



Full wwPDB EM Validation Report ⓘ

Aug 19, 2024 – 12:27 PM JST

PDB ID : 8XI5
EMDB ID : EMD-38371
Title : Structure of Eastern Equine Encephalitis VLP in complex with the receptor
VLDLR LA3-5
Authors : Cao, D.; Ma, B.; Cao, Z.; Xu, X.; Zhang, X.; Xiang, Y.
Deposited on : 2023-12-19
Resolution : 3.40 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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

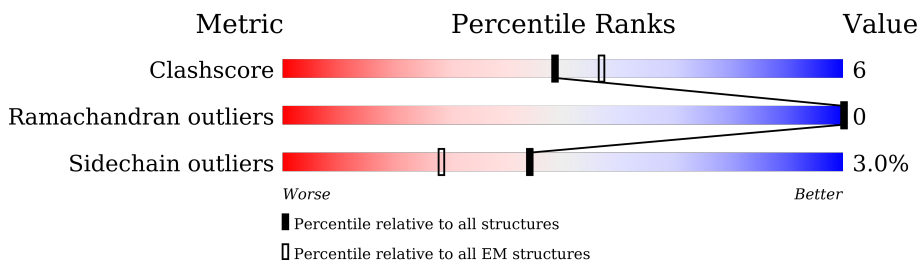
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



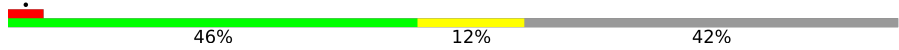
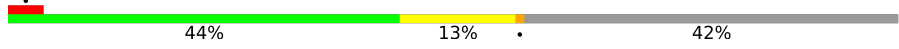
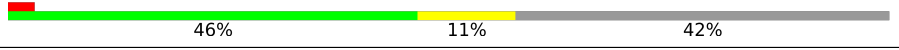
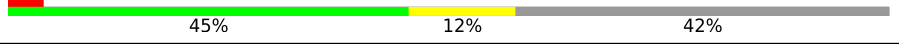

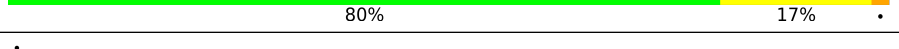
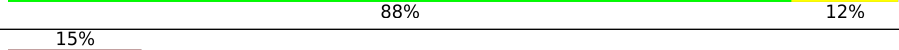
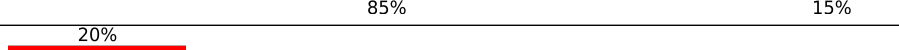
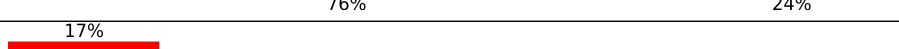

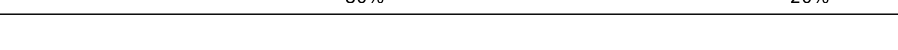
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	441	
1	D	441	
1	G	441	
1	J	441	
2	B	420	
2	E	420	
2	H	420	
2	K	420	

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Mol	Chain	Length	Quality of chain
3	C	261	 46% 12% 42%
3	F	261	 44% 13% 42%
3	I	261	 46% 11% 42%
3	L	261	 45% 12% 42%
4	M	41	 85% 12%
4	N	41	 93% 5%
4	O	41	 80% 17%
4	P	41	 88% 12%
5	Q	41	 15% 85% 15%
5	R	41	 20% 76% 24%
5	S	41	 17% 76% 24%
5	T	41	 22% 80% 20%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 33820 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 Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	441	3375	2155	560	640	20	0	0
1	D	441	3375	2155	560	640	20	0	0
1	G	441	3375	2155	560	640	20	0	0
1	J	441	3375	2155	560	640	20	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	SER	THR	conflict	UNP Q4QXJ7
A	237	VAL	ALA	conflict	UNP Q4QXJ7
A	246	LYS	ARG	conflict	UNP Q4QXJ7
A	311	PHE	SER	conflict	UNP Q4QXJ7
A	411	ILE	LEU	conflict	UNP Q4QXJ7
D	82	SER	THR	conflict	UNP Q4QXJ7
D	237	VAL	ALA	conflict	UNP Q4QXJ7
D	246	LYS	ARG	conflict	UNP Q4QXJ7
D	311	PHE	SER	conflict	UNP Q4QXJ7
D	411	ILE	LEU	conflict	UNP Q4QXJ7
G	82	SER	THR	conflict	UNP Q4QXJ7
G	237	VAL	ALA	conflict	UNP Q4QXJ7
G	246	LYS	ARG	conflict	UNP Q4QXJ7
G	311	PHE	SER	conflict	UNP Q4QXJ7
G	411	ILE	LEU	conflict	UNP Q4QXJ7
J	82	SER	THR	conflict	UNP Q4QXJ7
J	237	VAL	ALA	conflict	UNP Q4QXJ7
J	246	LYS	ARG	conflict	UNP Q4QXJ7
J	311	PHE	SER	conflict	UNP Q4QXJ7
J	411	ILE	LEU	conflict	UNP Q4QXJ7

- Molecule 2 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	420	3300	2088	599	589	24	0	0
2	E	420	3300	2088	599	589	24	0	0
2	H	420	3300	2088	599	589	24	0	0
2	K	420	3300	2088	599	589	24	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	LYS	GLU	conflict	UNP Q4QXJ7
E	206	LYS	GLU	conflict	UNP Q4QXJ7
H	206	LYS	GLU	conflict	UNP Q4QXJ7
K	206	LYS	GLU	conflict	UNP Q4QXJ7

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	151	1165	734	207	220	4	0	0
3	F	151	1165	734	207	220	4	0	0
3	I	151	1165	734	207	220	4	0	0
3	L	151	1165	734	207	220	4	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	50	SER	ASN	conflict	UNP Q4QXJ7
C	67	ASN	LYS	engineered mutation	UNP Q4QXJ7
F	50	SER	ASN	conflict	UNP Q4QXJ7
F	67	ASN	LYS	engineered mutation	UNP Q4QXJ7
I	50	SER	ASN	conflict	UNP Q4QXJ7
I	67	ASN	LYS	engineered mutation	UNP Q4QXJ7
L	50	SER	ASN	conflict	UNP Q4QXJ7
L	67	ASN	LYS	engineered mutation	UNP Q4QXJ7

- Molecule 4 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	41	Total	C	N	O	S	0	0
			303	176	50	71	6		
4	N	41	Total	C	N	O	S	0	0
			303	176	50	71	6		
4	O	41	Total	C	N	O	S	0	0
			303	176	50	71	6		
4	P	41	Total	C	N	O	S	0	0
			303	176	50	71	6		

- Molecule 5 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	41	Total	C	N	O	S	0	0
			310	176	59	69	6		
5	R	41	Total	C	N	O	S	0	0
			310	176	59	69	6		
5	S	41	Total	C	N	O	S	0	0
			310	176	59	69	6		
5	T	41	Total	C	N	O	S	0	0
			310	176	59	69	6		

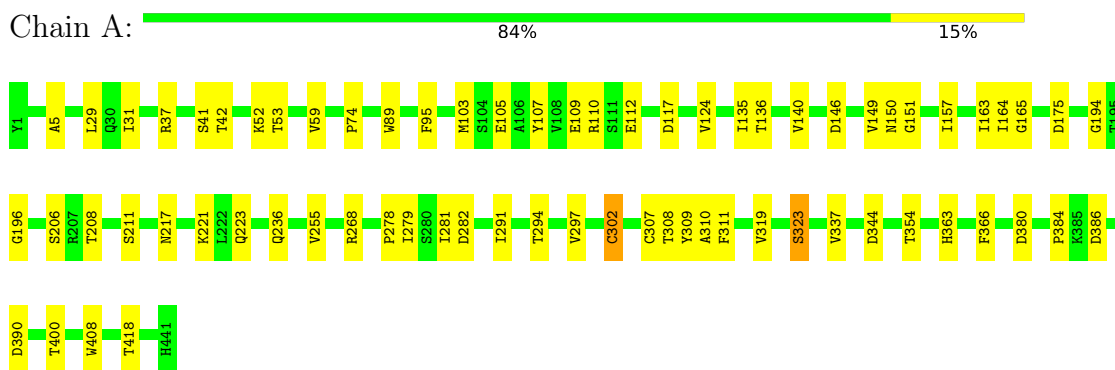
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	M	1	Total	Ca	0
			1	1	
6	N	1	Total	Ca	0
			1	1	
6	O	1	Total	Ca	0
			1	1	
6	P	1	Total	Ca	0
			1	1	
6	Q	1	Total	Ca	0
			1	1	
6	R	1	Total	Ca	0
			1	1	
6	S	1	Total	Ca	0
			1	1	
6	T	1	Total	Ca	0
			1	1	

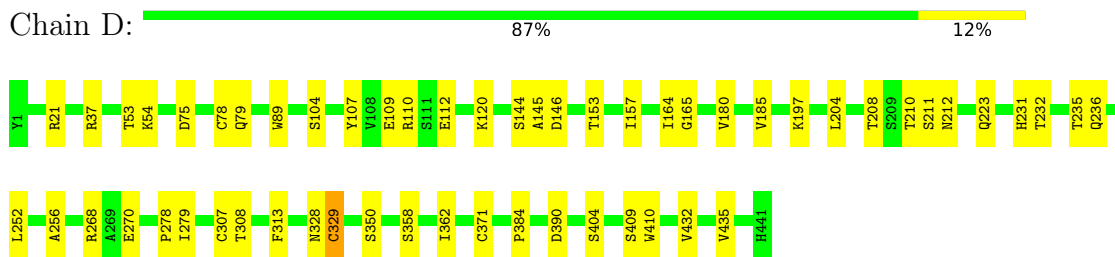
3 Residue-property plots

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.

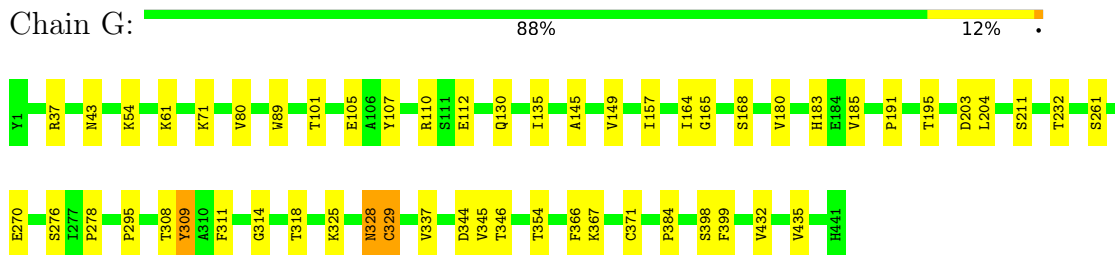
- Molecule 1: Spike glycoprotein E1



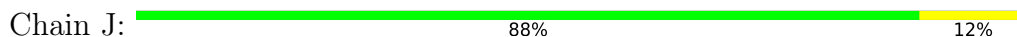
- Molecule 1: Spike glycoprotein E1

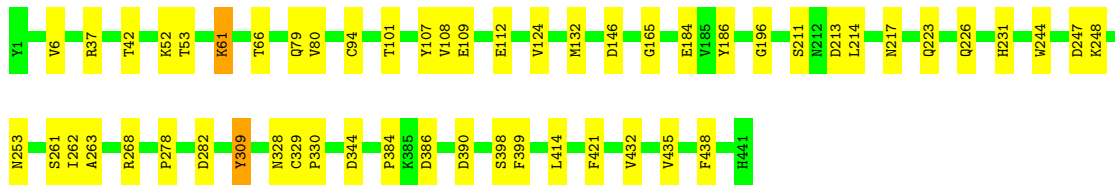


- Molecule 1: Spike glycoprotein E1

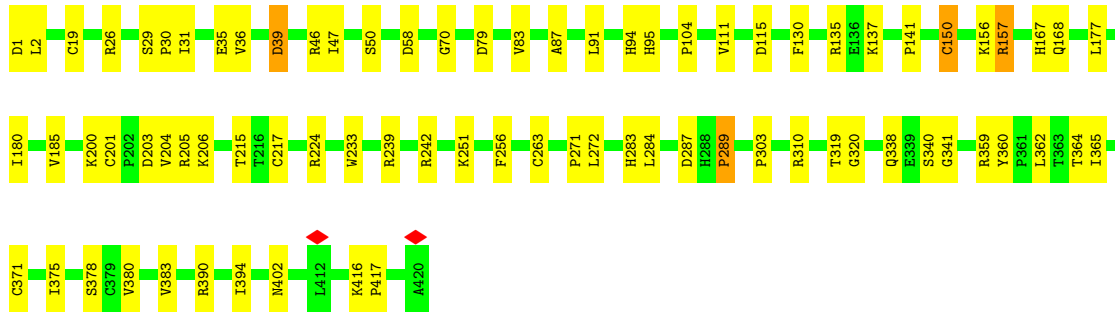
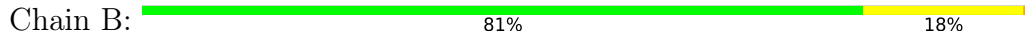


- Molecule 1: Spike glycoprotein E1

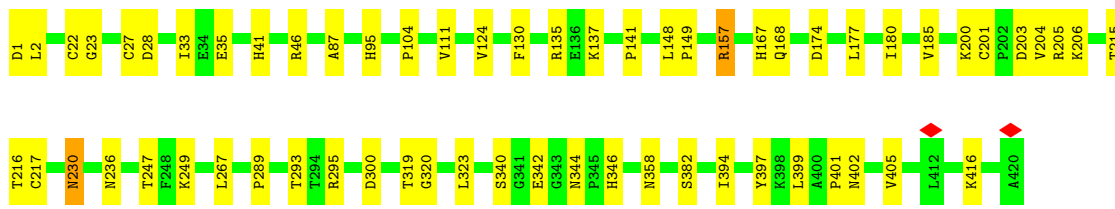
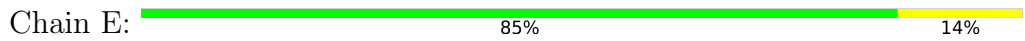




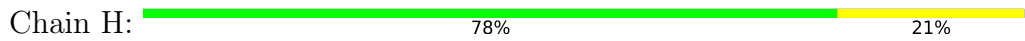
• Molecule 2: Spike glycoprotein E2



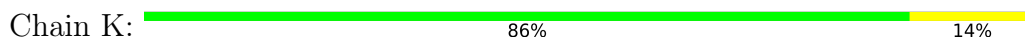
• Molecule 2: Spike glycoprotein E2

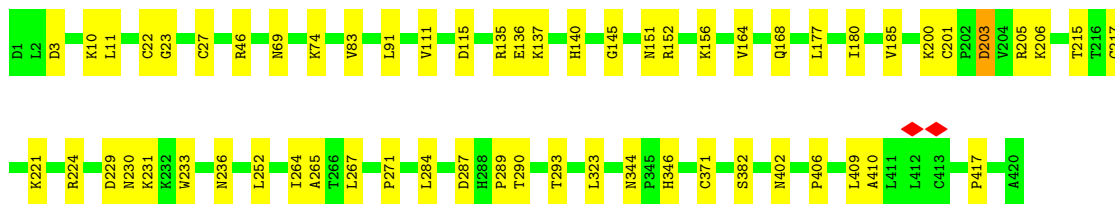


• Molecule 2: Spike glycoprotein E2

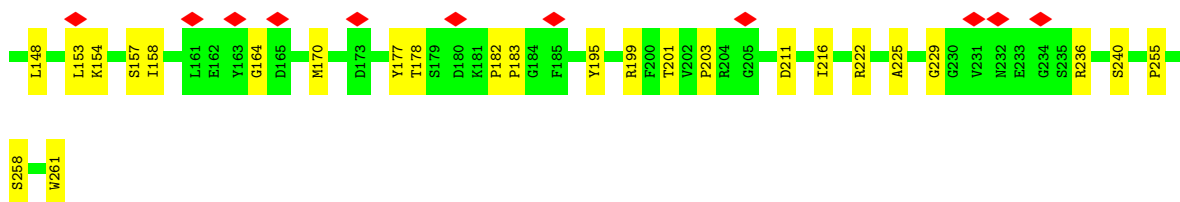
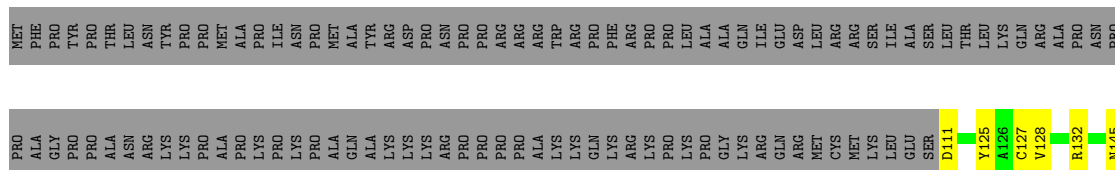


• Molecule 2: Spike glycoprotein E2

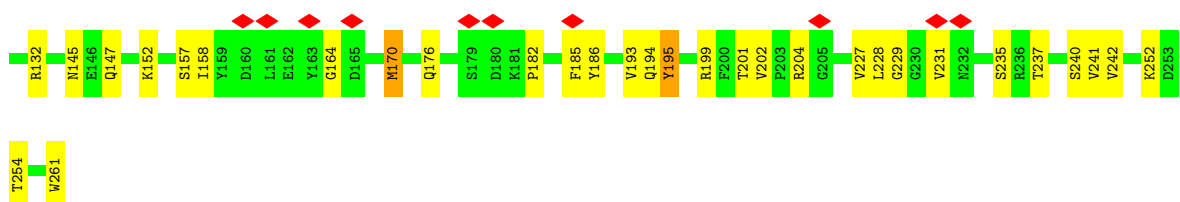
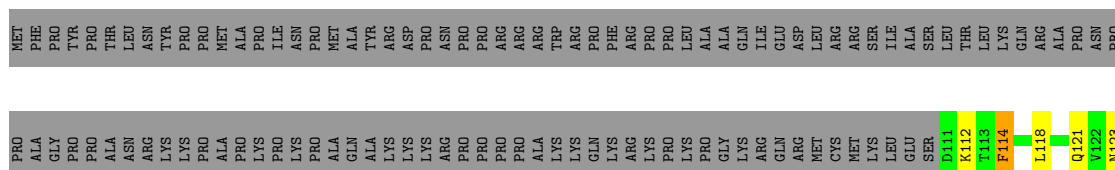




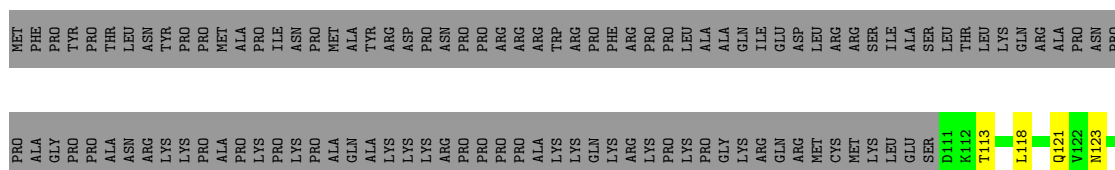
• Molecule 3: Capsid protein



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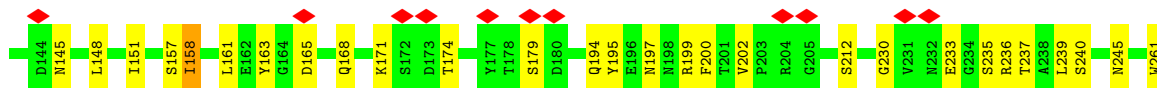
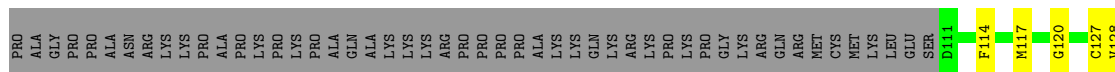


• Molecule 3: Capsid protein

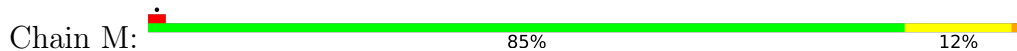




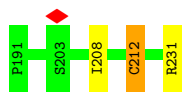
• Molecule 3: Capsid protein



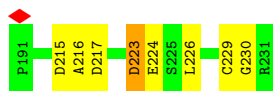
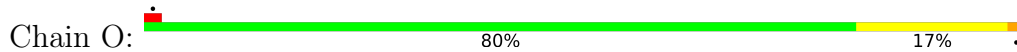
• Molecule 4: Very low-density lipoprotein receptor



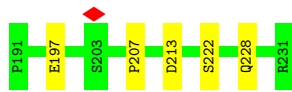
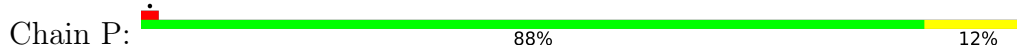
• Molecule 4: Very low-density lipoprotein receptor



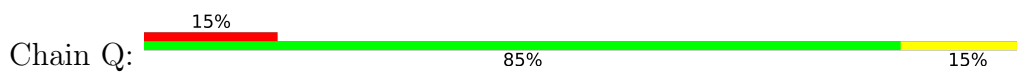
• Molecule 4: Very low-density lipoprotein receptor

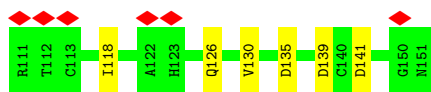


• Molecule 4: Very low-density lipoprotein receptor

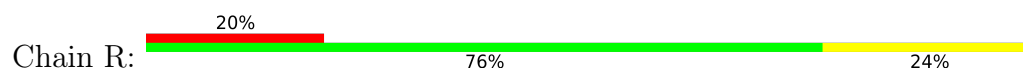


• Molecule 5: Very low-density lipoprotein receptor

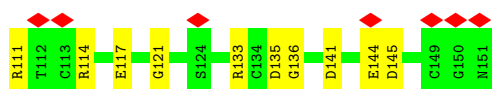
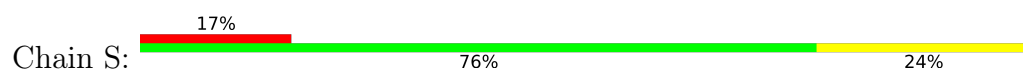




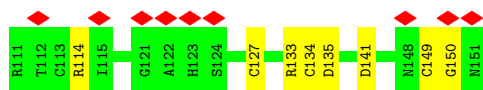
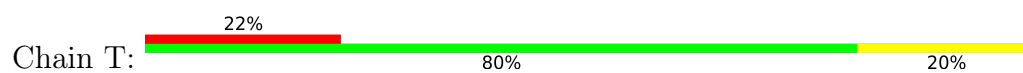
- Molecule 5: Very low-density lipoprotein receptor



- Molecule 5: Very low-density lipoprotein receptor



- Molecule 5: Very low-density lipoprotein receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.008	Depositor
Map size (\AA)	292.6, 292.6, 292.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.33, 1.33, 1.33	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:
CA

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	0.32	0/3469	0.55	0/4734
1	D	0.31	0/3469	0.54	0/4734
1	G	0.30	0/3469	0.53	0/4734
1	J	0.32	0/3469	0.58	2/4734 (0.0%)
2	B	0.30	0/3395	0.58	2/4630 (0.0%)
2	E	0.28	0/3395	0.56	1/4630 (0.0%)
2	H	0.28	0/3395	0.57	1/4630 (0.0%)
2	K	0.29	0/3395	0.57	1/4630 (0.0%)
3	C	0.27	0/1192	0.58	0/1615
3	F	0.27	0/1192	0.58	1/1615 (0.1%)
3	I	0.28	0/1192	0.54	0/1615
3	L	0.29	0/1192	0.64	2/1615 (0.1%)
4	M	0.24	0/308	0.48	0/417
4	N	0.25	0/308	0.48	0/417
4	O	0.26	0/308	0.52	0/417
4	P	0.25	0/308	0.57	0/417
5	Q	0.24	0/314	0.53	0/423
5	R	0.25	0/314	0.57	0/423
5	S	0.26	0/314	0.56	0/423
5	T	0.25	0/314	0.58	0/423
All	All	0.29	0/34712	0.56	10/47276 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	61	LYS	N-CA-C	-6.89	92.38	111.00
2	B	58	ASP	CB-CG-OD2	5.74	123.47	118.30
2	K	177	LEU	CA-CB-CG	5.72	128.46	115.30
2	B	177	LEU	CA-CB-CG	5.72	128.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	177	LEU	CA-CB-CG	5.71	128.43	115.30
2	E	177	LEU	CA-CB-CG	5.71	128.42	115.30
3	L	161	LEU	CA-CB-CG	5.61	128.20	115.30
1	J	414	LEU	CA-CB-CG	5.11	127.05	115.30
3	L	158	ILE	CG1-CB-CG2	-5.11	100.16	111.40
3	F	170	MET	CB-CG-SD	5.01	127.44	112.40

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	3375	0	3281	45	0
1	D	3375	0	3281	29	0
1	G	3375	0	3281	41	0
1	J	3375	0	3281	30	0
2	B	3300	0	3268	49	0
2	E	3300	0	3268	38	0
2	H	3300	0	3268	66	0
2	K	3300	0	3268	35	0
3	C	1165	0	1146	17	0
3	F	1165	0	1146	21	0
3	I	1165	0	1146	16	0
3	L	1165	0	1146	15	0
4	M	303	0	250	4	0
4	N	303	0	250	2	0
4	O	303	0	250	10	0
4	P	303	0	250	3	0
5	Q	310	0	258	6	0
5	R	310	0	260	15	0
5	S	310	0	258	13	0
5	T	310	0	258	6	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
All	All	33820	0	32814	415	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (415) 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:A:95:PHE:HB2	2:B:224:ARG:HG3	1.46	0.95
2:H:156:LYS:HE3	4:O:217:ASP:OD2	1.65	0.95
1:J:66:THR:HG22	1:J:101:THR:HG21	1.49	0.93
2:E:1:ASP:OD2	2:E:2:LEU:N	2.01	0.93
1:A:31:ILE:HG23	1:A:135:ILE:CD1	2.02	0.90
1:J:184:GLU:OE1	1:J:184:GLU:N	2.08	0.85
1:G:61:LYS:CE	5:S:136:GLY:O	2.26	0.84
2:H:199:CYS:HB2	2:H:205:ARG:HB3	1.59	0.84
1:G:308:THR:HG22	1:G:314:GLY:O	1.78	0.84
2:H:142:PRO:HG3	2:H:266:THR:HG22	1.59	0.83
1:A:31:ILE:HG23	1:A:135:ILE:HD11	1.58	0.83
2:H:206:LYS:NZ	5:S:135:ASP:OD2	2.12	0.82
2:K:156:LYS:NZ	4:P:213:ASP:OD2	2.11	0.82
3:C:255:PRO:HG2	3:C:258:SER:HB3	1.62	0.81
5:R:133:ARG:O	5:R:134:CYS:SG	2.39	0.81
2:B:1:ASP:OD2	2:B:2:LEU:N	2.13	0.80
2:H:197:TYR:CZ	2:H:207:GLY:HA3	2.19	0.77
1:G:61:LYS:NZ	5:S:136:GLY:HA3	2.00	0.77
2:E:203:ASP:OD2	5:Q:126:GLN:NE2	2.19	0.75
1:J:66:THR:HG22	1:J:101:THR:CG2	2.16	0.74
2:H:273:VAL:HG22	2:H:282:LEU:HD23	1.68	0.74
2:E:203:ASP:OD1	2:E:204:VAL:N	2.21	0.72
1:G:61:LYS:HZ3	5:S:136:GLY:HA3	1.55	0.72
2:B:203:ASP:OD1	2:B:204:VAL:N	2.21	0.70
1:G:308:THR:CG2	1:G:314:GLY:HA3	2.22	0.70
2:B:156:LYS:HE2	4:M:217:ASP:OD2	1.92	0.70
2:H:197:TYR:CE2	2:H:207:GLY:HA3	2.27	0.69
2:H:54:GLY:C	2:H:55:LEU:HD12	2.14	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:134:CYS:CB	5:R:149:CYS:SG	2.81	0.69
2:H:203:ASP:OD1	2:H:204:VAL:N	2.24	0.68
1:G:61:LYS:HE3	5:S:136:GLY:O	1.93	0.67
2:H:197:TYR:CE2	2:H:207:GLY:CA	2.78	0.67
2:K:206:LYS:NZ	5:T:135:ASP:OD2	2.28	0.67
1:G:37:ARG:HH21	1:G:130:GLN:HE21	1.42	0.67
2:E:206:LYS:NZ	5:Q:135:ASP:OD2	2.27	0.66
2:H:108:THR:HG22	2:H:125:ALA:HA	1.77	0.66
1:G:308:THR:HG22	1:G:314:GLY:HA3	1.77	0.65
4:O:226:LEU:N	4:O:226:LEU:HD23	2.12	0.64
1:A:59:VAL:HG22	1:A:103:MET:HB2	1.78	0.64
4:O:226:LEU:HD23	4:O:226:LEU:H	1.61	0.64
5:R:111:ARG:N	5:R:119:SER:HG	1.96	0.64
2:H:197:TYR:CZ	2:H:207:GLY:CA	2.81	0.63
2:H:108:THR:HB	2:H:124:VAL:O	1.98	0.63
2:H:390:ARG:HH22	2:H:416:LYS:HE2	1.64	0.62
4:O:223:ASP:OD1	4:O:223:ASP:N	2.32	0.62
2:H:108:THR:HG21	2:K:140:HIS:CG	2.35	0.62
1:J:244:TRP:HA	1:J:247:ASP:OD2	1.99	0.61
2:H:54:GLY:O	2:H:55:LEU:HD12	2.00	0.61
2:E:267:LEU:HD23	1:J:223:GLN:HE22	1.65	0.61
2:H:273:VAL:HG22	2:H:282:LEU:CD2	2.30	0.60
2:H:198:TYR:CD2	2:H:206:LYS:HB3	2.37	0.60
1:A:149:VAL:O	1:A:149:VAL:HG12	2.01	0.60
2:H:60:VAL:HG12	2:H:60:VAL:O	2.01	0.60
3:L:151:ILE:HG23	3:L:165:ASP:HB2	1.83	0.60
2:H:54:GLY:HA2	2:H:61:ASP:O	2.02	0.59
1:G:295:PRO:HB3	1:G:325:LYS:HG3	1.84	0.59
4:O:226:LEU:H	4:O:226:LEU:CD2	2.15	0.59
5:R:134:CYS:HB3	5:R:149:CYS:CB	2.33	0.59
2:H:136:GLU:HG2	2:H:290:THR:HG23	1.85	0.59
2:E:1:ASP:CG	2:E:2:LEU:H	2.02	0.59
1:G:112:GLU:OE2	2:H:46:ARG:NH2	2.35	0.59
1:J:112:GLU:OE2	2:K:46:ARG:NH2	2.36	0.59
2:E:401:PRO:HD2	3:F:176:GLN:HE22	1.67	0.58
2:H:197:TYR:CE2	2:H:207:GLY:N	2.71	0.58
1:G:309:TYR:HB3	1:G:384:PRO:HD3	1.85	0.58
1:D:180:VAL:HG22	1:D:185:VAL:HG12	1.86	0.58
3:I:182:PRO:O	3:I:186:TYR:OH	2.21	0.58
2:H:79:ASP:OD1	2:H:79:ASP:N	2.37	0.58
3:L:157:SER:OG	3:L:158:ILE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:231:VAL:HG22	3:F:261:TRP:HB2	1.87	0.57
1:D:307:CYS:SG	1:D:308:THR:N	2.78	0.57
2:H:108:THR:HA	2:H:126:HIS:H	1.68	0.57
5:T:149:CYS:SG	5:T:150:GLY:N	2.78	0.57
1:G:165:GLY:HA3	1:G:278:PRO:HG2	1.86	0.57
1:A:89:TRP:CZ3	2:B:70:GLY:HA2	2.40	0.57
2:H:205:ARG:O	2:H:205:ARG:HG3	2.05	0.57
2:K:406:PRO:HG2	2:K:409:LEU:HB2	1.86	0.57
2:K:83:VAL:HG22	2:K:111:VAL:HG12	1.85	0.57
2:K:229:ASP:OD2	2:K:231:LYS:HG2	2.04	0.56
1:A:221:LYS:NZ	1:A:223:GLN:OE1	2.38	0.56
1:D:268:ARG:NH1	1:D:270:GLU:OE2	2.38	0.56
2:H:287:ASP:OD1	2:H:287:ASP:N	2.38	0.56
3:I:157:SER:OG	3:I:158:ILE:N	2.38	0.56
2:K:287:ASP:OD1	2:K:287:ASP:N	2.37	0.56
4:O:226:LEU:O	4:O:230:GLY:HA2	2.06	0.56
1:G:89:TRP:CZ3	2:H:70:GLY:HA2	2.40	0.56
3:I:137:LEU:H	3:I:160:ASP:HB3	1.70	0.56
2:K:22:CYS:SG	2:K:23:GLY:N	2.79	0.56
4:M:213:ASP:OD1	4:M:213:ASP:N	2.39	0.56
1:D:362:ILE:HG21	1:D:404:SER:HA	1.86	0.55
1:J:309:TYR:HB3	1:J:384:PRO:HD3	1.88	0.55
1:J:398:SER:OG	1:J:399:PHE:N	2.38	0.55
1:A:95:PHE:HB2	2:B:224:ARG:CG	2.29	0.55
1:A:149:VAL:HG22	1:A:164:ILE:HG21	1.89	0.54
2:K:205:ARG:NH2	2:K:217:CYS:SG	2.80	0.54
5:R:134:CYS:HB3	5:R:149:CYS:SG	2.47	0.54
3:C:132:ARG:HA	3:C:164:GLY:HA3	1.90	0.54
3:L:168:GLN:HA	3:L:171:LYS:HG3	1.89	0.54
5:R:134:CYS:HB3	5:R:149:CYS:HB3	1.89	0.54
2:B:205:ARG:NH2	2:B:217:CYS:SG	2.80	0.54
2:E:22:CYS:SG	2:E:27:CYS:N	2.67	0.54
1:A:112:GLU:OE2	2:B:46:ARG:NH2	2.40	0.54
2:K:168:GLN:NE2	2:K:230:ASN:OD1	2.41	0.54
3:F:157:SER:OG	3:F:158:ILE:N	2.41	0.54
1:J:42:THR:HG22	1:J:124:VAL:HG12	1.90	0.54
5:R:135:ASP:OD1	5:R:135:ASP:N	2.40	0.54
3:F:185:PHE:HA	3:F:194:GLN:HG3	1.90	0.53
2:B:29:SER:OG	2:B:31:ILE:O	2.26	0.53
2:K:344:ASN:ND2	2:K:346:HIS:O	2.41	0.53
2:E:33:ILE:HG21	2:E:124:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:ARG:NH2	2:E:217:CYS:SG	2.81	0.53
2:K:410:ALA:HB1	2:K:417:PRO:HA	1.91	0.53
5:R:141:ASP:OD1	5:R:141:ASP:N	2.40	0.53
3:C:255:PRO:HG2	3:C:258:SER:CB	2.35	0.53
2:B:137:LYS:HB2	2:B:289:PRO:HG2	1.91	0.52
2:H:344:ASN:ND2	2:H:346:HIS:O	2.42	0.52
2:B:79:ASP:OD1	2:B:79:ASP:N	2.37	0.52
1:A:105:GLU:OE2	2:B:242:ARG:NH2	2.43	0.52
2:B:94:HIS:O	2:B:157:ARG:NH1	2.43	0.52
2:B:206:LYS:NZ	5:R:135:ASP:OD2	2.40	0.52
1:J:196:GLY:O	1:J:217:ASN:ND2	2.38	0.52
3:L:235:SER:OG	3:L:236:ARG:NH1	2.42	0.52
1:D:185:VAL:HG23	1:D:252:LEU:HB3	1.92	0.52
2:H:136:GLU:OE1	2:H:266:THR:OG1	2.25	0.52
1:A:146:ASP:OD2	1:A:146:ASP:N	2.40	0.52
3:L:195:TYR:HE1	3:L:197:ASN:HB2	1.75	0.52
3:C:157:SER:OG	3:C:158:ILE:N	2.43	0.52
2:H:112:GLY:HA3	2:H:121:THR:HG22	1.92	0.51
1:D:53:THR:HG21	1:D:236:GLN:HE22	1.74	0.51
3:F:132:ARG:HA	3:F:164:GLY:HA3	1.92	0.51
3:F:199:ARG:HH11	3:F:241:VAL:HG21	1.75	0.51
1:J:186:TYR:OH	1:J:248:LYS:HD2	2.10	0.51
2:H:52:MET:HB2	2:H:66:SER:HB2	1.92	0.51
5:T:141:ASP:OD1	5:T:141:ASP:N	2.40	0.51
1:G:329:CYS:SG	1:G:371:CYS:N	2.84	0.51
1:A:308:THR:HG23	1:A:310:ALA:H	1.73	0.51
1:G:308:THR:HG22	1:G:314:GLY:CA	2.40	0.51
1:J:253:ASN:HB3	1:J:262:ILE:HB	1.93	0.51
3:C:145:ASN:HB3	3:C:148:LEU:HB2	1.93	0.51
2:E:135:ARG:NH2	2:E:293:THR:OG1	2.41	0.51
1:A:337:VAL:HB	1:A:366:PHE:HB3	1.92	0.51
1:A:196:GLY:O	1:A:217:ASN:ND2	2.40	0.51
2:B:390:ARG:HH12	2:B:416:LYS:HB2	1.75	0.51
1:D:211:SER:OG	1:D:212:ASN:N	2.44	0.51
2:E:1:ASP:HA	4:N:212:CYS:O	2.11	0.51
3:C:240:SER:HB3	3:C:255:PRO:HD2	1.93	0.50
1:D:384:PRO:HD2	2:E:340:SER:HA	1.92	0.50
2:E:87:ALA:HB3	2:E:104:PRO:HG3	1.92	0.50
3:I:132:ARG:HA	3:I:164:GLY:HA3	1.93	0.50
3:C:127:CYS:SG	3:C:128:VAL:N	2.84	0.50
1:G:61:LYS:HE2	5:S:136:GLY:O	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ILE:HG13	1:G:157:ILE:HG21	1.93	0.50
2:H:135:ARG:NH2	2:H:326:THR:OG1	2.45	0.50
2:B:319:THR:OG1	2:B:320:GLY:N	2.45	0.50
4:P:222:SER:O	4:P:228:GLN:NE2	2.45	0.50
5:R:111:ARG:NH1	5:R:122:ALA:O	2.44	0.50
2:H:197:TYR:OH	2:H:207:GLY:HA3	2.11	0.50
1:A:110:ARG:NH2	1:A:211:SER:O	2.44	0.50
1:D:223:GLN:NE2	1:D:235:THR:OG1	2.45	0.49
2:E:344:ASN:ND2	2:E:346:HIS:O	2.45	0.49
3:F:186:TYR:HB2	3:F:193:VAL:HG23	1.95	0.49
3:L:233:GLU:HB2	3:L:237:THR:HA	1.93	0.49
3:C:111:ASP:N	3:C:111:ASP:OD1	2.45	0.49
3:F:201:THR:O	3:F:201:THR:OG1	2.30	0.49
1:A:309:TYR:HB2	1:A:384:PRO:HD3	1.94	0.49
2:B:87:ALA:HB3	2:B:104:PRO:HG3	1.94	0.49
3:F:123:ASN:N	3:F:123:ASN:OD1	2.45	0.49
3:F:158:ILE:HB	3:F:252:LYS:HD2	1.94	0.49
5:S:141:ASP:N	5:S:141:ASP:OD1	2.43	0.49
2:H:197:TYR:CZ	2:H:207:GLY:C	2.86	0.49
2:H:276:LYS:HD3	2:H:281:ILE:HD11	1.93	0.49
1:A:165:GLY:HA3	1:A:278:PRO:HG2	1.94	0.49
2:B:271:PRO:HB3	2:B:284:LEU:HD23	1.95	0.49
1:A:42:THR:HG22	1:A:124:VAL:HG12	1.95	0.49
3:C:177:TYR:HD1	3:C:222:ARG:HD3	1.78	0.49
2:H:63:ALA:O	2:H:78:ILE:HG13	2.12	0.49
2:K:136:GLU:HG2	2:K:290:THR:HG23	1.95	0.49
3:F:118:LEU:O	3:F:121:GLN:NE2	2.46	0.49
3:F:147:GLN:HG3	3:L:120:GLY:HA3	1.95	0.49
2:H:7:THR:OG1	2:H:8:GLN:OE1	2.31	0.48
3:C:201:THR:O	3:C:236:ARG:NH2	2.45	0.48
3:F:228:LEU:HD11	3:F:242:VAL:HG13	1.96	0.48
2:H:266:THR:O	2:H:329:ASN:ND2	2.46	0.48
1:J:165:GLY:HA3	1:J:278:PRO:HG2	1.95	0.48
2:K:22:CYS:SG	2:K:27:CYS:N	2.80	0.48
2:K:221:LYS:O	2:K:221:LYS:HG2	2.13	0.48
4:O:226:LEU:N	4:O:226:LEU:CD2	2.76	0.48
2:E:168:GLN:HB3	2:E:247:THR:HG22	1.95	0.48
2:E:319:THR:OG1	2:E:320:GLY:N	2.46	0.48
3:I:118:LEU:O	3:I:121:GLN:NE2	2.46	0.48
3:L:199:ARG:HB2	3:L:239:LEU:HB2	1.95	0.48
2:K:203:ASP:OD1	2:K:203:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:THR:HG22	1:D:210:THR:H	1.78	0.48
2:H:55:LEU:O	2:H:66:SER:OG	2.29	0.48
2:H:319:THR:OG1	2:H:320:GLY:N	2.47	0.48
1:A:135:ILE:HG13	1:A:157:ILE:HD11	1.95	0.48
1:G:191:PRO:O	1:G:195:THR:OG1	2.30	0.48
2:E:22:CYS:SG	2:E:23:GLY:N	2.82	0.48
3:I:154:LYS:HB2	3:I:163:TYR:HB2	1.96	0.47
3:L:145:ASN:HB3	3:L:148:LEU:HB2	1.95	0.47
1:A:135:ILE:HG13	1:A:157:ILE:CD1	2.44	0.47
1:A:302:CYS:HB2	1:A:319:VAL:HG22	1.96	0.47
2:B:30:PRO:O	2:B:50:SER:OG	2.32	0.47
2:B:150:CYS:HB3	2:B:263:CYS:HB2	1.80	0.47
2:B:340:SER:OG	2:B:341:GLY:N	2.47	0.47
1:G:203:ASP:OD1	1:G:203:ASP:N	2.47	0.47
2:E:33:ILE:HD11	2:E:111:VAL:HG22	1.96	0.47
1:G:318:THR:HG22	1:G:354:THR:HG22	1.96	0.47
2:K:271:PRO:HB3	2:K:284:LEU:HD23	1.96	0.47
3:L:128:VAL:O	3:L:174:THR:OG1	2.33	0.47
5:Q:118:ILE:HG12	5:Q:130:VAL:HG12	1.96	0.47
3:L:202:VAL:HG23	3:L:237:THR:HG23	1.96	0.47
1:A:307:CYS:SG	1:A:308:THR:N	2.88	0.47
1:J:211:SER:OG	1:J:213:ASP:OD1	2.32	0.47
2:H:382:SER:OG	2:H:383:VAL:N	2.48	0.47
1:G:110:ARG:NH2	1:G:211:SER:O	2.48	0.47
2:H:83:VAL:HG22	2:H:111:VAL:HG12	1.97	0.47
3:I:243:THR:OG1	3:I:244:TRP:N	2.48	0.47
5:S:135:ASP:OD1	5:S:135:ASP:N	2.43	0.47
1:A:311:PHE:H	2:B:338:GLN:HE21	1.62	0.47
2:H:151:ASN:OD1	2:H:151:ASN:N	2.48	0.47
2:B:168:GLN:HA	2:B:233:TRP:HD1	1.80	0.46
2:B:287:ASP:OD1	2:B:287:ASP:N	2.41	0.46
1:D:165:GLY:HA3	1:D:278:PRO:HG2	1.96	0.46
3:F:195:TYR:O	3:F:199:ARG:NH2	2.40	0.46
3:I:123:ASN:ND2	3:I:140:GLU:OE1	2.48	0.46
3:I:245:ASN:HB3	3:I:249:VAL:HG23	1.97	0.46
3:F:202:VAL:O	3:F:237:THR:OG1	2.33	0.46
1:G:308:THR:HG22	1:G:314:GLY:C	2.32	0.46
3:F:229:GLY:HA2	3:F:261:TRP:H	1.81	0.46
2:H:399:LEU:HB3	3:I:250:THR:HG21	1.98	0.46
1:J:432:VAL:HA	1:J:435:VAL:HG22	1.96	0.46
2:B:206:LYS:NZ	5:R:139:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:LYS:NZ	5:R:139:ASP:OD2	2.48	0.46
3:F:227:VAL:HA	3:F:241:VAL:HG12	1.97	0.46
1:A:52:LYS:NZ	1:A:109:GLU:OE2	2.41	0.46
3:F:182:PRO:O	3:F:186:TYR:OH	2.26	0.46
1:G:61:LYS:HZ1	5:S:136:GLY:HA3	1.77	0.46
5:Q:141:ASP:OD1	5:Q:141:ASP:N	2.41	0.46
1:A:255:VAL:HG13	2:B:303:PRO:HG3	1.98	0.46
2:E:168:GLN:NE2	2:E:230:ASN:OD1	2.49	0.46
2:E:394:ILE:HG23	2:E:416:LYS:HD3	1.97	0.46
4:O:215:ASP:O	4:O:224:GLU:OE1	2.33	0.46
5:S:121:GLY:N	5:S:144:GLU:OE2	2.47	0.46
2:B:46:ARG:HD3	2:B:256:PHE:HB2	1.97	0.46
2:E:397:TYR:HE1	2:E:405:VAL:HA	1.79	0.46
2:H:293:THR:HG22	2:H:305:ARG:HB2	1.97	0.46
5:S:133:ARG:NH2	5:S:145:ASP:OD1	2.49	0.46
1:D:313:PHE:HA	1:D:358:SER:HB2	1.98	0.46
1:G:180:VAL:HG22	1:G:185:VAL:HG12	1.98	0.46
1:J:390:ASP:OD1	1:J:390:ASP:N	2.49	0.46
1:D:112:GLU:OE1	2:E:46:ARG:NH2	2.39	0.46
3:C:203:PRO:HA	3:C:236:ARG:HH12	1.80	0.46
1:A:29:LEU:HD11	1:A:281:ILE:HD13	1.96	0.45
4:O:224:GLU:HA	4:O:229:CYS:SG	2.56	0.45
2:B:26:ARG:HE	2:B:26:ARG:HB2	1.69	0.45
2:H:168:GLN:HG2	2:H:169:PRO:HD2	1.99	0.45
1:D:54:LYS:HE2	1:D:54:LYS:HB2	1.72	0.45
1:J:263:ALA:HB1	1:J:268:ARG:HH21	1.81	0.45
1:A:151:GLY:O	1:A:163:ILE:CG2	2.64	0.45
2:E:95:HIS:HD1	2:E:157:ARG:HE	1.65	0.45
2:B:185:VAL:HG23	2:B:215:THR:HB	1.99	0.45
1:J:6:VAL:HA	1:J:278:PRO:HA	1.99	0.45
2:K:11:LEU:HD23	2:K:233:TRP:HZ3	1.82	0.45
3:L:179:SER:OG	3:L:245:ASN:O	2.35	0.45
5:S:114:ARG:HB3	5:S:117:GLU:HG3	1.98	0.45
2:E:185:VAL:HG23	2:E:215:THR:HB	1.99	0.45
5:R:134:CYS:CB	5:R:149:CYS:HG	2.21	0.45
5:T:134:CYS:HB3	5:T:149:CYS:HB2	1.67	0.45
1:A:344:ASP:OD2	1:A:344:ASP:N	2.49	0.45
1:D:78:CYS:SG	1:D:79:GLN:N	2.89	0.45
2:K:236:ASN:OD1	2:K:236:ASN:N	2.46	0.45
2:H:42:ALA:HB3	2:H:152:ARG:HH12	1.82	0.44
1:J:80:VAL:HG13	1:J:101:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:133:ARG:HD3	5:T:133:ARG:HA	1.86	0.44
1:D:110:ARG:HG3	1:D:204:LEU:HD21	1.99	0.44
2:H:143:GLU:HG3	2:H:144:HIS:N	2.31	0.44
4:M:211:VAL:HA	4:M:223:ASP:HB2	1.99	0.44
1:G:398:SER:OG	1:G:399:PHE:N	2.50	0.44
1:A:309:TYR:HE1	2:B:359:ARG:HH22	1.65	0.44
1:G:168:SER:HB3	1:G:276:SER:H	1.81	0.44
2:H:158:ALA:O	2:H:253:HIS:ND1	2.41	0.44
3:L:127:CYS:SG	3:L:128:VAL:N	2.91	0.44
2:B:36:VAL:HG22	2:B:47:ILE:HG23	1.99	0.44
4:M:229:CYS:HB3	4:M:231:ARG:HG2	1.99	0.44
2:H:65:MET:HE2	2:H:78:ILE:HG12	2.00	0.44
2:H:171:LEU:HD22	2:H:228:ILE:HG12	2.00	0.44
1:A:150:ASN:OD1	1:A:150:ASN:N	2.50	0.44
1:J:53:THR:HG22	1:J:108:VAL:HG22	1.98	0.44
1:G:71:LYS:NZ	1:G:105:GLU:OE2	2.51	0.44
2:H:249:LYS:HE3	2:H:249:LYS:HB3	1.75	0.44
1:A:136:THR:OG1	1:A:140:VAL:O	2.36	0.43
1:A:297:VAL:HG12	1:A:323:SER:HB2	2.00	0.43
1:D:145:ALA:HB3	1:D:157:ILE:HG12	1.99	0.43
2:H:185:VAL:HG23	2:H:215:THR:HB	1.99	0.43
1:J:52:LYS:NZ	1:J:109:GLU:OE2	2.51	0.43
2:K:164:VAL:O	2:K:252:LEU:N	2.51	0.43
2:B:206:LYS:NZ	5:R:139:ASP:CG	2.71	0.43
2:E:402:ASN:OD1	2:E:402:ASN:N	2.48	0.43
1:D:37:ARG:NH2	1:D:146:ASP:OD2	2.49	0.43
3:L:194:GLN:H	3:L:200:PHE:HB2	1.82	0.43
2:B:402:ASN:OD1	2:B:402:ASN:N	2.47	0.43
2:K:185:VAL:HG23	2:K:215:THR:HB	1.99	0.43
2:K:402:ASN:OD1	2:K:402:ASN:N	2.45	0.43
1:D:256:ALA:O	2:E:295:ARG:NH1	2.50	0.43
2:B:95:HIS:HD2	2:B:157:ARG:HE	1.65	0.43
3:C:216:ILE:HD12	3:C:225:ALA:HB3	1.99	0.43
2:B:206:LYS:CE	5:R:139:ASP:OD1	2.67	0.43
4:N:208:ILE:H	4:N:208:ILE:HG12	1.69	0.43
2:B:39:ASP:OD2	2:B:39:ASP:N	2.51	0.43
2:E:180:ILE:HA	2:E:185:VAL:HA	2.01	0.43
2:H:68:MET:HB3	2:H:73:GLN:HA	2.01	0.43
2:B:272:LEU:HB2	2:B:283:HIS:HB2	2.01	0.43
1:D:197:LYS:HA	1:D:197:LYS:HD3	1.83	0.43
2:B:402:ASN:HD22	3:C:178:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:204:ARG:NH2	3:F:235:SER:O	2.46	0.42
2:K:145:GLY:HA3	2:K:265:ALA:O	2.19	0.42
2:K:145:GLY:N	2:K:264:ILE:CG2	2.82	0.42
2:B:180:ILE:HA	2:B:185:VAL:HA	2.01	0.42
1:D:89:TRP:CH2	2:E:174:ASP:OD2	2.72	0.42
1:G:232:THR:O	1:G:232:THR:OG1	2.33	0.42
1:G:328:ASN:HD21	1:G:346:THR:HA	1.84	0.42
2:H:271:PRO:HB3	2:H:284:LEU:HD23	2.00	0.42
1:J:217:ASN:OD1	1:J:217:ASN:N	2.52	0.42
3:C:182:PRO:HA	3:C:183:PRO:HD2	1.86	0.42
2:K:180:ILE:HA	2:K:185:VAL:HA	2.01	0.42
2:E:130:PHE:HZ	2:E:141:PRO:HD3	1.84	0.42
2:E:300:ASP:OD2	2:E:300:ASP:N	2.49	0.42
1:J:132:MET:HA	1:J:146:ASP:HA	2.00	0.42
2:B:130:PHE:HZ	2:B:141:PRO:HD3	1.85	0.42
3:F:240:SER:HB2	3:F:254:THR:HG22	2.01	0.42
1:G:54:LYS:HB2	1:G:54:LYS:HE2	1.70	0.42
1:G:337:VAL:HB	1:G:366:PHE:HB3	2.01	0.42
1:D:350:SER:O	1:D:350:SER:OG	2.35	0.42
3:F:112:LYS:HZ1	3:F:114:PHE:HB2	1.85	0.42
2:H:180:ILE:HA	2:H:185:VAL:HA	2.01	0.42
2:K:151:ASN:OD1	2:K:151:ASN:N	2.50	0.42
4:P:197:GLU:HA	4:P:207:PRO:HA	2.01	0.42
3:C:211:ASP:OD2	3:C:211:ASP:N	2.52	0.42
2:E:148:LEU:HD23	2:E:149:PRO:HD2	2.02	0.42
2:E:204:VAL:HG21	5:Q:139:ASP:OD1	2.18	0.42
2:H:276:LYS:HB3	2:H:276:LYS:HE2	1.86	0.42
2:H:109:VAL:CG1	2:H:110:THR:N	2.82	0.42
1:A:390:ASP:OD1	1:A:390:ASP:N	2.49	0.42
2:B:380:VAL:HA	2:B:383:VAL:HG22	2.02	0.42
2:E:137:LYS:HB2	2:E:289:PRO:HG2	2.02	0.42
1:G:145:ALA:HB3	1:G:157:ILE:HD12	2.02	0.42
1:G:261:SER:O	1:G:270:GLU:N	2.52	0.42
1:J:146:ASP:OD2	1:J:146:ASP:N	2.53	0.42
2:H:236:ASN:OD1	2:H:236:ASN:N	2.49	0.42
3:I:132:ARG:HG2	3:I:161:LEU:HD11	2.02	0.42
3:I:168:GLN:NE2	3:I:169:CYS:SG	2.90	0.42
1:J:94:CYS:C	2:K:224:ARG:HE	2.22	0.42
4:O:216:ALA:HA	4:O:224:GLU:OE2	2.20	0.42
1:G:61:LYS:NZ	5:S:136:GLY:CA	2.77	0.41
1:G:432:VAL:HA	1:G:435:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:VAL:O	2:H:252:LEU:N	2.53	0.41
1:A:363:HIS:ND1	1:A:380:ASP:OD2	2.53	0.41
2:H:318:VAL:HG22	2:H:323:LEU:HD22	2.02	0.41
3:I:113:THR:HB	3:I:127:CYS:HA	2.02	0.41
3:L:230:GLY:O	3:L:237:THR:OG1	2.38	0.41
1:A:418:THR:HG21	2:B:375:ILE:HG12	2.03	0.41
1:D:432:VAL:HA	1:D:435:VAL:HG12	2.01	0.41
2:E:1:ASP:CG	2:E:2:LEU:N	2.62	0.41
1:G:135:ILE:HG13	1:G:157:ILE:CG2	2.50	0.41
2:K:69:ASN:HD21	2:K:74:LYS:HD2	1.85	0.41
2:K:135:ARG:NH2	2:K:293:THR:OG1	2.46	0.41
5:Q:135:ASP:OD1	5:Q:135:ASP:N	2.40	0.41
1:A:37:ARG:HD2	1:A:268:ARG:HD2	2.01	0.41
2:E:205:ARG:NH2	2:E:216:THR:OG1	2.54	0.41
1:G:43:ASN:N	1:G:43:ASN:OD1	2.53	0.41
2:K:267:LEU:HD12	2:K:267:LEU:HA	1.89	0.41
1:A:5:ALA:HB3	1:A:279:ILE:HD11	2.03	0.41
1:A:194:GLY:HA3	1:D:153:THR:HA	2.03	0.41
1:J:61:LYS:HD2	1:J:66:THR:HB	2.03	0.41
2:K:3:ASP:OD2	2:K:10:LYS:NZ	2.44	0.41
2:B:251:LYS:HE2	2:B:251:LYS:HB3	1.85	0.41
1:D:329:CYS:SG	1:D:371:CYS:N	2.94	0.41
5:T:135:ASP:OD1	5:T:135:ASP:N	2.54	0.41
3:C:229:GLY:HA2	3:C:261:TRP:HB3	2.01	0.41
2:E:236:ASN:OD1	2:E:236:ASN:N	2.51	0.41
1:J:37:ARG:HD2	1:J:268:ARG:HD2	2.02	0.41
1:A:291:ILE:O	1:A:294:THR:OG1	2.36	0.41
2:B:394:ILE:HD12	2:B:416:LYS:HD2	2.03	0.41
1:D:104:SER:HB2	1:D:232:THR:HG23	2.03	0.41
2:E:342:GLU:HB3	2:E:358:ASN:HD22	1.85	0.41
2:H:108:THR:HG21	2:K:140:HIS:ND1	2.35	0.41
2:H:365:ILE:HD13	2:H:365:ILE:HA	1.92	0.41
3:I:242:VAL:HA	3:I:252:LYS:HA	2.03	0.41
1:A:117:ASP:OD2	1:A:117:ASP:N	2.49	0.41
2:B:365:ILE:HD12	2:B:365:ILE:HA	1.99	0.41
1:D:164:ILE:HD13	1:D:279:ILE:HG22	2.02	0.41
2:H:95:HIS:HB2	2:H:157:ARG:HE	1.86	0.41
2:B:416:LYS:HA	2:B:417:PRO:HD3	1.89	0.40
1:D:104:SER:O	1:D:104:SER:OG	2.38	0.40
1:D:120:LYS:HB2	1:D:120:LYS:HE2	1.89	0.40
1:G:149:VAL:HG22	1:G:164:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:ILE:HD13	2:H:76:ILE:HA	1.89	0.40
1:A:74:PRO:HD2	1:A:107:TYR:HE1	1.86	0.40
1:A:206:SER:OG	1:A:208:THR:O	2.39	0.40
1:A:400:THR:O	1:A:400:THR:OG1	2.33	0.40
3:C:170:MET:HE2	3:C:170:MET:HB3	2.02	0.40
2:B:83:VAL:HG22	2:B:111:VAL:HG12	2.03	0.40
1:G:328:ASN:ND2	1:G:345:VAL:O	2.54	0.40
1:J:328:ASN:ND2	1:J:344:ASP:OD1	2.47	0.40
2:K:137:LYS:HB2	2:K:289:PRO:HG2	2.02	0.40
2:B:360:TYR:HB2	2:B:364:THR:HG23	2.03	0.40
1:G:80:VAL:HG13	1:G:101:THR:HG23	2.04	0.40
1:G:135:ILE:HD13	1:G:135:ILE:HA	1.88	0.40
3:I:171:LYS:HB2	3:I:171:LYS:HE3	1.90	0.40
1:A:53:THR:HG21	1:A:236:GLN:HE22	1.87	0.40
3:I:168:GLN:HA	3:I:171:LYS:HD2	2.02	0.40
1:J:112:GLU:H	1:J:112:GLU:HG2	1.71	0.40
1:J:330:PRO:HA	1:J:344:ASP:HA	2.04	0.40
2:K:145:GLY:CA	2:K:264:ILE:CG2	3.00	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	439/441 (100%)	412 (94%)	27 (6%)	0	100	100
1	D	439/441 (100%)	413 (94%)	26 (6%)	0	100	100
1	G	439/441 (100%)	414 (94%)	25 (6%)	0	100	100
1	J	439/441 (100%)	416 (95%)	23 (5%)	0	100	100
2	B	418/420 (100%)	377 (90%)	41 (10%)	0	100	100
2	E	418/420 (100%)	388 (93%)	30 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	418/420 (100%)	380 (91%)	38 (9%)	0	100	100
2	K	418/420 (100%)	383 (92%)	35 (8%)	0	100	100
3	C	149/261 (57%)	130 (87%)	19 (13%)	0	100	100
3	F	149/261 (57%)	127 (85%)	22 (15%)	0	100	100
3	I	149/261 (57%)	132 (89%)	17 (11%)	0	100	100
3	L	149/261 (57%)	131 (88%)	18 (12%)	0	100	100
4	M	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
4	N	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
4	O	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
4	P	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
5	Q	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
5	R	39/41 (95%)	32 (82%)	7 (18%)	0	100	100
5	S	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
5	T	39/41 (95%)	39 (100%)	0	0	100	100
All	All	4336/4816 (90%)	3995 (92%)	341 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	371/371 (100%)	363 (98%)	8 (2%)	52	75
1	D	371/371 (100%)	360 (97%)	11 (3%)	41	68
1	G	371/371 (100%)	362 (98%)	9 (2%)	49	74
1	J	371/371 (100%)	359 (97%)	12 (3%)	39	67
2	B	367/367 (100%)	350 (95%)	17 (5%)	27	57
2	E	367/367 (100%)	355 (97%)	12 (3%)	38	66
2	H	367/367 (100%)	359 (98%)	8 (2%)	52	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	367/367 (100%)	358 (98%)	9 (2%)	47	72
3	C	125/221 (57%)	120 (96%)	5 (4%)	31	60
3	F	125/221 (57%)	120 (96%)	5 (4%)	31	60
3	I	125/221 (57%)	122 (98%)	3 (2%)	49	74
3	L	125/221 (57%)	119 (95%)	6 (5%)	25	56
4	M	37/37 (100%)	36 (97%)	1 (3%)	44	70
4	N	37/37 (100%)	35 (95%)	2 (5%)	22	52
4	O	37/37 (100%)	36 (97%)	1 (3%)	44	70
4	P	37/37 (100%)	37 (100%)	0	100	100
5	Q	36/36 (100%)	36 (100%)	0	100	100
5	R	36/36 (100%)	35 (97%)	1 (3%)	43	70
5	S	36/36 (100%)	35 (97%)	1 (3%)	43	70
5	T	36/36 (100%)	34 (94%)	2 (6%)	21	51
All	All	3744/4128 (91%)	3631 (97%)	113 (3%)	44	68

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	175	ASP
1	A	282	ASP
1	A	302	CYS
1	A	323	SER
1	A	354	THR
1	A	386	ASP
1	A	408	TRP
2	B	19	CYS
2	B	35	GLU
2	B	39	ASP
2	B	91	LEU
2	B	115	ASP
2	B	135	ARG
2	B	150	CYS
2	B	157	ARG
2	B	167	HIS
2	B	200	LYS
2	B	201	CYS

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Mol	Chain	Res	Type
2	B	239	ARG
2	B	289	PRO
2	B	310	ARG
2	B	362	LEU
2	B	371	CYS
2	B	378	SER
3	C	125	TYR
3	C	153	LEU
3	C	154	LYS
3	C	195	TYR
3	C	199	ARG
1	D	21	ARG
1	D	75	ASP
1	D	107	TYR
1	D	109	GLU
1	D	144	SER
1	D	231	HIS
1	D	328	ASN
1	D	329	CYS
1	D	390	ASP
1	D	409	SER
1	D	410	TRP
2	E	28	ASP
2	E	35	GLU
2	E	41	HIS
2	E	157	ARG
2	E	167	HIS
2	E	200	LYS
2	E	201	CYS
2	E	230	ASN
2	E	249	LYS
2	E	323	LEU
2	E	382	SER
2	E	399	LEU
3	F	114	PHE
3	F	145	ASN
3	F	152	LYS
3	F	170	MET
3	F	195	TYR
1	G	107	TYR
1	G	183	HIS
1	G	204	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	309	TYR
1	G	311	PHE
1	G	328	ASN
1	G	329	CYS
1	G	344	ASP
1	G	367	LYS
2	H	19	CYS
2	H	28	ASP
2	H	65	MET
2	H	94	HIS
2	H	157	ARG
2	H	200	LYS
2	H	201	CYS
2	H	362	LEU
3	I	176	GLN
3	I	185	PHE
3	I	200	PHE
1	J	79	GLN
1	J	107	TYR
1	J	214	LEU
1	J	226	GLN
1	J	231	HIS
1	J	261	SER
1	J	282	ASP
1	J	309	TYR
1	J	329	CYS
1	J	386	ASP
1	J	421	PHE
1	J	438	PHE
2	K	91	LEU
2	K	115	ASP
2	K	152	ARG
2	K	200	LYS
2	K	201	CYS
2	K	203	ASP
2	K	323	LEU
2	K	371	CYS
2	K	382	SER
3	L	114	PHE
3	L	117	MET
3	L	163	TYR
3	L	212	SER

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Mol	Chain	Res	Type
3	L	240	SER
3	L	261	TRP
4	M	231	ARG
4	N	212	CYS
4	N	231	ARG
4	O	223	ASP
5	R	127	CYS
5	S	111	ARG
5	T	114	ARG
5	T	127	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	8	GLN
2	B	95	HIS
2	B	253	HIS
3	C	168	GLN
1	D	223	GLN
1	D	369	GLN
2	E	144	HIS
2	E	155	HIS
2	E	168	GLN
2	E	253	HIS
2	E	338	GLN
2	E	346	HIS
3	F	119	ASN
3	F	176	GLN
3	F	189	HIS
1	G	30	GLN
1	G	130	GLN
1	G	328	ASN
2	H	404	GLN
3	I	119	ASN
3	I	168	GLN
1	J	35	ASN
1	J	100	ASN
1	J	223	GLN
1	J	439	HIS
3	L	119	ASN
5	R	151	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

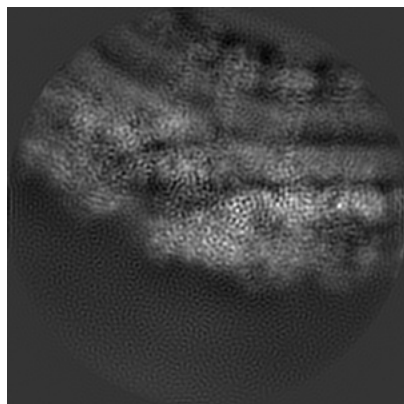
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38371. These allow visual inspection of the internal detail of the map and identification of artifacts.

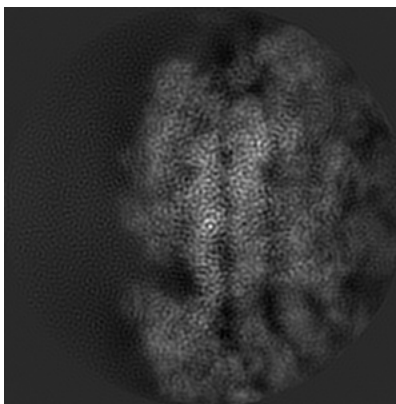
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

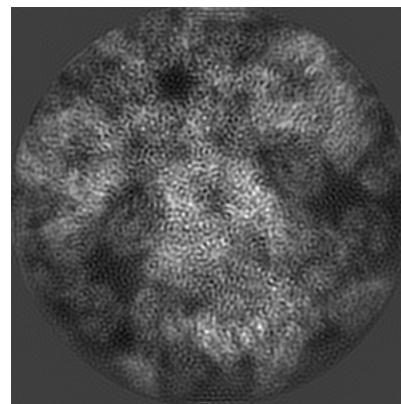
6.1.1 Primary map



X

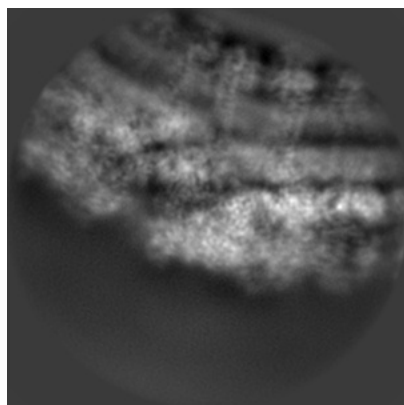


Y

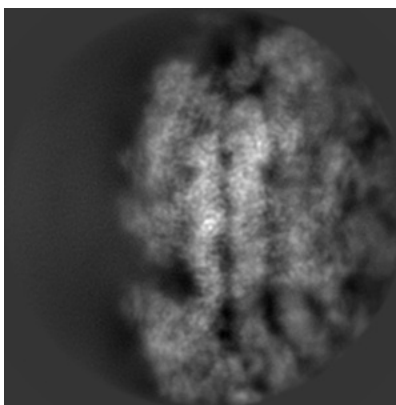


Z

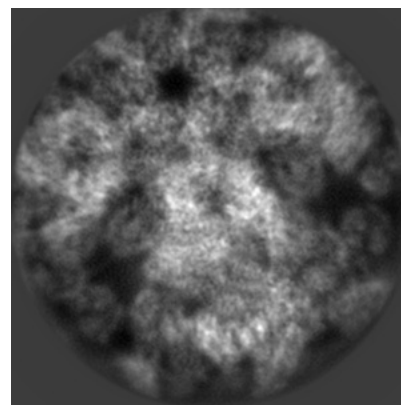
6.1.2 Raw map



X



Y

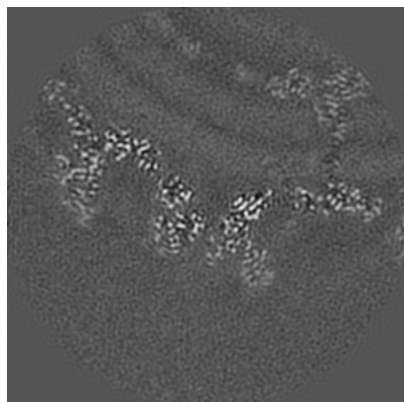


Z

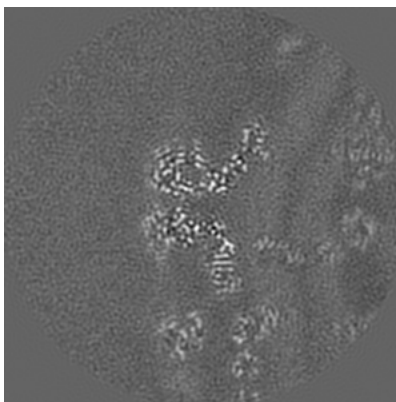
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

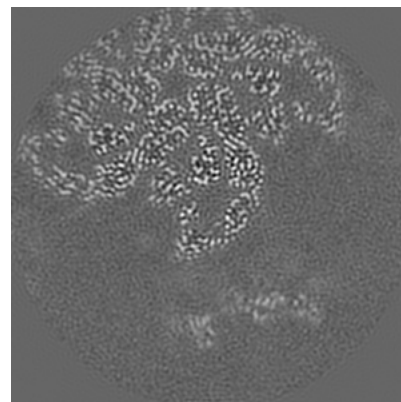
6.2.1 Primary map



X Index: 110

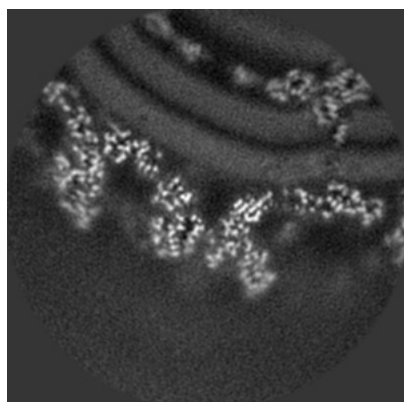


Y Index: 110

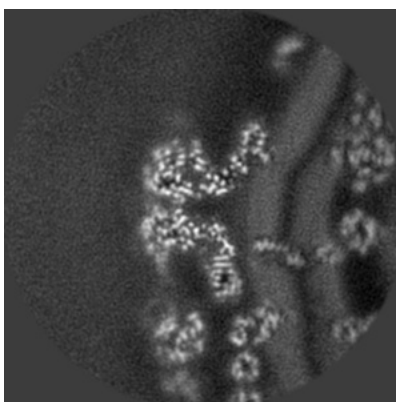


Z Index: 110

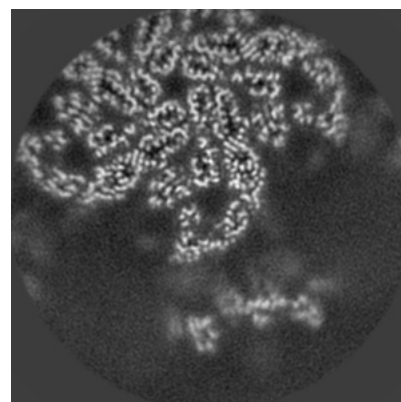
6.2.2 Raw map



X Index: 110



Y Index: 110

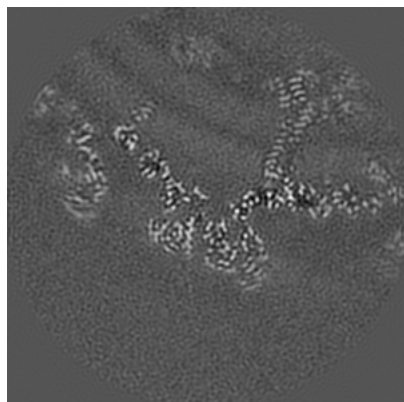


Z Index: 110

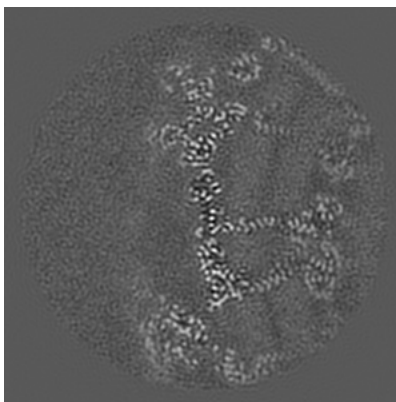
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

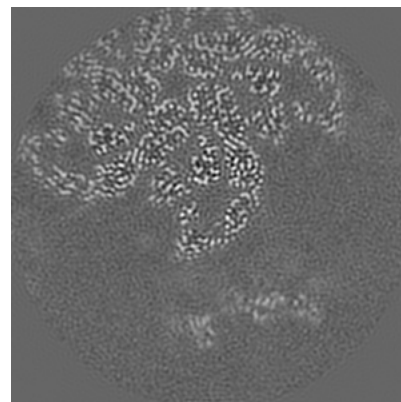
6.3.1 Primary map



X Index: 104

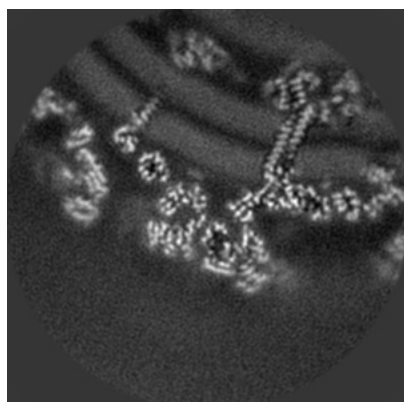


Y Index: 157

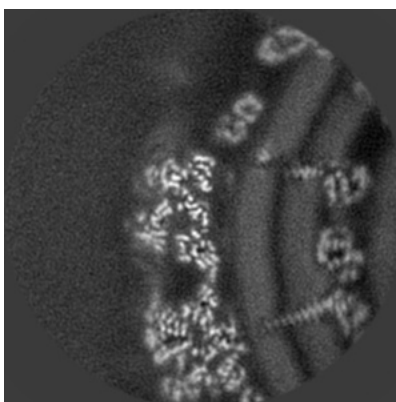


Z Index: 110

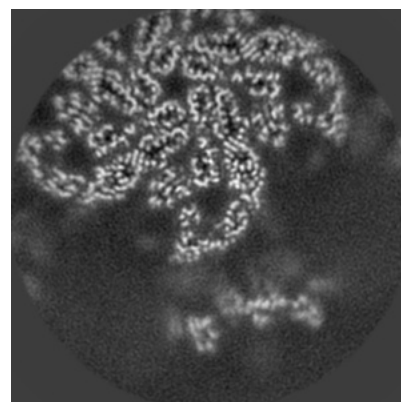
6.3.2 Raw map



X Index: 103



Y Index: 124

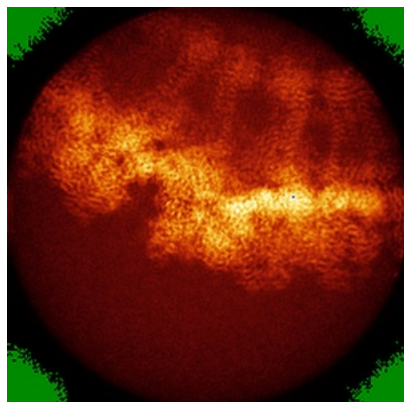


Z Index: 110

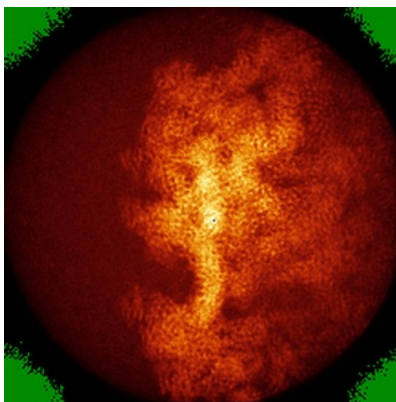
The images above show the largest variance slices of the map in three orthogonal directions.

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

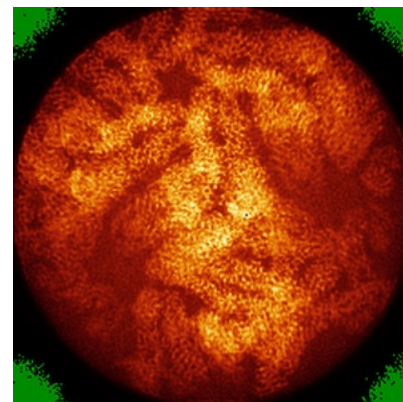
6.4.1 Primary map



X

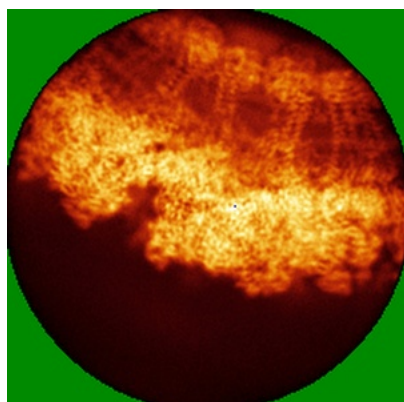


Y

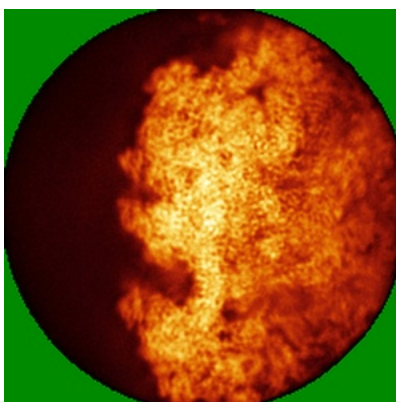


Z

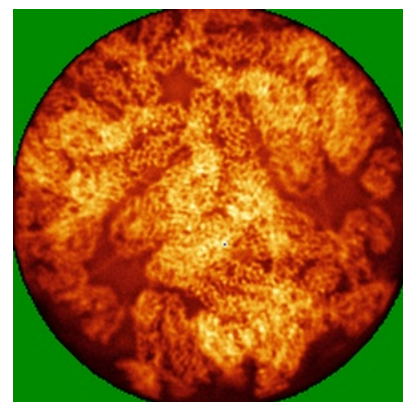
6.4.2 Raw map



X



Y

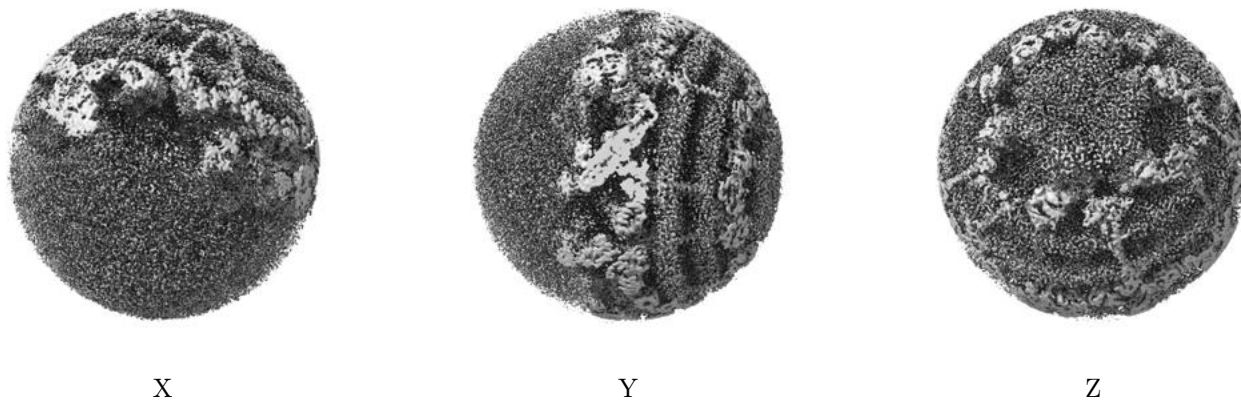


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

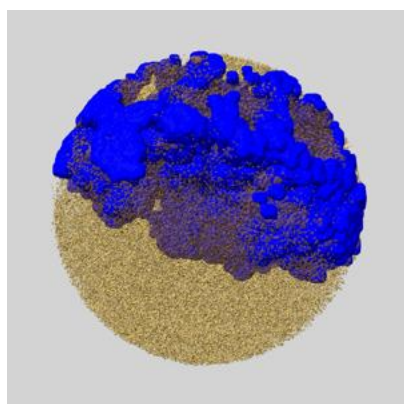
6.6 Mask visualisation [i](#)

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

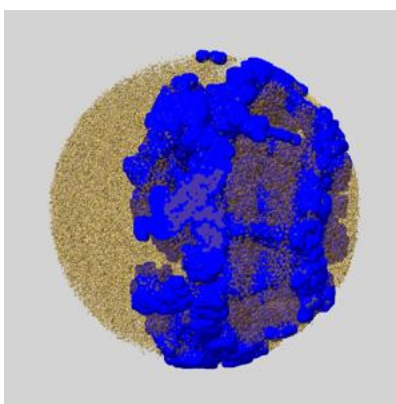
A mask typically either:

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

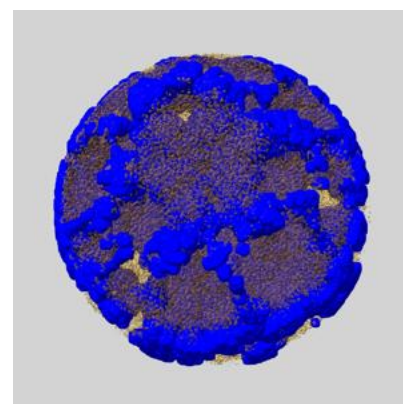
6.6.1 emd_38371_msk_1.map [i](#)



X



Y

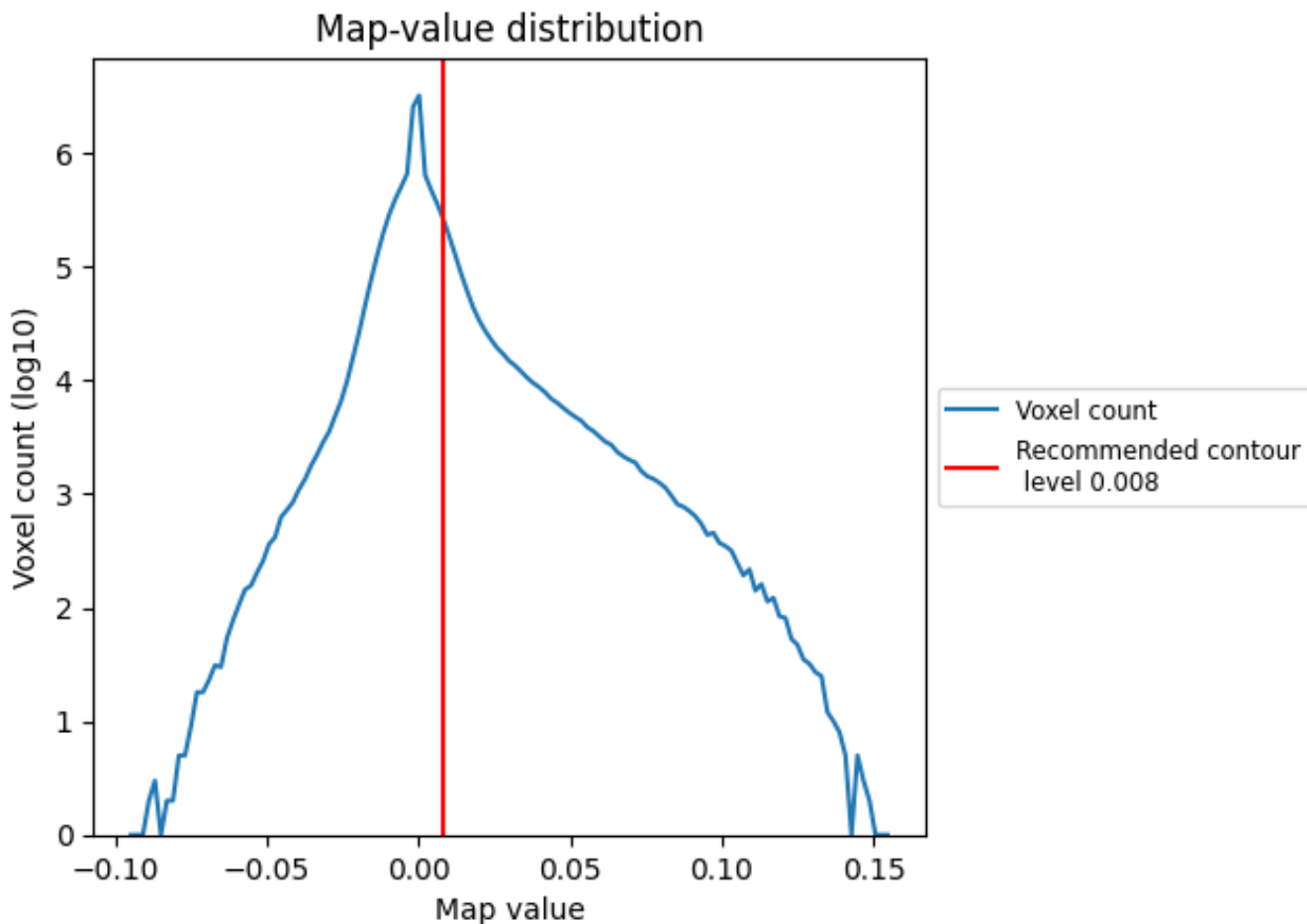


Z

7 Map analysis [i](#)

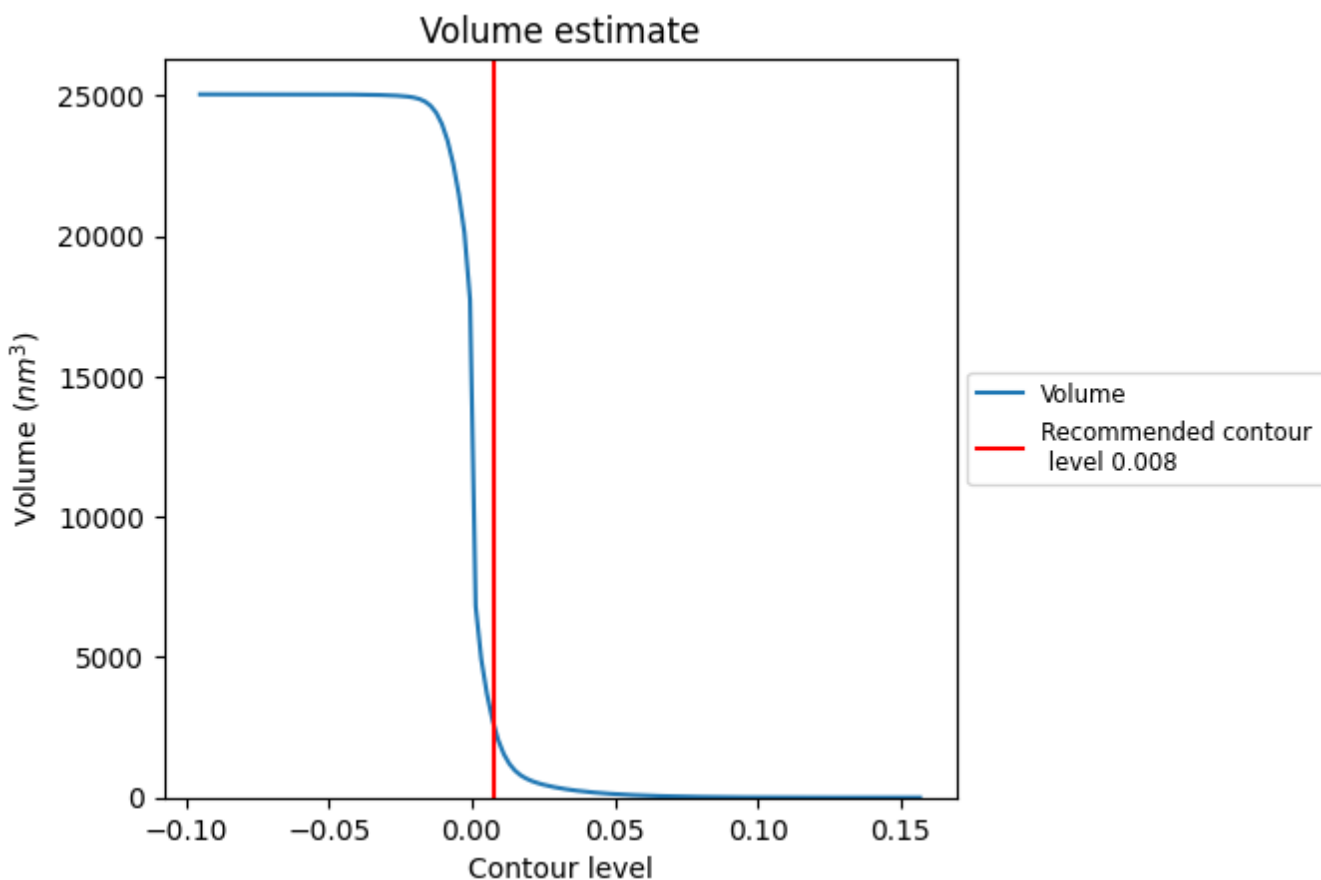
This section contains the results of statistical analysis of the map.

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.

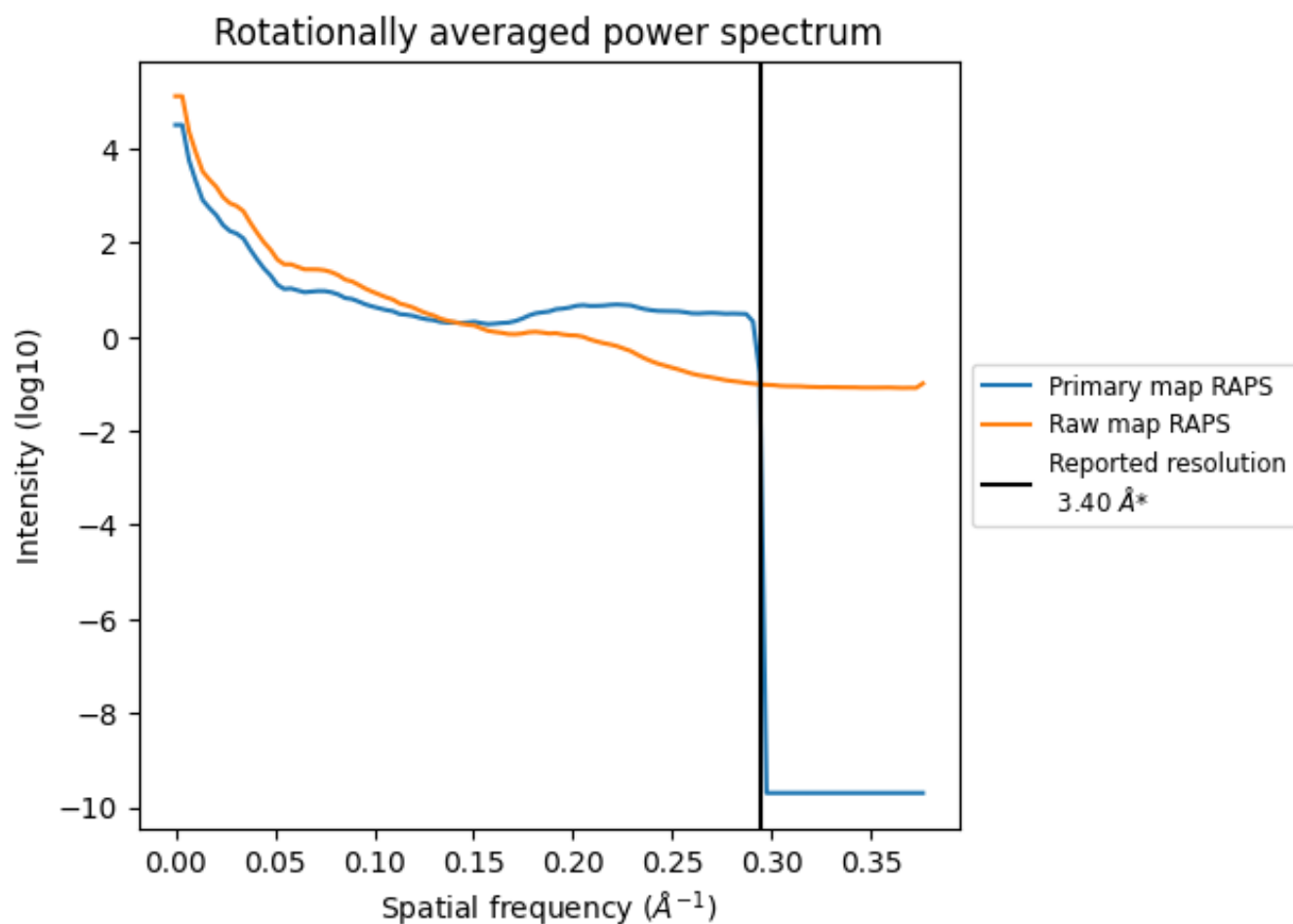
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2509 nm³; this corresponds to an approximate mass of 2266 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 [i](#)

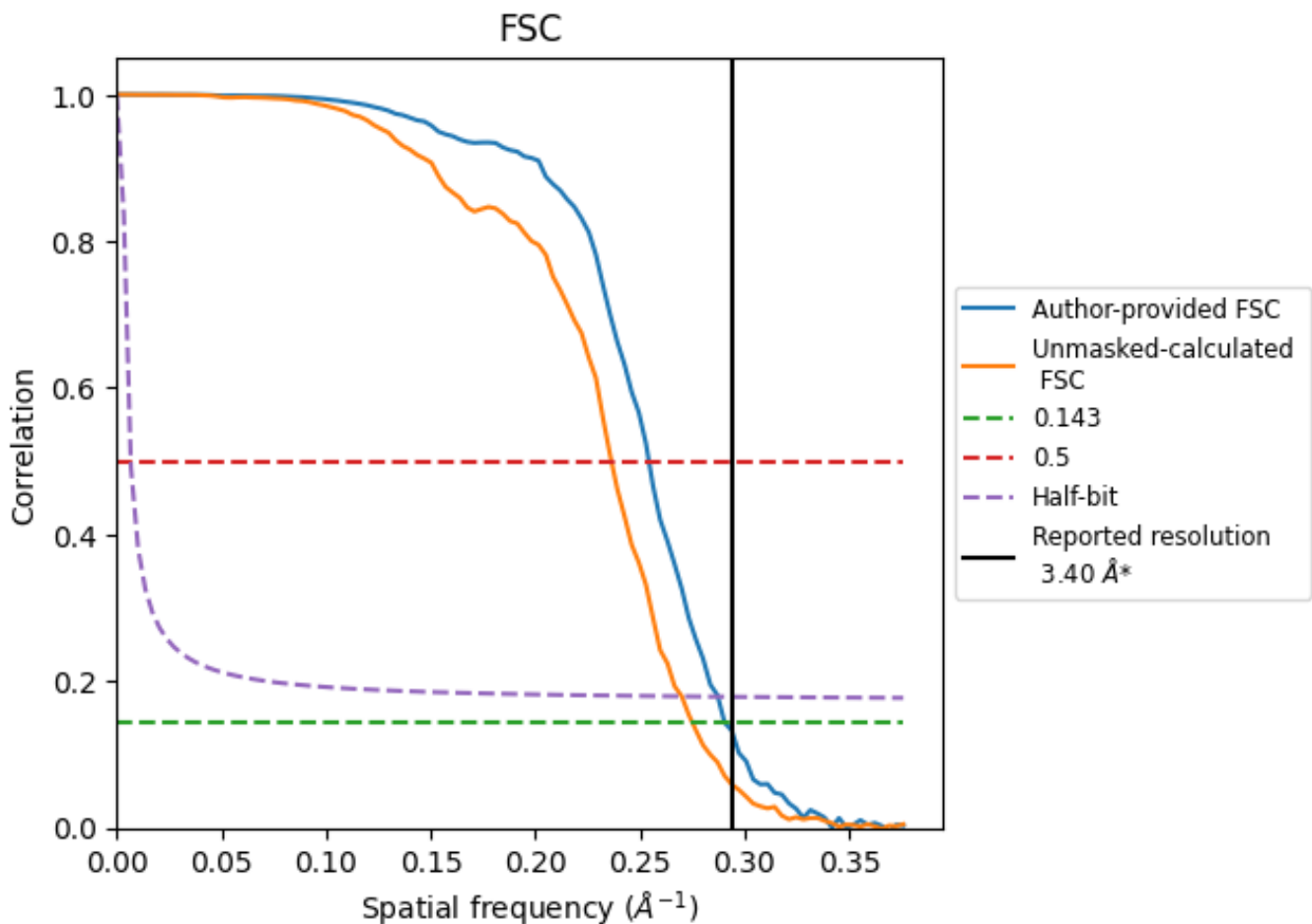


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

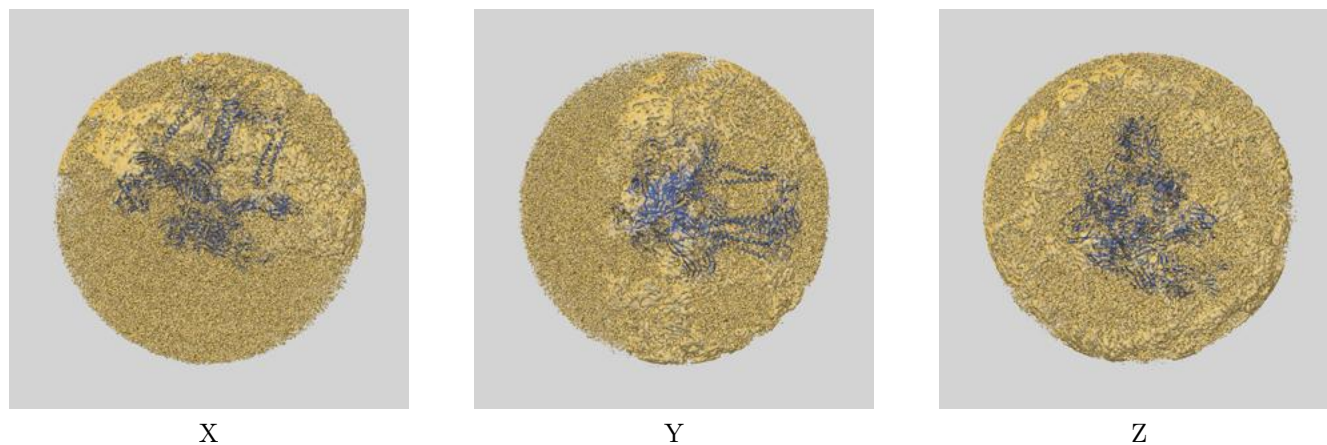
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	3.93	3.48
Unmasked-calculated*	3.63	4.23	3.70

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

9 Map-model fit [i](#)

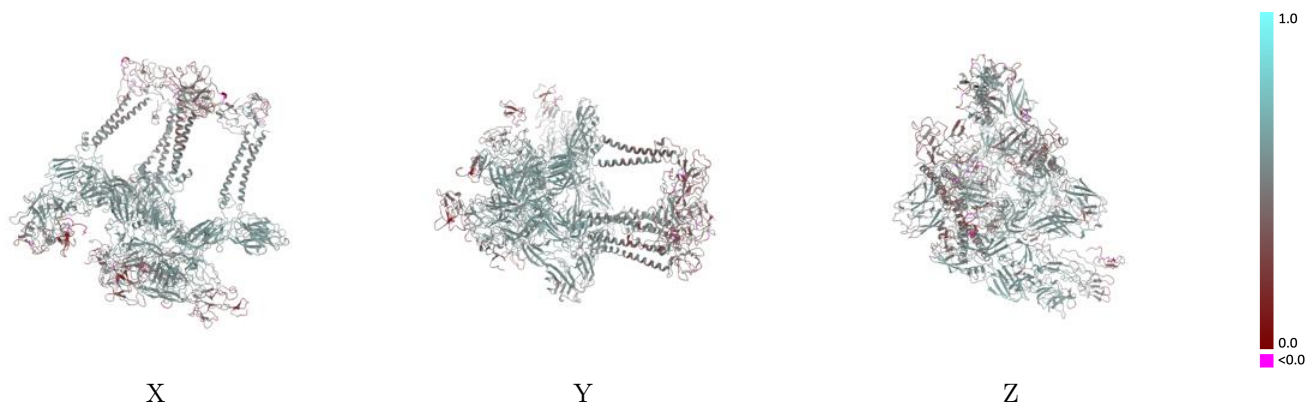
This section contains information regarding the fit between EMDB map EMD-38371 and PDB model 8XI5. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



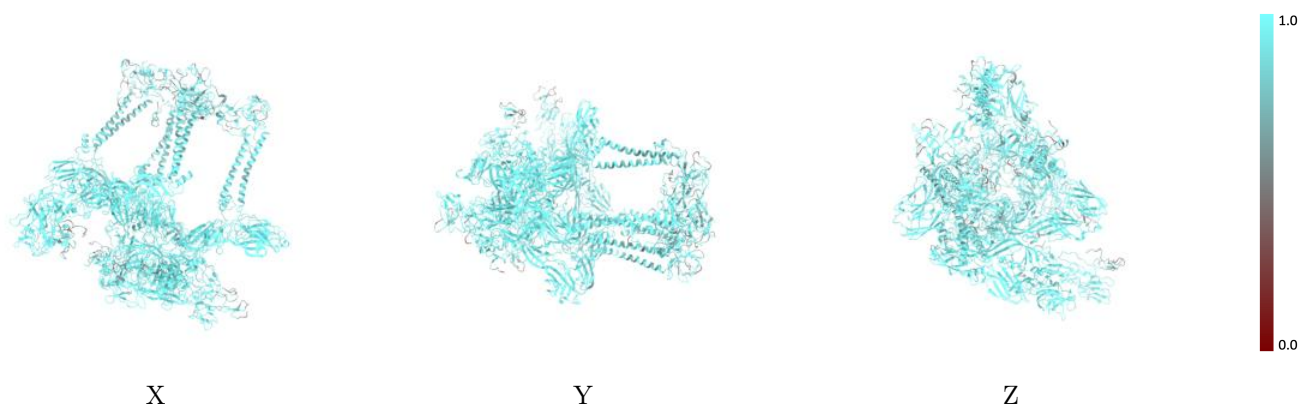
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



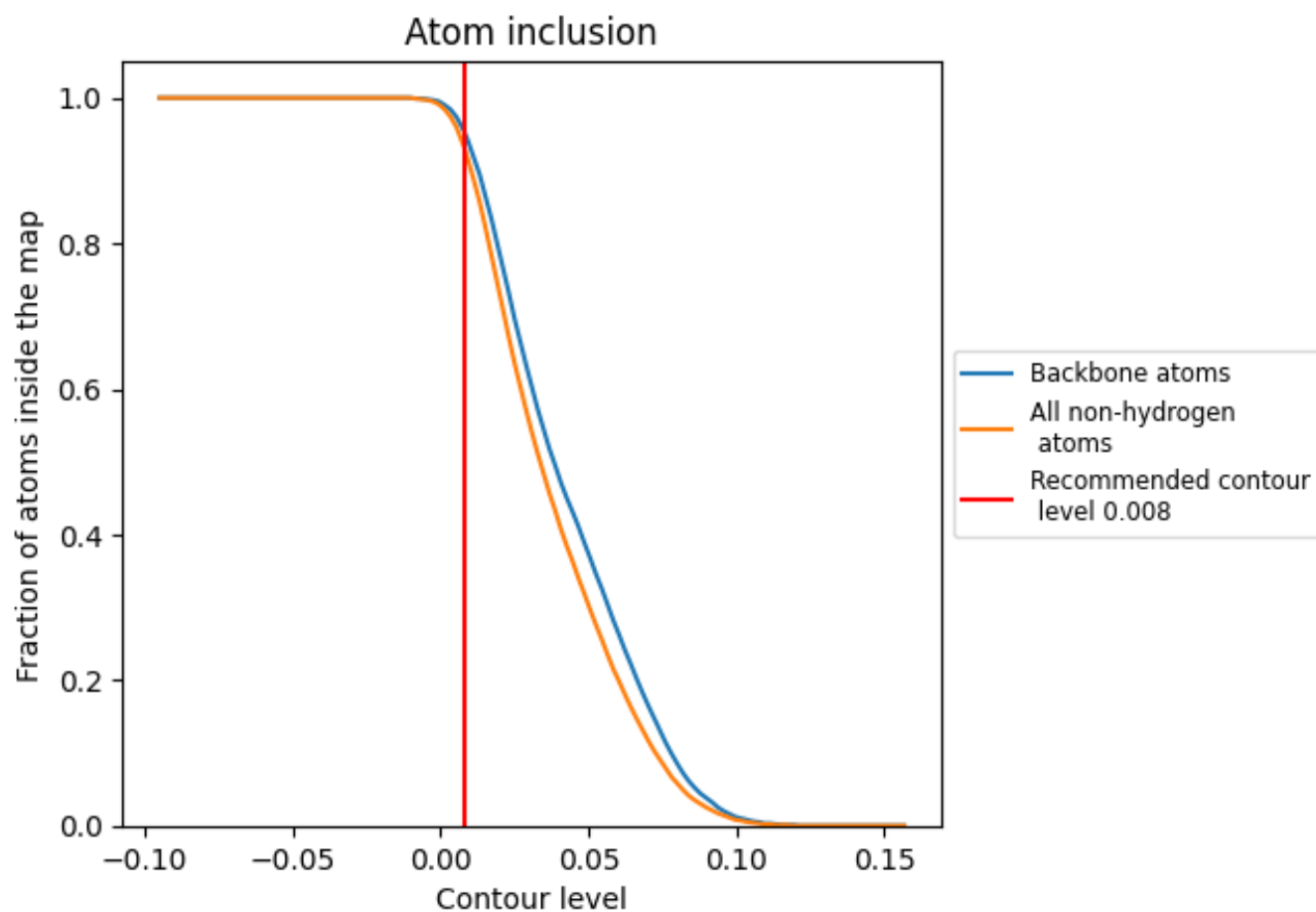
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.4930
A	 0.9710	 0.5410
B	 0.9560	 0.5150
C	 0.7790	 0.3430
D	 0.9770	 0.5430
E	 0.9690	 0.5300
F	 0.7860	 0.3750
G	 0.9730	 0.5230
H	 0.9620	 0.5170
I	 0.7990	 0.3580
J	 0.9760	 0.5460
K	 0.9720	 0.5270
L	 0.8380	 0.4070
M	 0.9000	 0.4030
N	 0.8800	 0.3930
O	 0.8470	 0.3750
P	 0.8940	 0.3920
Q	 0.6840	 0.2610
R	 0.6250	 0.2430
S	 0.7140	 0.2780
T	 0.6510	 0.2620

