wwPDB EM Validation Summary Report

Jul 21, 2021 – 11:12 am BST

PDB ID	:	7OBQ
EMDB ID	:	EMD-12799
Title	:	SRP-SR at the distal site conformation
Authors	:	Jomaa, A.; Ban, N.
Deposited on	:	2021-04-23
Resolution	:	3.90 Å(reported)
Based on initial model	:	6FRK

This is a wwPDB EM Validation Summary 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 following versions of software and data (see references ⓘ) were used in the production of this report:

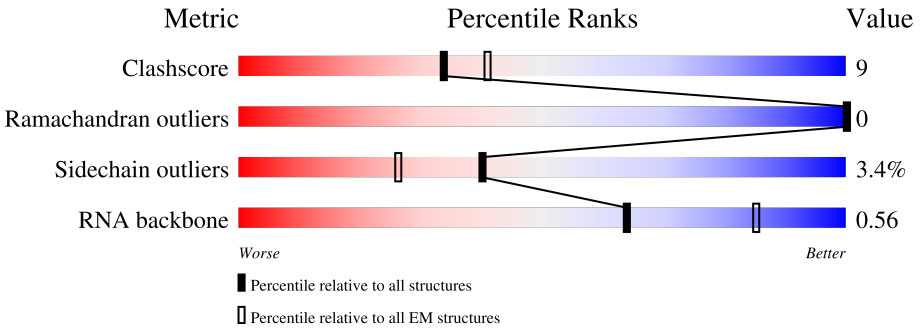
EMDB validation analysis	:	0.0.0.dev84
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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
RNA backbone	4643	859

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	1	249	39% 21% 6% 34%
2	q	144	22% 70% · 28%
3	s	62	26% 32% 68%
4	u	622	22% 69% · 29%
5	v	271	5% 72% · 26%
6	x	504	7% 75% · 22%
7	y	637	· 70% · 29%

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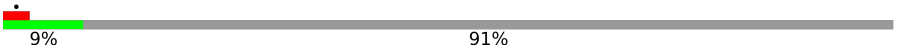
Mol	Chain	Length	Quality of chain
8	z	671	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 16668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	165	Total	C	N	O	P	0	0
			3542	1578	652	1147	165		

- Molecule 2 is a protein called Signal recognition particle 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	q	104	Total	C	N	O	S	0	0
			842	534	152	150	6		

- Molecule 3 is a protein called EM14S01-3B_G0054400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	s	20	Total	C	N	O	0	0
			100	60	20	20		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	1	UNK	MET	conflict	UNP A0A7I9EWR8
s	2	UNK	GLU	conflict	UNP A0A7I9EWR8
s	3	UNK	GLY	conflict	UNP A0A7I9EWR8
s	4	UNK	GLY	conflict	UNP A0A7I9EWR8
s	5	UNK	GLU	conflict	UNP A0A7I9EWR8
s	6	UNK	GLU	conflict	UNP A0A7I9EWR8
s	7	UNK	GLU	conflict	UNP A0A7I9EWR8
s	8	UNK	VAL	conflict	UNP A0A7I9EWR8
s	9	UNK	GLU	conflict	UNP A0A7I9EWR8
s	10	UNK	ARG	conflict	UNP A0A7I9EWR8
s	11	UNK	ILE	conflict	UNP A0A7I9EWR8
s	12	UNK	PRO	conflict	UNP A0A7I9EWR8
s	13	UNK	ASP	conflict	UNP A0A7I9EWR8
s	14	UNK	GLU	conflict	UNP A0A7I9EWR8
s	15	UNK	LEU	conflict	UNP A0A7I9EWR8

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Chain	Residue	Modelled	Actual	Comment	Reference
s	16	UNK	PHE	conflict	UNP A0A7I9EWR8
s	17	UNK	ASP	conflict	UNP A0A7I9EWR8
s	18	UNK	THR	conflict	UNP A0A7I9EWR8
s	19	UNK	LYS	conflict	UNP A0A7I9EWR8
s	20	UNK	LYS	conflict	UNP A0A7I9EWR8
s	21	UNK	LYS	conflict	UNP A0A7I9EWR8
s	22	UNK	HIS	conflict	UNP A0A7I9EWR8
s	23	UNK	LEU	conflict	UNP A0A7I9EWR8
s	24	UNK	LEU	conflict	UNP A0A7I9EWR8
s	25	UNK	ASP	conflict	UNP A0A7I9EWR8
s	26	UNK	LYS	conflict	UNP A0A7I9EWR8
s	27	UNK	LEU	conflict	UNP A0A7I9EWR8
s	28	UNK	ILE	conflict	UNP A0A7I9EWR8
s	29	UNK	ARG	conflict	UNP A0A7I9EWR8
s	30	UNK	VAL	conflict	UNP A0A7I9EWR8
s	31	UNK	GLY	conflict	UNP A0A7I9EWR8
s	32	UNK	ILE	conflict	UNP A0A7I9EWR8
s	33	UNK	ILE	conflict	UNP A0A7I9EWR8
s	34	UNK	LEU	conflict	UNP A0A7I9EWR8
s	35	UNK	VAL	conflict	UNP A0A7I9EWR8
s	36	UNK	LEU	conflict	UNP A0A7I9EWR8
s	37	UNK	LEU	conflict	UNP A0A7I9EWR8
s	38	UNK	ILE	conflict	UNP A0A7I9EWR8
s	39	UNK	TRP	conflict	UNP A0A7I9EWR8
s	40	UNK	GLY	conflict	UNP A0A7I9EWR8
s	41	UNK	THR	conflict	UNP A0A7I9EWR8
s	42	UNK	VAL	conflict	UNP A0A7I9EWR8
s	43	UNK	LEU	conflict	UNP A0A7I9EWR8
s	44	UNK	LEU	conflict	UNP A0A7I9EWR8
s	45	UNK	LEU	conflict	UNP A0A7I9EWR8
s	46	UNK	LYS	conflict	UNP A0A7I9EWR8
s	47	UNK	SER	conflict	UNP A0A7I9EWR8
s	48	UNK	ILE	conflict	UNP A0A7I9EWR8
s	49	UNK	PRO	conflict	UNP A0A7I9EWR8
s	50	UNK	HIS	conflict	UNP A0A7I9EWR8
s	51	UNK	HIS	conflict	UNP A0A7I9EWR8
s	52	UNK	SER	conflict	UNP A0A7I9EWR8
s	53	UNK	ASN	conflict	UNP A0A7I9EWR8
s	54	UNK	THR	conflict	UNP A0A7I9EWR8
s	55	UNK	PRO	conflict	UNP A0A7I9EWR8
s	56	UNK	ASP	conflict	UNP A0A7I9EWR8
s	57	UNK	TYR	conflict	UNP A0A7I9EWR8

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Chain	Residue	Modelled	Actual	Comment	Reference
s	58	UNK	GLN	conflict	UNP A0A7I9EWR8
s	59	UNK	GLU	conflict	UNP A0A7I9EWR8
s	60	UNK	PRO	conflict	UNP A0A7I9EWR8
s	61	UNK	ASN	conflict	UNP A0A7I9EWR8
s	62	UNK	SER	conflict	UNP A0A7I9EWR8

- Molecule 4 is a protein called Signal recognition particle subunit SRP68,Signal recognition particle subunit SRP68.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	u	441	Total	C	N	O	S	0	0
			3496	2190	640	651	15		

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	494A	UNK	SER	conflict	UNP Q00004
u	494B	UNK	ASP	conflict	UNP Q00004
u	494C	UNK	ALA	conflict	UNP Q00004
u	494D	UNK	GLY	conflict	UNP Q00004
u	494E	UNK	ALA	conflict	UNP Q00004
u	494F	UNK	PHE	conflict	UNP Q00004
u	494G	UNK	ARG	conflict	UNP Q00004
u	494H	UNK	ASN	conflict	UNP Q00004
u	494I	UNK	SER	conflict	UNP Q00004
u	494J	UNK	LEU	conflict	UNP Q00004
u	494K	UNK	LYS	conflict	UNP Q00004
u	494L	UNK	ASP	conflict	UNP Q00004
u	494M	UNK	LEU	conflict	UNP Q00004
u	494N	UNK	PRO	conflict	UNP Q00004
u	494O	UNK	ASP	conflict	UNP Q00004
u	494P	UNK	VAL	conflict	UNP Q00004
u	494Q	UNK	GLN	conflict	UNP Q00004
u	511	UNK	GLU	conflict	UNP Q00004
u	512	UNK	LEU	conflict	UNP Q00004
u	513	UNK	ILE	conflict	UNP Q00004
u	514	UNK	THR	conflict	UNP Q00004
u	515	UNK	GLN	conflict	UNP Q00004
u	516	UNK	VAL	conflict	UNP Q00004
u	517	UNK	ARG	conflict	UNP Q00004
u	518	UNK	SER	conflict	UNP Q00004
u	519	UNK	GLU	conflict	UNP Q00004

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Chain	Residue	Modelled	Actual	Comment	Reference
u	520	UNK	LYS	conflict	UNP Q00004
u	521	UNK	CYS	conflict	UNP Q00004
u	522	UNK	SER	conflict	UNP Q00004
u	523	UNK	LEU	conflict	UNP Q00004
u	524	UNK	GLN	conflict	UNP Q00004
u	525	UNK	ALA	conflict	UNP Q00004
u	526	UNK	ALA	conflict	UNP Q00004
u	527	UNK	ALA	conflict	UNP Q00004
u	528	UNK	ILE	conflict	UNP Q00004
u	529	UNK	LEU	conflict	UNP Q00004
u	530	UNK	ASP	conflict	UNP Q00004
u	531	UNK	ALA	conflict	UNP Q00004
u	532	UNK	SER	conflict	UNP Q00004
u	533	UNK	ASP	conflict	UNP Q00004
u	534	UNK	SER	conflict	UNP Q00004
u	535	UNK	HIS	conflict	UNP Q00004
u	536	UNK	GLN	conflict	UNP Q00004
u	537	UNK	PRO	conflict	UNP Q00004
u	538	UNK	GLU	conflict	UNP Q00004
u	539	UNK	THR	conflict	UNP Q00004
u	540	UNK	SER	conflict	UNP Q00004
u	541	UNK	SER	conflict	UNP Q00004
u	542	UNK	GLN	conflict	UNP Q00004
u	543	UNK	VAL	conflict	UNP Q00004
u	544	UNK	LYS	conflict	UNP Q00004
u	545	UNK	ASP	conflict	UNP Q00004
u	546	UNK	ASN	conflict	UNP Q00004
u	547	UNK	LYS	conflict	UNP Q00004
u	548	UNK	PRO	conflict	UNP Q00004
u	549	UNK	LEU	conflict	UNP Q00004
u	550	UNK	VAL	conflict	UNP Q00004
u	551	UNK	GLU	conflict	UNP Q00004
u	552	UNK	ARG	conflict	UNP Q00004
u	553	UNK	PHE	conflict	UNP Q00004
u	554	UNK	GLU	conflict	UNP Q00004
u	555	UNK	THR	conflict	UNP Q00004
u	556	UNK	PHE	conflict	UNP Q00004
u	557	UNK	CYS	conflict	UNP Q00004
u	558	UNK	LEU	conflict	UNP Q00004
u	559	UNK	ASP	conflict	UNP Q00004
u	560	UNK	PRO	conflict	UNP Q00004
u	561	UNK	SER	conflict	UNP Q00004

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Chain	Residue	Modelled	Actual	Comment	Reference
u	562	UNK	LEU	conflict	UNP Q00004
u	563	UNK	VAL	conflict	UNP Q00004
u	564	UNK	THR	conflict	UNP Q00004
u	565	UNK	LYS	conflict	UNP Q00004
u	566	UNK	GLN	conflict	UNP Q00004
u	567	UNK	ALA	conflict	UNP Q00004
u	568	UNK	ASN	conflict	UNP Q00004
u	569	UNK	LEU	conflict	UNP Q00004
u	570	UNK	VAL	conflict	UNP Q00004
u	571	UNK	HIS	conflict	UNP Q00004
u	572	UNK	PHE	conflict	UNP Q00004
u	573	UNK	PRO	conflict	UNP Q00004
u	574	UNK	PRO	conflict	UNP Q00004
u	575	UNK	GLY	conflict	UNP Q00004
u	576	UNK	PHE	conflict	UNP Q00004
u	577	UNK	GLN	conflict	UNP Q00004
u	578	UNK	PRO	conflict	UNP Q00004
u	579	UNK	ILE	conflict	UNP Q00004
u	580	UNK	PRO	conflict	UNP Q00004
u	581	UNK	CYS	conflict	UNP Q00004
u	582	UNK	LYS	conflict	UNP Q00004
u	583	UNK	PRO	conflict	UNP Q00004
u	584	UNK	LEU	conflict	UNP Q00004
u	585	UNK	PHE	conflict	UNP Q00004
u	586	UNK	PHE	conflict	UNP Q00004
u	587	UNK	ASP	conflict	UNP Q00004
u	588	UNK	LEU	conflict	UNP Q00004
u	589	UNK	ALA	conflict	UNP Q00004
u	590	UNK	LEU	conflict	UNP Q00004
u	591	UNK	ASN	conflict	UNP Q00004
u	592	UNK	HIS	conflict	UNP Q00004
u	593	UNK	VAL	conflict	UNP Q00004
u	594	UNK	ALA	conflict	UNP Q00004
u	595	UNK	PHE	conflict	UNP Q00004
u	596	UNK	PRO	conflict	UNP Q00004
u	597	UNK	PRO	conflict	UNP Q00004
u	598	UNK	LEU	conflict	UNP Q00004
u	599	UNK	GLU	conflict	UNP Q00004
u	600	UNK	ASP	conflict	UNP Q00004
u	601	UNK	LYS	conflict	UNP Q00004
u	602	UNK	LEU	conflict	UNP Q00004
u	603	UNK	GLU	conflict	UNP Q00004

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Chain	Residue	Modelled	Actual	Comment	Reference
u	604	UNK	GLN	conflict	UNP Q00004
u	605	UNK	LYS	conflict	UNP Q00004
u	606	UNK	THR	conflict	UNP Q00004
u	607	UNK	LYS	conflict	UNP Q00004
u	608	UNK	SER	conflict	UNP Q00004
u	609	UNK	GLY	conflict	UNP Q00004
u	610	UNK	LEU	conflict	UNP Q00004
u	611	UNK	THR	conflict	UNP Q00004
u	612	UNK	GLY	conflict	UNP Q00004
u	613	UNK	TYR	conflict	UNP Q00004
u	614	UNK	ILE	conflict	UNP Q00004
u	615	UNK	LYS	conflict	UNP Q00004
u	616	UNK	GLY	conflict	UNP Q00004
u	617	UNK	ILE	conflict	UNP Q00004
u	618	UNK	PHE	conflict	UNP Q00004
u	619	UNK	GLY	conflict	UNP Q00004
u	620	UNK	PHE	conflict	UNP Q00004
u	621	UNK	ARG	conflict	UNP Q00004
u	622	UNK	SER	conflict	UNP Q00004

- Molecule 5 is a protein called Signal recognition particle receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	v	201	Total	C	N	O	S	0	0
			1563	987	275	296	5		

- Molecule 6 is a protein called Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	x	393	Total	C	N	O	S	0	0
			3049	1931	517	579	22		

- Molecule 7 is a protein called SRP receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	y	454	Total	C	N	O	S	0	0
			3483	2204	610	651	18		

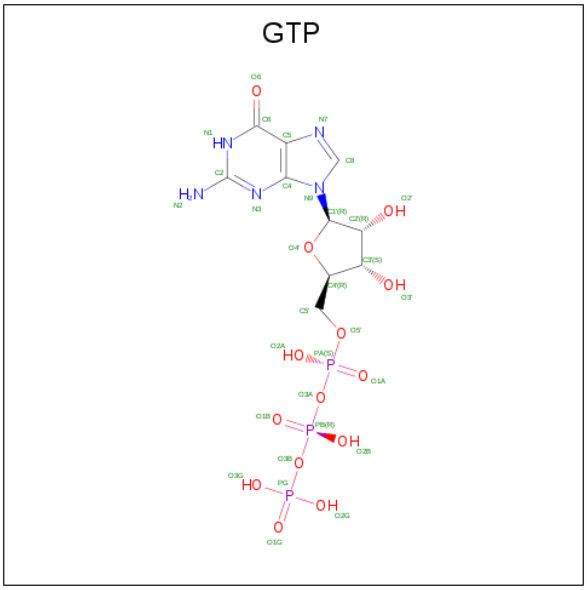
- Molecule 8 is a protein called Signal recognition particle subunit SRP72.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	z	62	Total	C	N	O	S	0	0
			494	309	96	88	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

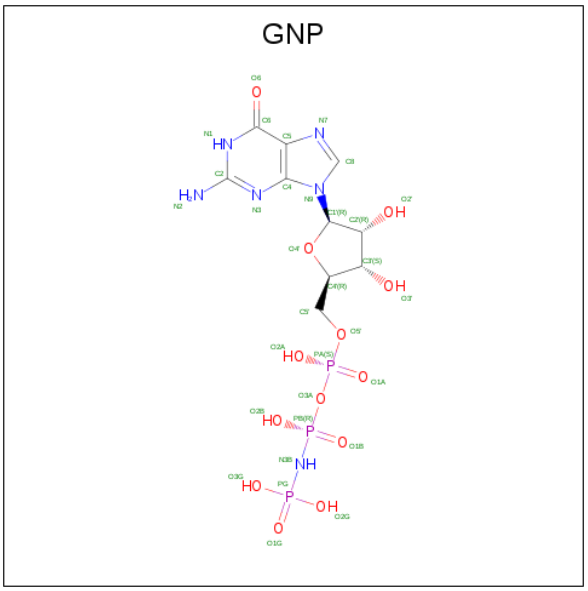
Mol	Chain	Residues	Atoms		AltConf
9	v	1	Total	Mg	0
			1	1	
9	x	1	Total	Mg	0
			1	1	
9	y	1	Total	Mg	0
			1	1	

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	v	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



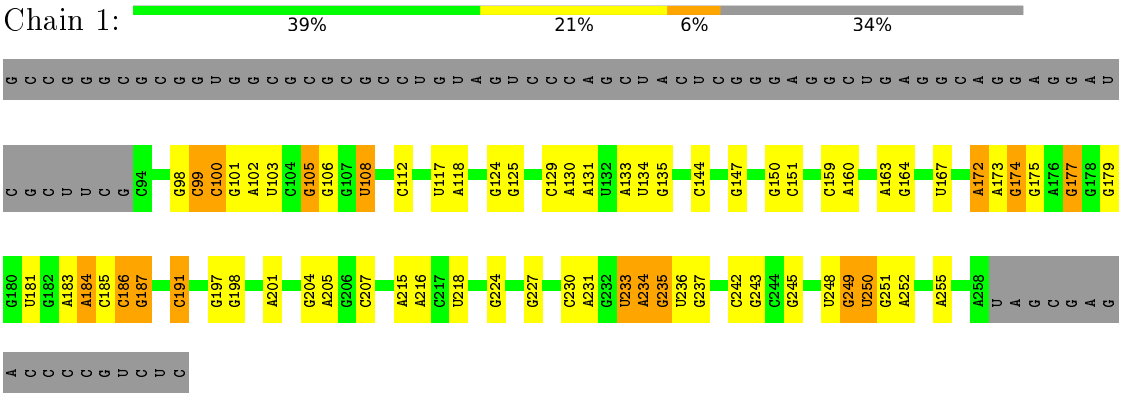
Mol	Chain	Residues	Atoms					AltConf
11	x	1	Total	C	N	O	P	0
			32	10	6	13	3	
11	y	1	Total	C	N	O	P	0
			32	10	6	13	3	

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.

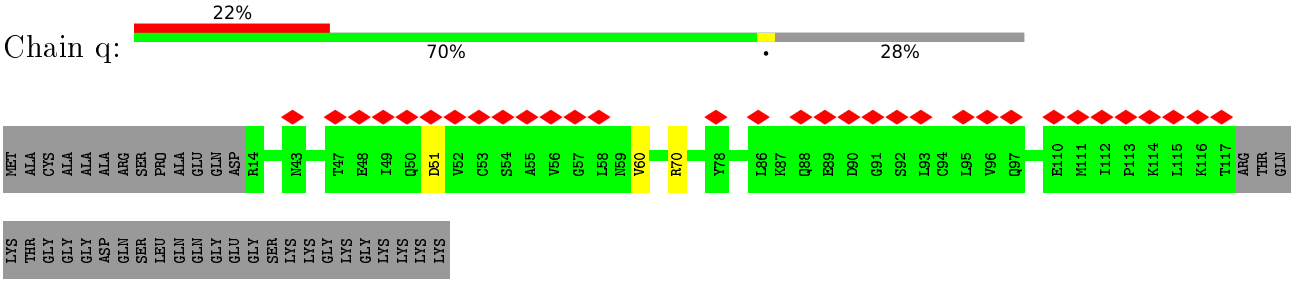
• Molecule 1: SRP RNA

Chain 1:



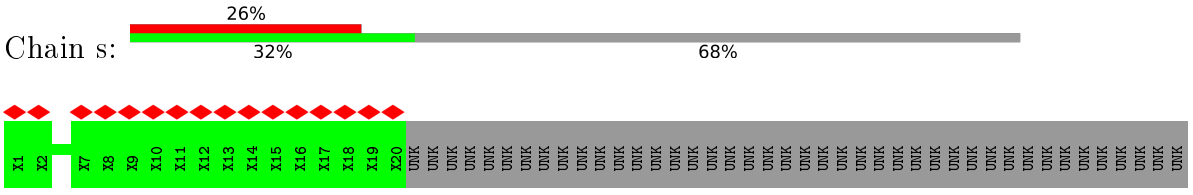
• Molecule 2: Signal recognition particle 19

Chain q:



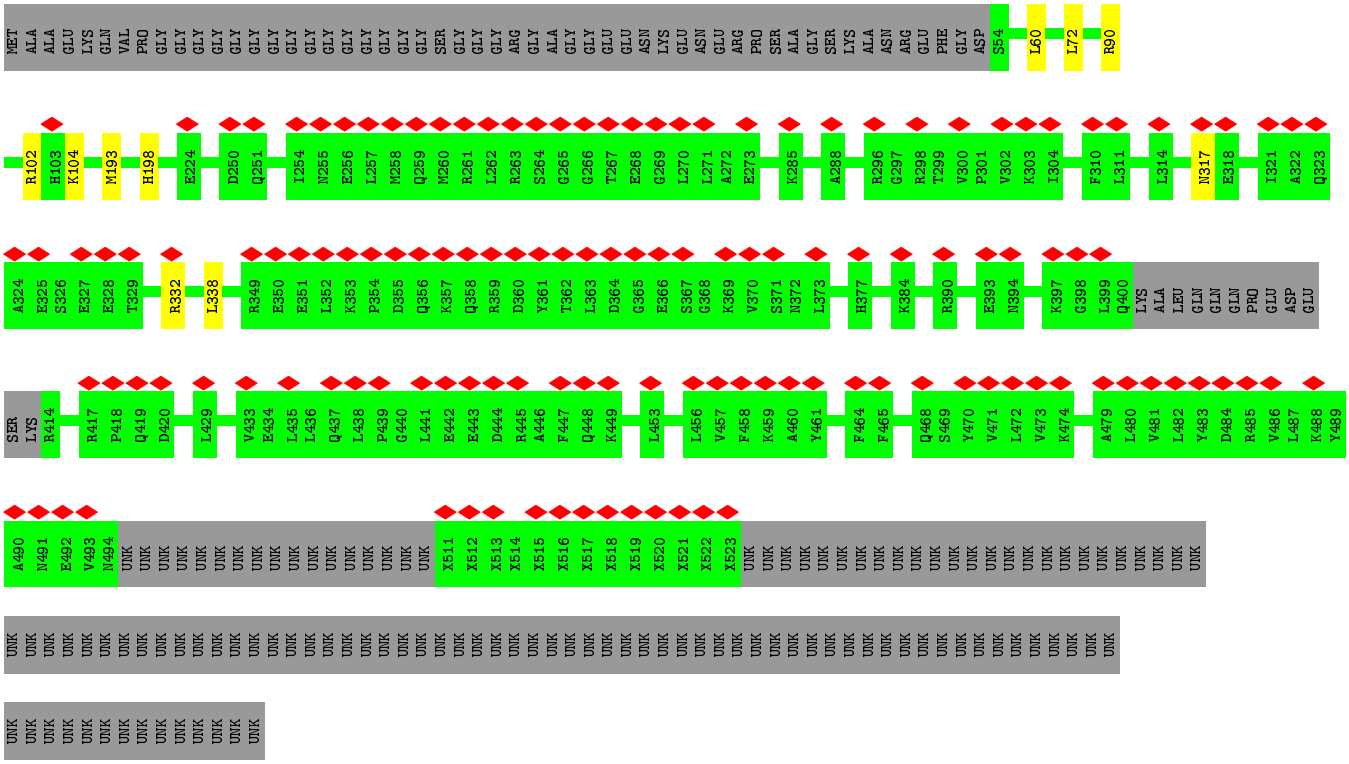
• Molecule 3: EM14S01-3B_G0054400.mRNA.1.CDS.1

Chain s:

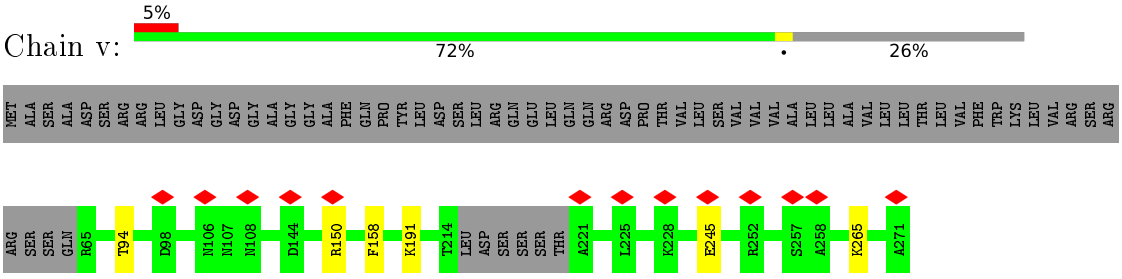


• Molecule 4: Signal recognition particle subunit SRP68,Signal recognition particle subunit SRP68

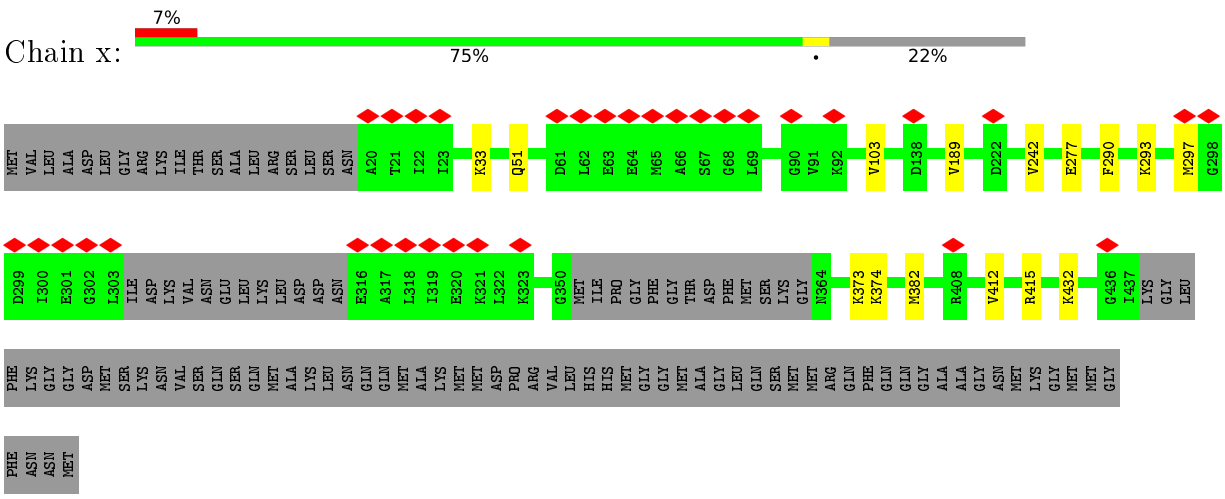
Chain u:



• Molecule 5: Signal recognition particle receptor subunit beta

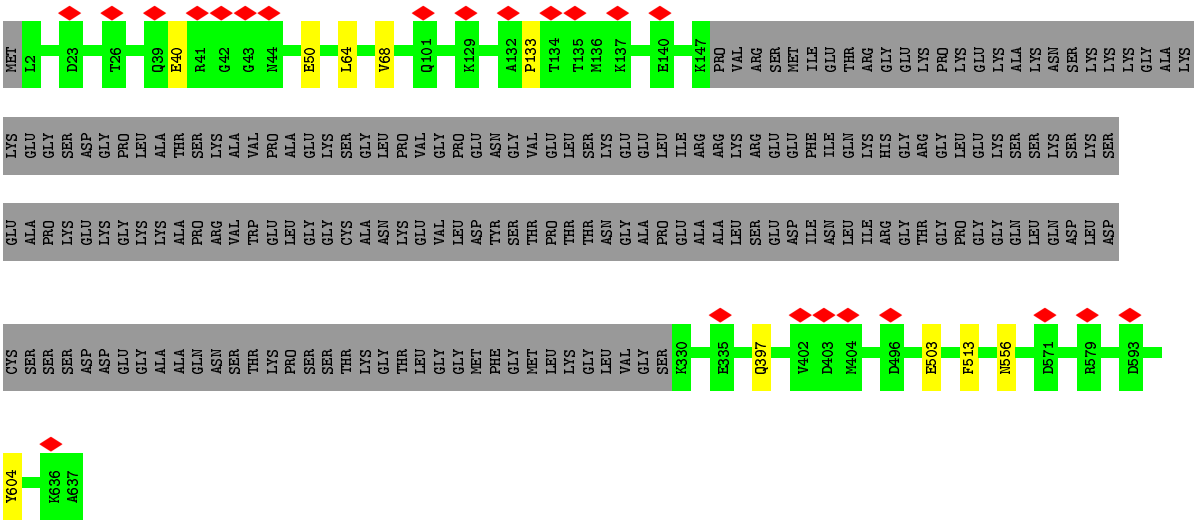


• Molecule 6: Signal recognition particle 54 kDa protein



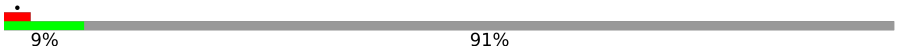
• Molecule 7: SRP receptor subunit alpha

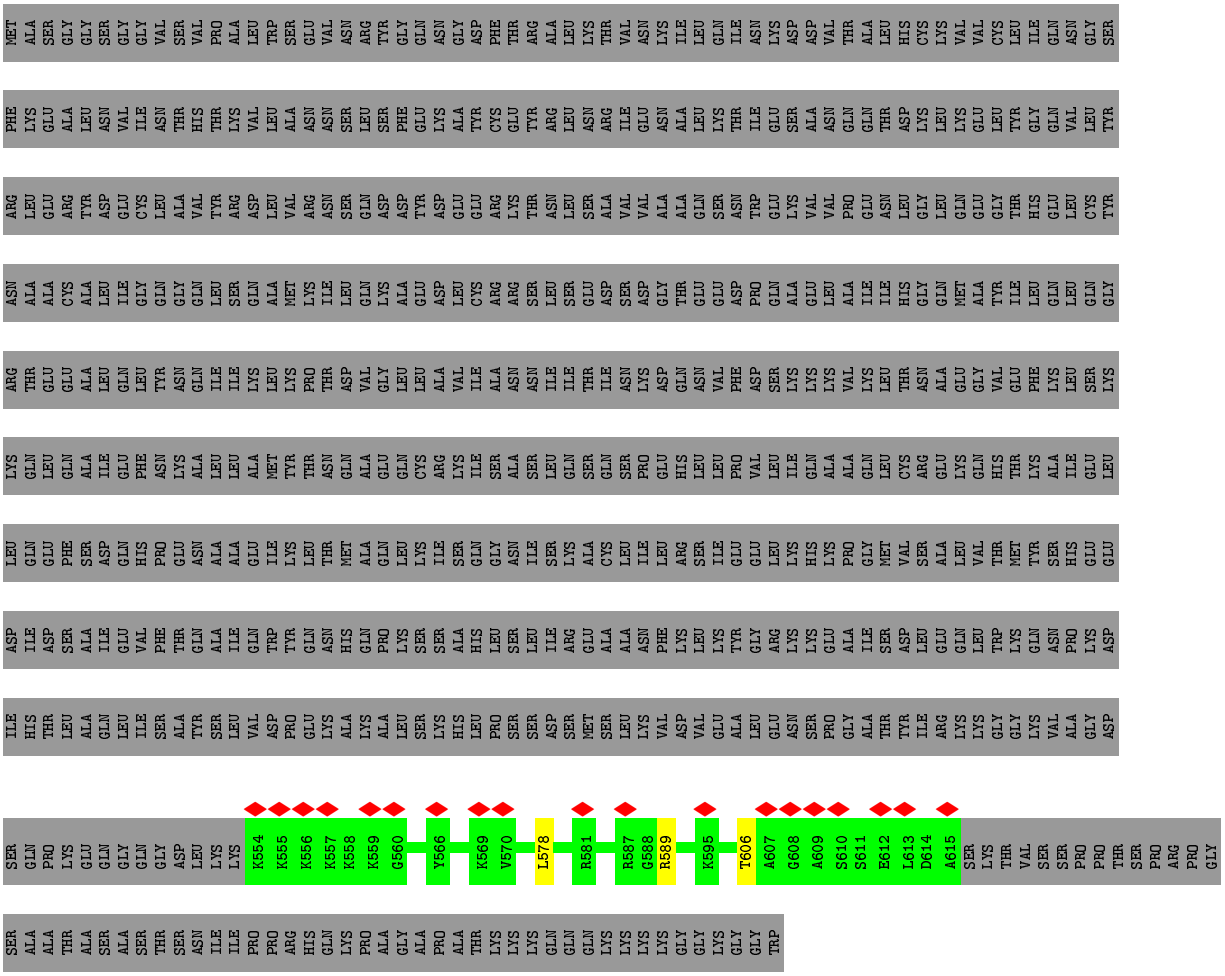
Chain y:



• Molecule 8: Signal recognition particle subunit SRP72

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155989	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, GTP, MG

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	1	0.15	0/3964	0.66	0/6183
2	q	0.24	0/856	0.50	0/1152
4	u	0.24	0/3479	0.48	0/4674
5	v	0.24	0/1584	0.48	0/2132
6	x	0.24	0/3091	0.42	0/4148
7	y	0.24	0/3532	0.47	1/4772 (0.0%)
8	z	0.24	0/503	0.51	0/665
All	All	0.22	0/17009	0.52	1/23726 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	y	133	PRO	N-CA-CB	5.76	110.21	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1	3542	0	1787	31	0
2	q	842	0	873	0	0
3	s	100	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	u	3496	0	3434	0	0
5	v	1563	0	1604	0	0
6	x	3049	0	3110	0	0
7	y	3483	0	3505	0	0
8	z	494	0	526	0	0
9	v	1	0	0	0	0
9	x	1	0	0	0	0
9	y	1	0	0	0	0
10	v	32	0	12	0	0
11	x	32	0	13	0	0
11	y	32	0	13	0	0
All	All	16668	0	14900	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 31 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)
1:1:108:U:H3	1:1:245:G:H1	1.34	0.75
1:1:103:U:OP2	1:1:251:G:N2	2.26	0.66
1:1:175:G:O2'	1:1:177:G:OP2	2.12	0.65
1:1:198:G:N2	1:1:201:A:OP2	2.33	0.56
1:1:183:A:N6	1:1:187:G:OP1	2.39	0.56

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	
2	q	102/144 (71%)	102 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	u	424/622 (68%)	418 (99%)	6 (1%)	0	100	100
5	v	197/271 (73%)	190 (96%)	7 (4%)	0	100	100
6	x	387/504 (77%)	384 (99%)	3 (1%)	0	100	100
7	y	450/637 (71%)	430 (96%)	20 (4%)	0	100	100
8	z	60/671 (9%)	52 (87%)	8 (13%)	0	100	100
All	All	1620/2849 (57%)	1576 (97%)	44 (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	
2	q	93/121 (77%)	90 (97%)	3 (3%)	39	63
4	u	353/410 (86%)	343 (97%)	10 (3%)	43	66
5	v	171/230 (74%)	165 (96%)	6 (4%)	36	62
6	x	330/420 (79%)	315 (96%)	15 (4%)	27	56
7	y	370/531 (70%)	361 (98%)	9 (2%)	49	69
8	z	51/570 (9%)	48 (94%)	3 (6%)	19	49
All	All	1368/2282 (60%)	1322 (97%)	46 (3%)	40	62

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	x	373	LYS
7	y	50	GLU
6	x	374	LYS
6	x	415	ARG
7	y	68	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
7	y	60	ASN
7	y	617	GLN
7	y	71	GLN
5	v	161	GLN
6	x	385	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	164/249 (65%)	35 (21%)	3 (1%)

5 of 35 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	98	G
1	1	99	C
1	1	100	C
1	1	102	A
1	1	105	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	99	C
1	1	234	A
1	1	236	U

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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
11	GNP	y	701	9	28,34,34	2.36	10 (35%)	30,54,54	1.86	4 (13%)
11	GNP	x	601	9	28,34,34	2.36	10 (35%)	30,54,54	1.83	4 (13%)
10	GTP	v	301	9	26,34,34	0.95	1 (3%)	33,54,54	1.99	7 (21%)

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
11	GNP	y	701	9	-	10/17/38/38	0/3/3/3
11	GNP	x	601	9	-	5/17/38/38	0/3/3/3
10	GTP	v	301	9	-	6/18/38/38	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	x	601	GNP	C4-N9	-7.47	1.37	1.47
11	y	701	GNP	C4-N9	-7.47	1.37	1.47
11	x	601	GNP	C5-C6	-4.63	1.44	1.52
11	y	701	GNP	C5-C6	-4.55	1.45	1.52
11	y	701	GNP	PB-O3A	4.42	1.64	1.59

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	x	601	GNP	C4-C5-N7	6.15	110.61	102.46
11	y	701	GNP	C4-C5-N7	6.12	110.58	102.46
10	v	301	GTP	N3-C2-N1	-5.24	120.23	127.22
11	y	701	GNP	C5-C6-N1	-5.07	111.93	118.19
11	x	601	GNP	C5-C6-N1	-5.07	111.93	118.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

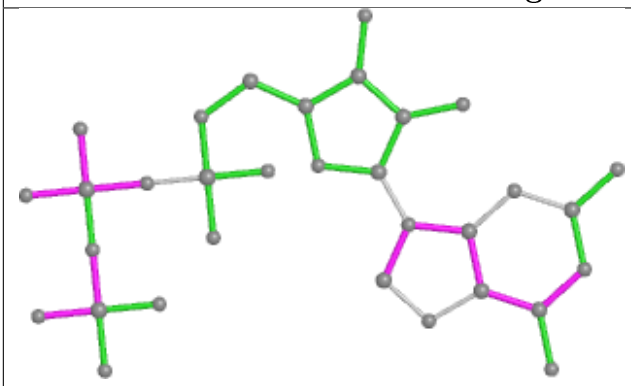
Mol	Chain	Res	Type	Atoms
10	v	301	GTP	C5'-O5'-PA-O1A
10	v	301	GTP	C5'-O5'-PA-O2A
11	x	601	GNP	PG-N3B-PB-O1B
11	x	601	GNP	PG-N3B-PB-O3A
11	x	601	GNP	C2'-C1'-N9-C4

There are no ring outliers.

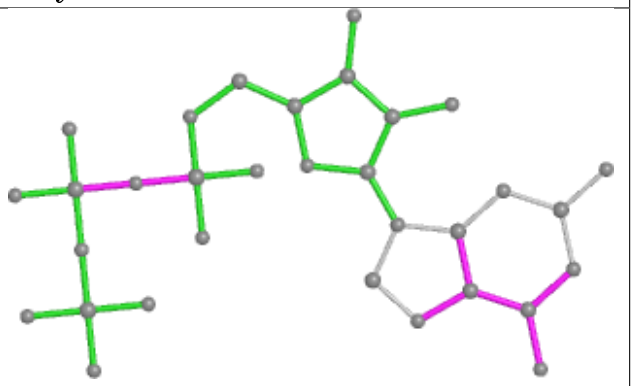
No monomer is involved in short contacts.

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 then 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.

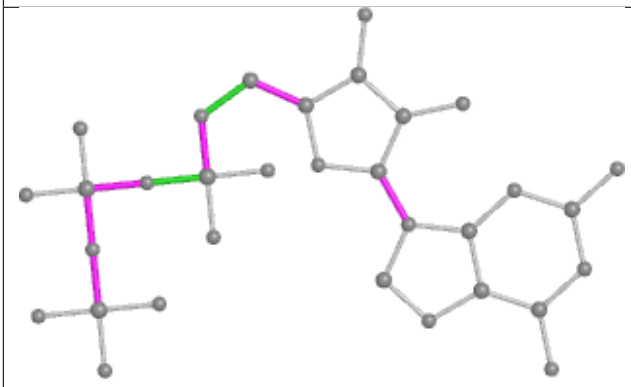
Ligand GNP y 701



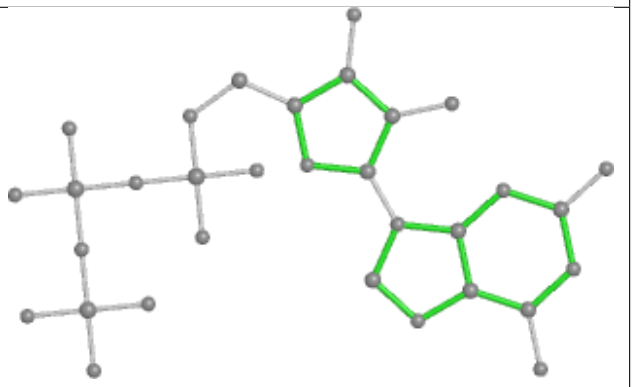
Bond lengths



Bond angles

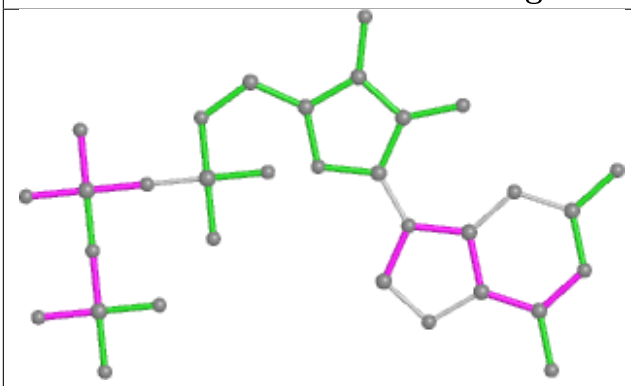


Torsions

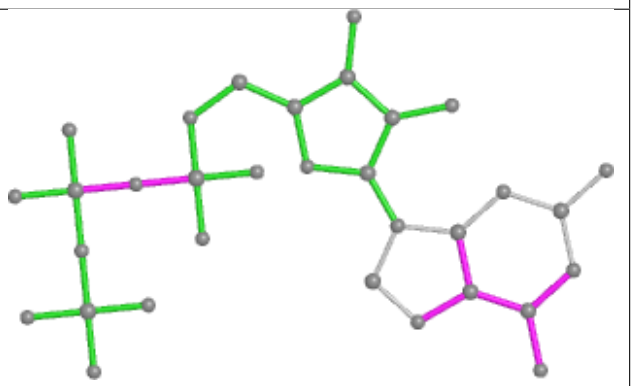


Rings

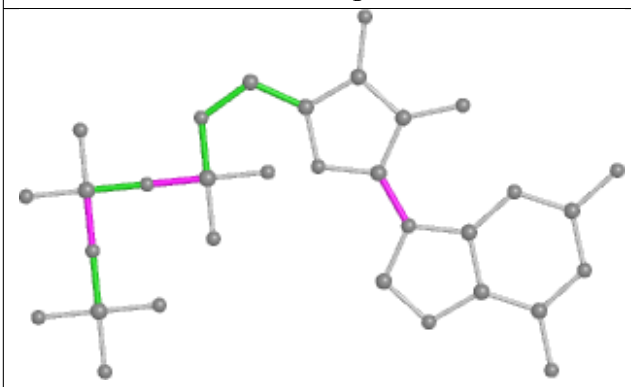
Ligand GNP x 601



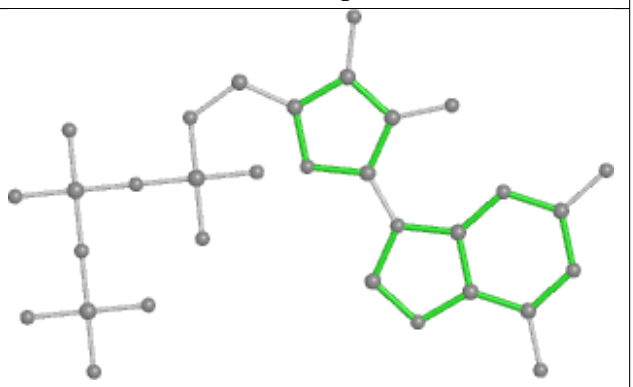
Bond lengths



Bond angles

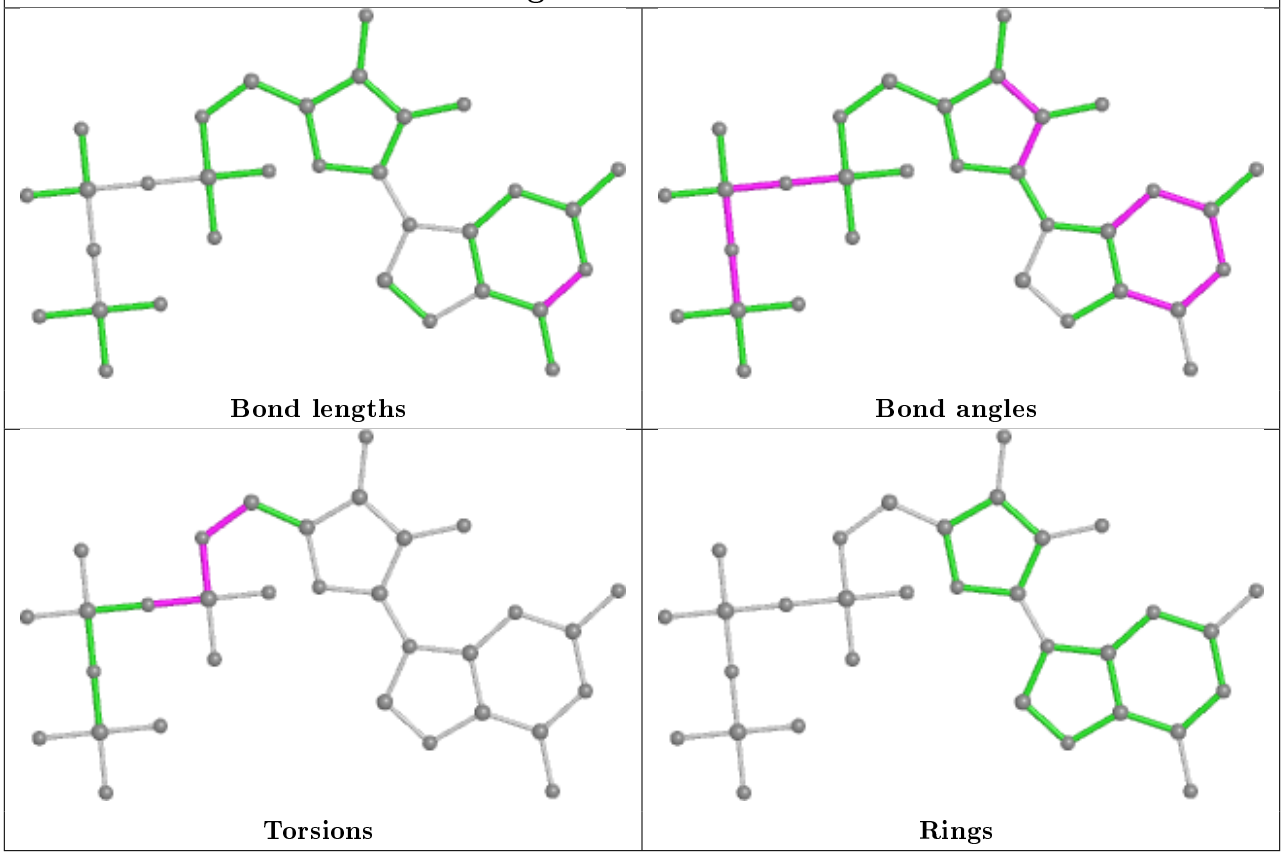


Torsions



Rings

Ligand GTP v 301



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.

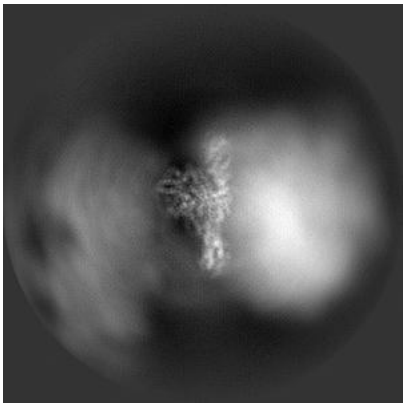
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12799. These allow visual inspection of the internal detail of the map and identification of artifacts.

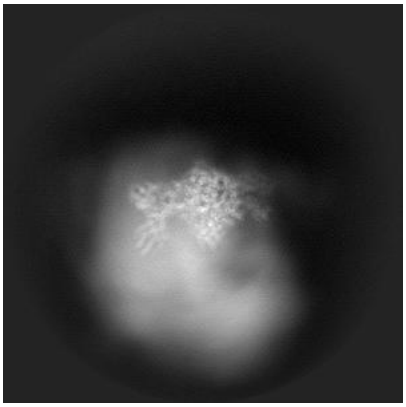
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

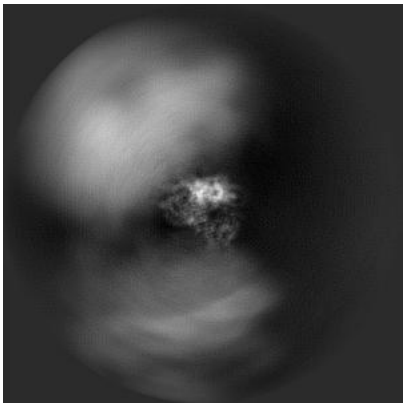
6.1.1 Primary map



X



Y

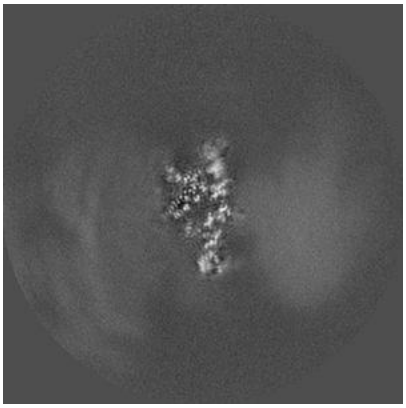


Z

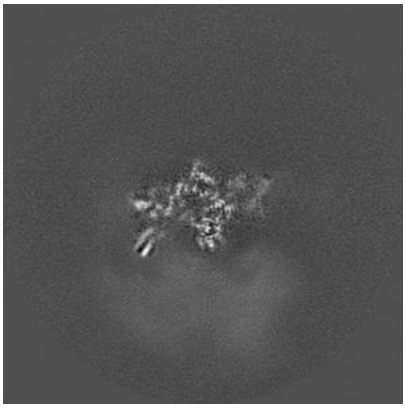
The images above show the map projected in three orthogonal directions.

6.2 Central slices

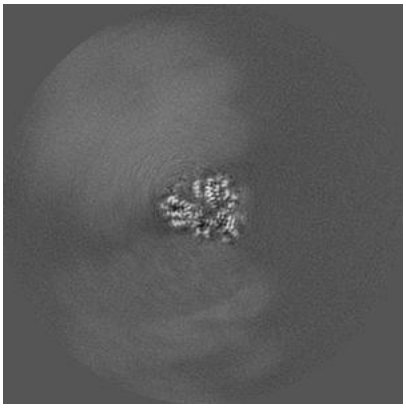
6.2.1 Primary map



X Index: 224



Y Index: 224

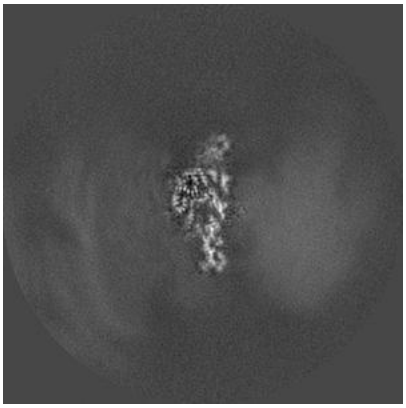


Z Index: 224

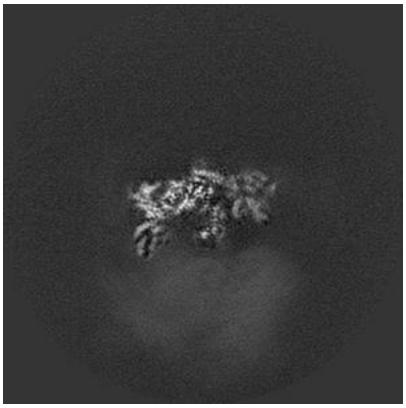
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

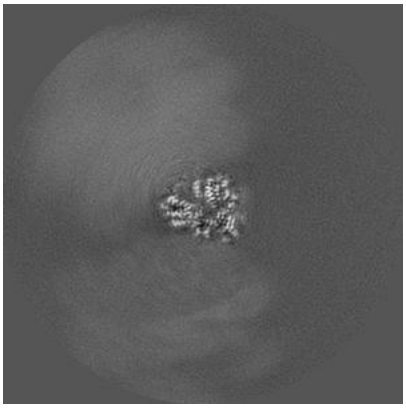
6.3.1 Primary map



X Index: 218



Y Index: 231



Z Index: 224

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

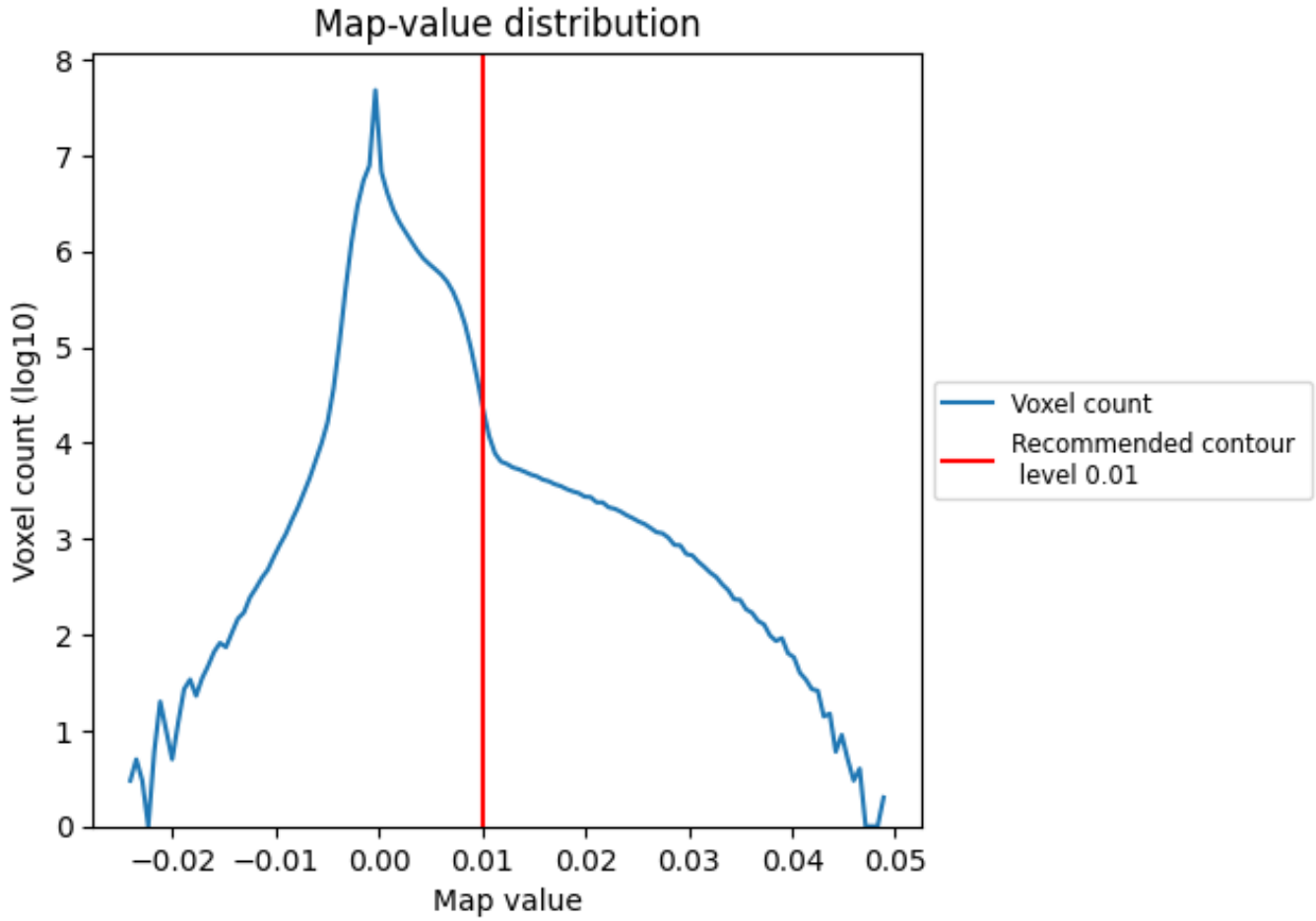
6.5 Mask visualisation (i)

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

7 Map analysis

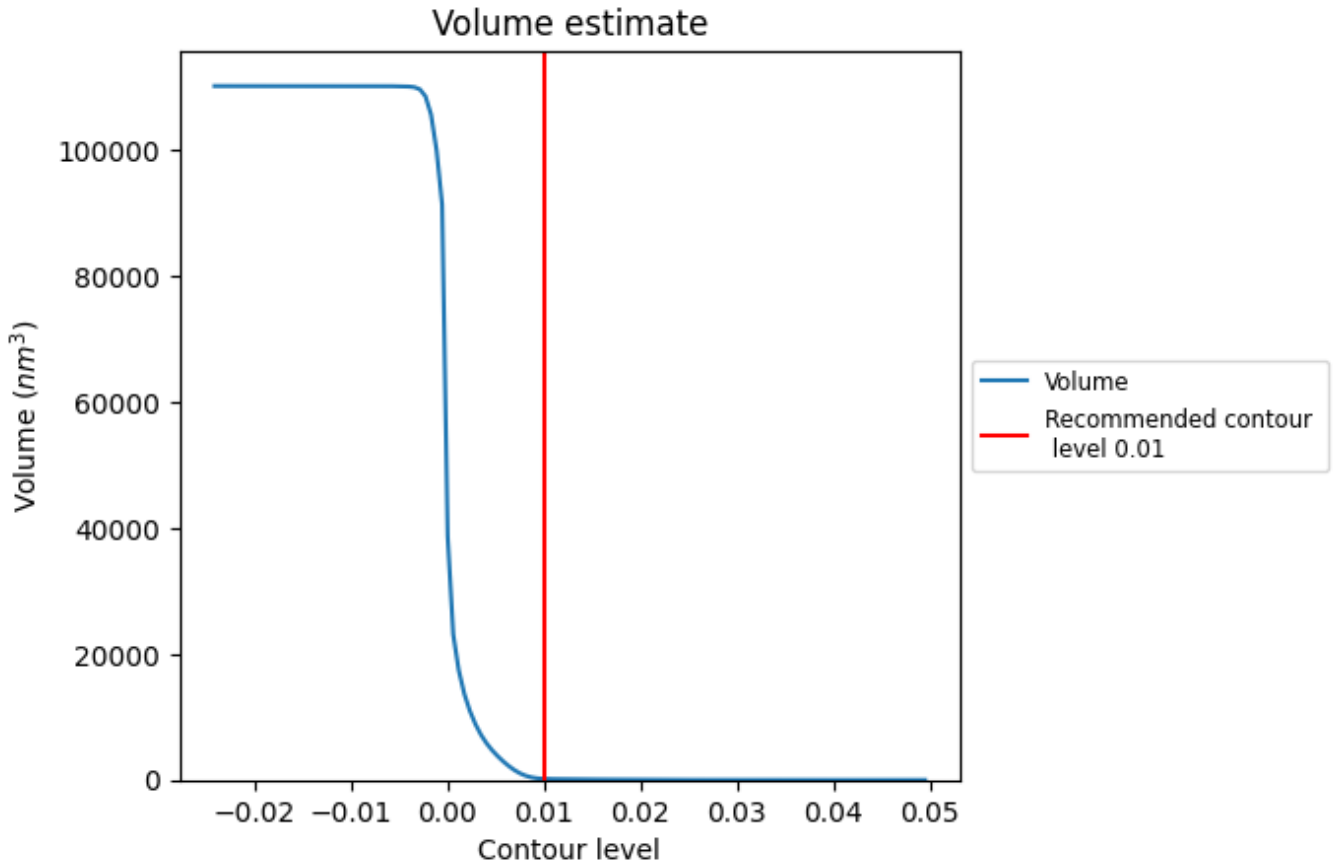
This section contains the results of statistical analysis of the map.

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.

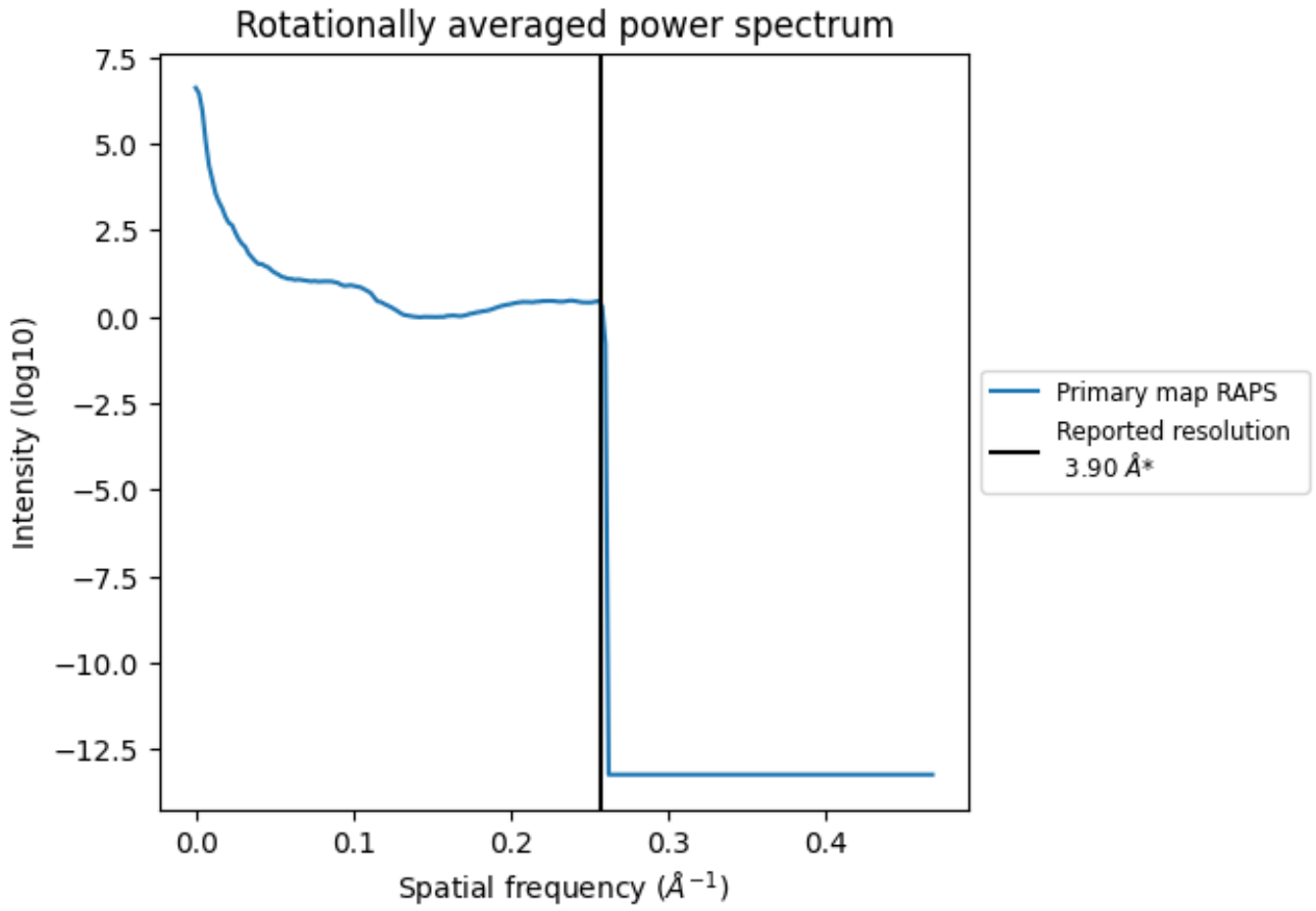
7.2 Volume estimate



The volume at the recommended contour level is 180 nm^3; this corresponds to an approximate mass of 163 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 0.256 $Å^{-1}$

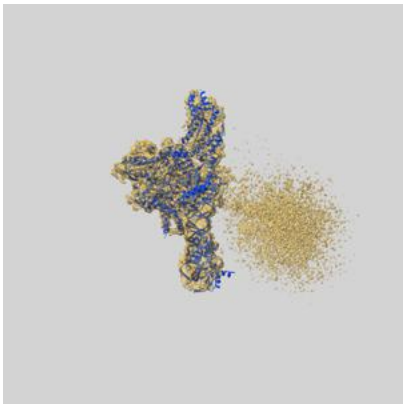
8 Fourier-Shell correlation

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

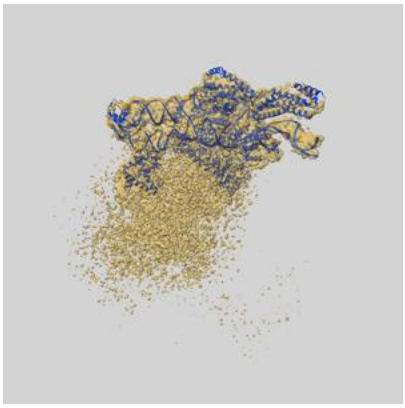
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12799 and PDB model 7OBQ. Per-residue inclusion information can be found in section 3 on page 12.

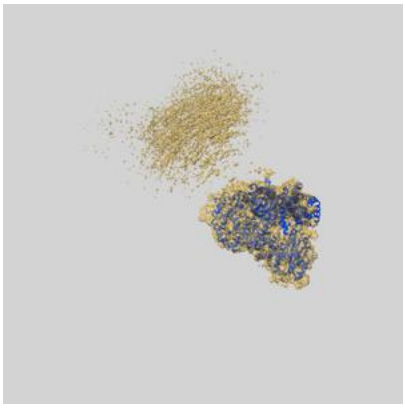
9.1 Map-model overlay



X



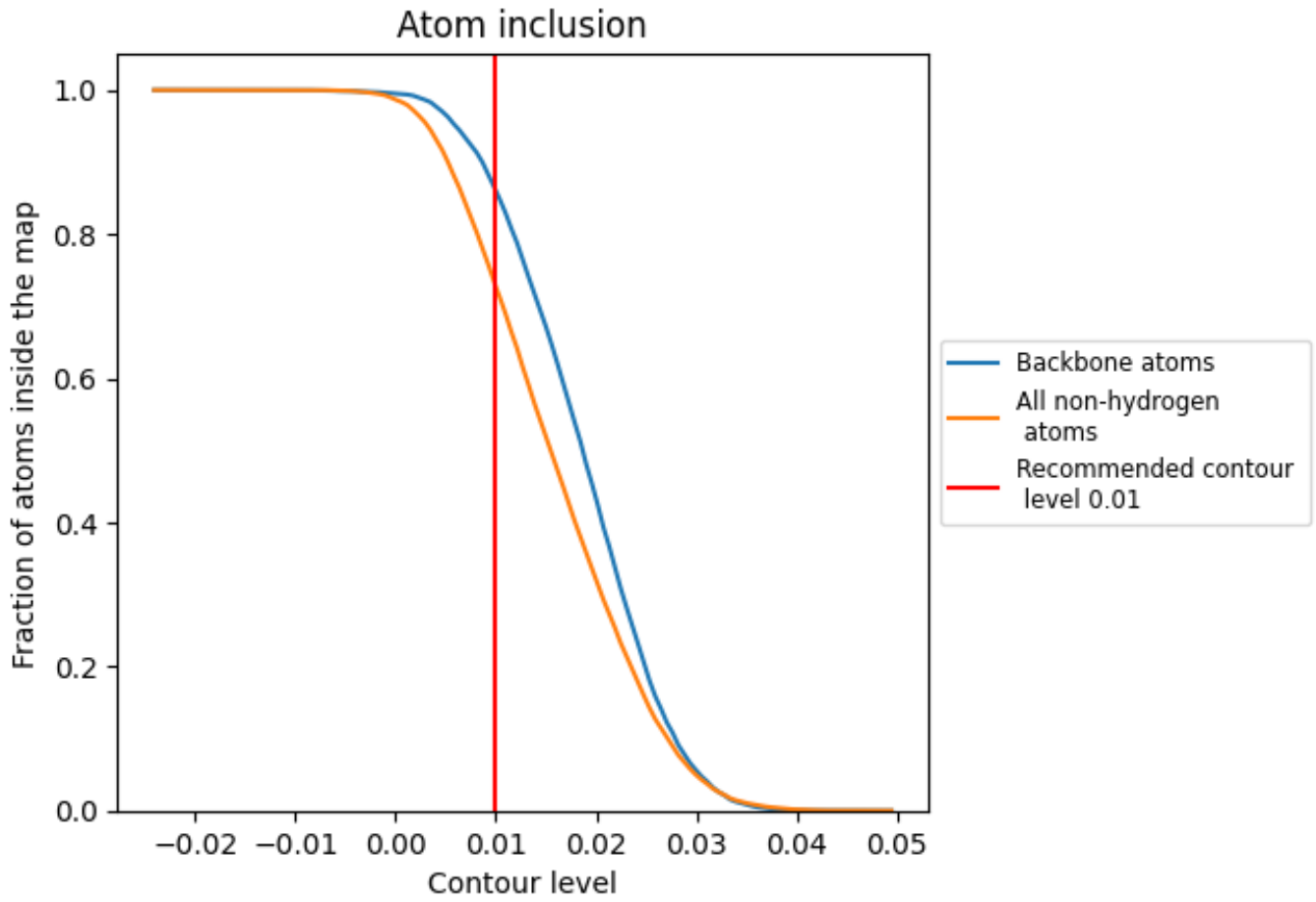
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.