



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:01 PM UTC

PDB ID : 6PXV / pdb_00006pxv
EMDB ID : EMD-20522
Title : Cryo-EM structure of full-length insulin receptor bound to 4 insulin. 3D refinement was focused on the extracellular region.
Authors : Uchikawa, E.; Choi, E.; Shang, G.J.; Yu, H.T.; Bai, X.C.
Deposited on : 2019-07-27
Resolution : 3.20 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:

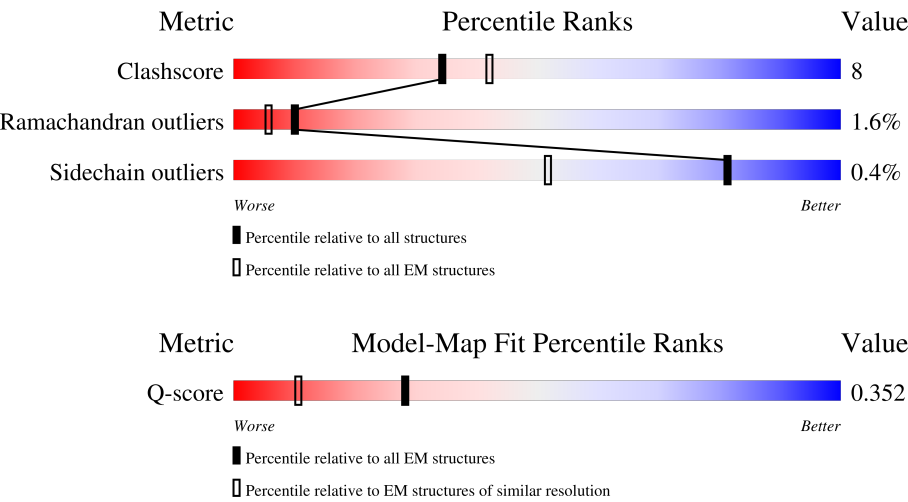
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	1354	
1	C	1354	
2	D	74	
2	E	74	

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Mol	Chain	Length	Quality of chain
2	F	74	14% 45% 14% 41%
2	G	74	14% 45% 15% 41%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14774 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	823	Total 6664	C 4231	N 1149	O 1236	S 48	0	0
1	C	823	Total 6664	C 4231	N 1149	O 1236	S 48	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	960	PHE	TYR	conflict	UNP P06213
A	962	THR	SER	conflict	UNP P06213
A	1120	ASN	ASP	conflict	UNP P06213
A	1333	ALA	ARG	conflict	UNP P06213
A	1334	ALA	ILE	conflict	UNP P06213
A	1335	ALA	LEU	conflict	UNP P06213
A	1337	ALA	LEU	conflict	UNP P06213
A	1344	LEU	-	expression tag	UNP P06213
A	1345	GLU	-	expression tag	UNP P06213
A	1346	SER	-	expression tag	UNP P06213
A	1347	SER	-	expression tag	UNP P06213
A	1348	GLY	-	expression tag	UNP P06213
A	1349	LEU	-	expression tag	UNP P06213
A	1350	GLU	-	expression tag	UNP P06213
A	1351	VAL	-	expression tag	UNP P06213
A	1352	LEU	-	expression tag	UNP P06213
A	1353	PHE	-	expression tag	UNP P06213
A	1354	GLN	-	expression tag	UNP P06213
C	960	PHE	TYR	conflict	UNP P06213
C	962	THR	SER	conflict	UNP P06213
C	1120	ASN	ASP	conflict	UNP P06213
C	1333	ALA	ARG	conflict	UNP P06213
C	1334	ALA	ILE	conflict	UNP P06213
C	1335	ALA	LEU	conflict	UNP P06213
C	1337	ALA	LEU	conflict	UNP P06213
C	1344	LEU	-	expression tag	UNP P06213

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1345	GLU	-	expression tag	UNP P06213
C	1346	SER	-	expression tag	UNP P06213
C	1347	SER	-	expression tag	UNP P06213
C	1348	GLY	-	expression tag	UNP P06213
C	1349	LEU	-	expression tag	UNP P06213
C	1350	GLU	-	expression tag	UNP P06213
C	1351	VAL	-	expression tag	UNP P06213
C	1352	LEU	-	expression tag	UNP P06213
C	1353	PHE	-	expression tag	UNP P06213
C	1354	GLN	-	expression tag	UNP P06213

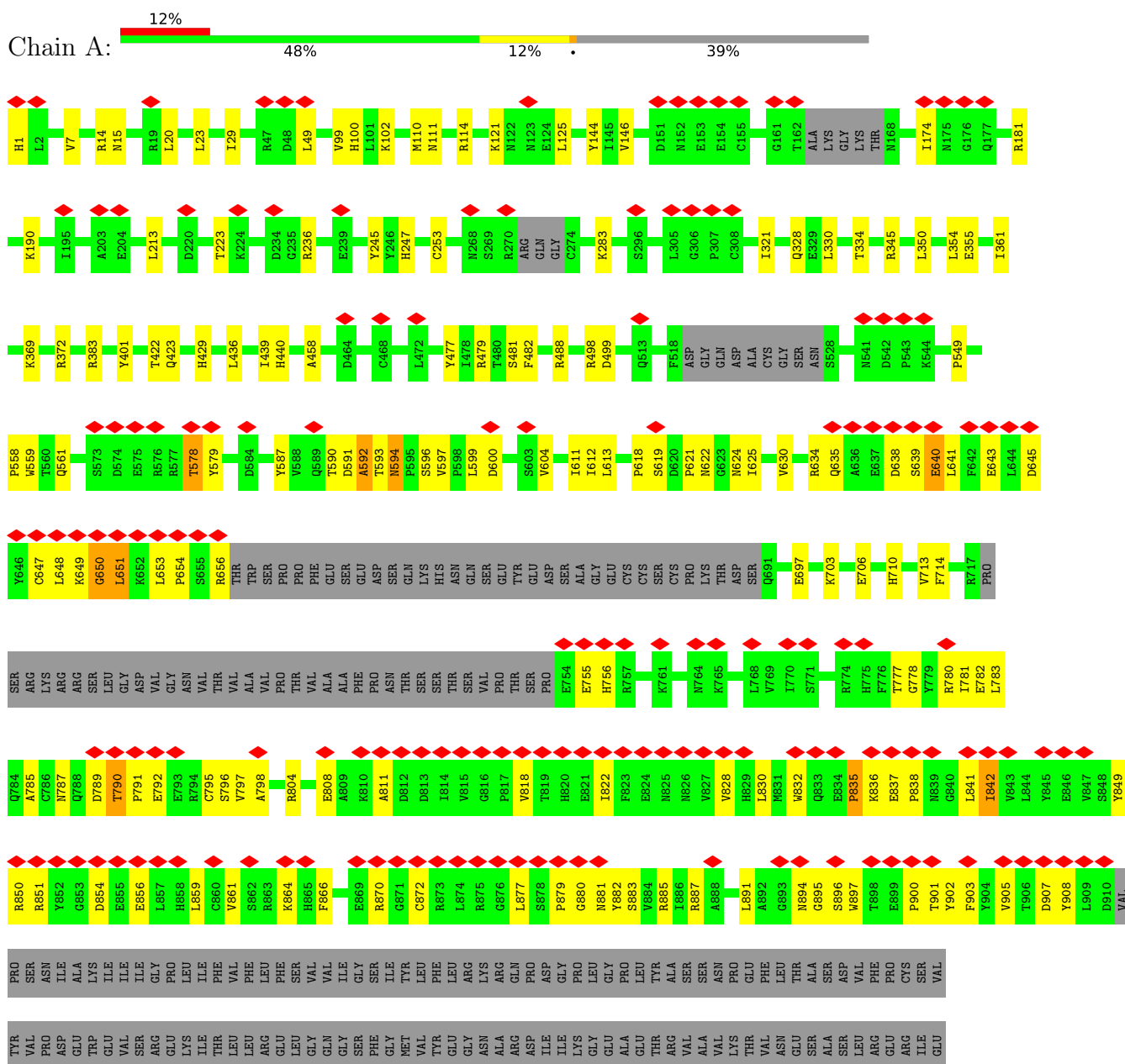
- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	48	Total	C	N	O	S	0	0
			376	238	61	71	6		
2	E	48	Total	C	N	O	S	0	0
			376	238	61	71	6		
2	F	44	Total	C	N	O	S	0	0
			347	220	56	65	6		
2	G	44	Total	C	N	O	S	0	0
			347	220	56	65	6		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

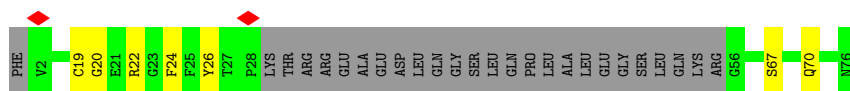
• Molecule 1: Insulin receptor



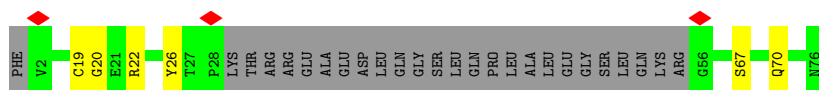


ASN	LYS	MET	TYR	PRO	GLU	VAL
GLY	ALA	ASP	ARG	THR	PHE	TYR
ALA	PRO	GLY	LYS	PRO	LEU	PRO
ALA	GLU	TYR	GLY	LEU	ASN	ASP
ALA	GLU	LEU	LYS	GLU	ALA	GLU
THR	GLU	ASP	GLY	MET	SER	TRP
ALA	GLU	ASP	GLY	GLY	VAL	GLU
PRO	LEU	GLN	LEU	ILE	VAL	GLU
PRO	GLU	PRO	PRO	PRO	MET	VAL
ARG	GLU	PRO	LEU	GLN	MET	VAL
SER	MET	ASP	PRO	MET	LYS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

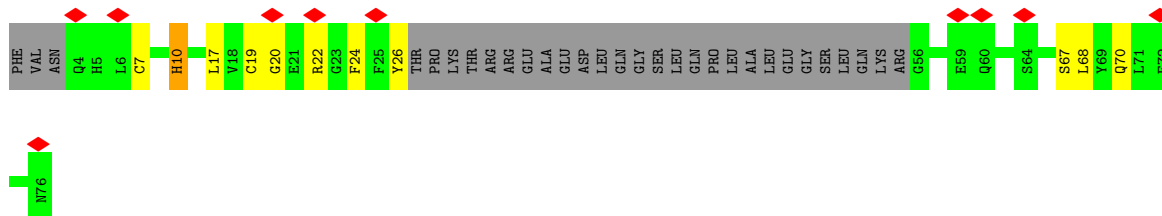
- Molecule 2: Insulin



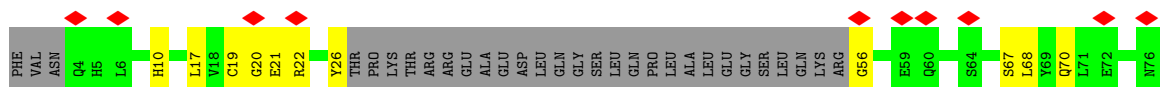
- Molecule 2: Insulin



- Molecule 2: Insulin



- Molecule 2: Insulin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	235707	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 IS (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	2/6828 (0.0%)	0.93	31/9258 (0.3%)
1	C	0.57	2/6828 (0.0%)	0.93	32/9258 (0.3%)
2	D	0.28	0/383	0.54	0/518
2	E	0.28	0/383	0.54	0/518
2	F	0.31	0/353	0.63	1/475 (0.2%)
2	G	0.31	0/353	0.61	1/475 (0.2%)
All	All	0.55	4/15128 (0.0%)	0.90	65/20502 (0.3%)

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	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	894	ASN	CA-C	5.43	1.59	1.52
1	A	894	ASN	CA-C	5.35	1.59	1.52
1	A	842	ILE	CG1-CD1	-5.20	1.31	1.51
1	C	842	ILE	CG1-CD1	-5.17	1.31	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ASN	CA-CB-CG	6.58	119.18	112.60
1	A	592	ALA	N-CA-C	6.57	119.70	109.52
1	C	639	SER	CA-C-N	6.56	129.72	120.28
1	C	639	SER	C-N-CA	6.56	129.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	881	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	639	SER	CA-C-N	6.53	129.69	120.28
1	A	639	SER	C-N-CA	6.53	129.69	120.28
1	C	901	THR	N-CA-C	-6.39	100.23	110.14
1	A	901	THR	N-CA-C	-6.38	100.26	110.14
1	C	789	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	789	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	854	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	854	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	795	CYS	CA-C-N	5.94	131.77	120.97
1	C	795	CYS	C-N-CA	5.94	131.77	120.97
1	A	795	CYS	CA-C-N	5.93	131.77	120.97
1	A	795	CYS	C-N-CA	5.93	131.77	120.97
1	C	578	THR	CA-C-N	5.90	132.82	121.54
1	C	578	THR	C-N-CA	5.90	132.82	121.54
1	A	578	THR	CA-C-N	5.87	132.76	121.54
1	A	578	THR	C-N-CA	5.87	132.76	121.54
1	A	894	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	894	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	593	THR	N-CA-C	5.85	118.59	109.52
1	C	907	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	818	VAL	N-CA-C	-5.78	98.72	107.73
1	C	818	VAL	N-CA-C	-5.78	98.72	107.73
1	A	907	ASP	CA-CB-CG	5.75	118.35	112.60
2	G	10	HIS	N-CA-C	-5.70	104.97	111.07
1	C	592	ALA	N-CA-C	5.67	118.80	109.85
1	C	624	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	624	ASN	CA-CB-CG	5.56	118.16	112.60
2	F	10	HIS	N-CA-C	-5.51	105.17	111.07
1	C	880	GLY	N-CA-C	5.50	117.67	111.85
1	A	880	GLY	N-CA-C	5.48	117.66	111.85
1	C	600	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	600	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	648	LEU	CA-C-N	5.35	131.77	121.54
1	A	648	LEU	C-N-CA	5.35	131.77	121.54
1	C	648	LEU	CA-C-N	5.35	131.75	121.54
1	C	648	LEU	C-N-CA	5.35	131.75	121.54
1	A	895	GLY	CA-C-N	5.25	131.56	121.54
1	A	895	GLY	C-N-CA	5.25	131.56	121.54
1	A	647	CYS	N-CA-C	-5.24	106.88	113.28
1	C	647	CYS	N-CA-C	-5.23	106.90	113.28
1	C	895	GLY	CA-C-N	5.23	131.53	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	895	GLY	C-N-CA	5.23	131.53	121.54
1	A	611	ILE	N-CA-CB	5.23	118.44	111.64
1	A	870	ARG	N-CA-C	-5.22	104.23	111.28
1	C	870	ARG	N-CA-C	-5.22	104.23	111.28
1	C	611	ILE	N-CA-CB	5.21	118.42	111.64
1	A	645	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	837	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	837	GLU	CB-CG-CD	5.19	121.42	112.60
1	C	787	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	787	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	650	GLY	CA-C-N	5.17	131.23	122.65
1	A	650	GLY	C-N-CA	5.17	131.23	122.65
1	C	645	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	650	GLY	CA-C-N	5.14	131.18	122.65
1	C	650	GLY	C-N-CA	5.14	131.18	122.65
1	A	835	PRO	CA-C-N	5.05	131.18	121.54
1	A	835	PRO	C-N-CA	5.05	131.18	121.54
1	C	835	PRO	CA-C-N	5.04	131.16	121.54
1	C	835	PRO	C-N-CA	5.04	131.16	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	578	THR	Peptide
1	C	578	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6664	0	6478	109	0
1	C	6664	0	6478	116	0
2	D	376	0	346	5	0
2	E	376	0	346	4	0
2	F	347	0	317	8	0
2	G	347	0	317	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14774	0	14282	235	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 8.

All (235) 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:C:482:PHE:CZ	1:C:593:THR:HG21	1.45	1.50
1:A:482:PHE:CZ	1:A:593:THR:HG21	1.58	1.36
1:A:482:PHE:CE1	1:A:593:THR:HB	1.60	1.33
1:C:482:PHE:CZ	1:C:593:THR:CG2	2.13	1.30
1:C:482:PHE:CE1	1:C:593:THR:CG2	2.14	1.30
1:A:482:PHE:HE1	1:A:593:THR:CB	1.45	1.28
1:C:482:PHE:CE1	1:C:593:THR:HB	1.74	1.23
1:C:482:PHE:HE1	1:C:593:THR:CB	1.52	1.21
1:A:559:TRP:HB2	1:A:592:ALA:HB2	1.25	1.14
1:C:482:PHE:CE1	1:C:593:THR:CB	2.29	1.12
1:A:482:PHE:CZ	1:A:593:THR:CG2	2.34	1.10
1:C:559:TRP:HB2	1:C:592:ALA:HB2	1.17	1.10
1:A:482:PHE:CE1	1:A:593:THR:CB	2.26	1.09
1:A:482:PHE:CE1	1:A:593:THR:CG2	2.35	1.08
1:A:559:TRP:HB2	1:A:592:ALA:CB	1.88	1.03
1:A:482:PHE:HZ	1:A:593:THR:HG21	0.91	1.02
1:C:482:PHE:HE1	1:C:593:THR:HB	1.06	0.97
1:A:482:PHE:HE1	1:A:593:THR:HB	0.80	0.94
1:C:482:PHE:CE1	1:C:593:THR:HG22	2.02	0.93
1:A:559:TRP:CB	1:A:592:ALA:HB2	2.04	0.88
1:C:482:PHE:HZ	1:C:593:THR:CG2	1.66	0.86
1:A:790:THR:HB	1:A:791:PRO:HD3	1.57	0.86
1:C:790:THR:HB	1:C:791:PRO:HD3	1.57	0.85
1:C:482:PHE:HE1	1:C:593:THR:CG2	1.69	0.85
1:C:482:PHE:HZ	1:C:593:THR:HG21	0.88	0.81
1:C:559:TRP:HB2	1:C:592:ALA:CB	2.07	0.78
1:A:755:GLU:HG2	1:A:756:HIS:N	1.99	0.76
1:A:755:GLU:HG2	1:A:756:HIS:H	1.51	0.75
1:C:755:GLU:HG2	1:C:756:HIS:N	1.99	0.75
1:C:350:LEU:O	1:C:354:LEU:HB2	1.88	0.74
1:A:350:LEU:O	1:A:354:LEU:HB2	1.88	0.72
1:C:755:GLU:HG2	1:C:756:HIS:H	1.51	0.72
1:C:599:LEU:HD11	1:C:619:SER:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:HD11	1:A:619:SER:HB3	1.72	0.72
1:A:885:ARG:HE	1:A:897:TRP:HB3	1.56	0.70
1:C:885:ARG:HE	1:C:897:TRP:HB3	1.56	0.69
1:A:590:THR:OG1	1:A:591:ASP:N	2.27	0.68
1:C:482:PHE:CZ	1:C:593:THR:HG22	2.14	0.67
1:C:590:THR:OG1	1:C:591:ASP:N	2.27	0.67
1:C:785:ALA:H	1:C:796:SER:HB3	1.60	0.66
1:A:651:LEU:HD23	1:A:651:LEU:H	1.62	0.64
1:A:785:ALA:H	1:A:796:SER:HB3	1.60	0.64
1:A:597:VAL:HG22	1:A:797:VAL:CG2	2.28	0.64
1:C:651:LEU:H	1:C:651:LEU:HD23	1.62	0.63
1:A:808:GLU:HB2	1:A:811:ALA:HB2	1.80	0.63
1:C:808:GLU:HB2	1:C:811:ALA:HB2	1.81	0.63
1:C:597:VAL:HG22	1:C:797:VAL:CG2	2.28	0.62
1:C:559:TRP:CB	1:C:592:ALA:HB2	2.10	0.62
1:C:879:PRO:HA	1:C:905:VAL:HG23	1.82	0.61
1:A:879:PRO:HA	1:A:905:VAL:HG23	1.82	0.61
1:C:223:THR:HG22	1:C:236:ARG:HG2	1.82	0.61
1:A:643:GLU:HA	1:A:864:LYS:HE3	1.82	0.60
1:A:223:THR:HG22	1:A:236:ARG:HG2	1.82	0.60
1:C:643:GLU:HA	1:C:864:LYS:HE3	1.82	0.60
1:C:593:THR:O	1:C:594:ASN:O	2.20	0.59
1:A:558:PRO:HB3	1:A:592:ALA:HA	1.84	0.59
1:C:422:THR:HG22	1:C:423:GLN:HG3	1.86	0.57
1:C:822:ILE:HG12	1:C:828:VAL:HG22	1.86	0.57
1:C:482:PHE:HA	1:C:591:ASP:OD1	2.05	0.57
1:A:634:ARG:HD2	1:A:777:THR:HG21	1.87	0.56
1:A:422:THR:HG22	1:A:423:GLN:HG3	1.86	0.56
1:A:593:THR:O	1:A:622:ASN:HB2	2.05	0.56
1:A:822:ILE:HG12	1:A:828:VAL:HG22	1.86	0.56
1:C:634:ARG:HD2	1:C:777:THR:HG21	1.87	0.56
1:C:885:ARG:NH1	1:C:900:PRO:HD3	2.21	0.56
1:A:604:VAL:HB	1:A:612:ILE:HG13	1.88	0.56
1:A:835:PRO:HD2	1:A:842:ILE:HD12	1.88	0.56
1:C:835:PRO:HD2	1:C:842:ILE:HD12	1.88	0.55
1:A:885:ARG:NH1	1:A:900:PRO:HD3	2.21	0.55
1:C:558:PRO:HB3	1:C:592:ALA:HA	1.88	0.55
1:C:499:ASP:OD1	1:C:703:LYS:NZ	2.37	0.55
1:C:604:VAL:HB	1:C:612:ILE:HG13	1.88	0.55
1:C:436:LEU:O	1:C:440:HIS:ND1	2.34	0.53
1:A:482:PHE:HA	1:A:591:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:THR:O	1:A:594:ASN:O	2.25	0.53
1:C:613:LEU:HD22	1:C:781:ILE:HG21	1.91	0.53
1:C:479:ARG:NH2	2:F:17:LEU:O	2.41	0.53
1:A:593:THR:O	1:A:594:ASN:C	2.51	0.52
1:A:477:TYR:HB3	1:A:488:ARG:HB2	1.92	0.52
1:C:355:GLU:OE2	1:C:383:ARG:NH2	2.33	0.52
1:C:477:TYR:HB3	1:C:488:ARG:HB2	1.92	0.52
1:A:110:MET:HE1	1:A:190:LYS:HD3	1.92	0.52
1:A:479:ARG:NH2	2:G:17:LEU:O	2.42	0.52
1:A:436:LEU:O	1:A:440:HIS:ND1	2.34	0.52
1:A:613:LEU:HD22	1:A:781:ILE:HG21	1.91	0.52
1:C:110:MET:HE1	1:C:190:LYS:HD3	1.92	0.52
1:C:593:THR:O	1:C:622:ASN:HB2	2.10	0.52
2:F:67:SER:OG	2:F:70:GLN:NE2	2.43	0.52
1:A:654:PRO:HG2	1:A:656:ARG:HH21	1.73	0.52
1:A:499:ASP:OD1	1:A:703:LYS:NZ	2.36	0.52
1:C:654:PRO:HG2	1:C:656:ARG:HH21	1.73	0.52
1:A:355:GLU:OE2	1:A:383:ARG:NH2	2.33	0.51
2:D:67:SER:OG	2:D:70:GLN:NE2	2.43	0.51
2:G:67:SER:OG	2:G:70:GLN:NE2	2.43	0.51
1:A:482:PHE:CE1	1:A:593:THR:HG22	2.41	0.51
1:A:597:VAL:HG22	1:A:797:VAL:HG23	1.92	0.51
1:C:154:GLU:OE2	2:G:56:GLY:N	2.44	0.51
1:C:597:VAL:HG22	1:C:797:VAL:HG23	1.92	0.51
1:A:23:LEU:HD11	1:A:29:ILE:HD11	1.93	0.51
1:A:247:HIS:HB2	1:A:283:LYS:HG2	1.93	0.50
1:A:635:GLN:HE21	1:A:780:ARG:HB2	1.76	0.50
2:E:67:SER:OG	2:E:70:GLN:NE2	2.43	0.50
1:A:597:VAL:HG22	1:A:797:VAL:HG22	1.93	0.50
1:C:593:THR:O	1:C:594:ASN:C	2.54	0.50
1:A:144:TYR:CE2	1:A:146:VAL:HG12	2.46	0.50
1:C:597:VAL:HG22	1:C:797:VAL:HG22	1.93	0.50
1:A:488:ARG:HE	2:G:68:LEU:HD21	1.77	0.50
1:A:630:VAL:HG22	1:A:783:LEU:HD13	1.94	0.50
1:C:482:PHE:CE1	1:C:593:THR:HG21	1.97	0.50
2:G:26:TYR:CD1	2:G:26:TYR:C	2.90	0.50
1:A:144:TYR:CE2	1:A:146:VAL:CG1	2.95	0.49
1:C:247:HIS:HB2	1:C:283:LYS:HG2	1.93	0.49
1:C:635:GLN:HE21	1:C:780:ARG:HB2	1.76	0.49
1:C:23:LEU:HD11	1:C:29:ILE:HD11	1.93	0.49
1:C:111:ASN:HD22	1:C:213:LEU:HD11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:VAL:HG22	1:C:783:LEU:HD13	1.94	0.49
1:A:640:GLU:CD	1:A:640:GLU:H	2.21	0.48
1:A:436:LEU:HD23	1:A:439:ILE:HD12	1.95	0.48
1:A:111:ASN:HD22	1:A:213:LEU:HD11	1.76	0.48
1:A:114:ARG:HH22	1:A:328:GLN:HE21	1.60	0.48
1:A:1:HIS:N	1:A:223:THR:O	2.37	0.48
1:A:481:SER:HB2	2:G:17:LEU:HD21	1.96	0.48
1:A:877:LEU:HD12	1:A:877:LEU:N	2.29	0.48
1:C:114:ARG:HH22	1:C:328:GLN:HE21	1.60	0.48
1:C:436:LEU:HD23	1:C:439:ILE:HD12	1.95	0.48
1:C:481:SER:HB2	2:F:17:LEU:HD21	1.96	0.48
1:C:640:GLU:CD	1:C:640:GLU:H	2.21	0.48
1:C:782:GLU:HG3	1:C:798:ALA:HB1	1.96	0.47
1:A:830:LEU:HB2	1:A:872:CYS:HB3	1.96	0.47
1:C:1:HIS:N	1:C:223:THR:O	2.37	0.47
1:C:144:TYR:CE2	1:C:146:VAL:HG12	2.49	0.47
2:E:67:SER:H	2:E:70:GLN:HE21	1.61	0.47
1:C:851:ARG:HB2	1:C:882:TYR:CE2	2.49	0.47
1:A:14:ARG:NH2	1:C:713:VAL:O	2.35	0.47
2:F:67:SER:H	2:F:70:GLN:HE21	1.61	0.47
1:A:559:TRP:HB2	1:A:592:ALA:HB3	1.88	0.47
1:A:481:SER:O	1:A:591:ASP:OD1	2.33	0.47
1:A:782:GLU:HG3	1:A:798:ALA:HB1	1.97	0.47
1:A:851:ARG:HB2	1:A:882:TYR:CE2	2.49	0.47
1:A:345:ARG:NH1	1:C:697:GLU:OE1	2.46	0.47
1:C:877:LEU:HD12	1:C:877:LEU:N	2.29	0.47
2:G:67:SER:H	2:G:70:GLN:HE21	1.61	0.47
2:D:67:SER:H	2:D:70:GLN:HE21	1.61	0.47
1:C:859:LEU:HD23	1:C:872:CYS:SG	2.55	0.47
2:E:19:CYS:SG	2:E:22:ARG:NH2	2.88	0.46
2:G:19:CYS:SG	2:G:22:ARG:NH2	2.88	0.46
1:A:706:GLU:O	1:A:710:HIS:ND1	2.45	0.46
2:D:19:CYS:SG	2:D:22:ARG:NH2	2.88	0.46
1:C:830:LEU:HB2	1:C:872:CYS:HB3	1.96	0.46
2:F:19:CYS:SG	2:F:22:ARG:NH2	2.88	0.46
1:C:334:THR:HA	1:C:361:ILE:HA	1.97	0.46
1:A:621:PRO:HB3	1:A:625:ILE:HD11	1.98	0.46
1:C:144:TYR:CE2	1:C:146:VAL:CG1	2.98	0.46
1:A:697:GLU:OE1	1:C:345:ARG:NH1	2.46	0.46
1:A:477:TYR:OH	2:G:21:GLU:OE2	2.34	0.46
1:C:481:SER:O	1:C:591:ASP:OD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:885:ARG:HH12	1:C:900:PRO:HD3	1.81	0.46
1:C:498:ARG:NH1	1:C:706:GLU:OE1	2.48	0.45
1:A:334:THR:HA	1:A:361:ILE:HA	1.97	0.45
1:A:859:LEU:HD23	1:A:872:CYS:SG	2.55	0.45
1:C:706:GLU:O	1:C:710:HIS:ND1	2.45	0.45
2:F:24:PHE:CD2	2:F:26:TYR:HB2	2.51	0.45
1:A:885:ARG:HH12	1:A:900:PRO:HD3	1.81	0.45
1:C:621:PRO:HB3	1:C:625:ILE:HD11	1.98	0.45
1:C:828:VAL:HG21	1:C:903:PHE:CE1	2.51	0.45
1:A:713:VAL:O	1:C:14:ARG:NH2	2.35	0.45
1:A:861:VAL:HG12	1:A:866:PHE:HB2	1.99	0.45
1:A:828:VAL:HG21	1:A:903:PHE:CE1	2.52	0.44
1:C:369:LYS:HG3	1:C:401:TYR:HB3	1.99	0.44
1:A:498:ARG:NH1	1:A:706:GLU:OE1	2.48	0.44
1:A:369:LYS:HG3	1:A:401:TYR:HB3	1.99	0.44
1:C:832:TRP:HH2	1:C:872:CYS:HB2	1.82	0.44
1:A:832:TRP:HH2	1:A:872:CYS:HB2	1.82	0.44
1:A:849:TYR:HA	1:A:883:SER:O	2.17	0.44
1:C:755:GLU:CG	1:C:756:HIS:H	2.27	0.44
1:A:641:LEU:HB3	1:A:841:LEU:HD21	1.99	0.44
2:F:7:CYS:O	2:F:10:HIS:HB2	2.18	0.44
1:C:641:LEU:HB3	1:C:841:LEU:HD21	1.99	0.44
1:C:850:ARG:NH2	1:C:856:GLU:HB2	2.33	0.43
1:C:849:TYR:HA	1:C:883:SER:O	2.17	0.43
1:C:861:VAL:HG12	1:C:866:PHE:HB2	1.99	0.43
1:C:102:LYS:HA	1:C:125:LEU:HA	2.00	0.43
1:A:651:LEU:H	1:A:651:LEU:CD2	2.30	0.43
1:A:710:HIS:HD2	1:A:714:PHE:HE2	1.66	0.43
1:A:144:TYR:HE2	1:A:146:VAL:HG12	1.83	0.43
1:C:429:HIS:CE1	1:C:458:ALA:HB2	2.54	0.43
1:A:832:TRP:CH2	1:A:872:CYS:HB2	2.54	0.43
1:A:850:ARG:NH2	1:A:856:GLU:HB2	2.33	0.43
1:A:596:SER:HB3	1:A:618:PRO:HB2	2.01	0.43
1:C:778:GLY:HA2	1:C:804:ARG:HA	2.01	0.43
1:C:832:TRP:CH2	1:C:872:CYS:HB2	2.54	0.43
1:A:174:ILE:HB	1:A:181:ARG:HH22	1.84	0.43
1:C:596:SER:HB3	1:C:618:PRO:HB2	2.01	0.42
1:C:710:HIS:HD2	1:C:714:PHE:HE2	1.66	0.42
1:C:790:THR:HB	1:C:791:PRO:CD	2.40	0.42
1:A:654:PRO:HB2	1:A:656:ARG:HE	1.84	0.42
1:C:593:THR:O	1:C:622:ASN:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:CE1	1:A:458:ALA:HB2	2.54	0.42
1:C:14:ARG:CZ	2:E:26:TYR:HB2	2.49	0.42
1:A:245:TYR:HB3	1:A:253:CYS:HB3	2.01	0.42
1:C:653:LEU:HD21	1:C:891:LEU:HD23	2.01	0.42
1:C:41:THR:OG1	1:C:67:TYR:O	2.29	0.42
1:A:102:LYS:HA	1:A:125:LEU:HA	2.01	0.42
1:C:654:PRO:HB2	1:C:656:ARG:HE	1.84	0.42
1:A:561:GLN:HE21	1:A:587:TYR:HB3	1.85	0.42
1:A:778:GLY:HA2	1:A:804:ARG:HA	2.01	0.42
1:C:321:ILE:HD11	1:C:330:LEU:HD12	2.01	0.42
1:A:593:THR:O	1:A:622:ASN:CB	2.67	0.41
1:A:653:LEU:HD21	1:A:891:LEU:HD23	2.01	0.41
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.93	0.41
1:C:558:PRO:CB	1:C:592:ALA:HA	2.50	0.41
1:C:514:ASN:OD1	1:C:514:ASN:N	2.51	0.41
1:C:174:ILE:HB	1:C:181:ARG:HH22	1.84	0.41
1:C:245:TYR:HB3	1:C:253:CYS:HB3	2.01	0.41
1:C:488:ARG:HE	2:F:68:LEU:HD21	1.84	0.41
1:A:15:ASN:HD21	2:D:24:PHE:H	1.68	0.41
1:C:887:ARG:HB2	1:C:897:TRP:CD2	2.56	0.41
1:A:321:ILE:HD11	1:A:330:LEU:HD12	2.01	0.41
1:A:14:ARG:CZ	2:D:26:TYR:HB2	2.51	0.41
1:C:561:GLN:HE21	1:C:587:TYR:HB3	1.85	0.41
1:C:598:PRO:HG2	1:C:783:LEU:HG	2.03	0.41
1:A:121:LYS:NZ	1:C:706:GLU:OE2	2.44	0.41
1:A:885:ARG:HE	1:A:897:TRP:CB	2.29	0.41
1:A:887:ARG:HB2	1:A:897:TRP:CD2	2.56	0.41
1:C:350:LEU:O	1:C:354:LEU:CB	2.65	0.41
1:A:345:ARG:HH21	1:A:372:ARG:HD2	1.86	0.41
1:C:99:VAL:HG12	1:C:100:HIS:CD2	2.56	0.41
1:A:882:TYR:O	1:A:902:TYR:HA	2.21	0.40
1:A:20:LEU:HD23	1:A:49:LEU:HD21	2.03	0.40
1:C:66:VAL:HB	1:C:98:MET:HE1	2.04	0.40
1:C:755:GLU:CG	1:C:756:HIS:N	2.77	0.40
1:A:99:VAL:HG12	1:A:100:HIS:CD2	2.56	0.40
1:C:882:TYR:O	1:C:902:TYR:HA	2.21	0.40
1:A:144:TYR:HE2	1:A:146:VAL:CG1	2.33	0.40
1:C:20:LEU:HD23	1:C:49:LEU:HD21	2.03	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	811/1354 (60%)	719 (89%)	80 (10%)	12 (2%)	8	37
1	C	811/1354 (60%)	719 (89%)	79 (10%)	13 (2%)	7	36
2	D	44/74 (60%)	41 (93%)	2 (4%)	1 (2%)	5	29
2	E	44/74 (60%)	41 (93%)	2 (4%)	1 (2%)	5	29
2	F	40/74 (54%)	37 (92%)	2 (5%)	1 (2%)	4	27
2	G	40/74 (54%)	37 (92%)	2 (5%)	1 (2%)	4	27
All	All	1790/3004 (60%)	1594 (89%)	167 (9%)	29 (2%)	10	36

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	649	LYS
1	A	790	THR
1	A	896	SER
1	C	649	LYS
1	C	790	THR
1	C	896	SER
1	A	579	TYR
1	A	638	ASP
1	C	579	TYR
1	C	594	ASN
1	C	638	ASP
1	A	650	GLY
1	C	650	GLY
1	A	594	ASN
1	A	792	GLU
1	C	792	GLU
1	A	836	LYS
1	A	908	TYR
1	C	590	THR
1	C	836	LYS

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Mol	Chain	Res	Type
1	C	908	TYR
1	A	838	PRO
1	C	838	PRO
1	A	549	PRO
2	D	20	GLY
2	E	20	GLY
2	F	20	GLY
2	G	20	GLY
1	C	549	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	751/1209 (62%)	748 (100%)	3 (0%)	84	86
1	C	751/1209 (62%)	748 (100%)	3 (0%)	84	86
2	D	43/65 (66%)	43 (100%)	0	100	100
2	E	43/65 (66%)	43 (100%)	0	100	100
2	F	39/65 (60%)	39 (100%)	0	100	100
2	G	39/65 (60%)	39 (100%)	0	100	100
All	All	1666/2678 (62%)	1660 (100%)	6 (0%)	81	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	640	GLU
1	A	651	LEU
1	C	7	VAL
1	C	640	GLU
1	C	651	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	32	HIS
1	A	100	HIS
1	A	175	ASN
1	A	209	HIS
1	A	264	HIS
1	A	313	HIS
1	A	337	ASN
1	A	546	GLN
1	A	561	GLN
1	A	635	GLN
1	A	894	ASN
1	C	15	ASN
1	C	32	HIS
1	C	100	HIS
1	C	175	ASN
1	C	209	HIS
1	C	264	HIS
1	C	313	HIS
1	C	337	ASN
1	C	546	GLN
1	C	561	GLN
1	C	635	GLN
1	C	894	ASN
2	D	3	ASN
2	D	70	GLN
2	E	3	ASN
2	E	70	GLN
2	F	70	GLN
2	G	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

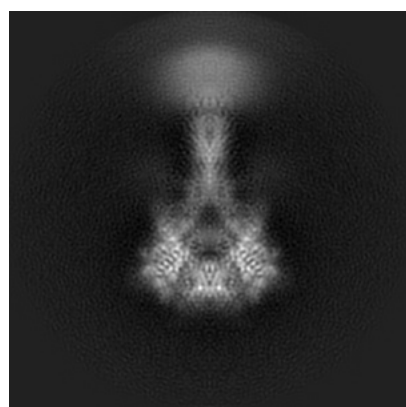
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20522. These allow visual inspection of the internal detail of the map and identification of artifacts.

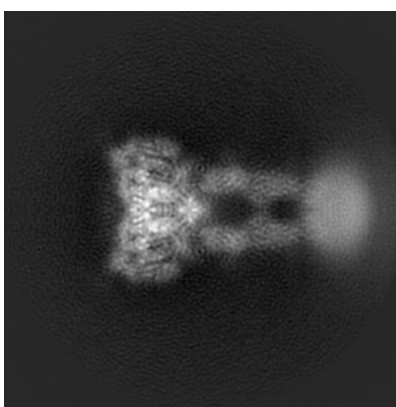
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

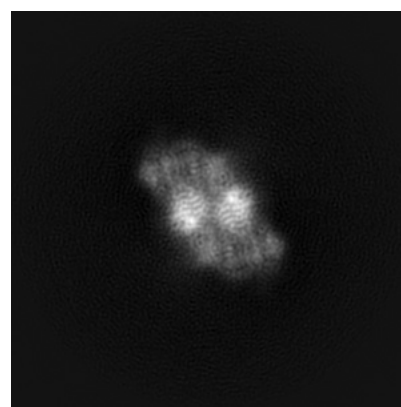
6.1.1 Primary map



X



Y

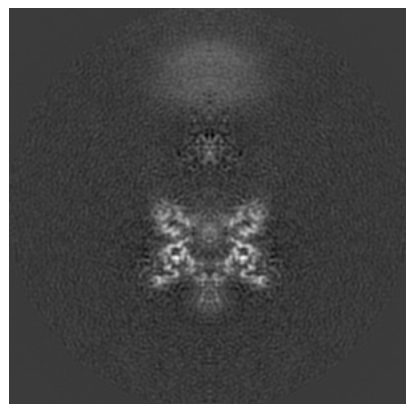


Z

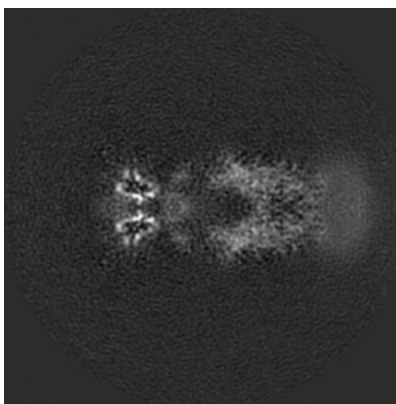
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

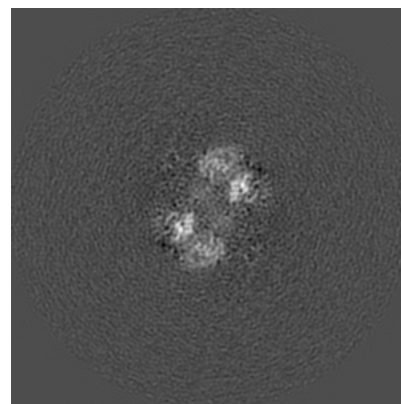
6.2.1 Primary map



X Index: 150



Y Index: 150

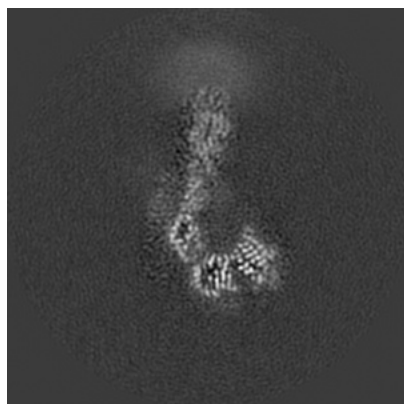


Z Index: 150

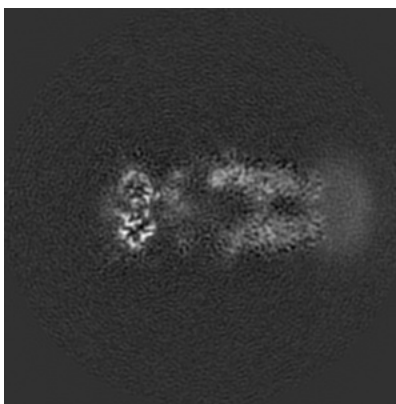
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

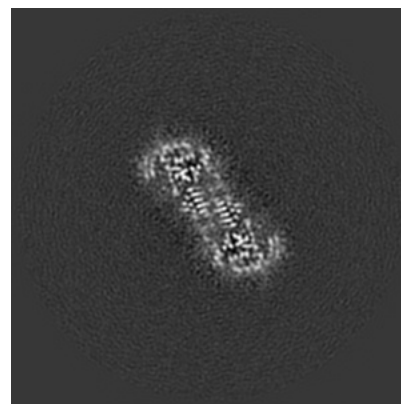
6.3.1 Primary map



X Index: 135



Y Index: 153

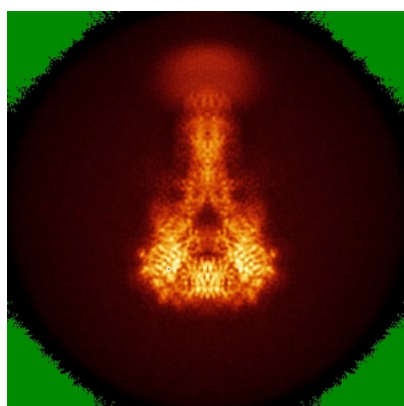


Z Index: 107

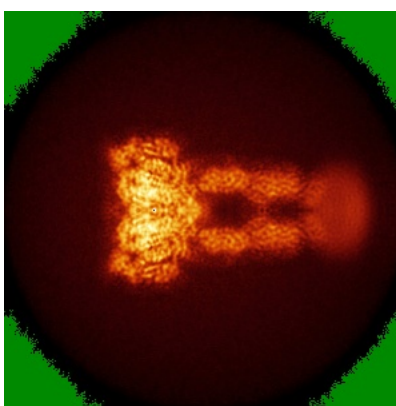
The images above show the largest variance slices of the map in three orthogonal directions.

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

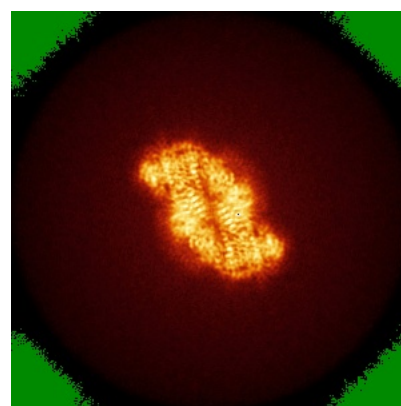
6.4.1 Primary map



X



Y

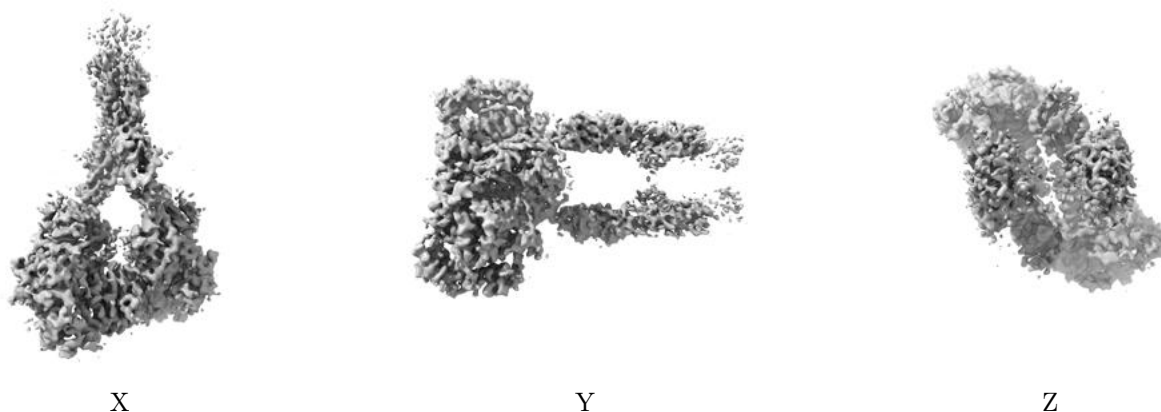


Z

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

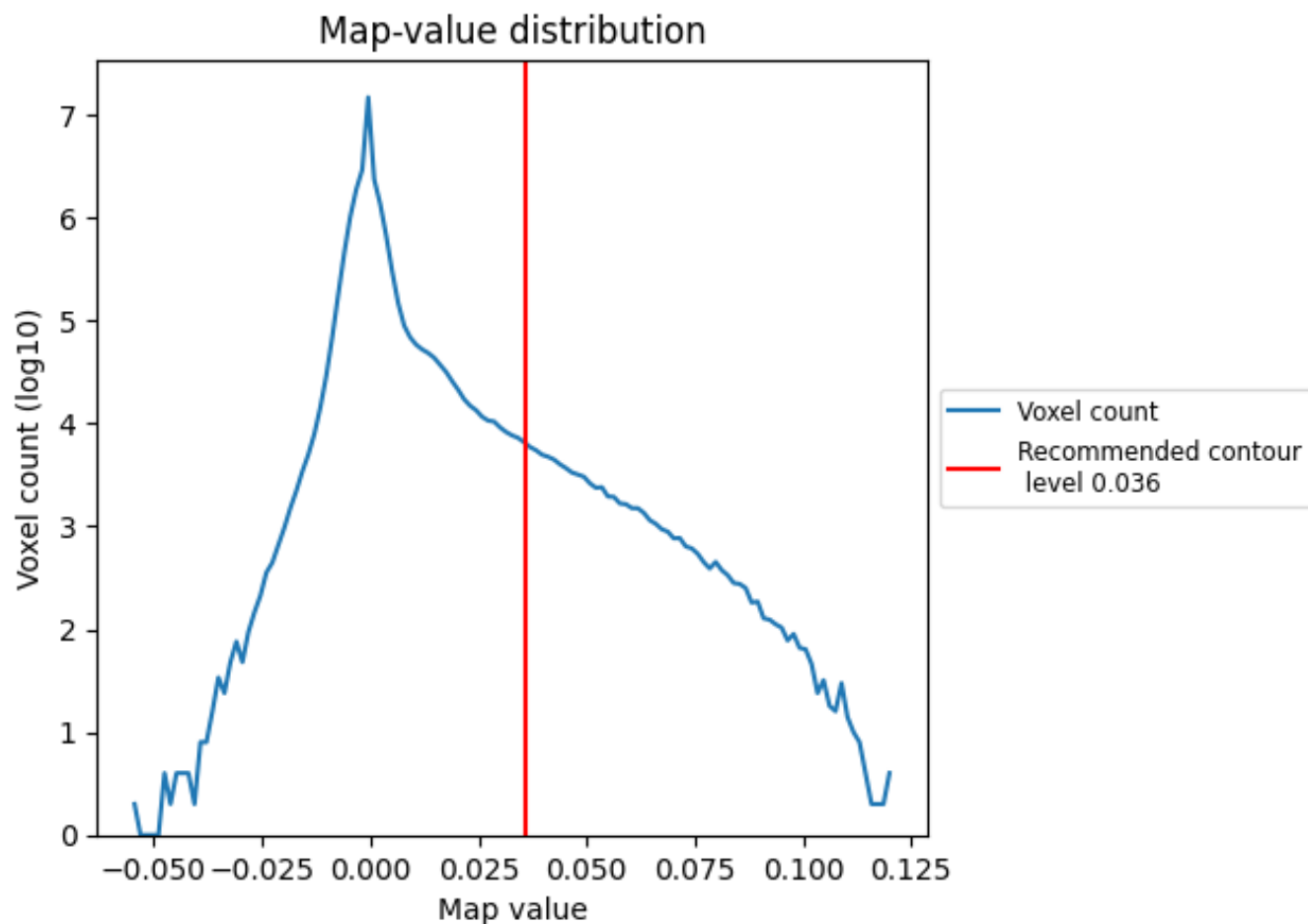
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

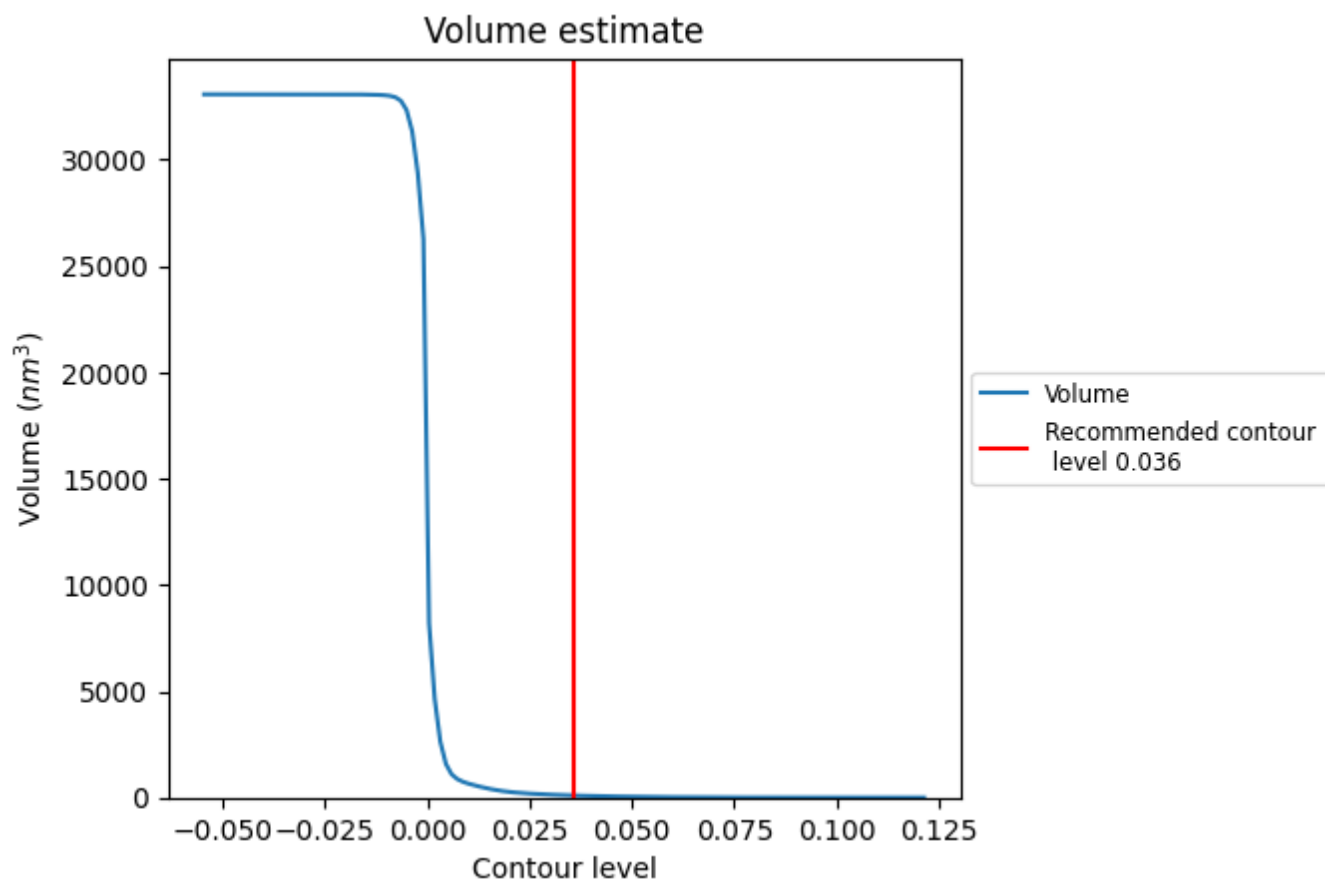
This section contains the results of statistical analysis of the map.

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.

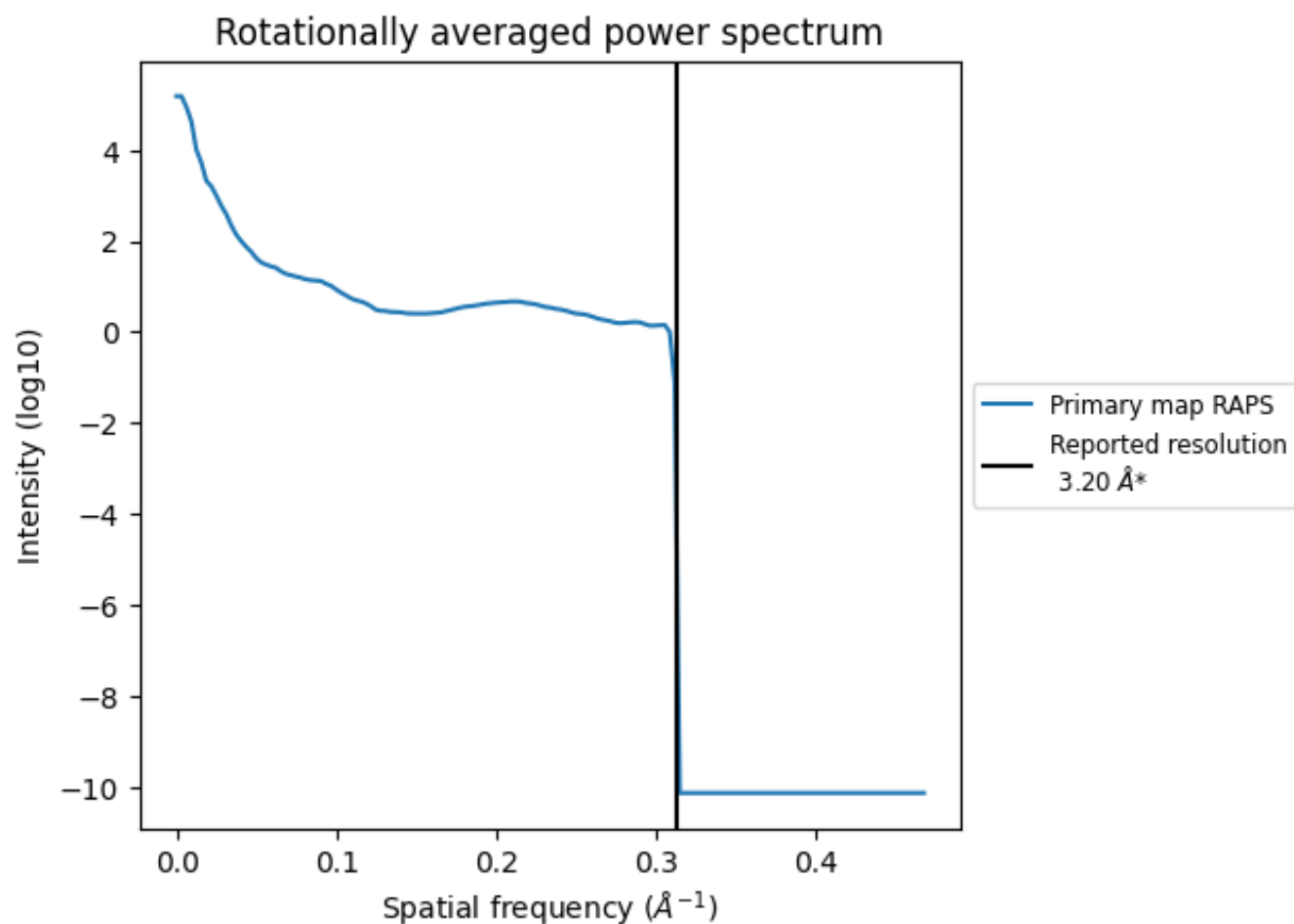
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; this corresponds to an approximate mass of 86 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 0.312 Å⁻¹

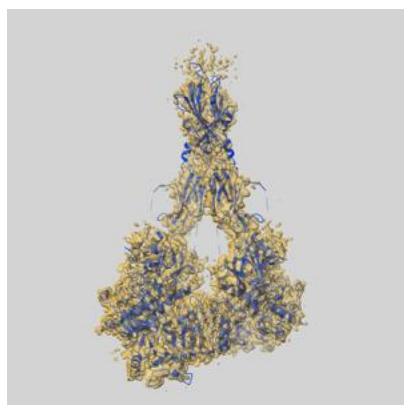
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

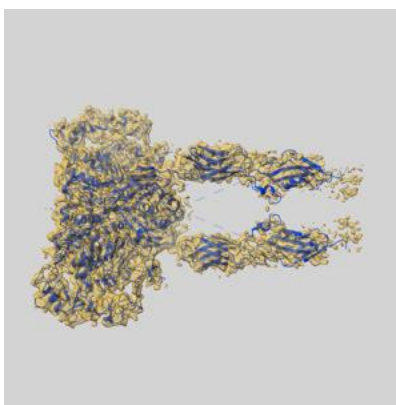
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20522 and PDB model 6PXV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

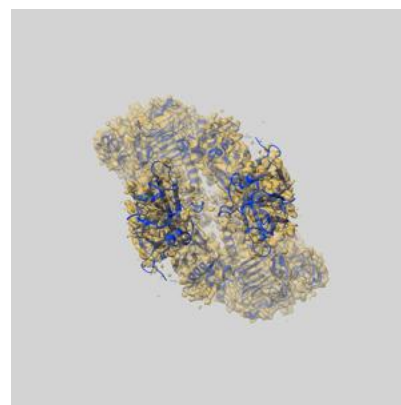
9.1 Map-model overlay [i](#)



X



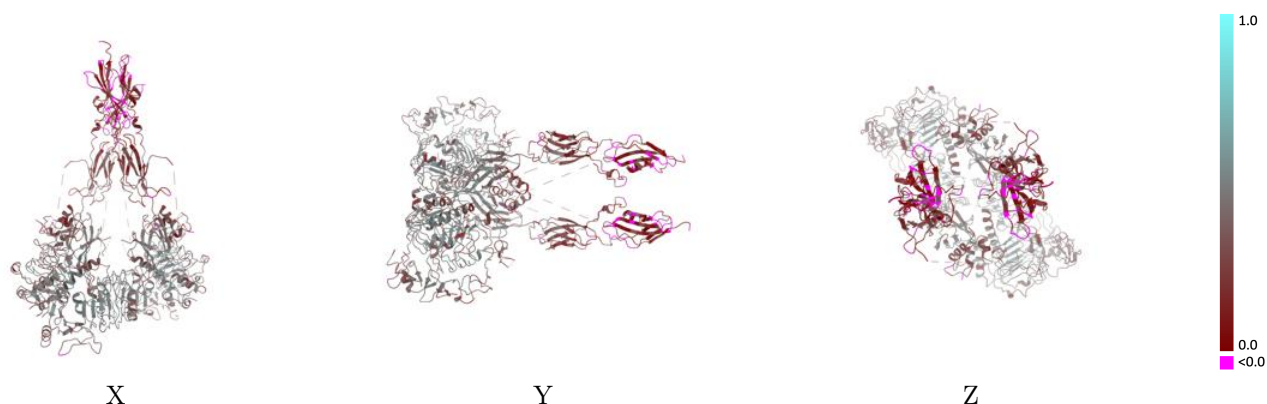
Y



Z

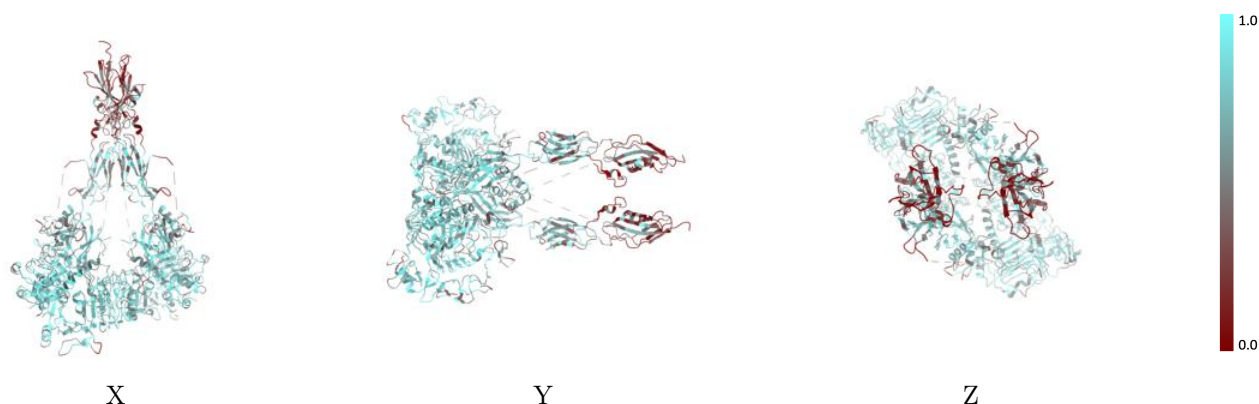
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



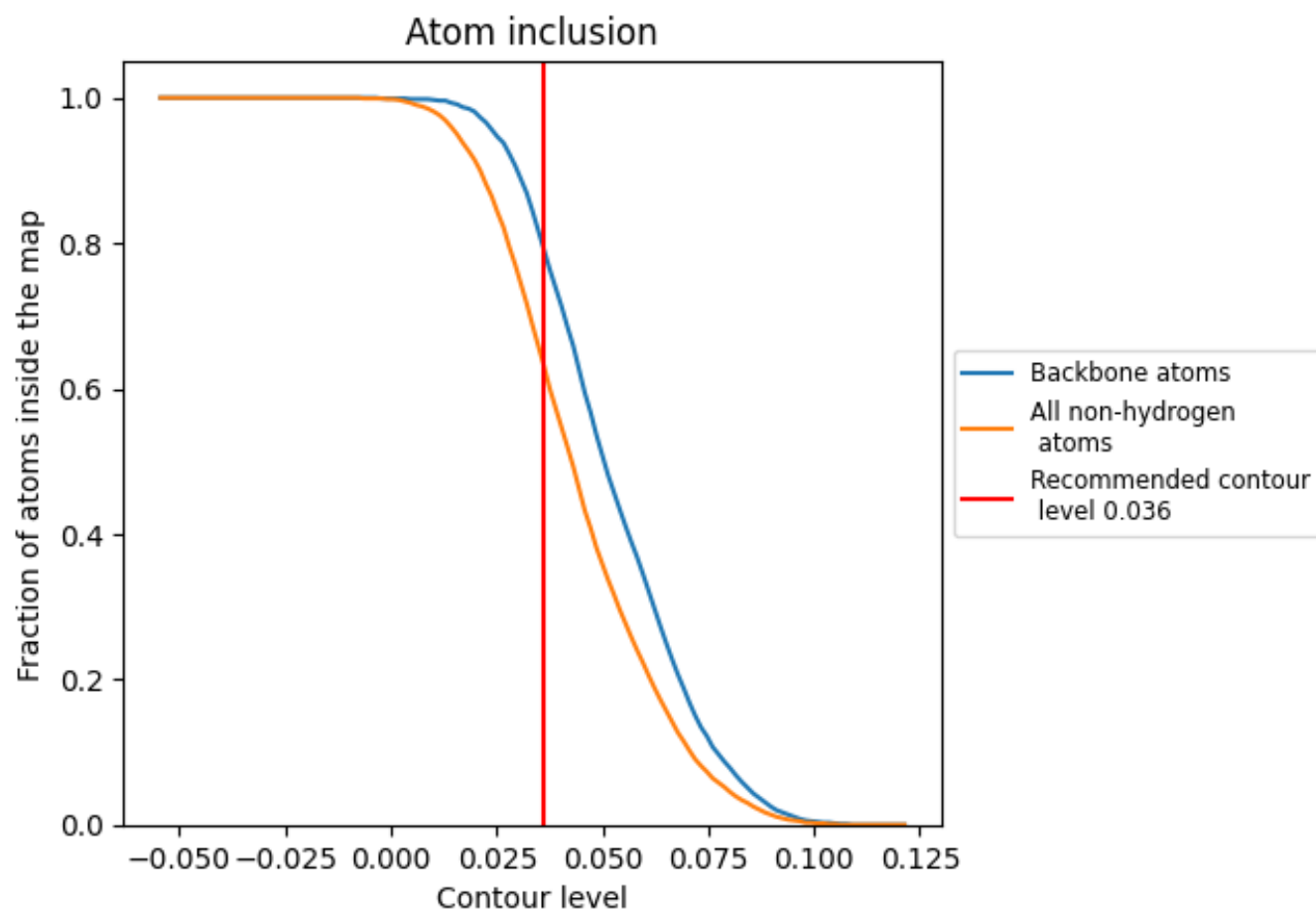
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 63% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6340	0.3520
A	0.6320	0.3540
C	0.6340	0.3530
D	0.7080	0.3970
E	0.6970	0.3940
F	0.5780	0.2860
G	0.5780	0.2840

1.0

0.0

<0.0