



# wwPDB EM Validation Summary Report ⓘ

Oct 8, 2022 – 08:18 PM EDT

PDB ID : 7UTZ  
EMDB ID : EMD-26795  
Title : Human thyrotropin analog TR1402 bound to human Thyrotropin receptor in complex with miniGs399 (composite structure)  
Authors : Faust, B.; Cheng, Y.; Manglik, A.  
Deposited on : 2022-04-28  
Resolution : 2.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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  
buster-report : 1.1.7 (2018)  
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

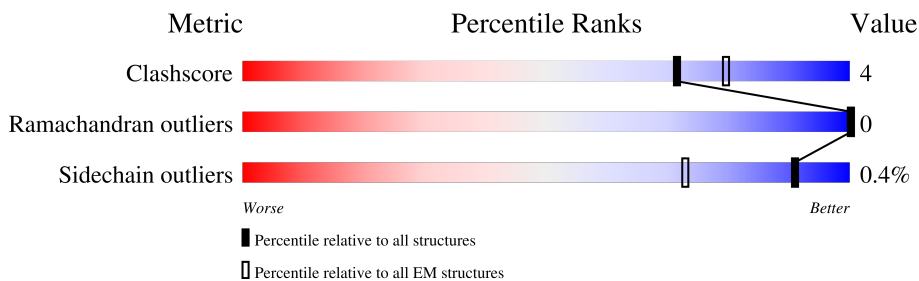
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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  $\geq 3$ , 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	701	
5	X	261	
6	Y	370	
7	Z	71	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 23845 atoms, of which 11798 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 analog TR1402.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	86	1273	404	620	120	116	13	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ARG	GLN	conflict	UNP P01215
A	14	ARG	GLU	conflict	UNP P01215
A	16	ARG	PRO	conflict	UNP P01215
A	20	ARG	GLN	conflict	UNP P01215

- Molecule 2 is a protein called Thyrotropin subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	109	1648	542	800	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	600	9460	3082	4739	754	849	36	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	14	ASP	-	expression tag	UNP A0A0A0MTJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
R	15	TYR	-	expression tag	UNP A0A0A0MTJ0
R	16	LYS	-	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	ASP	-	expression tag	UNP A0A0A0MTJ0
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

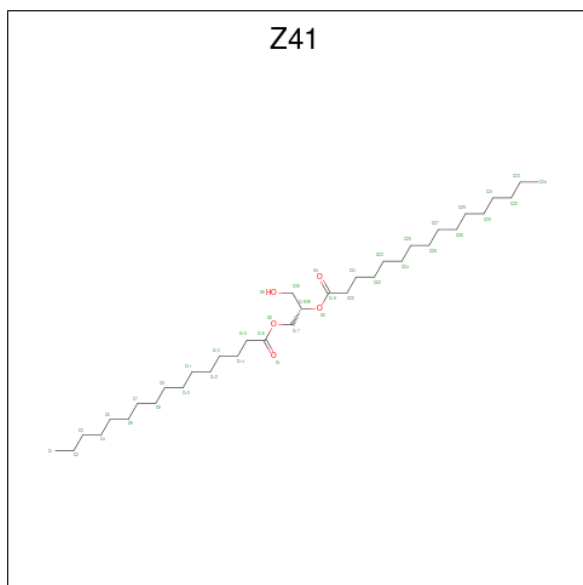
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
8	A	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	A	1	Total	C	H	N	O	0
			56	16	28	2	10	
8	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
8	R	1	Total	C	H	N	O	0
			112	32	56	4	20	
8	R	1	Total	C	H	N	O	0
			112	32	56	4	20	
8	R	1	Total	C	H	N	O	0
			112	32	56	4	20	
8	R	1	Total	C	H	N	O	0
			112	32	56	4	20	

- Molecule 9 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (three-letter code: Z41) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>5</sub>).

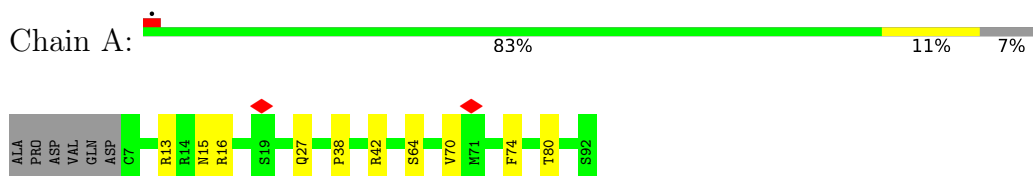


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	R	1	108	35	68	5	0

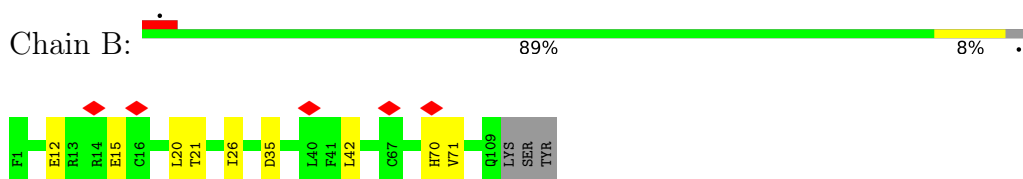
### 3 Residue-property plots

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.

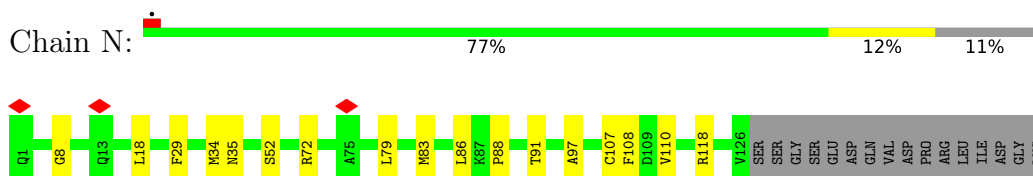
- Molecule 1: Glycoprotein hormones alpha chain analog TR1402



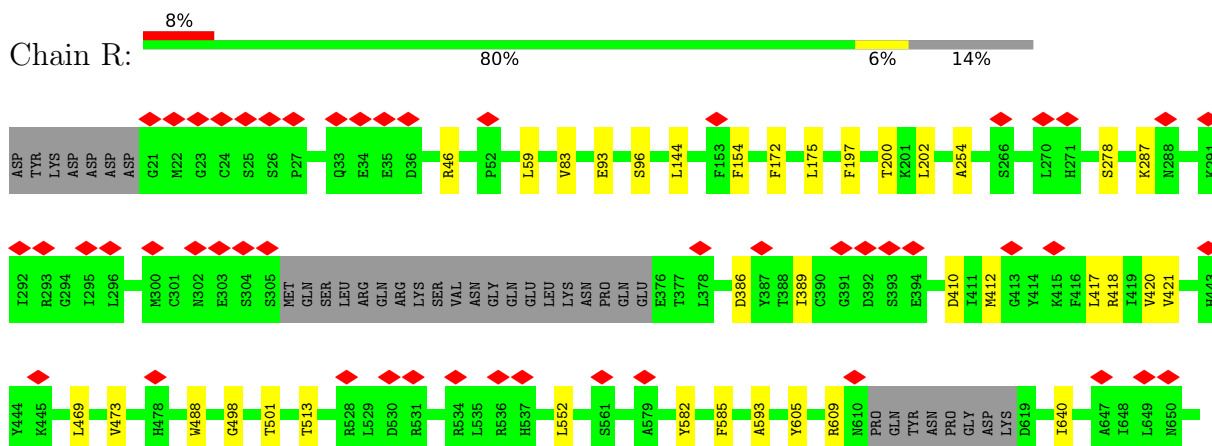
- Molecule 2: Thyrotropin subunit beta

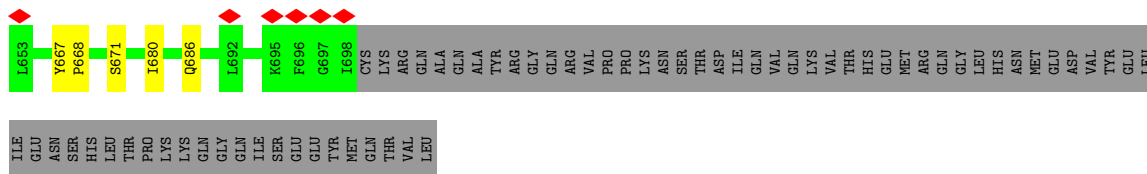


- Molecule 3: Nanobody 35

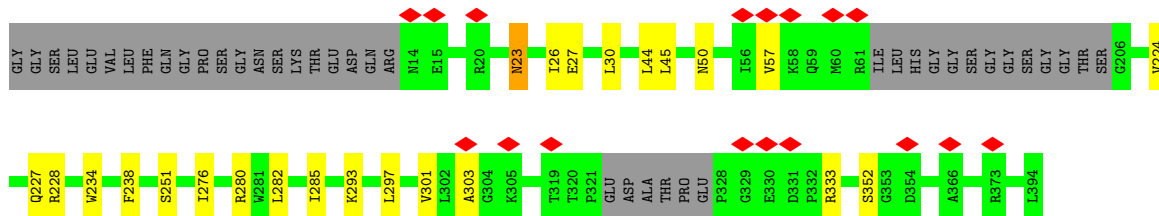
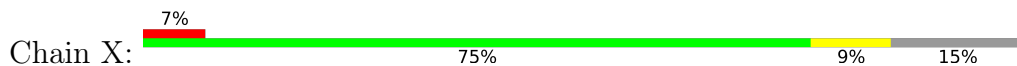


- Molecule 4: Thyrotropin receptor

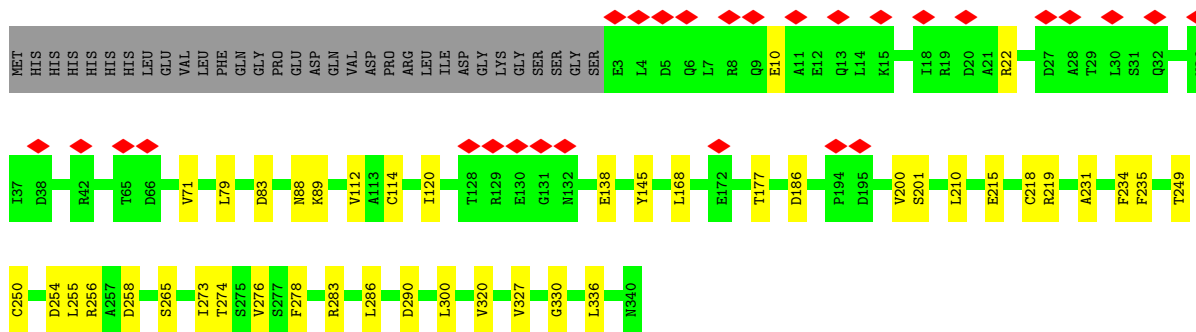
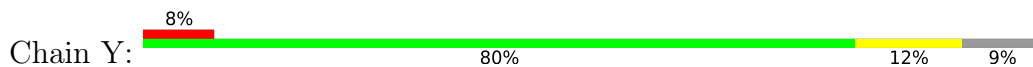




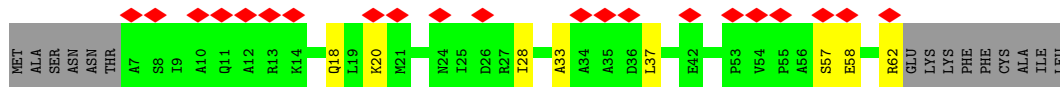
• Molecule 5: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



• 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375930	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.517	Depositor
Minimum map value	-1.237	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.596	Depositor
Map size (Å)	345.69598, 345.69598, 345.69598	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Z41, 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	0.27	0/668	0.63	0/903
2	B	0.27	0/871	0.55	0/1188
3	N	0.29	0/981	0.62	0/1329
4	R	0.26	0/4834	0.51	0/6580
5	X	0.29	0/1731	0.59	0/2344
6	Y	0.27	0/2648	0.61	0/3589
7	Z	0.29	0/435	0.55	0/587
All	All	0.27	0/12168	0.56	0/16520

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	X	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	X	303	ALA	Mainchain
5	X	352	SER	Mainchain

## 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	653	620	619	7	0
2	B	848	800	800	7	0
3	N	961	932	932	10	0
4	R	4721	4739	4736	23	0
5	X	1696	1590	1587	13	0
6	Y	2601	2509	2505	30	0
7	Z	429	442	441	7	0
8	A	28	28	26	0	0
8	B	14	14	13	0	0
8	R	56	56	52	0	0
9	R	40	68	0	0	0
All	All	12047	11798	11711	84	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 4.

The worst 5 of 84 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:71:VAL:HG21	6:Y:112:VAL:HG21	1.63	0.81
4:R:410:ASP:OD2	4:R:418:ARG:NH2	2.22	0.73
6:Y:215:GLU:OE2	6:Y:219:ARG:NH2	2.23	0.72
7:Z:57:SER:OG	7:Z:58:GLU:OE1	2.14	0.66
5:X:228:ARG:NH1	6:Y:186:ASP:OD1	2.30	0.65

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%)	81 (96%)	3 (4%)	0	100	100
2	B	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
3	N	124/142 (87%)	119 (96%)	5 (4%)	0	100	100
4	R	594/701 (85%)	574 (97%)	20 (3%)	0	100	100
5	X	215/261 (82%)	210 (98%)	5 (2%)	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	1514/1749 (87%)	1469 (97%)	45 (3%)	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	74/83 (89%)	74 (100%)	0	100	100
2	B	94/102 (92%)	94 (100%)	0	100	100
3	N	104/118 (88%)	104 (100%)	0	100	100
4	R	530/635 (84%)	528 (100%)	2 (0%)	91	96
5	X	158/228 (69%)	156 (99%)	2 (1%)	69	84
6	Y	281/309 (91%)	281 (100%)	0	100	100
7	Z	45/58 (78%)	44 (98%)	1 (2%)	52	71
All	All	1286/1533 (84%)	1281 (100%)	5 (0%)	91	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	46	ARG
4	R	287	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	X	23	ASN
5	X	280	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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
8	NAG	R	804	4	14,14,15	0.17	0	17,19,21	0.45	0
9	Z41	R	805	-	39,39,39	0.57	0	41,41,41	0.94	1 (2%)
8	NAG	R	801	4	14,14,15	0.25	0	17,19,21	0.54	0
8	NAG	R	802	4	14,14,15	0.31	0	17,19,21	0.46	0
8	NAG	A	101	1	14,14,15	0.22	0	17,19,21	0.40	0
8	NAG	A	102	1	14,14,15	0.21	0	17,19,21	0.51	0
8	NAG	B	201	2	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	R	803	4	14,14,15	0.18	0	17,19,21	0.45	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
8	NAG	R	804	4	-	2/6/23/26	0/1/1/1
9	Z41	R	805	-	-	8/41/41/41	-
8	NAG	R	801	4	-	1/6/23/26	0/1/1/1
8	NAG	R	802	4	-	0/6/23/26	0/1/1/1
8	NAG	A	101	1	-	2/6/23/26	0/1/1/1
8	NAG	A	102	1	-	1/6/23/26	0/1/1/1
8	NAG	B	201	2	-	2/6/23/26	0/1/1/1
8	NAG	R	803	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	805	Z41	O3-C19-C20	2.06	115.94	111.50

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

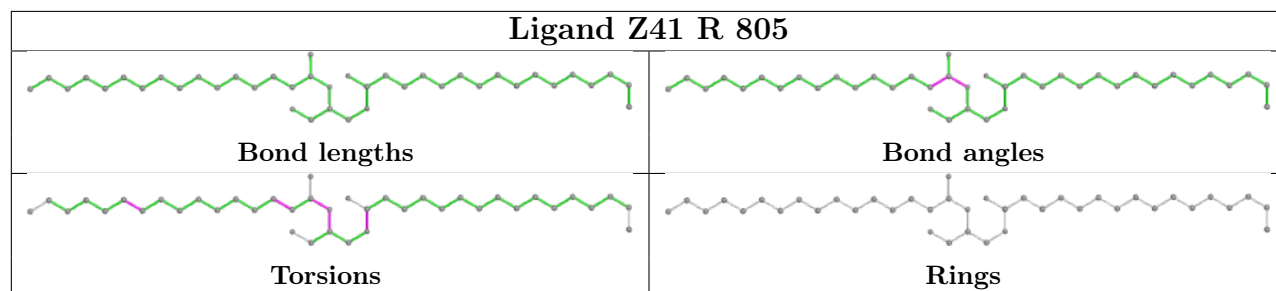
Mol	Chain	Res	Type	Atoms
9	R	805	Z41	C20-C19-O3-C18
9	R	805	Z41	O4-C19-O3-C18
8	R	804	NAG	C4-C5-C6-O6
8	R	804	NAG	O5-C5-C6-O6
8	A	101	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

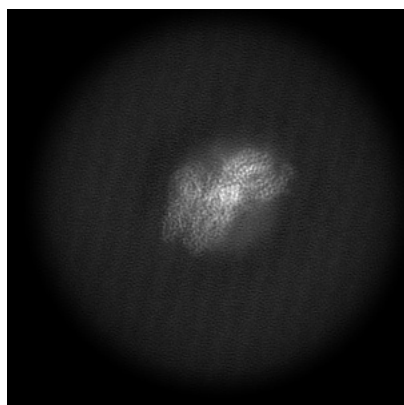
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26795. These allow visual inspection of the internal detail of the map and identification of artifacts.

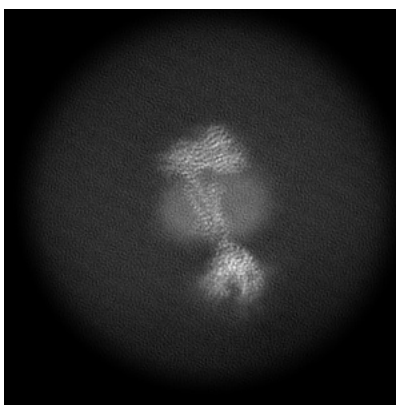
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

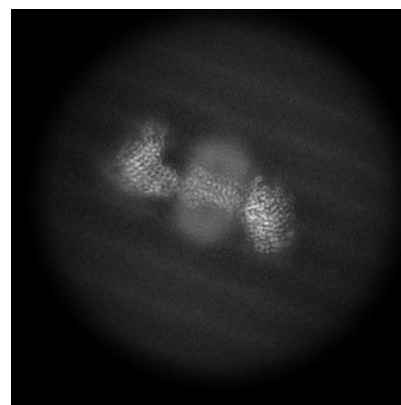
#### 6.1.1 Primary map



X



Y

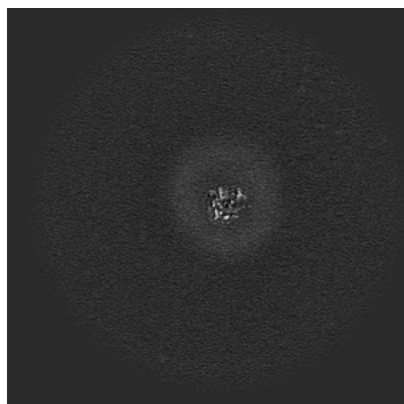


Z

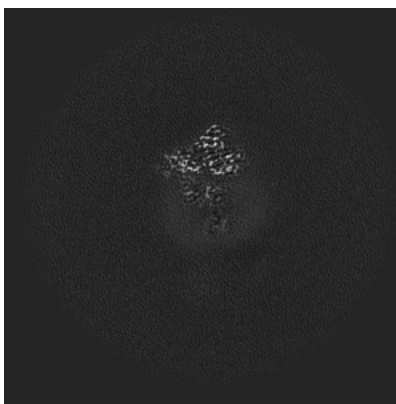
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

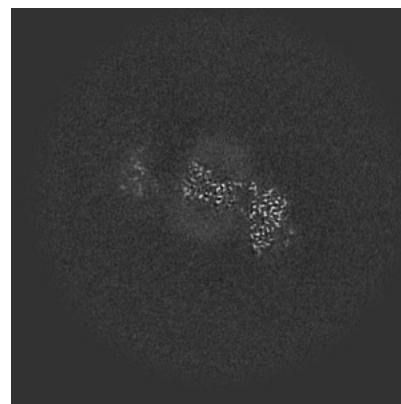
#### 6.2.1 Primary map



X Index: 208



Y Index: 208

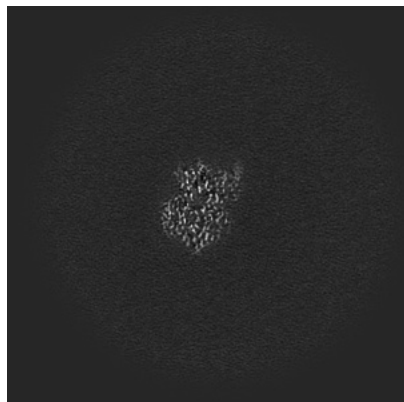


Z Index: 208

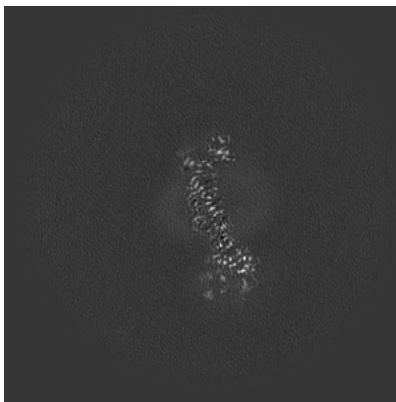
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

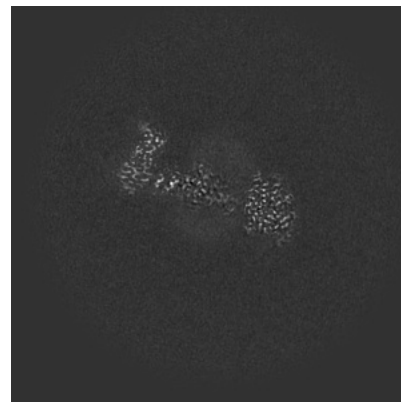
### 6.3.1 Primary map



X Index: 260



Y Index: 230

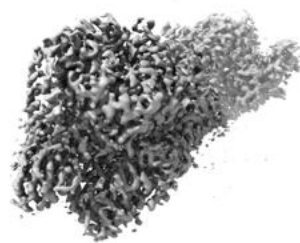


Z Index: 225

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

## 6.4 Orthogonal surface views [i](#)

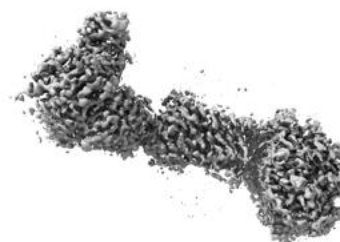
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.596. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

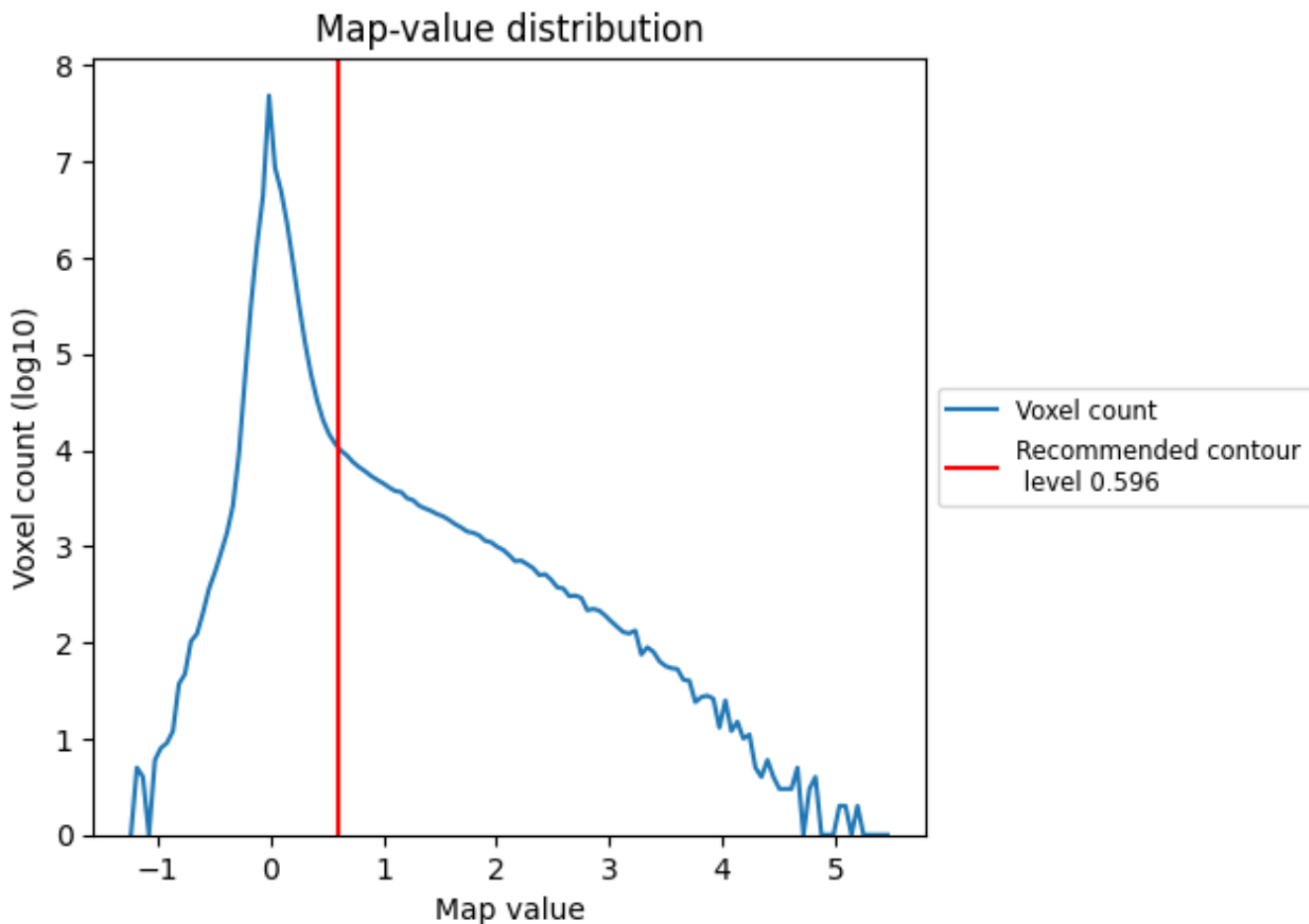
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

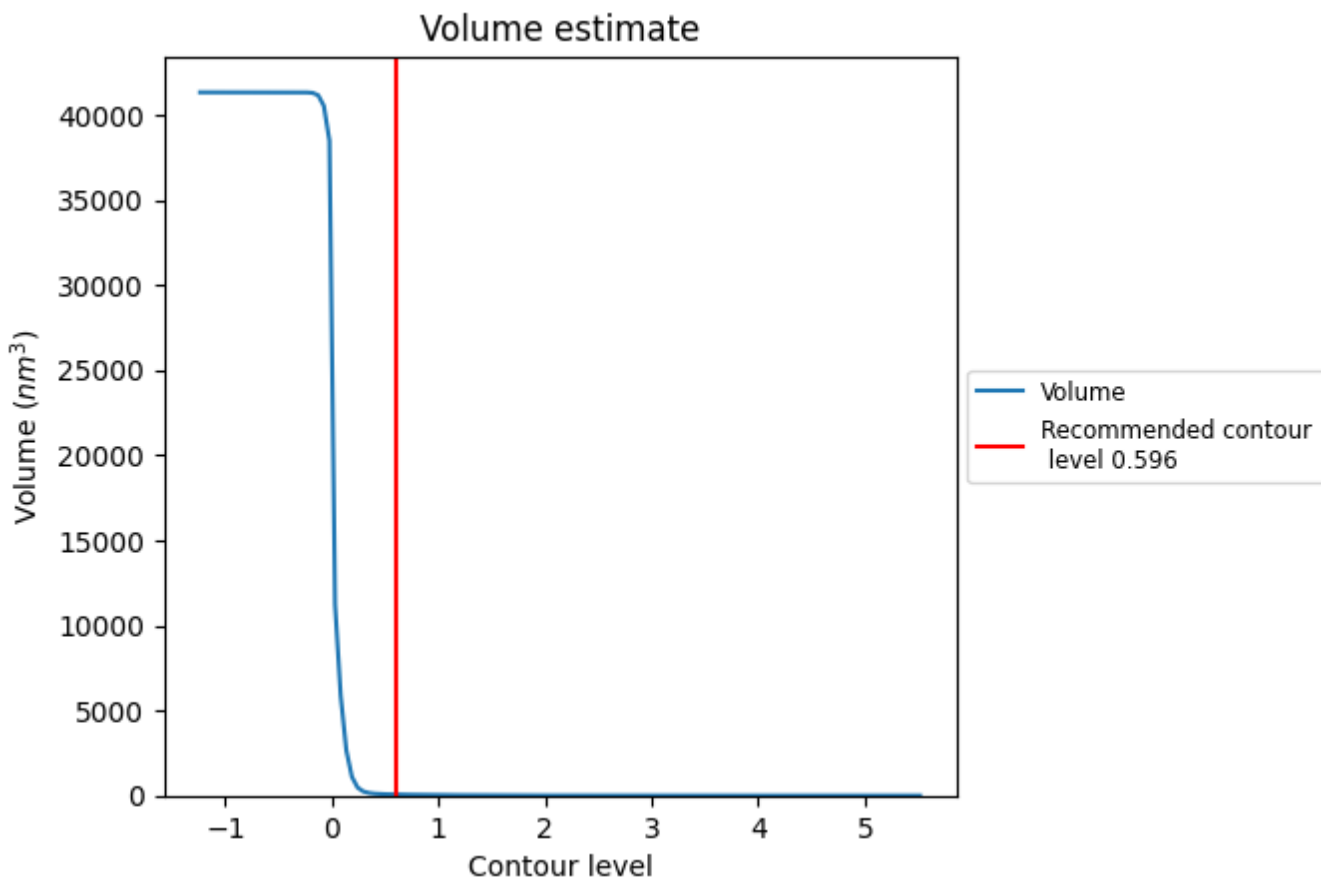
This section contains the results of statistical analysis of the map.

### 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](#)

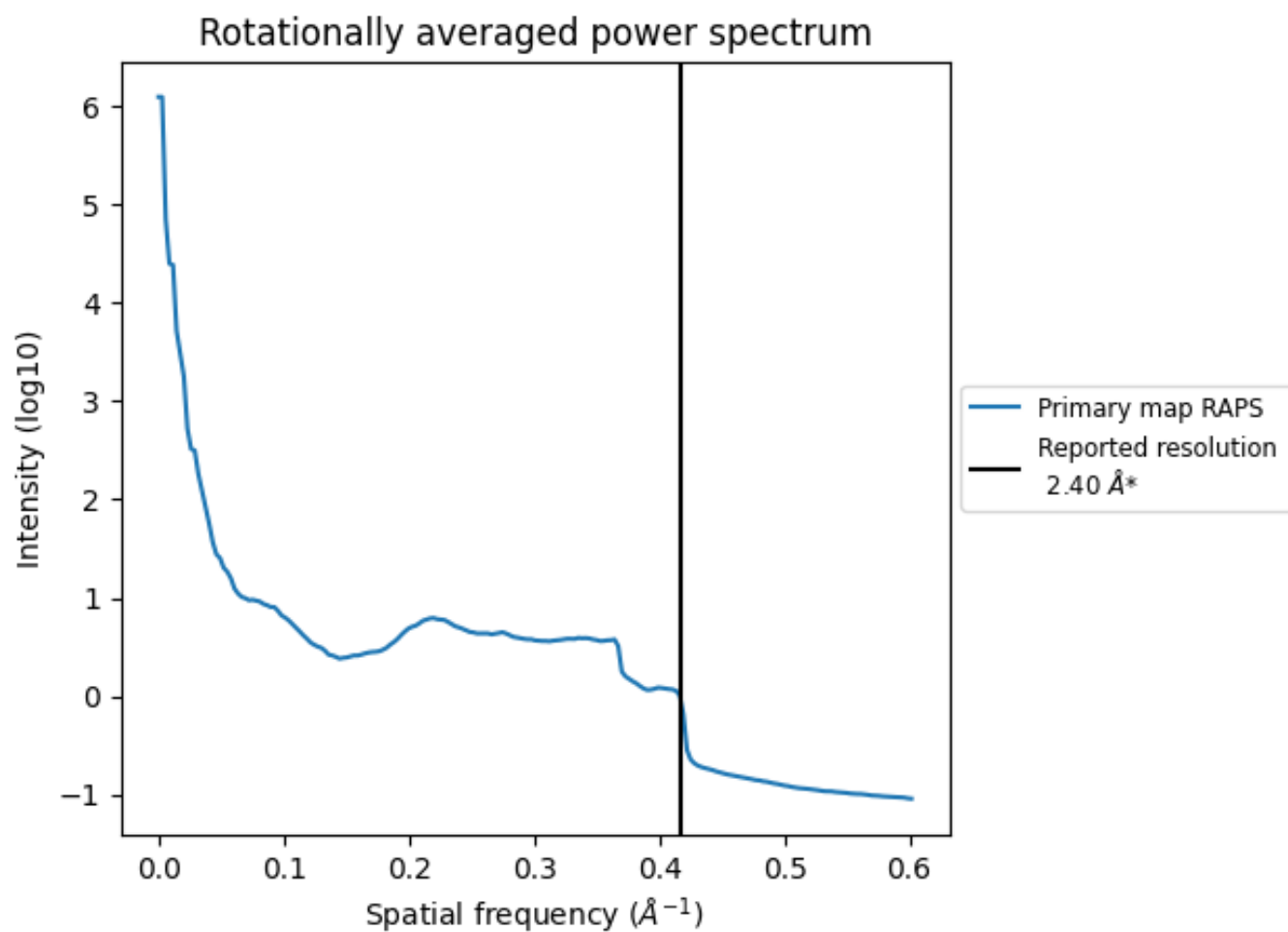


The volume at the recommended contour level is  $64 \text{ nm}^3$ ; this corresponds to an approximate mass of 58 kDa.

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  $0.417 \text{\AA}^{-1}$

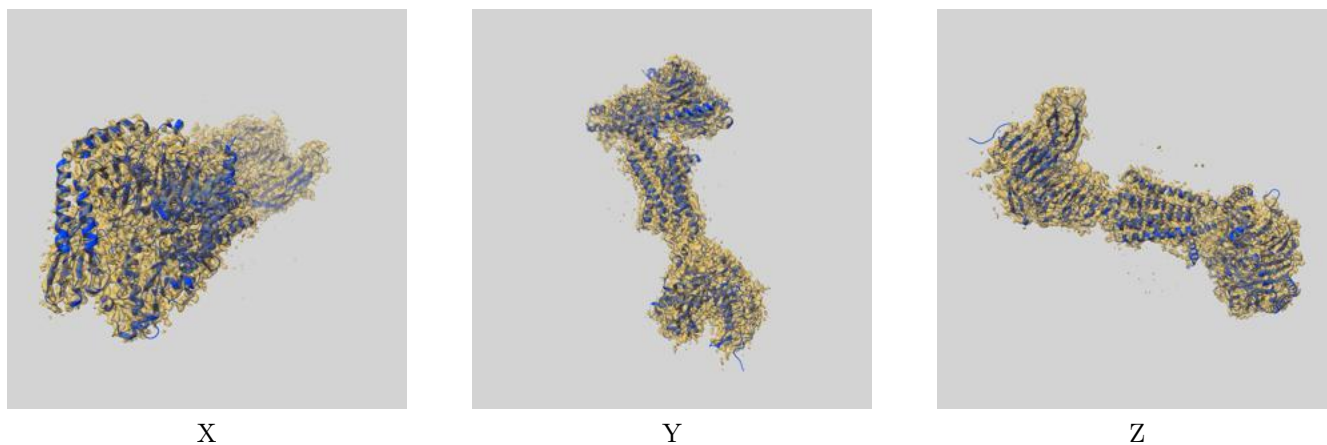
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

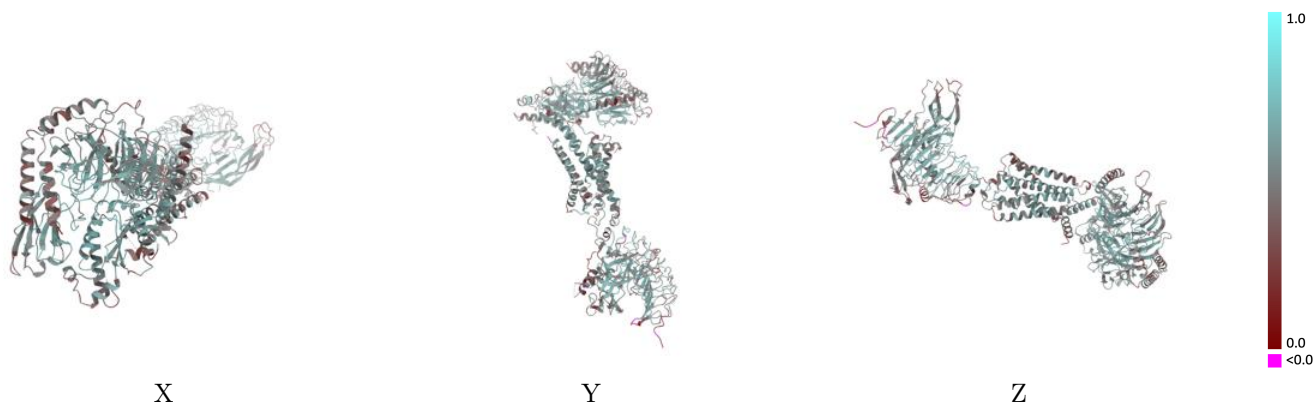
This section contains information regarding the fit between EMDB map EMD-26795 and PDB model 7UTZ. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



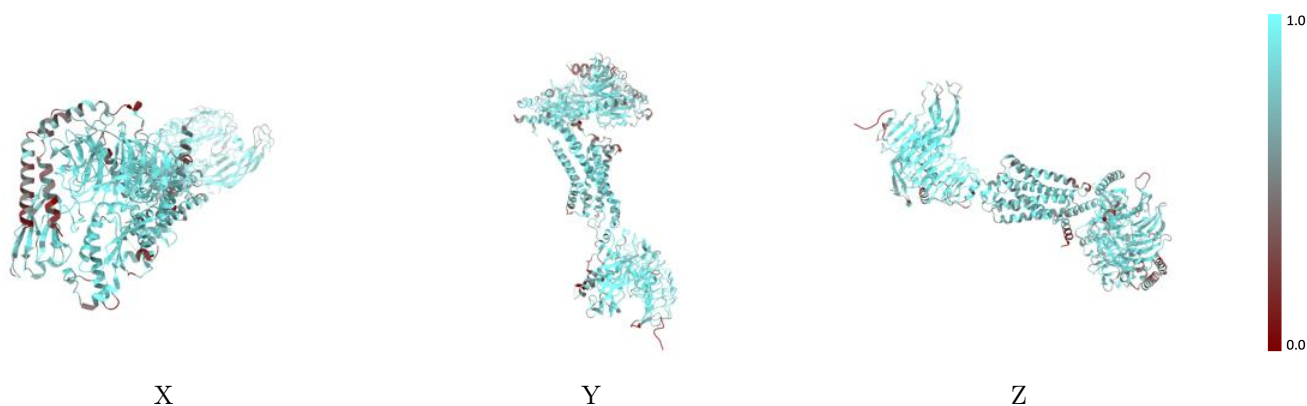
The images above show the 3D surface view of the map at the recommended contour level 0.596 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



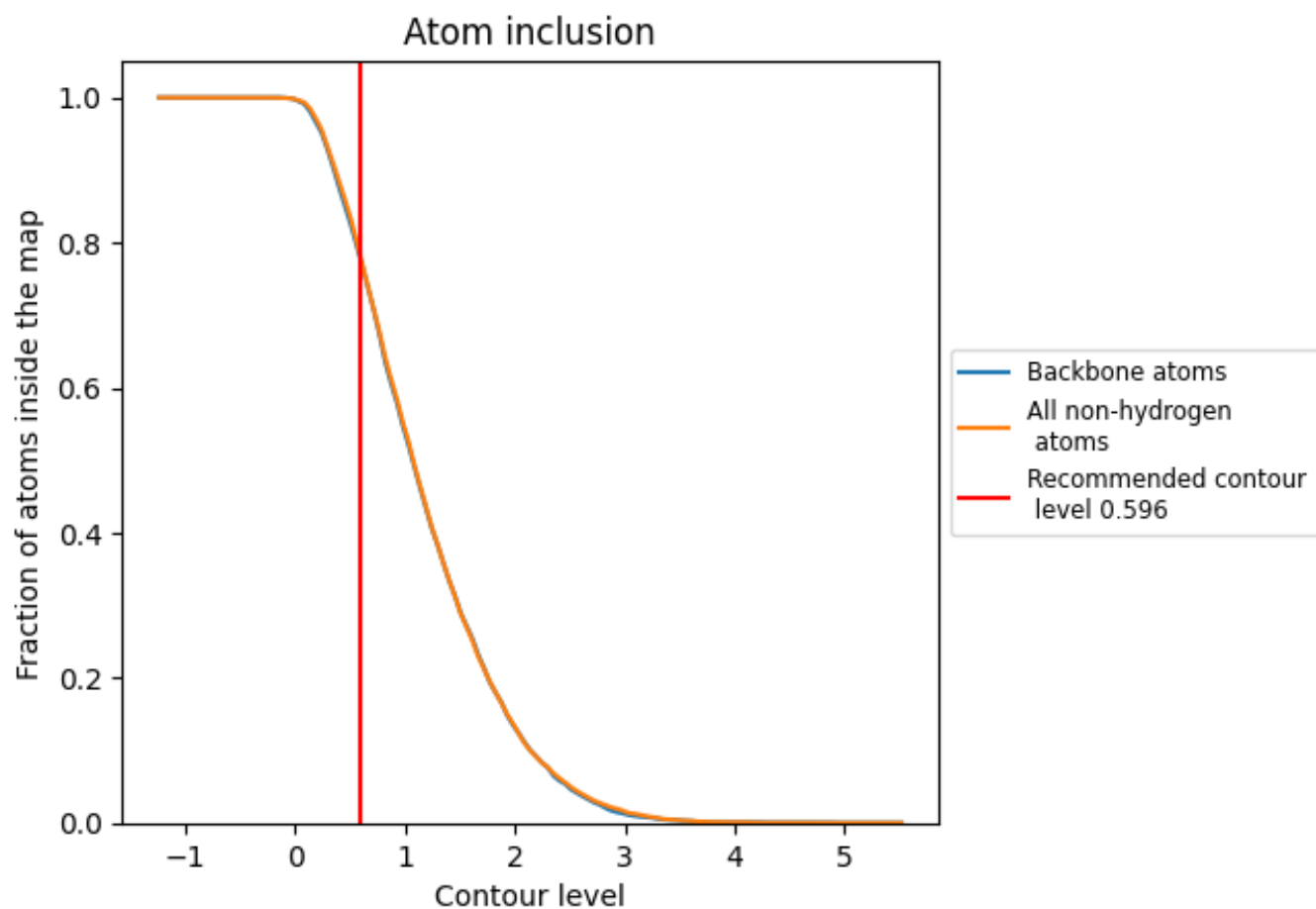
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.596).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.596) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7796	 0.5200
A	 0.8421	 0.5170
B	 0.8187	 0.5010
N	 0.8145	 0.5530
R	 0.7744	 0.5000
X	 0.8219	 0.5420
Y	 0.7930	 0.5520
Z	 0.5000	 0.4220

