WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:15 am GMT

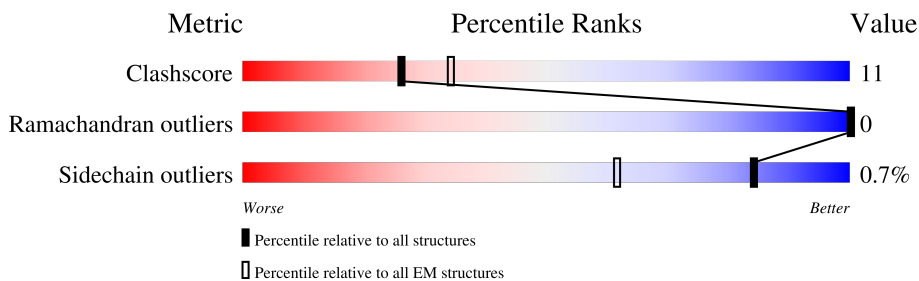|		
PDB ID	:	7AML
EMDB ID	:	EMD-11822
Title	:	RET/GDNF/GFRa1 extracellular complex Cryo-EM structure
Authors	:	Adams, S.E.; Earl, C.P.; Purkiss, A.G.; McDonald, N.Q.
Deposited on	:	2020-10-09
Resolution	:	3.50 Å(reported)
Based on initial model	:	7AB8

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 3.50 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		0.7%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 <=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	615	18% / 73% / 23% / •
1	D	615	18% / 74% / 22% / •
2	B	353	13% / 66% / 20% / 14%
2	E	353	12% / 66% / 20% / 14%
3	C	101	• / 71% / 26% / •
3	F	101	72% / 25% / •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 31456 atoms, of which 15438 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 Proto-oncogene tyrosine-protein kinase receptor Ret.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	596	Total	C	H	N	O	S	0	0
			9267	2963	4546	807	923	28		
1	D	596	Total	C	H	N	O	S	0	0
			9267	2963	4546	807	923	28		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	ARG	LYS	conflict	UNP A8E7C6
A	627	GLY	-	expression tag	UNP A8E7C6
A	628	SER	-	expression tag	UNP A8E7C6
A	629	GLU	-	expression tag	UNP A8E7C6
A	630	PHE	-	expression tag	UNP A8E7C6
A	631	GLU	-	expression tag	UNP A8E7C6
A	632	ASN	-	expression tag	UNP A8E7C6
A	633	LEU	-	expression tag	UNP A8E7C6
A	634	TYR	-	expression tag	UNP A8E7C6
A	635	PHE	-	expression tag	UNP A8E7C6
A	636	GLN	-	expression tag	UNP A8E7C6
D	505	ARG	LYS	conflict	UNP A8E7C6
D	627	GLY	-	expression tag	UNP A8E7C6
D	628	SER	-	expression tag	UNP A8E7C6
D	629	GLU	-	expression tag	UNP A8E7C6
D	630	PHE	-	expression tag	UNP A8E7C6
D	631	GLU	-	expression tag	UNP A8E7C6
D	632	ASN	-	expression tag	UNP A8E7C6
D	633	LEU	-	expression tag	UNP A8E7C6
D	634	TYR	-	expression tag	UNP A8E7C6
D	635	PHE	-	expression tag	UNP A8E7C6
D	636	GLN	-	expression tag	UNP A8E7C6

- Molecule 2 is a protein called GDNF family receptor alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	304	Total	C	H	N	O	S	0	0
			4719	1478	2334	427	448	32		
2	E	304	Total	C	H	N	O	S	0	0
			4719	1478	2334	427	448	32		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	352	GLY	-	expression tag	UNP Q98TT9
B	353	SER	-	expression tag	UNP Q98TT9
B	354	GLU	-	expression tag	UNP Q98TT9
B	355	PHE	-	expression tag	UNP Q98TT9
B	356	LEU	-	expression tag	UNP Q98TT9
B	357	GLU	-	expression tag	UNP Q98TT9
B	358	VAL	-	expression tag	UNP Q98TT9
B	359	LEU	-	expression tag	UNP Q98TT9
B	360	PHE	-	expression tag	UNP Q98TT9
B	361	GLN	-	expression tag	UNP Q98TT9
B	362	GLY	-	expression tag	UNP Q98TT9
B	363	PRO	-	expression tag	UNP Q98TT9
B	364	GLY	-	expression tag	UNP Q98TT9
B	365	GLY	-	expression tag	UNP Q98TT9
B	366	GLY	-	expression tag	UNP Q98TT9
B	367	GLU	-	expression tag	UNP Q98TT9
B	368	ASN	-	expression tag	UNP Q98TT9
B	369	LEU	-	expression tag	UNP Q98TT9
B	370	TYR	-	expression tag	UNP Q98TT9
B	371	PHE	-	expression tag	UNP Q98TT9
B	372	GLN	-	expression tag	UNP Q98TT9
E	352	GLY	-	expression tag	UNP Q98TT9
E	353	SER	-	expression tag	UNP Q98TT9
E	354	GLU	-	expression tag	UNP Q98TT9
E	355	PHE	-	expression tag	UNP Q98TT9
E	356	LEU	-	expression tag	UNP Q98TT9
E	357	GLU	-	expression tag	UNP Q98TT9
E	358	VAL	-	expression tag	UNP Q98TT9
E	359	LEU	-	expression tag	UNP Q98TT9
E	360	PHE	-	expression tag	UNP Q98TT9
E	361	GLN	-	expression tag	UNP Q98TT9
E	362	GLY	-	expression tag	UNP Q98TT9
E	363	PRO	-	expression tag	UNP Q98TT9
E	364	GLY	-	expression tag	UNP Q98TT9
E	365	GLY	-	expression tag	UNP Q98TT9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	366	GLY	-	expression tag	UNP Q98TT9
E	367	GLU	-	expression tag	UNP Q98TT9
E	368	ASN	-	expression tag	UNP Q98TT9
E	369	LEU	-	expression tag	UNP Q98TT9
E	370	TYR	-	expression tag	UNP Q98TT9
E	371	PHE	-	expression tag	UNP Q98TT9
E	372	GLN	-	expression tag	UNP Q98TT9

- Molecule 3 is a protein called Glial cell line-derived neurotrophic factor.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	98	1550	488	763	139	153	7	0	0
			Total	C	H	N	O	S		
3	F	98	1550	488	763	139	153	7	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	4	4	4	0
			Total	Ca	
4	D	4	4	4	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
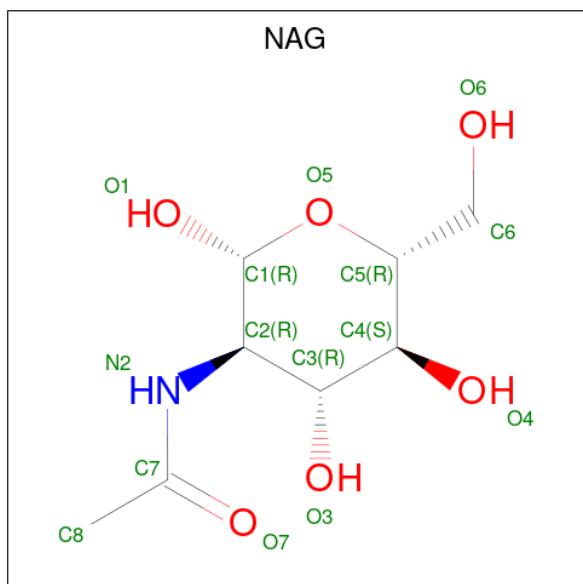
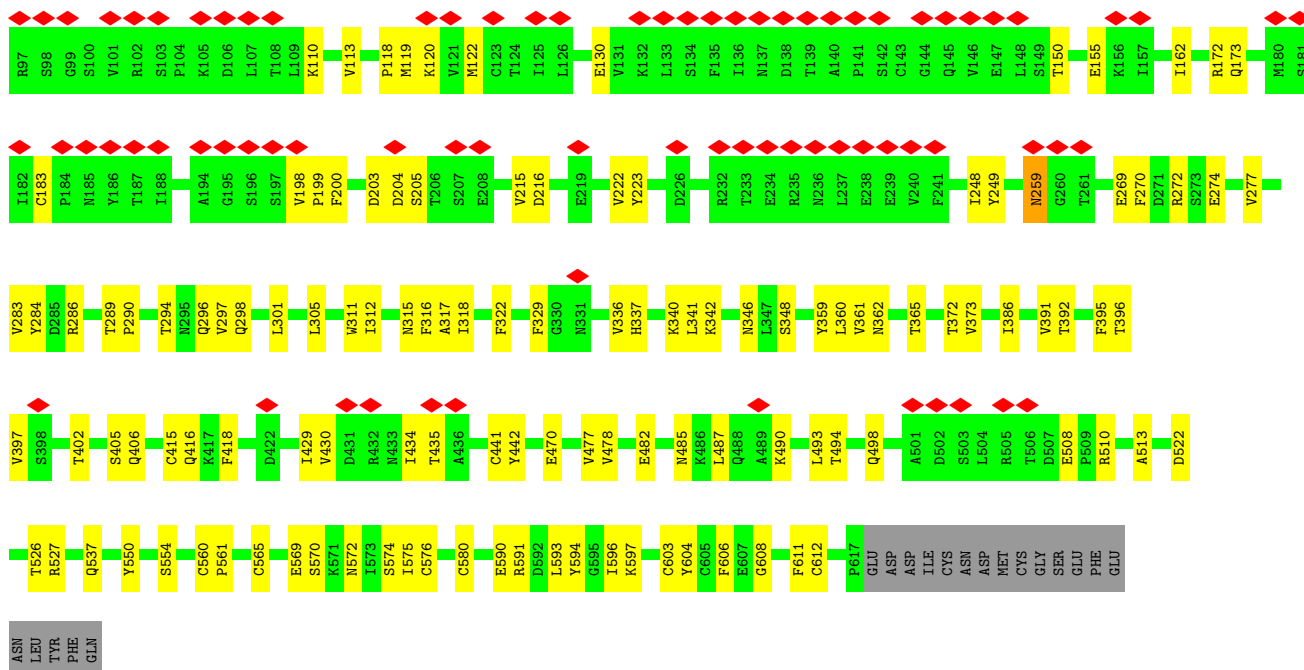| Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	A	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	D	1	Total 164	C 56	H 66	N 7	O 35	0
5	C	1	Total 24	C 8	H 10	N 1	O 5	0
5	F	1	Total 24	C 8	H 10	N 1	O 5	0

3   Residue-property plots (i)

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: Proto-oncogene tyrosine-protein kinase receptor Ret
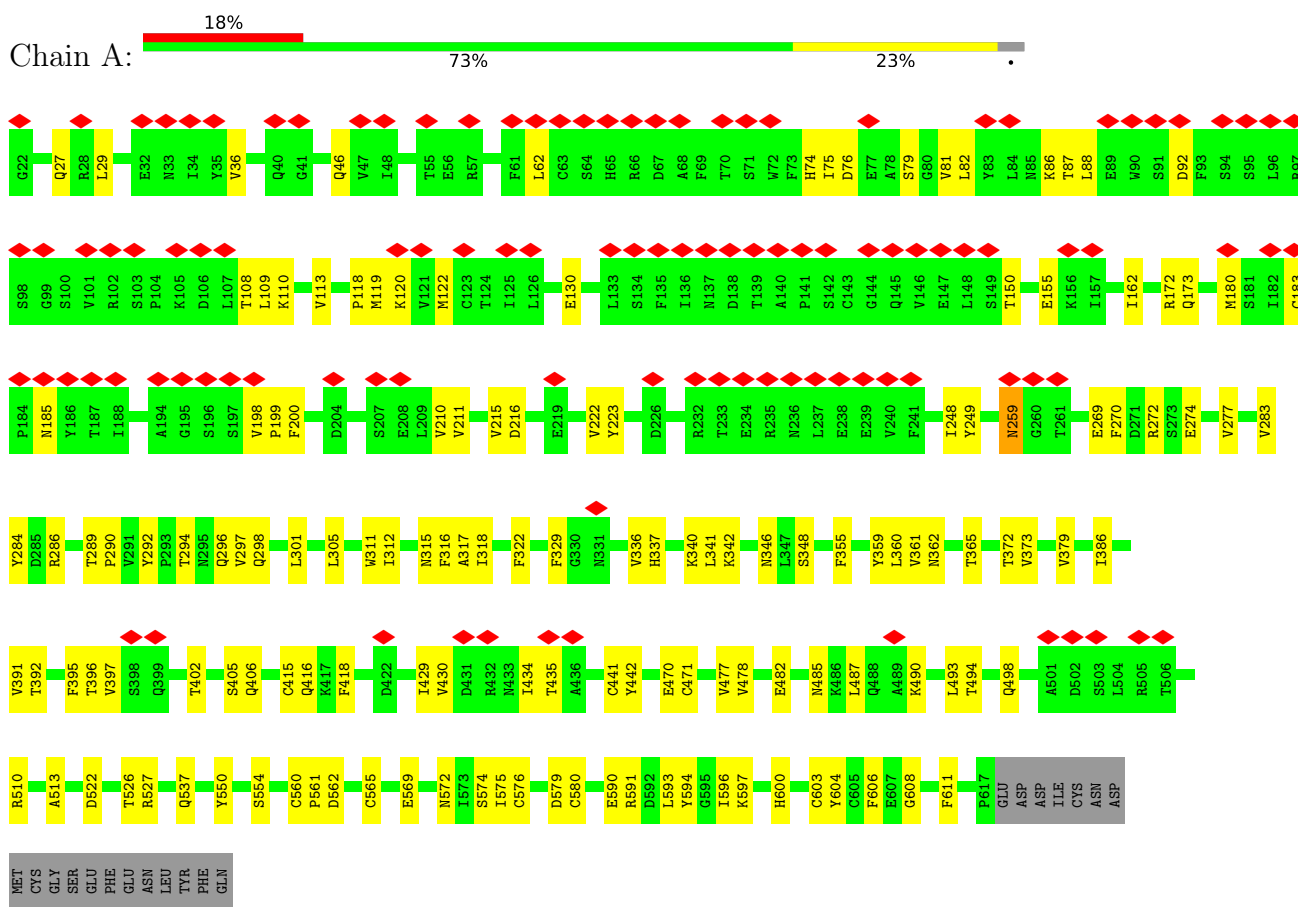
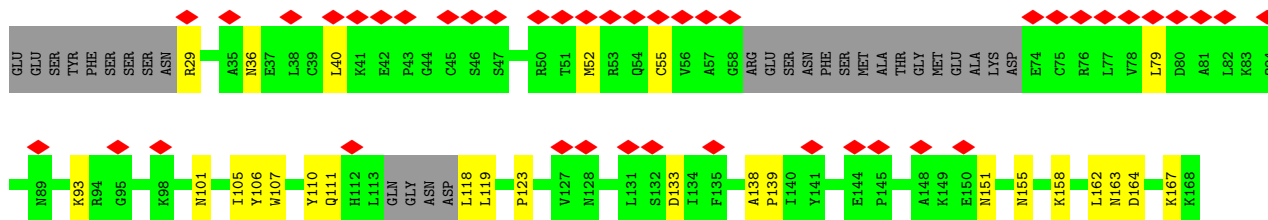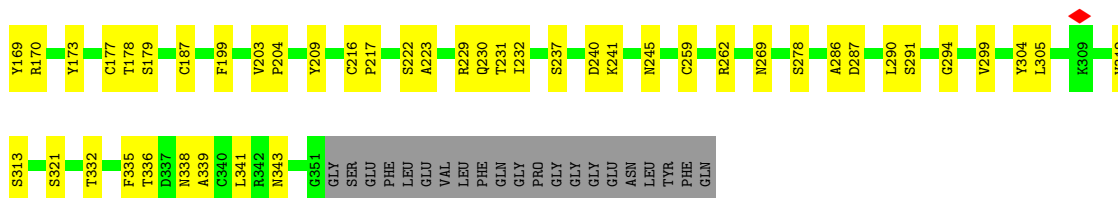• Molecule 1: Proto-oncogene tyrosine-protein kinase receptor Ret

• Molecule 2: GDNF family receptor alpha

Chain B:

• Molecule 2: GDNF family receptor alpha

Chain E:

Y169 R170 Y173 C177 T178 S179 C187 F199 V203 P204 Y209 C216 P217 S222 A223 R229 Q230 T231 I232 S237 D240 K241 N245 C259 R262 N269 S278 A286 D287 L290 S291 G294 V299 Y304 L305 K309 V312

S313 S321 T332 F335 T336 D337 N338 A339 C340 L341 R342 N343 G351 GLY SER GLU PHE LEU GLU VAL LEU PHE GLN GLY PRO GLY GLY GLU ASN LEU TYR PHE GLN

• Molecule 3: Glial cell line-derived neurotrophic factor

Chain C:

71%   26%

VAL LYS GLY Q138 C142 H148 L149 N150 D153 G157 Y158 R159 E163 L164 I165 G171 P172 C173 Y180 L184 L187 K192 L193 D194 K195 T201 C202 C203 R204 P205 I212 L215 D216 D217 S218 L219 E220 C232 V235

• Molecule 3: Glial cell line-derived neurotrophic factor

Chain F:

72%   25%

VAL LYS GLY Q138 C142 L143 L144 H148 L149 N150 D153 R159 E163 L164 I165 F166 R167 Y168 C169 C173 Y180 L184 L187 K192 L193 D194 K195 C203 R204 I212 L215 D216 D217 S218 L219 V235

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	382547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	48.6	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	46296	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.552	Depositor
Minimum map value	-2.321	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.269	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: NAG, 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	0.30	0/4823	0.49	0/6550
1	D	0.32	0/4823	0.50	0/6550
2	B	0.34	0/2429	0.47	0/3271
2	E	0.34	0/2429	0.47	0/3271
3	C	0.38	0/801	0.71	0/1077
3	F	0.40	0/801	0.70	0/1077
All	All	0.33	0/16106	0.51	0/21796

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	4721	4546	4555	102	0
1	D	4721	4546	4555	97	0
2	B	2385	2334	2334	52	0
2	E	2385	2334	2334	53	0
3	C	787	763	763	28	0
3	F	787	763	763	26	0
4	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	0	1	0
5	A	98	66	91	6	0
5	C	14	10	13	0	0
5	D	98	66	91	6	0
5	F	14	10	13	0	0
All	All	16018	15438	15512	354	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 11.

All (354) 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:274:GLU:N	1:A:346:ASN:OD1	2.04	0.91
1:D:274:GLU:N	1:D:346:ASN:OD1	2.04	0.90
2:E:269:ASN:OD1	2:E:291:SER:OG	1.94	0.86
2:B:269:ASN:OD1	2:B:291:SER:OG	1.94	0.84
2:B:151:ASN:O	2:B:155:ASN:ND2	2.13	0.81
3:F:180:TYR:CE2	3:F:184:LEU:HD11	2.16	0.81
2:E:151:ASN:O	2:E:155:ASN:ND2	2.13	0.80
3:C:180:TYR:CE2	3:C:184:LEU:HD11	2.16	0.80
2:E:338:ASN:OD1	2:E:339:ALA:N	2.16	0.78
2:B:338:ASN:OD1	2:B:339:ALA:N	2.16	0.78
1:D:27:GLN:NE2	1:D:29:LEU:O	2.20	0.74
1:A:27:GLN:NE2	1:A:29:LEU:O	2.20	0.74
2:B:87:LEU:HD21	2:B:109:ILE:HD13	1.71	0.70
2:E:269:ASN:ND2	2:E:287:ASP:OD1	2.26	0.69
2:B:269:ASN:ND2	2:B:287:ASP:OD1	2.26	0.68
3:C:159:ARG:O	3:C:217:ASP:N	2.26	0.68
3:F:159:ARG:O	3:F:217:ASP:N	2.26	0.68
1:D:203:ASP:OD1	1:D:205:SER:N	2.27	0.67
5:A:709:NAG:O7	5:A:709:NAG:O3	2.12	0.67
2:E:158:LYS:O	2:E:162:LEU:HD23	1.95	0.67
1:D:36:VAL:HA	1:D:88:LEU:HD13	1.76	0.67
1:A:62:LEU:HG	1:A:75:ILE:HD13	1.77	0.67
1:D:493:LEU:HD23	1:D:494:THR:N	2.10	0.67
1:D:290:PRO:O	1:D:296:GLN:NE2	2.28	0.66
5:D:709:NAG:O7	5:D:709:NAG:O3	2.11	0.66
1:A:290:PRO:O	1:A:296:GLN:NE2	2.28	0.66
2:B:158:LYS:O	2:B:162:LEU:HD23	1.95	0.66
1:A:36:VAL:HA	1:A:88:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:MET:CE	2:B:79:LEU:HD23	2.26	0.65
3:C:180:TYR:CZ	3:C:184:LEU:HD11	2.32	0.65
1:A:493:LEU:HD23	1:A:494:THR:N	2.10	0.65
1:D:62:LEU:HG	1:D:75:ILE:HD13	1.77	0.64
2:E:52:MET:CE	2:E:79:LEU:HD23	2.26	0.64
3:F:180:TYR:CZ	3:F:184:LEU:HD11	2.32	0.64
1:A:386:ILE:HB	1:A:487:LEU:HD23	1.80	0.64
2:B:170:ARG:HA	2:B:173:TYR:CE1	2.34	0.63
1:D:386:ILE:HB	1:D:487:LEU:HD23	1.80	0.63
2:B:216:CYS:HB2	2:B:217:PRO:HD2	1.81	0.63
2:E:262:ARG:NH1	2:E:294:GLY:O	2.30	0.62
2:E:216:CYS:HB2	2:E:217:PRO:HD2	1.82	0.62
2:E:170:ARG:HA	2:E:173:TYR:CE1	2.34	0.62
2:B:262:ARG:NH1	2:B:294:GLY:O	2.30	0.62
1:A:301:LEU:HD13	1:A:361:VAL:HG11	1.82	0.61
2:B:222:SER:O	2:B:223:ALA:C	2.37	0.61
2:B:338:ASN:HB3	2:B:341:LEU:HD13	1.82	0.61
1:A:569:GLU:OE2	1:A:576:CYS:HB3	2.00	0.61
1:D:301:LEU:HD13	1:D:361:VAL:HG11	1.82	0.60
2:E:259:CYS:SG	2:E:299:VAL:HG22	2.41	0.60
2:E:338:ASN:HB3	2:E:341:LEU:HD13	1.82	0.60
1:D:498:GLN:N	1:D:498:GLN:OE1	2.34	0.60
3:F:187:LEU:HD22	3:F:192:LYS:HE3	1.83	0.60
1:A:498:GLN:OE1	1:A:498:GLN:N	2.34	0.60
3:C:187:LEU:HD22	3:C:192:LYS:HE3	1.83	0.60
1:D:569:GLU:OE2	4:D:704:CA:CA	1.79	0.59
1:A:292:TYR:CE1	2:B:251:VAL:HG21	2.38	0.59
1:D:272:ARG:NE	1:D:348:SER:O	2.36	0.59
1:A:272:ARG:NE	1:A:348:SER:O	2.36	0.59
2:B:259:CYS:SG	2:B:299:VAL:HG22	2.41	0.59
1:A:318:ILE:HG21	1:A:359:TYR:CE2	2.38	0.58
2:B:332:THR:O	2:B:336:THR:N	2.37	0.58
2:E:332:THR:O	2:E:336:THR:N	2.37	0.58
1:A:537:GLN:N	1:A:554:SER:O	2.37	0.58
1:D:318:ILE:HG21	1:D:359:TYR:CE2	2.38	0.58
1:A:600:HIS:ND1	3:C:157:GLY:HA3	2.19	0.58
1:D:434:ILE:HG22	1:D:435:THR:N	2.19	0.57
1:A:434:ILE:HG22	1:A:435:THR:N	2.19	0.57
2:B:178:THR:HG22	2:B:178:THR:O	2.05	0.57
2:E:178:THR:O	2:E:178:THR:HG22	2.05	0.57
2:B:87:LEU:HD21	2:B:109:ILE:CD1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:ARG:CG	3:C:205:PRO:HD2	2.35	0.57
2:E:222:SER:O	2:E:223:ALA:C	2.41	0.57
2:B:231:THR:HG23	2:B:232:ILE:HG23	1.87	0.57
1:D:405:SER:OG	1:D:406:GLN:N	2.38	0.56
3:C:201:THR:HA	3:F:204:ARG:HD2	1.87	0.56
1:D:537:GLN:N	1:D:554:SER:O	2.37	0.56
2:B:133:ASP:OD1	2:B:286:ALA:HB3	2.06	0.56
2:B:162:LEU:HD13	3:C:165:ILE:HG23	1.88	0.56
2:E:231:THR:HG23	2:E:232:ILE:HG23	1.87	0.55
1:A:405:SER:OG	1:A:406:GLN:N	2.38	0.55
1:D:477:VAL:CG2	1:D:490:LYS:HD3	2.36	0.55
2:E:133:ASP:OD1	2:E:286:ALA:HB3	2.06	0.55
1:A:118:PRO:HB3	1:A:122:MET:HG2	1.89	0.55
1:A:477:VAL:CG2	1:A:490:LYS:HD3	2.37	0.55
1:A:395:PHE:O	1:A:396:THR:OG1	2.25	0.54
1:D:594:TYR:O	1:D:597:LYS:NZ	2.39	0.54
2:E:36:ASN:O	2:E:40:LEU:HD13	2.08	0.54
1:A:477:VAL:HG13	1:A:477:VAL:O	2.08	0.54
2:B:36:ASN:O	2:B:40:LEU:HD13	2.08	0.54
3:C:204:ARG:HG3	3:C:205:PRO:HD2	1.89	0.54
3:C:164:LEU:HD22	3:C:212:ILE:HD13	1.89	0.54
1:D:305:LEU:HD12	1:D:359:TYR:CE1	2.43	0.54
2:E:162:LEU:HD13	3:F:165:ILE:HG23	1.89	0.54
3:F:164:LEU:HD22	3:F:212:ILE:HD13	1.90	0.54
1:D:297:VAL:HG22	1:D:297:VAL:O	2.09	0.53
1:A:594:TYR:O	1:A:597:LYS:NZ	2.39	0.53
1:D:46:GLN:HB2	1:D:81:VAL:HG22	1.91	0.53
1:D:362:ASN:ND2	5:D:708:NAG:O7	2.42	0.53
1:A:46:GLN:HB2	1:A:81:VAL:HG22	1.91	0.53
1:D:477:VAL:O	1:D:477:VAL:HG13	2.08	0.53
1:A:362:ASN:ND2	5:A:708:NAG:O7	2.42	0.53
1:A:305:LEU:HD12	1:A:359:TYR:CE1	2.43	0.53
1:D:118:PRO:HB3	1:D:122:MET:HG2	1.89	0.53
1:A:150:THR:O	1:A:150:THR:HG22	2.08	0.53
1:A:297:VAL:O	1:A:297:VAL:HG22	2.08	0.53
1:A:336:VAL:O	1:A:336:VAL:HG13	2.08	0.53
1:D:150:THR:HG22	1:D:150:THR:O	2.08	0.53
1:D:119:MET:HG2	1:D:120:LYS:HG2	1.91	0.53
1:A:119:MET:HG2	1:A:120:LYS:HG2	1.91	0.52
2:E:312:VAL:HG23	2:E:335:PHE:O	2.09	0.52
1:D:336:VAL:HG13	1:D:336:VAL:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:VAL:HG23	2:B:335:PHE:O	2.09	0.52
1:A:560:CYS:O	1:A:579:ASP:OD2	2.28	0.52
1:D:482:GLU:OE1	1:D:485:ASN:N	2.34	0.52
2:B:229:ARG:NH2	2:B:304:TYR:O	2.43	0.52
2:E:138:ALA:N	2:E:139:PRO:CD	2.73	0.52
2:E:229:ARG:NH2	2:E:304:TYR:O	2.43	0.52
1:D:510:ARG:NH1	5:D:711:NAG:O4	2.39	0.51
1:A:86:LYS:NZ	1:A:87:THR:O	2.43	0.51
1:A:172:ARG:HG3	1:A:173:GLN:N	2.26	0.51
5:A:710:NAG:O7	5:A:710:NAG:O3	2.21	0.51
1:D:86:LYS:NZ	1:D:87:THR:O	2.43	0.51
1:A:415:CYS:HA	1:A:418:PHE:CE2	2.45	0.51
1:D:415:CYS:HA	1:D:418:PHE:CE2	2.45	0.51
1:D:86:LYS:NZ	1:D:92:ASP:OD2	2.41	0.51
5:D:710:NAG:O7	5:D:710:NAG:O3	2.21	0.51
2:B:230:GLN:NE2	3:C:219:LEU:O	2.34	0.51
1:D:395:PHE:O	1:D:396:THR:OG1	2.25	0.51
1:D:203:ASP:OD1	1:D:204:ASP:N	2.44	0.51
1:D:560:CYS:O	1:D:576:CYS:SG	2.69	0.51
2:B:138:ALA:N	2:B:139:PRO:CD	2.73	0.50
1:A:434:ILE:CG2	1:A:435:THR:N	2.75	0.50
3:F:235:VAL:HG23	3:F:235:VAL:OXT	2.12	0.50
3:F:215:LEU:HD11	3:F:219:LEU:C	2.32	0.50
3:C:215:LEU:HD11	3:C:219:LEU:C	2.32	0.50
1:A:560:CYS:O	1:A:576:CYS:SG	2.69	0.50
1:D:172:ARG:HG3	1:D:173:GLN:N	2.26	0.50
1:A:360:LEU:HD12	1:A:373:VAL:O	2.12	0.50
1:A:119:MET:HG2	1:A:120:LYS:N	2.27	0.50
1:D:360:LEU:HD12	1:D:373:VAL:O	2.12	0.50
2:E:163:ASN:OD1	2:E:164:ASP:N	2.45	0.50
2:B:106:TYR:CE1	2:B:123:PRO:HB3	2.47	0.50
2:E:240:ASP:OD1	2:E:241:LYS:N	2.41	0.49
1:A:429:ILE:HG12	1:A:442:TYR:CD1	2.47	0.49
2:B:173:TYR:CE1	2:B:199:PHE:CG	3.00	0.49
2:E:106:TYR:CE1	2:E:123:PRO:HB3	2.47	0.49
1:D:311:TRP:O	1:D:315:ASN:ND2	2.45	0.49
1:A:562:ASP:OD1	1:A:562:ASP:O	2.30	0.49
1:D:119:MET:HG2	1:D:120:LYS:N	2.27	0.49
1:D:434:ILE:CG2	1:D:435:THR:N	2.75	0.49
2:B:240:ASP:OD1	2:B:241:LYS:N	2.43	0.49
3:F:180:TYR:CE2	3:F:184:LEU:CD1	2.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:NZ	1:A:92:ASP:OD2	2.41	0.49
2:B:163:ASN:OD1	2:B:164:ASP:N	2.45	0.49
1:A:510:ARG:NH1	5:A:711:NAG:O4	2.40	0.49
2:E:173:TYR:CE1	2:E:199:PHE:CG	3.00	0.49
1:D:429:ILE:HG12	1:D:442:TYR:CD1	2.47	0.49
1:A:441:CYS:SG	1:A:470:GLU:OE1	2.71	0.48
1:D:441:CYS:SG	1:D:470:GLU:OE1	2.71	0.48
2:B:209:TYR:OH	2:B:290:LEU:HD12	2.13	0.48
2:B:162:LEU:CD1	3:C:165:ILE:HG23	2.43	0.48
2:E:209:TYR:OH	2:E:290:LEU:HD12	2.13	0.48
1:D:62:LEU:CG	1:D:75:ILE:HD13	2.44	0.48
1:D:522:ASP:O	1:D:526:THR:HG23	2.14	0.48
1:A:62:LEU:CG	1:A:75:ILE:HD13	2.44	0.47
1:D:283:VAL:HG12	1:D:284:TYR:N	2.29	0.47
3:F:164:LEU:HD13	3:F:212:ILE:HD12	1.96	0.47
3:F:173:CYS:SG	3:F:203:CYS:HB2	2.54	0.47
1:A:283:VAL:HG12	1:A:284:TYR:N	2.29	0.47
1:A:311:TRP:O	1:A:315:ASN:ND2	2.45	0.47
1:D:416:GLN:OE1	1:D:416:GLN:N	2.35	0.47
2:E:173:TYR:O	2:E:177:CYS:SG	2.73	0.47
2:E:230:GLN:OE1	3:F:219:LEU:HB3	2.15	0.47
1:A:575:ILE:HG23	1:A:575:ILE:O	2.15	0.47
2:B:173:TYR:O	2:B:177:CYS:SG	2.73	0.47
1:A:477:VAL:HG21	1:A:490:LYS:HD3	1.97	0.47
3:C:142:CYS:HA	3:C:171:GLY:HA3	1.96	0.47
3:C:164:LEU:HD13	3:C:212:ILE:HD12	1.96	0.47
2:E:278:SER:O	2:E:343:ASN:ND2	2.45	0.47
1:A:180:MET:O	1:A:180:MET:HG2	2.15	0.47
1:D:570:SER:O	1:D:570:SER:OG	2.27	0.47
3:C:148:HIS:NE2	3:C:163:GLU:OE1	2.47	0.47
1:A:606:PHE:O	1:A:608:GLY:N	2.48	0.46
1:D:301:LEU:HD12	1:D:337:HIS:CG	2.50	0.46
1:A:429:ILE:HG23	1:A:442:TYR:CE1	2.50	0.46
1:A:522:ASP:O	1:A:526:THR:HG23	2.14	0.46
1:D:477:VAL:HG21	1:D:490:LYS:HD3	1.97	0.46
1:D:575:ILE:HG23	1:D:575:ILE:O	2.15	0.46
3:F:148:HIS:NE2	3:F:163:GLU:OE1	2.47	0.46
1:A:113:VAL:O	1:A:113:VAL:HG13	2.16	0.46
1:A:301:LEU:HD12	1:A:337:HIS:CG	2.50	0.46
2:B:29:ARG:N	2:B:93:LYS:HZ1	2.13	0.46
1:A:298:GLN:HA	1:A:365:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:216:CYS:HB2	2:E:217:PRO:CD	2.45	0.46
1:A:402:THR:HG22	1:A:527:ARG:NH1	2.30	0.46
2:B:106:TYR:CZ	2:B:123:PRO:HB3	2.50	0.46
3:C:180:TYR:CE2	3:C:184:LEU:CD1	2.93	0.46
2:E:203:VAL:HG13	2:E:204:PRO:HD2	1.98	0.46
1:D:215:VAL:HG22	1:D:216:ASP:N	2.31	0.46
1:D:429:ILE:HG23	1:D:442:TYR:CE1	2.50	0.46
1:D:76:ASP:OD2	1:D:79:SER:HB3	2.16	0.46
1:D:110:LYS:HE2	1:D:130:GLU:HB3	1.98	0.46
2:E:29:ARG:N	2:E:93:LYS:HZ1	2.13	0.46
1:D:298:GLN:HA	1:D:365:THR:HG21	1.98	0.46
3:C:194:ASP:OD1	3:C:195:LYS:N	2.46	0.46
2:E:106:TYR:CZ	2:E:123:PRO:HB3	2.50	0.46
1:D:402:THR:HG22	1:D:527:ARG:NH1	2.31	0.46
1:D:606:PHE:O	1:D:608:GLY:N	2.48	0.46
1:A:76:ASP:OD2	1:A:79:SER:HB3	2.16	0.45
2:E:106:TYR:CE2	2:E:110:TYR:CD1	3.05	0.45
1:A:110:LYS:HE2	1:A:130:GLU:HB3	1.98	0.45
1:A:215:VAL:HG22	1:A:216:ASP:N	2.31	0.45
1:D:113:VAL:O	1:D:113:VAL:HG13	2.16	0.45
1:D:294:THR:O	1:D:294:THR:HG22	2.16	0.45
2:B:203:VAL:HG13	2:B:204:PRO:HD2	1.98	0.45
2:E:106:TYR:CZ	2:E:110:TYR:CD1	3.05	0.45
1:D:277:VAL:HG13	1:D:341:LEU:O	2.17	0.45
1:D:560:CYS:HB3	1:D:561:PRO:HD3	1.99	0.45
2:B:118:LEU:CD2	2:B:119:LEU:HD12	2.47	0.45
2:E:101:ASN:O	2:E:105:ILE:HG13	2.16	0.45
1:A:591:ARG:NH1	1:A:593:LEU:O	2.50	0.45
3:C:173:CYS:SG	3:C:203:CYS:HB2	2.57	0.45
1:D:591:ARG:NH1	1:D:593:LEU:O	2.50	0.45
3:F:150:ASN:HB2	3:F:153:ASP:OD2	2.16	0.45
1:A:604:TYR:CZ	1:A:611:PHE:HB2	2.52	0.45
3:C:150:ASN:HB2	3:C:153:ASP:OD2	2.16	0.45
3:C:194:ASP:O	3:C:195:LYS:HE2	2.16	0.45
3:C:164:LEU:HD13	3:C:212:ILE:CD1	2.47	0.45
1:A:277:VAL:HG13	1:A:341:LEU:O	2.17	0.45
1:A:416:GLN:OE1	1:A:416:GLN:N	2.35	0.45
2:B:133:ASP:OD1	2:B:287:ASP:N	2.50	0.45
2:B:106:TYR:CE2	2:B:110:TYR:CD1	3.05	0.44
2:E:118:LEU:CD2	2:E:119:LEU:HD12	2.47	0.44
2:E:245:ASN:ND2	2:E:321:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:ASP:O	3:F:195:LYS:HE2	2.16	0.44
2:B:101:ASN:O	2:B:105:ILE:HG13	2.16	0.44
2:B:216:CYS:HB2	2:B:217:PRO:CD	2.45	0.44
2:B:305:LEU:HD21	2:B:313:SER:HB3	1.99	0.44
1:A:294:THR:HG22	1:A:294:THR:O	2.16	0.44
1:D:155:GLU:OE1	1:D:155:GLU:N	2.46	0.44
1:D:604:TYR:CZ	1:D:611:PHE:HB2	2.52	0.44
3:F:164:LEU:HD13	3:F:212:ILE:CD1	2.47	0.44
1:A:277:VAL:HG11	1:A:340:LYS:HD3	1.99	0.44
1:D:478:VAL:O	1:D:490:LYS:CB	2.66	0.44
3:C:203:CYS:SG	3:C:232:CYS:SG	3.16	0.44
2:E:305:LEU:HD21	2:E:313:SER:HB3	1.99	0.44
3:F:187:LEU:HD22	3:F:192:LYS:CE	2.47	0.44
2:E:169:TYR:O	2:E:173:TYR:CD1	2.71	0.44
1:D:396:THR:HG22	1:D:397:VAL:N	2.33	0.44
2:B:106:TYR:CZ	2:B:110:TYR:CD1	3.05	0.44
3:F:148:HIS:CE1	3:F:163:GLU:OE1	2.71	0.44
3:C:165:ILE:HG13	3:C:165:ILE:O	2.18	0.44
2:B:245:ASN:ND2	2:B:321:SER:OG	2.50	0.44
1:A:560:CYS:HB3	1:A:561:PRO:HD3	1.99	0.43
1:A:590:GLU:HG3	1:A:591:ARG:N	2.33	0.43
1:D:317:ALA:N	1:D:342:LYS:O	2.43	0.43
2:E:133:ASP:OD1	2:E:287:ASP:N	2.50	0.43
3:C:148:HIS:CE1	3:C:163:GLU:OE1	2.71	0.43
1:A:155:GLU:OE1	1:A:155:GLU:N	2.46	0.43
1:A:292:TYR:CZ	2:B:251:VAL:HG21	2.53	0.43
2:B:52:MET:O	2:B:55:CYS:N	2.52	0.43
1:A:81:VAL:HG12	1:A:82:LEU:N	2.34	0.43
1:A:162:ILE:O	1:A:249:TYR:N	2.52	0.43
1:D:75:ILE:HG13	1:D:82:LEU:HD12	2.00	0.43
1:D:222:VAL:HG12	1:D:223:TYR:N	2.33	0.43
2:E:167:LYS:NZ	3:F:164:LEU:HD11	2.33	0.43
2:B:169:TYR:O	2:B:173:TYR:CD1	2.71	0.43
3:F:165:ILE:HG13	3:F:165:ILE:O	2.18	0.43
1:A:74:HIS:C	1:A:75:ILE:HD12	2.39	0.43
5:A:706:NAG:O7	5:A:706:NAG:H3	2.19	0.43
1:D:478:VAL:O	1:D:490:LYS:HB2	2.18	0.43
1:A:62:LEU:CD1	1:A:75:ILE:HD13	2.49	0.43
1:A:396:THR:HG22	1:A:397:VAL:N	2.33	0.43
1:A:569:GLU:CD	1:A:576:CYS:HB3	2.38	0.43
1:D:62:LEU:CD1	1:D:75:ILE:HD13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:GLU:HG3	1:D:591:ARG:N	2.33	0.43
1:A:198:VAL:HG13	1:A:199:PRO:HD2	2.00	0.43
1:A:513:ALA:HB2	1:A:574:SER:HB3	1.99	0.43
2:E:52:MET:CE	2:E:79:LEU:CD2	2.97	0.43
2:E:179:SER:O	2:E:187:CYS:HA	2.19	0.43
1:A:222:VAL:HG12	1:A:223:TYR:N	2.33	0.42
2:B:52:MET:CE	2:B:79:LEU:CD2	2.97	0.42
3:C:164:LEU:HG	3:C:165:ILE:N	2.34	0.42
1:D:277:VAL:HG11	1:D:340:LYS:HD3	1.99	0.42
1:A:361:VAL:O	1:A:372:THR:HG22	2.20	0.42
1:D:81:VAL:HG12	1:D:82:LEU:N	2.34	0.42
2:B:179:SER:O	2:B:187:CYS:HA	2.19	0.42
1:D:198:VAL:HG12	1:D:200:PHE:CD2	2.55	0.42
1:D:223:TYR:CE2	1:D:248:ILE:HD11	2.54	0.42
2:E:52:MET:O	2:E:55:CYS:N	2.52	0.42
1:D:162:ILE:O	1:D:249:TYR:N	2.52	0.42
3:F:164:LEU:HG	3:F:165:ILE:N	2.34	0.42
1:A:198:VAL:HG12	1:A:200:PHE:CD2	2.55	0.42
1:D:513:ALA:HB2	1:D:574:SER:HB3	2.00	0.42
5:D:706:NAG:O7	5:D:706:NAG:H3	2.19	0.42
5:D:710:NAG:HO3	5:D:710:NAG:C7	2.27	0.42
1:A:259:ASN:OD1	1:A:259:ASN:C	2.58	0.42
1:A:223:TYR:CE2	1:A:248:ILE:HD11	2.55	0.42
1:A:289:THR:HG21	1:A:322:PHE:CE1	2.55	0.42
1:D:361:VAL:O	1:D:372:THR:HG22	2.20	0.42
1:D:74:HIS:C	1:D:75:ILE:HD12	2.39	0.42
5:A:709:NAG:HO3	5:A:709:NAG:C7	2.25	0.42
1:D:198:VAL:HG13	1:D:199:PRO:HD2	2.00	0.42
3:C:187:LEU:HD22	3:C:192:LYS:CE	2.47	0.42
1:A:75:ILE:HG13	1:A:82:LEU:HD12	2.01	0.41
1:D:289:THR:HG21	1:D:322:PHE:CE1	2.55	0.41
1:A:286:ARG:HD3	1:A:329:PHE:CE1	2.56	0.41
3:F:194:ASP:OD1	3:F:195:LYS:N	2.46	0.41
1:A:478:VAL:O	1:A:490:LYS:HB2	2.20	0.41
1:A:482:GLU:OE1	1:A:485:ASN:N	2.34	0.41
3:C:204:ARG:HG2	3:C:205:PRO:HD2	2.03	0.41
3:F:144:LEU:HD11	3:F:167:ARG:HB3	2.02	0.41
1:A:362:ASN:HA	1:A:372:THR:HG22	2.02	0.41
1:A:478:VAL:O	1:A:490:LYS:CB	2.68	0.41
1:D:603:CYS:SG	1:D:604:TYR:N	2.94	0.41
2:B:332:THR:HG22	2:B:336:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:LEU:CD1	3:F:165:ILE:HG23	2.50	0.41
1:A:391:VAL:HG12	1:A:392:THR:N	2.36	0.41
1:D:110:LYS:HA	1:D:110:LYS:HD3	1.89	0.41
1:A:312:ILE:HG23	1:A:316:PHE:CD2	2.55	0.41
1:A:429:ILE:HG22	1:A:430:VAL:N	2.35	0.41
1:D:259:ASN:OD1	1:D:259:ASN:C	2.58	0.41
2:B:338:ASN:O	2:B:342:ARG:NE	2.48	0.41
1:A:603:CYS:SG	1:A:604:TYR:N	2.94	0.41
1:D:362:ASN:HA	1:D:372:THR:HG22	2.02	0.41
2:E:52:MET:HE3	2:E:79:LEU:HD23	1.99	0.41
2:E:107:TRP:O	2:E:111:GLN:HB3	2.21	0.41
1:A:108:THR:O	1:A:109:LEU:HD23	2.20	0.41
1:A:317:ALA:N	1:A:342:LYS:O	2.43	0.41
1:D:312:ILE:HG23	1:D:316:PHE:CD2	2.55	0.41
1:D:429:ILE:HG22	1:D:430:VAL:N	2.35	0.41
2:B:107:TRP:O	2:B:111:GLN:HB3	2.21	0.41
2:E:52:MET:HE3	2:E:79:LEU:CD2	2.51	0.41
1:D:550:TYR:OH	1:D:596:ILE:HG13	2.21	0.41
2:E:29:ARG:N	2:E:93:LYS:NZ	2.69	0.41
1:D:75:ILE:HG13	1:D:82:LEU:CD1	2.51	0.40
2:B:98:LYS:O	2:B:98:LYS:HG3	2.21	0.40
1:A:75:ILE:HG13	1:A:82:LEU:CD1	2.51	0.40
1:A:110:LYS:HD3	1:A:110:LYS:HA	1.89	0.40
1:A:172:ARG:CG	1:A:173:GLN:N	2.84	0.40
1:A:441:CYS:SG	1:A:471:CYS:N	2.94	0.40
1:D:269:GLU:HB3	1:D:270:PHE:CD1	2.57	0.40
2:E:230:GLN:NE2	3:F:219:LEU:O	2.46	0.40
1:A:210:VAL:HG12	1:A:211:VAL:N	2.36	0.40
1:A:269:GLU:HB3	1:A:270:PHE:CD1	2.57	0.40
1:A:355:PHE:CZ	1:A:379:VAL:HG11	2.56	0.40
1:D:172:ARG:CG	1:D:173:GLN:N	2.84	0.40
1:D:75:ILE:HG22	1:D:76:ASP:N	2.36	0.40
1:D:391:VAL:HG12	1:D:392:THR:N	2.36	0.40
1:D:508:GLU:O	1:D:510:ARG:N	2.53	0.40
2:E:232:ILE:O	2:E:237:SER:OG	2.40	0.40
2:E:332:THR:HG22	2:E:336:THR:CG2	2.51	0.40
1:A:550:TYR:OH	1:A:596:ILE:HG13	2.21	0.40
1:D:286:ARG:HD3	1:D:329:PHE:CE1	2.55	0.40
1:D:603:CYS:HA	1:D:612:CYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	594/615 (97%)	559 (94%)	35 (6%)	0	100	100
1	D	594/615 (97%)	559 (94%)	35 (6%)	0	100	100
2	B	298/353 (84%)	279 (94%)	19 (6%)	0	100	100
2	E	298/353 (84%)	278 (93%)	20 (7%)	0	100	100
3	C	96/101 (95%)	96 (100%)	0	0	100	100
3	F	96/101 (95%)	90 (94%)	6 (6%)	0	100	100
All	All	1976/2138 (92%)	1861 (94%)	115 (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	535/553 (97%)	529 (99%)	6 (1%)	73	88
1	D	535/553 (97%)	530 (99%)	5 (1%)	78	90
2	B	272/312 (87%)	272 (100%)	0	100	100
2	E	272/312 (87%)	272 (100%)	0	100	100
3	C	90/92 (98%)	90 (100%)	0	100	100
3	F	90/92 (98%)	88 (98%)	2 (2%)	52	78
All	All	1794/1914 (94%)	1781 (99%)	13 (1%)	84	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	CYS
1	A	185	ASN
1	A	259	ASN
1	A	565	CYS
1	A	572	ASN
1	A	580	CYS
1	D	183	CYS
1	D	259	ASN
1	D	565	CYS
1	D	572	ASN
1	D	580	CYS
3	F	142	CYS
3	F	169	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	D	296	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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	$\#\|Z\| > 2$
5	NAG	D	710	1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	A	705	1	14,14,15	0.24	0	17,19,21	0.39	0
5	NAG	D	709	1	14,14,15	0.29	0	17,19,21	0.34	0
5	NAG	A	709	1	14,14,15	0.29	0	17,19,21	0.35	0
5	NAG	D	705	1	14,14,15	0.24	0	17,19,21	0.38	0
5	NAG	A	711	1	14,14,15	0.25	0	17,19,21	0.37	0
5	NAG	D	708	1	14,14,15	0.28	0	17,19,21	0.33	0
5	NAG	D	706	1	14,14,15	0.24	0	17,19,21	0.53	0
5	NAG	D	711	1	14,14,15	0.24	0	17,19,21	0.38	0
5	NAG	A	708	1	14,14,15	0.28	0	17,19,21	0.33	0
5	NAG	A	707	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	C	301	3	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	A	706	1	14,14,15	0.23	0	17,19,21	0.54	0
5	NAG	A	710	1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	F	301	3	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	D	707	1	14,14,15	0.41	0	17,19,21	0.51	0

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
5	NAG	D	710	1	-	2/6/23/26	0/1/1/1
5	NAG	A	705	1	-	3/6/23/26	0/1/1/1
5	NAG	D	709	1	-	2/6/23/26	0/1/1/1
5	NAG	A	709	1	-	2/6/23/26	0/1/1/1
5	NAG	D	705	1	-	3/6/23/26	0/1/1/1
5	NAG	A	711	1	-	4/6/23/26	0/1/1/1
5	NAG	D	708	1	-	1/6/23/26	0/1/1/1
5	NAG	D	706	1	-	1/6/23/26	0/1/1/1
5	NAG	D	711	1	-	4/6/23/26	0/1/1/1
5	NAG	A	708	1	-	1/6/23/26	0/1/1/1
5	NAG	A	707	1	-	1/6/23/26	0/1/1/1
5	NAG	C	301	3	-	2/6/23/26	0/1/1/1

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	706	1	-	1/6/23/26	0/1/1/1
5	NAG	A	710	1	-	2/6/23/26	0/1/1/1
5	NAG	F	301	3	-	2/6/23/26	0/1/1/1
5	NAG	D	707	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	709	NAG	C1-C2-N2-C7
5	D	709	NAG	C1-C2-N2-C7
5	C	301	NAG	C4-C5-C6-O6
5	F	301	NAG	C4-C5-C6-O6
5	C	301	NAG	O5-C5-C6-O6
5	F	301	NAG	O5-C5-C6-O6
5	A	710	NAG	C1-C2-N2-C7
5	D	710	NAG	C1-C2-N2-C7
5	A	705	NAG	C8-C7-N2-C2
5	A	705	NAG	O7-C7-N2-C2
5	A	711	NAG	C8-C7-N2-C2
5	A	711	NAG	O7-C7-N2-C2
5	D	705	NAG	C8-C7-N2-C2
5	D	705	NAG	O7-C7-N2-C2
5	D	711	NAG	C8-C7-N2-C2
5	D	711	NAG	O7-C7-N2-C2
5	A	705	NAG	O5-C5-C6-O6
5	D	705	NAG	O5-C5-C6-O6
5	A	708	NAG	O5-C5-C6-O6
5	D	708	NAG	O5-C5-C6-O6
5	A	706	NAG	C3-C2-N2-C7
5	D	706	NAG	C3-C2-N2-C7
5	A	711	NAG	C4-C5-C6-O6
5	D	711	NAG	C4-C5-C6-O6
5	A	707	NAG	C3-C2-N2-C7
5	A	709	NAG	C3-C2-N2-C7
5	A	710	NAG	C3-C2-N2-C7
5	D	707	NAG	C3-C2-N2-C7
5	D	709	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	D	710	NAG	C3-C2-N2-C7
5	D	711	NAG	O5-C5-C6-O6
5	A	711	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	710	NAG	2	0
5	D	709	NAG	1	0
5	A	709	NAG	2	0
5	A	711	NAG	1	0
5	D	708	NAG	1	0
5	D	706	NAG	1	0
5	D	711	NAG	1	0
5	A	708	NAG	1	0
5	A	706	NAG	1	0
5	A	710	NAG	1	0

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-11822. 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 ⓘ
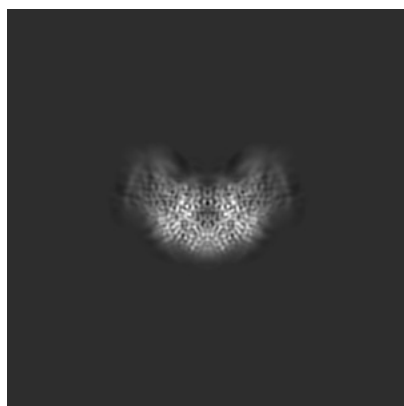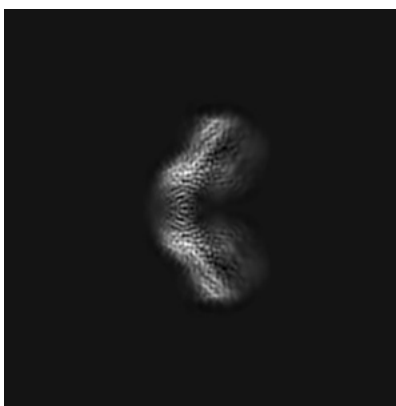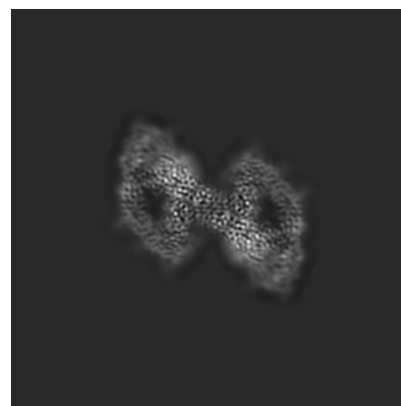
6.1.1　Primary map

| X | Y | Z |

6.1.2　Raw map

| X | Y | Z |
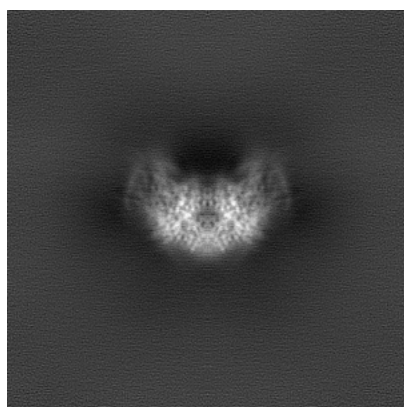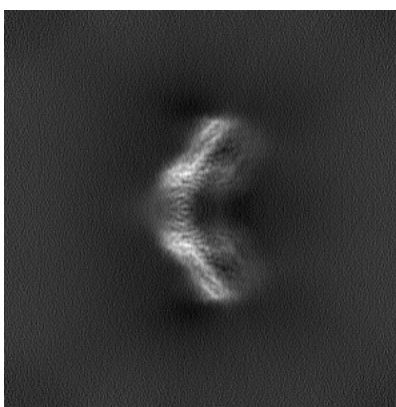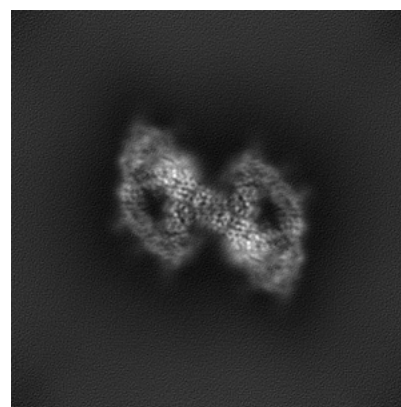
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
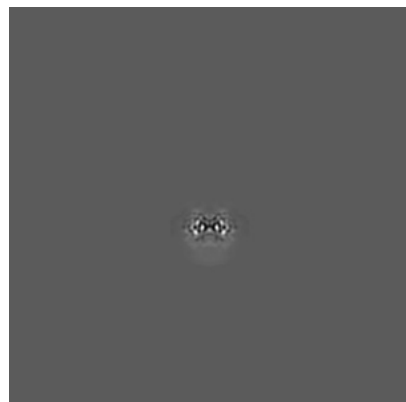
6.2.1 Primary map
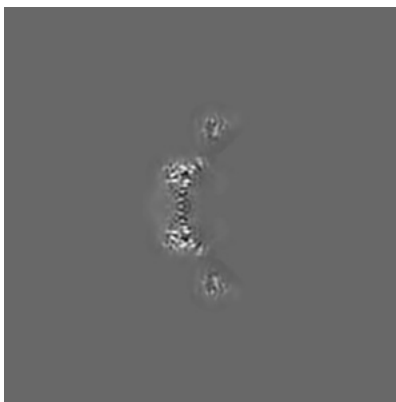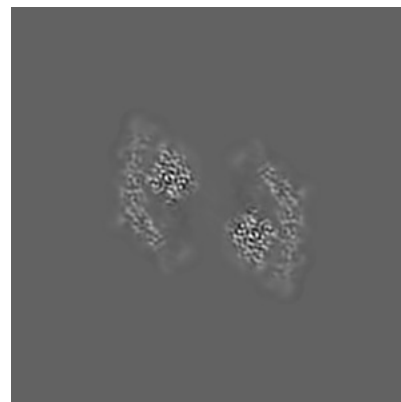
| X Index: 160 | Y Index: 160 | Z Index: 160 |

6.2.2 Raw map
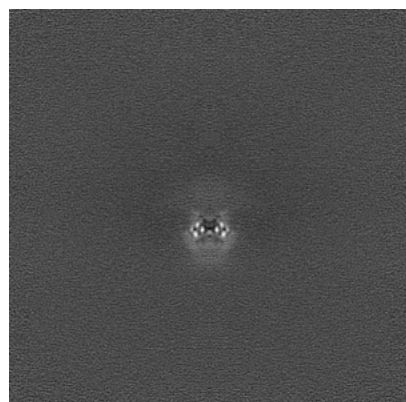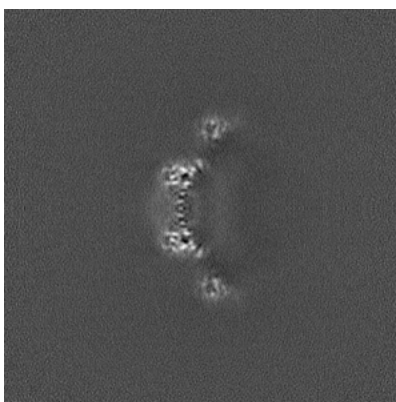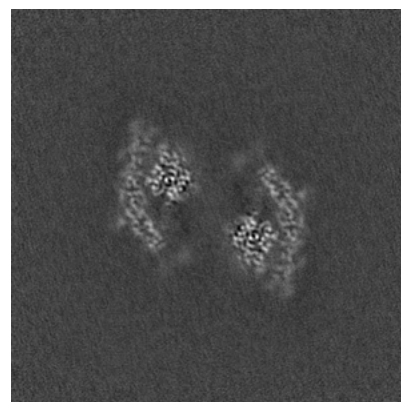
| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

6.3   Largest variance slices ⓘ
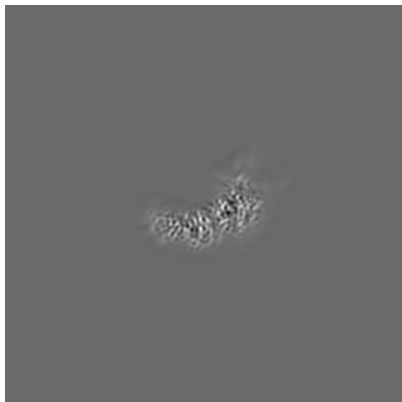
6.3.1   Primary map
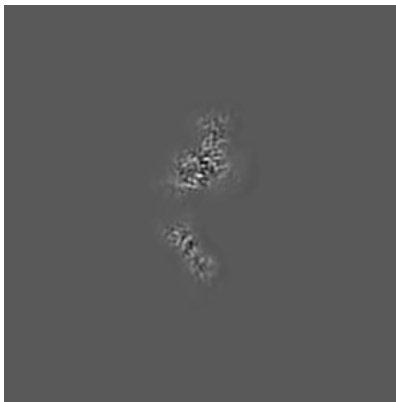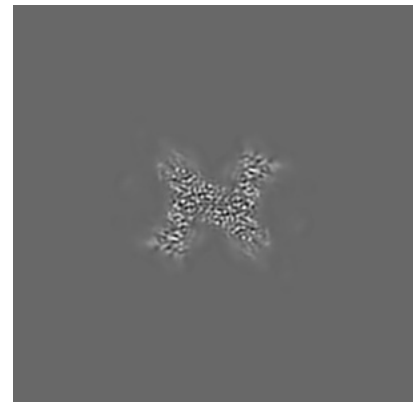
X Index: 131   Y Index: 138   Z Index: 145

6.3.2   Raw map
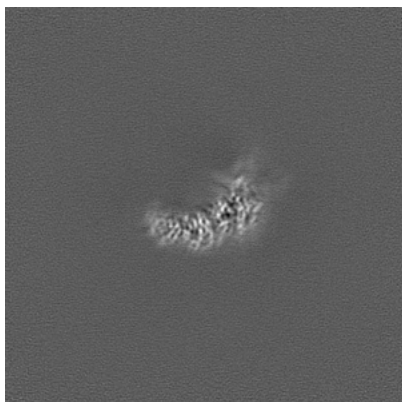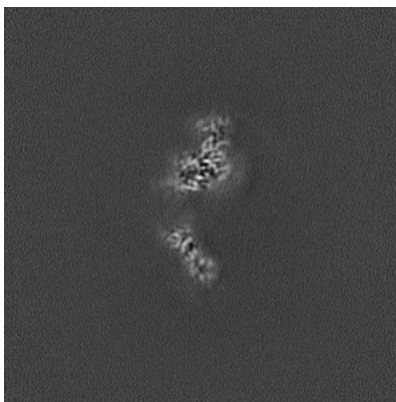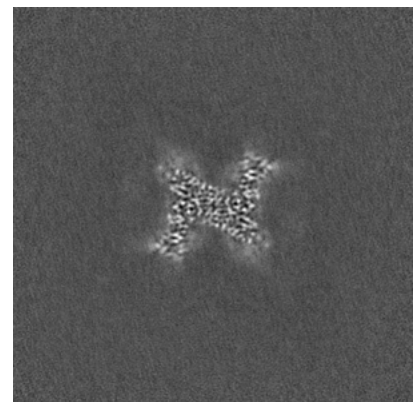
X Index: 131   Y Index: 138   Z Index: 144

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
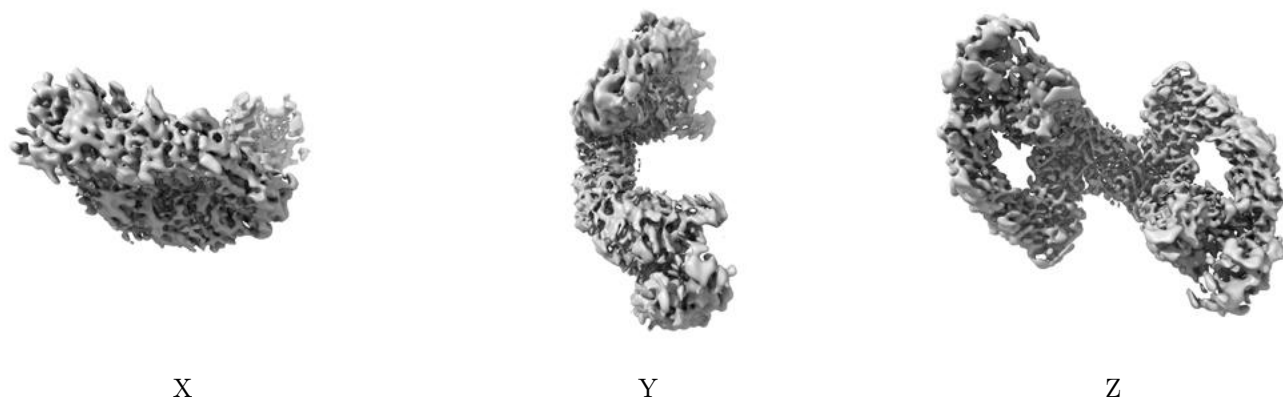
The images above show the 3D surface view of the map at the recommended contour level 0.269. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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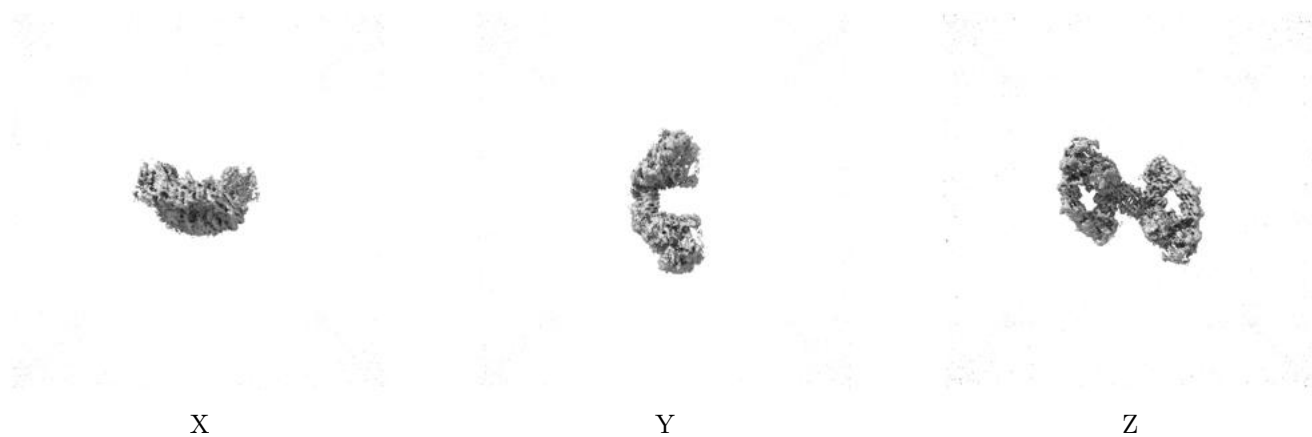
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

6.5.1 emd_11822_msk_1.map ⓘ

X   Y   Z
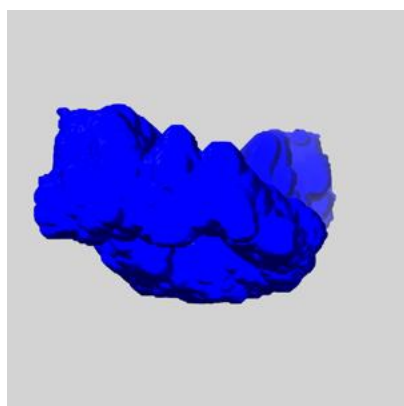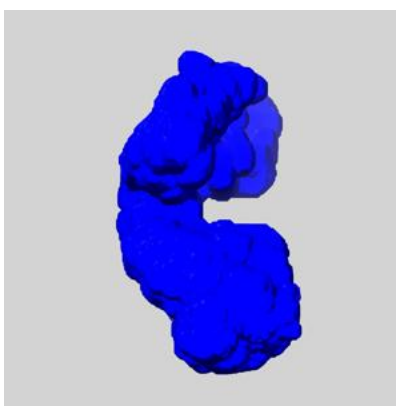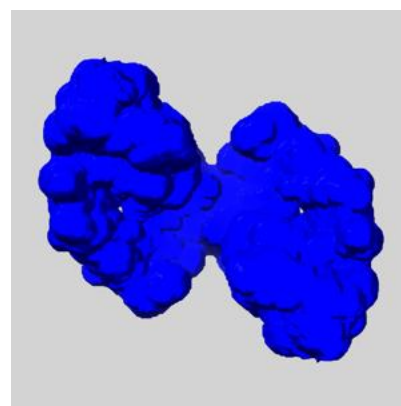
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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 ⓘ
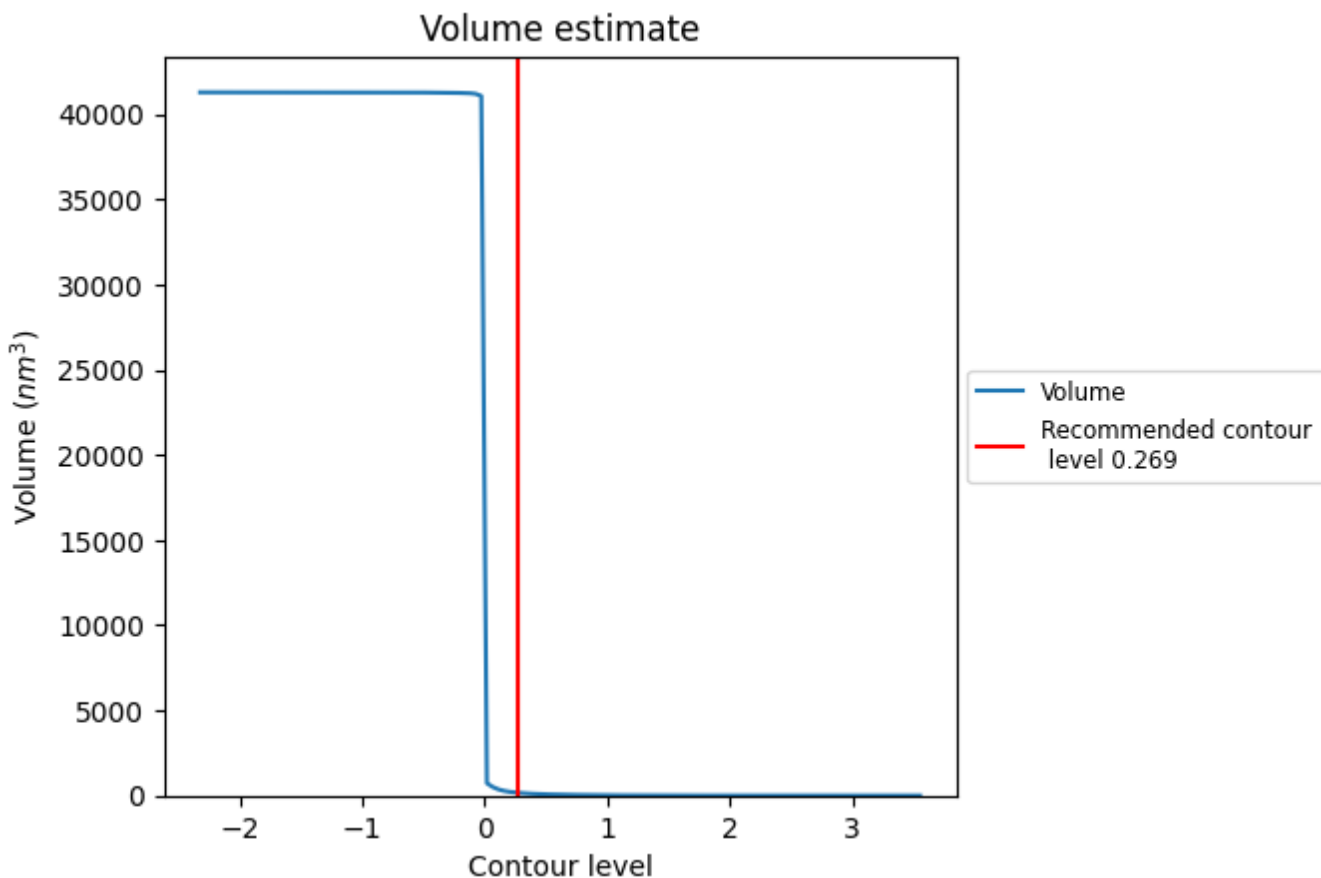
The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 kDa.

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)
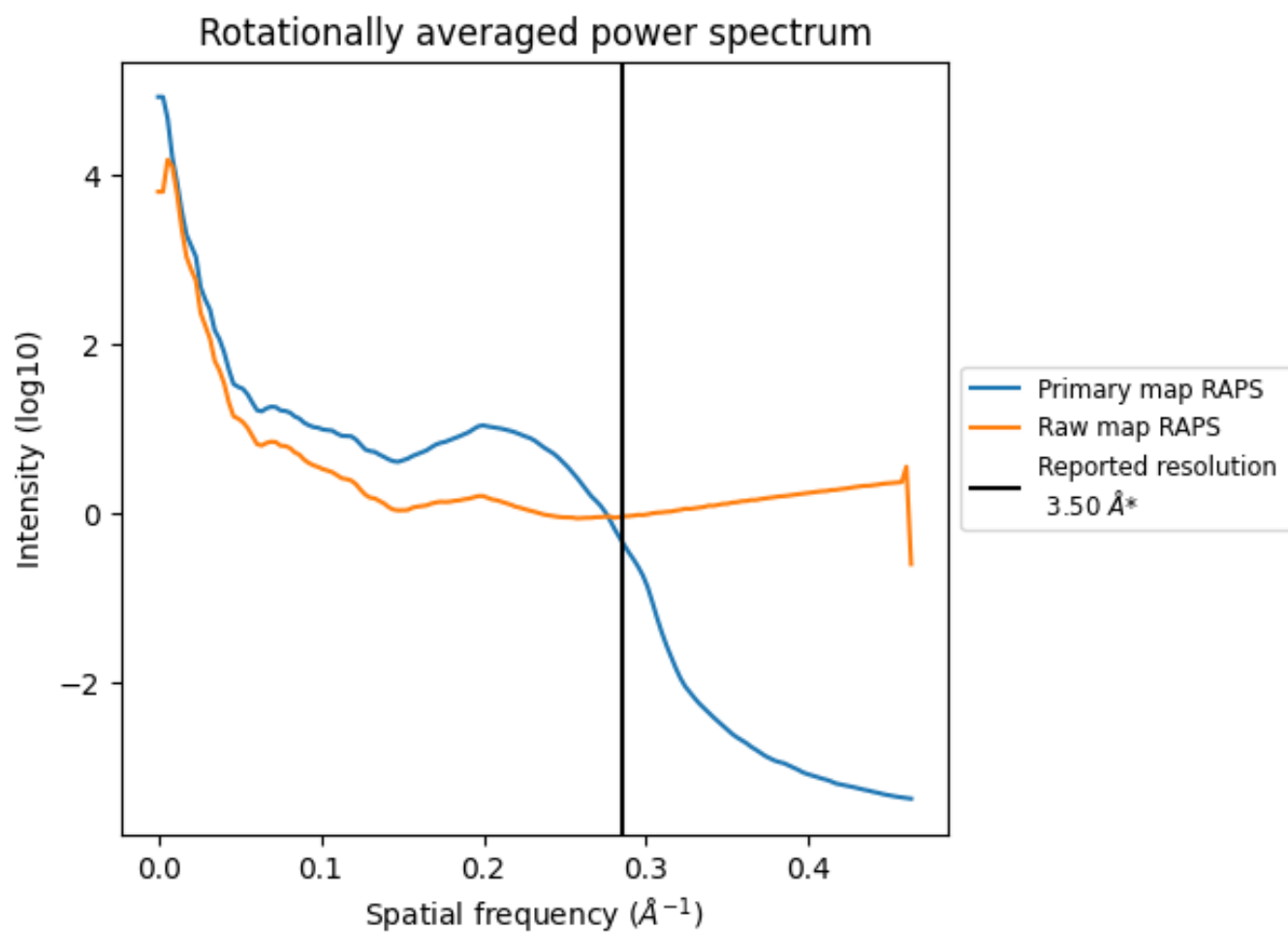
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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)
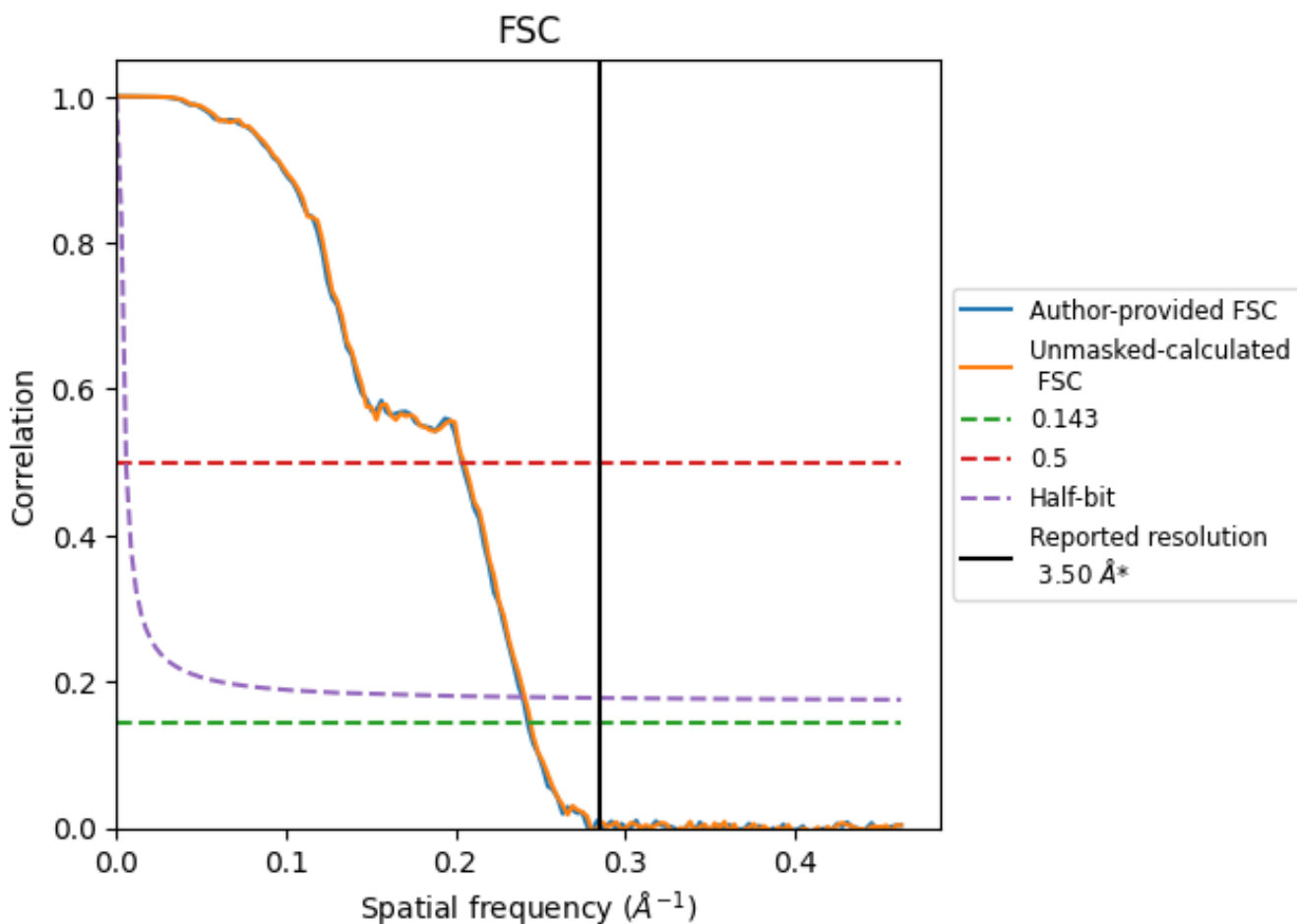
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	4.12	4.90	4.18
Unmasked-calculated*	4.09	4.88	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.5 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.5 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11822 and PDB model 7AML. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)

X　　　　　　　　　　　Y　　　　　　　　　　　Z
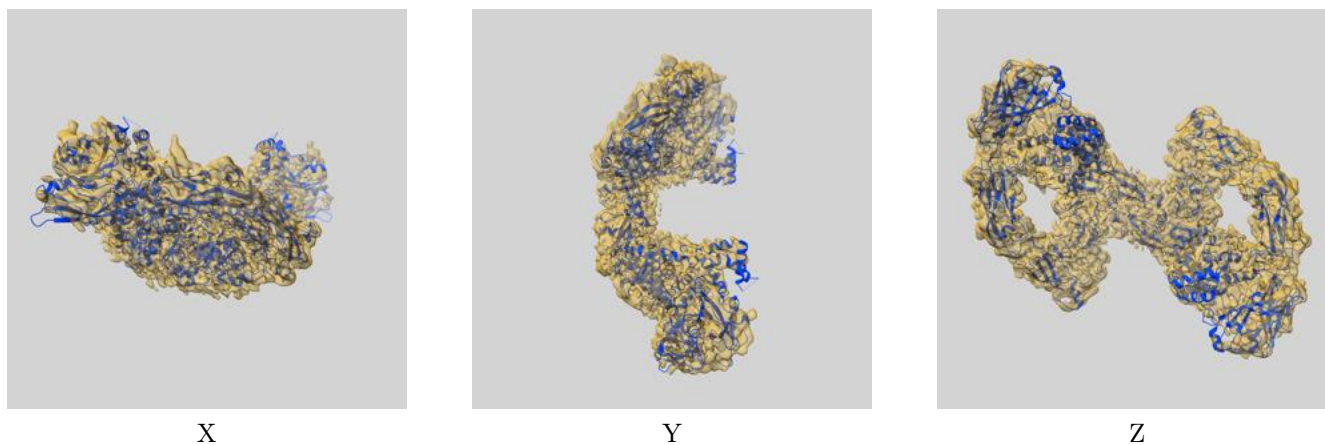
The images above show the 3D surface view of the map at the recommended contour level 0.269 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

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

9.3　Atom inclusion mapped to coordinate model ⓘ
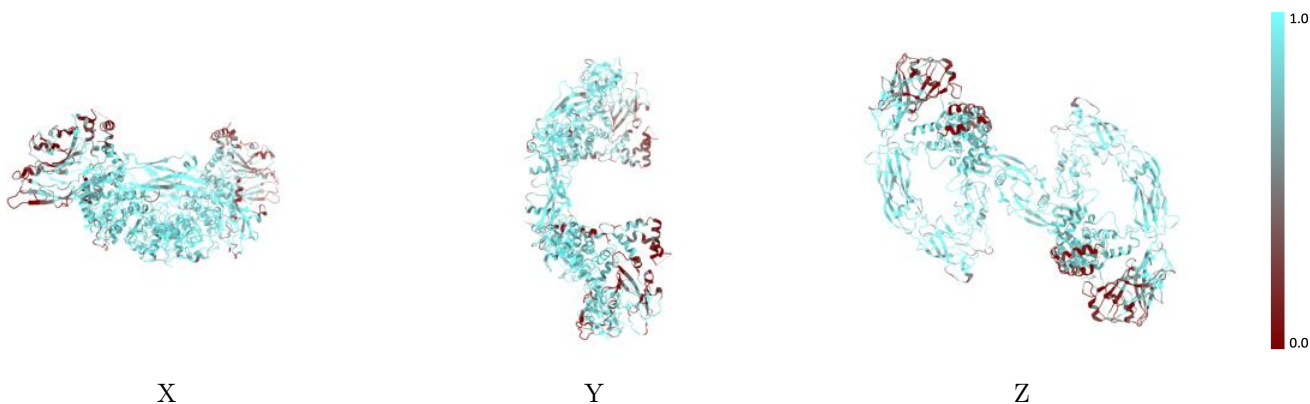
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.269).

9.4　Atom inclusion ⓘ
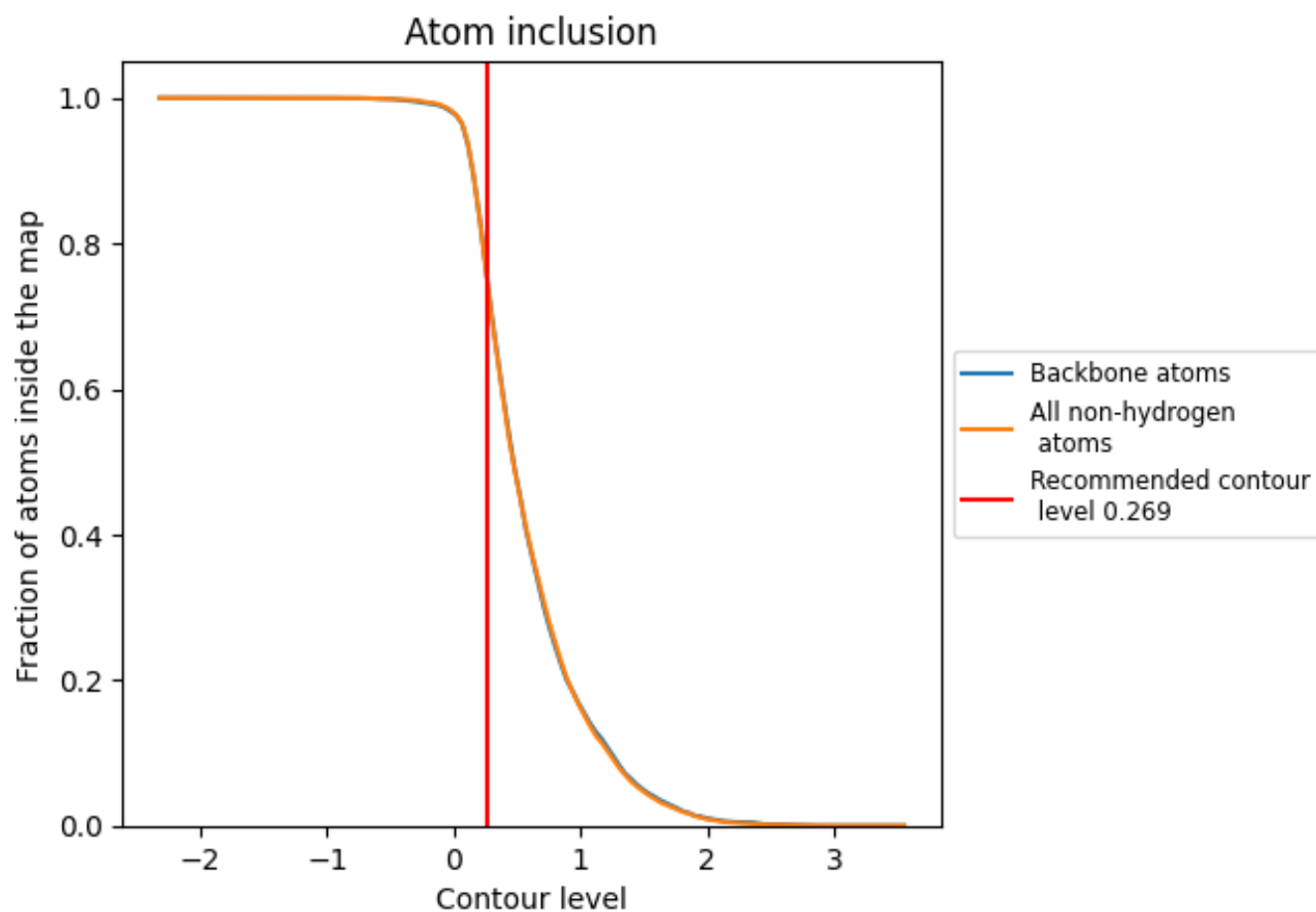
At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.269) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7406	0.3300
A	0.7145	0.3240
B	0.7544	0.3370
C	0.8780	0.3760
D	0.7126	0.3230
E	0.7415	0.3230
F	0.8615	0.3570

1.0

0.0
<0.0