



wwPDB EM Validation Summary Report ⓘ

Sep 23, 2026 – 02:05 am BST

PDB ID : 29IX / pdb_000029ix
EMDB ID : EMD-57202
Title : Human monosomes with bound toxin NT-2, focus on 60S subunit. NT-2 added to purified ribosomes as control.
Authors : Rabl, J.; Karousis, E.D.
Deposited on : 2026-03-15
Resolution : 2.20 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

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

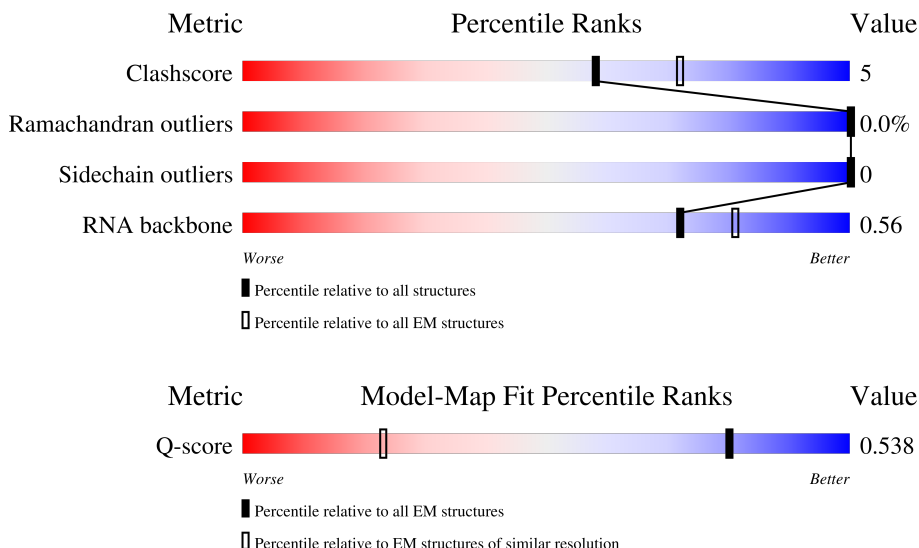
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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.



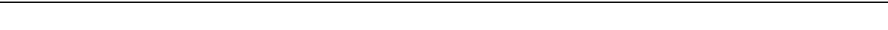
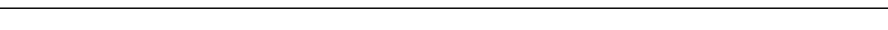
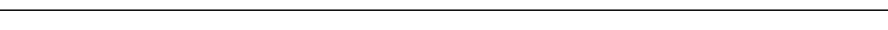
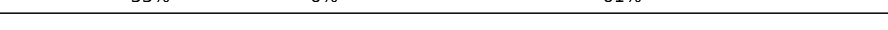
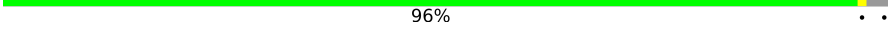
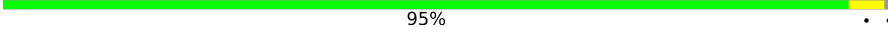
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	AA	248	 81% 10% 9%
2	AB	266	 73% 8% 19%
3	AC	192	 86% 13% .

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Mol	Chain	Length	Quality of chain
4	AD	214	 87% 8% .
5	AE	178	 80% 16% .
6	AF	211	 92% 6% .
7	AG	215	 55% 8% 37%
8	AH	204	 93% 6%
9	AI	203	 78% 21% .
10	AJ	184	 74% 8% 18%
11	AK	188	 94% 6% .
12	AL	196	 76% . 20%
13	AM	176	 92% 7% .
14	AN	160	 92% 7% .
15	AO	128	 68% 11% 21%
16	AP	140	 89% . 6%
17	AQ	157	 33% 6% 61%
18	AR	156	 70% 6% 24%
19	AS	145	 90% . . 8%
20	AT	136	 90% 10% .
21	AU	148	 88% 11% .
22	AV	159	 60% . 37%
23	AW	115	 75% 6% 19%
24	AX	125	 74% 13% 13%
25	AY	135	 96% . .
26	AZ	110	 95% . .
27	Aa	117	 85% 5% 9%
28	Ab	123	 90% 8% . .

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Mol	Chain	Length	Quality of chain
29	Ac	105	 90% 8% .
30	Ad	97	 89% 11%
31	Ae	70	 86% 13% .
32	Af	51	 94% . .
33	Ag	128	 40% . 59%
34	Ah	106	 94% . .
35	Ai	92	 92% 7% .
36	Aj	137	 86% 5% 9%
37	BA	403	 84% 13% .
38	BB	427	 77% 7% 16%
39	BC	297	 87% 12% .
40	BD	288	 66% 9% 25%
41	DA	5069	 44% 21% . 31%
42	DB	120	 78% 20% . .
43	DC	157	 59% 32% 9% .
44	DD	257	 84% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	PUT	DA	5101	-	-	X	-
48	PUT	DA	5102	-	-	X	-
48	PUT	DA	5103	-	-	X	-
49	SPD	DA	5107	-	-	X	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 237999 atoms, of which 95223 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 Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AA	225	Total	C	H	N	O	S	0	0
			3866	1202	1996	358	301	9		

- Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	216	Total	C	H	N	O	S	0	0
			3640	1121	1884	339	292	4		

- Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	AC	190	Total	C	H	N	O	S	0	0
			3119	956	1601	284	272	6		

- Molecule 4 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	205	Total	C	H	N	O	S	0	0
			3362	1053	1701	321	274	13		

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	AE	171	Total	C	H	N	O	S	0	0
			2783	867	1412	256	242	6		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	AF	207	Total	C	H	N	O	S	0	0
			3452	1046	1779	346	277	4		

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	AG	136	Total	C	H	N	O	S	0	0
			2307	719	1187	215	179	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	AH	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 9 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AI	201	Total	C	H	N	O	S	0	0
			3444	1063	1794	321	261	5		

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AJ	151	Total	C	H	N	O	S	0	0
			2474	765	1250	238	212	9		

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AK	187	Total	C	H	N	O	S	0	0
			3141	944	1628	314	250	5		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AL	156	Total	C	H	N	O	S	0	0
			2740	812	1438	279	202	9		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AM	175	Total	C	H	N	O	S	0	0
			2943	925	1490	283	235	10		

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AN	159	Total	C	H	N	O	S	0	0
			2664	823	1366	252	217	6		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AO	101	Total	C	H	N	O	S	0	0
			1675	529	850	144	150	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AP	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 17 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AQ	62	Total	C	H	N	O	S	0	0
			1052	332	533	101	83	3		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	AR	119	Total	C	H	N	O	S	0	0
			2029	624	1053	183	168	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	AS	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	AT	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	AU	147	Total	C	H	N	O	S	0	0
			2373	736	1210	237	187	3		

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	AV	100	Total	C	H	N	O	S	0	0
			1687	505	876	177	125	4		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	93	Total	C	H	N	O	S	0	0
			1490	462	764	129	129	6		

- Molecule 24 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	109	Total	C	H	N	O	S	0	0
			1848	569	947	173	157	2		

- Molecule 25 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	130	Total	C	H	N	O	S	0	0
			2236	676	1166	221	168	5		

- Molecule 26 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	AZ	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	144	3		

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Aa	106	Total	C	H	N	O	S	0	0
			1778	530	933	174	135	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Ab	122	Total	C	H	N	O	S	0	0
			2163	641	1148	205	168	1		

- Molecule 29 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Ac	102	Total	C	H	N	O	S	0	0
			1750	521	918	177	129	5		

- Molecule 30 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Ad	86	Total	C	H	N	O	S	0	0
			1441	434	736	155	111	5		

- Molecule 31 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Ae	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 32 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Af	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 33 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Ag	52	Total	C	H	N	O	S	0	0
			896	267	466	90	67	6		

- Molecule 34 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Ah	103	Total	C	H	N	O	S	0	0
			1754	528	912	172	136	6		

- Molecule 35 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	Ai	91	Total	C	H	N	O	S	0	0
			1464	445	757	136	119	7		

- Molecule 36 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	Aj	125	Total	C	H	N	O	S	0	0
			2071	622	1069	207	168	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	BA	396	Total	C	H	N	O	S	0	0
			6537	2037	3339	601	546	14		

- Molecule 38 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BB	359	Total	C	H	N	O	S	0	0
			5898	1802	3036	572	475	13		

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	BC	293	Total	C	H	N	O	S	0	0
			4807	1510	2421	435	427	14		

- Molecule 40 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	BD	216	Total	C	H	N	O	S	0	0
			3625	1119	1888	329	285	4		

- Molecule 41 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	DA	3483	Total	C	H	N	O	P	0	0
			112180	33315	37450	13662	24271	3482		

- Molecule 42 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	DB	119	Total	C	H	N	O	P	0	0
			3823	1132	1285	454	834	118		

- Molecule 43 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	DC	156	Total	C	H	N	O	P	0	0
			4989	1481	1674	585	1094	155		

- Molecule 44 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	DD	246	Total	C	H	N	O	S	0	0
			3867	1183	1979	387	312	6		

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	AD	1	Total	Mg	0
			1	1	
45	AJ	1	Total	Mg	0
			1	1	
45	AP	1	Total	Mg	0
			1	1	
45	AY	1	Total	Mg	0
			1	1	
45	AZ	1	Total	Mg	0
			1	1	
45	Ad	1	Total	Mg	0
			1	1	
45	BA	2	Total	Mg	0
			2	2	
45	DA	171	Total	Mg	0
			171	171	
45	DB	2	Total	Mg	0
			2	2	
45	DC	3	Total	Mg	0
			3	3	

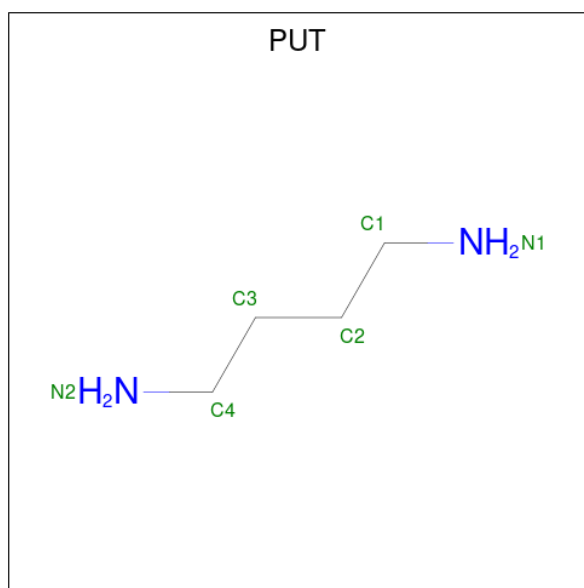
- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
46	AM	1	Total K 1 1	0
46	AN	1	Total K 1 1	0
46	AP	1	Total K 1 1	0
46	DA	40	Total K 40 40	0
46	DD	2	Total K 2 2	0

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

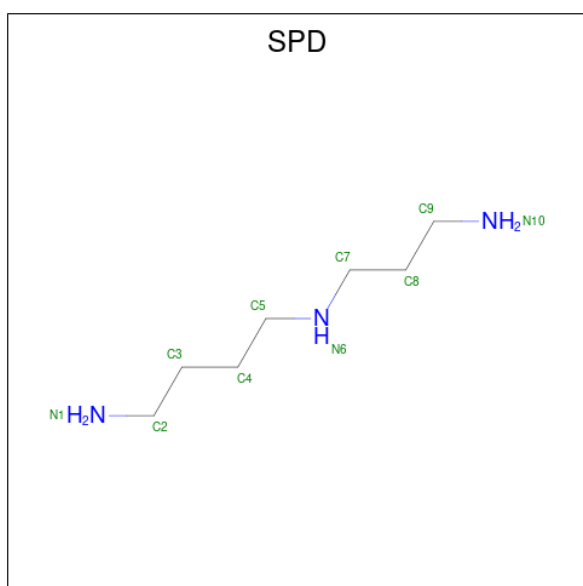
Mol	Chain	Residues	Atoms	AltConf
47	Aa	1	Total Zn 1 1	0
47	Ad	1	Total Zn 1 1	0
47	Ag	1	Total Zn 1 1	0
47	Ah	1	Total Zn 1 1	0
47	Ai	1	Total Zn 1 1	0

- Molecule 48 is 1,4-DIAMINOBTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



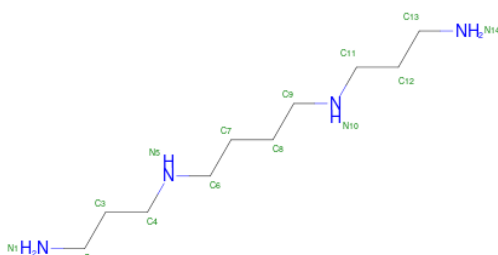
Mol	Chain	Residues	Atoms			AltConf
48	DA	1	Total	C	N	0
			6	4	2	
48	DA	1	Total	C	N	0
			6	4	2	
48	DA	1	Total	C	N	0
			6	4	2	
48	DB	1	Total	C	N	0
			6	4	2	

- Molecule 49 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



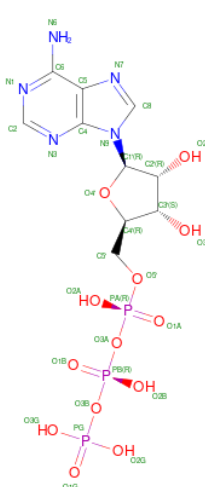
Mol	Chain	Residues	Atoms				AltConf
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	
49	DA	1	Total	C	H	N	0
			12	7	2	3	

- Molecule 50 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



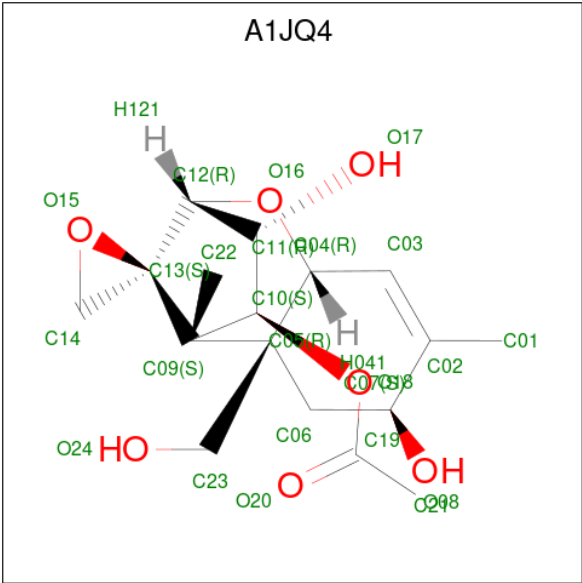
Mol	Chain	Residues	Atoms				AltConf
50	DA	1	Total 23	C 10	H 9	N 4	0
50	DA	1	Total 23	C 10	H 9	N 4	0
50	DA	1	Total 23	C 10	H 9	N 4	0
50	DA	1	Total 23	C 10	H 9	N 4	0

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms						AltConf
51	DA	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 52 is Toxin NT-2 (CCD ID: A1JQ4) (formula: C₁₇H₂₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
52	DA	1	Total	C	H	O	0
			48	17	24	7	

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	AA	117	Total	O	0
			117	117	
53	AB	133	Total	O	0
			133	133	
53	AC	128	Total	O	0
			128	128	
53	AD	91	Total	O	0
			91	91	
53	AE	141	Total	O	0
			141	141	
53	AF	95	Total	O	0
			95	95	
53	AG	70	Total	O	0
			70	70	

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Mol	Chain	Residues	Atoms		AltConf
53	AH	112	Total 112	O 112	0
53	AI	110	Total 110	O 110	0
53	AJ	47	Total 47	O 47	0
53	AK	93	Total 93	O 93	0
53	AL	51	Total 51	O 51	0
53	AM	115	Total 115	O 115	0
53	AN	85	Total 85	O 85	0
53	AO	73	Total 73	O 73	0
53	AP	67	Total 67	O 67	0
53	AQ	38	Total 38	O 38	0
53	AR	63	Total 63	O 63	0
53	AS	53	Total 53	O 53	0
53	AT	70	Total 70	O 70	0
53	AU	68	Total 68	O 68	0
53	AV	48	Total 48	O 48	0
53	AW	37	Total 37	O 37	0
53	AX	63	Total 63	O 63	0
53	AY	79	Total 79	O 79	0
53	AZ	56	Total 56	O 56	0
53	Aa	56	Total 56	O 56	0
53	Ab	77	Total 77	O 77	0

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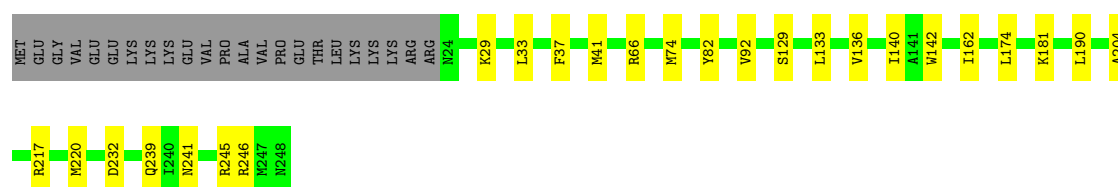
Mol	Chain	Residues	Atoms		AltConf
53	Ac	70	Total 70	O 70	0
53	Ad	54	Total 54	O 54	0
53	Ae	63	Total 63	O 63	0
53	Af	24	Total 24	O 24	0
53	Ag	25	Total 25	O 25	0
53	Ah	53	Total 53	O 53	0
53	Ai	40	Total 40	O 40	0
53	Aj	63	Total 63	O 63	0
53	BA	174	Total 174	O 174	0
53	BB	163	Total 163	O 163	0
53	BC	165	Total 165	O 165	0
53	BD	116	Total 116	O 116	0
53	DA	6364	Total 6364	O 6364	0
53	DB	202	Total 202	O 202	0
53	DC	232	Total 232	O 232	0
53	DD	100	Total 100	O 100	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

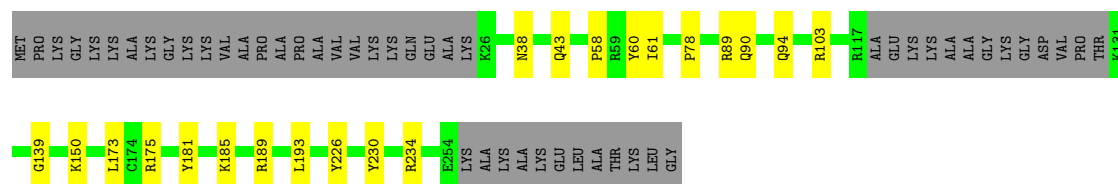
- Molecule 1: Large ribosomal subunit protein uL30

Chain AA: 



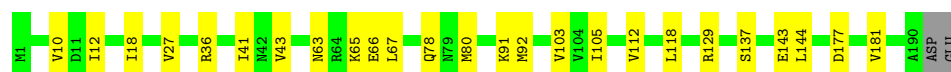
- Molecule 2: 60S ribosomal protein L7a

Chain AB: 



- Molecule 3: 60S ribosomal protein L9

Chain AC: 



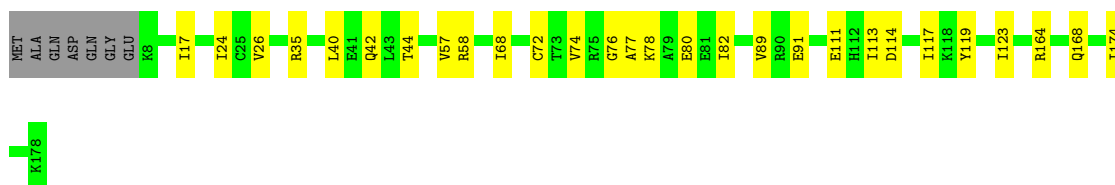
- Molecule 4: Ribosomal protein uL16-like

Chain AD: 



- Molecule 5: 60S ribosomal protein L11

Chain AE: 



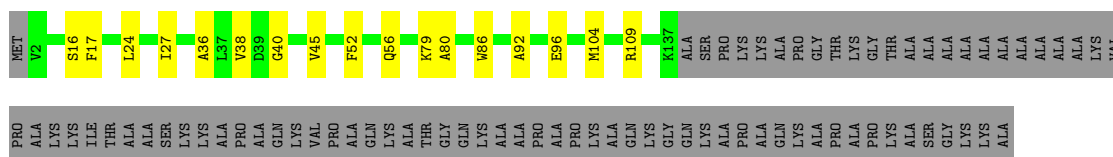
- Molecule 6: 60S ribosomal protein L13

Chain AF: 92% 6% .



- Molecule 7: 60S ribosomal protein L14

Chain AG: 55% 8% 37%



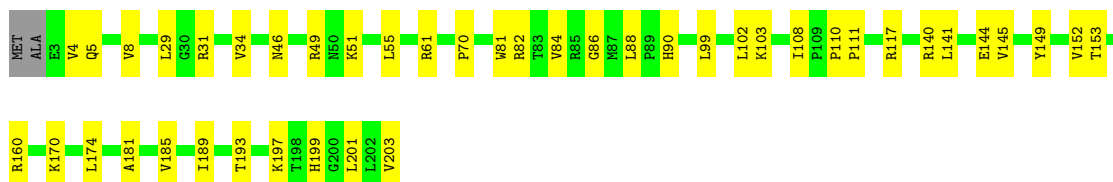
- Molecule 8: 60S ribosomal protein L15

Chain AH: 93% 6%



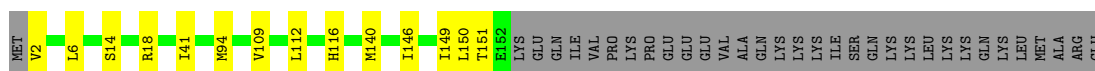
- Molecule 9: 60S ribosomal protein L13a

Chain AI: 78% 21% .



- Molecule 10: 60S ribosomal protein L17

Chain AJ: 74% 8% 18%



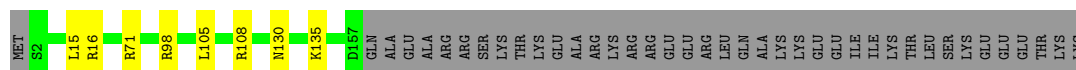
- Molecule 11: 60S ribosomal protein L18

Chain AK: 94% 6% .



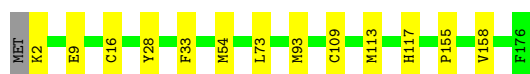
- Molecule 12: 60S ribosomal protein L19

Chain AL: 76% 20%



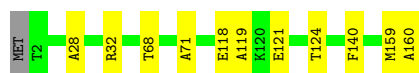
- Molecule 13: 60S ribosomal protein L18a

Chain AM: 92% 7%



- Molecule 14: 60S ribosomal protein L21

Chain AN: 92% 7%



- Molecule 15: 60S ribosomal protein L22

Chain AO: 68% 11% 21%



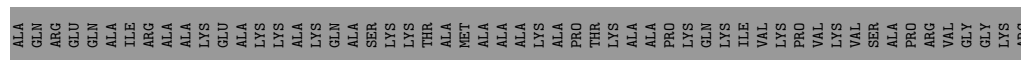
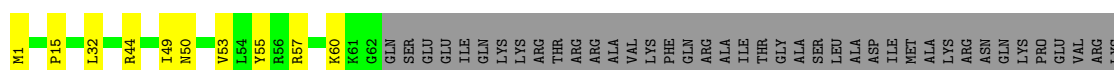
- Molecule 16: 60S ribosomal protein L23

Chain AP: 89% 6%



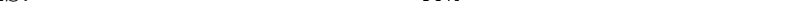
- Molecule 17: 60S ribosomal protein L24

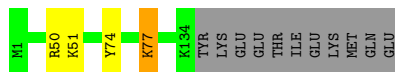
Chain AQ: 33% 6% 61%

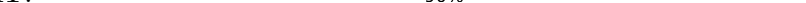


- Molecule 18: 60S ribosomal protein L23a

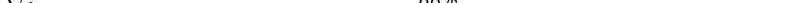
MET	ALA	PRO	LYS	ALA	LYS	LYS	GLU	ALA	PRO	ALA	PRO	PRO	PRO	LYS	ALA	ALA	GLU	ALA	LYS	ALA	LYS	ALA	ALA	LEU	LYS	ALA	ALA	LYS	LYS	LYS	ALA	VAL	VAL	LEU	LYS	GLY	VAL	HIS	HIS	SER	SER	HIS	LYS	K38	T42	R47	F79	P80	L81	T82	I90	I99	Q111	K114	K115
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

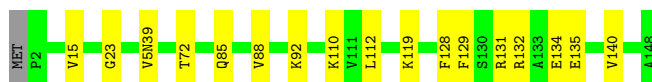
- Chain AS:  90% .. 8%



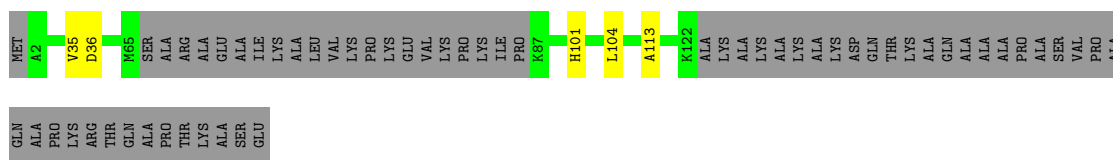
- Chain AT:  90% 10%



- Chain AU: 

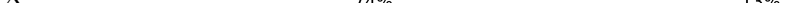


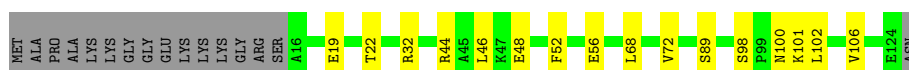
- Chain AV: 60% 3% 37%



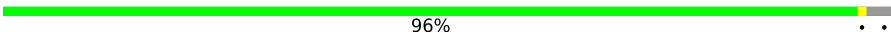
- Chain AW: 75% 6% 19%

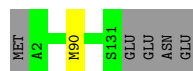


- Chain AX: 

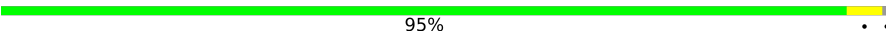


- Molecule 25: 60S ribosomal protein L32

Chain AY:  96% ..



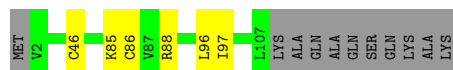
- Molecule 26: Large ribosomal subunit protein eL33

Chain AZ:  95% ..



- Molecule 27: 60S ribosomal protein L34

Chain Aa:  85% 5% 9%



- Molecule 28: 60S ribosomal protein L35

Chain Ab:  90% 8% ..



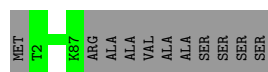
- Molecule 29: 60S ribosomal protein L36

Chain Ac:  90% 8% .



- Molecule 30: Large ribosomal subunit protein eL37

Chain Ad:  89% 11%

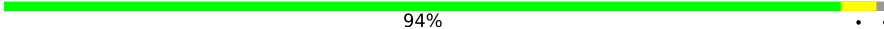


- Molecule 31: 60S ribosomal protein L38

Chain Ae:  86% 13% .



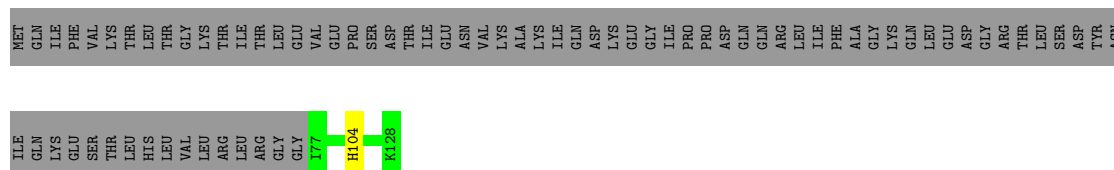
- Molecule 32: 60S ribosomal protein L39

Chain Af:  94%

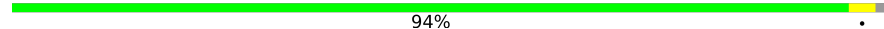


- Molecule 33: Large ribosomal subunit protein eL40

Chain Ag:  40% 59%

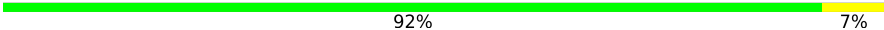


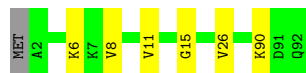
- Molecule 34: 60S ribosomal protein L36a

Chain Ah:  94%



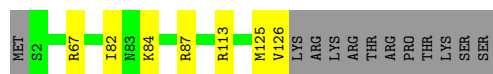
- Molecule 35: 60S ribosomal protein L37a

Chain Ai:  92% 7%



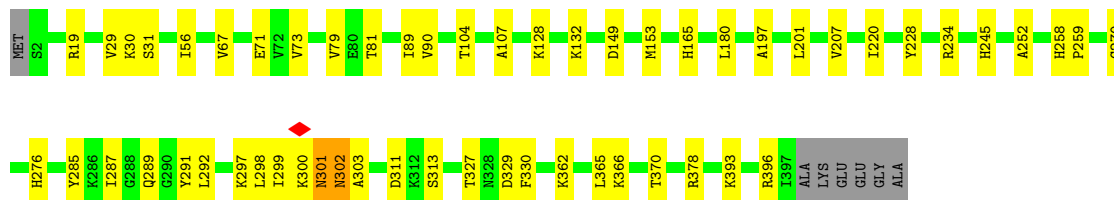
- Molecule 36: 60S ribosomal protein L28

Chain Aj:  86% 5% 9%



- Molecule 37: Large ribosomal subunit protein uL3

Chain BA:  84% 13%



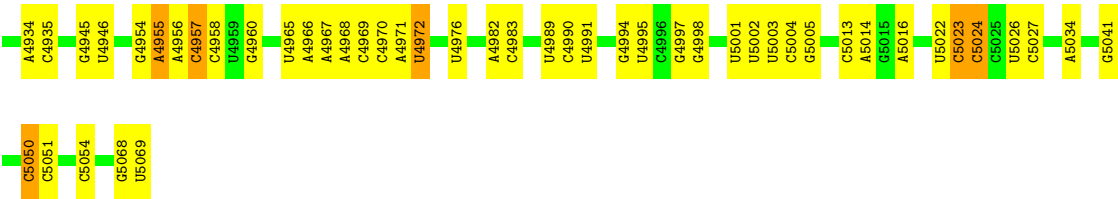
- Molecule 38: 60S ribosomal protein L4

Chain BB:  77% 7% 16%

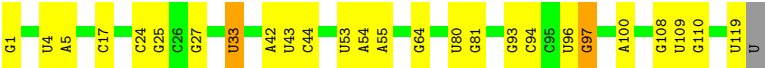
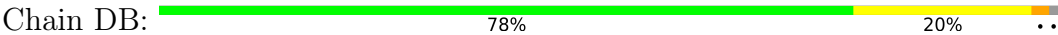




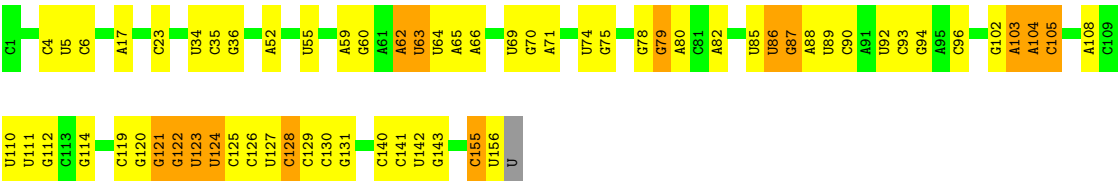
C	C	A4597	U4497	C4411	U4312	A4212	G	U	A3867	U	U3770	A3656	G
G	C	U4498	U4498	A4415	A4313	A4213	G	G	G3868	G	C3771	U3657	C
C	C	U4499	U4499	A4416	C4314	A4213	C	U	C3869	A	C3772	U3657	C
C	C	U4500	U4500	C4417	A4315	A4220	C	A	A3662	C	U3773	A3662	U
C	C	C4504	C4504	C4418	A4323	C4221	G	A	A3663	C	U3774	A3663	C
C	C	C4505	C4505	U4419	A4323	C4223	C	A	A3664	C	U3775	A3664	C
C	C	U4512	U4512	U4420	G4329	A4224	C	U	A3665	C	C3776	C3665	C
C	C	A4513	U4513	C4421	G4330	A4225	C	A	G3669	U	C3777	C3669	U
C	C	G4519	U4519	A4422	C4331	U4226	C	A	G3672	C	U3778	G3672	C
C	C	U4520	U4520	A4423	C4332	U4227	C	G	C3673	C	A3776	C3673	C
C	C	U4521	U4521	A4424	A4339	U4228	A	U	A3692	C	C3777	A3692	C
C	C	U4522	U4522	A4428	U4340	U4229	G	G	U3693	C	C3778	U3693	C
C	C	A4523	A4523	U4431	C4342	U4232	G	A	U3694	C	C3779	U3694	C
C	C	U4524	U4524	U4431	C4342	A4233	G	A	U3695	C	C3780	U3695	C
C	C	C4525	C4525	C4434	G4347	U4238	C	G	A3784	C	C3781	A3784	C
C	C	U4529	U4529	U4440	A4348	A4239	U	C	A3785	C	C3782	A3785	C
C	C	U4530	U4530	U4441	C4349	A4240	C	C	G3792	C	C3783	G3792	C
C	C	U4531	U4531	U4442	C4350	U4241	C	C	A3791	C	C3784	A3791	C
C	C	U4532	U4532	C4443	U4351	U4242	C	C	A3792	C	C3785	A3792	C
C	C	C4444	C4444	C4444	U4352	C4243	C	C	A3793	C	C3786	A3793	C
C	C	A4535	U4535	U4455	U4353	A4244	C	C	A3794	C	C3787	A3794	C
C	C	U4536	U4536	C4447	U4354	U4245	C	C	A3795	C	C3788	A3795	C
C	C	C4537	C4537	U4448	G4355	G4245	C	C	A3796	C	C3789	A3796	C
C	C	U4538	U4538	A4449	G4356	A4253	G	C	A3797	C	C3790	A3797	C
C	C	A4548	U4548	U4455	U4361	U4254	U	C	A3798	C	C3791	A3798	C
C	C	U4549	U4549	C4456	A4256	A4255	G	C	A3799	C	C3792	A3799	C
C	C	U4550	U4550	U4457	G4370	A4257	A	C	A3800	C	C3793	A3800	C
C	C	U4551	U4551	C4458	C4373	C4258	A	C	A3801	C	C3794	A3801	C
C	C	U4552	U4552	U4459	U4260	U4259	U	C	A3802	C	C3795	A3802	C
C	C	C4560	C4560	U4460	A4376	U4261	C	C	A3803	C	C3796	A3803	C
C	C	C4563	U4563	U4464	C4377	C4262	C	C	A3804	C	C3797	A3804	C
C	C	U4564	U4564	U4465	A4378	C4263	C	C	A3805	C	C3798	A3805	C
C	C	U4565	U4565	C4466	A4379	U4264	C	C	A3806	C	C3799	A3806	C
C	C	U4566	U4566	U4469	A4380	U4265	U	C	A3807	C	C3800	A3807	C
C	C	U4567	U4567	C4470	C4387	U4266	A	C	A3808	C	C3801	A3808	C
C	C	A4571	U4571	U4471	A4390	A4268	U	C	A3809	C	C3802	A3809	C
C	C	U4572	U4572	G4475	G4391	A4273	C	C	A3810	C	C3803	A3810	C
C	C	G4573	G4573	C4476	G4392	A4274	C	C	A3811	C	C3804	A3811	C
C	C	U4576	U4576	A4477	A4393	G4275	A	C	A3812	C	C3805	A3812	C
C	C	U4577	U4577	C4478	U4395	U4281	C	C	A3813	C	C3806	A3813	C
C	C	U4578	U4578	U4484	A4396	A4281	C	C	A3814	C	C3807	A3814	C
C	C	U4579	U4579	C4485	G4400	G4291	U	C	A3815	C	C3808	A3815	C
C	C	A4584	U4584	C4486	G4401	U4292	U	C	A3816	C	C3809	A3816	C
C	C	U4585	U4585	A4487	C4402	U4293	U	C	A3817	C	C3810	A3817	C
C	C	U4590	U4590	U4488	U4403	U4296	C	C	A3818	C	C3811	A3818	C
C	C	U4591	U4591	C4489	U4404	U4297	C	C	A3819	C	C3812	A3819	C
C	C	U4701	U4701	U4493	G4405	U4299	C	C	A3820	C	C3813	A3820	C
C	C	C4702	C4702	C4494	U4406	U4305	C	C	A3821	C	C3814	A3821	C
C	C	U4703	U4703	C4495	G4407	U4306	C	C	A3822	C	C3815	A3822	C
C	C	A4705	C4596	A4496	G4410	U4307	C	C	A3823	C	C3816	A3823	C



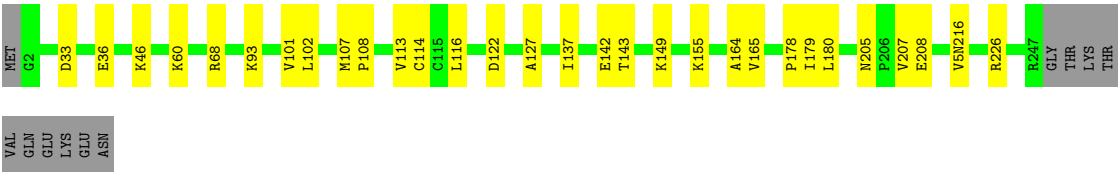
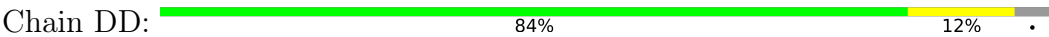
• Molecule 42: 5S rRNA



• Molecule 43: 5.8S rRNA



• Molecule 44: Large ribosomal subunit protein uL2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	616107	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 ($e^-/\text{\AA}^2$)	60.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.134	Depositor
Minimum map value	-0.599	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	414.72, 414.72, 414.72	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.648, 0.648, 0.648	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, HIC, PUT, UR3, 1MA, B8T, UY1, PSU, ATP, SPD, MLZ, 6MZ, OMU, V5N, OMG, A1JQ4, SPM, K, A2M, MG, ZN, OMC

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	AA	0.24	0/1905	0.44	0/2539
2	AB	0.27	0/1787	0.48	0/2408
3	AC	0.20	0/1537	0.42	0/2066
4	AD	0.19	0/1700	0.39	0/2270
5	AE	0.21	0/1394	0.49	0/1863
6	AF	0.19	0/1704	0.38	0/2282
7	AG	0.20	0/1142	0.42	0/1527
8	AH	0.17	0/1746	0.38	0/2338
9	AI	0.21	0/1682	0.45	0/2250
10	AJ	0.26	0/1250	0.53	0/1678
11	AK	0.28	1/1537 (0.1%)	0.41	1/2052 (0.0%)
12	AL	0.25	0/1318	0.46	0/1745
13	AM	0.23	0/1493	0.43	0/2003
14	AN	0.25	0/1326	0.45	0/1770
15	AO	0.22	0/839	0.48	0/1126
16	AP	0.35	1/993 (0.1%)	0.45	0/1332
17	AQ	0.34	0/532	0.50	0/708
18	AR	0.21	0/993	0.42	0/1334
19	AS	0.37	1/1132 (0.1%)	0.44	1/1504 (0.1%)
20	AT	0.16	0/1130	0.36	0/1507
21	AU	0.21	0/1179	0.40	0/1573
22	AV	0.21	0/824	0.46	0/1086
23	AW	0.20	0/736	0.42	0/988
24	AX	0.21	0/916	0.44	0/1234
25	AY	0.15	0/1088	0.35	0/1451
26	AZ	0.19	0/895	0.39	0/1198
27	Aa	0.16	0/855	0.37	0/1140
28	Ab	0.21	0/1023	0.44	0/1351
29	Ac	0.20	0/843	0.40	0/1115
30	Ad	0.28	0/720	0.41	0/952
31	Ae	0.18	0/575	0.38	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Af	0.22	0/454	0.48	0/599
33	Ag	0.16	0/425	0.37	0/561
34	Ah	0.13	0/855	0.30	0/1128
35	Ai	0.16	0/717	0.36	0/953
36	Aj	0.23	0/1017	0.44	0/1364
37	BA	0.23	0/3253	0.50	2/4352 (0.0%)
38	BB	0.19	0/2916	0.40	0/3917
39	BC	0.18	0/2432	0.38	0/3256
40	BD	0.16	0/1771	0.35	0/2377
41	DA	0.16	12/80842 (0.0%)	0.31	0/126109
42	DB	0.12	0/2836	0.27	0/4421
43	DC	0.20	1/3631 (0.0%)	0.32	0/5657
44	DD	0.19	0/1913	0.41	0/2563
All	All	0.19	16/139856 (0.0%)	0.35	4/206408 (0.0%)

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
2	AB	0	1
10	AJ	0	1
12	AL	0	1
15	AO	0	1
18	AR	0	1
26	AZ	0	1
28	Ab	0	2
29	Ac	0	1
All	All	0	9

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AK	59	PRO	CA-C	8.16	1.57	1.52
41	DA	2815	A2M	O3'-P	6.61	1.62	1.56
41	DA	4523	A2M	O3'-P	6.43	1.62	1.56
41	DA	3830	A2M	O3'-P	6.41	1.62	1.56
16	AP	11	GLY	N-CA	6.40	1.52	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AK	59	PRO	O-C-N	8.50	125.14	121.15
37	BA	301	ASN	N-CA-C	-7.72	98.39	110.36
19	AS	77	LYS	CA-C-O	5.98	126.56	119.56
37	BA	302	ASN	N-CA-CB	-5.46	107.94	114.17

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	89	ARG	Sidechain
10	AJ	18	ARG	Sidechain
12	AL	71	ARG	Sidechain
15	AO	113	ARG	Sidechain
18	AR	47	ARG	Sidechain

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	AA	1870	1996	1996	19	0
2	AB	1756	1884	1884	13	0
3	AC	1518	1601	1601	16	0
4	AD	1661	1701	1701	10	0
5	AE	1371	1412	1412	21	0
6	AF	1673	1779	1779	8	0
7	AG	1120	1187	1187	14	0
8	AH	1701	1749	1749	8	0
9	AI	1650	1794	1794	32	0
10	AJ	1224	1250	1250	8	0
11	AK	1513	1628	1628	7	0
12	AL	1302	1438	1438	4	0
13	AM	1453	1490	1490	10	0
14	AN	1298	1366	1366	9	0
15	AO	825	850	850	11	0
16	AP	979	1039	1039	3	0
17	AQ	519	533	533	7	0
18	AR	976	1053	1053	7	0
19	AS	1115	1205	1205	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AT	1107	1182	1182	8	0
21	AU	1163	1210	1206	13	0
22	AV	811	876	876	4	0
23	AW	726	764	764	6	0
24	AX	901	947	946	9	0
25	AY	1070	1166	1165	2	0
26	AZ	876	912	912	3	0
27	Aa	845	933	933	5	0
28	Ab	1015	1148	1148	8	0
29	Ac	832	918	917	6	0
30	Ad	705	736	736	0	0
31	Ae	569	637	637	5	0
32	Af	444	483	483	2	0
33	Ag	430	466	465	1	0
34	Ah	842	912	912	2	0
35	Ai	707	757	756	6	0
36	Aj	1002	1069	1068	6	0
37	BA	3198	3339	3339	47	0
38	BB	2862	3036	3036	22	0
39	BC	2386	2421	2421	25	0
40	BD	1737	1888	1888	18	0
41	DA	74730	37450	37836	654	0
42	DB	2538	1285	1286	12	0
43	DC	3315	1674	1685	44	0
44	DD	1888	1979	1976	22	0
45	AD	1	0	0	0	0
45	AJ	1	0	0	0	0
45	AP	1	0	0	0	0
45	AY	1	0	0	0	0
45	AZ	1	0	0	0	0
45	Ad	1	0	0	0	0
45	BA	2	0	0	0	0
45	DA	171	0	0	0	0
45	DB	2	0	0	0	0
45	DC	3	0	0	0	0
46	AM	1	0	0	0	0
46	AN	1	0	0	0	0
46	AP	1	0	0	0	0
46	DA	40	0	0	0	0
46	DD	2	0	0	0	0
47	Aa	1	0	0	0	0
47	Ad	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	Ag	1	0	0	0	0
47	Ah	1	0	0	0	0
47	Ai	1	0	0	0	0
48	DA	18	0	36	14	0
48	DB	6	0	0	0	0
49	DA	40	8	76	23	0
50	DA	56	36	104	9	0
51	DA	31	12	12	2	0
52	DA	24	24	0	0	0
53	AA	117	0	0	1	0
53	AB	133	0	0	0	0
53	AC	128	0	0	0	0
53	AD	91	0	0	0	0
53	AE	141	0	0	0	0
53	AF	95	0	0	0	0
53	AG	70	0	0	0	0
53	AH	112	0	0	0	0
53	AI	110	0	0	1	0
53	AJ	47	0	0	0	0
53	AK	93	0	0	0	0
53	AL	51	0	0	0	0
53	AM	115	0	0	0	0
53	AN	85	0	0	0	0
53	AO	73	0	0	0	0
53	AP	67	0	0	0	0
53	AQ	38	0	0	0	0
53	AR	63	0	0	2	0
53	AS	53	0	0	0	0
53	AT	70	0	0	0	0
53	AU	68	0	0	1	0
53	AV	48	0	0	0	0
53	AW	37	0	0	0	0
53	AX	63	0	0	0	0
53	AY	79	0	0	0	0
53	AZ	56	0	0	0	0
53	Aa	56	0	0	0	0
53	Ab	77	0	0	2	0
53	Ac	70	0	0	0	0
53	Ad	54	0	0	0	0
53	Ae	63	0	0	0	0
53	Af	24	0	0	0	0
53	Ag	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	Ah	53	0	0	0	0
53	Ai	40	0	0	0	0
53	Aj	63	0	0	0	0
53	BA	174	0	0	1	0
53	BB	163	0	0	0	0
53	BC	165	0	0	0	0
53	BD	116	0	0	0	0
53	DA	6364	0	0	7	0
53	DB	202	0	0	0	0
53	DC	232	0	0	0	0
53	DD	100	0	0	0	0
All	All	142776	95223	95756	1071	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 5.

The worst 5 of 1071 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)
41:DA:1534:A2M:O4'	41:DA:1534:A2M:C1'	1.64	1.23
41:DA:3718:A2M:O4'	41:DA:3718:A2M:C1'	1.63	1.22
41:DA:370:U:O4	48:DA:5103:PUT:H41	1.86	0.76
41:DA:2050:G:H21	49:DA:5107:SPD:H72	1.51	0.76
9:AI:86:GLY:O	49:DA:5107:SPD:H92	1.86	0.75

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AA	223/248 (90%)	220 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	212/266 (80%)	205 (97%)	7 (3%)	0	100	100
3	AC	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
4	AD	201/214 (94%)	198 (98%)	3 (2%)	0	100	100
5	AE	169/178 (95%)	166 (98%)	3 (2%)	0	100	100
6	AF	205/211 (97%)	197 (96%)	8 (4%)	0	100	100
7	AG	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
8	AH	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
9	AI	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
10	AJ	149/184 (81%)	145 (97%)	4 (3%)	0	100	100
11	AK	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
12	AL	154/196 (79%)	153 (99%)	1 (1%)	0	100	100
13	AM	173/176 (98%)	170 (98%)	3 (2%)	0	100	100
14	AN	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
15	AO	99/128 (77%)	93 (94%)	6 (6%)	0	100	100
16	AP	129/140 (92%)	129 (100%)	0	0	100	100
17	AQ	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
18	AR	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
19	AS	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
20	AT	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
21	AU	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	19
22	AV	96/159 (60%)	93 (97%)	3 (3%)	0	100	100
23	AW	91/115 (79%)	88 (97%)	3 (3%)	0	100	100
24	AX	107/125 (86%)	105 (98%)	2 (2%)	0	100	100
25	AY	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
26	AZ	107/110 (97%)	107 (100%)	0	0	100	100
27	Aa	104/117 (89%)	103 (99%)	1 (1%)	0	100	100
28	Ab	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
29	Ac	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
30	Ad	84/97 (87%)	84 (100%)	0	0	100	100
31	Ae	67/70 (96%)	67 (100%)	0	0	100	100
32	Af	48/51 (94%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Ag	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
34	Ah	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
35	Ai	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
36	Aj	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
37	BA	393/403 (98%)	380 (97%)	12 (3%)	1 (0%)	36	42
38	BB	357/427 (84%)	349 (98%)	8 (2%)	0	100	100
39	BC	291/297 (98%)	287 (99%)	4 (1%)	0	100	100
40	BD	210/288 (73%)	204 (97%)	6 (3%)	0	100	100
44	DD	243/257 (95%)	233 (96%)	10 (4%)	0	100	100
All	All	6272/7187 (87%)	6130 (98%)	140 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	BA	303	ALA
21	AU	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	194/215 (90%)	194 (100%)	0	100	100
2	AB	189/223 (85%)	189 (100%)	0	100	100
3	AC	169/171 (99%)	169 (100%)	0	100	100
4	AD	175/181 (97%)	175 (100%)	0	100	100
5	AE	144/149 (97%)	144 (100%)	0	100	100
6	AF	173/177 (98%)	173 (100%)	0	100	100
7	AG	116/161 (72%)	116 (100%)	0	100	100
8	AH	171/172 (99%)	171 (100%)	0	100	100
9	AI	173/174 (99%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	132/163 (81%)	132 (100%)	0	100	100
11	AK	164/165 (99%)	164 (100%)	0	100	100
12	AL	139/175 (79%)	139 (100%)	0	100	100
13	AM	156/157 (99%)	156 (100%)	0	100	100
14	AN	139/140 (99%)	139 (100%)	0	100	100
15	AO	91/115 (79%)	91 (100%)	0	100	100
16	AP	101/107 (94%)	101 (100%)	0	100	100
17	AQ	54/126 (43%)	54 (100%)	0	100	100
18	AR	107/133 (80%)	107 (100%)	0	100	100
19	AS	124/135 (92%)	124 (100%)	0	100	100
20	AT	117/118 (99%)	117 (100%)	0	100	100
21	AU	119/120 (99%)	119 (100%)	0	100	100
22	AV	82/126 (65%)	82 (100%)	0	100	100
23	AW	78/97 (80%)	78 (100%)	0	100	100
24	AX	99/110 (90%)	99 (100%)	0	100	100
25	AY	116/121 (96%)	116 (100%)	0	100	100
26	AZ	88/89 (99%)	88 (100%)	0	100	100
27	Aa	92/100 (92%)	92 (100%)	0	100	100
28	Ab	109/110 (99%)	109 (100%)	0	100	100
29	Ac	86/89 (97%)	86 (100%)	0	100	100
30	Ad	73/80 (91%)	73 (100%)	0	100	100
31	Ae	64/65 (98%)	64 (100%)	0	100	100
32	Af	47/48 (98%)	47 (100%)	0	100	100
33	Ag	47/115 (41%)	47 (100%)	0	100	100
34	Ah	91/94 (97%)	91 (100%)	0	100	100
35	Ai	74/75 (99%)	74 (100%)	0	100	100
36	Aj	109/121 (90%)	109 (100%)	0	100	100
37	BA	344/348 (99%)	344 (100%)	0	100	100
38	BB	299/348 (86%)	299 (100%)	0	100	100
39	BC	247/250 (99%)	247 (100%)	0	100	100
40	BD	192/252 (76%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DD	188/198 (95%)	188 (100%)	0	100	100
All	All	5472/6113 (90%)	5472 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
32	Af	17	GLN
37	BA	301	ASN
32	Af	19	GLN
36	Aj	100	ASN
37	BA	376	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
41	DA	3467/5069 (68%)	529 (15%)	11 (0%)
42	DB	118/120 (98%)	9 (7%)	0
43	DC	155/157 (98%)	28 (18%)	0
All	All	3740/5346 (69%)	566 (15%)	11 (0%)

5 of 566 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
41	DA	39	A
41	DA	42	A
41	DA	48	G
41	DA	58	G
41	DA	59	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	DA	2252	G
41	DA	2562	G
41	DA	4893	A
41	DA	4142	C
41	DA	1590	C

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

122 non-standard protein/DNA/RNA residues 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$
41	PSU	DA	4403	41	18,21,22	1.17	2 (11%)	22,30,33	1.37	3 (13%)
41	OMU	DA	4498	41,45	19,22,23	0.71	0	26,31,34	1.22	4 (15%)
41	PSU	DA	4552	41	18,21,22	1.16	2 (11%)	22,30,33	1.37	3 (13%)
41	PSU	DA	3695	41	18,21,22	1.18	3 (16%)	22,30,33	1.15	2 (9%)
41	5MC	DA	3782	41,45	18,22,23	3.57	7 (38%)	26,32,35	1.04	2 (7%)
41	OMC	DA	2351	41,45	19,22,23	3.10	8 (42%)	26,31,34	0.94	2 (7%)
41	OMG	DA	4623	41	23,26,27	2.51	7 (30%)	33,38,41	1.87	10 (30%)
41	PSU	DA	4673	41,45	18,21,22	1.18	2 (11%)	22,30,33	1.32	3 (13%)
41	PSU	DA	4471	41	18,21,22	1.22	3 (16%)	22,30,33	1.34	3 (13%)
41	A2M	DA	398	41	22,25,26	3.37	9 (40%)	31,36,39	2.87	14 (45%)
41	PSU	DA	1792	41	18,21,22	1.17	2 (11%)	22,30,33	1.37	3 (13%)
41	PSU	DA	4353	41	18,21,22	1.15	1 (5%)	22,30,33	1.44	3 (13%)
33	MLZ	Ag	98	33	8,9,10	0.78	0	4,9,11	0.83	0
41	PSU	DA	1536	41	18,21,22	1.16	2 (11%)	22,30,33	1.40	3 (13%)
41	PSU	DA	3844	41	18,21,22	1.21	2 (11%)	22,30,33	1.28	3 (13%)
41	OMG	DA	2364	41,45	23,26,27	2.50	7 (30%)	33,38,41	1.92	9 (27%)
21	V5N	AU	39	21	9,11,12	1.46	1 (11%)	9,14,16	2.14	3 (33%)
41	PSU	DA	4532	41	18,21,22	1.17	2 (11%)	22,30,33	1.36	3 (13%)
41	OMG	DA	4637	41	23,26,27	2.48	6 (26%)	33,38,41	1.85	10 (30%)
41	OMU	DA	4620	41	19,22,23	0.63	0	26,31,34	1.20	4 (15%)
41	B8T	DA	1859	41	19,22,23	0.99	1 (5%)	26,31,34	0.74	1 (3%)
41	PSU	DA	4628	41	18,21,22	1.20	2 (11%)	22,30,33	1.29	3 (13%)
41	A2M	DA	4571	41	22,25,26	3.28	9 (40%)	31,36,39	2.79	18 (58%)
41	UR3	DA	4530	41	19,22,23	3.07	8 (42%)	26,32,35	1.46	3 (11%)
41	PSU	DA	4312	41	18,21,22	1.16	2 (11%)	22,30,33	1.42	3 (13%)
41	OMG	DA	3744	41	23,26,27	2.49	7 (30%)	33,38,41	1.87	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	DA	3920	41,45	18,21,22	1.19	2 (11%)	22,30,33	1.26	3 (13%)
41	PSU	DA	3884	41	18,21,22	1.17	2 (11%)	22,30,33	1.40	3 (13%)
41	PSU	DA	3637	46,41	18,21,22	1.06	1 (5%)	22,30,33	1.44	4 (18%)
41	OMC	DA	2804	41	19,22,23	3.12	8 (42%)	26,31,34	0.70	0
41	PSU	DA	1862	41	18,21,22	1.13	2 (11%)	22,30,33	1.44	3 (13%)
41	OMG	DA	1316	41	23,26,27	2.50	7 (30%)	33,38,41	1.87	9 (27%)
41	6MZ	DA	4220	41	22,25,26	3.81	9 (40%)	30,36,39	2.38	10 (33%)
41	PSU	DA	4420	41	18,21,22	1.15	2 (11%)	22,30,33	1.17	2 (9%)
44	V5N	DD	216	44	9,11,12	1.45	1 (11%)	9,14,16	1.89	3 (33%)
41	A2M	DA	3785	41	22,25,26	3.43	10 (45%)	31,36,39	2.67	12 (38%)
41	PSU	DA	4442	41	18,21,22	1.19	3 (16%)	22,30,33	1.13	2 (9%)
41	A2M	DA	2787	41	22,25,26	3.44	9 (40%)	31,36,39	2.49	9 (29%)
41	OMG	DA	4370	41	23,26,27	2.52	7 (30%)	33,38,41	1.90	9 (27%)
41	PSU	DA	4457	41	18,21,22	1.19	2 (11%)	22,30,33	1.21	3 (13%)
41	PSU	DA	4576	41	18,21,22	1.20	2 (11%)	22,30,33	1.19	3 (13%)
41	OMG	DA	3627	41	23,26,27	2.52	7 (30%)	33,38,41	1.92	10 (30%)
41	PSU	DA	4423	41	18,21,22	1.16	1 (5%)	22,30,33	1.42	3 (13%)
41	OMC	DA	3808	41	19,22,23	3.15	8 (42%)	26,31,34	0.75	0
41	A2M	DA	4523	41,45	22,25,26	3.41	9 (40%)	31,36,39	2.85	12 (38%)
43	OMG	DC	75	43	23,26,27	2.52	7 (30%)	33,38,41	1.91	9 (27%)
41	A2M	DA	1534	41,45	22,25,26	3.55	9 (40%)	31,36,39	2.63	10 (32%)
41	OMG	DA	4618	41	23,26,27	2.51	7 (30%)	33,38,41	1.95	10 (30%)
41	PSU	DA	4579	41	18,21,22	1.10	2 (11%)	22,30,33	1.20	3 (13%)
41	PSU	DA	2632	41	18,21,22	1.23	3 (16%)	22,30,33	1.26	3 (13%)
41	OMC	DA	3887	41	19,22,23	3.13	8 (42%)	26,31,34	0.76	0
41	PSU	DA	1744	41	18,21,22	1.18	2 (11%)	22,30,33	1.42	3 (13%)
41	OMG	DA	2424	41	23,26,27	2.52	7 (30%)	33,38,41	1.87	10 (30%)
41	OMU	DA	4306	41	19,22,23	0.81	1 (5%)	26,31,34	1.14	3 (11%)
41	OMC	DA	2824	41	19,22,23	3.17	8 (42%)	26,31,34	0.71	0
41	PSU	DA	1683	46,41	18,21,22	1.13	2 (11%)	22,30,33	1.40	3 (13%)
41	OMC	DA	2365	41	19,22,23	3.13	8 (42%)	26,31,34	0.70	0
41	OMG	DA	1625	41	23,26,27	2.52	7 (30%)	33,38,41	1.88	9 (27%)
43	PSU	DC	69	43	18,21,22	1.17	3 (16%)	22,30,33	1.13	2 (9%)
41	PSU	DA	4361	41	18,21,22	1.14	2 (11%)	22,30,33	1.42	3 (13%)
41	PSU	DA	4296	41	18,21,22	1.22	2 (11%)	22,30,33	1.33	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	DA	1871	41,45	22,25,26	3.44	9 (40%)	31,36,39	2.72	12 (38%)
41	OMC	DA	2422	41,45	19,22,23	3.18	8 (42%)	26,31,34	0.71	0
41	PSU	DA	3639	41	18,21,22	1.28	3 (16%)	22,30,33	1.31	3 (13%)
41	PSU	DA	4689	41	18,21,22	1.15	1 (5%)	22,30,33	1.33	3 (13%)
41	OMG	DA	1522	41	23,26,27	2.51	7 (30%)	33,38,41	1.92	10 (30%)
41	PSU	DA	3851	41	18,21,22	1.22	3 (16%)	22,30,33	1.31	3 (13%)
41	OMC	DA	3841	41	19,22,23	3.13	8 (42%)	26,31,34	0.64	0
41	PSU	DA	2839	41	18,21,22	1.15	1 (5%)	22,30,33	1.33	3 (13%)
41	OMG	DA	4196	41	23,26,27	2.53	6 (26%)	33,38,41	1.90	7 (21%)
41	PSU	DA	5001	41	18,21,22	1.21	2 (11%)	22,30,33	1.23	3 (13%)
41	OMU	DA	4227	41	19,22,23	0.71	0	26,31,34	1.21	4 (15%)
41	A2M	DA	3830	41	22,25,26	3.39	9 (40%)	31,36,39	2.69	13 (41%)
41	PSU	DA	1779	41	18,21,22	1.19	2 (11%)	22,30,33	1.35	3 (13%)
41	PSU	DA	3822	41	18,21,22	1.24	2 (11%)	22,30,33	1.15	3 (13%)
41	PSU	DA	4299	41	18,21,22	1.13	1 (5%)	22,30,33	1.39	3 (13%)
41	A2M	DA	2815	41	22,25,26	3.36	9 (40%)	31,36,39	2.72	15 (48%)
41	PSU	DA	4972	41	18,21,22	1.18	2 (11%)	22,30,33	1.30	3 (13%)
41	5MC	DA	4447	46,41	18,22,23	3.51	7 (38%)	26,32,35	1.16	2 (7%)
41	PSU	DA	1781	41	18,21,22	1.17	2 (11%)	22,30,33	1.40	3 (13%)
41	A2M	DA	2401	41	22,25,26	3.41	9 (40%)	31,36,39	2.69	13 (41%)
41	PSU	DA	2508	41	18,21,22	1.15	1 (5%)	22,30,33	1.43	3 (13%)
43	PSU	DC	55	43	18,21,22	1.17	1 (5%)	22,30,33	1.43	3 (13%)
37	HIC	BA	245	37	10,11,12	0.51	0	8,14,16	0.51	0
41	A2M	DA	400	41	22,25,26	3.40	9 (40%)	31,36,39	2.81	12 (38%)
41	PSU	DA	4493	46,41	18,21,22	1.17	2 (11%)	22,30,33	1.40	3 (13%)
41	OMC	DA	3701	46,41	19,22,23	3.09	8 (42%)	26,31,34	0.74	0
41	OMC	DA	3869	41	19,22,23	3.13	8 (42%)	26,31,34	0.76	0
41	OMC	DA	1881	41,45	19,22,23	3.15	8 (42%)	26,31,34	0.80	0
41	OMG	DA	4499	41	23,26,27	2.53	6 (26%)	33,38,41	1.98	8 (24%)
41	A2M	DA	1323	41	22,25,26	3.39	9 (40%)	31,36,39	2.74	13 (41%)
41	OMU	DA	3925	41	19,22,23	0.72	0	26,31,34	1.23	4 (15%)
41	OMG	DA	3899	41,45	23,26,27	2.51	7 (30%)	33,38,41	1.89	10 (30%)
41	1MA	DA	1322	41,45	21,25,26	2.91	5 (23%)	31,37,40	2.13	8 (25%)
41	PSU	DA	4431	41	18,21,22	1.18	1 (5%)	22,30,33	1.41	3 (13%)
41	UY1	DA	3818	46,41	19,22,23	4.30	6 (31%)	22,31,34	2.03	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	DA	1326	41	22,25,26	3.43	9 (40%)	31,36,39	2.75	13 (41%)
41	OMG	DA	4392	41	23,26,27	2.50	7 (30%)	33,38,41	1.90	10 (30%)
41	OMC	DA	2861	41	19,22,23	3.18	8 (42%)	26,31,34	0.67	0
41	PSU	DA	1782	41	18,21,22	1.17	2 (11%)	22,30,33	1.40	3 (13%)
41	PSU	DA	1860	41	18,21,22	1.21	1 (5%)	22,30,33	1.57	3 (13%)
41	OMG	DA	3792	41	23,26,27	2.52	7 (30%)	33,38,41	1.92	9 (27%)
41	OMG	DA	4494	41	23,26,27	2.51	7 (30%)	33,38,41	1.89	9 (27%)
41	A2M	DA	3825	41	22,25,26	3.42	9 (40%)	31,36,39	2.77	13 (41%)
41	OMG	DA	3669	41	23,26,27	2.53	7 (30%)	33,38,41	1.96	11 (33%)
41	PSU	DA	4293	41	18,21,22	1.16	2 (11%)	22,30,33	1.41	3 (13%)
41	OMG	DA	4228	41	23,26,27	2.48	8 (34%)	33,38,41	1.99	10 (30%)
41	OMC	DA	4456	41	19,22,23	3.14	8 (42%)	26,31,34	0.74	0
41	A2M	DA	1524	41	22,25,26	3.37	8 (36%)	31,36,39	2.89	12 (38%)
41	OMU	DA	2415	41	19,22,23	0.79	1 (5%)	26,31,34	1.13	3 (11%)
41	A2M	DA	2363	41,45	22,25,26	3.36	9 (40%)	31,36,39	2.69	13 (41%)
41	PSU	DA	4521	41,45	18,21,22	1.20	2 (11%)	22,30,33	1.34	3 (13%)
41	OMC	DA	1340	41	19,22,23	3.12	8 (42%)	26,31,34	0.69	0
41	PSU	DA	3715	41	18,21,22	1.31	3 (16%)	22,30,33	1.25	3 (13%)
41	PSU	DA	4500	41	18,21,22	1.15	3 (16%)	22,30,33	1.34	3 (13%)
41	A2M	DA	3718	41	22,25,26	3.40	9 (40%)	31,36,39	2.75	13 (41%)
41	OMU	DA	2837	41	19,22,23	0.74	0	26,31,34	1.26	3 (11%)
41	PSU	DA	224	41	18,21,22	1.20	2 (11%)	22,30,33	1.29	3 (13%)
41	PSU	DA	1677	41	18,21,22	1.29	4 (22%)	22,30,33	1.38	3 (13%)
41	OMC	DA	4536	41	19,22,23	3.14	8 (42%)	26,31,34	0.78	0
41	A2M	DA	3867	41	22,25,26	3.41	9 (40%)	31,36,39	2.78	14 (45%)
41	OMG	DA	2876	41	23,26,27	2.55	7 (30%)	33,38,41	1.97	9 (27%)

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
41	PSU	DA	4403	41	-	0/7/25/26	0/2/2/2
41	OMU	DA	4498	41,45	-	1/9/27/28	0/2/2/2
41	PSU	DA	4552	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	3695	41	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	5MC	DA	3782	41,45	-	0/7/25/26	0/2/2/2
41	OMC	DA	2351	41,45	-	4/9/27/28	0/2/2/2
41	OMG	DA	4623	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4673	41,45	-	0/7/25/26	0/2/2/2
41	PSU	DA	4471	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	398	41	-	2/9/27/28	0/3/3/3
41	PSU	DA	1792	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4353	41	-	0/7/25/26	0/2/2/2
33	MLZ	Ag	98	33	-	2/7/8/10	-
41	PSU	DA	1536	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	3844	41	-	1/7/25/26	0/2/2/2
41	OMG	DA	2364	41,45	-	0/9/27/28	0/3/3/3
21	V5N	AU	39	21	-	2/9/10/12	0/1/1/1
41	PSU	DA	4532	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4637	41	-	1/9/27/28	0/3/3/3
41	OMU	DA	4620	41	-	0/9/27/28	0/2/2/2
41	B8T	DA	1859	41	-	1/7/27/28	0/2/2/2
41	PSU	DA	4628	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	4571	41	-	1/9/27/28	0/3/3/3
41	UR3	DA	4530	41	-	2/7/25/26	0/2/2/2
41	PSU	DA	4312	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	3744	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	3920	41,45	-	0/7/25/26	0/2/2/2
41	PSU	DA	3884	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	3637	46,41	-	0/7/25/26	0/2/2/2
41	OMC	DA	2804	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	1862	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	1316	41	-	0/9/27/28	0/3/3/3
41	6MZ	DA	4220	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4420	41	-	3/7/25/26	0/2/2/2
44	V5N	DD	216	44	-	1/9/10/12	0/1/1/1
41	A2M	DA	3785	41	-	3/9/27/28	0/3/3/3
41	PSU	DA	4442	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	2787	41	-	3/9/27/28	0/3/3/3
41	OMG	DA	4370	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	4457	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4576	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	3627	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4423	41	-	0/7/25/26	0/2/2/2
41	OMC	DA	3808	41	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A2M	DA	4523	41,45	-	1/9/27/28	0/3/3/3
43	OMG	DC	75	43	-	0/9/27/28	0/3/3/3
41	A2M	DA	1534	41,45	-	3/9/27/28	0/3/3/3
41	OMG	DA	4618	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	4579	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	2632	41	-	0/7/25/26	0/2/2/2
41	OMC	DA	3887	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	1744	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	2424	41	-	0/9/27/28	0/3/3/3
41	OMU	DA	4306	41	-	0/9/27/28	0/2/2/2
41	OMC	DA	2824	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	1683	46,41	-	0/7/25/26	0/2/2/2
41	OMC	DA	2365	41	-	0/9/27/28	0/2/2/2
41	OMG	DA	1625	41	-	0/9/27/28	0/3/3/3
43	PSU	DC	69	43	-	0/7/25/26	0/2/2/2
41	PSU	DA	4361	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4296	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	1871	41,45	-	0/9/27/28	0/3/3/3
41	OMC	DA	2422	41,45	-	2/9/27/28	0/2/2/2
41	PSU	DA	3639	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4689	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	1522	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	3851	41	-	0/7/25/26	0/2/2/2
41	OMC	DA	3841	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	2839	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4196	41	-	0/9/27/28	0/3/3/3
41	PSU	DA	5001	41	-	0/7/25/26	0/2/2/2
41	OMU	DA	4227	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	3830	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	1779	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	3822	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4299	41	-	0/7/25/26	0/2/2/2
41	A2M	DA	2815	41	-	1/9/27/28	0/3/3/3
41	PSU	DA	4972	41	-	0/7/25/26	0/2/2/2
41	5MC	DA	4447	46,41	-	4/7/25/26	0/2/2/2
41	PSU	DA	1781	41	-	1/7/25/26	0/2/2/2
41	A2M	DA	2401	41	-	2/9/27/28	0/3/3/3
41	PSU	DA	2508	41	-	0/7/25/26	0/2/2/2
43	PSU	DC	55	43	-	0/7/25/26	0/2/2/2
37	HIC	BA	245	37	-	1/5/6/8	0/1/1/1
41	A2M	DA	400	41	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	DA	4493	46,41	-	0/7/25/26	0/2/2/2
41	OMC	DA	3701	46,41	-	4/9/27/28	0/2/2/2
41	OMC	DA	3869	41	-	0/9/27/28	0/2/2/2
41	OMC	DA	1881	41,45	-	0/9/27/28	0/2/2/2
41	OMG	DA	4499	41	-	0/9/27/28	0/3/3/3
41	A2M	DA	1323	41	-	3/9/27/28	0/3/3/3
41	OMU	DA	3925	41	-	0/9/27/28	0/2/2/2
41	OMG	DA	3899	41,45	-	0/9/27/28	0/3/3/3
41	1MA	DA	1322	41,45	-	1/7/25/26	0/3/3/3
41	PSU	DA	4431	41	-	0/7/25/26	0/2/2/2
41	UY1	DA	3818	46,41	-	1/9/27/28	0/2/2/2
41	A2M	DA	1326	41	-	1/9/27/28	0/3/3/3
41	OMG	DA	4392	41	-	0/9/27/28	0/3/3/3
41	OMC	DA	2861	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	1782	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	1860	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	3792	41	-	2/9/27/28	0/3/3/3
41	OMG	DA	4494	41	-	1/9/27/28	0/3/3/3
41	A2M	DA	3825	41	-	1/9/27/28	0/3/3/3
41	OMG	DA	3669	41	-	2/9/27/28	0/3/3/3
41	PSU	DA	4293	41	-	0/7/25/26	0/2/2/2
41	OMG	DA	4228	41	-	0/9/27/28	0/3/3/3
41	OMC	DA	4456	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	1524	41	-	1/9/27/28	0/3/3/3
41	OMU	DA	2415	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	2363	41,45	-	0/9/27/28	0/3/3/3
41	PSU	DA	4521	41,45	-	1/7/25/26	0/2/2/2
41	OMC	DA	1340	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	3715	41	-	0/7/25/26	0/2/2/2
41	PSU	DA	4500	41	-	3/7/25/26	0/2/2/2
41	A2M	DA	3718	41	-	1/9/27/28	0/3/3/3
41	OMU	DA	2837	41	-	0/9/27/28	0/2/2/2
41	PSU	DA	224	41	-	3/7/25/26	0/2/2/2
41	PSU	DA	1677	41	-	0/7/25/26	0/2/2/2
41	OMC	DA	4536	41	-	0/9/27/28	0/2/2/2
41	A2M	DA	3867	41	-	3/9/27/28	0/3/3/3
41	OMG	DA	2876	41	-	1/9/27/28	0/3/3/3

The worst 5 of 575 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	DA	4220	6MZ	C6-N6	12.13	1.47	1.34
41	DA	3818	UY1	C6-C5	12.11	1.49	1.35
41	DA	3818	UY1	C2-N1	9.77	1.49	1.36
41	DA	1534	A2M	O4'-C1'	9.40	1.64	1.42
41	DA	3782	5MC	C6-C5	9.31	1.49	1.34

The worst 5 of 641 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	DA	1524	A2M	N6-C6-N1	-6.75	103.56	118.35
41	DA	3867	A2M	C5-C4-N3	-6.33	118.49	126.75
41	DA	1524	A2M	C5-C4-N3	-6.26	118.58	126.75
41	DA	1534	A2M	C5-C4-N3	-6.20	118.66	126.75
41	DA	1326	A2M	C5-C4-N3	-6.19	118.68	126.75

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Ag	98	MLZ	O-C-CA-CB
37	BA	245	HIC	O-C-CA-CB
44	DD	216	V5N	O-C-CA-CB
41	DA	224	PSU	C2'-C1'-C5-C4
41	DA	398	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

44 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	DA	4498	OMU	3	0
41	DA	4552	PSU	1	0
41	DA	3782	5MC	1	0
41	DA	2351	OMC	1	0
41	DA	4673	PSU	1	0
41	DA	4637	OMG	1	0
41	DA	4620	OMU	1	0
41	DA	1859	B8T	3	0
41	DA	3744	OMG	1	0
41	DA	3785	A2M	2	0
41	DA	3808	OMC	1	0
41	DA	1534	A2M	1	0
41	DA	4579	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	DA	2632	PSU	1	0
41	DA	2424	OMG	1	0
41	DA	4306	OMU	1	0
41	DA	1871	A2M	1	0
41	DA	4689	PSU	1	0
41	DA	4196	OMG	1	0
41	DA	2815	A2M	2	0
41	DA	4972	PSU	1	0
41	DA	4447	5MC	2	0
37	BA	245	HIC	1	0
41	DA	3869	OMC	1	0
41	DA	4499	OMG	3	0
41	DA	1323	A2M	1	0
41	DA	3925	OMU	1	0
41	DA	1322	1MA	1	0
41	DA	1326	A2M	4	0
41	DA	4392	OMG	1	0
41	DA	1860	PSU	1	0
41	DA	3792	OMG	1	0
41	DA	3825	A2M	3	0
41	DA	3669	OMG	1	0
41	DA	4456	OMC	1	0
41	DA	1524	A2M	1	0
41	DA	2415	OMU	1	0
41	DA	1340	OMC	2	0
41	DA	4500	PSU	1	0
41	DA	3718	A2M	5	0
41	DA	2837	OMU	1	0
41	DA	4536	OMC	4	0
41	DA	3867	A2M	2	0
41	DA	2876	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 248 ligands modelled in this entry, 234 are monoatomic - leaving 14 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	$\# Z > 2$
49	SPD	DA	5105	-	9,9,9	0.66	0	8,8,8	1.42	1 (12%)
50	SPM	DA	5111	-	13,13,13	0.55	0	12,12,12	0.93	0
48	PUT	DA	5101	-	5,5,5	0.19	0	4,4,4	0.43	0
51	ATP	DA	5112	-	29,33,33	0.32	0	44,52,52	0.87	3 (6%)
52	A1JQ4	DA	5324	46	27,27,27	2.83	9 (33%)	37,46,46	3.28	16 (43%)
49	SPD	DA	5104	-	9,9,9	0.84	0	8,8,8	1.37	1 (12%)
48	PUT	DB	10000	-	5,5,5	0.28	0	4,4,4	0.34	0
48	PUT	DA	5103	-	5,5,5	0.21	0	4,4,4	0.37	0
49	SPD	DA	5106	-	9,9,9	0.47	0	8,8,8	1.52	1 (12%)
50	SPM	DA	5109	-	13,13,13	0.61	0	12,12,12	0.89	0
50	SPM	DA	5108	-	13,13,13	0.61	0	12,12,12	0.86	0
50	SPM	DA	5110	-	13,13,13	0.54	0	12,12,12	0.97	0
48	PUT	DA	5102	-	5,5,5	0.26	0	4,4,4	0.29	0
49	SPD	DA	5107	-	9,9,9	0.42	0	8,8,8	1.35	1 (12%)

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
49	SPD	DA	5105	-	-	3/7/7/7	-
50	SPM	DA	5111	-	-	8/11/11/11	-
48	PUT	DA	5101	-	-	0/3/3/3	-
51	ATP	DA	5112	-	-	10/22/38/38	0/3/3/3
52	A1JQ4	DA	5324	46	-	6/7/72/72	0/5/4/4
49	SPD	DA	5104	-	-	3/7/7/7	-
48	PUT	DB	10000	-	-	1/3/3/3	-
48	PUT	DA	5103	-	-	1/3/3/3	-
49	SPD	DA	5106	-	-	6/7/7/7	-
50	SPM	DA	5109	-	-	1/11/11/11	-
50	SPM	DA	5108	-	-	1/11/11/11	-
50	SPM	DA	5110	-	-	2/11/11/11	-
48	PUT	DA	5102	-	-	1/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	SPD	DA	5107	-	-	6/7/7/7	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	DA	5324	A1JQ4	C09-C10	11.19	1.70	1.55
52	DA	5324	A1JQ4	C07-C02	4.11	1.54	1.51
52	DA	5324	A1JQ4	O16-C04	3.67	1.50	1.45
52	DA	5324	A1JQ4	O18-C19	3.30	1.42	1.35
52	DA	5324	A1JQ4	C23-C05	3.14	1.58	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	DA	5324	A1JQ4	O15-C13-C09	11.13	132.96	118.00
52	DA	5324	A1JQ4	O15-C13-C12	-7.79	100.79	115.59
52	DA	5324	A1JQ4	C13-C09-C05	5.66	110.28	106.90
52	DA	5324	A1JQ4	C14-C13-C09	5.30	137.16	127.57
52	DA	5324	A1JQ4	C01-C02-C07	4.73	119.22	115.93

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	DA	5105	SPD	C8-C7-N6-C5
49	DA	5106	SPD	C4-C5-N6-C7
49	DA	5107	SPD	C4-C5-N6-C7
51	DA	5112	ATP	C5'-O5'-PA-O2A
51	DA	5112	ATP	O4'-C1'-N9-C8

There are no ring outliers.

10 monomers are involved in 48 short contacts:

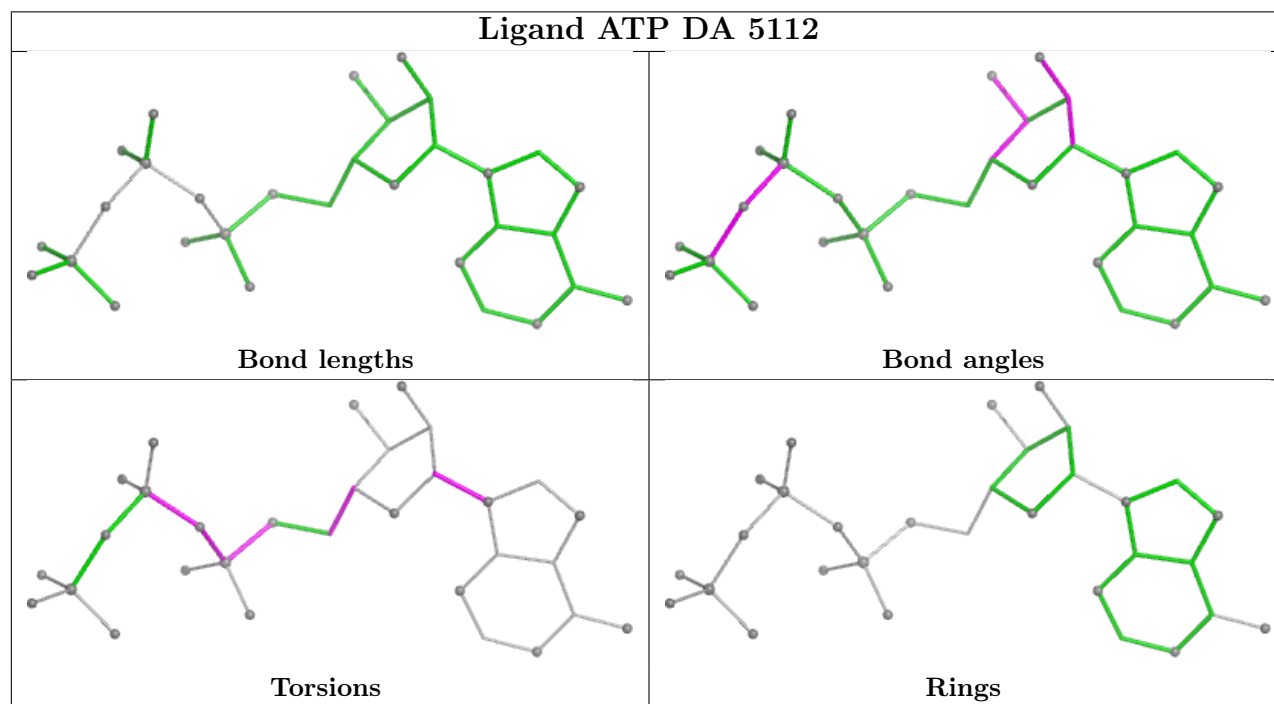
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	DA	5105	SPD	1	0
50	DA	5111	SPM	8	0
48	DA	5101	PUT	4	0
51	DA	5112	ATP	2	0
49	DA	5104	SPD	1	0
48	DA	5103	PUT	4	0
49	DA	5106	SPD	4	0

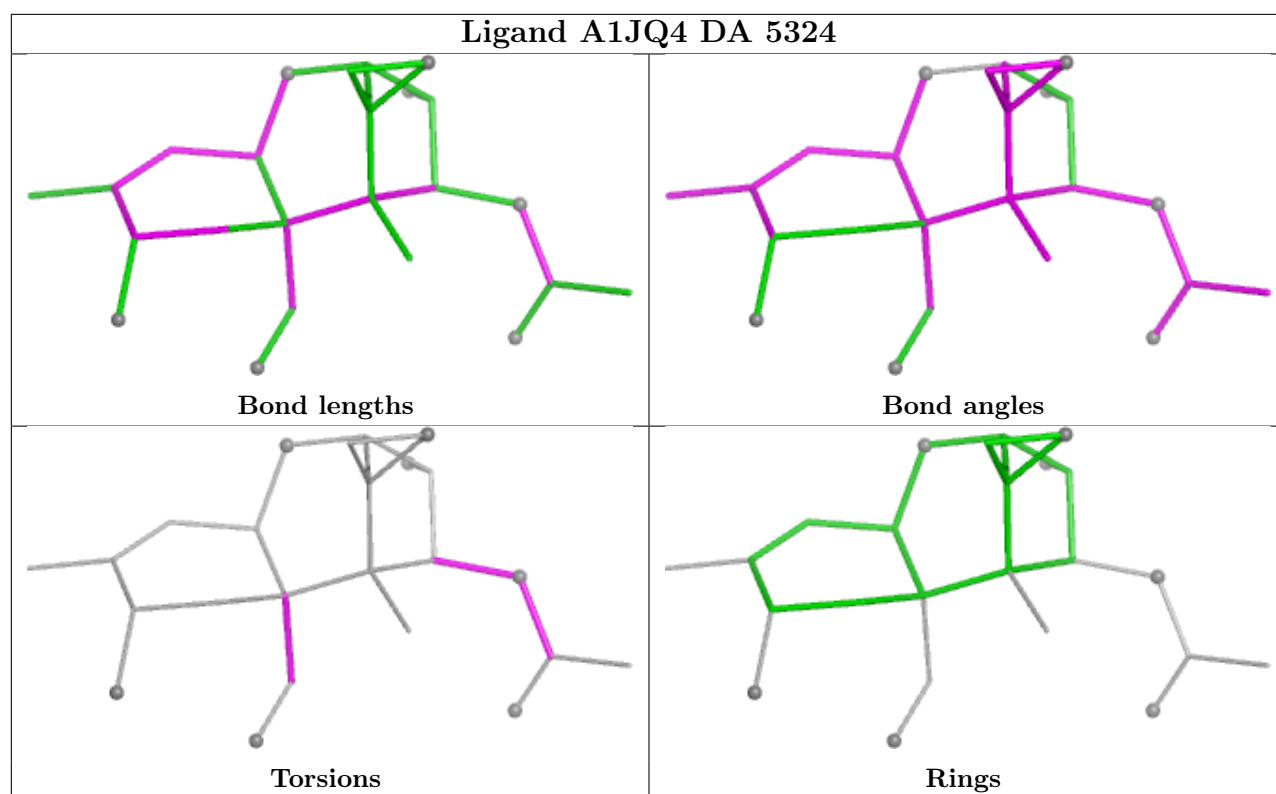
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	DA	5108	SPM	1	0
48	DA	5102	PUT	6	0
49	DA	5107	SPD	17	0

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.

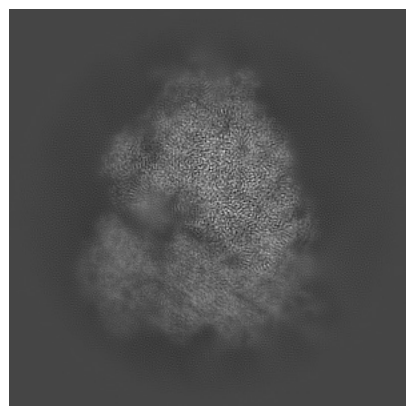
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57202. These allow visual inspection of the internal detail of the map and identification of artifacts.

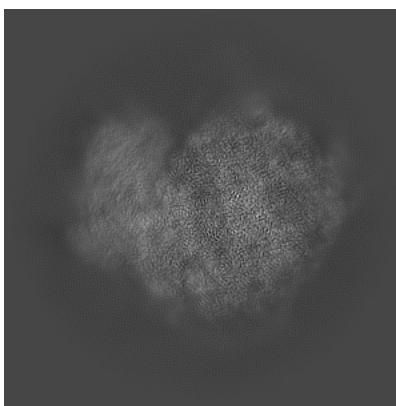
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

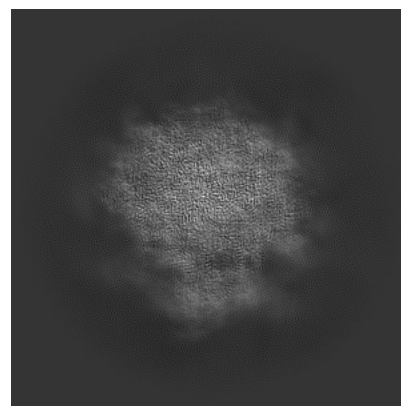
6.1.1 Primary map



X

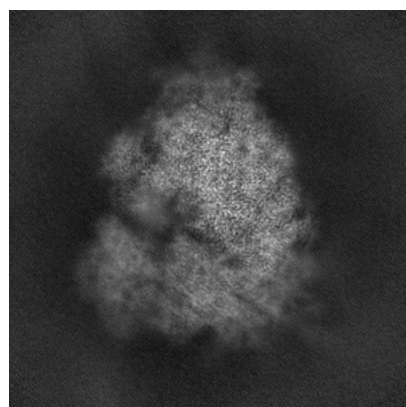


Y

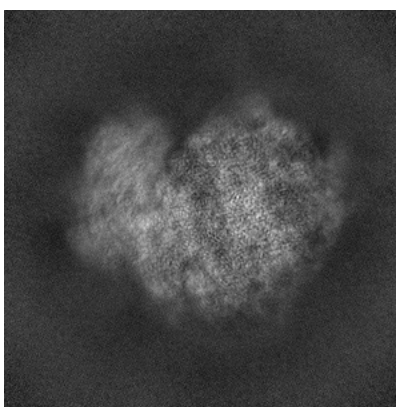


Z

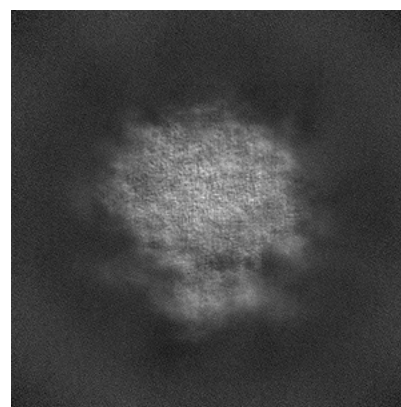
6.1.2 Raw map



X



Y

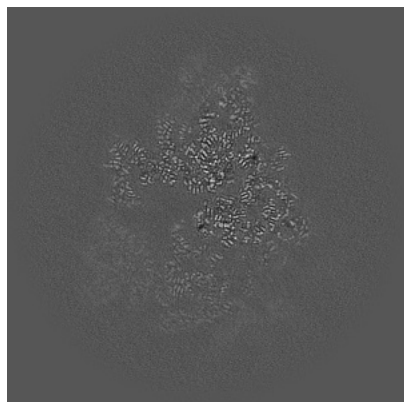


Z

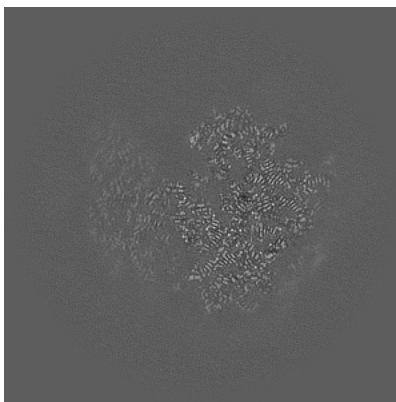
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

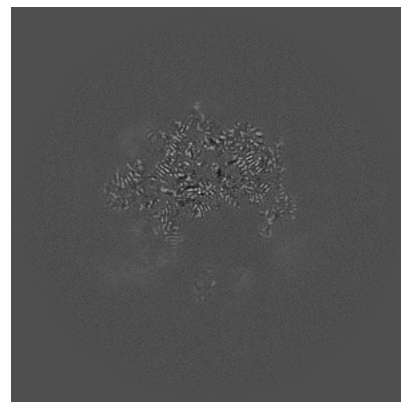
6.2.1 Primary map



X Index: 320

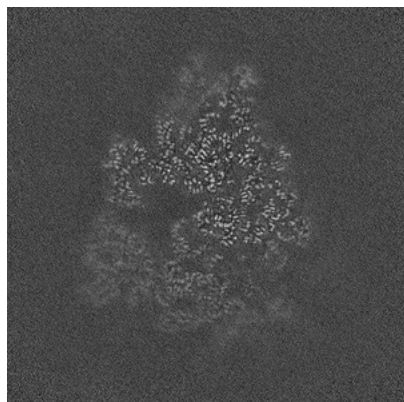


Y Index: 320

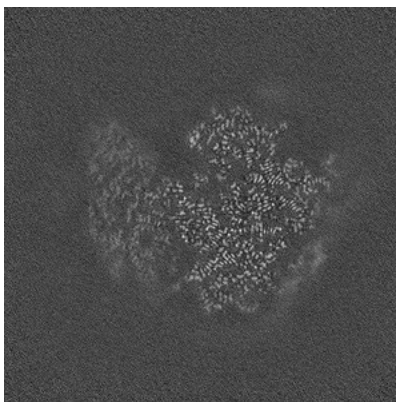


Z Index: 320

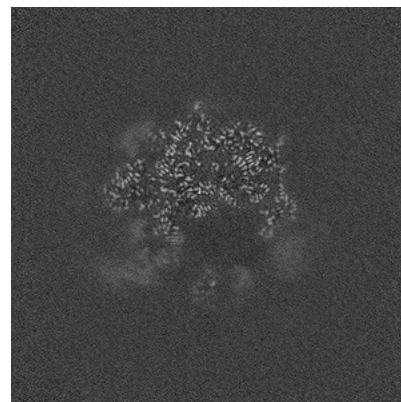
6.2.2 Raw map



X Index: 320



Y Index: 320

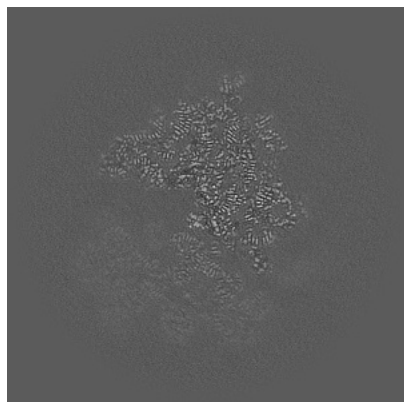


Z Index: 320

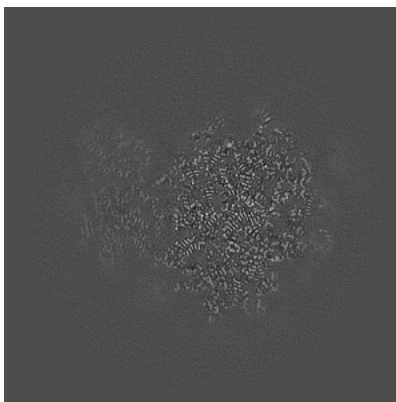
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

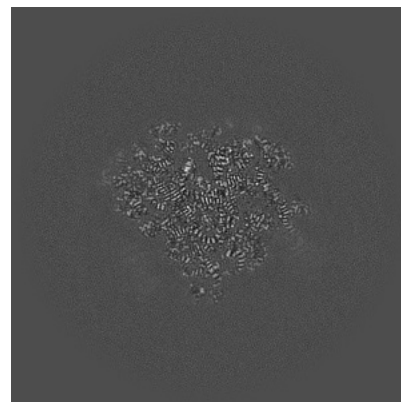
6.3.1 Primary map



X Index: 286

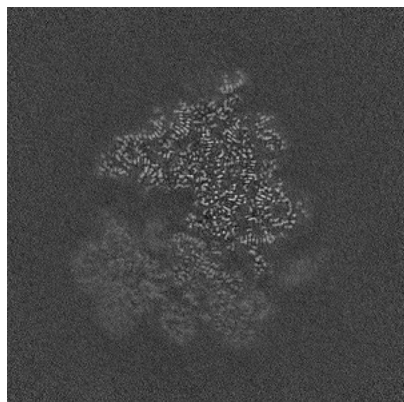


Y Index: 339

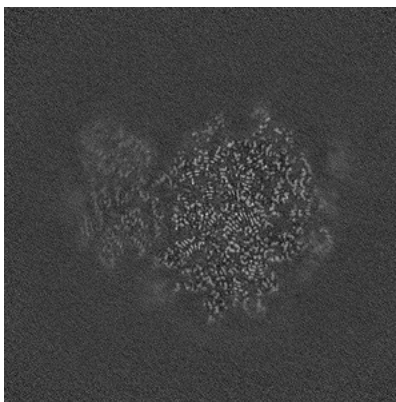


Z Index: 365

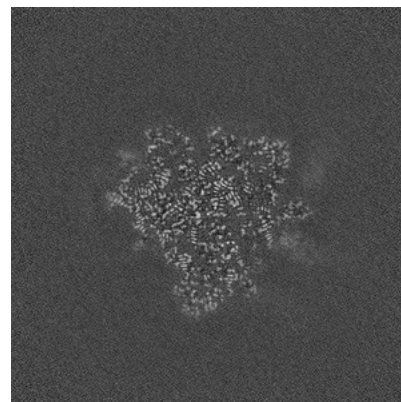
6.3.2 Raw map



X Index: 285



Y Index: 339

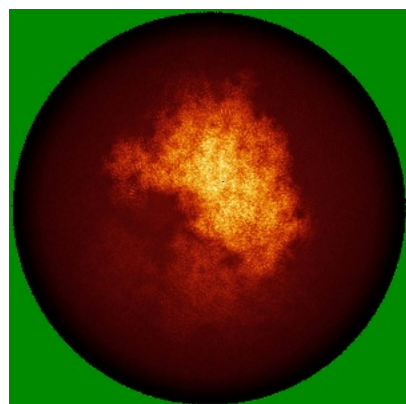


Z Index: 386

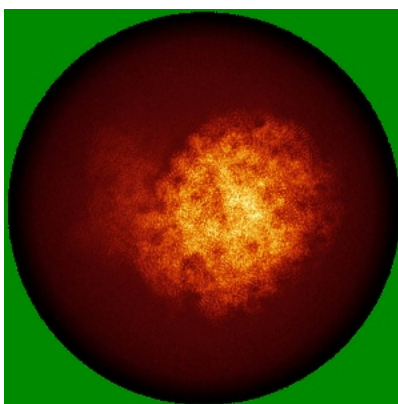
The images above show the largest variance slices of the map in three orthogonal directions.

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

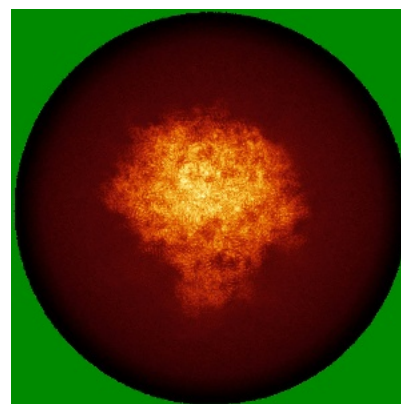
6.4.1 Primary map



X

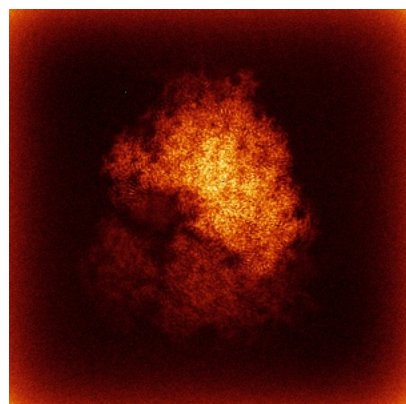


Y

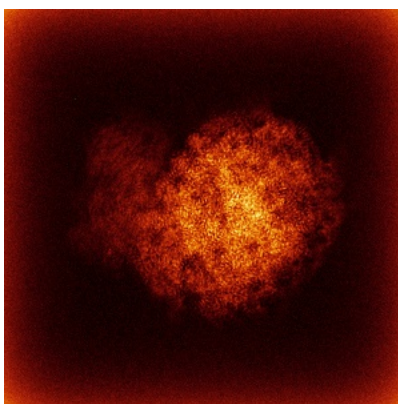


Z

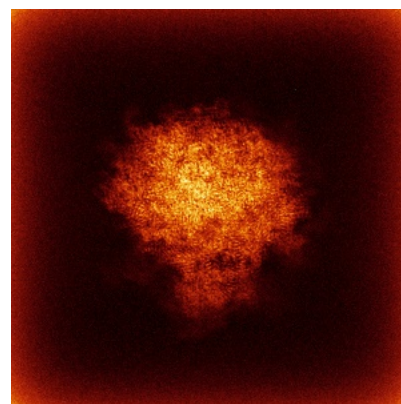
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



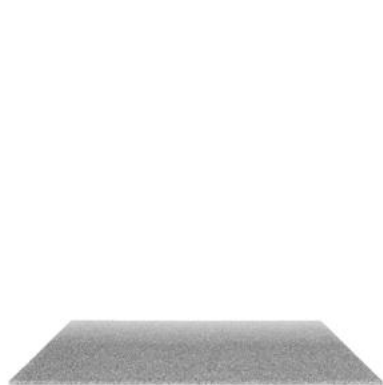
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

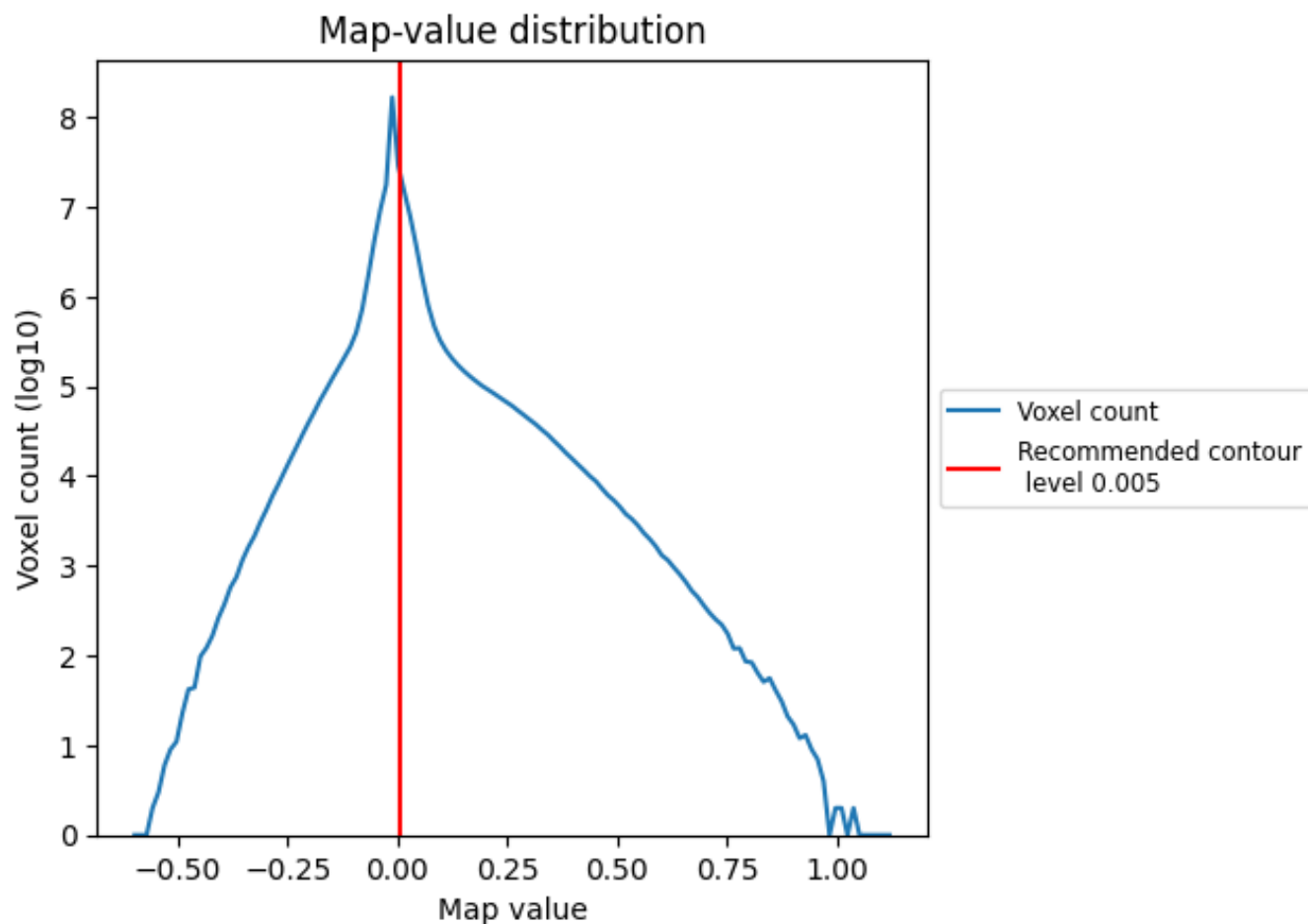
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

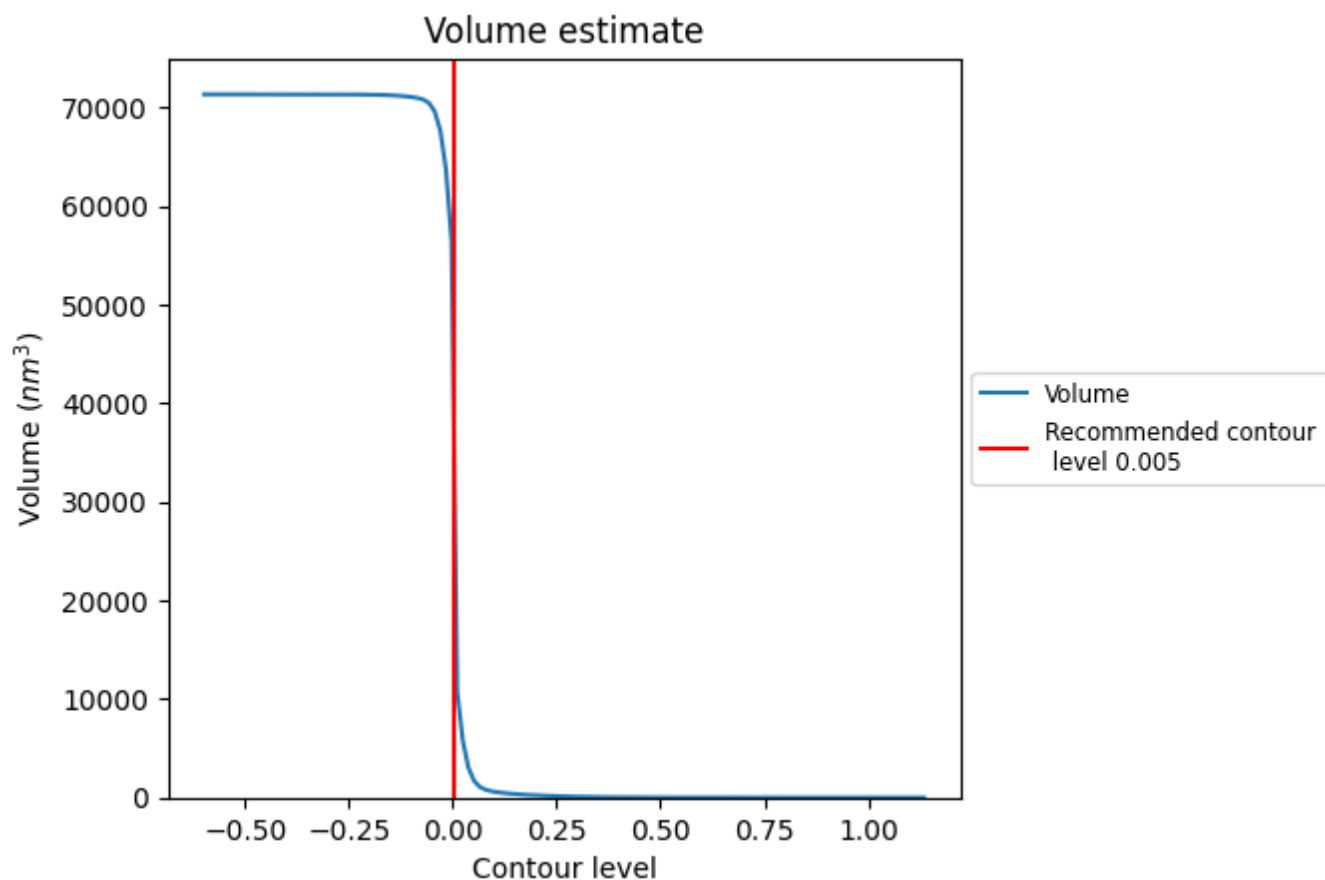
This section contains the results of statistical analysis of the map.

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.

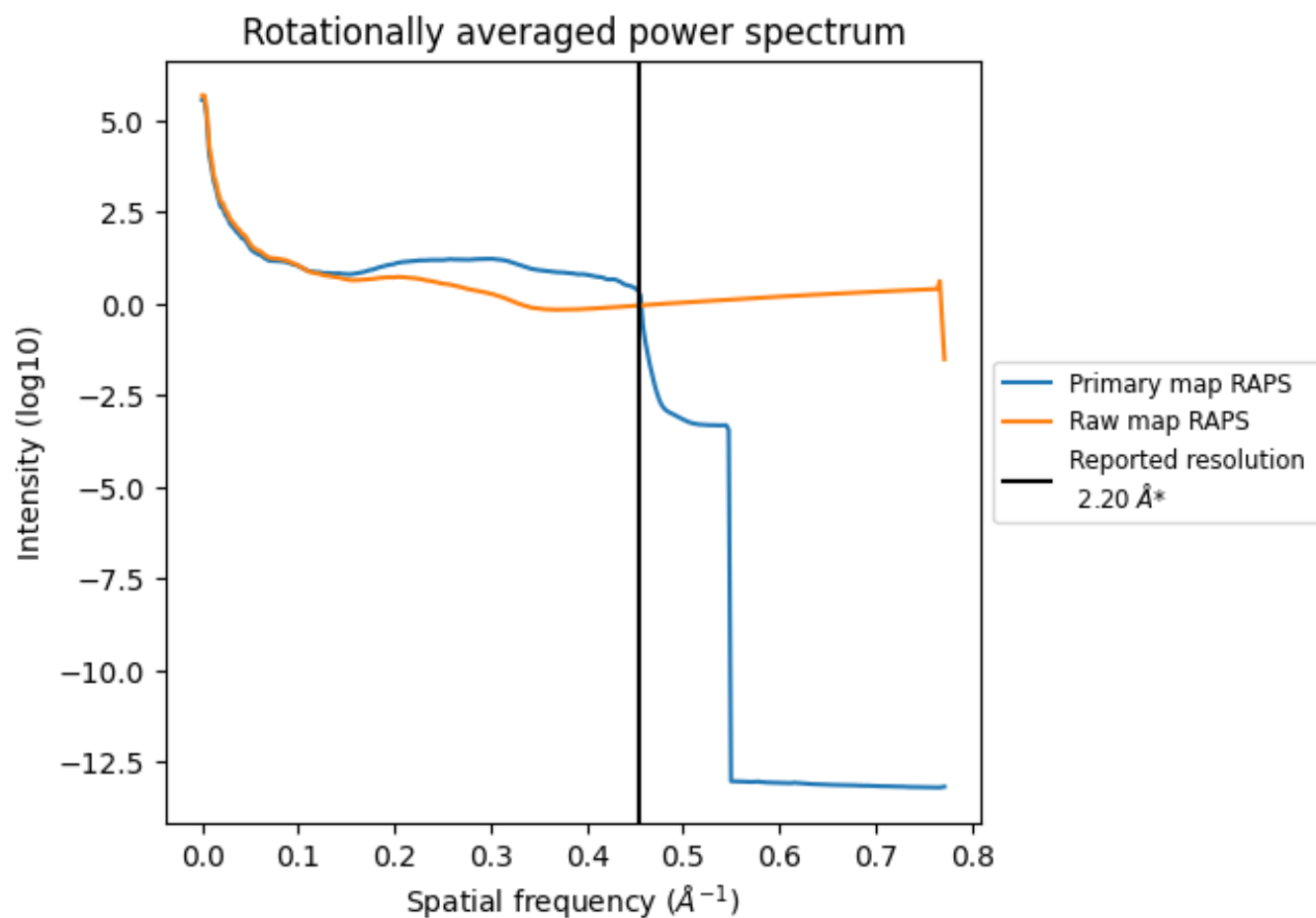
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29576 nm³; this corresponds to an approximate mass of 26717 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 ⓘ

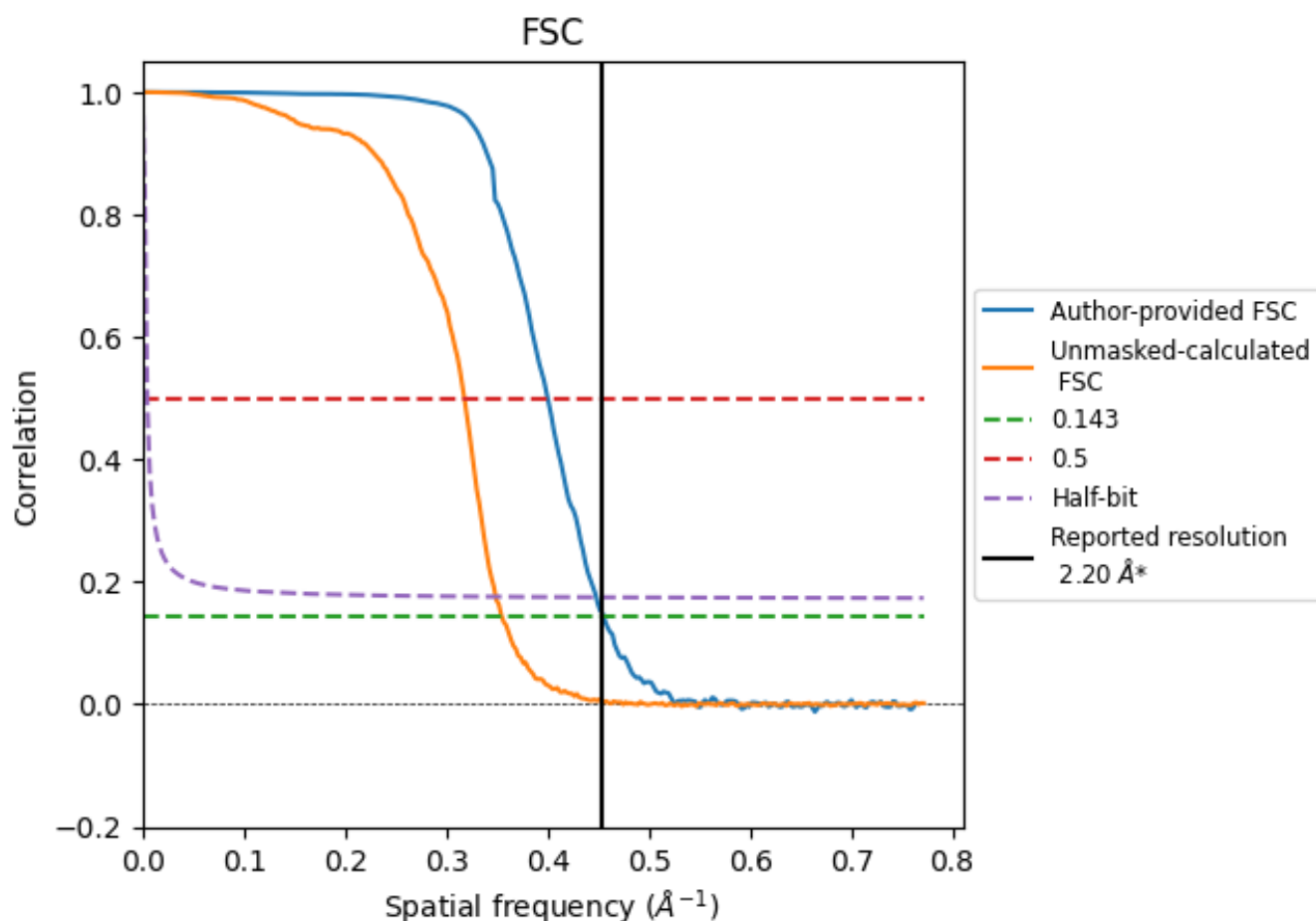


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.455 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

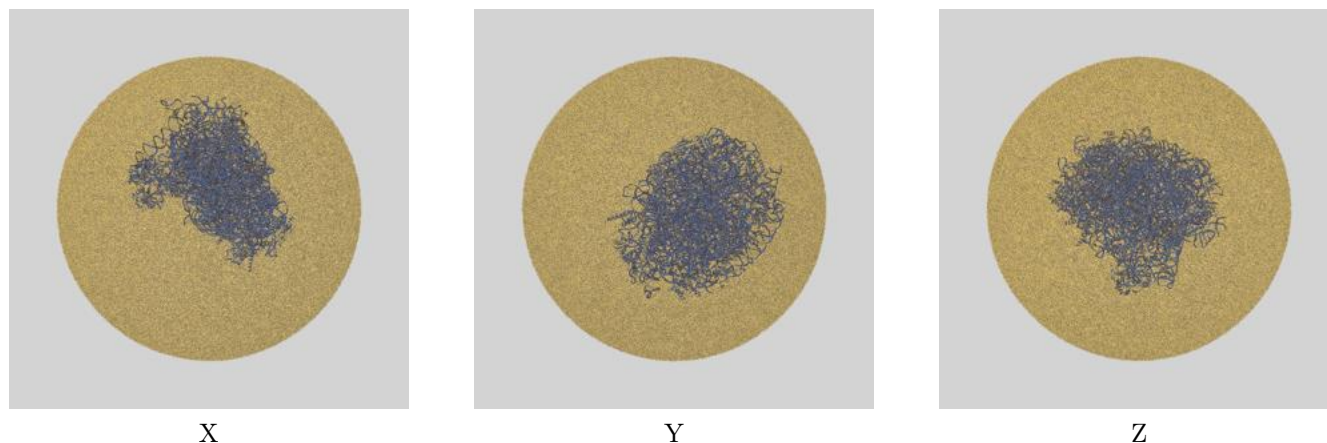
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.19	2.50	2.23
Unmasked-calculated*	2.82	3.14	2.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.82 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

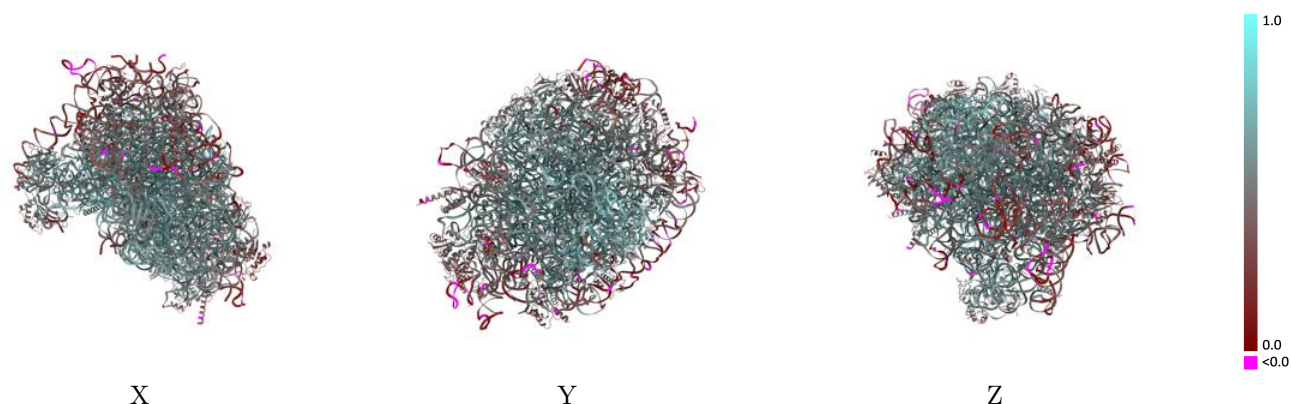
This section contains information regarding the fit between EMDB map EMD-57202 and PDB model 29IX. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



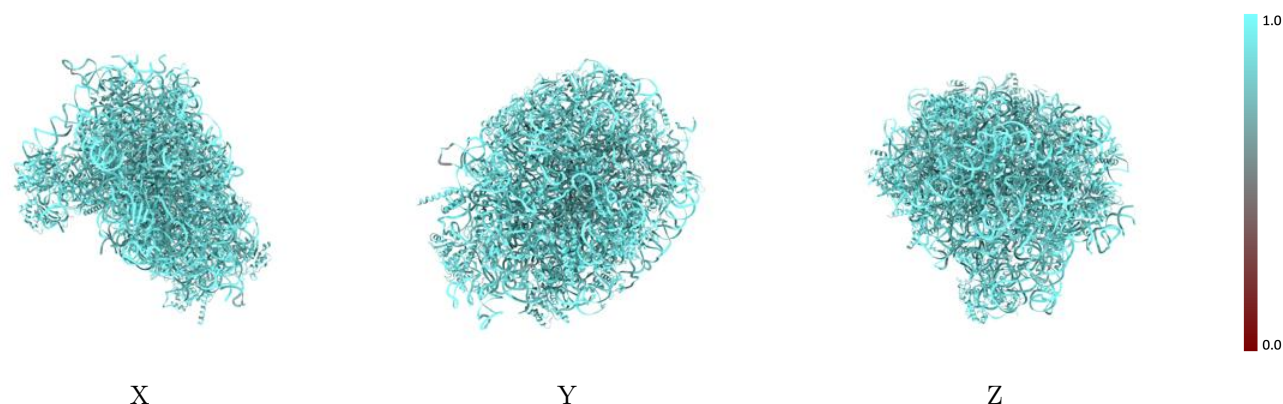
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



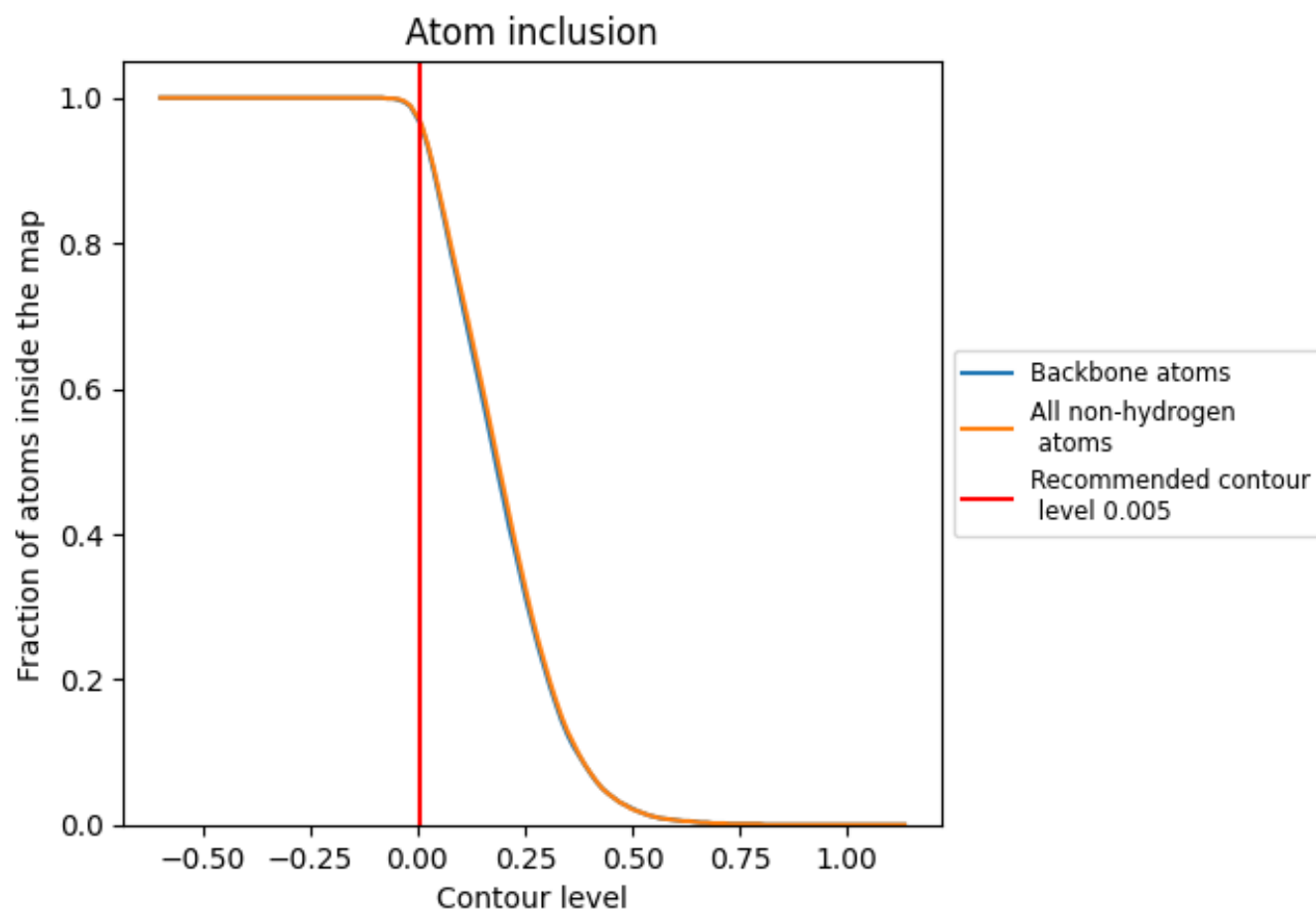
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.5380
AA	 0.9700	 0.5560
AB	 0.9410	 0.4140
AC	 0.9440	 0.4550
AD	 0.9750	 0.6050
AE	 0.9460	 0.4440
AF	 0.9720	 0.5480
AG	 0.9340	 0.3770
AH	 0.9900	 0.6260
AI	 0.9610	 0.5270
AJ	 0.9840	 0.6240
AK	 0.9900	 0.6240
AL	 0.9560	 0.4940
AM	 0.9790	 0.5480
AN	 0.9640	 0.5610
AO	 0.8700	 0.2790
AP	 0.9790	 0.5830
AQ	 0.9720	 0.5080
AR	 0.9610	 0.5130
AS	 0.9830	 0.6190
AT	 0.8900	 0.3360
AU	 0.9910	 0.6220
AV	 0.9610	 0.4720
AW	 0.9270	 0.3720
AX	 0.9700	 0.5130
AY	 0.9860	 0.6330
AZ	 0.9870	 0.5780
Aa	 0.9630	 0.4880
Ab	 0.9650	 0.5500
Ac	 0.9740	 0.4790
Ad	 0.9940	 0.6620
Ae	 0.8800	 0.3210
Af	 0.9810	 0.6120
Ag	 0.9740	 0.5270
Ah	 0.9850	 0.6300



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Chain	Atom inclusion	Q-score
Ai	 0.9650	 0.5510
Aj	 0.9780	 0.5800
BA	 0.9590	 0.5230
BB	 0.9830	 0.6080
BC	 0.9640	 0.5010
BD	 0.9430	 0.4060
DA	 0.9710	 0.5400
DB	 0.9950	 0.6070
DC	 0.9740	 0.5610
DD	 0.9830	 0.6140