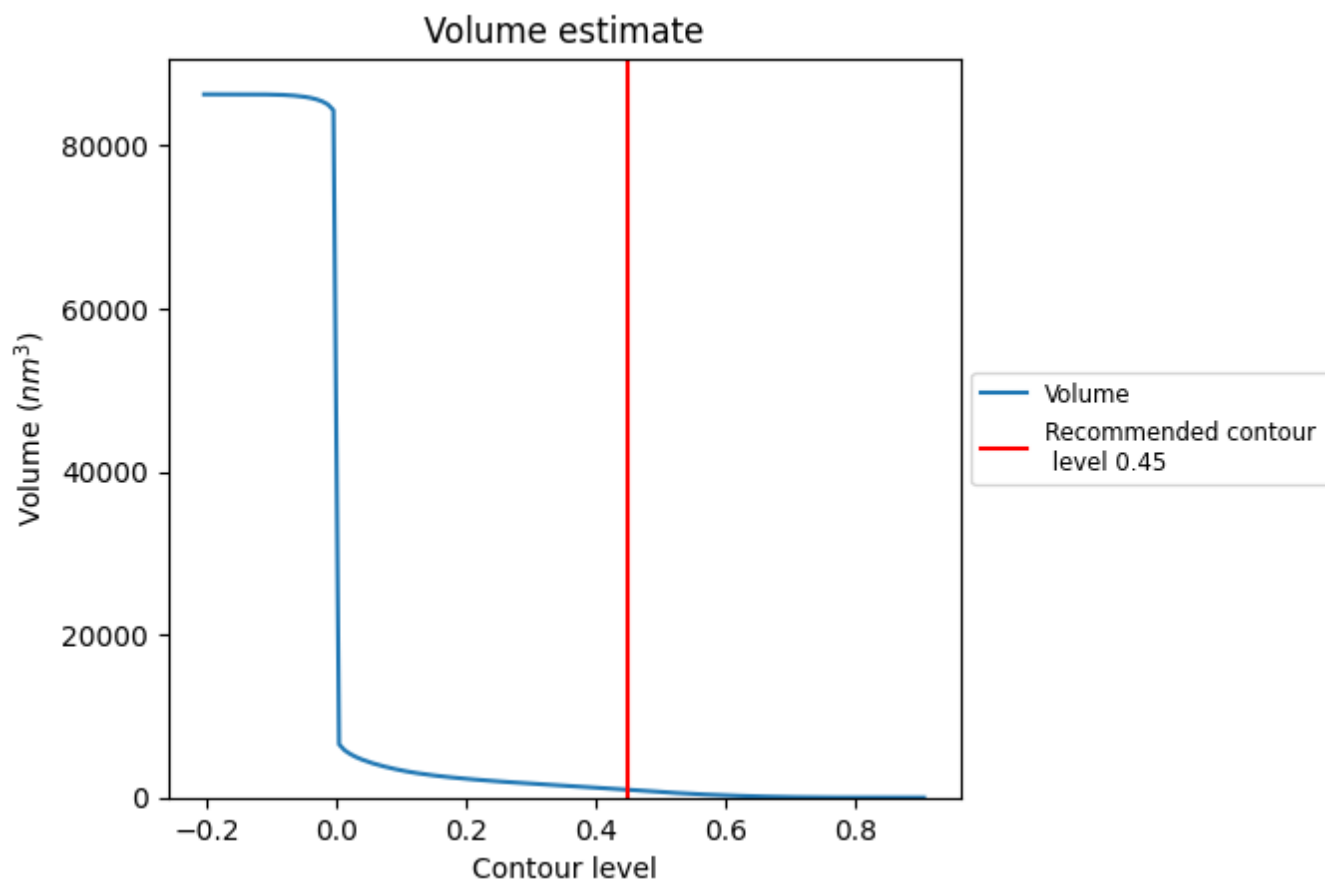
This section contains the results of statistical analysis of the map.

### 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.

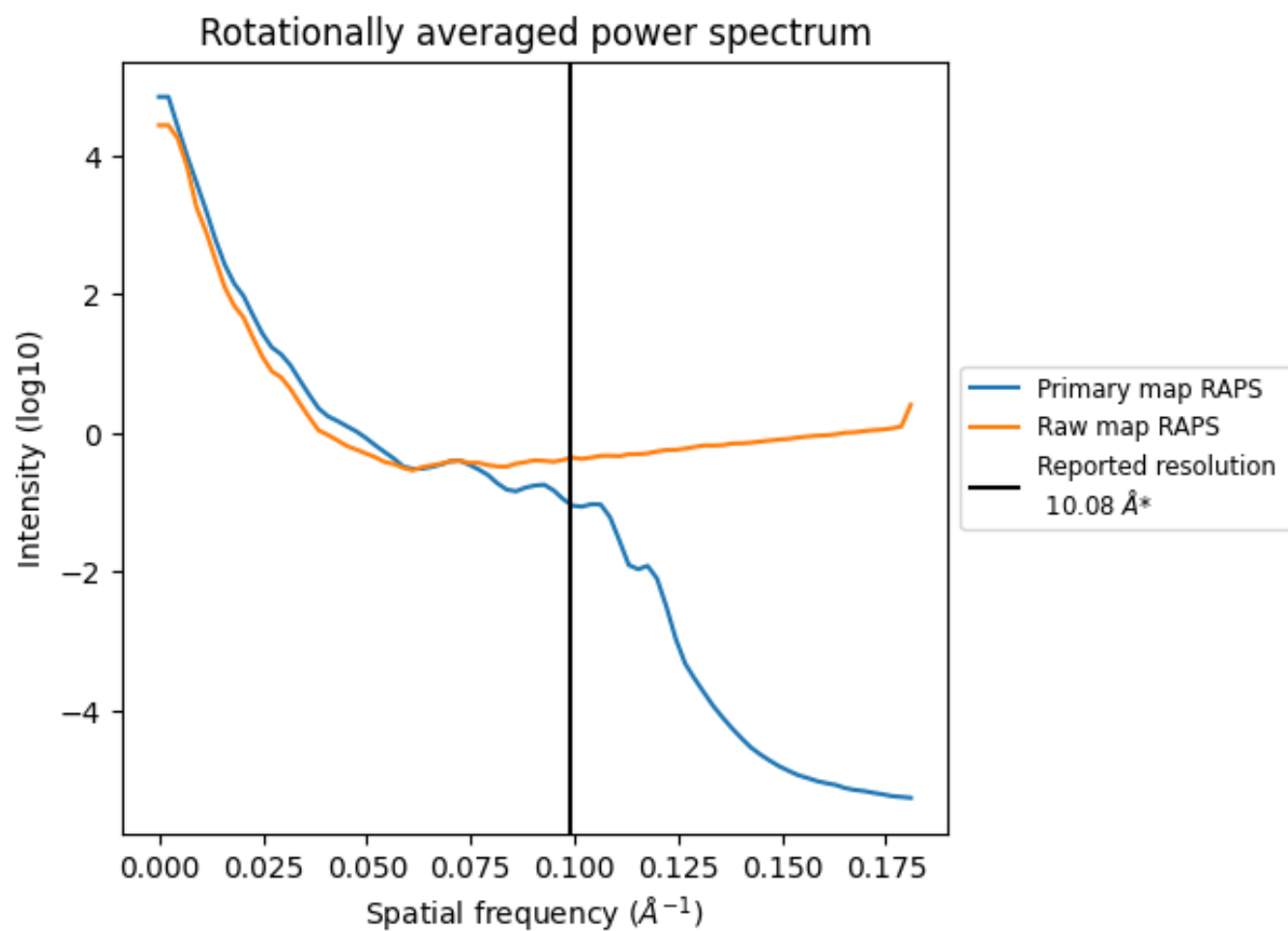
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 968 nm<sup>3</sup>; this corresponds to an approximate mass of 874 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 ⓘ

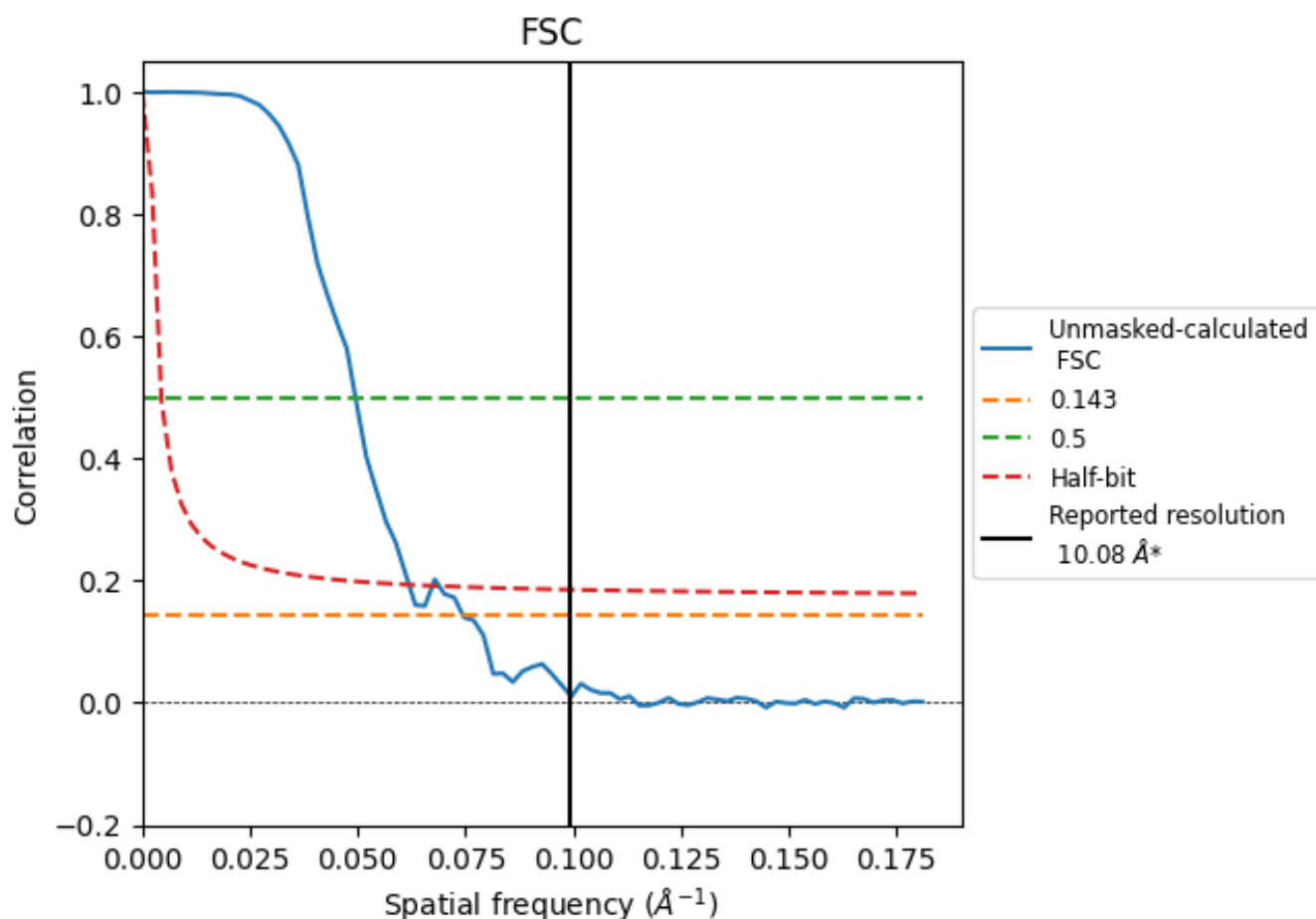


\*Reported resolution corresponds to spatial frequency of 0.099 Å<sup>-1</sup>

## 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 0.099  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

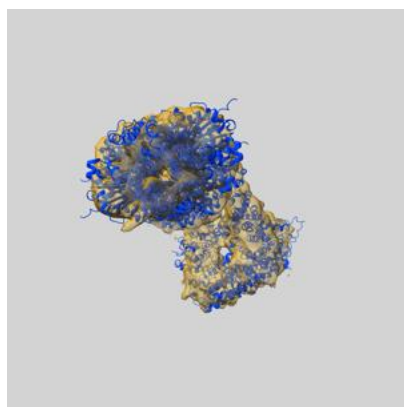
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	13.44	20.20	16.16

\*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 13.44 differs from the reported value 10.08 by more than 10 %

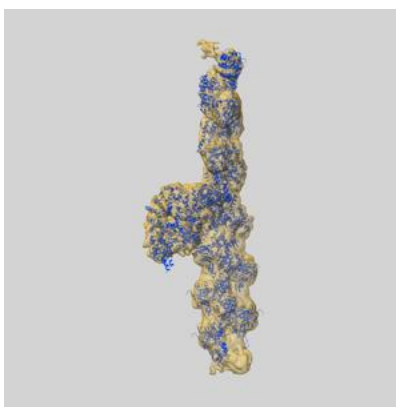
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39097 and PDB model 8YAE. Per-residue inclusion information can be found in section 3 on page 6.

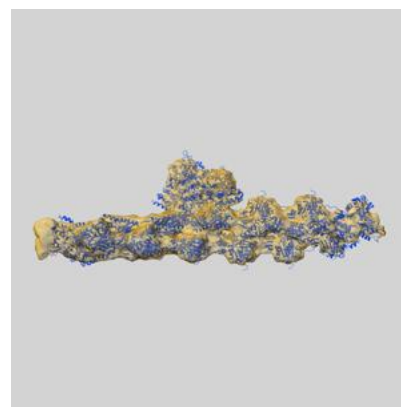
### 9.1 Map-model overlay [i](#)



X



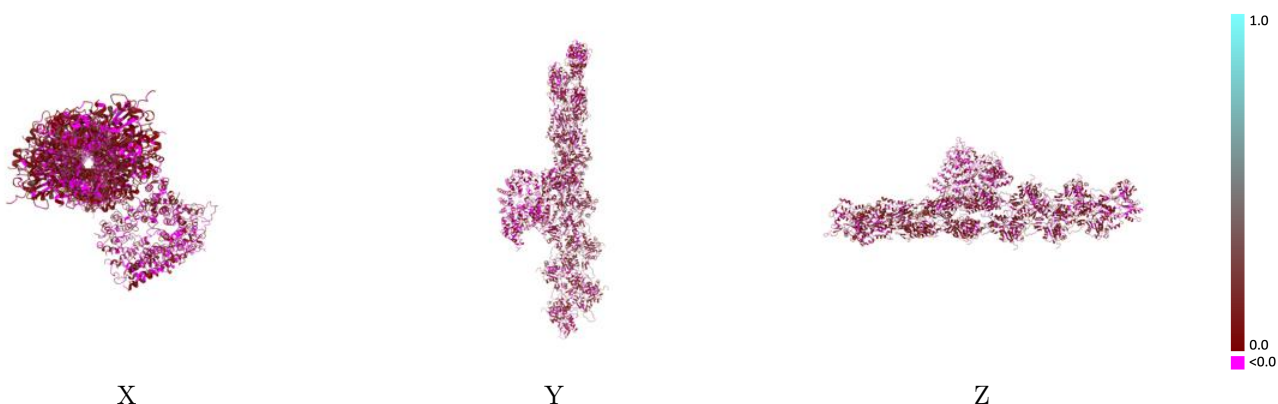
Y



Z

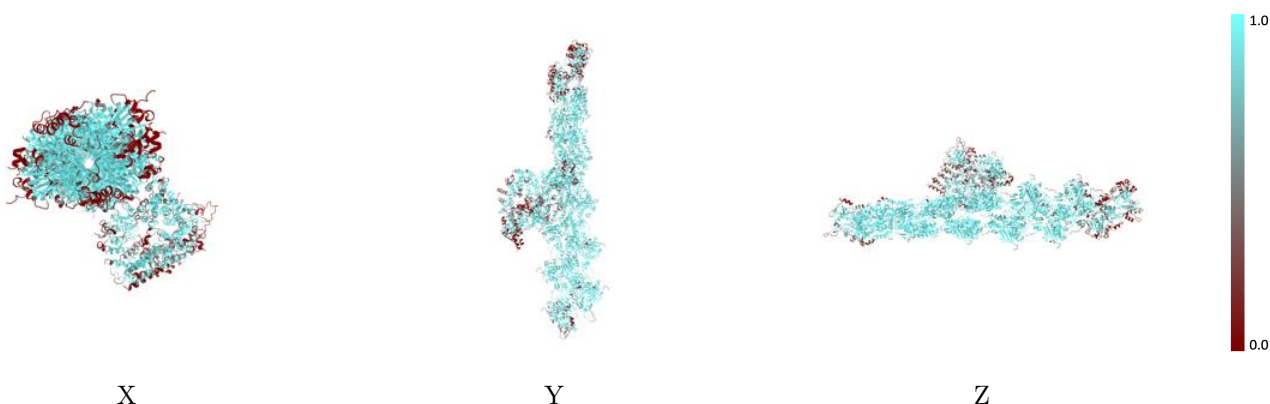
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



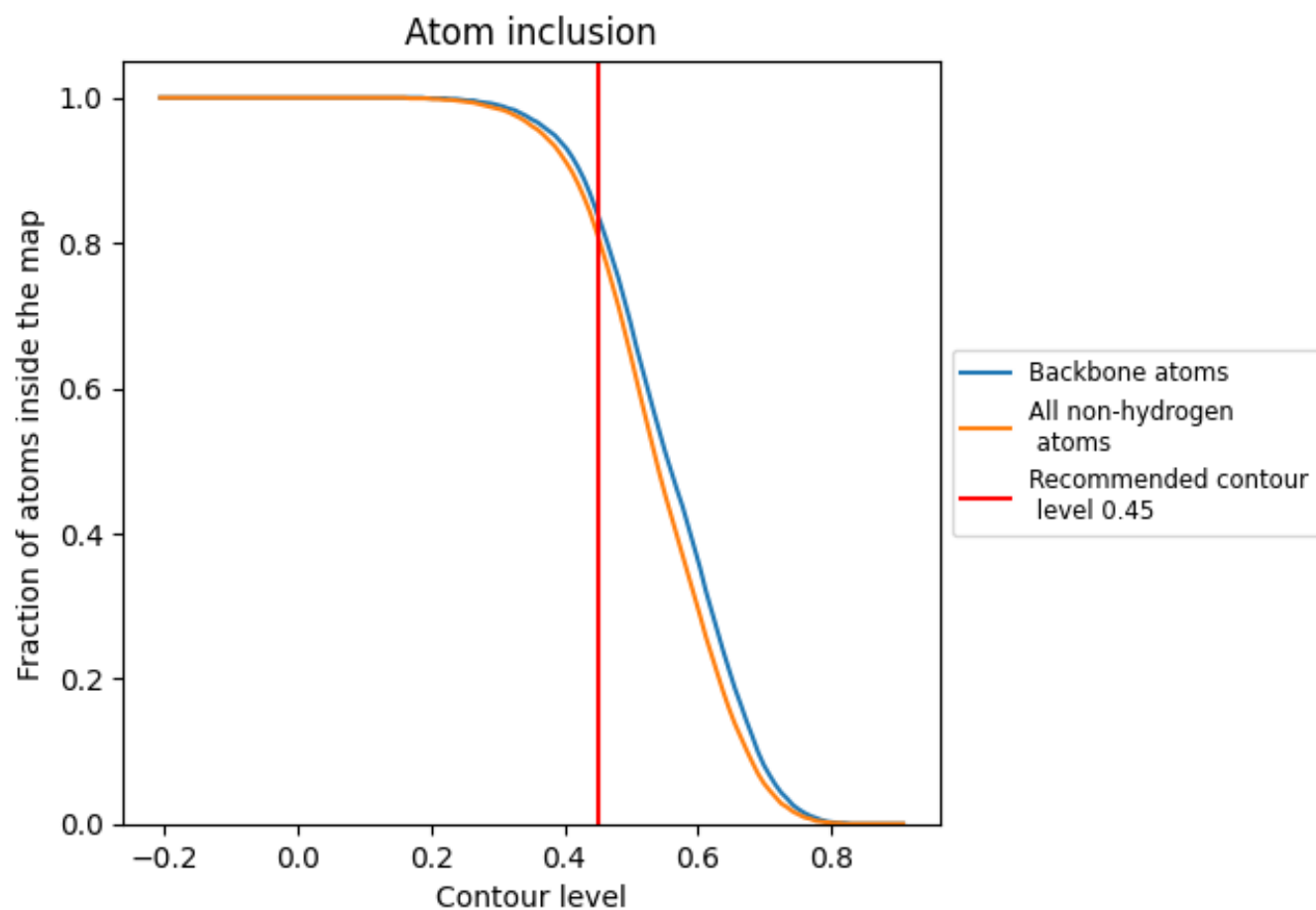
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8100	<div></div> 0.0850
A	<div></div> 0.6460	<div></div> 0.0450
B	<div></div> 0.9440	<div></div> 0.1040
C	<div></div> 0.9580	<div></div> 0.1160
D	<div></div> 0.9530	<div></div> 0.1140
E	<div></div> 0.9540	<div></div> 0.0960
F	<div></div> 0.9580	<div></div> 0.1100
G	<div></div> 0.8990	<div></div> 0.0970
H	<div></div> 0.7520	<div></div> 0.0770
I	<div></div> 0.9270	<div></div> 0.1050
J	<div></div> 0.8650	<div></div> 0.0940
K	<div></div> 0.9220	<div></div> 0.1050
L	<div></div> 0.5020	<div></div> 0.0600
M	<div></div> 0.5750	<div></div> 0.0790
N	<div></div> 0.9580	<div></div> 0.1020

1.0

0.0

<0.0