



Full wwPDB EM Validation Report ⓘ

Oct 8, 2022 – 05:54 PM EDT

PDB ID : 7T9I
EMDB ID : EMD-25758
Title : Native human TSH bound to human Thyrotropin receptor in complex with miniGs399 (composite structure)
Authors : Faust, B.; Cheng, Y.; Manglik, A.
Deposited on : 2021-12-19
Resolution : 2.90 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

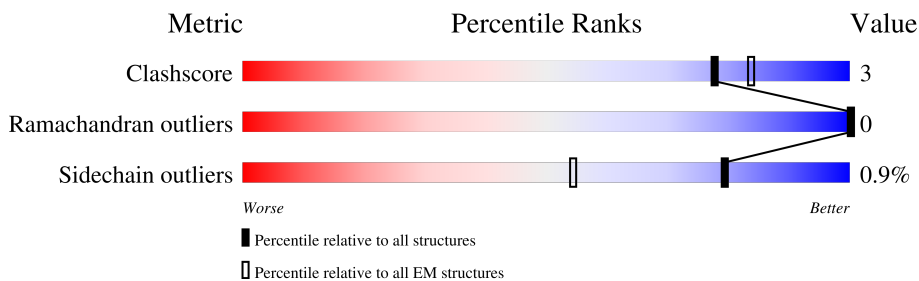
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	92	
2	B	112	
3	N	142	
4	R	702	
5	X	261	
6	Y	370	
7	Z	71	
8	C	2	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 23613 atoms, of which 11641 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 Glycoprotein hormones alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	86	1205	389	572	112	119	13	0	0

- Molecule 2 is a protein called Thyrotropin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	109	1636	539	791	137	155	14	0	0

- Molecule 3 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	N	126	1893	599	932	168	188	6	0	0

- Molecule 4 is a protein called Thyrotropin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	R	596	9416	3067	4721	750	842	36	0	0

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	13	ASP	-	expression tag	UNP A0A0A0MTJ0
R	14	TYR	-	expression tag	UNP A0A0A0MTJ0
R	15	LYS	-	expression tag	UNP A0A0A0MTJ0
R	16	ASP	-	expression tag	UNP A0A0A0MTJ0
R	17	ASP	-	expression tag	UNP A0A0A0MTJ0
R	18	ASP	-	expression tag	UNP A0A0A0MTJ0
R	19	ASP	-	expression tag	UNP A0A0A0MTJ0
R	20	GLY	-	expression tag	UNP A0A0A0MTJ0
R	21	THR	-	expression tag	UNP A0A0A0MTJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	ALA	deletion	UNP A0A0A0MTJ0
R	?	-	LEU	deletion	UNP A0A0A0MTJ0
R	?	-	ASN	deletion	UNP A0A0A0MTJ0
R	?	-	SER	deletion	UNP A0A0A0MTJ0
R	?	-	PRO	deletion	UNP A0A0A0MTJ0
R	?	-	LEU	deletion	UNP A0A0A0MTJ0
R	?	-	HIS	deletion	UNP A0A0A0MTJ0
R	?	-	GLN	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	TYR	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	ASN	deletion	UNP A0A0A0MTJ0
R	?	-	LEU	deletion	UNP A0A0A0MTJ0
R	?	-	GLY	deletion	UNP A0A0A0MTJ0
R	?	-	ASP	deletion	UNP A0A0A0MTJ0
R	?	-	SER	deletion	UNP A0A0A0MTJ0
R	?	-	ILE	deletion	UNP A0A0A0MTJ0
R	?	-	VAL	deletion	UNP A0A0A0MTJ0
R	?	-	GLY	deletion	UNP A0A0A0MTJ0
R	?	-	TYR	deletion	UNP A0A0A0MTJ0
R	?	-	LYS	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	LYS	deletion	UNP A0A0A0MTJ0
R	?	-	SER	deletion	UNP A0A0A0MTJ0
R	?	-	LYS	deletion	UNP A0A0A0MTJ0
R	?	-	PHE	deletion	UNP A0A0A0MTJ0
R	?	-	GLN	deletion	UNP A0A0A0MTJ0
R	?	-	ASP	deletion	UNP A0A0A0MTJ0
R	?	-	THR	deletion	UNP A0A0A0MTJ0
R	?	-	HIS	deletion	UNP A0A0A0MTJ0
R	?	-	ASN	deletion	UNP A0A0A0MTJ0
R	?	-	ASN	deletion	UNP A0A0A0MTJ0
R	?	-	ALA	deletion	UNP A0A0A0MTJ0
R	?	-	HIS	deletion	UNP A0A0A0MTJ0
R	?	-	TYR	deletion	UNP A0A0A0MTJ0
R	?	-	TYR	deletion	UNP A0A0A0MTJ0
R	?	-	VAL	deletion	UNP A0A0A0MTJ0
R	?	-	PHE	deletion	UNP A0A0A0MTJ0
R	?	-	PHE	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	GLN	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	ASP	deletion	UNP A0A0A0MTJ0
R	?	-	GLU	deletion	UNP A0A0A0MTJ0
R	?	-	ILE	deletion	UNP A0A0A0MTJ0
R	?	-	ILE	deletion	UNP A0A0A0MTJ0
R	?	-	GLY	deletion	UNP A0A0A0MTJ0
R	?	-	PHE	deletion	UNP A0A0A0MTJ0

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	X	221	3286	1089	1590	310	290	7	0	0

There are 95 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-7	GLY	-	expression tag	UNP P63092
X	-6	GLY	-	expression tag	UNP P63092
X	-5	SER	-	expression tag	UNP P63092
X	-4	LEU	-	expression tag	UNP P63092
X	-3	GLU	-	expression tag	UNP P63092
X	-2	VAL	-	expression tag	UNP P63092
X	-1	LEU	-	expression tag	UNP P63092
X	0	PHE	-	expression tag	UNP P63092
X	1	GLN	-	expression tag	UNP P63092
X	2	GLY	-	expression tag	UNP P63092
X	3	PRO	-	expression tag	UNP P63092
X	4	SER	-	expression tag	UNP P63092
X	5	GLY	-	expression tag	UNP P63092
X	6	ASN	-	expression tag	UNP P63092
X	7	SER	-	expression tag	UNP P63092
X	8	LYS	-	expression tag	UNP P63092
X	9	THR	-	expression tag	UNP P63092
X	10	GLU	-	expression tag	UNP P63092
X	11	ASP	-	expression tag	UNP P63092
X	12	GLN	-	expression tag	UNP P63092
X	13	ARG	-	expression tag	UNP P63092
X	14	ASN	-	expression tag	UNP P63092
X	15	GLU	-	expression tag	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
X	16	GLU	-	expression tag	UNP P63092
X	17	LYS	-	expression tag	UNP P63092
X	18	ALA	-	expression tag	UNP P63092
X	19	GLN	-	expression tag	UNP P63092
X	20	ARG	-	expression tag	UNP P63092
X	21	GLU	-	expression tag	UNP P63092
X	22	ALA	-	expression tag	UNP P63092
X	23	ASN	-	expression tag	UNP P63092
X	24	LYS	-	expression tag	UNP P63092
X	25	LYS	-	expression tag	UNP P63092
X	26	ILE	-	expression tag	UNP P63092
X	27	GLU	-	expression tag	UNP P63092
X	28	LYS	-	expression tag	UNP P63092
X	29	GLN	-	expression tag	UNP P63092
X	30	LEU	-	expression tag	UNP P63092
X	31	GLN	-	expression tag	UNP P63092
X	32	LYS	-	expression tag	UNP P63092
X	33	ASP	-	expression tag	UNP P63092
X	34	LYS	-	expression tag	UNP P63092
X	35	GLN	-	expression tag	UNP P63092
X	36	VAL	-	expression tag	UNP P63092
X	37	TYR	-	expression tag	UNP P63092
X	38	ARG	-	expression tag	UNP P63092
X	39	ALA	-	expression tag	UNP P63092
X	40	THR	-	expression tag	UNP P63092
X	41	HIS	-	expression tag	UNP P63092
X	42	ARG	-	expression tag	UNP P63092
X	43	LEU	-	expression tag	UNP P63092
X	44	LEU	-	expression tag	UNP P63092
X	45	LEU	-	expression tag	UNP P63092
X	46	LEU	-	expression tag	UNP P63092
X	47	GLY	-	expression tag	UNP P63092
X	48	ALA	-	expression tag	UNP P63092
X	49	ASP	-	expression tag	UNP P63092
X	50	ASN	-	expression tag	UNP P63092
X	51	SER	-	expression tag	UNP P63092
X	52	GLY	-	expression tag	UNP P63092
X	53	LYS	-	expression tag	UNP P63092
X	54	SER	-	expression tag	UNP P63092
X	55	THR	-	expression tag	UNP P63092
X	56	ILE	-	expression tag	UNP P63092
X	57	VAL	-	expression tag	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
X	58	LYS	-	expression tag	UNP P63092
X	59	GLN	-	expression tag	UNP P63092
X	60	MET	-	expression tag	UNP P63092
X	61	ARG	-	expression tag	UNP P63092
X	193	ILE	-	expression tag	UNP P63092
X	194	LEU	-	expression tag	UNP P63092
X	195	HIS	-	expression tag	UNP P63092
X	196	GLY	-	expression tag	UNP P63092
X	197	GLY	-	expression tag	UNP P63092
X	198	SER	-	expression tag	UNP P63092
X	199	GLY	-	expression tag	UNP P63092
X	200	GLY	-	expression tag	UNP P63092
X	201	SER	-	expression tag	UNP P63092
X	202	GLY	-	expression tag	UNP P63092
X	203	GLY	-	expression tag	UNP P63092
X	249	ASP	ALA	conflict	UNP P63092
X	252	ASP	SER	conflict	UNP P63092
X	?	-	ASN	deletion	UNP P63092
X	?	-	MET	deletion	UNP P63092
X	?	-	VAL	deletion	UNP P63092
X	?	-	ILE	deletion	UNP P63092
X	?	-	ARG	deletion	UNP P63092
X	?	-	GLU	deletion	UNP P63092
X	?	-	ASP	deletion	UNP P63092
X	?	-	ASN	deletion	UNP P63092
X	?	-	GLN	deletion	UNP P63092
X	?	-	THR	deletion	UNP P63092
X	308	LEU	ILE	conflict	UNP P63092
X	372	ALA	ILE	conflict	UNP P63092
X	375	ILE	VAL	conflict	UNP P63092

- Molecule 6 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	Y	338	5110	1604	2509	467	509	21	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-29	MET	-	initiating methionine	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-28	HIS	-	expression tag	UNP P62873
Y	-27	HIS	-	expression tag	UNP P62873
Y	-26	HIS	-	expression tag	UNP P62873
Y	-25	HIS	-	expression tag	UNP P62873
Y	-24	HIS	-	expression tag	UNP P62873
Y	-23	HIS	-	expression tag	UNP P62873
Y	-22	LEU	-	expression tag	UNP P62873
Y	-21	GLU	-	expression tag	UNP P62873
Y	-20	VAL	-	expression tag	UNP P62873
Y	-19	LEU	-	expression tag	UNP P62873
Y	-18	PHE	-	expression tag	UNP P62873
Y	-17	GLN	-	expression tag	UNP P62873
Y	-16	GLY	-	expression tag	UNP P62873
Y	-15	PRO	-	expression tag	UNP P62873
Y	-14	GLU	-	expression tag	UNP P62873
Y	-13	ASP	-	expression tag	UNP P62873
Y	-12	GLN	-	expression tag	UNP P62873
Y	-11	VAL	-	expression tag	UNP P62873
Y	-10	ASP	-	expression tag	UNP P62873
Y	-9	PRO	-	expression tag	UNP P62873
Y	-8	ARG	-	expression tag	UNP P62873
Y	-7	LEU	-	expression tag	UNP P62873
Y	-6	ILE	-	expression tag	UNP P62873
Y	-5	ASP	-	expression tag	UNP P62873
Y	-4	GLY	-	expression tag	UNP P62873
Y	-3	LYS	-	expression tag	UNP P62873
Y	-2	GLY	-	expression tag	UNP P62873
Y	-1	SER	-	expression tag	UNP P62873
Y	0	SER	-	expression tag	UNP P62873
Y	1	GLY	-	expression tag	UNP P62873

- Molecule 7 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

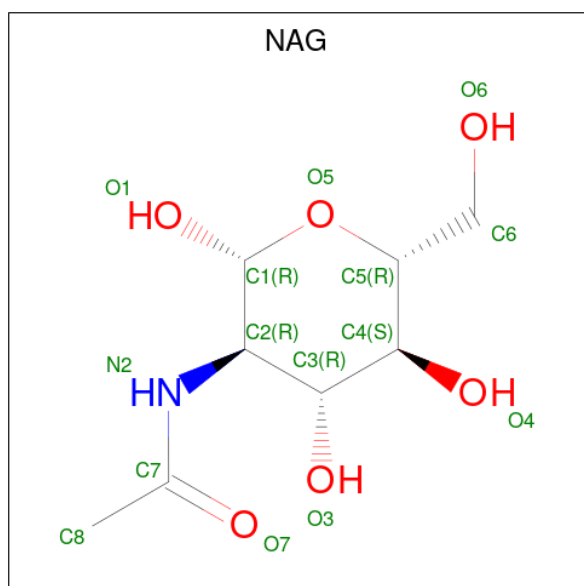
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	Z	56	871	269	442	76	81	3	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	C	2	28	16	2	10	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

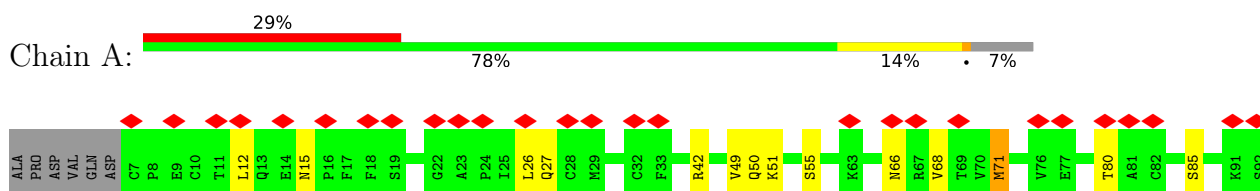


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
9	A	1	28	8	14	1	5	0
9	B	1	28	8	14	1	5	0
9	R	1	112	32	56	4	20	0
9	R	1	112	32	56	4	20	0
9	R	1	112	32	56	4	20	0
9	R	1	112	32	56	4	20	0

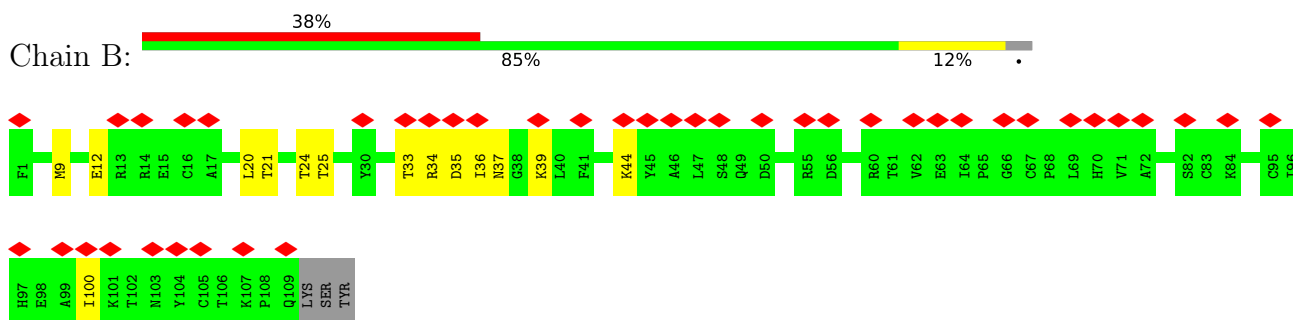
3 Residue-property plots

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.

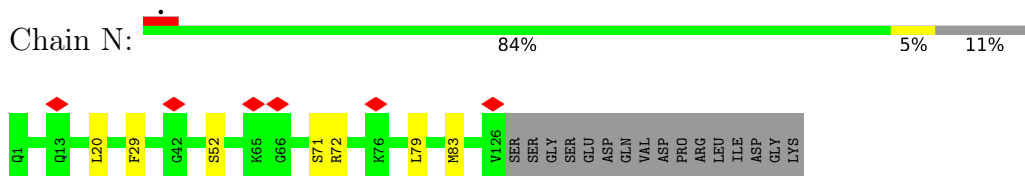
- Molecule 1: Glycoprotein hormones alpha chain



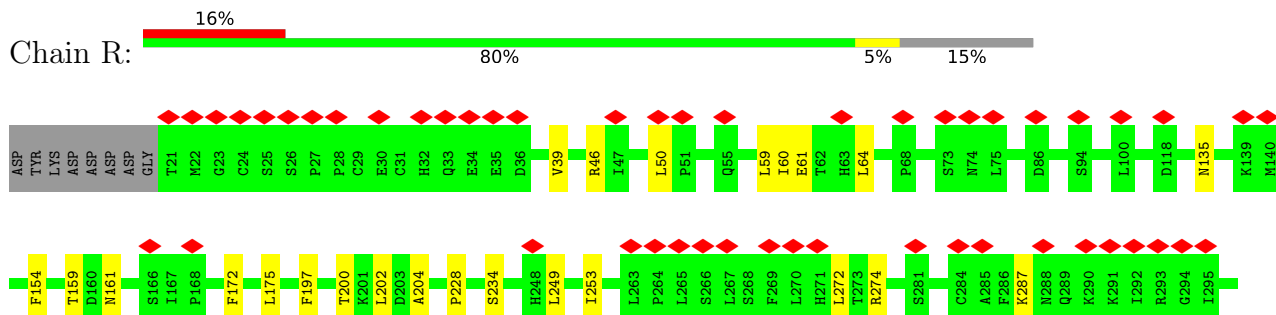
- Molecule 2: Thyrotropin subunit beta

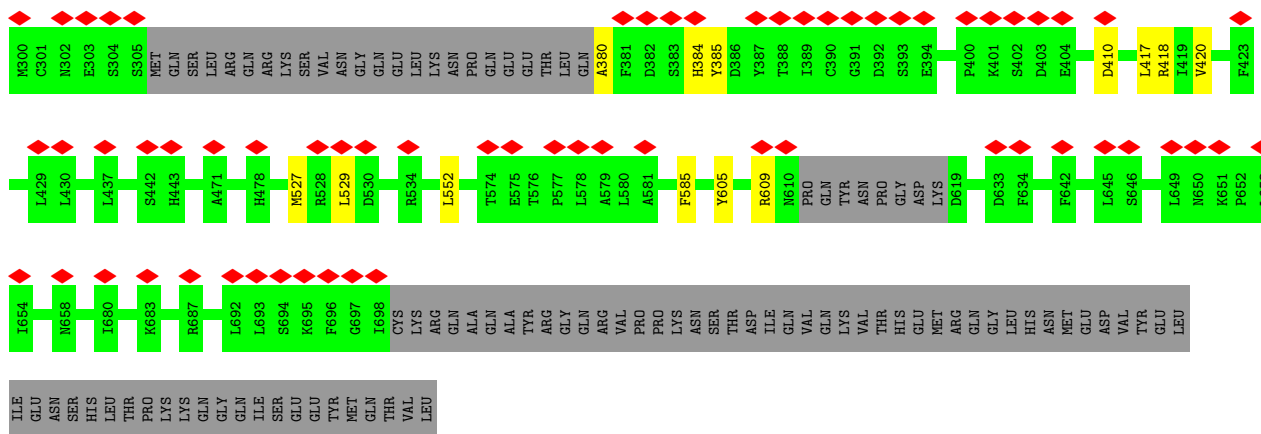


- Molecule 3: Nanobody 35

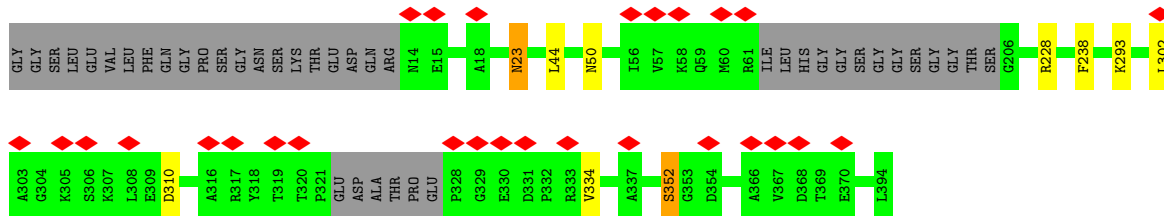
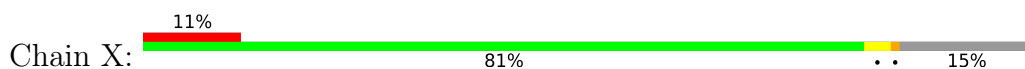


- Molecule 4: Thyrotropin receptor

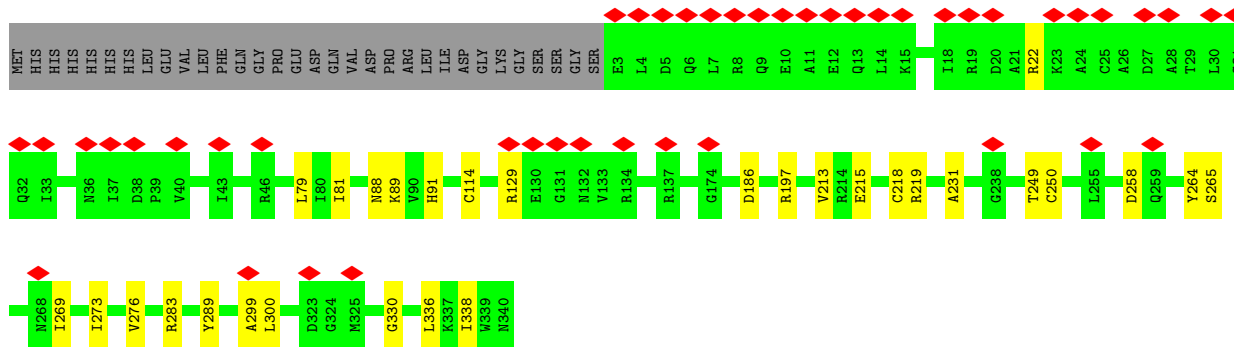
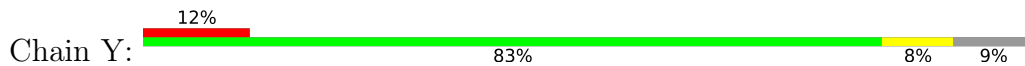




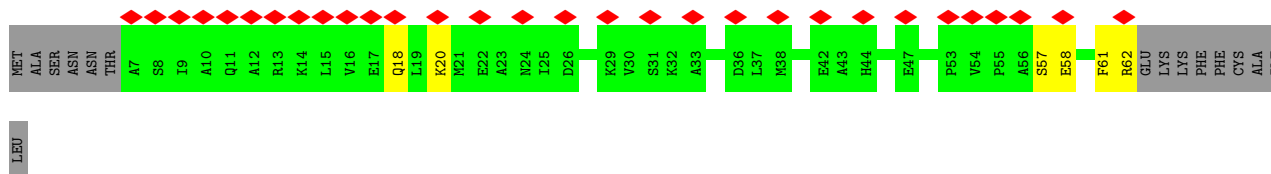
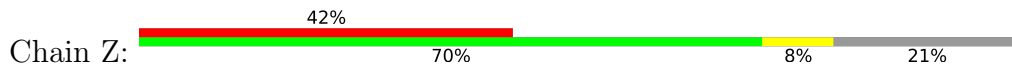
• Molecule 5: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



• Molecule 6: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



• Molecule 7: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	77	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.803	Depositor
Minimum map value	-0.321	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.327	Depositor
Map size (Å)	338.944, 338.944, 338.944	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.662, 0.662, 0.662	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

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	0.53	0/647	0.86	1/879 (0.1%)
2	B	0.34	0/868	0.72	0/1184
3	N	0.32	0/981	0.66	0/1329
4	R	0.28	0/4808	0.55	0/6544
5	X	0.33	0/1731	0.65	0/2344
6	Y	0.28	0/2648	0.65	0/3589
7	Z	0.32	0/435	0.67	0/587
All	All	0.32	0/12118	0.63	1/16456 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	15	ASN	CB-CA-C	-5.20	99.99	110.40

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	633	572	587	10	0
2	B	845	791	791	11	0
3	N	961	932	932	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	4695	4721	4719	19	0
5	X	1696	1590	1587	7	0
6	Y	2601	2509	2505	20	0
7	Z	429	442	441	4	0
8	C	28	0	25	3	0
9	A	14	14	13	0	0
9	B	14	14	13	0	0
9	R	56	56	52	0	0
All	All	11972	11641	11665	68	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 3.

All (68) 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)
6:Y:218:CYS:O	7:Z:18:GLN:NE2	2.14	0.80
5:X:23:ASN:OD1	6:Y:88:ASN:OD1	2.02	0.77
4:R:410:ASP:OD2	4:R:418:ARG:NH2	2.25	0.69
7:Z:57:SER:OG	7:Z:58:GLU:OE1	2.14	0.65
6:Y:338:ILE:HG21	7:Z:61:PHE:CE2	2.32	0.64
6:Y:22:ARG:NE	6:Y:258:ASP:O	2.31	0.63
4:R:60:ILE:HG22	4:R:61:GLU:HG3	1.80	0.62
6:Y:215:GLU:OE2	6:Y:219:ARG:NH2	2.32	0.62
4:R:605:TYR:OH	4:R:609:ARG:NH1	2.33	0.62
2:B:44:LYS:HE2	4:R:204:ALA:HB2	1.82	0.61
6:Y:330:GLY:HA2	6:Y:336:LEU:HD23	1.81	0.61
5:X:228:ARG:NH1	6:Y:186:ASP:OD1	2.34	0.60
1:A:42:ARG:NH2	2:B:12:GLU:OE1	2.35	0.59
2:B:20:LEU:HD23	2:B:21:THR:N	2.18	0.58
5:X:44:LEU:HD22	5:X:238:PHE:CG	2.39	0.58
4:R:154:PHE:CE1	4:R:175:LEU:HD21	2.39	0.58
6:Y:197:ARG:O	6:Y:213:VAL:HG12	2.03	0.58
3:N:52:SER:O	3:N:72:ARG:NH1	2.38	0.56
1:A:71:MET:O	1:A:71:MET:HE2	2.04	0.56
1:A:50:GLN:O	8:C:1:NAG:H81	2.06	0.56
4:R:197:PHE:HB3	4:R:202:LEU:HD11	1.90	0.54
4:R:380:ALA:O	4:R:384:HIS:ND1	2.38	0.54
6:Y:250:CYS:SG	6:Y:273:ILE:HD13	2.48	0.54
6:Y:81:ILE:HG22	6:Y:91:HIS:HB2	1.90	0.53
1:A:27:GLN:NE2	2:B:37:ASN:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:79:LEU:HD11	6:Y:114:CYS:HB3	1.90	0.52
2:B:33:THR:O	2:B:34:ARG:NH2	2.42	0.52
3:N:29:PHE:O	3:N:72:ARG:NH2	2.44	0.51
5:X:302:LEU:HD21	5:X:334:VAL:HG23	1.92	0.51
6:Y:88:ASN:OD1	6:Y:89:LYS:N	2.44	0.50
6:Y:283:ARG:HD3	6:Y:300:LEU:HD12	1.93	0.50
4:R:172:PHE:HB2	4:R:200:THR:HG21	1.94	0.50
1:A:49:VAL:HG12	4:R:135:ASN:OD1	2.12	0.49
1:A:12:LEU:HD22	1:A:26:LEU:HB3	1.95	0.49
4:R:39:VAL:HG11	4:R:50:LEU:HD12	1.95	0.49
6:Y:283:ARG:CD	6:Y:300:LEU:HD12	2.43	0.48
1:A:71:MET:C	1:A:71:MET:SD	2.92	0.48
3:N:71:SER:O	3:N:79:LEU:HD12	2.14	0.48
5:X:50:ASN:O	5:X:293:LYS:NZ	2.44	0.48
4:R:552:LEU:HD21	4:R:585:PHE:HE2	1.77	0.48
2:B:35:ASP:N	2:B:35:ASP:OD1	2.47	0.47
2:B:36:ILE:O	2:B:39:LYS:NZ	2.34	0.47
2:B:24:THR:OG1	2:B:25:THR:N	2.48	0.47
7:Z:20:LYS:HE3	7:Z:20:LYS:HA	1.95	0.47
6:Y:231:ALA:HB1	6:Y:276:VAL:HG22	1.95	0.47
6:Y:330:GLY:CA	6:Y:336:LEU:HD23	2.45	0.46
6:Y:249:THR:HG22	6:Y:265:SER:HB3	1.97	0.45
4:R:417:LEU:HA	4:R:420:VAL:HG12	1.98	0.45
2:B:9:MET:CE	2:B:24:THR:HG21	2.47	0.44
4:R:234:SER:OG	4:R:253:ILE:HG22	2.17	0.44
5:X:310:ASP:N	5:X:310:ASP:OD1	2.50	0.44
2:B:9:MET:HE3	2:B:24:THR:HG21	2.00	0.43
5:X:352:SER:O	5:X:352:SER:OG	2.33	0.43
8:C:1:NAG:H4	8:C:2:NAG:H2	1.65	0.42
1:A:66:ASN:HB2	1:A:68:VAL:HG13	2.01	0.42
4:R:228:PRO:O	4:R:249:LEU:HD23	2.20	0.42
1:A:71:MET:O	1:A:71:MET:SD	2.78	0.42
2:B:100:ILE:HG23	4:R:60:ILE:HG21	2.01	0.41
4:R:159:THR:O	4:R:161:ASN:ND2	2.53	0.41
4:R:272:LEU:HD11	4:R:274:ARG:O	2.20	0.41
6:Y:269:ILE:HG21	6:Y:289:TYR:CE2	2.55	0.41
8:C:1:NAG:H3	8:C:1:NAG:H82	2.02	0.41
4:R:59:LEU:HD13	4:R:64:LEU:HD11	2.02	0.41
1:A:49:VAL:HG13	1:A:49:VAL:O	2.21	0.41
4:R:527:MET:O	4:R:529:LEU:N	2.53	0.41
6:Y:81:ILE:O	6:Y:81:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:20:LEU:HD11	3:N:83:MET:SD	2.61	0.40
6:Y:264:TYR:OH	6:Y:299:ALA:O	2.21	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	84/92 (91%)	74 (88%)	10 (12%)	0	100	100
2	B	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
3	N	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
4	R	590/702 (84%)	570 (97%)	20 (3%)	0	100	100
5	X	215/261 (82%)	208 (97%)	7 (3%)	0	100	100
6	Y	336/370 (91%)	328 (98%)	8 (2%)	0	100	100
7	Z	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
All	All	1510/1750 (86%)	1455 (96%)	55 (4%)	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	72/83 (87%)	67 (93%)	5 (7%)	15	41
2	B	93/102 (91%)	93 (100%)	0	100	100
3	N	104/118 (88%)	104 (100%)	0	100	100
4	R	528/636 (83%)	525 (99%)	3 (1%)	86	96
5	X	158/228 (69%)	156 (99%)	2 (1%)	69	90
6	Y	281/309 (91%)	280 (100%)	1 (0%)	91	97
7	Z	45/58 (78%)	44 (98%)	1 (2%)	52	81
All	All	1281/1534 (84%)	1269 (99%)	12 (1%)	79	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	55	SER
1	A	71	MET
1	A	80	THR
1	A	85	SER
4	R	46	ARG
4	R	287	LYS
4	R	385	TYR
5	X	23	ASN
5	X	352	SER
6	Y	129	ARG
7	Z	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	1	8,1	14,14,15	0.33	0	17,19,21	1.38	4 (23%)
8	NAG	C	2	8	14,14,15	0.39	0	17,19,21	0.79	1 (5%)

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
8	NAG	C	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1	NAG	C1-O5-C5	2.49	115.56	112.19
8	C	1	NAG	O5-C5-C6	-2.47	103.34	107.20
8	C	2	NAG	C1-O5-C5	2.36	115.39	112.19
8	C	1	NAG	O5-C1-C2	-2.17	107.86	111.29
8	C	1	NAG	O4-C4-C5	2.04	114.37	109.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

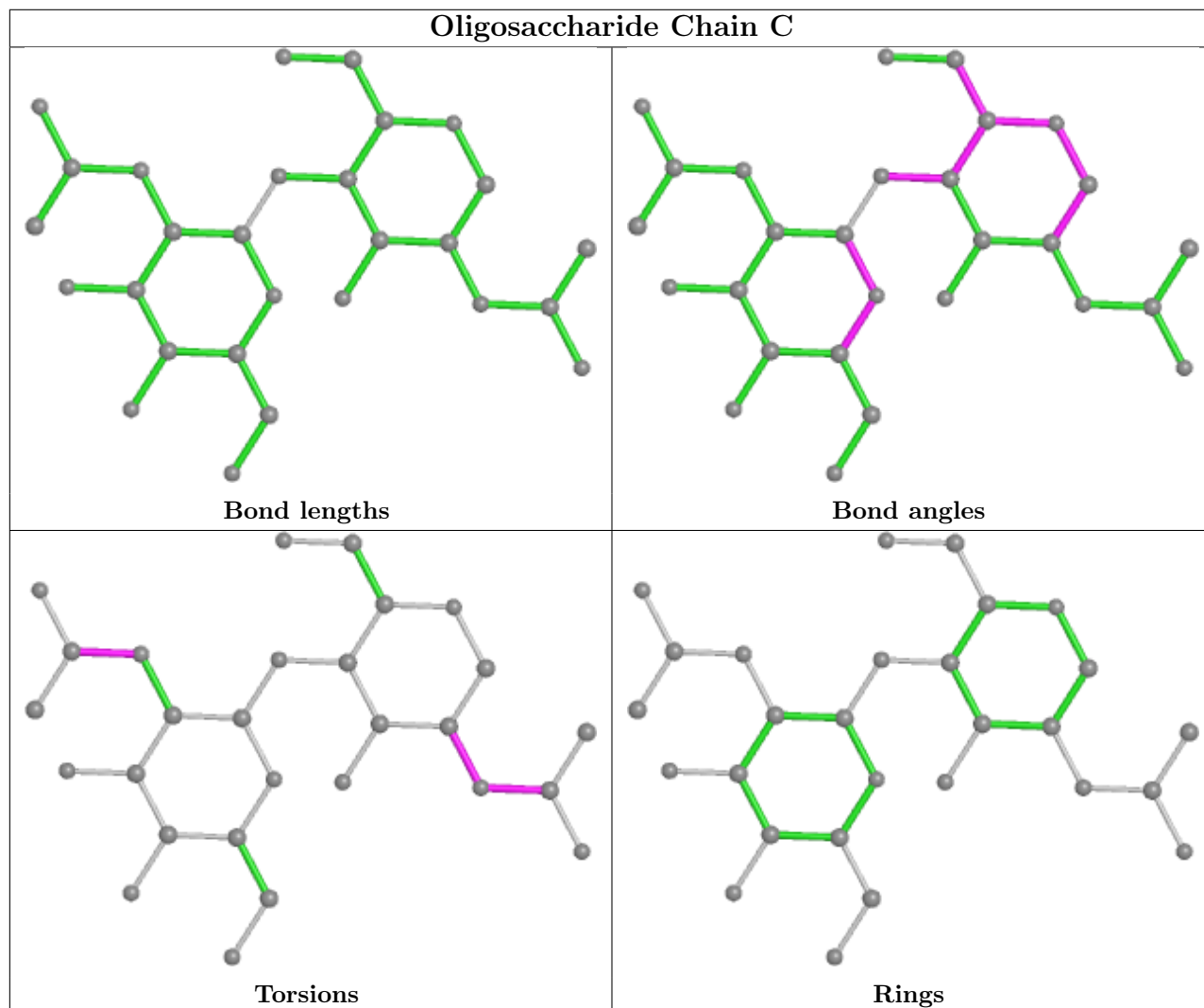
Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C8-C7-N2-C2
8	C	1	NAG	O7-C7-N2-C2
8	C	2	NAG	C8-C7-N2-C2
8	C	2	NAG	O7-C7-N2-C2
8	C	1	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1	NAG	3	0
8	C	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	NAG	R	803	4	14,14,15	0.19	0	17,19,21	0.44	0
9	NAG	A	101	1	14,14,15	0.25	0	17,19,21	1.28	2 (11%)
9	NAG	B	201	2	14,14,15	0.23	0	17,19,21	0.43	0
9	NAG	R	801	4	14,14,15	0.26	0	17,19,21	0.53	0
9	NAG	R	804	4	14,14,15	0.17	0	17,19,21	0.45	0
9	NAG	R	802	4	14,14,15	0.30	0	17,19,21	0.46	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
9	NAG	R	803	4	-	0/6/23/26	0/1/1/1
9	NAG	A	101	1	-	1/6/23/26	0/1/1/1
9	NAG	B	201	2	-	2/6/23/26	0/1/1/1
9	NAG	R	801	4	-	1/6/23/26	0/1/1/1
9	NAG	R	804	4	-	2/6/23/26	0/1/1/1
9	NAG	R	802	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	101	NAG	C1-O5-C5	2.63	115.76	112.19
9	A	101	NAG	O5-C1-C2	-2.62	107.14	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	R	804	NAG	C4-C5-C6-O6
9	B	201	NAG	O5-C5-C6-O6
9	R	804	NAG	O5-C5-C6-O6
9	B	201	NAG	C4-C5-C6-O6
9	A	101	NAG	O5-C5-C6-O6
9	R	801	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

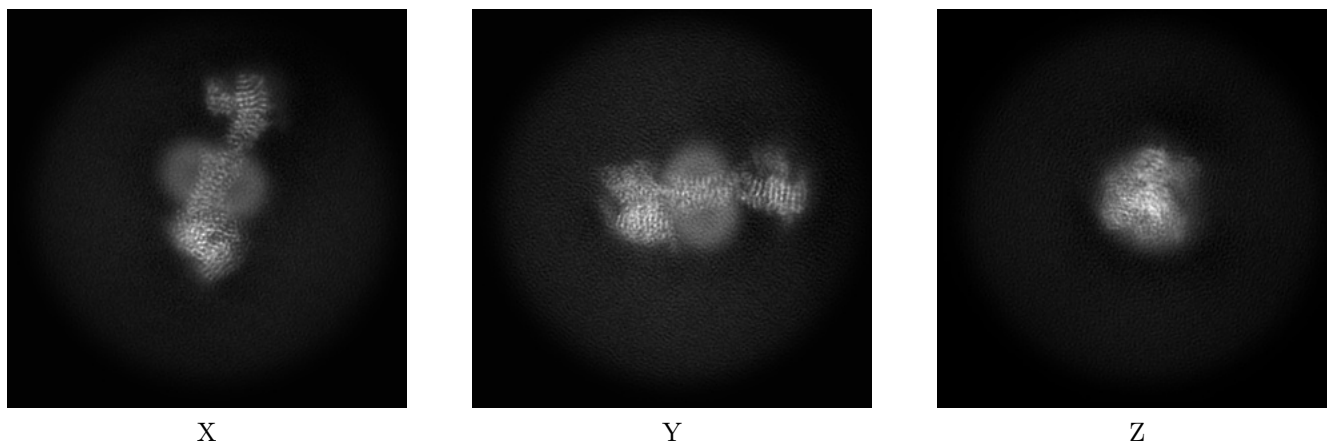
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25758. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

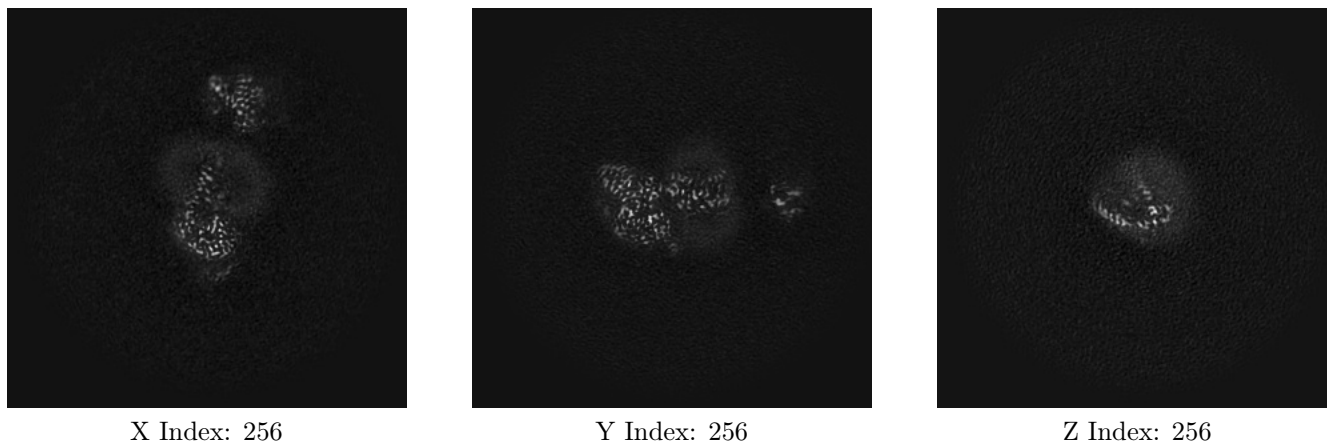
6.1.1 Primary map



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

6.2 Central slices [i](#)

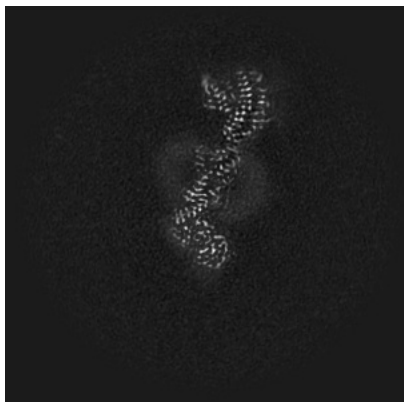
6.2.1 Primary map



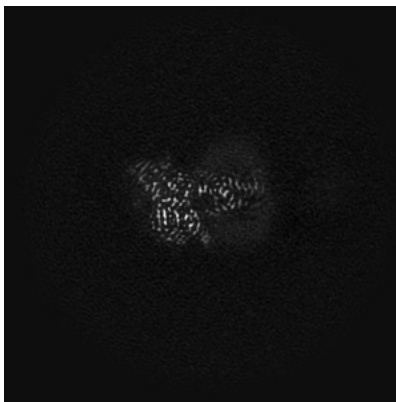
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

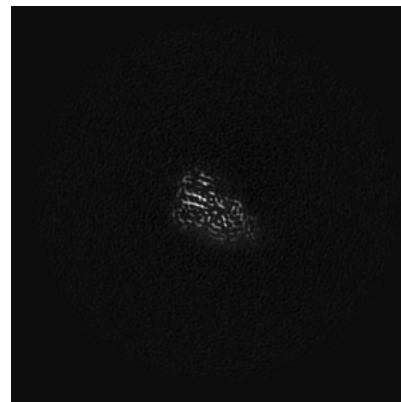
6.3.1 Primary map



X Index: 275



Y Index: 249



Z Index: 228

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

6.4 Orthogonal surface views [i](#)

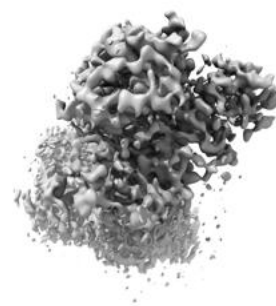
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.327. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

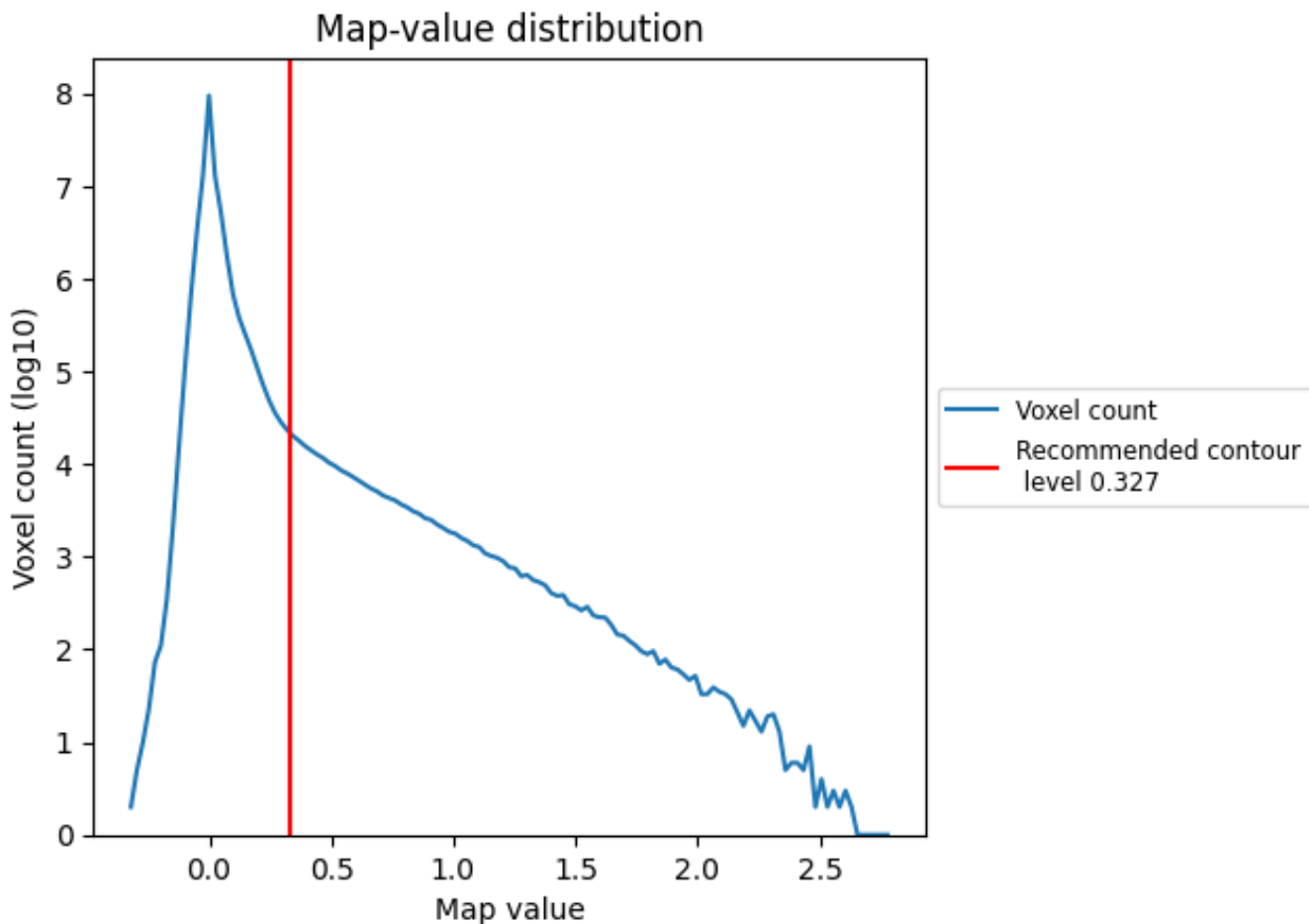
6.5 Mask visualisation

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

7 Map analysis [i](#)

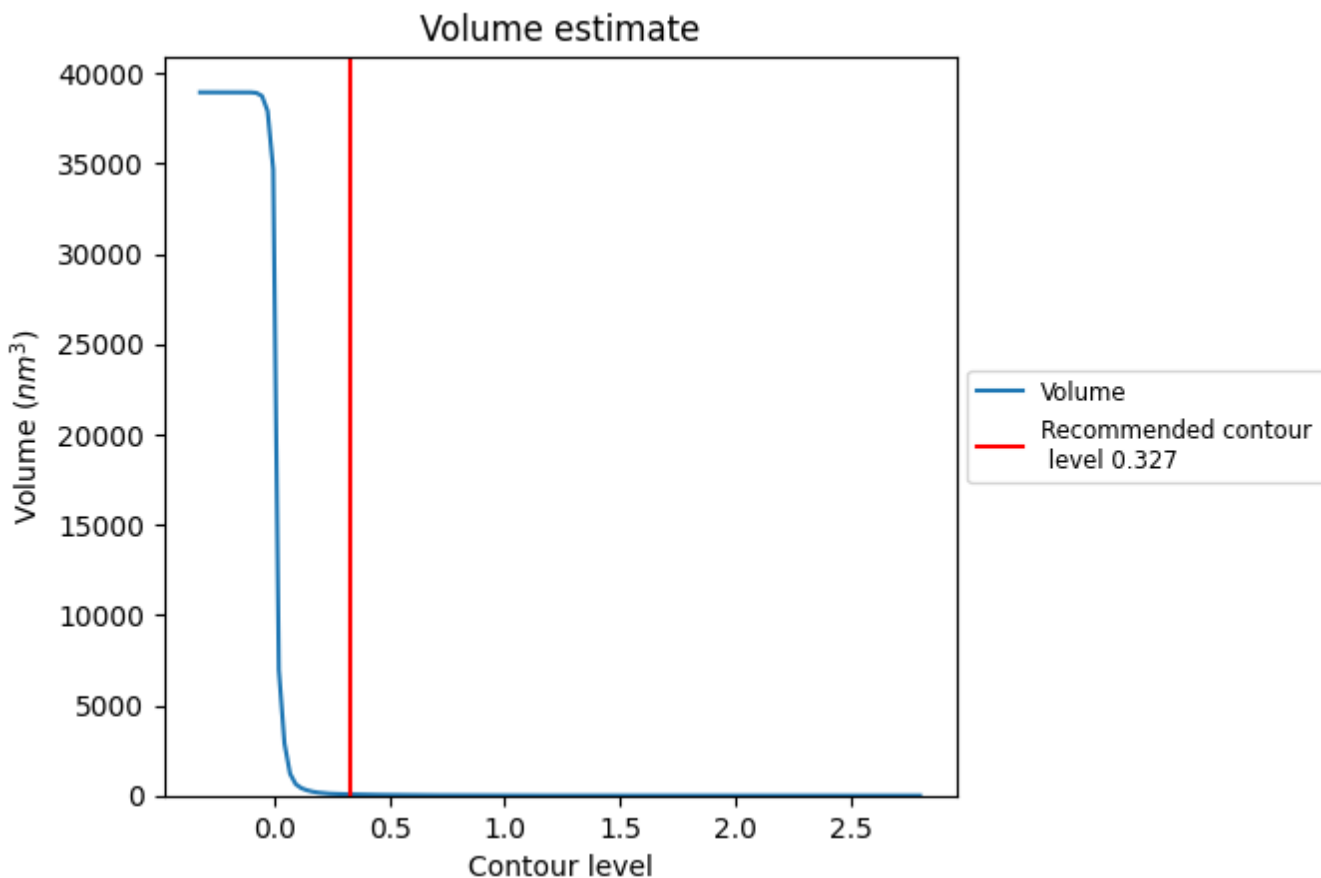
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

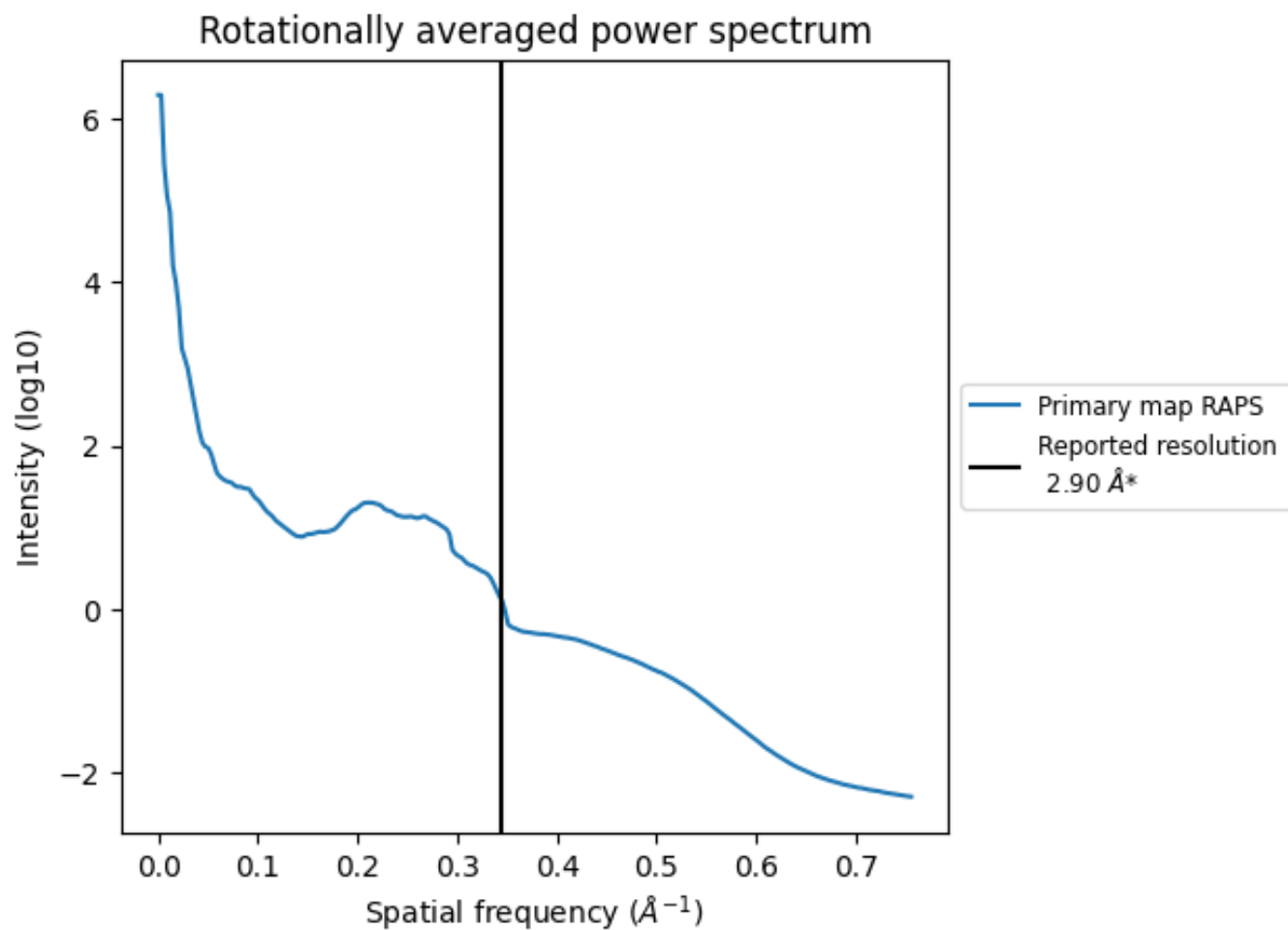
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm³; this corresponds to an approximate mass of 61 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 0.345 Å⁻¹

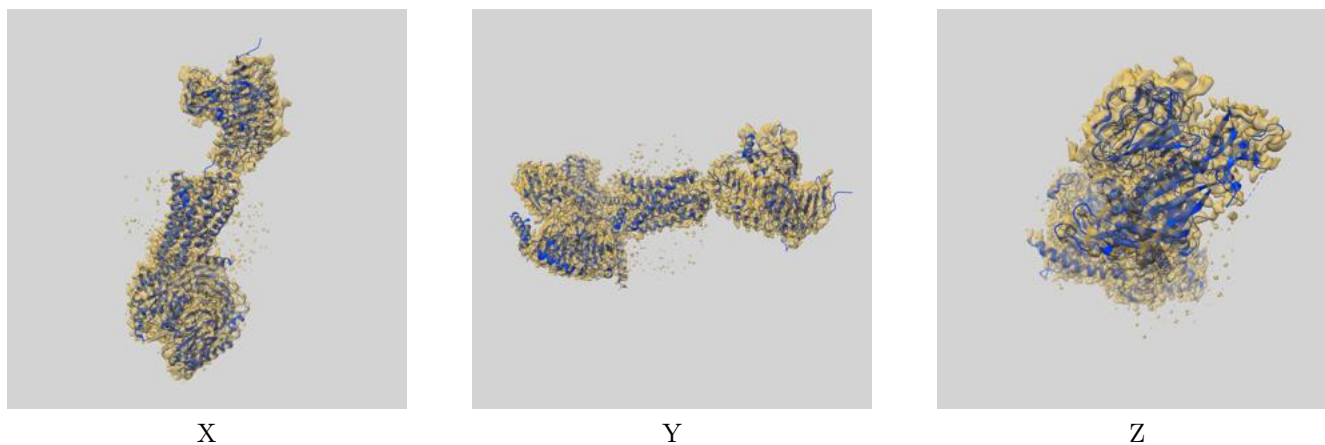
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

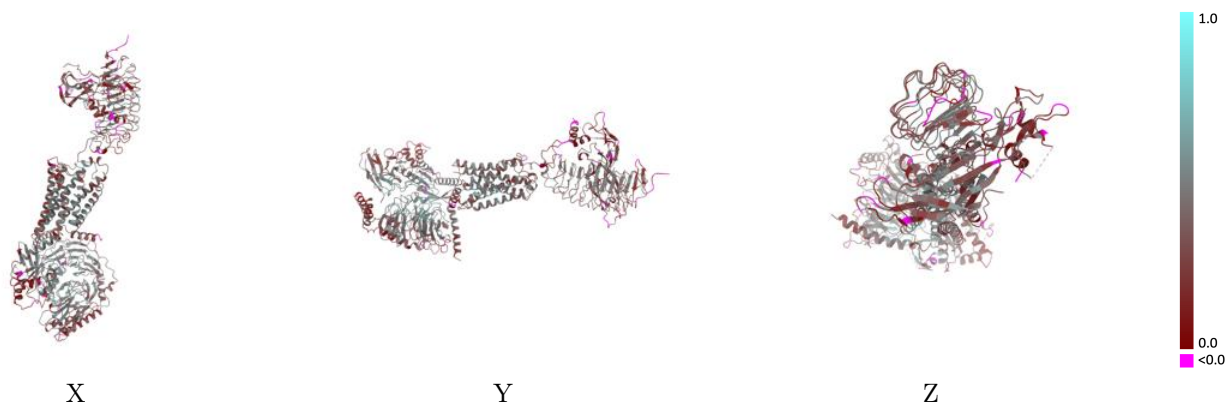
This section contains information regarding the fit between EMDB map EMD-25758 and PDB model 7T9I. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



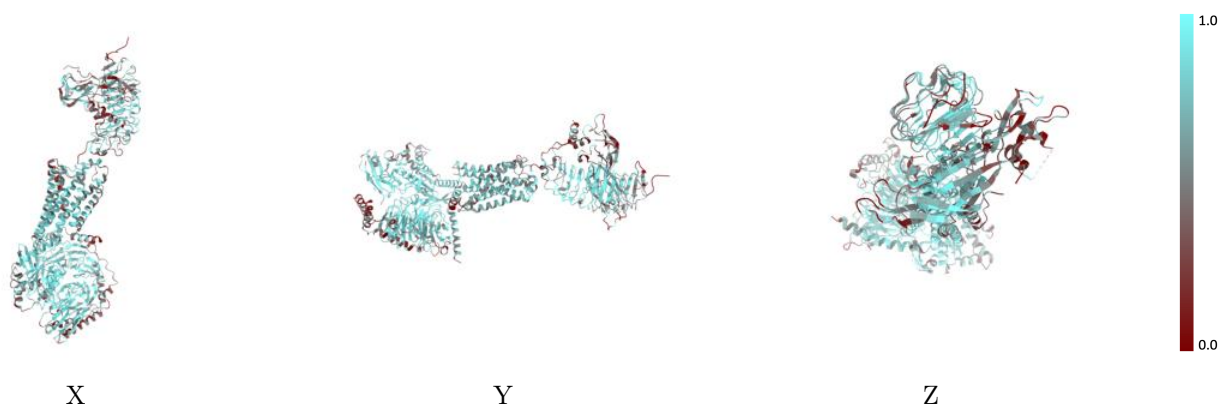
The images above show the 3D surface view of the map at the recommended contour level 0.327 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



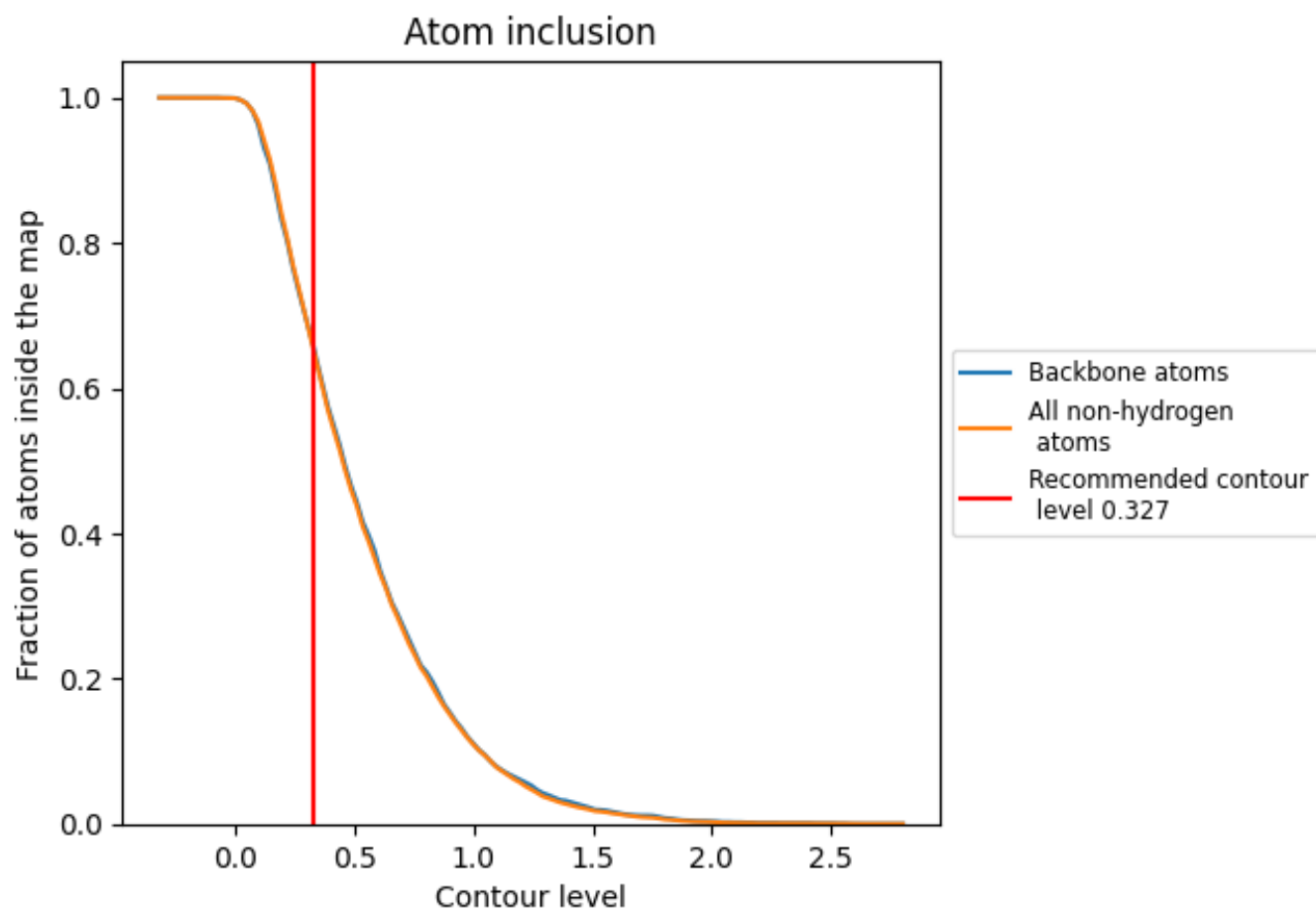
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.327).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 65% 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 (0.327) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6525	 0.3750
A	 0.5479	 0.2940
B	 0.5018	 0.2820
C	 0.5000	 0.2660
N	 0.7836	 0.4420
R	 0.6243	 0.3660
X	 0.7735	 0.3920
Y	 0.7355	 0.4260
Z	 0.3626	 0.2560

