



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:22 PM UTC

PDB ID : 9FLV / pdb_00009flv
EMDB ID : EMD-50540
Title : CryoEM structure of the fragment-5 (2393-2807) in the grappling hook protein A (GhpA) in the bacterium Aureispira sp. CCB-QB1
Authors : Lien, Y.-W.; Amendola, D.; Lee, K.S.; Bartlau, N.; Xu, J.; Furusawa, G.; Polz, M.F.; Stocker, R.; Weiss, G.L.; Pilhofer, M.
Deposited on : 2024-06-05
Resolution : 3.60 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:

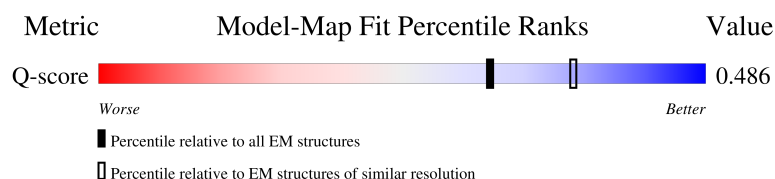
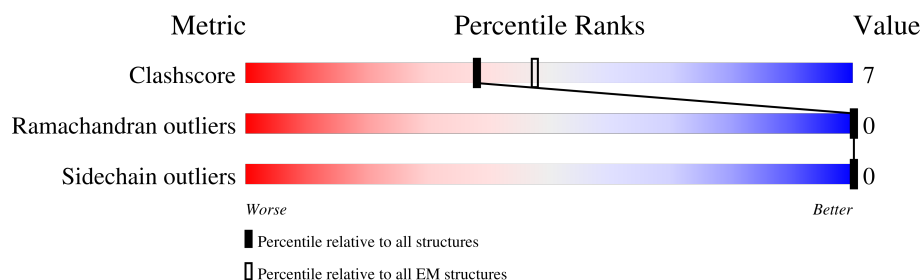
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

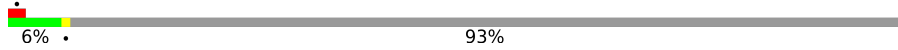
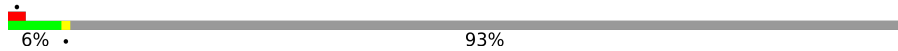
The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



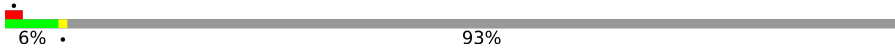
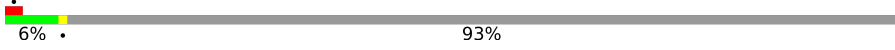
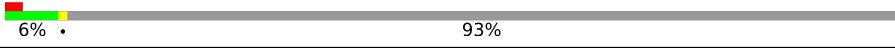
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	5898	 6% . 93%
1	B	5898	 6% . 93%
1	C	5898	 6% . 93%
1	D	5898	 6% . 93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	5898	 93%
1	F	5898	 93%
1	G	5898	 93%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20818 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 The grappling hook protein A (GhpA) in the bacterium *Aureispira* sp. CCB-QB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		
1	B	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		
1	C	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		
1	D	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		
1	E	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		
1	F	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		
1	G	415	Total	C	N	O	S	0	0
			2974	1836	488	636	14		

















TLE	TYR	CYS	ASP	THR	ALA	LEU	VAL	THR	THR	ILE	ASP	VAL	GLN	GLY	GLY	THR	THR	GLU	CYS	ASN	PHE	PRO	ASN	ASN	MET	ILE	THR	THR	PRO	ASN	ASN	ASP	ASP	ALA	ASN	GLU	THR	PHE	PHE	ILE	VAL	PRO	PRO	CYS	CYS	LEU	LEU	ASP	GLY	GLY	LEU	GLU	GLY	GLY	THR	THR	LYS	PHE	ALA	ALA	VAL	VAL	ASN	ASN	ARG	TRP	GLY	ASP	ASP	LEU	MET	MET	TYR	TYR	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	ASN	ASP	ASP	ASN	ASN	TYR	LYS	ASN	ASN	ASP	TRP	GLY	GLY	THR	HIS	ASN	GLY	VAL	PRO	VAL	PRO	PRO	ASP	ALA	ALA	THR	TYR	PHE	TYR	ILE	MET	GLU	LEU	ALA	ALA	ASP	GLY	GLN	ARG	PHE	GLN	GLY	PHE	VAL	GLU	VAL	ARG	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: The grappling hook protein A (GhpA) in the bacterium *Aureispira* sp. CCB-QB1

Chain C: 6% 93%

MET	GLN	ILE	GLN	ARG	HIS	SER	PHE	LYS	TRP	ILE	LEU	TYR	GLY	PHE	LEU	CYS	TRP	MET	THR	SER	PHE	VAL	GLN	ALA	GLN	THR	PRO	LEU	THR	ASN	ALA	THR	PRO	ALA	GLU	GLY	PHE	ILE	GLY	GLU	GLN	VAL	CYS	PHE	THR	PRO	VAL	THR	THR	GLY	ALA	PRO	GLY	GLY	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

TYR	VAL	ARG	LEU	ILE	VAL	PRO	THR	PRO	GLY	PHE	THR	PHE	ASP	ASN	ALA	SER	PHE	GLY	GLY	SER	SER	ILE	GLN	THR	VAL	GLN	ASN	LEU	GLY	VAL	ILE	VAL	SER	SER	GLY	ALA	PRO	ASN	ASN	ASN	PHE	VAL	VAL	ILE	ILE	ASP	PRO	ILE	ALA	GLN	SER	SER	THR	THR	SER	ASP	THR	ILE	PHE	ALA	ALA	PRO	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY SER THR VAL ILE LEU LEU GLU TYR PRO THR VAL GLY SER MET VAL GLN GLY GLY VAL SER SER LEU CYS MET THR VAL ASP PRO ALA ALA THR THR ILE GLY VAL VAL VAL ASP ILE CYS THR GLN GLY VAL TYR PHE GLY ASP THR THR THR GLY ASN GLY PRO ILE

ALA	GLY	ALA	ALA	ASN	GLU	CYS	GLU	PRO	ILE	ILE	PRO	PRO	ILE	LEU	PHE	ARG	PHE	ASP	LYS	LYS	VAL	ASN	GLY	SER	ASP	GLY	VAL	TYR	ASN	ASN	GLU	VAL	PRO	GLY	GLY	GLY	ALA	SER	LEU	CYS	HIS	ILE	ILE	HIS	GLN	TYR	GLU	GLU	LEU	ASN	ILE	ASP	ILE	ALA	ALA	ALA	GLY	GLY	THR	LEU	ASN	GLY	PRO	ILE	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

SER	ASP	THR	LEU	GLU	ILE	CYS	ASP	ASP	THR	ASP	ILE	ASN	ASN	GLY	ALA	THR	VAL	ASN	VAL	PRO	GLY	ASN	PRO	SER	GLN	SER	SER	ASP	THR	VAL	VAL	THR	THR	HIS	VAL	GLU	HIS	VAL	LEU	LEU	GLY	HIS	THR	ASN	ASN	THR	VAL	SER	PRO	VAL	THR	THR	ILE	GLY	GLN	THR	VAL	LEU	TYR	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ILE	GLY	ALA	ALA	GLU	ILE	THR	GLU	TYR	THR	ALA	ALA	GLY	LEU	THR	ALA	ALA	SER	ILE	THR	PHE	ILE	VAL	PRO	PRO	ASP	GLY	MET	ILE	TYR	ASN	PRO	ALA	ALA	SER	LEU	THR	TRP	ALA	GLY	THR	THR	PRO	VAL	VAL	ILE	ILE	VAL	VAL	PRO	GLY	GLY	THR	GLY	SER	THR	VAL	THR	THR	VAL	ASP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

HIS	THR	GLN	ASN	GLY	ALA	ASN	ILE	LEU	PRO	CYS	SER	PRO	SER	LEU	GLN	TYR	THR	ALA	ASP	VAL	ASN	GLN	THR	TYR	ALA	ASN	GLY	ASP	PRO	VAL	LEU	SER	ARG	ASP	ARG	LEU	THR	HIS	SER	SER	THR	LEU	THR	TYR	ASP	LEU	VAL	GLY	ALA	ALA	THR	GLY	CYS	THR	THR	SER	SER	ALA	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	PRO	ILE	ASP	VAL	ILE	ASP	PHE	GLN	LYS	THR	VAL	ASN	ASN	SER	PRO	PRO	THR	GLY	GLY	ARG	ASN	GLY	GLN	TRP	TRP	PRO	GLY	ASP	VAL	VAL	GLN	TYR	ARG	LEU	GLU	LEU	LEU	GLN	ILE	PRO	SER	PRO	PHE	PRO	LEU	PRO	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

HIS	ASP	VAL	ALA	SER	LEU	ALA	ALA	THR	PHE	GLY	GLY	ASP	VAL	PHE	ARG	ASP	PRO	ALA	THR	CYS	TRP	ASN	THR	ALA	VAL	THR	TYR	THR	ARG	ASP	ILE	PRO	THR	THR	ASN	SER	LEU	ILE	LEU	ASP	PHE	GLY	ASP	VAL	VAL	THR	GLY	CYS	VAL	ASP	ILE	VAL	LEU	LEU	LIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASP	ILE	PRO	PRO	THR	THR	PRO	LEU	ASP	ALA	ALA	GLY	LEU	PHE	HIS	SER	ASN	PHE	MET	GLN	VAL	ASN	SER	ASP	ASN	SER	THR	THR	ALA	ALA	ASN	ASN	ILE	THR	THR	SER	SER	ALA	LEU	LEU	THR	THR	GLN	VAL	GLY	ALA	PRO	PRO	ASP	LEU	LEU	GLU	LEU	LEU	THR	THR	LYS	GLY	ILE	ILE	VAL	SER	SER	ASP	ASN	ASN	PRO	PRO	ASN	ASN	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	ILE	SER	PRO	THR	VAL	VAL	PRO	PRO	PRO	ASP	GLY	ASN	ALA	THR	ASP	SER	SER	ALA	GLY	ASP	GLN	LEU	PHE	PHE	ASP	ILE	THR	ILE	ILE	GLU	ASN	VAL	GLY	GLY	ALA	ALA	ALA	GLY	TYR	ASP	VAL	VAL	GLN	VAL	ARG	ASP	VAL	ASP	ALA	PRO	PRO	PRO	GLU	LEU	THR	ASN	CYS	ALA	ALA	LEU	VAL	VAL	ALA	PRO	ASN	PRO	PRO	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

ASP	ASN	THR	ALA	GLU	VAL	ASP	TRP	SER	THR	ARG	GLY	VAL	LYS	PHE	PRO	VAL	GLU	ASP	ALA	ASN	GLY	ARG	ILE	ALA	ASP	PRO	THR	MET	ASN	LYS	VAL	VAL	ASP	Tyr	ILE	PHE	PRO	ASN	Thr	Ser	Asn	Thr	Thr	Asn	Thr	Gln	Ala	Ala	Ile	Ser	Gly	Val	Val	Val	Tyr	Thr
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU GLN LEU LEU ASN ASN PRO GLY GLY GLN ASP VAL THR LEU VAL VAL GLN ASP VAL VAL ALA PHE VAL ALA ALA VAL ASP SER ILE VAL ILE CYS SER ASN SER SER SER THR ILE ILE THR SER ILE GLY GLY GLY PHE PRO ALA ALA VAL VAL GLN SER GLY ALA THR ILE THR









PRO	ALA	ILE	TYR	CYS	THR	ASP	ASP	ILE	ASP	VAL	GLN	GLY	GLY	THR	THR	GLU	CYS	PHE	ASN	ASN	ASP	ASP	ALA	ASN	GLN	GLU	THR	THR	LYS	PHE	VAL	VAL	TYR	ASN	ARG	THR	GLY	ASP	LEU	MET	
THR	GLU	ASN	ASP	ASN	LYS	ASN	ASP	GLY	THR	HIS	ASN	GLY	VAL	VAL	PRO	VAL	PRO	ASP	ALA	THR	THR	PHE	THR	ILE	MET	GLU	LEU	ALA	ASP	GLY	GLN	ARG	PHE	GLN	GLY	PHE	VAL	VAL	GLU	VAL	ARG

- Molecule 1: The grappling hook protein A (GhpA) in the bacterium *Aureispira* sp. CCB-QB1

[illegible]







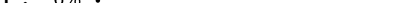










- Chain F:  6% 93%

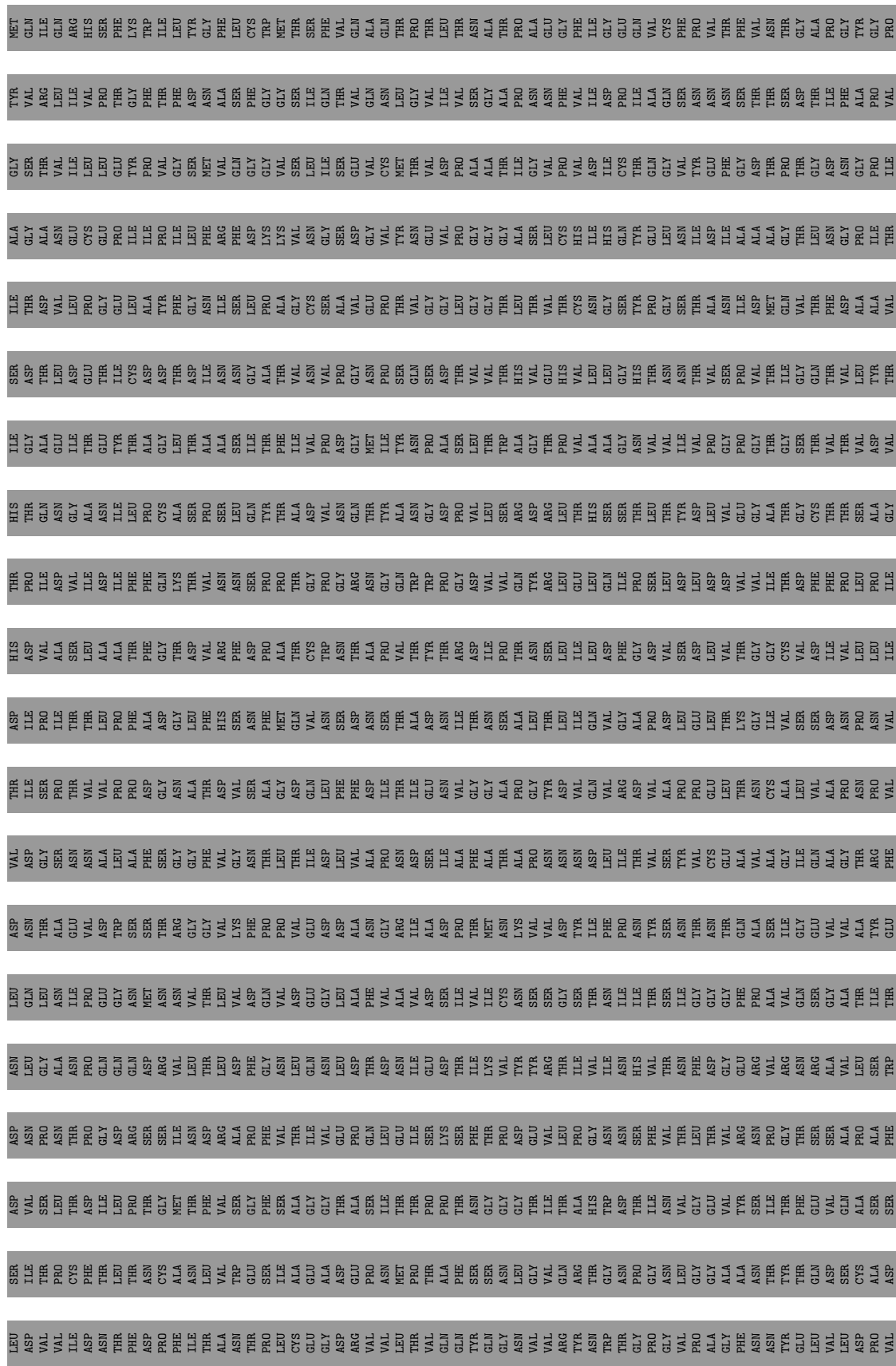








- Molecule 1: The grappling hook protein A (GhpA) in the bacterium *Aureispira* sp. CCB-QB1











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	33957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.442	Depositor
Minimum map value	-3.682	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.126	Depositor
Recommended contour level	1	Depositor
Map size (Å)	319.50003, 319.50003, 319.50003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	1.00	1/3038 (0.0%)	1.41	68/4209 (1.6%)
1	B	1.00	1/3038 (0.0%)	1.42	68/4209 (1.6%)
1	C	1.00	1/3038 (0.0%)	1.41	68/4209 (1.6%)
1	D	1.00	1/3038 (0.0%)	1.41	68/4209 (1.6%)
1	E	1.00	1/3038 (0.0%)	1.42	68/4209 (1.6%)
1	F	1.00	1/3038 (0.0%)	1.42	68/4209 (1.6%)
1	G	1.00	1/3038 (0.0%)	1.41	68/4209 (1.6%)
All	All	1.00	7/21266 (0.0%)	1.41	476/29463 (1.6%)

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
1	F	0	1
1	G	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2434	SER	CA-CB	-5.46	1.44	1.53
1	D	2434	SER	CA-CB	-5.45	1.44	1.53
1	A	2434	SER	CA-CB	-5.45	1.44	1.53
1	F	2434	SER	CA-CB	-5.45	1.44	1.53
1	G	2434	SER	CA-CB	-5.44	1.44	1.53
1	B	2434	SER	CA-CB	-5.41	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2434	SER	CA-CB	-5.41	1.44	1.53

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2405	PHE	CA-CB-CG	8.93	122.73	113.80
1	D	2405	PHE	CA-CB-CG	8.92	122.72	113.80
1	G	2405	PHE	CA-CB-CG	8.92	122.72	113.80
1	A	2405	PHE	CA-CB-CG	8.91	122.71	113.80
1	E	2405	PHE	CA-CB-CG	8.90	122.70	113.80
1	C	2405	PHE	CA-CB-CG	8.89	122.69	113.80
1	F	2405	PHE	CA-CB-CG	8.89	122.69	113.80
1	B	2763	ASP	CA-CB-CG	8.62	121.22	112.60
1	D	2763	ASP	CA-CB-CG	8.58	121.18	112.60
1	F	2763	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	2763	ASP	CA-CB-CG	8.56	121.16	112.60
1	C	2763	ASP	CA-CB-CG	8.56	121.16	112.60
1	G	2763	ASP	CA-CB-CG	8.55	121.15	112.60
1	E	2763	ASP	CA-CB-CG	8.54	121.14	112.60
1	B	2676	GLY	CA-C-N	8.24	128.27	119.78
1	B	2676	GLY	C-N-CA	8.24	128.27	119.78
1	E	2676	GLY	CA-C-N	8.23	128.25	119.78
1	E	2676	GLY	C-N-CA	8.23	128.25	119.78
1	G	2676	GLY	CA-C-N	8.20	128.22	119.78
1	G	2676	GLY	C-N-CA	8.20	128.22	119.78
1	A	2676	GLY	CA-C-N	8.19	128.22	119.78
1	A	2676	GLY	C-N-CA	8.19	128.22	119.78
1	F	2676	GLY	CA-C-N	8.19	128.22	119.78
1	F	2676	GLY	C-N-CA	8.19	128.22	119.78
1	C	2676	GLY	CA-C-N	8.19	128.21	119.78
1	C	2676	GLY	C-N-CA	8.19	128.21	119.78
1	D	2676	GLY	CA-C-N	8.17	128.19	119.78
1	D	2676	GLY	C-N-CA	8.17	128.19	119.78
1	B	2642	PRO	CB-CA-C	-7.96	101.61	111.64
1	D	2642	PRO	CB-CA-C	-7.95	101.62	111.64
1	F	2642	PRO	CB-CA-C	-7.94	101.64	111.64
1	A	2642	PRO	CB-CA-C	-7.93	101.65	111.64
1	G	2642	PRO	CB-CA-C	-7.93	101.65	111.64
1	E	2642	PRO	CB-CA-C	-7.93	101.65	111.64
1	C	2642	PRO	CB-CA-C	-7.92	101.67	111.64
1	B	2686	ASN	CA-C-N	7.71	127.72	119.78
1	B	2686	ASN	C-N-CA	7.71	127.72	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2646	THR	CA-C-N	7.71	127.72	119.78
1	F	2646	THR	C-N-CA	7.71	127.72	119.78
1	E	2646	THR	CA-C-N	7.69	127.70	119.78
1	E	2646	THR	C-N-CA	7.69	127.70	119.78
1	A	2646	THR	CA-C-N	7.69	127.70	119.78
1	A	2646	THR	C-N-CA	7.69	127.70	119.78
1	D	2646	THR	CA-C-N	7.68	127.69	119.78
1	D	2646	THR	C-N-CA	7.68	127.69	119.78
1	C	2686	ASN	CA-C-N	7.68	127.69	119.78
1	C	2686	ASN	C-N-CA	7.68	127.69	119.78
1	A	2686	ASN	CA-C-N	7.67	127.68	119.78
1	A	2686	ASN	C-N-CA	7.67	127.68	119.78
1	F	2686	ASN	CA-C-N	7.67	127.68	119.78
1	F	2686	ASN	C-N-CA	7.67	127.68	119.78
1	G	2646	THR	CA-C-N	7.67	127.68	119.78
1	G	2646	THR	C-N-CA	7.67	127.68	119.78
1	B	2646	THR	CA-C-N	7.66	127.67	119.78
1	B	2646	THR	C-N-CA	7.66	127.67	119.78
1	D	2686	ASN	CA-C-N	7.66	127.67	119.78
1	D	2686	ASN	C-N-CA	7.66	127.67	119.78
1	G	2686	ASN	CA-C-N	7.65	127.66	119.78
1	G	2686	ASN	C-N-CA	7.65	127.66	119.78
1	C	2646	THR	CA-C-N	7.65	127.66	119.78
1	C	2646	THR	C-N-CA	7.65	127.66	119.78
1	E	2686	ASN	CA-C-N	7.65	127.66	119.78
1	E	2686	ASN	C-N-CA	7.65	127.66	119.78
1	B	2487	SER	N-CA-C	7.42	122.57	112.55
1	F	2487	SER	N-CA-C	7.41	122.55	112.55
1	G	2765	ILE	N-CA-C	7.41	118.48	108.11
1	A	2487	SER	N-CA-C	7.40	122.55	112.55
1	D	2487	SER	N-CA-C	7.40	122.53	112.55
1	C	2487	SER	N-CA-C	7.39	122.53	112.55
1	G	2487	SER	N-CA-C	7.39	122.53	112.55
1	F	2765	ILE	N-CA-C	7.38	118.45	108.11
1	E	2487	SER	N-CA-C	7.38	122.52	112.55
1	C	2765	ILE	N-CA-C	7.38	118.44	108.11
1	B	2765	ILE	N-CA-C	7.38	118.44	108.11
1	A	2765	ILE	N-CA-C	7.37	118.43	108.11
1	D	2428	GLY	CA-C-N	7.37	127.35	119.76
1	D	2428	GLY	C-N-CA	7.37	127.35	119.76
1	D	2765	ILE	N-CA-C	7.37	118.43	108.11
1	G	2428	GLY	CA-C-N	7.36	127.34	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2428	GLY	C-N-CA	7.36	127.34	119.76
1	B	2428	GLY	CA-C-N	7.36	127.34	119.76
1	B	2428	GLY	C-N-CA	7.36	127.34	119.76
1	E	2765	ILE	N-CA-C	7.36	118.41	108.11
1	A	2428	GLY	CA-C-N	7.34	127.32	119.76
1	A	2428	GLY	C-N-CA	7.34	127.32	119.76
1	F	2428	GLY	CA-C-N	7.34	127.32	119.76
1	F	2428	GLY	C-N-CA	7.34	127.32	119.76
1	C	2428	GLY	CA-C-N	7.33	127.31	119.76
1	C	2428	GLY	C-N-CA	7.33	127.31	119.76
1	E	2428	GLY	CA-C-N	7.32	127.30	119.76
1	E	2428	GLY	C-N-CA	7.32	127.30	119.76
1	F	2725	GLY	CA-C-N	7.14	127.59	120.52
1	F	2725	GLY	C-N-CA	7.14	127.59	120.52
1	G	2725	GLY	CA-C-N	7.11	127.56	120.52
1	G	2725	GLY	C-N-CA	7.11	127.56	120.52
1	A	2725	GLY	CA-C-N	7.10	127.55	120.52
1	A	2725	GLY	C-N-CA	7.10	127.55	120.52
1	E	2725	GLY	CA-C-N	7.09	127.54	120.52
1	E	2725	GLY	C-N-CA	7.09	127.54	120.52
1	B	2725	GLY	CA-C-N	7.09	127.54	120.52
1	B	2725	GLY	C-N-CA	7.09	127.54	120.52
1	F	2639	THR	O-C-N	-7.09	115.12	123.06
1	D	2639	THR	O-C-N	-7.09	115.12	123.06
1	A	2639	THR	O-C-N	-7.08	115.13	123.06
1	B	2639	THR	O-C-N	-7.08	115.13	123.06
1	D	2725	GLY	CA-C-N	7.08	127.53	120.52
1	D	2725	GLY	C-N-CA	7.08	127.53	120.52
1	C	2639	THR	O-C-N	-7.08	115.13	123.06
1	G	2639	THR	O-C-N	-7.07	115.14	123.06
1	C	2725	GLY	CA-C-N	7.07	127.52	120.52
1	C	2725	GLY	C-N-CA	7.07	127.52	120.52
1	E	2639	THR	O-C-N	-7.07	115.15	123.06
1	D	2728	ALA	CA-C-N	6.93	126.89	120.03
1	D	2728	ALA	C-N-CA	6.93	126.89	120.03
1	B	2728	ALA	CA-C-N	6.92	126.88	120.03
1	B	2728	ALA	C-N-CA	6.92	126.88	120.03
1	A	2728	ALA	CA-C-N	6.91	126.87	120.03
1	A	2728	ALA	C-N-CA	6.91	126.87	120.03
1	C	2728	ALA	CA-C-N	6.91	126.87	120.03
1	C	2728	ALA	C-N-CA	6.91	126.87	120.03
1	E	2728	ALA	CA-C-N	6.91	126.87	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2728	ALA	C-N-CA	6.91	126.87	120.03
1	F	2728	ALA	CA-C-N	6.88	126.84	120.03
1	F	2728	ALA	C-N-CA	6.88	126.84	120.03
1	G	2728	ALA	CA-C-N	6.88	126.84	120.03
1	G	2728	ALA	C-N-CA	6.88	126.84	120.03
1	F	2758	SER	CA-C-N	6.76	126.46	119.56
1	F	2758	SER	C-N-CA	6.76	126.46	119.56
1	D	2758	SER	CA-C-N	6.74	126.44	119.56
1	D	2758	SER	C-N-CA	6.74	126.44	119.56
1	A	2758	SER	CA-C-N	6.74	126.43	119.56
1	A	2758	SER	C-N-CA	6.74	126.43	119.56
1	B	2758	SER	CA-C-N	6.71	126.41	119.56
1	B	2758	SER	C-N-CA	6.71	126.41	119.56
1	C	2758	SER	CA-C-N	6.71	126.40	119.56
1	C	2758	SER	C-N-CA	6.71	126.40	119.56
1	E	2758	SER	CA-C-N	6.71	126.40	119.56
1	E	2758	SER	C-N-CA	6.71	126.40	119.56
1	G	2758	SER	CA-C-N	6.70	126.40	119.56
1	G	2758	SER	C-N-CA	6.70	126.40	119.56
1	G	2526	ALA	CA-C-N	6.69	126.38	119.82
1	G	2526	ALA	C-N-CA	6.69	126.38	119.82
1	F	2526	ALA	CA-C-N	6.67	126.36	119.82
1	F	2526	ALA	C-N-CA	6.67	126.36	119.82
1	B	2526	ALA	CA-C-N	6.66	126.35	119.82
1	B	2526	ALA	C-N-CA	6.66	126.35	119.82
1	A	2526	ALA	CA-C-N	6.66	126.34	119.82
1	A	2526	ALA	C-N-CA	6.66	126.34	119.82
1	C	2526	ALA	CA-C-N	6.65	126.33	119.82
1	C	2526	ALA	C-N-CA	6.65	126.33	119.82
1	D	2526	ALA	CA-C-N	6.65	126.33	119.82
1	D	2526	ALA	C-N-CA	6.65	126.33	119.82
1	E	2526	ALA	CA-C-N	6.64	126.33	119.82
1	E	2526	ALA	C-N-CA	6.64	126.33	119.82
1	B	2564	ASN	CA-C-N	6.55	126.73	120.31
1	B	2564	ASN	C-N-CA	6.55	126.73	120.31
1	F	2564	ASN	CA-C-N	6.55	126.73	120.31
1	F	2564	ASN	C-N-CA	6.55	126.73	120.31
1	G	2437	GLN	N-CA-C	-6.54	104.88	112.92
1	D	2564	ASN	CA-C-N	6.53	126.71	120.31
1	D	2564	ASN	C-N-CA	6.53	126.71	120.31
1	E	2480	GLN	CA-C-N	6.52	126.70	120.31
1	E	2480	GLN	C-N-CA	6.52	126.70	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2437	GLN	N-CA-C	-6.52	104.90	112.92
1	E	2564	ASN	CA-C-N	6.51	126.69	120.31
1	E	2564	ASN	C-N-CA	6.51	126.69	120.31
1	A	2564	ASN	CA-C-N	6.51	126.69	120.31
1	A	2564	ASN	C-N-CA	6.51	126.69	120.31
1	F	2437	GLN	N-CA-C	-6.51	104.91	112.92
1	A	2437	GLN	N-CA-C	-6.51	104.92	112.92
1	B	2437	GLN	N-CA-C	-6.50	104.92	112.92
1	C	2437	GLN	N-CA-C	-6.50	104.92	112.92
1	D	2437	GLN	N-CA-C	-6.50	104.93	112.92
1	E	2717	SER	N-CA-C	6.49	118.71	108.79
1	G	2564	ASN	CA-C-N	6.48	126.66	120.31
1	G	2564	ASN	C-N-CA	6.48	126.66	120.31
1	C	2480	GLN	CA-C-N	6.48	126.66	120.31
1	C	2480	GLN	C-N-CA	6.48	126.66	120.31
1	D	2480	GLN	CA-C-N	6.48	126.66	120.31
1	D	2480	GLN	C-N-CA	6.48	126.66	120.31
1	G	2717	SER	N-CA-C	6.48	118.71	108.79
1	A	2717	SER	N-CA-C	6.48	118.70	108.79
1	C	2438	ASN	CA-C-N	6.48	126.85	119.92
1	C	2438	ASN	C-N-CA	6.48	126.85	119.92
1	C	2717	SER	N-CA-C	6.47	118.69	108.79
1	C	2564	ASN	CA-C-N	6.47	126.65	120.31
1	C	2564	ASN	C-N-CA	6.47	126.65	120.31
1	B	2717	SER	N-CA-C	6.46	118.68	108.79
1	F	2717	SER	N-CA-C	6.46	118.68	108.79
1	A	2480	GLN	CA-C-N	6.45	126.63	120.31
1	A	2480	GLN	C-N-CA	6.45	126.63	120.31
1	D	2717	SER	N-CA-C	6.45	118.66	108.79
1	A	2438	ASN	CA-C-N	6.45	126.82	119.92
1	A	2438	ASN	C-N-CA	6.45	126.82	119.92
1	D	2438	ASN	CA-C-N	6.44	126.81	119.92
1	D	2438	ASN	C-N-CA	6.44	126.81	119.92
1	E	2438	ASN	CA-C-N	6.44	126.81	119.92
1	E	2438	ASN	C-N-CA	6.44	126.81	119.92
1	B	2480	GLN	CA-C-N	6.44	126.62	120.31
1	B	2480	GLN	C-N-CA	6.44	126.62	120.31
1	B	2438	ASN	CA-C-N	6.44	126.81	119.92
1	B	2438	ASN	C-N-CA	6.44	126.81	119.92
1	G	2480	GLN	CA-C-N	6.44	126.62	120.31
1	G	2480	GLN	C-N-CA	6.44	126.62	120.31
1	F	2480	GLN	CA-C-N	6.43	126.61	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2480	GLN	C-N-CA	6.43	126.61	120.31
1	G	2438	ASN	CA-C-N	6.43	126.80	119.92
1	G	2438	ASN	C-N-CA	6.43	126.80	119.92
1	F	2438	ASN	CA-C-N	6.41	126.78	119.92
1	F	2438	ASN	C-N-CA	6.41	126.78	119.92
1	D	2398	SER	CA-C-N	6.29	126.25	120.03
1	D	2398	SER	C-N-CA	6.29	126.25	120.03
1	F	2398	SER	CA-C-N	6.28	126.24	120.03
1	F	2398	SER	C-N-CA	6.28	126.24	120.03
1	B	2398	SER	CA-C-N	6.27	126.24	120.03
1	B	2398	SER	C-N-CA	6.27	126.24	120.03
1	E	2398	SER	CA-C-N	6.26	126.23	120.03
1	E	2398	SER	C-N-CA	6.26	126.23	120.03
1	G	2398	SER	CA-C-N	6.25	126.21	120.03
1	G	2398	SER	C-N-CA	6.25	126.21	120.03
1	A	2398	SER	CA-C-N	6.24	126.21	120.03
1	A	2398	SER	C-N-CA	6.24	126.21	120.03
1	C	2649	ILE	CA-C-N	6.24	126.21	119.78
1	C	2649	ILE	C-N-CA	6.24	126.21	119.78
1	C	2398	SER	CA-C-N	6.24	126.20	120.03
1	C	2398	SER	C-N-CA	6.24	126.20	120.03
1	F	2649	ILE	CA-C-N	6.24	126.20	119.78
1	F	2649	ILE	C-N-CA	6.24	126.20	119.78
1	E	2649	ILE	CA-C-N	6.22	126.19	119.78
1	E	2649	ILE	C-N-CA	6.22	126.19	119.78
1	G	2649	ILE	CA-C-N	6.22	126.19	119.78
1	G	2649	ILE	C-N-CA	6.22	126.19	119.78
1	A	2649	ILE	CA-C-N	6.21	126.18	119.78
1	A	2649	ILE	C-N-CA	6.21	126.18	119.78
1	B	2649	ILE	CA-C-N	6.20	126.17	119.78
1	B	2649	ILE	C-N-CA	6.20	126.17	119.78
1	D	2649	ILE	CA-C-N	6.18	126.15	119.78
1	D	2649	ILE	C-N-CA	6.18	126.15	119.78
1	F	2608	ASN	CA-C-N	6.07	126.04	120.03
1	F	2608	ASN	C-N-CA	6.07	126.04	120.03
1	C	2608	ASN	CA-C-N	6.04	126.01	120.03
1	C	2608	ASN	C-N-CA	6.04	126.01	120.03
1	E	2608	ASN	CA-C-N	6.04	126.01	120.03
1	E	2608	ASN	C-N-CA	6.04	126.01	120.03
1	E	2401	LEU	CA-C-N	6.04	126.38	119.92
1	E	2401	LEU	C-N-CA	6.04	126.38	119.92
1	B	2608	ASN	CA-C-N	6.03	126.00	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2608	ASN	C-N-CA	6.03	126.00	120.03
1	A	2608	ASN	CA-C-N	6.03	126.00	120.03
1	A	2608	ASN	C-N-CA	6.03	126.00	120.03
1	F	2401	LEU	CA-C-N	6.02	126.36	119.92
1	F	2401	LEU	C-N-CA	6.02	126.36	119.92
1	G	2608	ASN	CA-C-N	6.00	125.97	120.03
1	G	2608	ASN	C-N-CA	6.00	125.97	120.03
1	D	2608	ASN	CA-C-N	6.00	125.97	120.03
1	D	2608	ASN	C-N-CA	6.00	125.97	120.03
1	G	2401	LEU	CA-C-N	6.00	126.34	119.92
1	G	2401	LEU	C-N-CA	6.00	126.34	119.92
1	A	2401	LEU	CA-C-N	5.99	126.33	119.92
1	A	2401	LEU	C-N-CA	5.99	126.33	119.92
1	C	2401	LEU	CA-C-N	5.98	126.32	119.92
1	C	2401	LEU	C-N-CA	5.98	126.32	119.92
1	D	2401	LEU	CA-C-N	5.98	126.31	119.92
1	D	2401	LEU	C-N-CA	5.98	126.31	119.92
1	E	2643	THR	CA-C-N	5.98	125.89	119.85
1	E	2643	THR	C-N-CA	5.98	125.89	119.85
1	F	2799	GLU	N-CA-C	-5.97	102.06	109.64
1	B	2401	LEU	CA-C-N	5.96	126.30	119.92
1	B	2401	LEU	C-N-CA	5.96	126.30	119.92
1	B	2799	GLU	N-CA-C	-5.96	102.07	109.64
1	B	2643	THR	CA-C-N	5.95	125.86	119.85
1	B	2643	THR	C-N-CA	5.95	125.86	119.85
1	A	2643	THR	CA-C-N	5.95	125.85	119.85
1	A	2643	THR	C-N-CA	5.95	125.85	119.85
1	A	2799	GLU	N-CA-C	-5.95	102.09	109.64
1	C	2799	GLU	N-CA-C	-5.94	102.10	109.64
1	G	2799	GLU	N-CA-C	-5.94	102.10	109.64
1	G	2643	THR	CA-C-N	5.93	125.84	119.85
1	G	2643	THR	C-N-CA	5.93	125.84	119.85
1	D	2799	GLU	N-CA-C	-5.93	102.11	109.64
1	E	2799	GLU	N-CA-C	-5.93	102.11	109.64
1	D	2643	THR	CA-C-N	5.92	125.83	119.85
1	D	2643	THR	C-N-CA	5.92	125.83	119.85
1	C	2643	THR	CA-C-N	5.92	125.83	119.85
1	C	2643	THR	C-N-CA	5.92	125.83	119.85
1	F	2643	THR	CA-C-N	5.92	125.83	119.85
1	F	2643	THR	C-N-CA	5.92	125.83	119.85
1	A	2543	ASN	CA-CB-CG	5.87	118.47	112.60
1	D	2543	ASN	CA-CB-CG	5.87	118.47	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2486	ASN	N-CA-C	-5.85	95.45	107.67
1	C	2486	ASN	N-CA-C	-5.85	95.45	107.67
1	F	2543	ASN	CA-CB-CG	5.85	118.45	112.60
1	E	2486	ASN	N-CA-C	-5.84	95.46	107.67
1	D	2486	ASN	N-CA-C	-5.84	95.47	107.67
1	A	2486	ASN	N-CA-C	-5.83	95.48	107.67
1	E	2543	ASN	CA-CB-CG	5.83	118.43	112.60
1	G	2486	ASN	N-CA-C	-5.83	95.50	107.67
1	F	2486	ASN	N-CA-C	-5.81	95.52	107.67
1	G	2543	ASN	CA-CB-CG	5.81	118.41	112.60
1	C	2543	ASN	CA-CB-CG	5.81	118.41	112.60
1	B	2543	ASN	CA-CB-CG	5.78	118.38	112.60
1	G	2432	PHE	CA-CB-CG	5.78	119.58	113.80
1	E	2432	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	2432	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	2432	PHE	CA-CB-CG	5.73	119.53	113.80
1	D	2432	PHE	CA-CB-CG	5.73	119.53	113.80
1	C	2432	PHE	CA-CB-CG	5.73	119.53	113.80
1	F	2432	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	2432	PHE	CA-C-O	-5.66	114.65	120.54
1	C	2432	PHE	CA-C-O	-5.66	114.66	120.54
1	E	2432	PHE	CA-C-O	-5.64	114.67	120.54
1	D	2432	PHE	CA-C-O	-5.63	114.68	120.54
1	G	2432	PHE	CA-C-O	-5.63	114.69	120.54
1	A	2432	PHE	CA-C-O	-5.63	114.69	120.54
1	F	2432	PHE	CA-C-O	-5.61	114.70	120.54
1	C	2703	LEU	N-CA-C	5.55	118.49	109.06
1	F	2642	PRO	CA-C-O	-5.55	115.29	121.23
1	B	2703	LEU	N-CA-C	5.55	118.49	109.06
1	D	2703	LEU	N-CA-C	5.54	118.48	109.06
1	A	2703	LEU	N-CA-C	5.54	118.48	109.06
1	G	2703	LEU	N-CA-C	5.54	118.47	109.06
1	F	2703	LEU	N-CA-C	5.54	118.47	109.06
1	E	2703	LEU	N-CA-C	5.53	118.47	109.06
1	C	2642	PRO	CA-C-O	-5.53	115.31	121.23
1	E	2642	PRO	CA-C-O	-5.52	115.33	121.23
1	B	2642	PRO	CA-C-O	-5.51	115.33	121.23
1	E	2703	LEU	CA-C-N	-5.51	113.21	122.29
1	E	2703	LEU	C-N-CA	-5.51	113.21	122.29
1	C	2703	LEU	CA-C-N	-5.50	113.21	122.29
1	C	2703	LEU	C-N-CA	-5.50	113.21	122.29
1	A	2642	PRO	CA-C-O	-5.50	115.34	121.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2774	VAL	CA-C-N	5.50	126.72	119.84
1	D	2774	VAL	C-N-CA	5.50	126.72	119.84
1	G	2642	PRO	CA-C-O	-5.50	115.34	121.23
1	B	2703	LEU	CA-C-N	-5.49	113.22	122.29
1	B	2703	LEU	C-N-CA	-5.49	113.22	122.29
1	B	2774	VAL	CA-C-N	5.49	126.70	119.84
1	B	2774	VAL	C-N-CA	5.49	126.70	119.84
1	D	2703	LEU	CA-C-N	-5.49	113.23	122.29
1	D	2703	LEU	C-N-CA	-5.49	113.23	122.29
1	A	2703	LEU	CA-C-N	-5.49	113.23	122.29
1	A	2703	LEU	C-N-CA	-5.49	113.23	122.29
1	G	2703	LEU	CA-C-N	-5.48	113.24	122.29
1	G	2703	LEU	C-N-CA	-5.48	113.24	122.29
1	F	2703	LEU	CA-C-N	-5.48	113.25	122.29
1	F	2703	LEU	C-N-CA	-5.48	113.25	122.29
1	A	2774	VAL	CA-C-N	5.47	126.68	119.84
1	A	2774	VAL	C-N-CA	5.47	126.68	119.84
1	E	2774	VAL	CA-C-N	5.47	126.68	119.84
1	E	2774	VAL	C-N-CA	5.47	126.68	119.84
1	D	2642	PRO	CA-C-O	-5.47	115.38	121.23
1	C	2774	VAL	CA-C-N	5.46	126.67	119.84
1	C	2774	VAL	C-N-CA	5.46	126.67	119.84
1	F	2774	VAL	CA-C-N	5.46	126.67	119.84
1	F	2774	VAL	C-N-CA	5.46	126.67	119.84
1	G	2774	VAL	CA-C-N	5.45	126.65	119.84
1	G	2774	VAL	C-N-CA	5.45	126.65	119.84
1	E	2477	ALA	CA-C-N	5.43	125.40	120.03
1	E	2477	ALA	C-N-CA	5.43	125.40	120.03
1	G	2477	ALA	CA-C-N	5.42	125.40	120.03
1	G	2477	ALA	C-N-CA	5.42	125.40	120.03
1	C	2477	ALA	CA-C-N	5.41	125.38	120.03
1	C	2477	ALA	C-N-CA	5.41	125.38	120.03
1	A	2477	ALA	CA-C-N	5.39	125.36	120.03
1	A	2477	ALA	C-N-CA	5.39	125.36	120.03
1	E	2735	SER	CB-CA-C	-5.38	109.91	117.23
1	G	2510	ALA	CA-C-N	5.38	125.71	119.47
1	G	2510	ALA	C-N-CA	5.38	125.71	119.47
1	F	2735	SER	CB-CA-C	-5.38	109.92	117.23
1	B	2477	ALA	CA-C-N	5.37	125.35	120.03
1	B	2477	ALA	C-N-CA	5.37	125.35	120.03
1	A	2735	SER	CB-CA-C	-5.36	109.94	117.23
1	G	2735	SER	CB-CA-C	-5.36	109.94	117.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2735	SER	CB-CA-C	-5.36	109.94	117.23
1	D	2477	ALA	CA-C-N	5.36	125.33	120.03
1	D	2477	ALA	C-N-CA	5.36	125.33	120.03
1	D	2735	SER	CB-CA-C	-5.36	109.94	117.23
1	F	2510	ALA	CA-C-N	5.36	125.68	119.47
1	F	2510	ALA	C-N-CA	5.36	125.68	119.47
1	E	2629	CYS	CA-C-N	5.35	125.11	119.76
1	E	2629	CYS	C-N-CA	5.35	125.11	119.76
1	D	2510	ALA	CA-C-N	5.35	125.68	119.47
1	D	2510	ALA	C-N-CA	5.35	125.68	119.47
1	F	2477	ALA	CA-C-N	5.34	125.32	120.03
1	F	2477	ALA	C-N-CA	5.34	125.32	120.03
1	A	2629	CYS	CA-C-N	5.34	125.10	119.76
1	A	2629	CYS	C-N-CA	5.34	125.10	119.76
1	E	2510	ALA	CA-C-N	5.34	125.67	119.47
1	E	2510	ALA	C-N-CA	5.34	125.67	119.47
1	B	2735	SER	CB-CA-C	-5.34	109.97	117.23
1	C	2629	CYS	CA-C-N	5.34	125.10	119.76
1	C	2629	CYS	C-N-CA	5.34	125.10	119.76
1	F	2629	CYS	CA-C-N	5.34	125.10	119.76
1	F	2629	CYS	C-N-CA	5.34	125.10	119.76
1	D	2629	CYS	CA-C-N	5.33	125.09	119.76
1	D	2629	CYS	C-N-CA	5.33	125.09	119.76
1	C	2796	CYS	CA-C-N	5.32	125.22	119.85
1	C	2796	CYS	C-N-CA	5.32	125.22	119.85
1	A	2510	ALA	CA-C-N	5.32	125.64	119.47
1	A	2510	ALA	C-N-CA	5.32	125.64	119.47
1	F	2796	CYS	CA-C-N	5.32	125.22	119.85
1	F	2796	CYS	C-N-CA	5.32	125.22	119.85
1	B	2629	CYS	CA-C-N	5.31	125.07	119.76
1	B	2629	CYS	C-N-CA	5.31	125.07	119.76
1	B	2796	CYS	CA-C-N	5.31	125.21	119.85
1	B	2796	CYS	C-N-CA	5.31	125.21	119.85
1	E	2705	ILE	N-CA-C	5.31	115.54	108.11
1	G	2629	CYS	CA-C-N	5.31	125.07	119.76
1	G	2629	CYS	C-N-CA	5.31	125.07	119.76
1	G	2796	CYS	CA-C-N	5.30	125.21	119.85
1	G	2796	CYS	C-N-CA	5.30	125.21	119.85
1	C	2510	ALA	CA-C-N	5.30	125.62	119.47
1	C	2510	ALA	C-N-CA	5.30	125.62	119.47
1	B	2510	ALA	CA-C-N	5.30	125.62	119.47
1	B	2510	ALA	C-N-CA	5.30	125.62	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2705	ILE	N-CA-C	5.30	115.53	108.11
1	G	2705	ILE	N-CA-C	5.30	115.53	108.11
1	B	2705	ILE	N-CA-C	5.29	115.52	108.11
1	D	2705	ILE	N-CA-C	5.29	115.51	108.11
1	G	2603	ILE	CB-CA-C	-5.29	105.56	111.80
1	F	2705	ILE	N-CA-C	5.28	115.51	108.11
1	A	2796	CYS	CA-C-N	5.28	125.19	119.85
1	A	2796	CYS	C-N-CA	5.28	125.19	119.85
1	C	2705	ILE	N-CA-C	5.28	115.50	108.11
1	E	2796	CYS	CA-C-N	5.28	125.18	119.85
1	E	2796	CYS	C-N-CA	5.28	125.18	119.85
1	C	2603	ILE	CB-CA-C	-5.26	105.59	111.80
1	D	2796	CYS	CA-C-N	5.26	125.16	119.85
1	D	2796	CYS	C-N-CA	5.26	125.16	119.85
1	G	2405	PHE	CB-CA-C	-5.25	100.25	109.71
1	A	2603	ILE	CB-CA-C	-5.25	105.60	111.80
1	E	2603	ILE	CB-CA-C	-5.25	105.60	111.80
1	F	2405	PHE	CB-CA-C	-5.25	100.27	109.71
1	B	2405	PHE	CB-CA-C	-5.24	100.28	109.71
1	D	2603	ILE	CB-CA-C	-5.24	105.62	111.80
1	D	2405	PHE	CB-CA-C	-5.24	100.29	109.71
1	A	2405	PHE	CB-CA-C	-5.23	100.29	109.71
1	B	2603	ILE	CB-CA-C	-5.23	105.63	111.80
1	F	2603	ILE	CB-CA-C	-5.23	105.63	111.80
1	E	2405	PHE	CB-CA-C	-5.23	100.29	109.71
1	C	2405	PHE	CB-CA-C	-5.23	100.30	109.71
1	E	2570	ASN	N-CA-C	-5.15	103.25	110.35
1	F	2570	ASN	N-CA-C	-5.14	103.25	110.35
1	C	2575	ARG	N-CA-C	5.13	117.54	111.33
1	A	2570	ASN	N-CA-C	-5.13	103.27	110.35
1	G	2570	ASN	N-CA-C	-5.13	103.27	110.35
1	C	2570	ASN	N-CA-C	-5.13	103.28	110.35
1	D	2570	ASN	N-CA-C	-5.13	103.28	110.35
1	A	2575	ARG	N-CA-C	5.12	117.53	111.33
1	E	2575	ARG	N-CA-C	5.12	117.52	111.33
1	B	2570	ASN	N-CA-C	-5.12	103.29	110.35
1	G	2575	ARG	N-CA-C	5.12	117.52	111.33
1	C	2712	GLN	N-CA-C	5.11	117.04	107.99
1	F	2712	GLN	N-CA-C	5.09	117.01	107.99
1	A	2712	GLN	N-CA-C	5.09	117.00	107.99
1	F	2575	ARG	N-CA-C	5.09	117.49	111.33
1	D	2712	GLN	N-CA-C	5.09	117.00	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2461	ASN	N-CA-C	-5.09	107.12	113.38
1	D	2461	ASN	N-CA-C	-5.09	107.12	113.38
1	G	2461	ASN	N-CA-C	-5.09	107.12	113.38
1	D	2575	ARG	N-CA-C	5.09	117.48	111.33
1	E	2461	ASN	N-CA-C	-5.09	107.12	113.38
1	E	2641	HIS	CB-CA-C	-5.08	101.28	109.67
1	B	2575	ARG	N-CA-C	5.08	117.48	111.33
1	B	2712	GLN	N-CA-C	5.08	116.98	107.99
1	B	2461	ASN	N-CA-C	-5.08	107.13	113.38
1	A	2461	ASN	N-CA-C	-5.08	107.14	113.38
1	G	2712	GLN	N-CA-C	5.08	116.98	107.99
1	A	2641	HIS	CB-CA-C	-5.07	101.30	109.67
1	B	2641	HIS	CB-CA-C	-5.07	101.30	109.67
1	D	2641	HIS	CB-CA-C	-5.07	101.30	109.67
1	F	2461	ASN	N-CA-C	-5.07	107.14	113.38
1	F	2641	HIS	CB-CA-C	-5.07	101.31	109.67
1	G	2641	HIS	CB-CA-C	-5.07	101.31	109.67
1	C	2641	HIS	CB-CA-C	-5.06	101.31	109.67
1	E	2712	GLN	N-CA-C	5.05	116.93	107.99

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2755	ARG	Sidechain
1	B	2755	ARG	Sidechain
1	C	2755	ARG	Sidechain
1	D	2755	ARG	Sidechain
1	E	2755	ARG	Sidechain
1	F	2755	ARG	Sidechain
1	G	2755	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	2974	0	2834	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2974	0	2834	57	0
1	C	2974	0	2834	56	0
1	D	2974	0	2834	57	0
1	E	2974	0	2834	57	0
1	F	2974	0	2834	58	0
1	G	2974	0	2834	60	0
All	All	20818	0	19838	302	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 7.

All (302) 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)
1:F:2748:THR:CG2	1:G:2760:ASN:O	1.80	1.30
1:B:2748:THR:CG2	1:C:2760:ASN:O	1.79	1.28
1:A:2760:ASN:O	1:G:2748:THR:CG2	1.82	1.28
1:A:2748:THR:CG2	1:B:2760:ASN:O	1.82	1.27
1:D:2748:THR:CG2	1:E:2760:ASN:O	1.80	1.27
1:C:2748:THR:CG2	1:D:2760:ASN:O	1.83	1.24
1:E:2748:THR:CG2	1:F:2760:ASN:O	1.85	1.24
1:E:2393:TYR:CE2	1:E:2461:ASN:HB3	1.76	1.21
1:C:2393:TYR:CE2	1:C:2461:ASN:HB3	1.76	1.21
1:D:2393:TYR:CE2	1:D:2461:ASN:HB3	1.76	1.20
1:A:2393:TYR:CE2	1:A:2461:ASN:HB3	1.76	1.19
1:G:2393:TYR:CE2	1:G:2461:ASN:HB3	1.76	1.19
1:F:2393:TYR:CE2	1:F:2461:ASN:HB3	1.76	1.19
1:B:2393:TYR:CE2	1:B:2461:ASN:HB3	1.76	1.19
1:E:2748:THR:HG21	1:F:2760:ASN:O	0.92	1.09
1:B:2573:VAL:O	1:B:2640:LEU:HD12	1.52	1.09
1:F:2573:VAL:O	1:F:2640:LEU:HD12	1.52	1.08
1:A:2573:VAL:O	1:A:2640:LEU:HD12	1.52	1.08
1:C:2573:VAL:O	1:C:2640:LEU:HD12	1.52	1.08
1:G:2573:VAL:O	1:G:2640:LEU:HD12	1.52	1.07
1:E:2573:VAL:O	1:E:2640:LEU:HD12	1.52	1.07
1:C:2748:THR:HG21	1:D:2760:ASN:O	0.89	1.06
1:D:2573:VAL:O	1:D:2640:LEU:HD12	1.52	1.06
1:A:2748:THR:HG21	1:B:2760:ASN:O	0.89	1.05
1:A:2760:ASN:O	1:G:2748:THR:HG21	0.89	1.04
1:D:2748:THR:HG21	1:E:2760:ASN:O	0.87	1.04
1:F:2748:THR:HG21	1:G:2760:ASN:O	0.87	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2748:THR:HG21	1:C:2760:ASN:O	0.86	1.03
1:F:2748:THR:HG22	1:G:2760:ASN:ND2	1.75	1.01
1:B:2748:THR:HG22	1:C:2760:ASN:ND2	1.76	1.00
1:A:2748:THR:HG22	1:B:2760:ASN:ND2	1.78	0.99
1:F:2755:ARG:HG2	1:F:2765:ILE:HG12	1.46	0.98
1:G:2755:ARG:HG2	1:G:2765:ILE:HG12	1.46	0.98
1:C:2748:THR:HG22	1:D:2760:ASN:ND2	1.78	0.98
1:A:2755:ARG:HG2	1:A:2765:ILE:HG12	1.46	0.98
1:E:2755:ARG:HG2	1:E:2765:ILE:HG12	1.46	0.98
1:E:2748:THR:HG22	1:F:2760:ASN:ND2	1.79	0.98
1:D:2748:THR:HG22	1:E:2760:ASN:ND2	1.79	0.97
1:A:2760:ASN:ND2	1:G:2748:THR:HG22	1.80	0.96
1:B:2755:ARG:HG2	1:B:2765:ILE:HG12	1.45	0.96
1:D:2755:ARG:HG2	1:D:2765:ILE:HG12	1.46	0.96
1:B:2748:THR:HG21	1:C:2760:ASN:C	1.92	0.95
1:C:2755:ARG:HG2	1:C:2765:ILE:HG12	1.46	0.95
1:F:2748:THR:HG21	1:G:2760:ASN:C	1.92	0.94
1:D:2748:THR:HG21	1:E:2760:ASN:C	1.93	0.93
1:A:2748:THR:HG21	1:B:2760:ASN:C	1.94	0.93
1:A:2760:ASN:C	1:G:2748:THR:HG21	1.95	0.91
1:C:2748:THR:HG21	1:D:2760:ASN:C	1.95	0.91
1:B:2748:THR:HG22	1:C:2760:ASN:CG	1.99	0.88
1:E:2748:THR:HG21	1:F:2760:ASN:C	1.98	0.87
1:D:2748:THR:HG22	1:E:2760:ASN:CG	2.00	0.87
1:F:2748:THR:HG22	1:G:2760:ASN:CG	1.99	0.86
1:A:2748:THR:HG22	1:B:2760:ASN:CG	2.00	0.86
1:C:2748:THR:HG22	1:D:2760:ASN:CG	2.02	0.84
1:E:2748:THR:HG22	1:F:2760:ASN:CG	2.03	0.84
1:F:2748:THR:CG2	1:G:2760:ASN:ND2	2.40	0.83
1:A:2748:THR:CG2	1:B:2760:ASN:ND2	2.42	0.82
1:B:2748:THR:CG2	1:C:2760:ASN:ND2	2.41	0.82
1:A:2760:ASN:CG	1:G:2748:THR:HG22	2.03	0.82
1:C:2748:THR:CG2	1:D:2760:ASN:ND2	2.43	0.82
1:E:2748:THR:CG2	1:F:2760:ASN:ND2	2.42	0.81
1:D:2748:THR:CG2	1:E:2760:ASN:ND2	2.43	0.81
1:A:2760:ASN:ND2	1:G:2748:THR:CG2	2.45	0.79
1:B:2748:THR:CG2	1:C:2760:ASN:CG	2.58	0.77
1:F:2748:THR:CG2	1:G:2760:ASN:CG	2.58	0.76
1:D:2748:THR:CG2	1:E:2760:ASN:CG	2.59	0.75
1:A:2748:THR:CG2	1:B:2760:ASN:CG	2.58	0.75
1:E:2748:THR:CG2	1:F:2760:ASN:CG	2.60	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2748:THR:CG2	1:D:2760:ASN:CG	2.60	0.74
1:A:2760:ASN:CG	1:G:2748:THR:CG2	2.61	0.74
1:F:2748:THR:HG22	1:G:2760:ASN:HD21	1.51	0.73
1:E:2748:THR:HG22	1:F:2760:ASN:HD21	1.52	0.73
1:B:2748:THR:HG22	1:C:2760:ASN:HD21	1.53	0.71
1:C:2748:THR:HG22	1:D:2760:ASN:HD21	1.53	0.71
1:C:2393:TYR:CZ	1:C:2461:ASN:HB3	2.26	0.71
1:B:2393:TYR:CZ	1:B:2461:ASN:HB3	2.26	0.71
1:A:2393:TYR:CZ	1:A:2461:ASN:HB3	2.26	0.70
1:A:2748:THR:HG22	1:B:2760:ASN:HD21	1.54	0.70
1:D:2393:TYR:CZ	1:D:2461:ASN:HB3	2.26	0.70
1:E:2393:TYR:CZ	1:E:2461:ASN:HB3	2.26	0.70
1:F:2393:TYR:CZ	1:F:2461:ASN:HB3	2.26	0.70
1:A:2760:ASN:HD21	1:G:2748:THR:HG22	1.55	0.69
1:D:2748:THR:HG22	1:E:2760:ASN:HD21	1.55	0.69
1:G:2393:TYR:CZ	1:G:2461:ASN:HB3	2.26	0.69
1:G:2393:TYR:CE2	1:G:2461:ASN:CB	2.69	0.68
1:C:2393:TYR:CE2	1:C:2461:ASN:CB	2.69	0.66
1:D:2393:TYR:CE2	1:D:2461:ASN:CB	2.69	0.64
1:F:2393:TYR:CE2	1:F:2461:ASN:CB	2.69	0.63
1:E:2393:TYR:CE2	1:E:2461:ASN:CB	2.69	0.63
1:A:2755:ARG:HG2	1:A:2765:ILE:CG1	2.25	0.62
1:B:2755:ARG:HG2	1:B:2765:ILE:CG1	2.25	0.62
1:C:2437:GLN:O	1:C:2437:GLN:HG2	2.00	0.62
1:B:2437:GLN:HG2	1:B:2437:GLN:O	2.00	0.62
1:A:2393:TYR:CE2	1:A:2461:ASN:CB	2.69	0.62
1:G:2755:ARG:HG2	1:G:2765:ILE:CG1	2.25	0.62
1:D:2437:GLN:O	1:D:2437:GLN:HG2	2.00	0.61
1:C:2755:ARG:HG2	1:C:2765:ILE:CG1	2.25	0.61
1:F:2755:ARG:HG2	1:F:2765:ILE:CG1	2.25	0.61
1:F:2437:GLN:O	1:F:2437:GLN:HG2	2.00	0.61
1:A:2437:GLN:O	1:A:2437:GLN:HG2	2.00	0.61
1:D:2755:ARG:HG2	1:D:2765:ILE:CG1	2.25	0.61
1:E:2437:GLN:O	1:E:2437:GLN:HG2	2.00	0.61
1:E:2755:ARG:HG2	1:E:2765:ILE:CG1	2.25	0.61
1:C:2573:VAL:O	1:C:2640:LEU:CD1	2.41	0.60
1:G:2437:GLN:HG2	1:G:2437:GLN:O	2.00	0.60
1:G:2755:ARG:NE	1:G:2763:ASP:OD1	2.32	0.60
1:D:2755:ARG:NE	1:D:2763:ASP:OD1	2.32	0.60
1:F:2679:GLY:HA2	1:G:2684:LEU:HD13	1.84	0.60
1:A:2684:LEU:HD13	1:G:2679:GLY:HA2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2393:TYR:CE2	1:B:2461:ASN:CB	2.69	0.59
1:F:2755:ARG:NE	1:F:2763:ASP:OD1	2.32	0.59
1:B:2755:ARG:NE	1:B:2763:ASP:OD1	2.32	0.59
1:E:2755:ARG:NE	1:E:2763:ASP:OD1	2.32	0.58
1:F:2678:ASN:OD1	1:G:2689:VAL:HG23	2.03	0.58
1:F:2573:VAL:O	1:F:2640:LEU:CD1	2.41	0.57
1:C:2679:GLY:HA2	1:D:2684:LEU:HD13	1.84	0.57
1:A:2679:GLY:HA2	1:B:2684:LEU:HD13	1.87	0.57
1:C:2704:PHE:CD1	1:C:2704:PHE:C	2.83	0.57
1:B:2704:PHE:C	1:B:2704:PHE:CD1	2.83	0.57
1:C:2755:ARG:NE	1:C:2763:ASP:OD1	2.32	0.57
1:D:2679:GLY:HA2	1:E:2684:LEU:HD13	1.85	0.57
1:E:2679:GLY:HA2	1:F:2684:LEU:HD13	1.87	0.57
1:E:2704:PHE:CD1	1:E:2704:PHE:C	2.83	0.57
1:B:2679:GLY:HA2	1:C:2684:LEU:HD13	1.85	0.57
1:D:2704:PHE:CD1	1:D:2704:PHE:C	2.83	0.57
1:G:2704:PHE:C	1:G:2704:PHE:CD1	2.83	0.57
1:G:2573:VAL:O	1:G:2640:LEU:CD1	2.41	0.56
1:B:2678:ASN:OD1	1:C:2689:VAL:HG23	2.05	0.56
1:A:2748:THR:HG22	1:B:2760:ASN:OD1	2.06	0.56
1:A:2755:ARG:NE	1:A:2763:ASP:OD1	2.32	0.56
1:F:2704:PHE:CD1	1:F:2704:PHE:C	2.83	0.56
1:F:2678:ASN:OD1	1:G:2689:VAL:CG2	2.53	0.56
1:A:2689:VAL:HG23	1:G:2678:ASN:OD1	2.06	0.56
1:B:2678:ASN:OD1	1:C:2689:VAL:CG2	2.54	0.56
1:C:2678:ASN:OD1	1:D:2689:VAL:HG23	2.06	0.55
1:D:2573:VAL:O	1:D:2640:LEU:CD1	2.41	0.55
1:A:2573:VAL:O	1:A:2640:LEU:CD1	2.41	0.55
1:A:2704:PHE:CD1	1:A:2704:PHE:C	2.83	0.55
1:F:2748:THR:HG22	1:G:2760:ASN:OD1	2.07	0.55
1:B:2748:THR:HG22	1:C:2760:ASN:OD1	2.06	0.55
1:D:2748:THR:HG22	1:E:2760:ASN:OD1	2.06	0.55
1:D:2678:ASN:OD1	1:E:2689:VAL:HG23	2.06	0.54
1:A:2689:VAL:CG2	1:G:2678:ASN:OD1	2.55	0.54
1:A:2760:ASN:OD1	1:G:2748:THR:HG22	2.08	0.54
1:D:2678:ASN:OD1	1:E:2689:VAL:CG2	2.56	0.54
1:E:2678:ASN:OD1	1:F:2689:VAL:HG23	2.07	0.54
1:A:2678:ASN:OD1	1:B:2689:VAL:HG23	2.08	0.54
1:C:2678:ASN:OD1	1:D:2689:VAL:CG2	2.55	0.54
1:E:2748:THR:HG22	1:F:2760:ASN:OD1	2.08	0.54
1:E:2678:ASN:OD1	1:F:2689:VAL:CG2	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2393:TYR:HE2	1:G:2461:ASN:HB3	1.61	0.53
1:A:2678:ASN:OD1	1:B:2689:VAL:CG2	2.57	0.53
1:D:2760:ASN:HB2	1:D:2782:GLN:HE22	1.74	0.53
1:A:2393:TYR:HE2	1:A:2461:ASN:HB3	1.61	0.53
1:A:2489:ILE:CD1	1:A:2495:LEU:HA	2.39	0.53
1:G:2489:ILE:CD1	1:G:2495:LEU:HA	2.39	0.53
1:B:2760:ASN:HB2	1:B:2782:GLN:HE22	1.74	0.52
1:E:2760:ASN:HB2	1:E:2782:GLN:HE22	1.74	0.52
1:F:2760:ASN:HB2	1:F:2782:GLN:HE22	1.74	0.52
1:B:2489:ILE:CD1	1:B:2495:LEU:HA	2.39	0.52
1:C:2760:ASN:HB2	1:C:2782:GLN:HE22	1.74	0.52
1:F:2489:ILE:CD1	1:F:2495:LEU:HA	2.39	0.52
1:G:2760:ASN:HB2	1:G:2782:GLN:HE22	1.74	0.52
1:E:2573:VAL:O	1:E:2640:LEU:CD1	2.41	0.52
1:C:2489:ILE:CD1	1:C:2495:LEU:HA	2.39	0.52
1:D:2489:ILE:CD1	1:D:2495:LEU:HA	2.39	0.52
1:E:2489:ILE:CD1	1:E:2495:LEU:HA	2.39	0.52
1:A:2760:ASN:HB2	1:A:2782:GLN:HE22	1.74	0.52
1:B:2573:VAL:O	1:B:2640:LEU:CD1	2.41	0.52
1:C:2748:THR:HG22	1:D:2760:ASN:OD1	2.09	0.51
1:F:2393:TYR:HE2	1:F:2461:ASN:HB3	1.61	0.51
1:B:2393:TYR:HE2	1:B:2461:ASN:HB3	1.61	0.49
1:C:2430:ASN:O	1:C:2431:GLY:C	2.55	0.49
1:E:2430:ASN:O	1:E:2431:GLY:C	2.55	0.49
1:F:2430:ASN:O	1:F:2431:GLY:C	2.55	0.49
1:D:2430:ASN:O	1:D:2431:GLY:C	2.55	0.49
1:B:2430:ASN:O	1:B:2431:GLY:C	2.56	0.48
1:G:2430:ASN:O	1:G:2431:GLY:C	2.55	0.48
1:A:2430:ASN:O	1:A:2431:GLY:C	2.55	0.47
1:B:2748:THR:HG21	1:C:2760:ASN:CG	2.38	0.47
1:C:2748:THR:HG21	1:D:2760:ASN:CG	2.39	0.47
1:E:2393:TYR:HE2	1:E:2461:ASN:HB3	1.61	0.47
1:E:2748:THR:HG21	1:F:2760:ASN:CG	2.37	0.47
1:C:2747:THR:OG1	1:C:2748:THR:N	2.48	0.47
1:E:2747:THR:OG1	1:E:2748:THR:N	2.48	0.46
1:F:2747:THR:OG1	1:F:2748:THR:N	2.48	0.46
1:A:2747:THR:OG1	1:A:2748:THR:N	2.48	0.46
1:A:2760:ASN:CG	1:G:2748:THR:HG21	2.40	0.46
1:A:2766:THR:OG1	1:A:2767:THR:N	2.48	0.46
1:D:2748:THR:HG21	1:E:2760:ASN:CG	2.39	0.46
1:B:2766:THR:OG1	1:B:2767:THR:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2747:THR:OG1	1:G:2748:THR:N	2.48	0.46
1:G:2766:THR:OG1	1:G:2767:THR:N	2.48	0.46
1:B:2747:THR:OG1	1:B:2748:THR:N	2.48	0.46
1:D:2747:THR:OG1	1:D:2748:THR:N	2.48	0.46
1:A:2784:GLY:O	1:A:2805:SER:HA	2.16	0.46
1:C:2393:TYR:HE2	1:C:2461:ASN:HB3	1.61	0.45
1:G:2784:GLY:O	1:G:2805:SER:HA	2.16	0.45
1:C:2766:THR:OG1	1:C:2767:THR:N	2.48	0.45
1:F:2779:THR:O	1:F:2782:GLN:NE2	2.50	0.45
1:B:2784:GLY:O	1:B:2805:SER:HA	2.16	0.45
1:F:2748:THR:HG21	1:G:2760:ASN:CG	2.38	0.45
1:G:2779:THR:O	1:G:2782:GLN:NE2	2.50	0.45
1:D:2575:ARG:HA	1:D:2640:LEU:HD11	1.98	0.45
1:A:2673:ASN:ND2	1:A:2704:PHE:CE2	2.85	0.45
1:E:2575:ARG:HA	1:E:2640:LEU:HD11	1.98	0.45
1:A:2748:THR:HG21	1:B:2760:ASN:CG	2.37	0.45
1:F:2575:ARG:N	1:F:2640:LEU:HD11	2.32	0.45
1:A:2575:ARG:HA	1:A:2640:LEU:HD11	1.98	0.45
1:B:2673:ASN:ND2	1:B:2704:PHE:CE2	2.85	0.45
1:B:2779:THR:O	1:B:2782:GLN:NE2	2.50	0.45
1:E:2575:ARG:N	1:E:2640:LEU:HD11	2.32	0.45
1:E:2779:THR:O	1:E:2782:GLN:NE2	2.50	0.45
1:C:2575:ARG:HA	1:C:2640:LEU:HD11	1.98	0.45
1:D:2673:ASN:ND2	1:D:2704:PHE:CE2	2.85	0.45
1:F:2784:GLY:O	1:F:2805:SER:HA	2.16	0.45
1:G:2575:ARG:HA	1:G:2640:LEU:HD11	1.98	0.45
1:A:2575:ARG:N	1:A:2640:LEU:HD11	2.32	0.44
1:E:2673:ASN:ND2	1:E:2704:PHE:CE2	2.85	0.44
1:F:2575:ARG:HA	1:F:2640:LEU:HD11	1.98	0.44
1:G:2575:ARG:N	1:G:2640:LEU:HD11	2.32	0.44
1:G:2673:ASN:ND2	1:G:2704:PHE:CE2	2.85	0.44
1:B:2486:ASN:O	1:B:2489:ILE:HG13	2.18	0.44
1:C:2779:THR:O	1:C:2782:GLN:NE2	2.50	0.44
1:F:2486:ASN:O	1:F:2489:ILE:HG13	2.18	0.44
1:F:2673:ASN:ND2	1:F:2704:PHE:CE2	2.85	0.44
1:A:2760:ASN:HD22	1:A:2762:ILE:HG13	1.83	0.44
1:A:2779:THR:O	1:A:2782:GLN:NE2	2.50	0.44
1:C:2486:ASN:O	1:C:2489:ILE:HG13	2.18	0.44
1:F:2766:THR:OG1	1:F:2767:THR:N	2.48	0.44
1:B:2575:ARG:HA	1:B:2640:LEU:HD11	1.98	0.44
1:B:2679:GLY:O	1:B:2680:PHE:C	2.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2760:ASN:HD22	1:E:2762:ILE:HG13	1.83	0.44
1:A:2691:GLN:HB3	1:A:2692:PRO:HD3	2.00	0.44
1:B:2575:ARG:N	1:B:2640:LEU:HD11	2.32	0.44
1:C:2673:ASN:ND2	1:C:2704:PHE:CE2	2.85	0.44
1:C:2679:GLY:O	1:C:2680:PHE:C	2.61	0.44
1:C:2784:GLY:O	1:C:2805:SER:HA	2.16	0.44
1:D:2575:ARG:N	1:D:2640:LEU:HD11	2.32	0.44
1:D:2784:GLY:O	1:D:2805:SER:HA	2.16	0.44
1:A:2748:THR:CB	1:B:2760:ASN:O	2.61	0.44
1:B:2691:GLN:HB3	1:B:2692:PRO:HD3	2.00	0.44
1:D:2679:GLY:O	1:D:2680:PHE:C	2.61	0.44
1:D:2766:THR:OG1	1:D:2767:THR:N	2.48	0.44
1:B:2748:THR:CB	1:C:2760:ASN:O	2.60	0.44
1:C:2575:ARG:N	1:C:2640:LEU:HD11	2.32	0.44
1:D:2486:ASN:O	1:D:2489:ILE:HG13	2.18	0.44
1:F:2748:THR:CB	1:G:2760:ASN:O	2.61	0.44
1:E:2766:THR:OG1	1:E:2767:THR:N	2.48	0.44
1:G:2691:GLN:HB3	1:G:2692:PRO:HD3	2.00	0.44
1:A:2486:ASN:O	1:A:2489:ILE:HG13	2.18	0.43
1:D:2393:TYR:HE2	1:D:2461:ASN:HB3	1.61	0.43
1:G:2486:ASN:O	1:G:2489:ILE:HG13	2.18	0.43
1:C:2760:ASN:HD22	1:C:2762:ILE:HG13	1.83	0.43
1:D:2760:ASN:HD22	1:D:2762:ILE:HG13	1.83	0.43
1:D:2779:THR:O	1:D:2782:GLN:NE2	2.50	0.43
1:B:2760:ASN:HD22	1:B:2762:ILE:HG13	1.83	0.43
1:E:2419:THR:OG1	1:E:2420:VAL:N	2.51	0.43
1:E:2486:ASN:O	1:E:2489:ILE:HG13	2.18	0.43
1:G:2393:TYR:O	1:G:2394:PRO:C	2.62	0.43
1:F:2691:GLN:HB3	1:F:2692:PRO:HD3	2.00	0.43
1:G:2760:ASN:HD22	1:G:2762:ILE:HG13	1.83	0.43
1:C:2691:GLN:HB3	1:C:2692:PRO:HD3	2.00	0.43
1:E:2784:GLY:O	1:E:2805:SER:HA	2.16	0.43
1:F:2760:ASN:HD22	1:F:2762:ILE:HG13	1.83	0.43
1:C:2499:THR:OG1	1:C:2500:SER:N	2.52	0.43
1:F:2419:THR:OG1	1:F:2420:VAL:N	2.51	0.43
1:B:2499:THR:OG1	1:B:2500:SER:N	2.52	0.42
1:E:2499:THR:OG1	1:E:2500:SER:N	2.52	0.42
1:A:2499:THR:OG1	1:A:2500:SER:N	2.52	0.42
1:D:2419:THR:OG1	1:D:2420:VAL:N	2.51	0.42
1:D:2691:GLN:HB3	1:D:2692:PRO:HD3	2.00	0.42
1:D:2393:TYR:O	1:D:2394:PRO:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2691:GLN:HB3	1:E:2692:PRO:HD3	2.00	0.42
1:F:2393:TYR:O	1:F:2394:PRO:C	2.62	0.42
1:A:2684:LEU:CD1	1:G:2679:GLY:HA2	2.48	0.42
1:D:2499:THR:OG1	1:D:2500:SER:N	2.52	0.42
1:C:2419:THR:OG1	1:C:2420:VAL:N	2.51	0.42
1:D:2748:THR:CB	1:E:2760:ASN:O	2.61	0.42
1:E:2393:TYR:O	1:E:2394:PRO:C	2.62	0.42
1:E:2679:GLY:O	1:E:2680:PHE:C	2.61	0.42
1:F:2679:GLY:HA2	1:G:2684:LEU:CD1	2.48	0.42
1:C:2393:TYR:O	1:C:2394:PRO:C	2.62	0.42
1:F:2499:THR:OG1	1:F:2500:SER:N	2.52	0.42
1:B:2419:THR:OG1	1:B:2420:VAL:N	2.51	0.41
1:B:2393:TYR:O	1:B:2394:PRO:C	2.62	0.41
1:A:2393:TYR:O	1:A:2394:PRO:C	2.62	0.41
1:A:2760:ASN:O	1:G:2748:THR:CB	2.63	0.41
1:F:2490:CYS:O	1:F:2491:ASN:C	2.63	0.41
1:D:2490:CYS:O	1:D:2491:ASN:C	2.63	0.41
1:E:2490:CYS:O	1:E:2491:ASN:C	2.64	0.41
1:G:2499:THR:OG1	1:G:2500:SER:N	2.52	0.41
1:G:2679:GLY:O	1:G:2680:PHE:C	2.61	0.41
1:E:2424:TYR:CZ	1:E:2437:GLN:HB2	2.57	0.40
1:F:2424:TYR:CZ	1:F:2437:GLN:HB2	2.57	0.40
1:G:2490:CYS:O	1:G:2491:ASN:C	2.63	0.40
1:B:2424:TYR:CZ	1:B:2437:GLN:HB2	2.57	0.40
1:G:2419:THR:OG1	1:G:2420:VAL:N	2.51	0.40
1:C:2683:ASN:OD1	1:C:2683:ASN:N	2.47	0.40
1:F:2679:GLY:O	1:F:2680:PHE:C	2.61	0.40
1:D:2646:THR:HA	1:D:2647:PRO:HD3	1.90	0.40
1:G:2646:THR:HA	1:G:2647:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
1	B	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
1	C	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
1	D	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
1	E	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
1	F	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
1	G	413/5898 (7%)	409 (99%)	4 (1%)	0	100	100
All	All	2891/41286 (7%)	2863 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/4919 (7%)	343 (100%)	0	100	100
1	B	343/4919 (7%)	343 (100%)	0	100	100
1	C	343/4919 (7%)	343 (100%)	0	100	100
1	D	343/4919 (7%)	343 (100%)	0	100	100
1	E	343/4919 (7%)	343 (100%)	0	100	100
1	F	343/4919 (7%)	343 (100%)	0	100	100
1	G	343/4919 (7%)	343 (100%)	0	100	100
All	All	2401/34433 (7%)	2401 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2438	ASN
1	A	2536	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2582	ASN
1	A	2607	GLN
1	A	2608	ASN
1	A	2686	ASN
1	A	2760	ASN
1	A	2782	GLN
1	B	2438	ASN
1	B	2536	ASN
1	B	2606	GLN
1	B	2686	ASN
1	B	2760	ASN
1	B	2782	GLN
1	C	2438	ASN
1	C	2536	ASN
1	C	2582	ASN
1	C	2606	GLN
1	C	2607	GLN
1	C	2608	ASN
1	C	2686	ASN
1	C	2760	ASN
1	C	2782	GLN
1	D	2438	ASN
1	D	2536	ASN
1	D	2582	ASN
1	D	2607	GLN
1	D	2608	ASN
1	D	2686	ASN
1	D	2760	ASN
1	D	2782	GLN
1	E	2438	ASN
1	E	2536	ASN
1	E	2582	ASN
1	E	2607	GLN
1	E	2608	ASN
1	E	2686	ASN
1	E	2760	ASN
1	E	2782	GLN
1	F	2438	ASN
1	F	2536	ASN
1	F	2582	ASN
1	F	2606	GLN
1	F	2607	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	2608	ASN
1	F	2686	ASN
1	F	2760	ASN
1	F	2782	GLN
1	G	2438	ASN
1	G	2536	ASN
1	G	2582	ASN
1	G	2607	GLN
1	G	2608	ASN
1	G	2686	ASN
1	G	2760	ASN
1	G	2782	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.

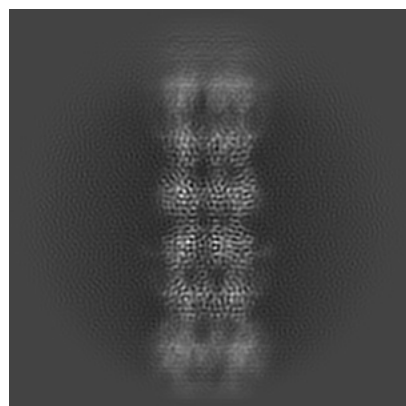
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50540. These allow visual inspection of the internal detail of the map and identification of artifacts.

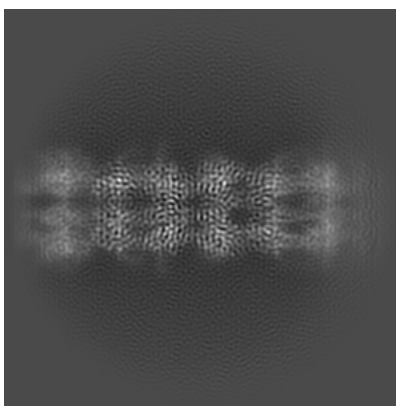
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

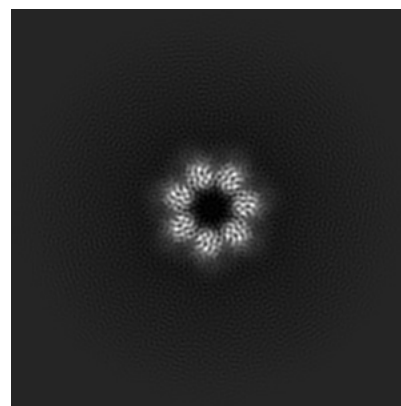
6.1.1 Primary map



X

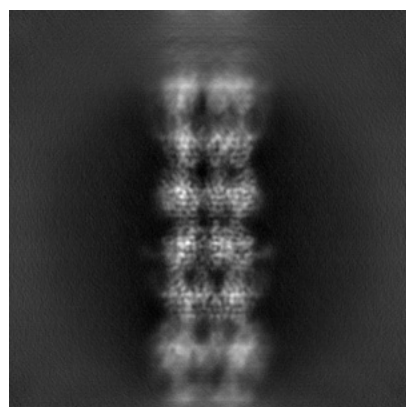


Y

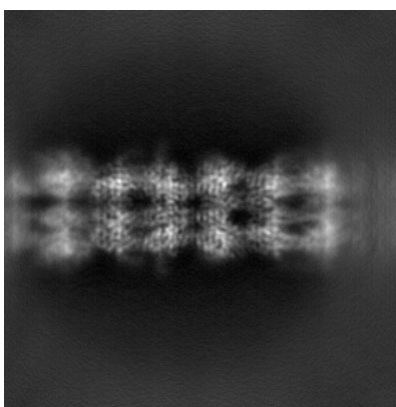


Z

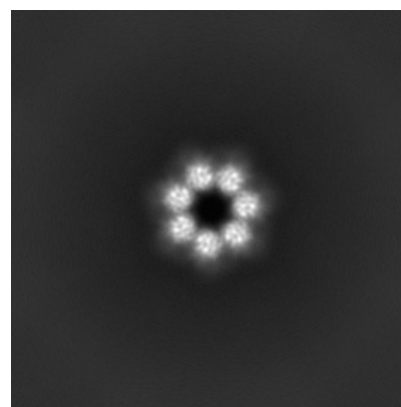
6.1.2 Raw map



X



Y

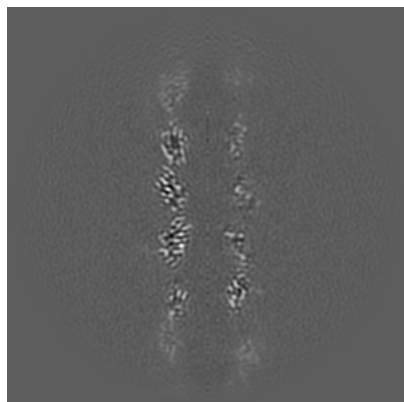


Z

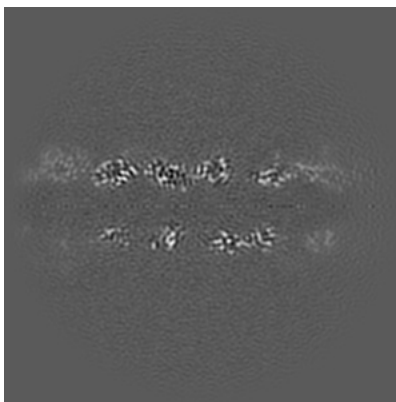
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

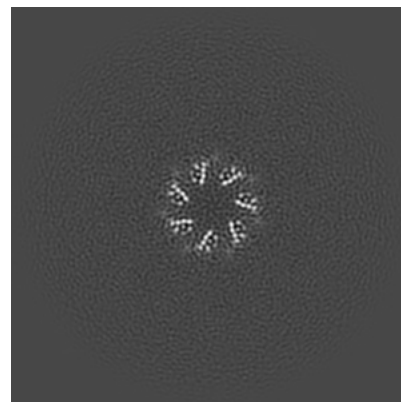
6.2.1 Primary map



X Index: 150

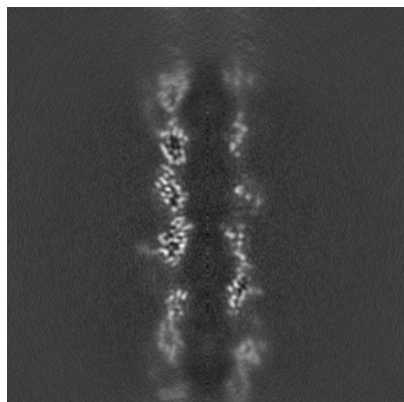


Y Index: 150

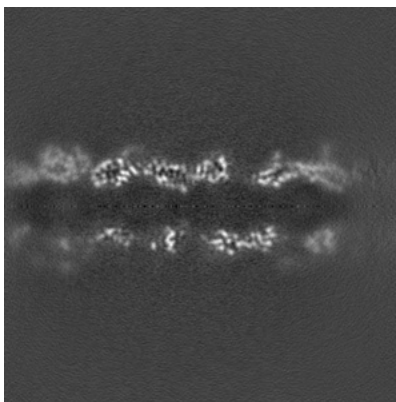


Z Index: 150

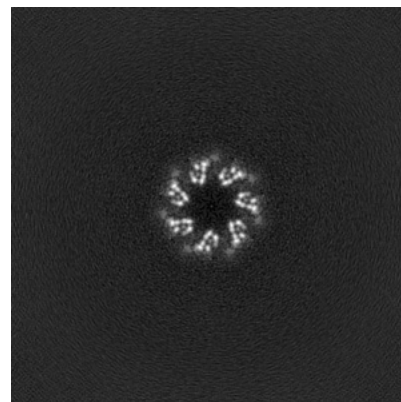
6.2.2 Raw map



X Index: 150



Y Index: 150

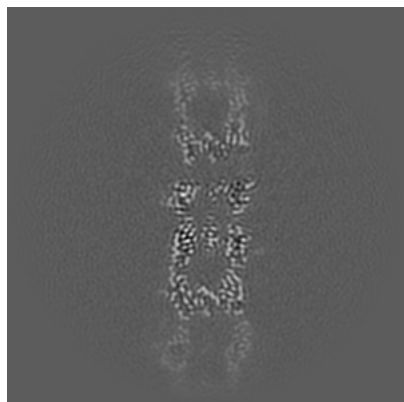


Z Index: 150

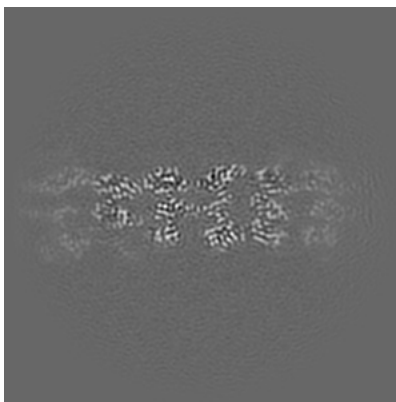
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

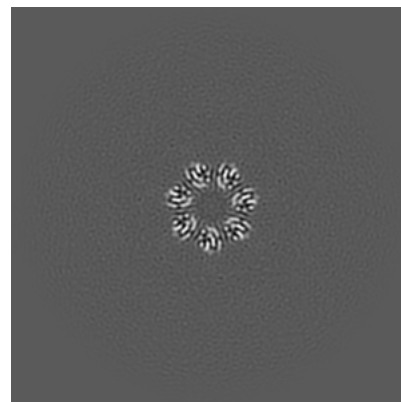
6.3.1 Primary map



X Index: 167

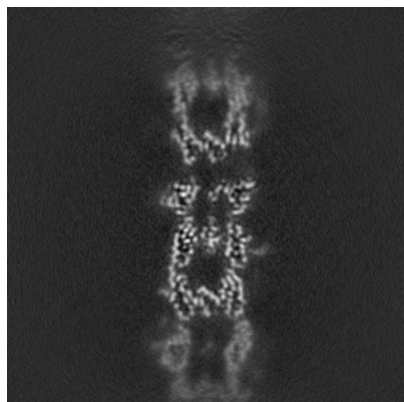


Y Index: 130

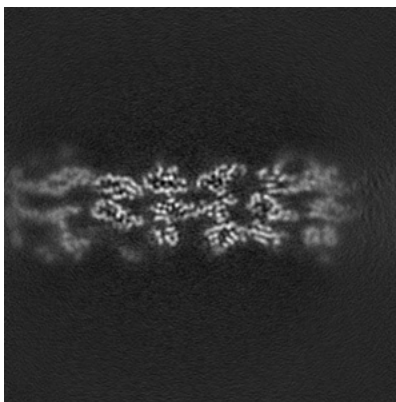


Z Index: 125

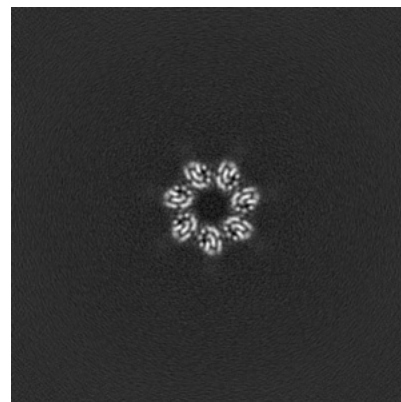
6.3.2 Raw map



X Index: 167



Y Index: 129

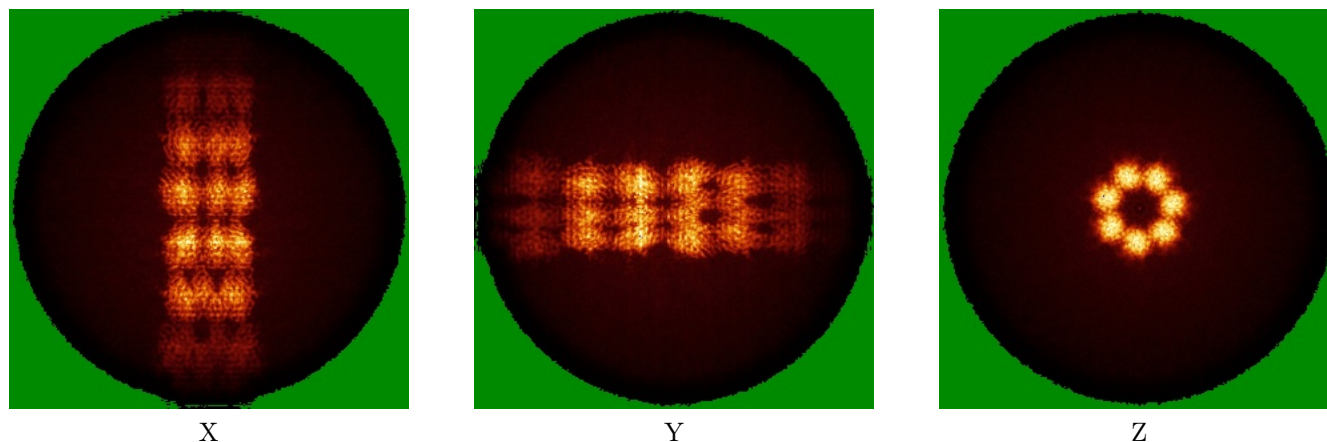


Z Index: 125

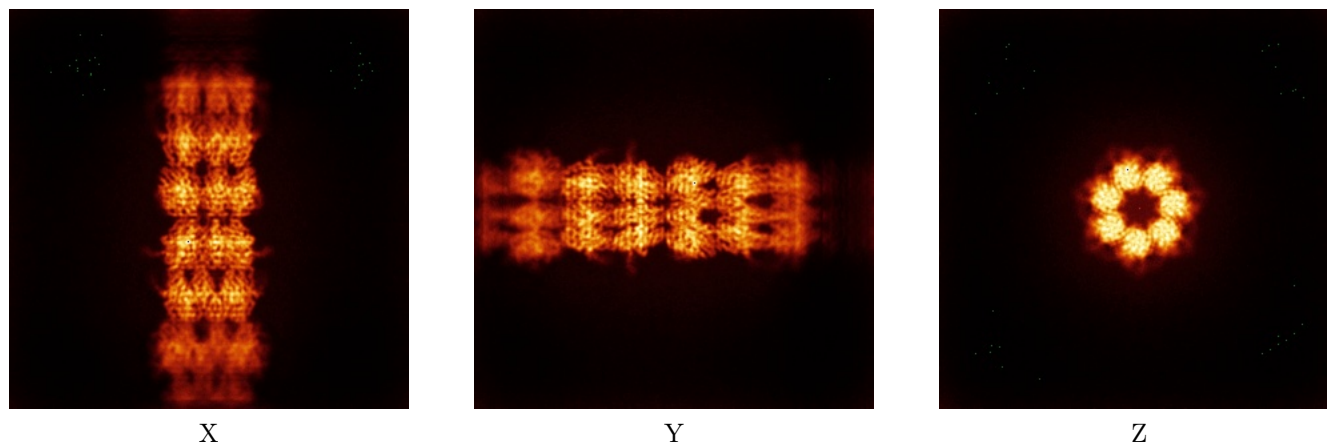
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

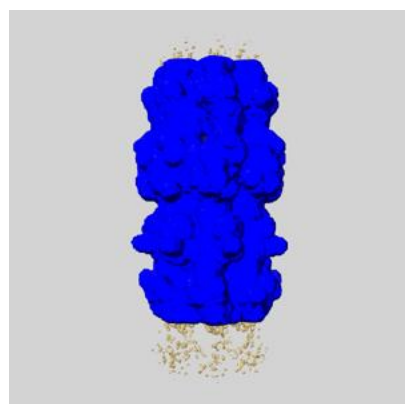
6.6 Mask visualisation [i](#)

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

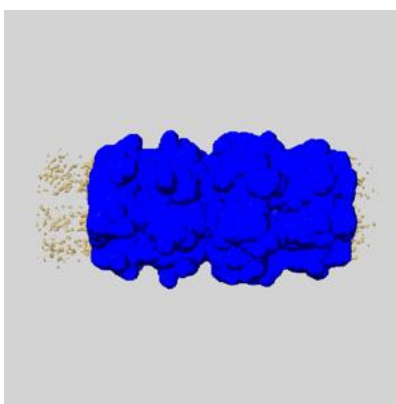
A mask typically either:

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

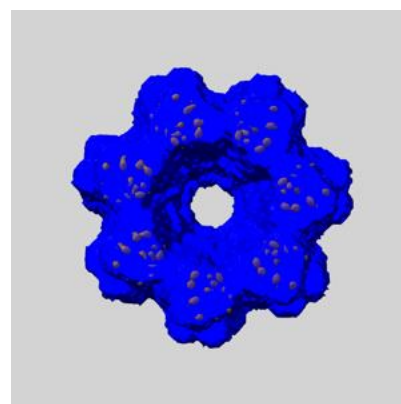
6.6.1 emd_50540_msk_1.map [i](#)



X



Y

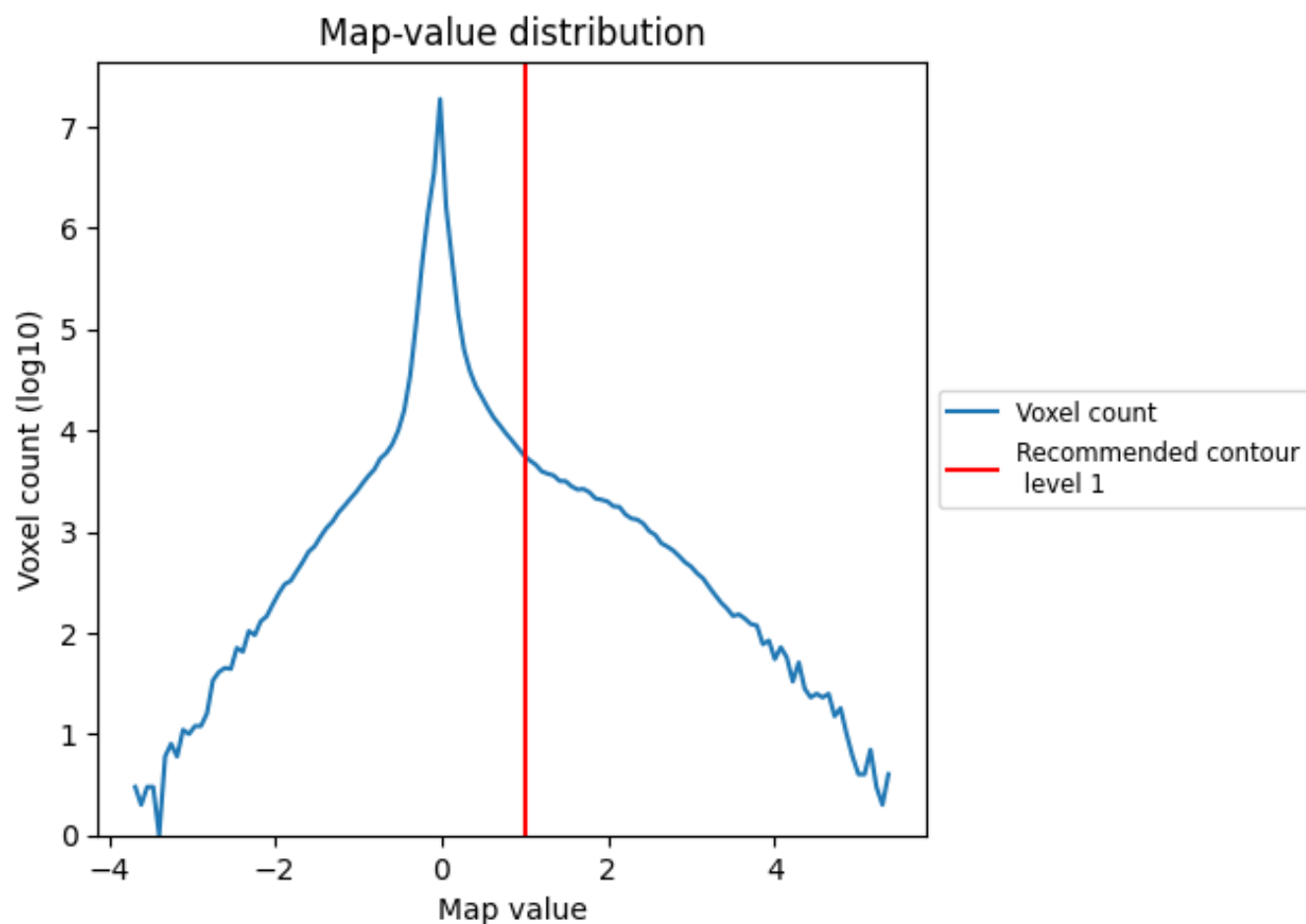


Z

7 Map analysis [i](#)

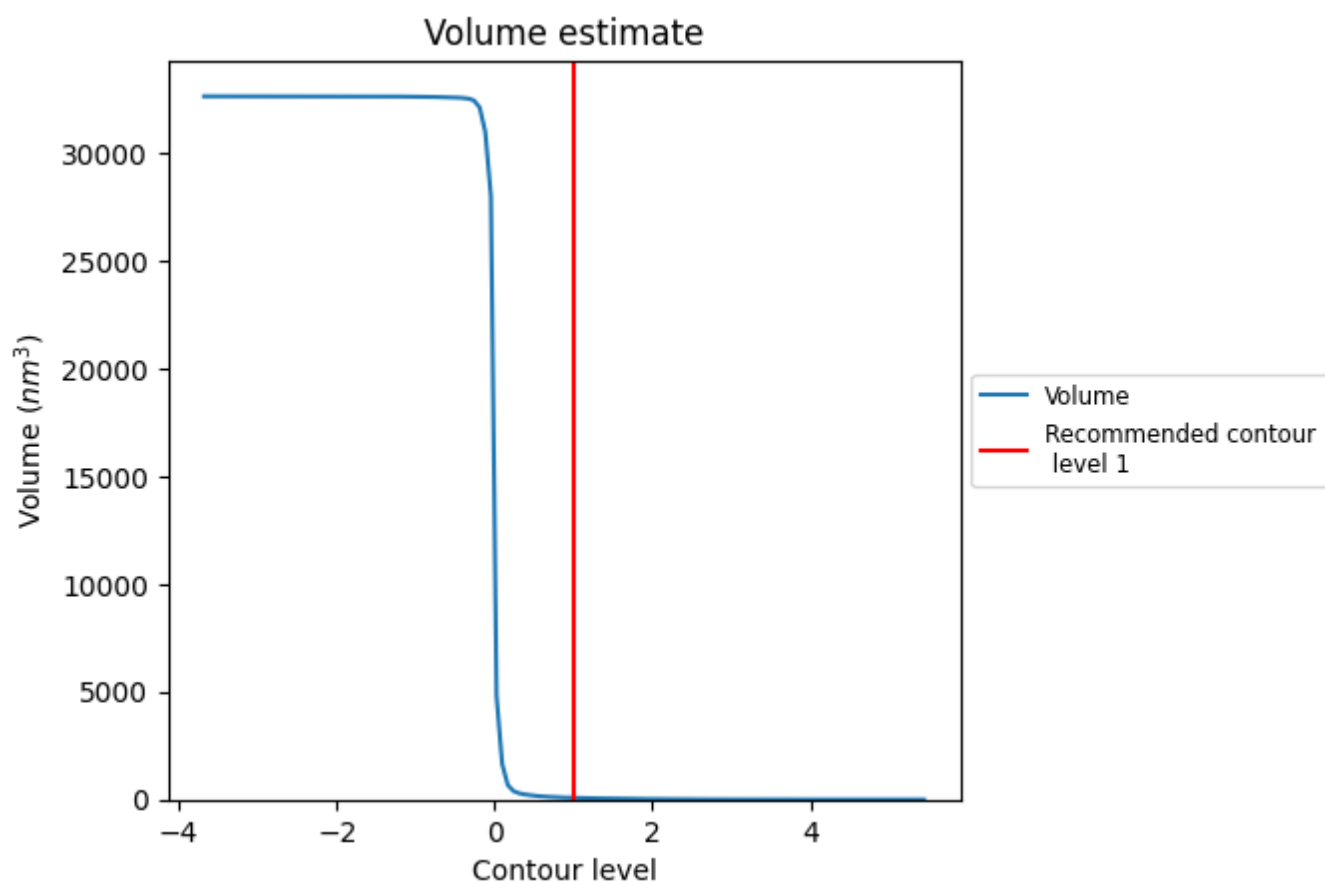
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

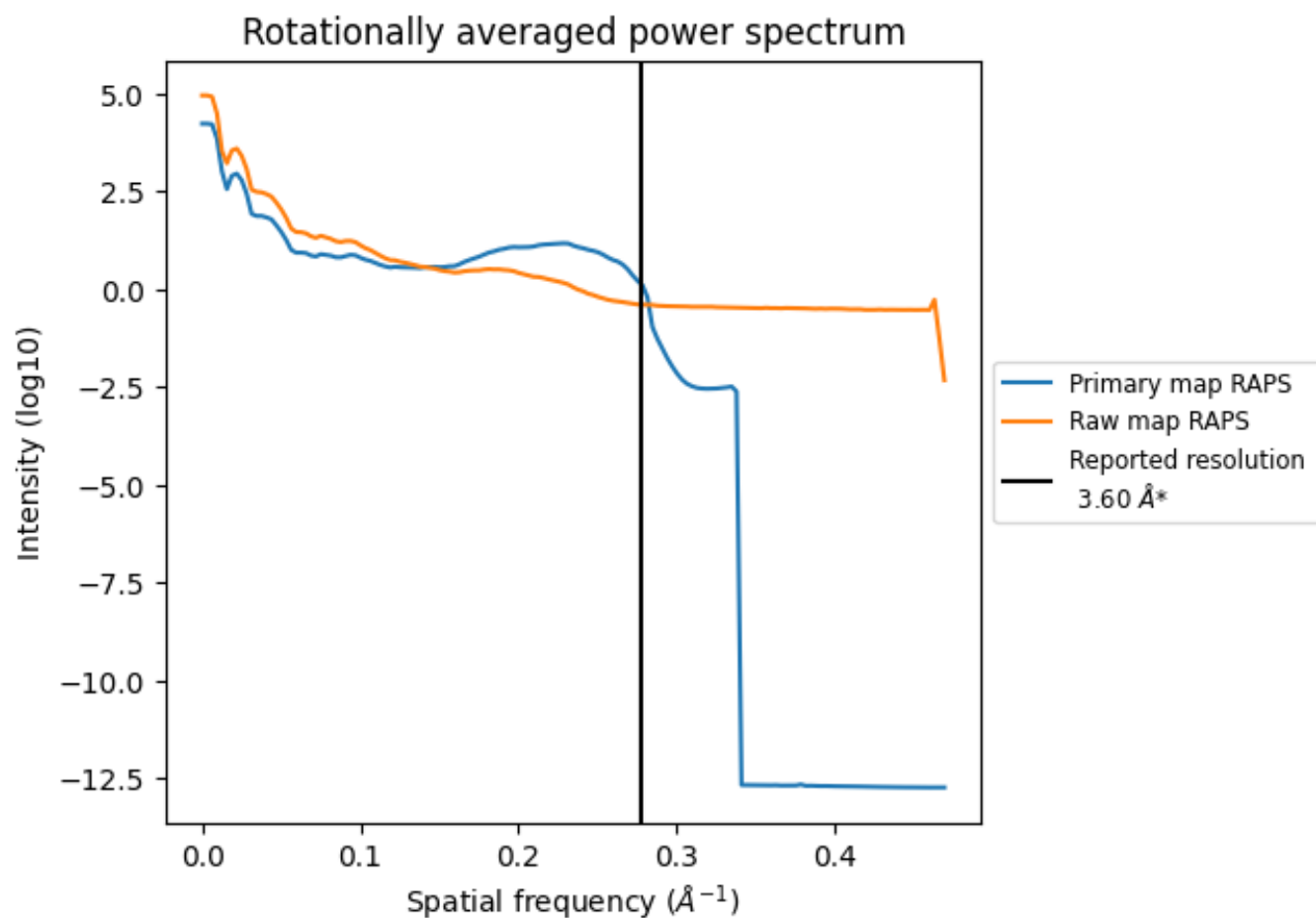
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 72 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 ⓘ

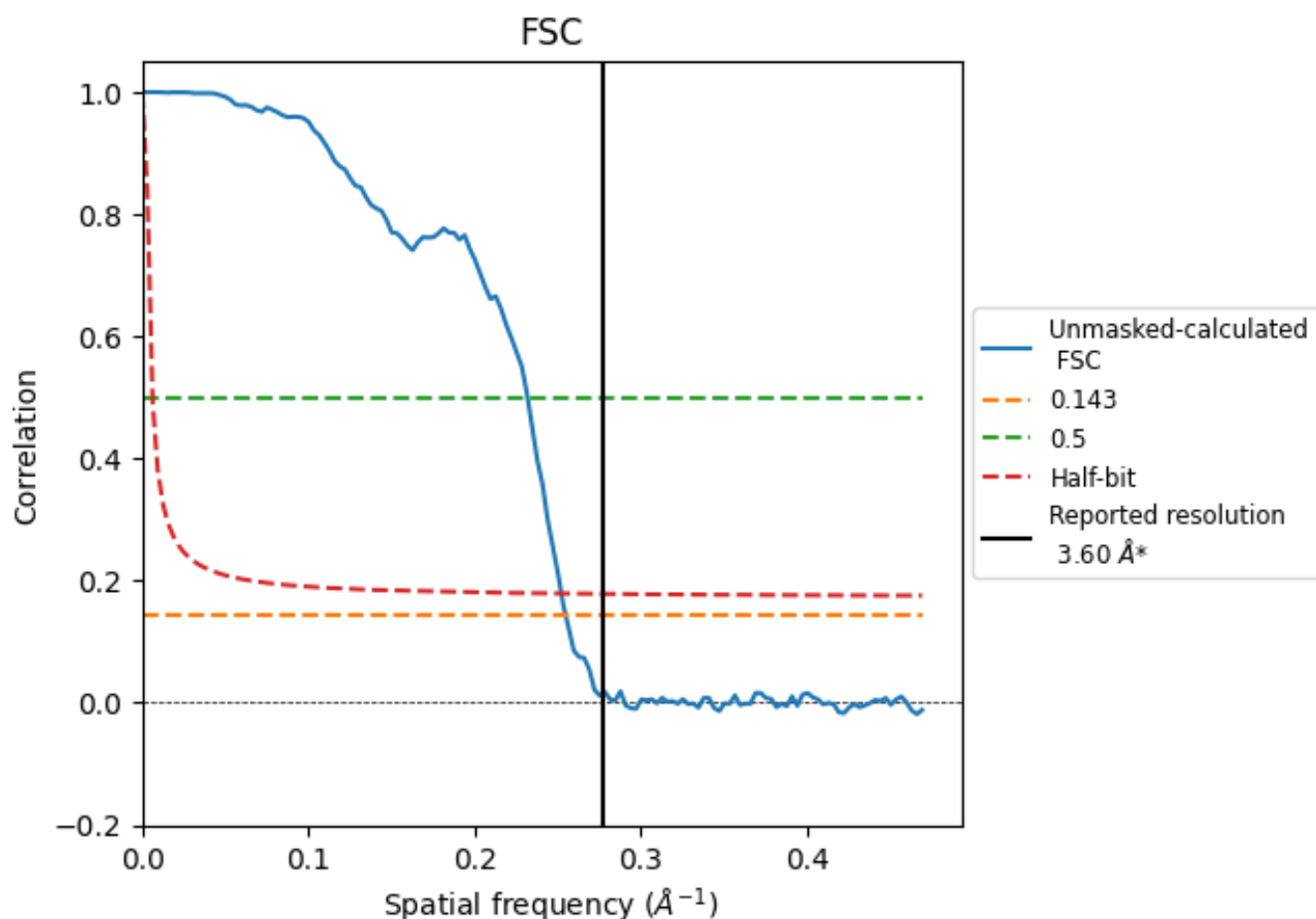


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

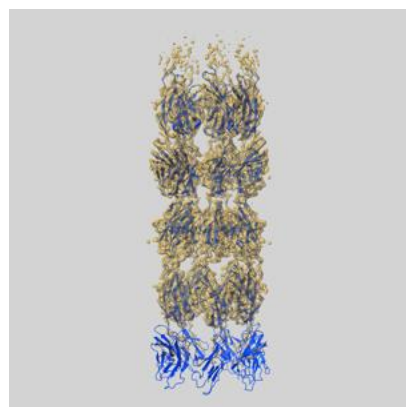
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	4.31	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

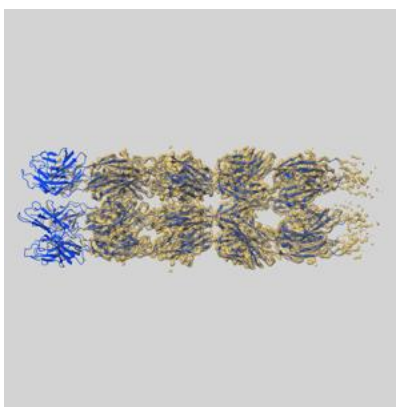
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50540 and PDB model 9FLV. Per-residue inclusion information can be found in section [3](#) on page [5](#).

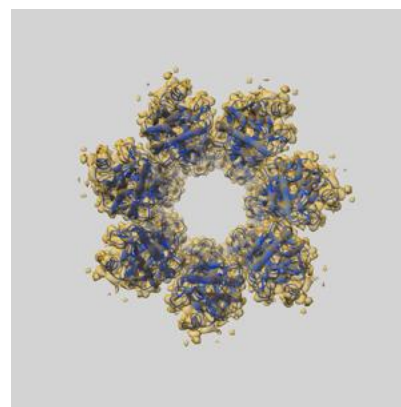
9.1 Map-model overlay [i](#)



X



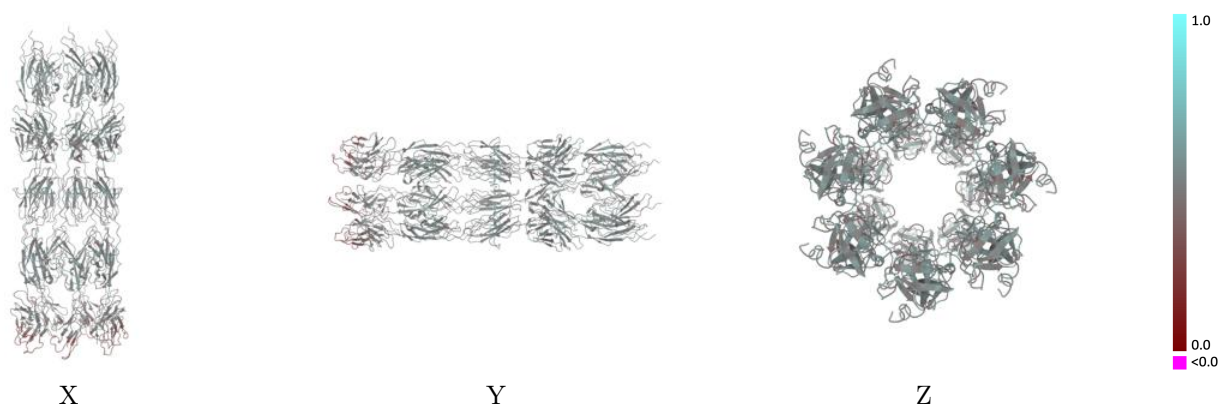
Y



Z

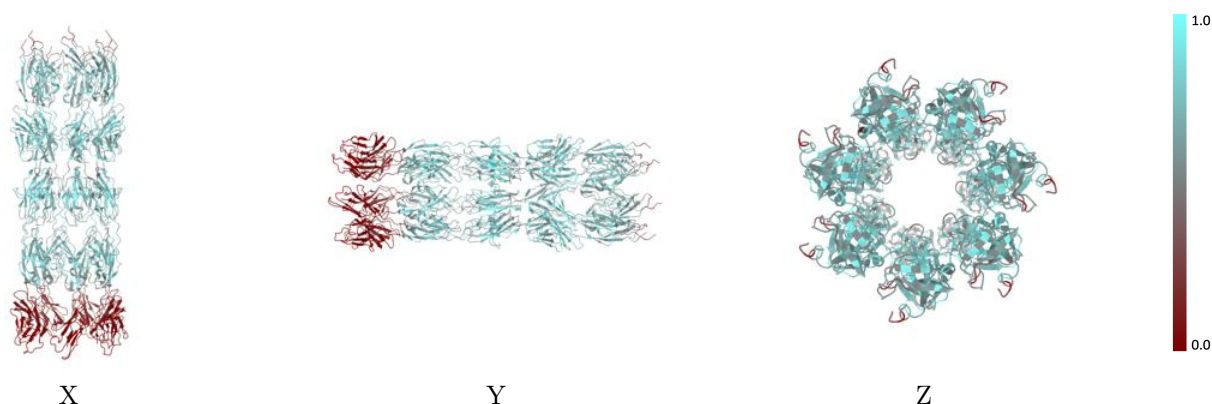
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



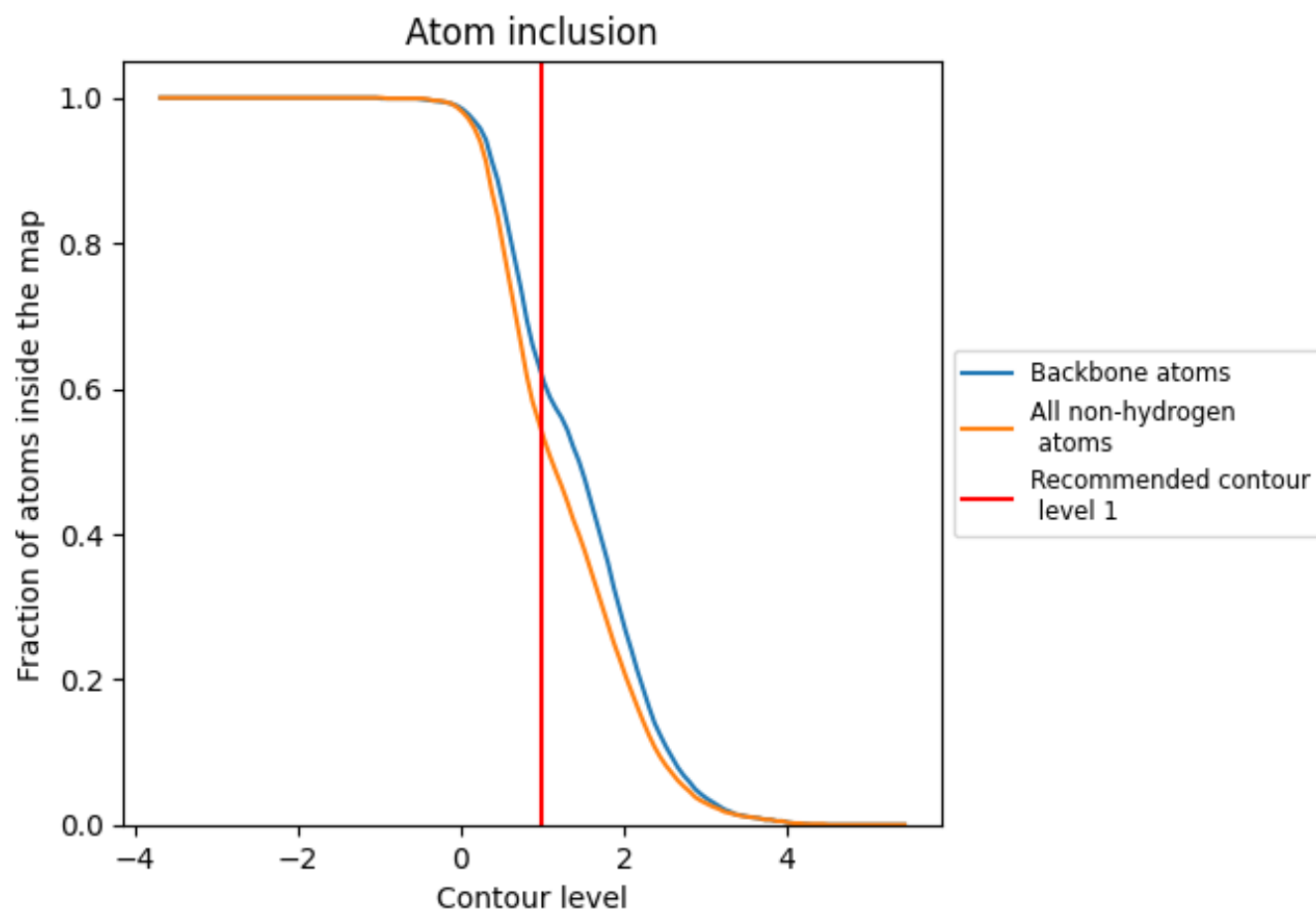
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 54% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5380	0.4860
A	0.5390	0.4860
B	0.5380	0.4850
C	0.5360	0.4850
D	0.5370	0.4860
E	0.5380	0.4860
F	0.5370	0.4860
G	0.5370	0.4850

1.0

0.0

<0.0