



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:31 PM UTC

PDB ID : 8I10 / pdb_00008i10
EMDB ID : EMD-35115
Title : Structure of beta-arrestin2 in complex with a phosphopeptide corresponding to the human Vasopressin V2 receptor, V2R (Local refine)
Authors : Maharana, J.; Sarma, P.; Yadav, M.K.; Banerjee, R.; Shukla, A.K.
Deposited on : 2023-01-12
Resolution : 3.96 Å(reported)
Based on initial model : 8GOC

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
Mogul : 2022.3.0, CSD as543be (2022)
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

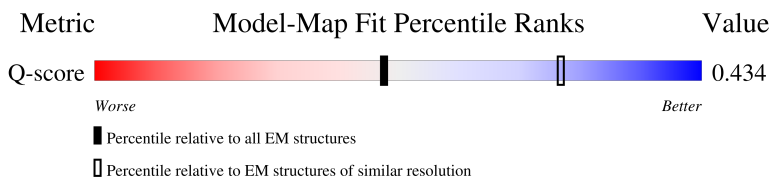
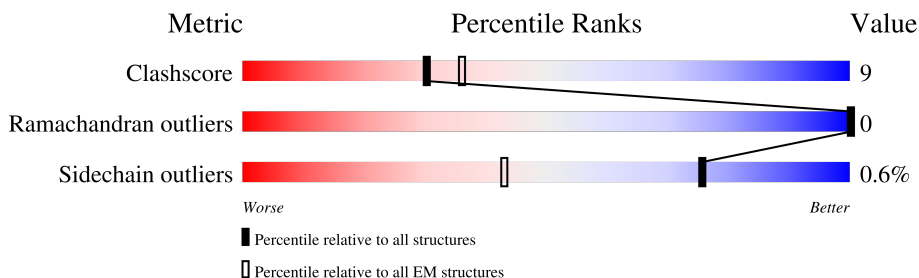
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 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	7646 (3.46 - 4.46)

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	420	
1	B	420	
1	C	420	
2	D	237	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	237	 38% 11% 51%
2	M	237	 41% 9% 50%
3	E	215	 43% 5% 51%
3	L	215	 38% 12% 50%
3	N	215	 40% 9% 50%
4	G	29	 10% 10% 10% 69%
4	U	29	 7% 14% 10% 69%
4	V	29	 10% 14% 7% 69%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13196 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 Beta-arrestin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2641	1691	462	486	2		
1	B	343	Total	C	N	O	S	0	0
			2632	1690	461	479	2		
1	C	343	Total	C	N	O	S	0	0
			2603	1665	459	477	2		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	CYS	engineered mutation	UNP P32120
A	60	VAL	CYS	engineered mutation	UNP P32120
A	69	CYS	LEU	engineered mutation	UNP P32120
A	126	SER	CYS	engineered mutation	UNP P32120
A	141	LEU	CYS	engineered mutation	UNP P32120
A	151	VAL	CYS	engineered mutation	UNP P32120
A	243	VAL	CYS	engineered mutation	UNP P32120
A	252	VAL	CYS	engineered mutation	UNP P32120
A	270	SER	CYS	engineered mutation	UNP P32120
A	278	PHE	LEU	engineered mutation	UNP P32120
A	280	ALA	SER	engineered mutation	UNP P32120
B	17	GLY	CYS	engineered mutation	UNP P32120
B	60	VAL	CYS	engineered mutation	UNP P32120
B	69	CYS	LEU	engineered mutation	UNP P32120
B	126	SER	CYS	engineered mutation	UNP P32120
B	141	LEU	CYS	engineered mutation	UNP P32120
B	151	VAL	CYS	engineered mutation	UNP P32120
B	243	VAL	CYS	engineered mutation	UNP P32120
B	252	VAL	CYS	engineered mutation	UNP P32120
B	270	SER	CYS	engineered mutation	UNP P32120
B	278	PHE	LEU	engineered mutation	UNP P32120
B	280	ALA	SER	engineered mutation	UNP P32120
C	17	GLY	CYS	engineered mutation	UNP P32120
C	60	VAL	CYS	engineered mutation	UNP P32120

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	CYS	LEU	engineered mutation	UNP P32120
C	126	SER	CYS	engineered mutation	UNP P32120
C	141	LEU	CYS	engineered mutation	UNP P32120
C	151	VAL	CYS	engineered mutation	UNP P32120
C	243	VAL	CYS	engineered mutation	UNP P32120
C	252	VAL	CYS	engineered mutation	UNP P32120
C	270	SER	CYS	engineered mutation	UNP P32120
C	278	PHE	LEU	engineered mutation	UNP P32120
C	280	ALA	SER	engineered mutation	UNP P32120

- Molecule 2 is a protein called Fab30 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	119	Total	C	N	O	S	0	0
			908	578	154	173	3		
2	H	117	Total	C	N	O	S	0	0
			897	571	153	170	3		
2	M	118	Total	C	N	O	S	0	0
			892	566	152	171	3		

- Molecule 3 is a protein called Fab30 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	105	Total	C	N	O	S	0	0
			786	497	129	157	3		
3	L	107	Total	C	N	O	S	0	0
			803	509	132	159	3		
3	N	107	Total	C	N	O	S	0	0
			797	503	132	159	3		

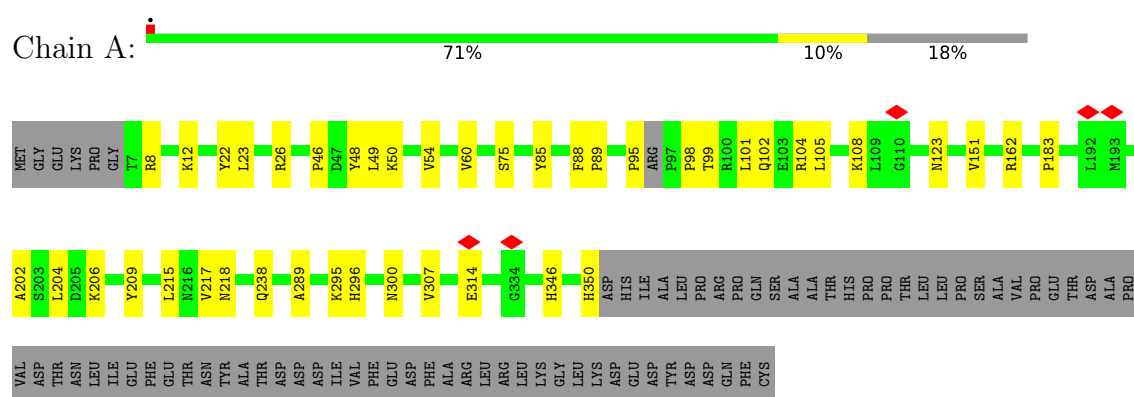
- Molecule 4 is a protein called Vasopressin V2 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	9	Total	C	N	O	P	0	0
			79	35	10	29	5		
4	U	9	Total	C	N	O	P	0	0
			79	35	10	29	5		
4	V	9	Total	C	N	O	P	0	0
			79	35	10	29	5		

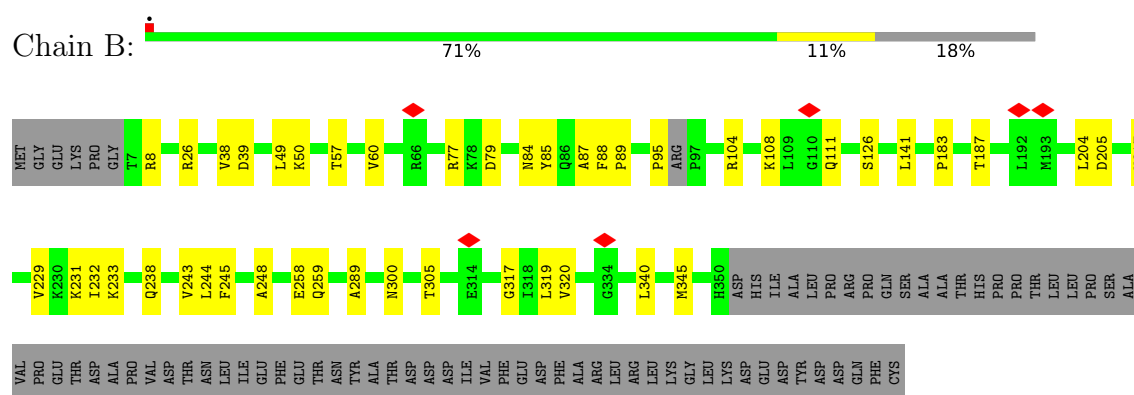
3 Residue-property plots

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.

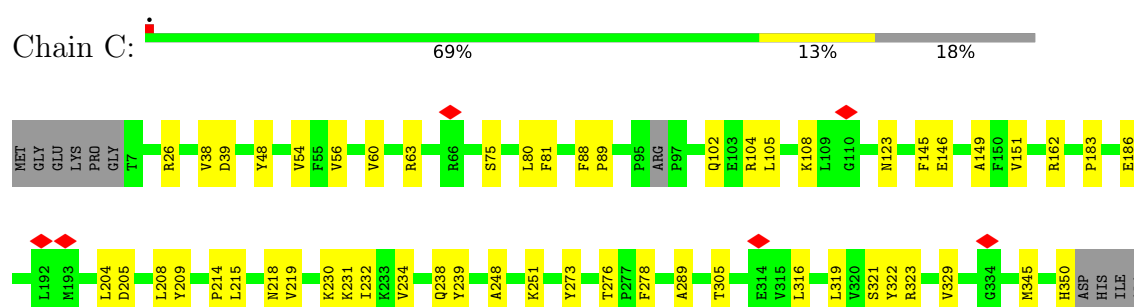
• Molecule 1: Beta-arrestin-2



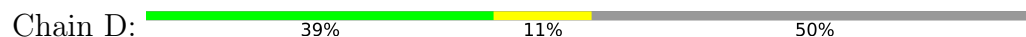
• Molecule 1: Beta-arrestin-2



• Molecule 1: Beta-arrestin-2

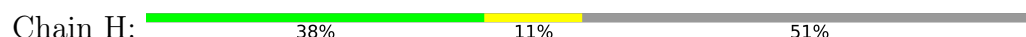


- Molecule 2: Fab30 Heavy Chain



VAL	THR	VAL	PRO	SER	SER	LEU	GLY	GLN	THR	TYR	ILE	THR	GLY	CYS	ASN	ASN	HIS	LYS	PRO	SER	ASN	THR	LYS	VAL	ASP	GLU	PRO	LYS	LYS	VAL	VAL	GLU	PRO	LYS	SER	CYS	ASP	LYS	HIS	HIS	HIS	HIS													
PHE	PRO	ALA	PRO	SER	SER	LYS	THR	SER	GLY	GLY	THR	THR	ALA	LEU	GLY	CYS	LEU	VAL	LYS	ASP	TYR	PHE	PRO	GLU	PRO	VAL	THR	VAL	VAL	SER	TRP	ASN	SER	GLY	ALA	LEU	THR	GLY	THR	HIS	PHE	PRO	ALA	VAL	LEU	GLN	SER	GLY	LEU	TYR	SER	GLY	PRO	SER	VAL
GLU	ILE	SER	GLU	G6	L7	G11	V15	L21	R22	C25	A26	A27	F30	N31	S35	W39	P44	G45	K46	D65	S66	V67	R70	F71	T72	D76	I77	S78	R79	N80	Q85	M86	N87	S88	W113	S123	ALA	SER	THR	LYS	GLY	PRO	SER	SER	VAL										

- Molecule 2: Fab30 Heavy Chain



GLU	ILE	SER	GLU	V5	Q6	L7	V8	E9	S10	G11	V15	L21	R22	C25	W39	V40	R41	L48	D65	V67	F71	I72	I73	S74	A75	K79	R80	T81	A82	L83	L84	R85	R86	D93	C99	D111	Y112	V121	SER	SER	ALA	LEU	GLN	SER	GLY	LEU	THR	LYS	GLY	PRO
VAL	THR	VAL	VAL	VAL	PRO	SER	SER	SER	LEU	GLY	GLN	THR	ILE	CYS	ASN	VAL	HIS	PRO	SER	ASN	LYS	LYS	VAL	GLU	PRO	LYS	CYS	ASP	GLY	LYS	THR	HIS	HIS	HIS	THR	PHE	PRO	ALA	VAL	LEU	GLN	SER	GLY	LEU	THR	LYS	LEU	SER		

- Molecule 2: Fab30 Heavy Chain

[illegible]

- Molecule 3: Fab30 Light Chain



THR	SER
PRO	D2
ARG	P9
GLU	L12
ALA	S15
LYS	D18
VAL	S32
GLN	P45
TRP	L79
LYS	Q80
ASP	Q91
ASN	Y92
GLN	K93
GLY	Y94
ASN	T103
SER	E106
THR	ILE
GLU	ARG
GLN	LYS
ASP	THR
LYS	VAL
ASP	ALA
THR	ALA
THR	PRO
SER	SER
LEU	VAL
SER	PHE
SER	ILE
THR	PHE
LEU	PRO
THR	PRO
LEU	SER
SER	ASP
LYS	SER
ALA	GLN
ASP	LEU
TYR	LYS
GLU	LYS
LYS	GLY
HIS	THR
LYS	ALA
VAL	SER
THR	VAL
ALA	VAL
CYS	CYS
GLU	LEU
VAL	LEU
THR	ASN
HIS	ASN
THR	THR

GLY
LEU
SER
SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLU
CYS

- Molecule 3: Fab30 Light Chain

Chain L:  38% 12% 50%

SER
D2
I3
T6
P9
L12
S15
D18
C24
R25
S29
A53
W36
L55
V59
R62
R67
F72
I73
L74
T75
I76
L79
E82
D83
Y92
K93
Y94
K108
ARG
THR
VAL
ALA
PRO
TYR
SER
LEU
PHE
ILE
PHE
THR
PRO
THR

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

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

- Molecule 3: Fab30 Light Chain

Chain N:  40% 9% 50%

SER
D2
I3
T6
S15
D18
R25
Q28
S29
W36
R67
S68
G69
D71
F72
T73
L74
T75
L79
Q80
F84
K93
Y94
I107
K108
ARG
THR
VAL
SER
ALA
THR
PRO
SER
VAL
PHE
ILE
PHE
PRO
PRO
SER
ASP
SER
GLN
ALA
LEU
SER
LYS
THR
GLY
ALA

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

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

- Molecule 4: Vasopressin V2 receptor

Chain G:  10% 10% 10% 69%

ALA
ARG
GLY
ARG
TPQ
PRO
PRO
SEP
GLY
PRO
GLN
ASP
GLU
SEP
CYS
T359
T360
A361
S362
S363
S364
L365
A366
K367
ASP
THR
SER
SER

- Molecule 4: Vasopressin V2 receptor

Chain U:  7% 14% 10% 69%

ALA
ARG
GLY
ARG
TPQ
PRO
PRO
SEP
GLY
PRO
GLN
ASP
GLU
SEP
CYS
T359
T360
A361
S362
S363
S364
L365
A366
K367
ASP
THR
SER
SER

- Molecule 4: Vasopressin V2 receptor

Chain V:  10% 14% 7% 69%

ALA
ARG
GLY
ARG
TPQ
PRO
PRO
SEP
GLY
PRO
GLN
ASP
GLU
SEP
CYS
T359
T360
A361
S362
S363
S364
L365
A366
K367
ASP
THR
SER
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	92018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.704	Depositor
Minimum map value	-1.129	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	419.832, 419.832, 419.832	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1662, 1.1662, 1.1662	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

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	0.21	0/2704	0.47	0/3683
1	B	0.21	0/2695	0.48	0/3668
1	C	0.22	0/2662	0.48	0/3626
2	D	0.28	0/932	0.54	0/1268
2	H	0.25	0/921	0.54	0/1253
2	M	0.24	0/916	0.52	0/1248
3	E	0.19	0/804	0.53	0/1095
3	L	0.23	0/821	0.53	0/1117
3	N	0.21	0/815	0.53	0/1109
4	G	0.18	0/25	0.51	0/30
4	U	0.23	0/25	0.64	0/30
4	V	0.91	0/25	1.35	0/30
All	All	0.22	0/13345	0.50	0/18157

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2641	0	2607	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2632	0	2610	38	0
1	C	2603	0	2570	44	0
2	D	908	0	847	23	0
2	H	897	0	834	20	0
2	M	892	0	813	19	0
3	E	786	0	751	11	0
3	L	803	0	775	20	0
3	N	797	0	757	16	0
4	G	79	0	56	11	0
4	U	79	0	56	7	0
4	V	79	0	56	9	0
All	All	13196	0	12732	232	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 9.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:21:LEU:HD12	2:M:22:ARG:H	1.29	0.95
1:A:183:PRO:HG2	1:A:204:LEU:HB2	1.49	0.94
1:B:233:LYS:HG2	1:B:258:GLU:HG2	1.52	0.90
3:E:91:GLN:HE22	3:E:94:TYR:H	1.23	0.87
1:C:104:ARG:HG2	4:V:365:LEU:HD11	1.56	0.85
2:H:73:ILE:HD12	2:H:84:LEU:HB3	1.60	0.84
2:M:22:ARG:HH22	2:M:83:TYR:HD2	1.28	0.81
1:C:105:LEU:HD22	4:V:365:LEU:HD13	1.62	0.81
1:A:88:PHE:CD2	1:A:89:PRO:HA	2.21	0.75
1:C:54:VAL:HG22	1:C:151:VAL:HG12	1.68	0.75
1:A:85:TYR:HE2	1:A:95:PRO:CD	2.00	0.74
1:B:104:ARG:HD2	4:U:365:LEU:HD11	1.69	0.73
3:N:93:LYS:HG2	3:N:94:TYR:CE1	2.25	0.72
3:L:6:THR:HG23	3:L:25:ARG:HB3	1.72	0.71
1:B:88:PHE:CD1	1:B:89:PRO:HA	2.26	0.71
1:B:183:PRO:HG2	1:B:204:LEU:HB2	1.71	0.71
1:B:88:PHE:HD1	1:B:89:PRO:HA	1.56	0.70
1:C:80:LEU:HD13	1:C:316:LEU:HB3	1.74	0.69
2:M:73:ILE:HD13	2:M:84:LEU:HB3	1.74	0.69
2:H:67:VAL:HB	2:H:71:PHE:CD2	2.28	0.68
3:L:62:ARG:HH12	3:L:83:ASP:CG	2.04	0.66
2:D:67:VAL:HB	2:D:71:PHE:CD2	2.31	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD13	1:B:88:PHE:HE2	1.61	0.65
1:C:108:LYS:NZ	4:V:363:SEP:OG	2.27	0.65
4:U:365:LEU:HD12	4:U:366:ALA:N	2.14	0.63
2:D:72:THR:HG22	2:D:85:GLN:HB3	1.80	0.62
1:A:104:ARG:HD2	4:G:365:LEU:HD21	1.79	0.62
2:H:111:ASP:OD1	2:H:112:TYR:N	2.32	0.62
3:N:6:THR:CG2	3:N:25:ARG:HB3	2.29	0.62
2:H:21:LEU:HD23	2:H:22:ARG:N	2.15	0.62
3:N:93:LYS:HG2	3:N:94:TYR:CD1	2.34	0.61
1:B:233:LYS:HG2	1:B:258:GLU:CG	2.28	0.61
1:A:206:LYS:HB2	1:A:209:TYR:CE2	2.36	0.61
2:D:21:LEU:HD22	2:D:86:MET:HE1	1.82	0.61
1:C:239:TYR:HE2	1:C:251:LYS:HD2	1.66	0.60
3:L:82:GLU:OE1	3:L:82:GLU:N	2.35	0.60
1:A:307:VAL:HG23	1:A:314:GLU:HG2	1.83	0.60
4:U:365:LEU:HD12	4:U:366:ALA:H	1.67	0.60
3:E:9:PRO:HG2	3:E:12:LEU:HD22	1.84	0.59
1:C:239:TYR:HE1	1:C:323:ARG:HG3	1.66	0.59
3:L:36:TRP:CG	3:L:74:LEU:HD12	2.37	0.59
1:C:209:TYR:HE2	1:C:215:LEU:HA	1.68	0.58
2:M:21:LEU:HD12	2:M:22:ARG:N	2.11	0.58
1:C:88:PHE:HD2	1:C:89:PRO:HA	1.69	0.57
1:C:104:ARG:CG	4:V:365:LEU:HD11	2.32	0.57
1:C:26:ARG:HH12	4:V:360:TPO:HG21	1.68	0.57
1:A:300:ASN:OD1	1:A:300:ASN:N	2.34	0.57
1:C:39:ASP:OD2	1:C:102:GLN:NE2	2.29	0.57
1:B:26:ARG:NH1	4:U:360:TPO:HG21	2.19	0.57
2:H:21:LEU:HD23	2:H:22:ARG:H	1.70	0.57
1:C:183:PRO:HG2	1:C:204:LEU:HB2	1.85	0.56
2:D:15:VAL:HG22	2:D:21:LEU:HD12	1.88	0.56
2:D:27:ALA:HB3	2:D:80:ASN:OD1	2.05	0.56
2:D:85:GLN:OE1	2:D:87:ASN:HB2	2.06	0.55
3:N:15:SER:N	3:N:18:ASP:OD2	2.30	0.55
1:B:258:GLU:OE1	1:B:259:GLN:N	2.39	0.55
1:A:108:LYS:HZ2	4:G:365:LEU:N	2.04	0.55
1:B:8:ARG:HG3	1:B:8:ARG:HH11	1.72	0.54
3:L:29:SER:O	3:L:29:SER:OG	2.17	0.54
1:B:111:GLN:N	1:B:111:GLN:OE1	2.40	0.54
1:A:54:VAL:HG22	1:A:151:VAL:HG12	1.90	0.54
2:H:15:VAL:HG23	2:H:21:LEU:HD12	1.90	0.54
1:A:98:PRO:HA	1:A:102:GLN:NE2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:VAL:CG2	1:C:81:PHE:HB3	2.38	0.54
2:D:87:ASN:OD1	2:D:88:SER:N	2.41	0.54
3:N:36:TRP:CD2	3:N:74:LEU:HD12	2.43	0.53
1:B:300:ASN:OD1	1:B:300:ASN:N	2.40	0.53
2:D:21:LEU:HD23	2:D:22:ARG:N	2.24	0.53
3:E:32:SER:O	3:E:32:SER:OG	2.27	0.53
2:M:34:SER:O	2:M:34:SER:OG	2.21	0.53
2:H:79:LYS:HG3	2:H:81:THR:HG23	1.91	0.53
2:D:31:ASN:O	2:D:35:SER:OG	2.22	0.52
3:L:55:LEU:HD21	3:L:59:VAL:HB	1.90	0.52
1:A:183:PRO:HG2	1:A:204:LEU:CB	2.33	0.52
2:H:21:LEU:HD22	2:H:86:MET:HE1	1.91	0.52
1:B:231:LYS:O	1:B:232:ILE:HD13	2.10	0.52
1:A:209:TYR:CE1	1:A:215:LEU:HG	2.44	0.51
1:B:231:LYS:HB3	1:B:258:GLU:OE2	2.10	0.51
3:E:15:SER:N	3:E:18:ASP:OD2	2.30	0.51
1:C:186:GLU:OE1	1:C:186:GLU:N	2.43	0.51
1:A:108:LYS:NZ	4:G:365:LEU:H	2.08	0.51
3:L:74:LEU:HD23	3:L:75:THR:N	2.26	0.51
2:M:9:GLU:OE2	2:M:99:CYS:N	2.44	0.51
2:D:85:GLN:HE22	2:D:87:ASN:HB2	1.76	0.51
1:A:108:LYS:NZ	4:G:365:LEU:N	2.59	0.51
3:N:67:ARG:HG2	3:N:72:PHE:CE2	2.46	0.51
3:E:91:GLN:NE2	3:E:94:TYR:H	2.00	0.50
2:M:25:CYS:HB2	2:M:39:TRP:CZ2	2.46	0.50
2:M:70:ARG:HG2	2:M:87:ASN:O	2.11	0.50
1:C:63:ARG:NH1	1:C:146:GLU:OE2	2.44	0.50
1:C:239:TYR:HE1	1:C:323:ARG:CG	2.25	0.50
1:C:239:TYR:CE1	1:C:323:ARG:HG3	2.46	0.50
2:D:70:ARG:O	2:D:87:ASN:HB3	2.11	0.50
3:L:76:ILE:HG21	3:L:79:LEU:HD13	1.93	0.50
1:A:238:GLN:NE2	1:A:289:ALA:HB3	2.27	0.49
1:A:48:TYR:OH	1:A:162:ARG:NH1	2.46	0.49
1:C:209:TYR:CE2	1:C:215:LEU:HA	2.46	0.49
3:L:9:PRO:HG2	3:L:12:LEU:HD23	1.95	0.49
1:C:231:LYS:O	1:C:232:ILE:HD13	2.12	0.49
1:A:99:THR:OG1	1:A:102:GLN:HG3	2.12	0.49
1:C:56:VAL:HG12	1:C:149:ALA:HB2	1.94	0.48
1:A:26:ARG:NH1	4:G:360:TPO:HG21	2.27	0.48
1:B:85:TYR:HE1	1:B:95:PRO:HD2	1.77	0.48
1:C:26:ARG:NH1	4:V:360:TPO:HG21	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:LEU:HD13	2:D:30:PHE:HE2	1.78	0.48
3:E:91:GLN:NE2	3:E:94:TYR:O	2.47	0.48
2:D:85:GLN:HE22	2:D:87:ASN:CA	2.27	0.48
3:L:67:ARG:HG2	3:L:72:PHE:CE1	2.48	0.48
2:M:22:ARG:NH2	2:M:83:TYR:HD2	2.06	0.48
1:C:239:TYR:CE2	1:C:251:LYS:HD2	2.49	0.48
2:H:11:GLY:O	2:H:21:LEU:HD21	2.14	0.48
1:A:8:ARG:HH12	4:G:364:SEP:HA	1.79	0.48
1:A:85:TYR:CD1	1:A:85:TYR:C	2.92	0.47
3:E:9:PRO:O	3:E:103:THR:HG23	2.14	0.47
1:B:183:PRO:HB2	1:B:340:LEU:HD13	1.97	0.47
1:C:230:LYS:N	1:C:329:VAL:O	2.46	0.47
2:H:25:CYS:HB2	2:H:39:TRP:CZ2	2.49	0.47
3:L:2:ASP:OD1	3:L:3:ILE:N	2.47	0.47
3:L:36:TRP:CD2	3:L:74:LEU:HD12	2.49	0.47
1:B:204:LEU:CD2	1:B:217:VAL:HG12	2.44	0.47
1:C:305:THR:OG1	1:C:319:LEU:HD23	2.15	0.47
1:A:300:ASN:ND2	1:A:346:HIS:NE2	2.62	0.47
1:B:238:GLN:NE2	1:B:289:ALA:HB3	2.29	0.47
1:B:77:ARG:HH12	1:B:79:ASP:CG	2.22	0.47
1:C:234:VAL:HG21	1:C:273:TYR:HD1	1.80	0.47
2:D:11:GLY:O	2:D:21:LEU:HD21	2.15	0.47
1:B:39:ASP:N	1:B:39:ASP:OD1	2.45	0.46
2:D:7:LEU:HD13	2:D:30:PHE:CE2	2.50	0.46
3:N:25:ARG:NH2	3:N:71:ASP:OD2	2.48	0.46
2:H:41:ARG:NH2	2:H:93:ASP:HA	2.31	0.46
3:L:62:ARG:NH1	3:L:83:ASP:OD2	2.49	0.46
1:C:104:ARG:HG2	4:V:365:LEU:CD1	2.38	0.46
1:C:218:ASN:OD1	1:C:219:VAL:N	2.49	0.46
3:E:91:GLN:HE22	3:E:94:TYR:N	2.04	0.46
3:L:15:SER:N	3:L:18:ASP:OD2	2.42	0.46
3:N:74:LEU:HD23	3:N:75:THR:N	2.30	0.46
1:B:108:LYS:NZ	4:U:363:SEP:OG	2.49	0.46
1:A:295:LYS:HE3	4:G:360:TPO:O3P	2.15	0.46
3:E:91:GLN:OE1	3:E:93:LYS:N	2.46	0.46
3:L:93:LYS:C	3:L:94:TYR:HD2	2.24	0.46
2:M:41:ARG:HH22	2:M:93:ASP:HA	1.80	0.46
1:C:238:GLN:NE2	1:C:289:ALA:HB3	2.32	0.45
2:H:9:GLU:OE2	2:H:99:CYS:N	2.49	0.45
2:M:80:ASN:OD1	2:M:80:ASN:O	2.34	0.45
2:M:79:LYS:HD2	2:M:79:LYS:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:TYR:HE1	1:B:95:PRO:CD	2.30	0.45
3:E:79:LEU:HD23	3:E:80:GLN:N	2.31	0.45
4:G:360:TPO:HG21	4:G:360:TPO:O1P	2.17	0.45
2:D:21:LEU:O	2:D:86:MET:HE3	2.17	0.45
2:M:41:ARG:NH2	2:M:93:ASP:HA	2.32	0.45
3:L:67:ARG:HG2	3:L:72:PHE:CD1	2.52	0.45
3:N:84:PHE:CZ	3:N:107:ILE:HG23	2.52	0.45
1:A:49:LEU:HD13	1:A:88:PHE:HE1	1.82	0.44
3:N:36:TRP:CG	3:N:74:LEU:HD12	2.52	0.44
1:A:108:LYS:HZ1	4:G:364:SEP:HB2	1.83	0.44
3:N:79:LEU:HD23	3:N:80:GLN:N	2.33	0.44
1:B:319:LEU:HD12	1:B:320:VAL:N	2.33	0.44
1:C:205:ASP:OD2	1:C:209:TYR:OH	2.29	0.44
1:A:12:LYS:HZ2	4:G:359:TPO:HG22	1.81	0.44
3:N:67:ARG:NH2	3:N:69:GLY:O	2.50	0.44
1:A:101:LEU:O	1:A:105:LEU:HD23	2.17	0.44
2:D:44:PRO:O	2:D:46:LYS:NZ	2.45	0.44
4:V:363:SEP:O	4:V:364:SEP:CB	2.65	0.44
1:A:85:TYR:HE2	1:A:95:PRO:HD2	1.79	0.44
2:H:48:LEU:H	2:H:48:LEU:HD23	1.82	0.44
3:L:93:LYS:HG3	3:L:94:TYR:CE2	2.53	0.44
4:U:359:TPO:O	4:U:360:TPO:C	2.64	0.44
1:A:123:ASN:ND2	1:A:123:ASN:O	2.50	0.43
1:A:350:HIS:ND1	1:A:350:HIS:N	2.66	0.43
1:B:85:TYR:HE2	1:B:87:ALA:HA	1.82	0.43
1:B:104:ARG:CD	4:U:365:LEU:HD11	2.43	0.43
1:B:204:LEU:HD22	1:B:217:VAL:HG12	2.01	0.43
1:C:208:LEU:C	1:C:209:TYR:HD1	2.26	0.43
2:H:15:VAL:CG2	2:H:21:LEU:HD12	2.49	0.43
1:C:345:MET:HE2	1:C:345:MET:HB3	1.93	0.43
2:H:21:LEU:HB3	2:H:86:MET:HE2	2.01	0.43
2:D:21:LEU:C	2:D:86:MET:HE3	2.44	0.43
1:A:46:PRO:HA	1:A:49:LEU:HD21	2.01	0.43
2:M:41:ARG:HD3	2:M:51:VAL:HB	2.01	0.43
1:A:202:ALA:HA	1:A:218:ASN:O	2.19	0.43
1:B:244:LEU:HD23	1:B:245:PHE:H	1.84	0.43
2:M:79:LYS:HG3	2:M:81:THR:HG23	2.01	0.43
3:N:93:LYS:HG2	3:N:94:TYR:HE1	1.81	0.42
1:B:57:THR:HG22	1:B:84:ASN:OD1	2.20	0.42
1:C:38:VAL:HG12	1:C:38:VAL:O	2.20	0.42
1:C:321:SER:C	1:C:322:TYR:HD1	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:363:SEP:O	4:V:364:SEP:HB2	2.19	0.42
1:B:141:LEU:HD23	1:B:141:LEU:H	1.84	0.42
1:B:243:VAL:HG22	1:B:317:GLY:O	2.18	0.42
1:A:104:ARG:CD	4:G:365:LEU:HD21	2.48	0.42
1:B:229:VAL:HG11	1:B:232:ILE:HD11	2.01	0.42
1:A:22:TYR:C	1:A:23:LEU:HD12	2.44	0.42
3:N:28:GLN:OE1	3:N:29:SER:N	2.53	0.42
3:L:33:ALA:HB1	3:L:92:TYR:CD1	2.54	0.42
1:A:49:LEU:CD1	1:A:88:PHE:HE1	2.33	0.42
1:B:319:LEU:HD12	1:B:320:VAL:H	1.85	0.42
3:L:24:CYS:HB2	3:L:36:TRP:CH2	2.55	0.42
1:C:214:PRO:HA	1:C:276:THR:HG22	2.02	0.41
1:C:350:HIS:ND1	1:C:350:HIS:N	2.67	0.41
2:M:51:VAL:HG22	2:M:67:VAL:HG21	2.01	0.41
3:N:3:ILE:HD11	3:N:94:TYR:HD2	1.83	0.41
1:A:99:THR:H	1:A:102:GLN:CD	2.28	0.41
3:L:79:LEU:HD12	3:L:79:LEU:HA	1.82	0.41
2:M:31:ASN:O	2:M:35:SER:HB2	2.20	0.41
1:C:60:VAL:HG12	1:C:145:PHE:CD1	2.56	0.41
2:H:75:ALA:HA	2:H:82:ALA:HA	2.02	0.41
2:D:25:CYS:HB2	2:D:39:TRP:CZ2	2.56	0.41
1:A:49:LEU:HD12	1:A:50:LYS:N	2.35	0.41
2:H:66:SER:OG	2:H:67:VAL:HG13	2.21	0.41
2:M:39:TRP:CH2	2:M:99:CYS:HB3	2.55	0.41
1:B:248:ALA:HA	1:C:75:SER:O	2.21	0.41
1:C:278:PHE:CG	2:M:33:TYR:CE1	3.08	0.41
2:D:85:GLN:NE2	2:D:87:ASN:HB2	2.34	0.41
2:H:39:TRP:CH2	2:H:99:CYS:HB3	2.55	0.41
1:A:204:LEU:CD2	1:A:217:VAL:HG12	2.51	0.41
1:B:38:VAL:HG12	1:B:38:VAL:O	2.21	0.41
1:B:126:SER:OG	1:B:305:THR:HG21	2.20	0.41
1:C:48:TYR:OH	1:C:162:ARG:NH1	2.54	0.41
1:C:208:LEU:O	1:C:209:TYR:HD1	2.04	0.41
2:H:65:ASP:OD1	2:H:65:ASP:N	2.54	0.41
1:B:88:PHE:CD1	1:B:89:PRO:CA	3.00	0.41
2:D:76:ASP:OD2	2:D:78:SER:N	2.50	0.40
1:C:278:PHE:CD1	1:C:278:PHE:C	2.99	0.40
3:N:25:ARG:CZ	3:N:25:ARG:HB2	2.52	0.40
1:B:49:LEU:HD12	1:B:50:LYS:N	2.37	0.40
1:B:345:MET:HE2	1:B:345:MET:HB3	1.77	0.40
1:A:75:SER:O	1:C:248:ALA:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:O	1:C:123:ASN:CG	2.64	0.40
2:D:71:PHE:CD2	2:D:71:PHE:N	2.88	0.40
2:D:113:TRP:CE3	3:E:45:PRO:HD2	2.56	0.40
1:A:206:LYS:HB2	1:A:209:TYR:HE2	1.85	0.40
2:H:6:GLN:HG3	2:H:7:LEU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/420 (81%)	317 (94%)	22 (6%)	0	100	100
1	B	339/420 (81%)	320 (94%)	19 (6%)	0	100	100
1	C	339/420 (81%)	323 (95%)	16 (5%)	0	100	100
2	D	117/237 (49%)	109 (93%)	8 (7%)	0	100	100
2	H	115/237 (48%)	110 (96%)	5 (4%)	0	100	100
2	M	116/237 (49%)	106 (91%)	10 (9%)	0	100	100
3	E	103/215 (48%)	94 (91%)	9 (9%)	0	100	100
3	L	105/215 (49%)	97 (92%)	8 (8%)	0	100	100
3	N	105/215 (49%)	95 (90%)	10 (10%)	0	100	100
4	G	3/29 (10%)	2 (67%)	1 (33%)	0	100	100
4	U	3/29 (10%)	2 (67%)	1 (33%)	0	100	100
4	V	3/29 (10%)	3 (100%)	0	0	100	100
All	All	1687/2703 (62%)	1578 (94%)	109 (6%)	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	287/376 (76%)	285 (99%)	2 (1%)	76	79
1	B	284/376 (76%)	281 (99%)	3 (1%)	65	74
1	C	279/376 (74%)	279 (100%)	0	100	100
2	D	91/200 (46%)	90 (99%)	1 (1%)	65	74
2	H	89/200 (44%)	88 (99%)	1 (1%)	65	74
2	M	87/200 (44%)	87 (100%)	0	100	100
3	E	86/190 (45%)	85 (99%)	1 (1%)	63	73
3	L	88/190 (46%)	88 (100%)	0	100	100
3	N	86/190 (45%)	86 (100%)	0	100	100
4	G	2/16 (12%)	2 (100%)	0	100	100
4	U	2/16 (12%)	2 (100%)	0	100	100
4	V	2/16 (12%)	2 (100%)	0	100	100
All	All	1383/2346 (59%)	1375 (99%)	8 (1%)	76	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	296	HIS
1	B	60	VAL
1	B	187	THR
1	B	205	ASP
2	D	65	ASP
3	E	18	ASP
2	H	15	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	GLN
1	A	211	HIS
1	A	220	HIS
1	B	112	HIS
1	B	249	GLN
1	C	163	ASN
1	C	249	GLN
2	D	85	GLN
2	D	104	GLN
2	M	85	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TPO	V	359	4	8,10,11	0.69	0	10,14,16	1.03	1 (10%)
4	SEP	G	364	4	8,9,10	1.62	1 (12%)	7,12,14	1.60	1 (14%)
4	SEP	G	362	4	8,9,10	1.60	1 (12%)	7,12,14	1.19	1 (14%)
4	TPO	G	360	4	8,10,11	0.64	0	10,14,16	1.01	1 (10%)
4	SEP	G	363	4	8,9,10	1.61	1 (12%)	7,12,14	1.31	1 (14%)
4	TPO	V	360	4	8,10,11	0.61	0	10,14,16	1.21	2 (20%)
4	SEP	V	362	4	8,9,10	1.60	1 (12%)	7,12,14	1.22	1 (14%)
4	SEP	V	364	4	8,9,10	0.70	0	7,12,14	0.66	0
4	TPO	U	360	4	8,10,11	0.59	0	10,14,16	1.10	1 (10%)
4	SEP	V	363	4	8,9,10	1.61	1 (12%)	7,12,14	1.38	1 (14%)
4	SEP	U	363	4	8,9,10	1.60	1 (12%)	7,12,14	1.26	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SEP	U	364	4	8,9,10	1.61	1 (12%)	7,12,14	1.66	1 (14%)
4	TPO	U	359	4	8,10,11	0.70	0	10,14,16	1.08	1 (10%)
4	SEP	U	362	4	8,9,10	1.59	1 (12%)	7,12,14	0.85	0
4	TPO	G	359	4	8,10,11	0.66	0	10,14,16	1.20	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPO	V	359	4	-	3/9/11/13	-
4	SEP	G	364	4	-	1/6/8/10	-
4	SEP	G	362	4	-	0/6/8/10	-
4	TPO	G	360	4	-	2/9/11/13	-
4	SEP	G	363	4	-	2/6/8/10	-
4	TPO	V	360	4	-	1/9/11/13	-
4	SEP	V	362	4	-	0/6/8/10	-
4	SEP	V	364	4	-	2/6/8/10	-
4	TPO	U	360	4	-	0/9/11/13	-
4	SEP	V	363	4	-	3/6/8/10	-
4	SEP	U	363	4	-	2/6/8/10	-
4	SEP	U	364	4	-	1/6/8/10	-
4	TPO	U	359	4	-	3/9/11/13	-
4	SEP	U	362	4	-	3/6/8/10	-
4	TPO	G	359	4	-	6/9/11/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	364	SEP	P-O1P	3.54	1.61	1.50
4	U	364	SEP	P-O1P	3.53	1.61	1.50
4	V	363	SEP	P-O1P	3.53	1.61	1.50
4	U	362	SEP	P-O1P	3.52	1.61	1.50
4	U	363	SEP	P-O1P	3.50	1.61	1.50
4	G	362	SEP	P-O1P	3.50	1.61	1.50
4	V	362	SEP	P-O1P	3.48	1.61	1.50
4	G	363	SEP	P-O1P	3.48	1.61	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	364	SEP	OG-CB-CA	3.93	111.97	108.14
4	G	364	SEP	OG-CB-CA	3.72	111.77	108.14
4	V	363	SEP	OG-CB-CA	2.91	110.98	108.14
4	V	362	SEP	OG-CB-CA	2.64	110.72	108.14
4	V	360	TPO	O-C-CA	-2.59	118.12	124.77
4	G	362	SEP	OG-CB-CA	2.53	110.61	108.14
4	G	363	SEP	OG-CB-CA	2.53	110.61	108.14
4	G	360	TPO	O-C-CA	-2.51	118.31	124.77
4	U	360	TPO	O-C-CA	-2.51	118.32	124.77
4	G	359	TPO	O-C-CA	-2.47	118.42	124.77
4	U	359	TPO	O-C-CA	-2.42	118.55	124.77
4	V	359	TPO	O-C-CA	-2.40	118.59	124.77
4	U	363	SEP	OG-CB-CA	2.36	110.44	108.14
4	V	360	TPO	P-OG1-CB	-2.01	117.87	123.33
4	G	359	TPO	P-OG1-CB	-2.00	117.88	123.33

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	359	TPO	N-CA-CB-OG1
4	G	360	TPO	C-CA-CB-CG2
4	G	363	SEP	N-CA-CB-OG
4	U	359	TPO	N-CA-CB-CG2
4	U	359	TPO	N-CA-CB-OG1
4	U	359	TPO	C-CA-CB-CG2
4	U	362	SEP	CB-OG-P-O2P
4	U	362	SEP	CB-OG-P-O3P
4	U	363	SEP	N-CA-CB-OG
4	U	363	SEP	CA-CB-OG-P
4	U	364	SEP	N-CA-CB-OG
4	V	359	TPO	N-CA-CB-CG2
4	V	359	TPO	N-CA-CB-OG1
4	V	359	TPO	C-CA-CB-CG2
4	V	363	SEP	N-CA-CB-OG
4	V	363	SEP	CA-CB-OG-P
4	V	364	SEP	N-CA-CB-OG
4	V	364	SEP	C-CA-CB-OG
4	G	364	SEP	N-CA-CB-OG
4	G	359	TPO	CB-OG1-P-O1P
4	U	362	SEP	CB-OG-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	V	363	SEP	CB-OG-P-O3P
4	G	363	SEP	CA-CB-OG-P
4	G	359	TPO	CB-OG1-P-O2P
4	G	359	TPO	CB-OG1-P-O3P
4	G	359	TPO	C-CA-CB-CG2
4	G	359	TPO	O-C-CA-CB
4	V	360	TPO	O-C-CA-CB
4	G	360	TPO	N-CA-CB-CG2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	364	SEP	2	0
4	G	360	TPO	3	0
4	V	360	TPO	2	0
4	V	364	SEP	2	0
4	U	360	TPO	2	0
4	V	363	SEP	3	0
4	U	363	SEP	1	0
4	U	359	TPO	1	0
4	G	359	TPO	1	0

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.

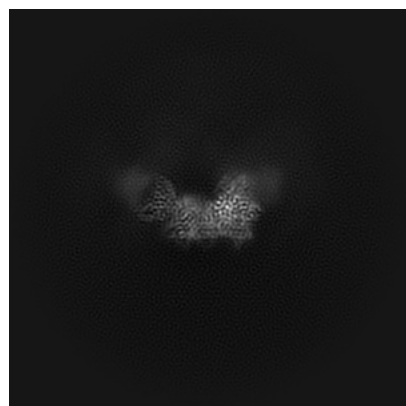
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35115. These allow visual inspection of the internal detail of the map and identification of artifacts.

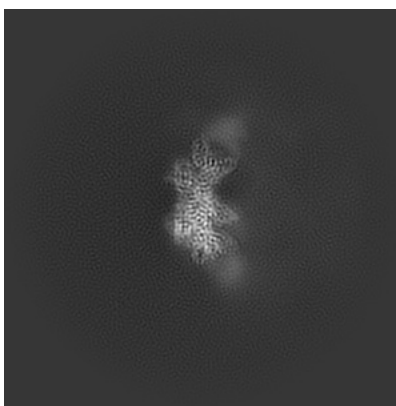
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

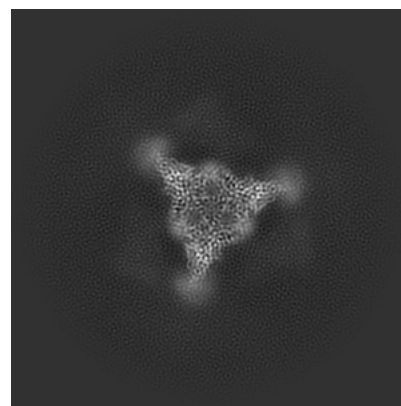
6.1.1 Primary map



X

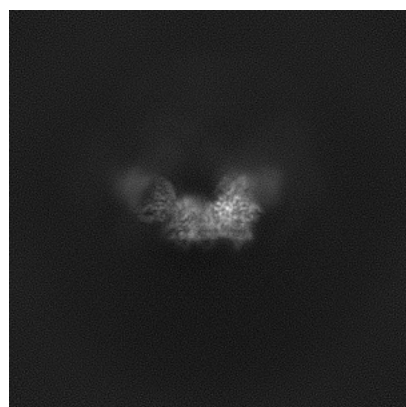


Y

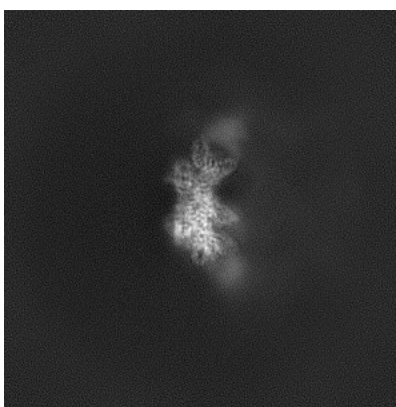


Z

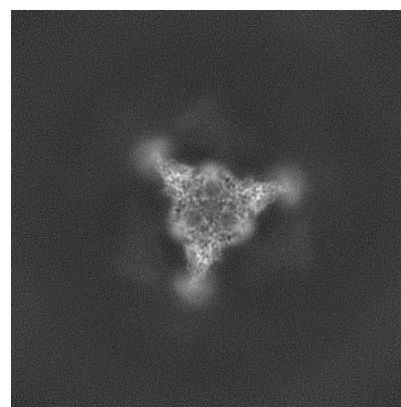
6.1.2 Raw map



X



Y



Z

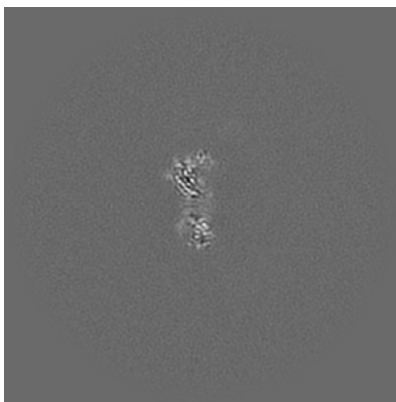
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

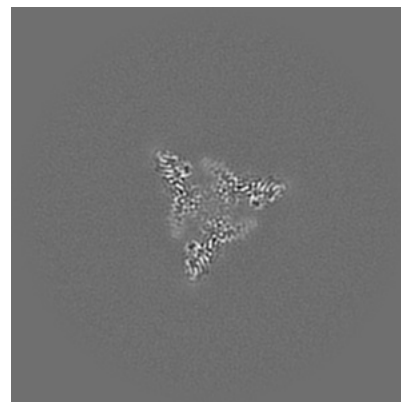
6.2.1 Primary map



X Index: 180



Y Index: 180

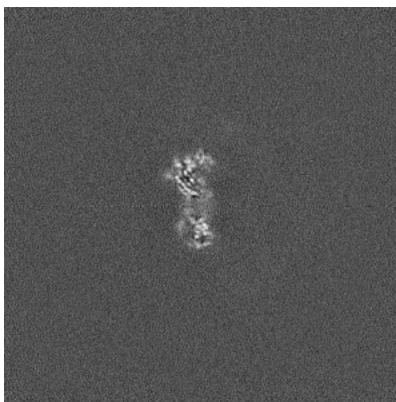


Z Index: 180

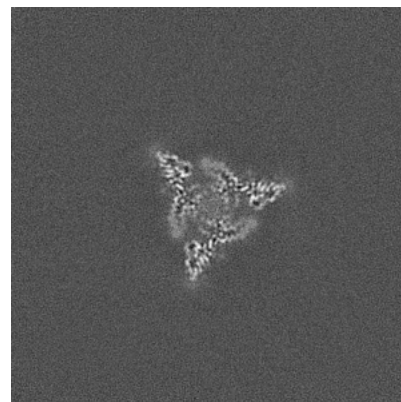
6.2.2 Raw map



X Index: 180



Y Index: 180

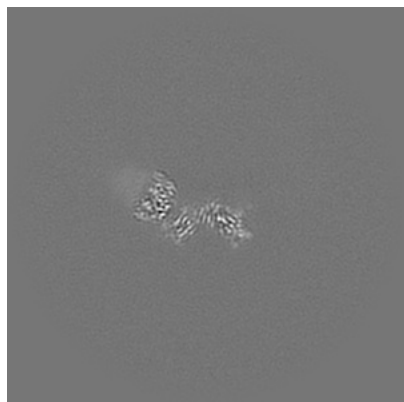


Z Index: 180

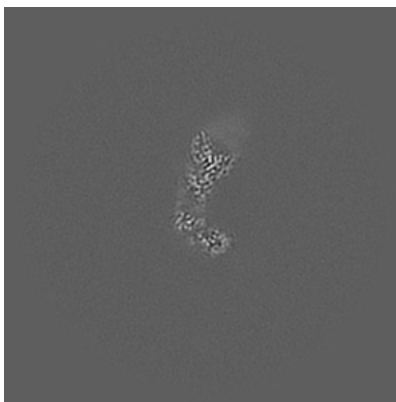
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

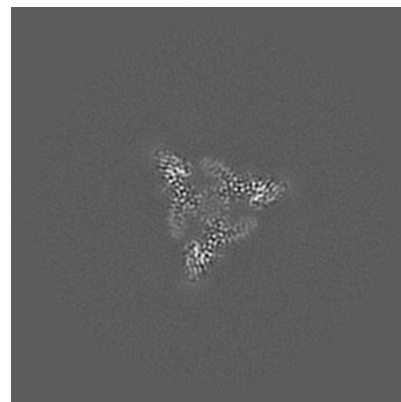
6.3.1 Primary map



X Index: 169

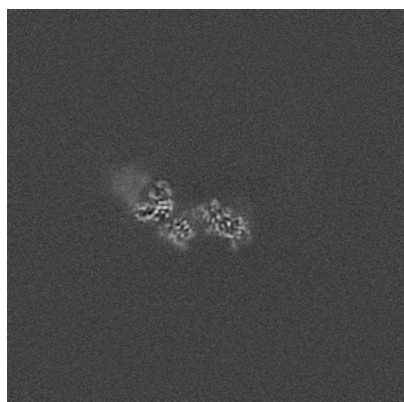


Y Index: 199

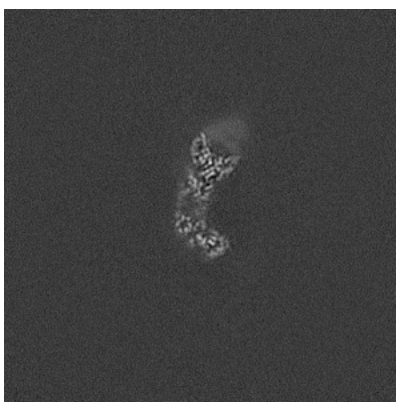


Z Index: 181

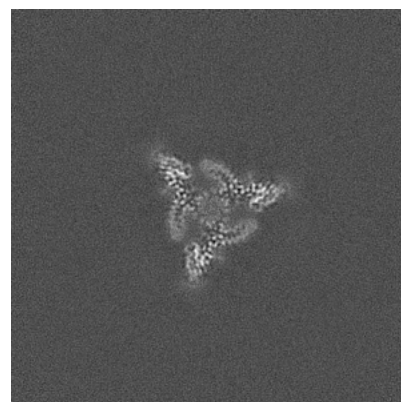
6.3.2 Raw map



X Index: 166



Y Index: 198

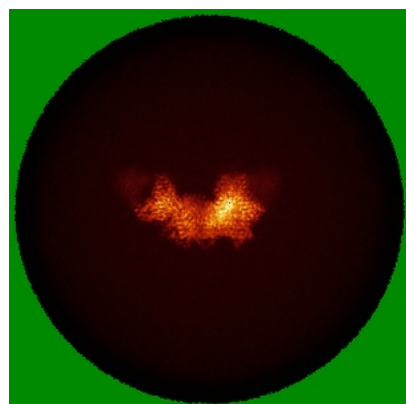


Z Index: 181

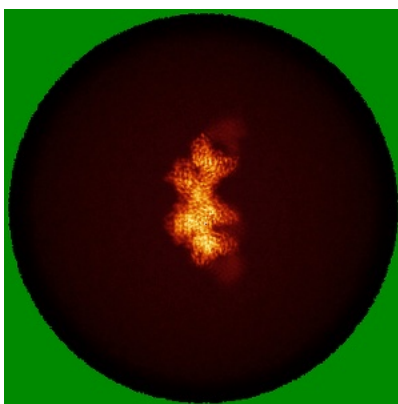
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

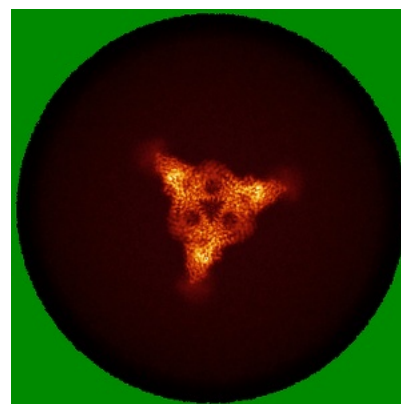
6.4.1 Primary map



X

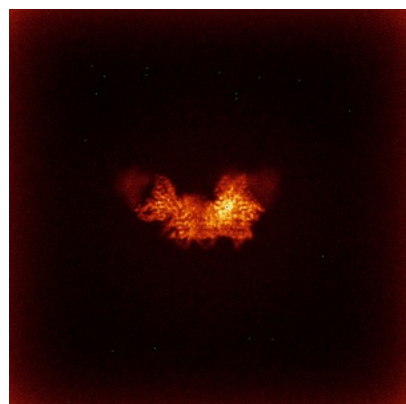


Y

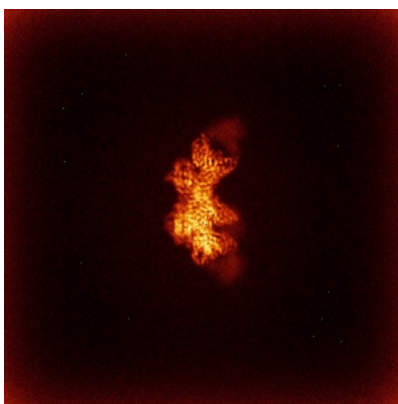


Z

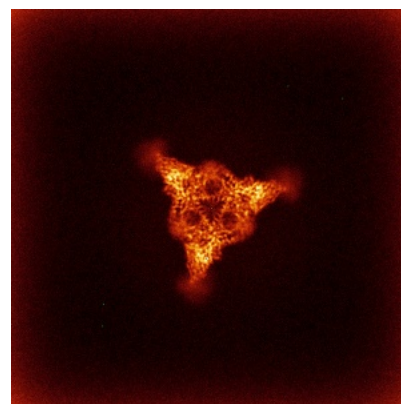
6.4.2 Raw map



X



Y

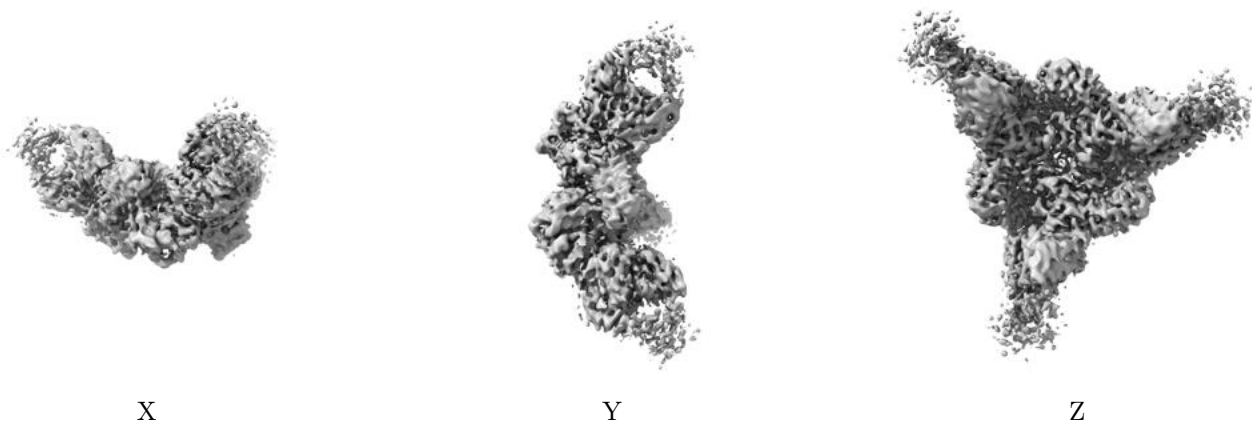


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

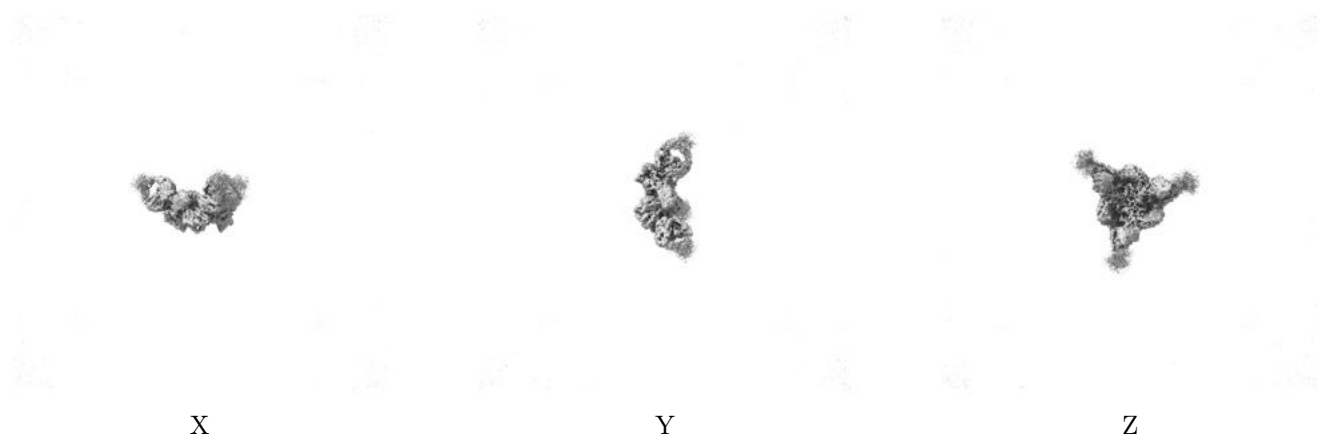
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

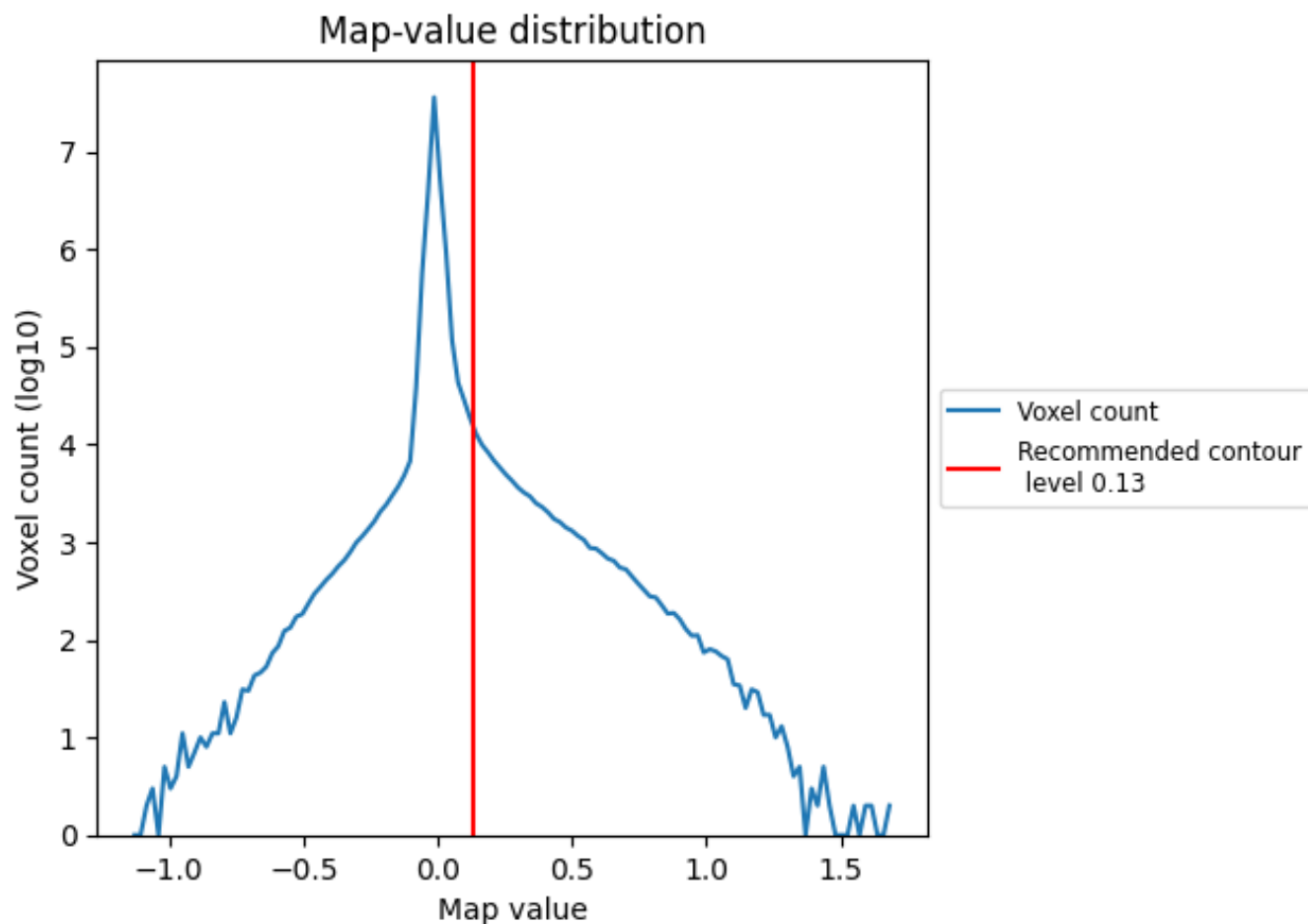
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

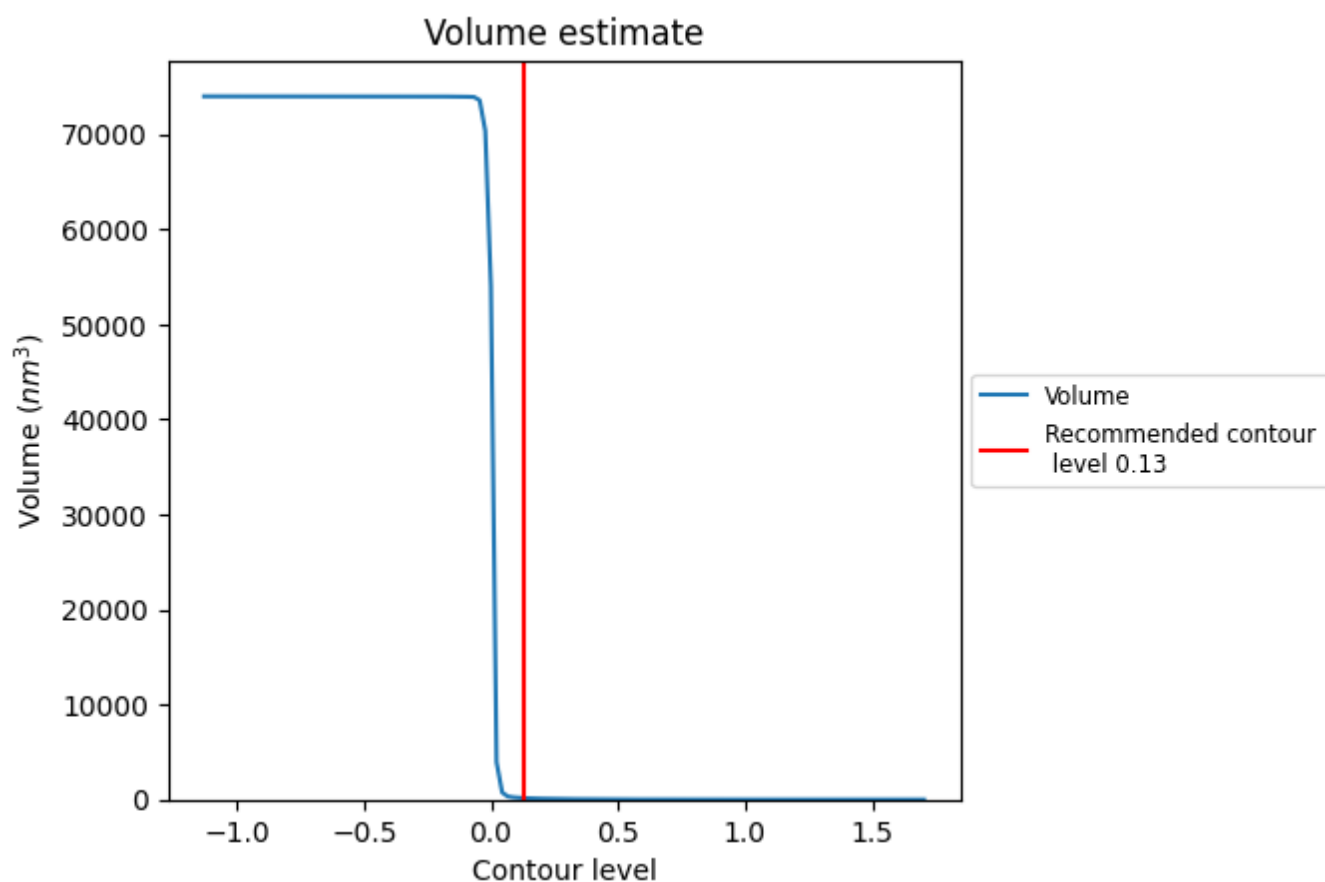
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

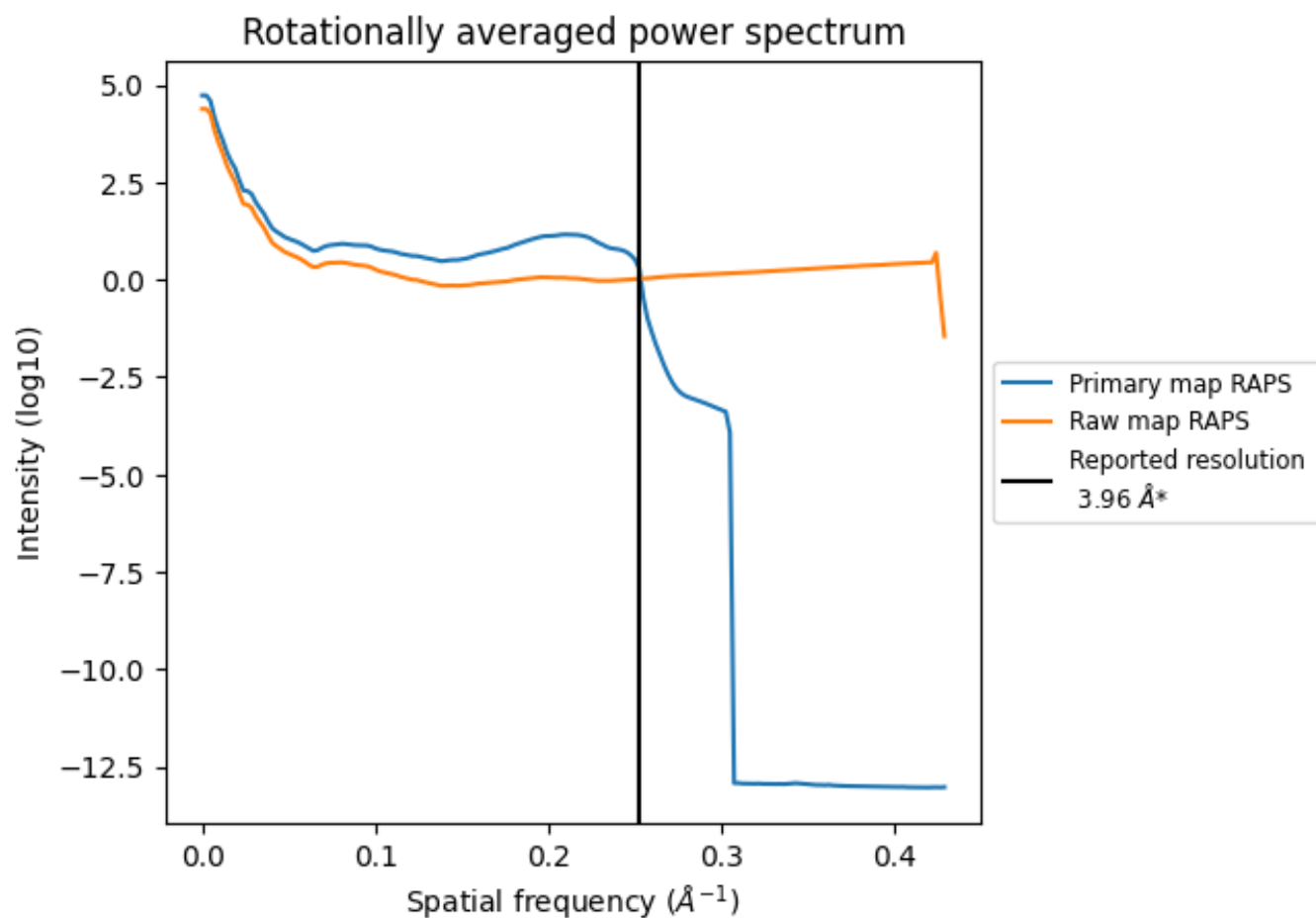
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 ⓘ

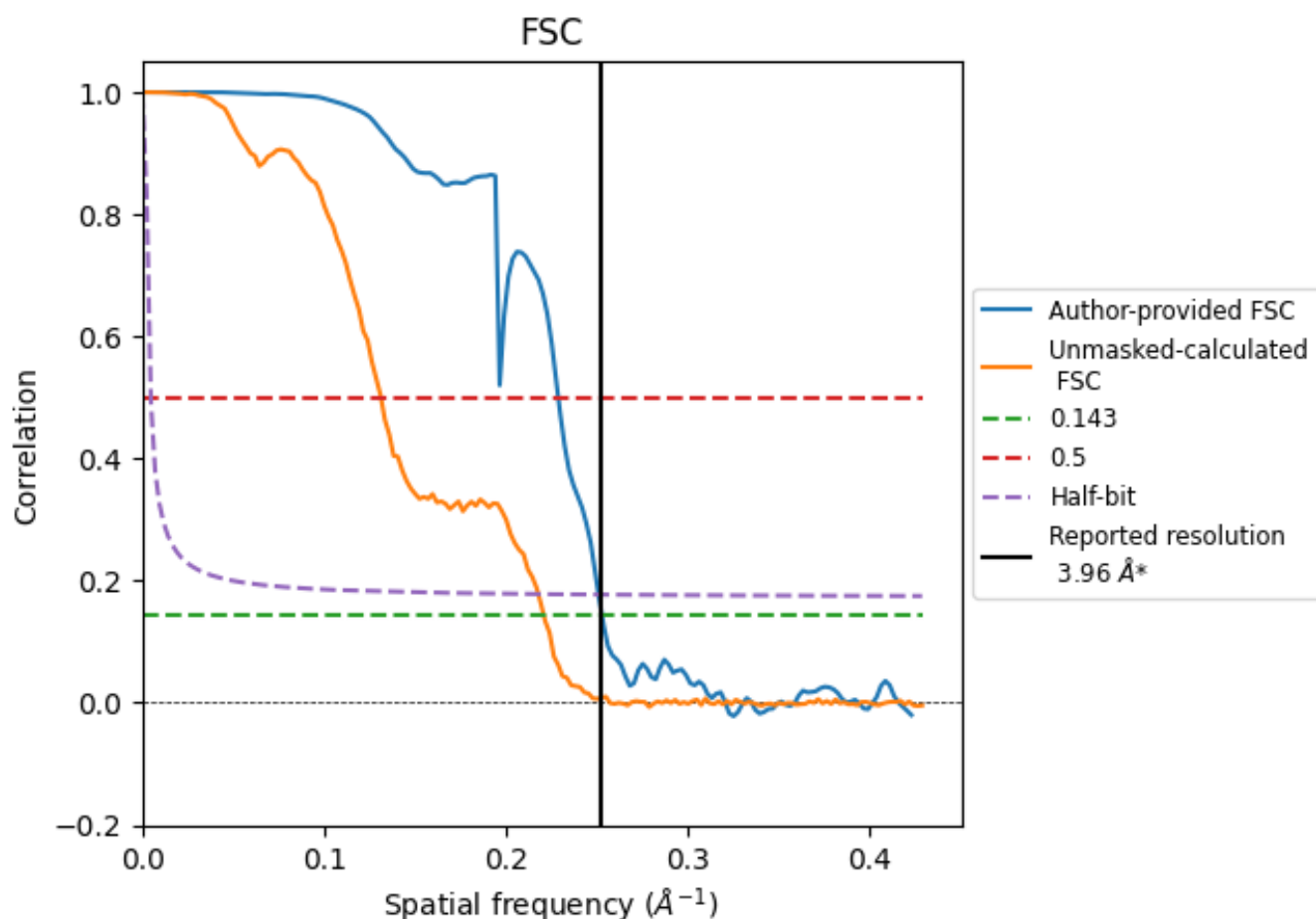


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 $0.253 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	3.96	4.37	3.99
Unmasked-calculated*	4.53	7.62	4.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.53 differs from the reported value 3.96 by more than 10 %

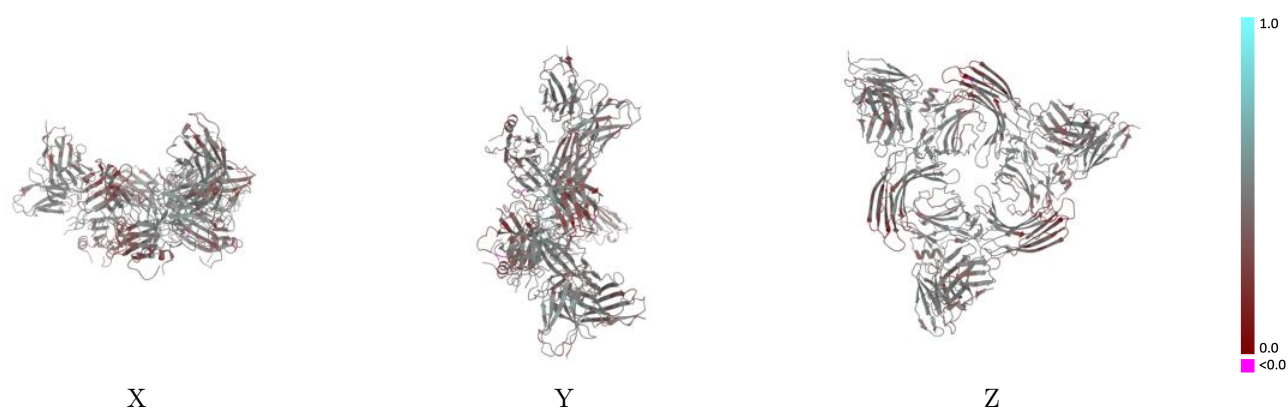
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35115 and PDB model 8I10. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

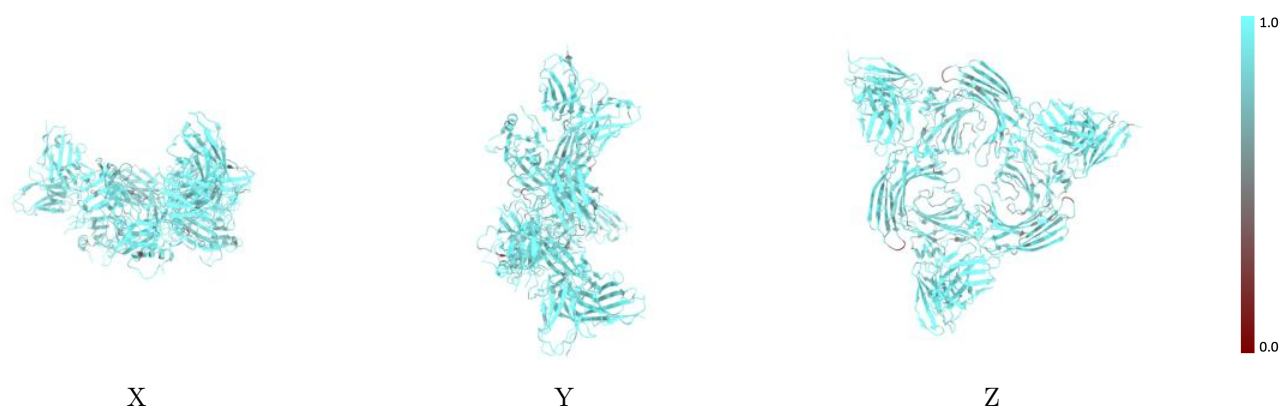
This section was not generated.

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



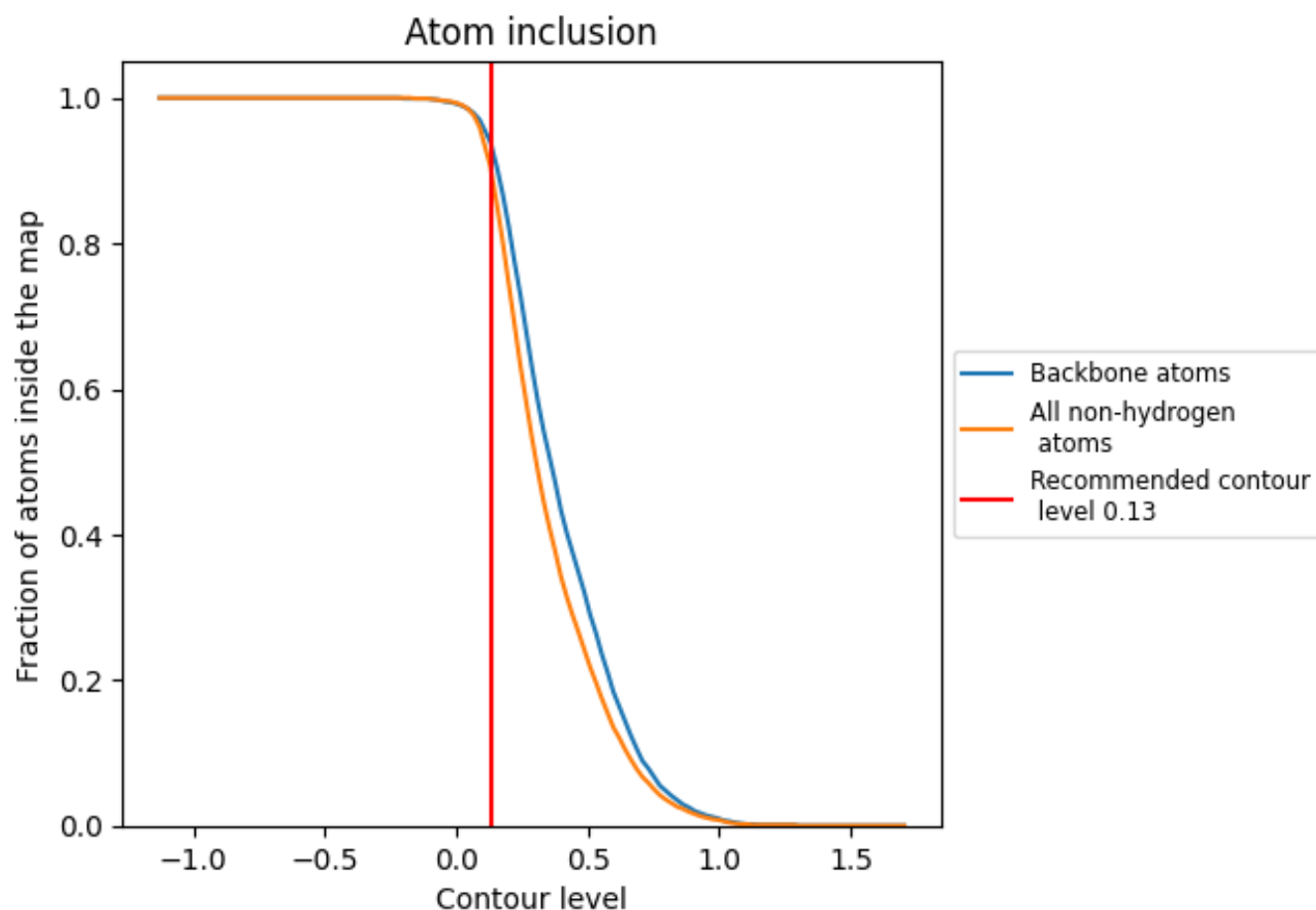
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9050	0.4340
A	0.8860	0.4200
B	0.8800	0.4150
C	0.8880	0.4230
D	0.9360	0.4490
E	0.9400	0.4600
G	0.9620	0.4680
H	0.9370	0.4470
L	0.9250	0.4570
M	0.9340	0.4530
N	0.9220	0.4560
U	0.9750	0.4740
V	0.9620	0.4820

