



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:24 PM UTC

PDB ID : 9E13 / pdb_00009e13
EMDB ID : EMD-47382
Title : Full-length human dynein-1 in phi-like conformation bound to a Lis1 dimer under Lis1 condition
Authors : Yang, J.; Zhang, K.
Deposited on : 2024-10-21
Resolution : 4.50 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:

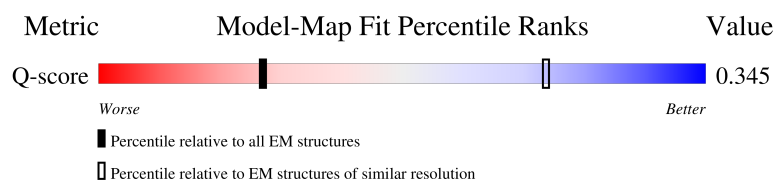
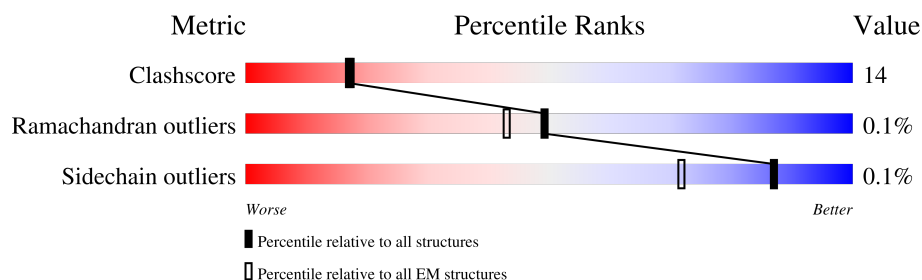
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




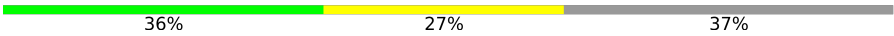








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	
1	B	4646	
2	C	638	
2	D	638	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	492	
3	F	492	
4	G	96	
4	H	96	
5	I	89	
5	J	89	
6	K	113	
6	L	113	
7	O	410	
7	P	410	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94479 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 protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4542	Total	C	N	O	S	0	0
			36692	23323	6381	6822	166		
1	B	4521	Total	C	N	O	S	0	0
			36527	23221	6349	6791	166		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		
2	D	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		
3	F	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
4	H	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
5	J	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

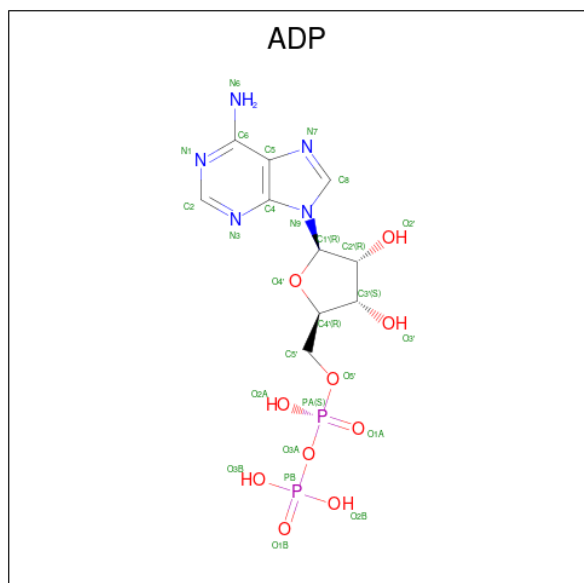
- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
6	L	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 7 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
7	P	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



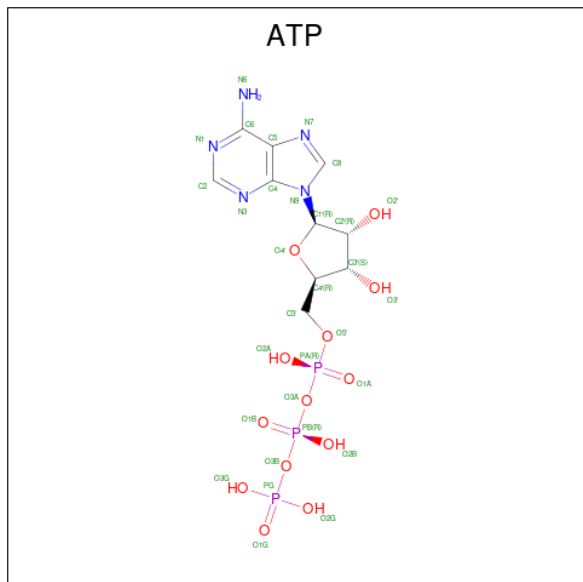
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Mg	0
			2	2	

Continued on next page...

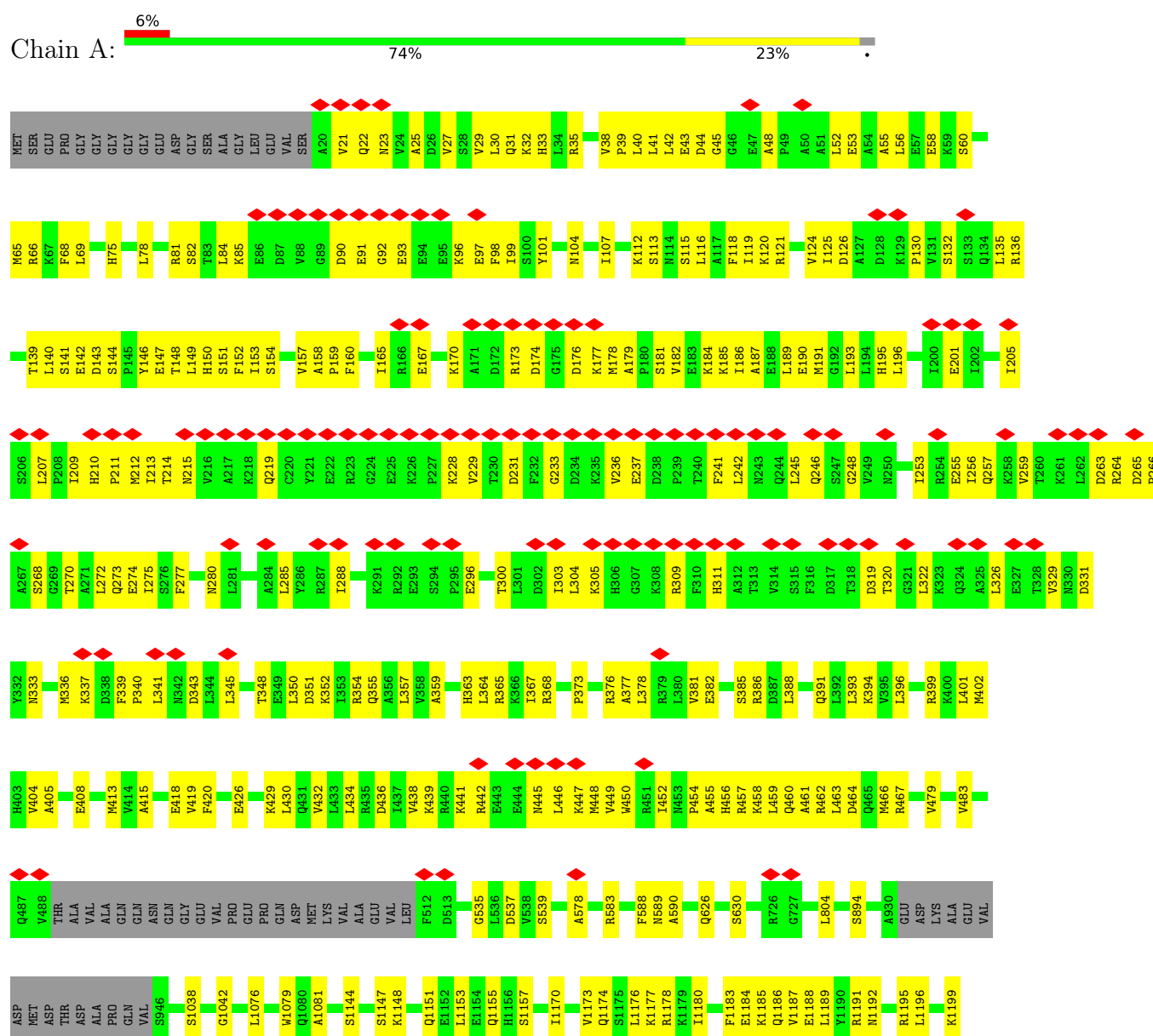
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	B	2	2	2	0

3 Residue-property plots

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

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

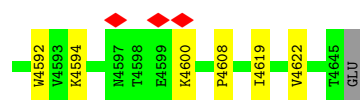




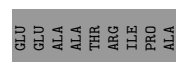
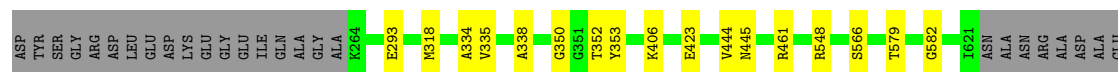
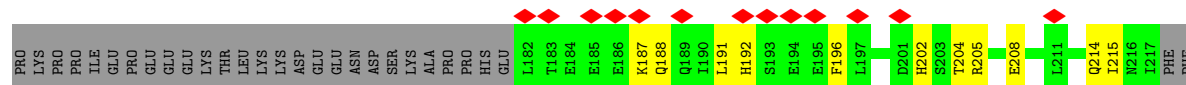
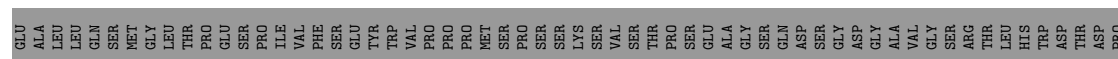
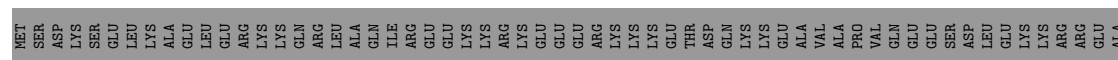




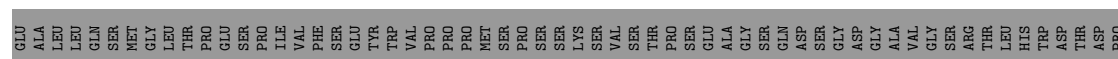
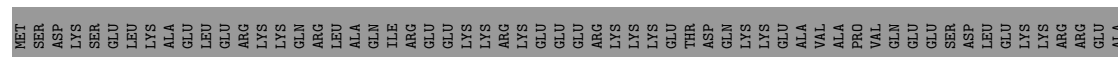
GLU	K4457	H4187	T4039	G3874	L3708	M3524	N3431	S3560	P3287	R3221	T3110	D2973
ASP	G4458	I4190	L4042	M3875	V3716	R3525	E3432	S3560	A3288	L3222	S3111	E2974
LEU	T4459	M4043	M4043	L3876	D3723	I3541	E3433	I3563	V3289	R3223	K3112	D2975
ALA	R4195	S4052	S4052	H3877	V3724	Q3542	E3434	R3364	E3291	Q3227	M3113	L2976
TYR	M4473	E4056	E4056	D3878	D3723	Q3542	M3436	M3367	E3291	E3228	L3115	R2977
ALA	M4478	E4056	E4056	D3879	V3724	Q3542	I3437	I3367	A3292	L3229	E3116	K2989
GLU	E4478	E4056	E4056	F3883	K3727	A3548	R3438	K3568	A3292	E3230	D3124	D2995
THR	D4481	Q4065	Q4065	A3884	L3731	E3551	D3439	K3569	Q3293	V3231	Y3125	D2996
GLY	L4212	L4066	L4066	M3885	L3753	Y3552	L3440	K3370	N3294	E3232	D3124	S2997
LYS	R4213	E4075	E4075	L3886	L3753	L3553	E3441	E3371	A3295	K3233	Y3129	S2997
ARG	S4214	E4075	E4075	L3887	L3753	L3553	A3442	M3372	V3296	N3237	Y3130	D2998
THR	A4215	Q4079	Q4079	L3887	L3753	L3553	S4443	S3373	K3297	D3238	D3131	L3000
THR	C4217	K4082	K4082	L3887	L3753	L3553	I3444	M3374	K3297	K3239	K3132	D3001
ASP	D4217	K4082	K4082	L3887	L3753	L3553	R3445	P3376	I3299	L3240	Q3135	G3003
THR	D4220	R4092	R4092	L3887	L3753	L3553	R3446	S3376	K3300	K3241	P3136	F3004
SER	L4223	R4092	R4092	L3887	L3753	L3553	K3447	Y3377	K3301	K3243	P3137	L3005
ASP	L4223	R4092	R4092	L3887	L3753	L3553	K3448	M3378	Q3302	K3244	R3140	E3006
GLY	M4095	M4095	M4095	L3887	L3753	L3553	Y3451	Y3379	H3303	K3245	R3140	K3007
ARG	L4096	L4096	L4096	L3887	L3753	L3553	A3452	E3380	H3303	K3245	I3143	M3008
M4377	V4099	V4099	V4099	L3887	L3753	L3553	I3455	I3381	L3304	D3246	I3143	L3012
R4378	H4100	H4100	H4100	L3887	L3753	L3553	E3457	V3382	L3304	Q3247	V3144	L3012
H4381	L4101	L4101	L4101	L3887	L3753	L3553	A3458	M3383	E3306	E3249	V3148	V3017
S4385	M4105	M4105	M4105	L3887	L3753	L3553	Q3459	R3384	R3307	A3250	F3149	L3020
L4388	L4106	L4106	L4106	L3887	L3753	L3553	A3459	A3386	R3308	K3251	L3154	D3024
H4389	P4118	P4118	P4118	L3887	L3753	L3553	K3462	S3385	R3309	K3252	L3154	E3025
L4398	F4125	F4125	F4125	L3887	L3753	L3553	L3461	L3387	M3310	K3253	L3161	T3031
K4399	M4128	M4128	M4128	L3887	L3753	L3553	K3462	A3388	A3311	N3256	T3172	Q3032
R4400	L4138	L4138	L4138	L3887	L3753	L3553	K3462	C3389	N3312	S3257	P3173	G3033
F4411	L4138	L4138	L4138	L3887	L3753	L3553	K3462	G3390	P3313	Q3258	K3174	C3033
F4412	L4138	L4138	L4138	L3887	L3753	L3553	K3462	P3391	P3313	I3260	H3175	E3035
F4413	L4138	L4138	L4138	L3887	L3753	L3553	K3462	M3395	A3315	I3260	D3178	E3035
F4414	L4138	L4138	L4138	L3887	L3753	L3553	K3462	Q3399	L3319	Q3263	H3182	K3039
F4415	L4138	L4138	L4138	L3887	L3753	L3553	K3462	Y3402	A3320	L3264	Y3183	M3043
F4416	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3403	E3322	H3265	A3184	L3044
F4417	L4138	L4138	L4138	L3887	L3753	L3553	K3462	D3404	M3405	Q3267	L3044	D3045
F4418	L4138	L4138	L4138	L3887	L3753	L3553	K3462	M3405	M3405	E3269	F3187	S3046
F4419	L4138	L4138	L4138	L3887	L3753	L3553	K3462	L3406	T3332	V3270	R3191	E3049
F4420	L4138	L4138	L4138	L3887	L3753	L3553	K3462	V3409	D3333	I3271	E3195	S3072
F4421	L4138	L4138	L4138	L3887	L3753	L3553	K3462	E3410	T3334	A3272	I3208	K3076
F4422	L4138	L4138	L4138	L3887	L3753	L3553	K3462	F3411	Q3337	I3271	T3211	F3094
F4423	L4138	L4138	L4138	L3887	L3753	L3553	K3462	R3413	K3336	K3276	Q3214	G3095
F4424	L4138	L4138	L4138	L3887	L3753	L3553	K3462	L3416	T3338	S3277	D3096	K3097
F4425	L4138	L4138	L4138	L3887	L3753	L3553	K3462	E3420	R3399	S3277	E3216	S3098
F4426	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	E3217	T3099
F4427	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4428	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4429	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4430	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4431	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4432	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4433	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4434	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4435	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4436	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4437	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4438	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4439	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4440	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4441	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4442	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4443	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4444	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4445	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4446	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4447	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4448	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4449	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4450	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4451	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4452	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4453	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4454	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4455	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4456	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4457	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4458	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107
F4459	L4138	L4138	L4138	L3887	L3753	L3553	K3462	A3420	S3340	K3278	R3218	K3107

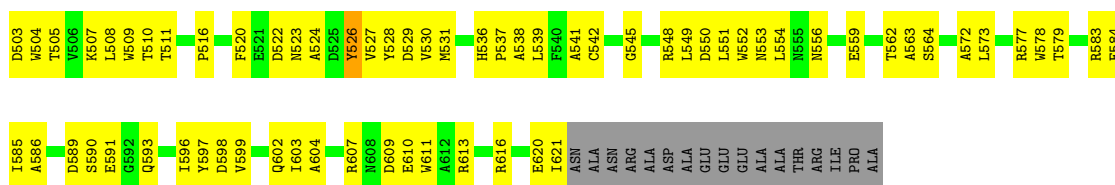


• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

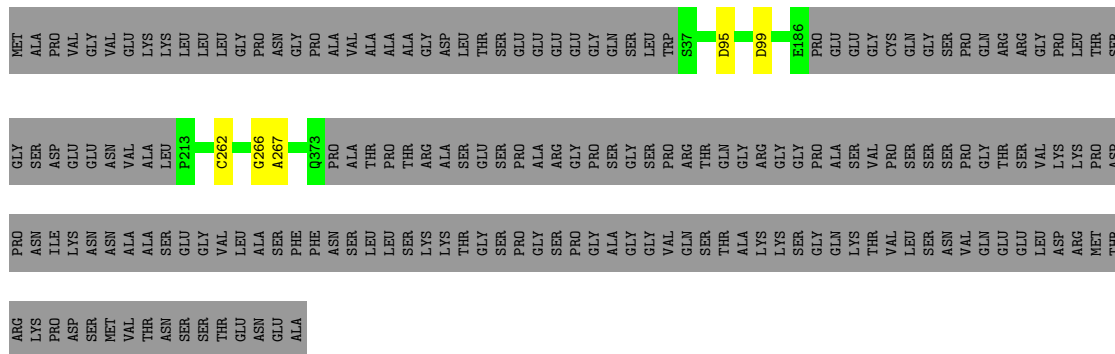


• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

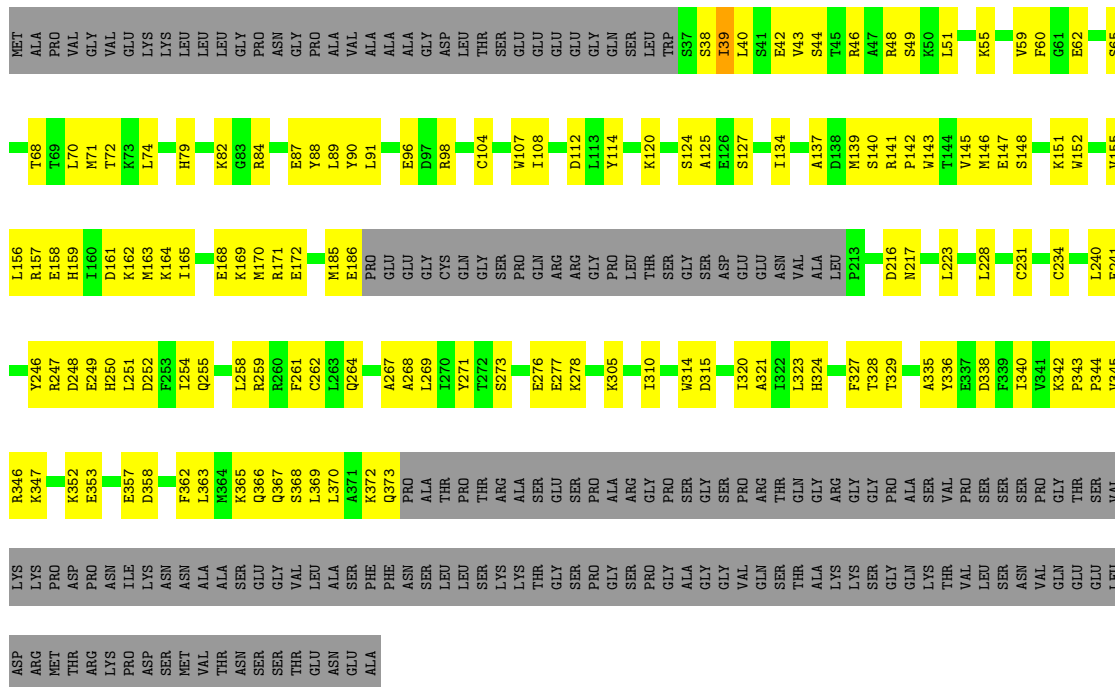




- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

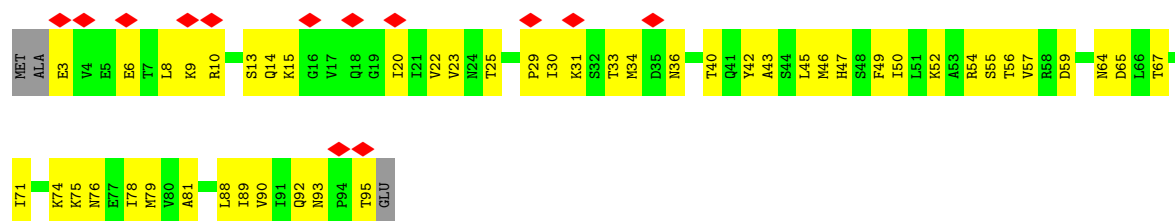


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2

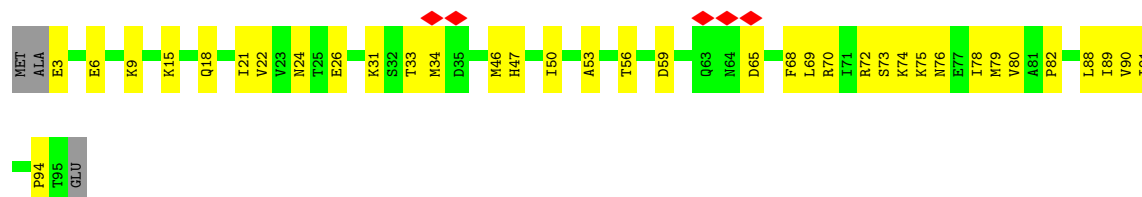


- Molecule 4: Dynein light chain roadblock-type 1

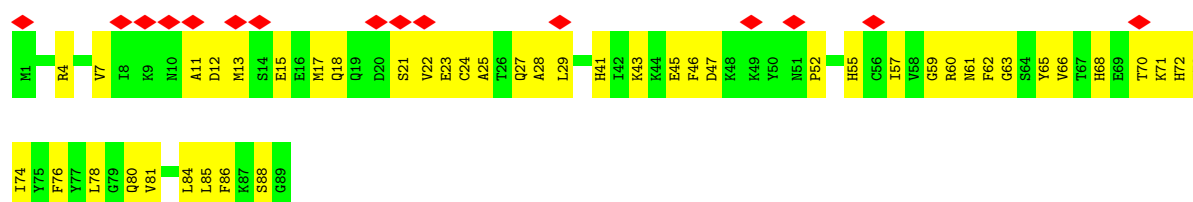




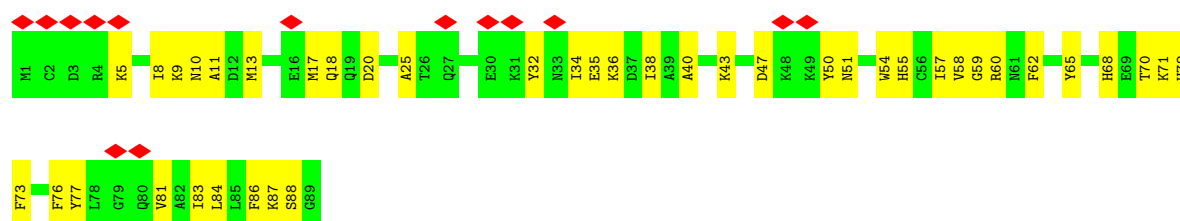
• Molecule 4: Dynein light chain roadblock-type 1



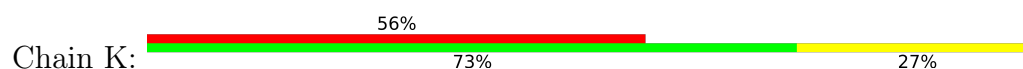
• Molecule 5: Dynein light chain 1, cytoplasmic



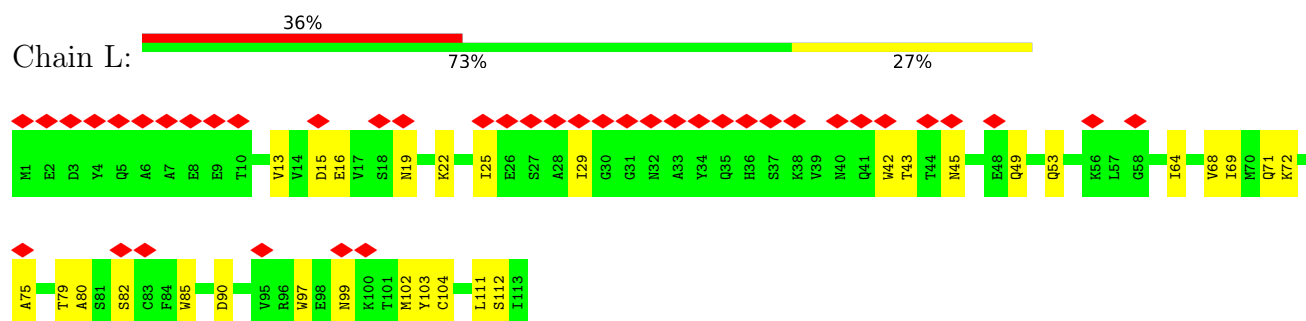
• Molecule 5: Dynein light chain 1, cytoplasmic



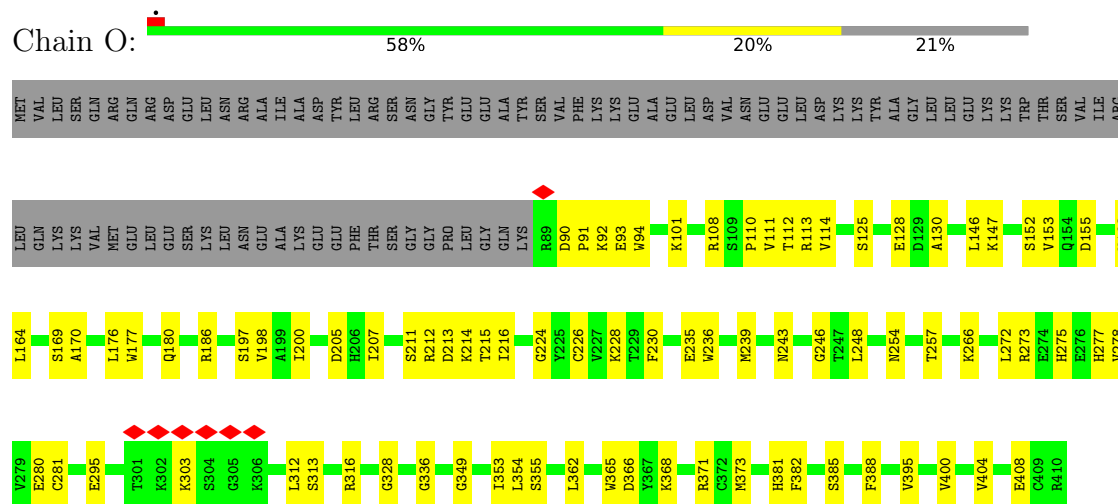
• Molecule 6: Dynein light chain Tctex-type 1



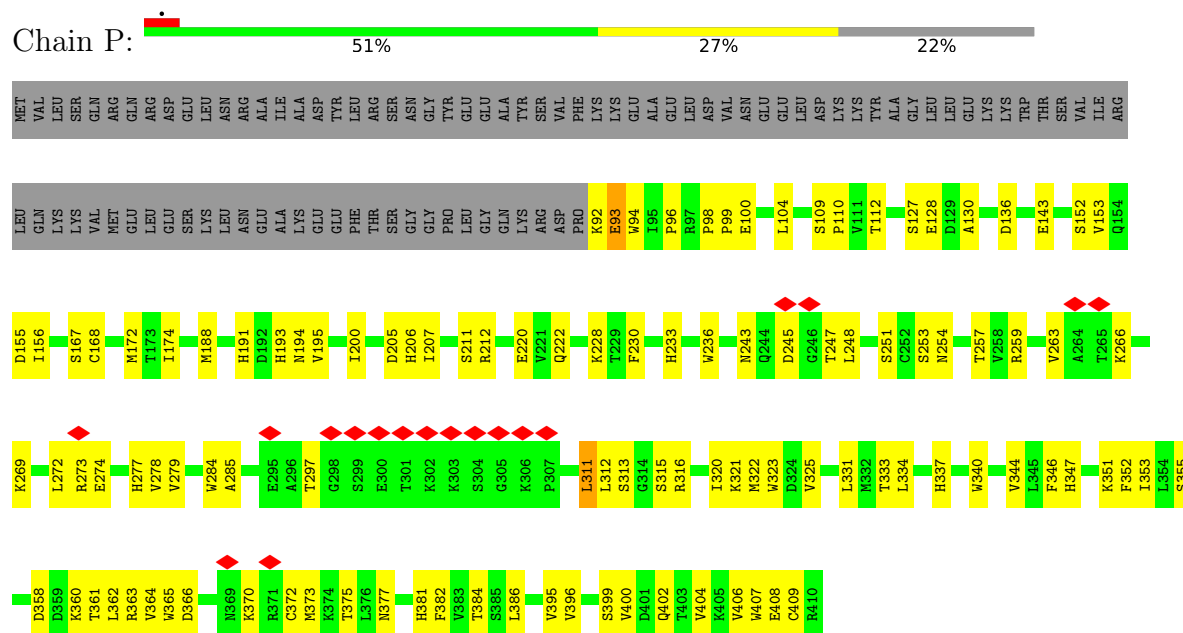
- Molecule 6: Dynein light chain Tctex-type 1



- Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta



- Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.743	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	729.12, 729.12, 729.12	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.736, 1.736, 1.736	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	2/37419 (0.0%)	0.43	15/50625 (0.0%)
1	B	0.20	1/37248 (0.0%)	0.41	3/50392 (0.0%)
2	C	0.23	0/3195	0.46	1/4351 (0.0%)
2	D	0.20	0/3195	0.46	0/4351
3	E	0.20	0/2573	0.42	0/3473
3	F	0.18	0/2573	0.38	0/3473
4	G	0.17	0/752	0.44	0/1017
4	H	0.16	0/752	0.40	0/1017
5	I	0.35	0/744	0.78	0/997
5	J	0.21	0/744	0.48	0/997
6	K	0.17	0/888	0.46	0/1203
6	L	0.12	0/888	0.33	0/1203
7	O	0.17	0/2624	0.42	0/3555
7	P	0.16	0/2597	0.42	1/3518 (0.0%)
All	All	0.20	3/96192 (0.0%)	0.42	20/130172 (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
1	A	0	4
1	B	0	2
2	D	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3242	LYS	C-O	-9.86	1.11	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3242	LYS	C-O	-7.30	1.15	1.24
1	A	1801	PRO	CA-C	6.87	1.55	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3242	LYS	O-C-N	-11.27	110.47	122.07
1	A	3242	LYS	O-C-N	-8.21	111.42	122.43
1	A	3262	GLU	N-CA-C	-7.84	102.73	111.28
1	A	3438	ARG	N-CA-C	-6.66	102.90	111.02
1	A	3250	ALA	N-CA-C	-6.52	104.25	111.82

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	LEU	Peptide
1	A	3223	ARG	Sidechain
1	A	3242	LYS	Mainchain
1	A	3446	ARG	Sidechain
1	B	3219	ARG	Sidechain

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	A	36692	0	36962	814	0
1	B	36527	0	36805	994	0
2	C	3112	0	2964	20	0
2	D	3112	0	2964	163	0
3	E	2518	0	2525	3	0
3	F	2518	0	2525	114	0
4	G	742	0	768	48	0
4	H	742	0	768	33	0
5	I	728	0	714	56	0
5	J	728	0	714	46	0
6	K	872	0	846	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	872	0	846	25	0
7	O	2557	0	2487	66	0
7	P	2531	0	2463	89	0
8	A	81	0	36	2	0
8	B	81	0	36	6	0
9	A	31	0	12	2	0
9	B	31	0	12	2	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
All	All	94479	0	94447	2368	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 14.

The worst 5 of 2368 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:B:3426:ASN:HA	1:B:3429:LYS:CE	1.28	1.56
1:B:3426:ASN:CA	1:B:3429:LYS:HE3	1.09	1.34
1:B:3426:ASN:HA	1:B:3429:LYS:CD	1.78	1.13
1:B:3426:ASN:N	1:B:3429:LYS:HE3	1.67	1.07
1:B:3256:MET:HG2	1:B:3433:VAL:HG21	1.42	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4530/4646 (98%)	4368 (96%)	157 (4%)	5 (0%)	48	83
1	B	4507/4646 (97%)	4365 (97%)	137 (3%)	5 (0%)	48	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	390/638 (61%)	363 (93%)	27 (7%)	0	100	100
2	D	390/638 (61%)	365 (94%)	25 (6%)	0	100	100
3	E	307/492 (62%)	296 (96%)	11 (4%)	0	100	100
3	F	307/492 (62%)	291 (95%)	14 (5%)	2 (1%)	18	55
4	G	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
4	H	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
5	I	87/89 (98%)	73 (84%)	14 (16%)	0	100	100
5	J	87/89 (98%)	83 (95%)	3 (3%)	1 (1%)	11	45
6	K	111/113 (98%)	110 (99%)	1 (1%)	0	100	100
6	L	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
7	O	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
7	P	317/410 (77%)	297 (94%)	19 (6%)	1 (0%)	36	71
All	All	11646/12968 (90%)	11197 (96%)	435 (4%)	14 (0%)	49	83

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	3270	VAL
1	A	3271	ILE
1	A	3384	ARG
1	A	3444	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	4044/4125 (98%)	4036 (100%)	8 (0%)	87	85
1	B	4028/4125 (98%)	4021 (100%)	7 (0%)	87	85
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	279 (100%)	0	100	100
4	G	87/89 (98%)	87 (100%)	0	100	100
4	H	87/89 (98%)	87 (100%)	0	100	100
5	I	78/78 (100%)	78 (100%)	0	100	100
5	J	78/78 (100%)	78 (100%)	0	100	100
6	K	97/97 (100%)	97 (100%)	0	100	100
6	L	97/97 (100%)	97 (100%)	0	100	100
7	O	287/364 (79%)	287 (100%)	0	100	100
7	P	284/364 (78%)	284 (100%)	0	100	100
All	All	10413/11464 (91%)	10398 (100%)	15 (0%)	87	88

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3454	LEU
1	B	3436	MET
1	B	3243	MET
1	B	3440	LEU
1	B	3428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1056	GLN
1	B	2464	GLN
7	O	381	HIS
3	F	115	HIS
1	B	1186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
8	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
8	ADP	B	4701	10	28,29,29	1.38	4 (14%)	43,45,45	1.84	8 (18%)
8	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
9	ATP	A	4702	10	32,33,33	0.40	0	48,52,52	0.29	0
8	ADP	B	4703	-	28,29,29	1.39	4 (14%)	43,45,45	1.90	8 (18%)
8	ADP	A	4701	10	28,29,29	1.38	5 (17%)	43,45,45	1.82	9 (20%)
9	ATP	B	4702	10	32,33,33	0.48	0	48,52,52	0.29	0
8	ADP	B	4704	-	28,29,29	1.37	4 (14%)	43,45,45	1.84	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	4703	-	-	5/16/32/32	0/3/3/3
8	ADP	B	4701	10	-	3/16/32/32	0/3/3/3
8	ADP	A	4704	-	-	1/16/32/32	0/3/3/3
9	ATP	A	4702	10	-	4/22/38/38	0/3/3/3
8	ADP	B	4703	-	-	6/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	4701	10	-	0/16/32/32	0/3/3/3
9	ATP	B	4702	10	-	4/22/38/38	0/3/3/3
8	ADP	B	4704	-	-	3/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4703	ADP	C5-C4	4.72	1.47	1.39
8	A	4704	ADP	C5-C4	4.70	1.47	1.39
8	B	4703	ADP	C5-C4	4.65	1.47	1.39
8	A	4701	ADP	C5-C4	4.55	1.47	1.39
8	B	4701	ADP	C5-C4	4.52	1.47	1.39

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4703	ADP	C5-C4-N3	-6.28	118.07	126.72
8	A	4703	ADP	C5-C4-N3	-6.01	118.45	126.72
8	A	4704	ADP	C5-C4-N3	-5.96	118.50	126.72
8	B	4701	ADP	C5-C4-N3	-5.86	118.65	126.72
8	B	4704	ADP	C5-C4-N3	-5.85	118.66	126.72

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4703	ADP	C5'-O5'-PA-O1A
8	A	4703	ADP	C5'-O5'-PA-O3A
8	B	4701	ADP	C5'-O5'-PA-O1A
8	B	4701	ADP	C5'-O5'-PA-O2A
8	B	4701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

7 monomers are involved in 12 short contacts:

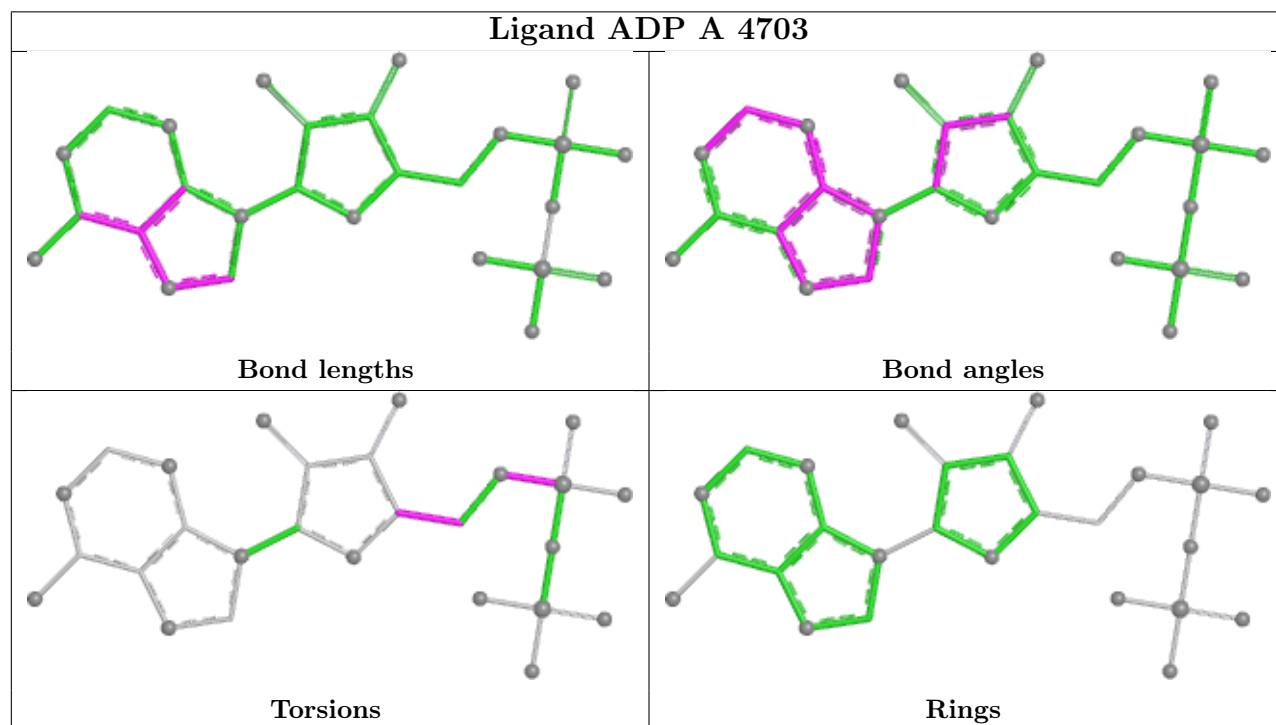
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	4701	ADP	3	0
8	A	4704	ADP	1	0
9	A	4702	ATP	2	0
8	B	4703	ADP	2	0

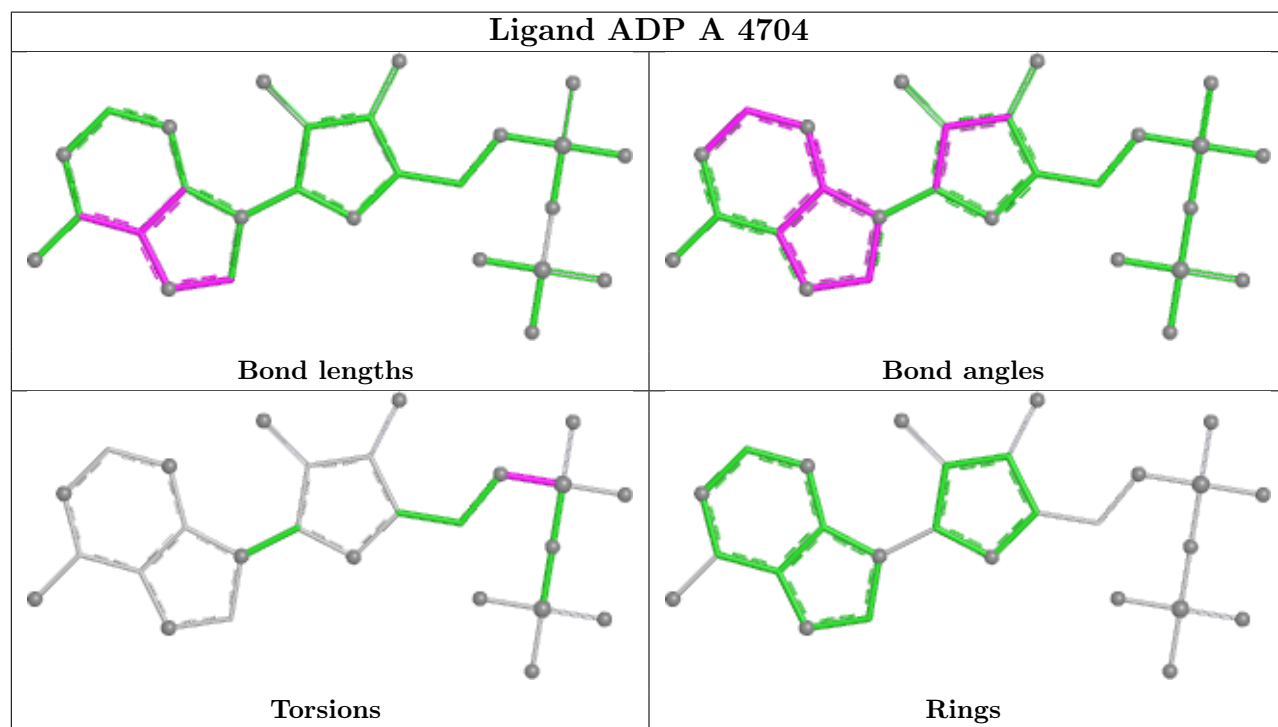
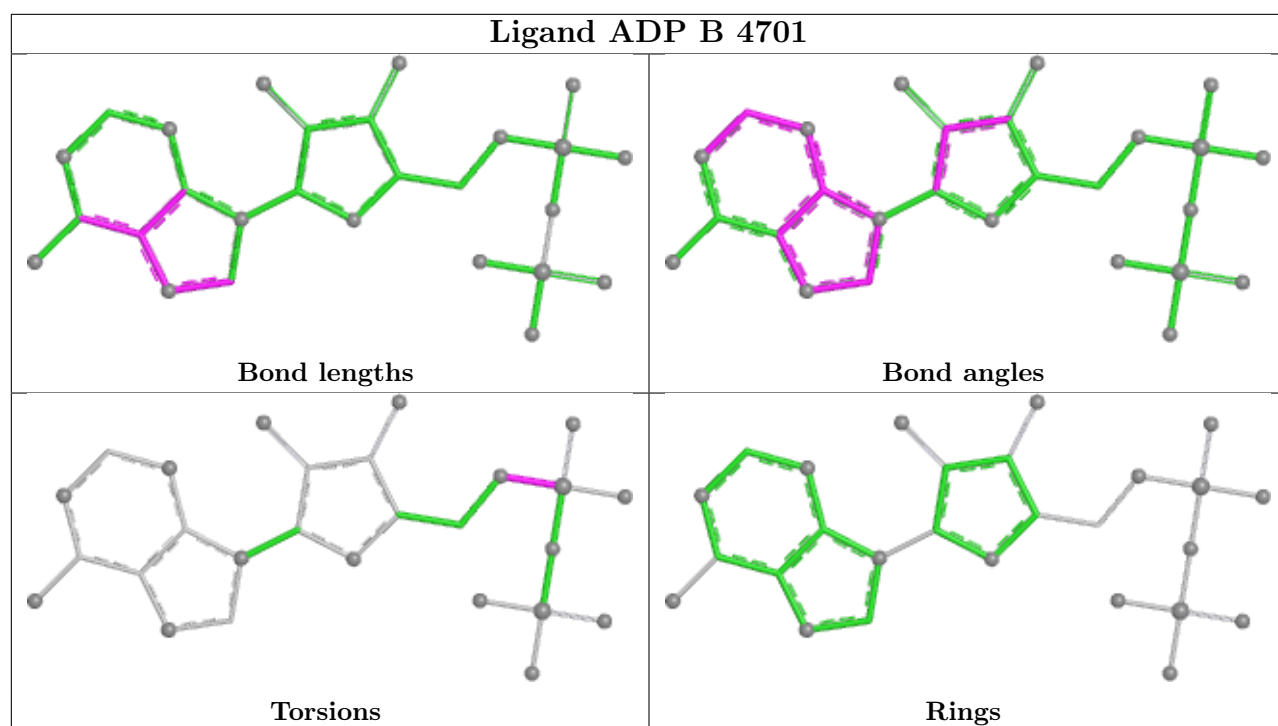
Continued on next page...

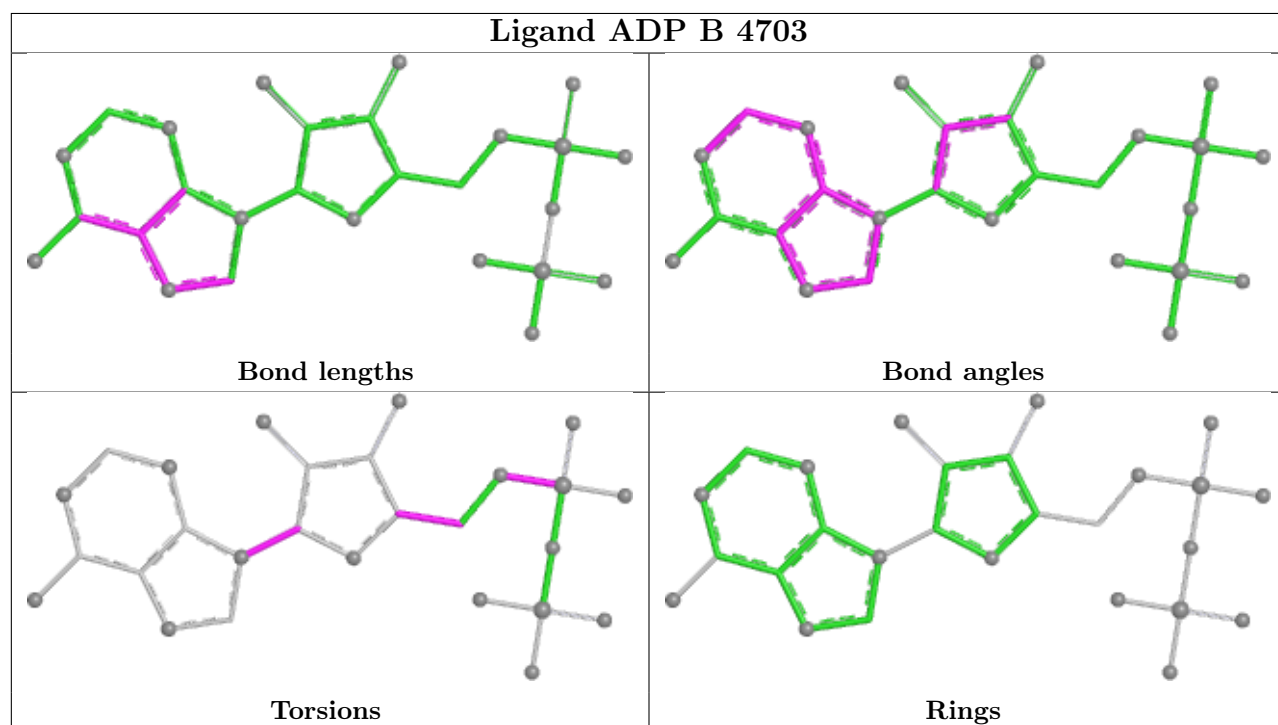
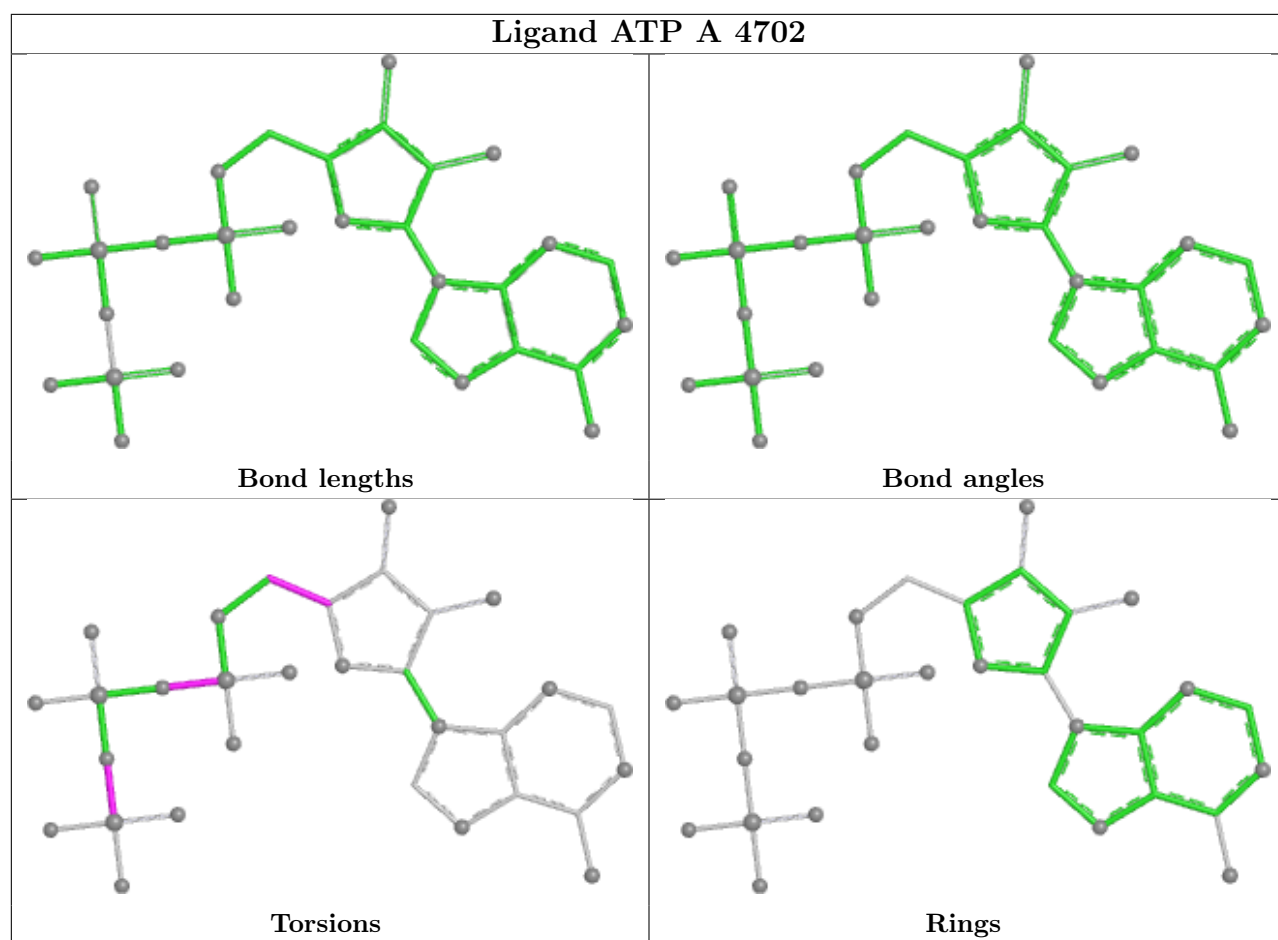
Continued from previous page...

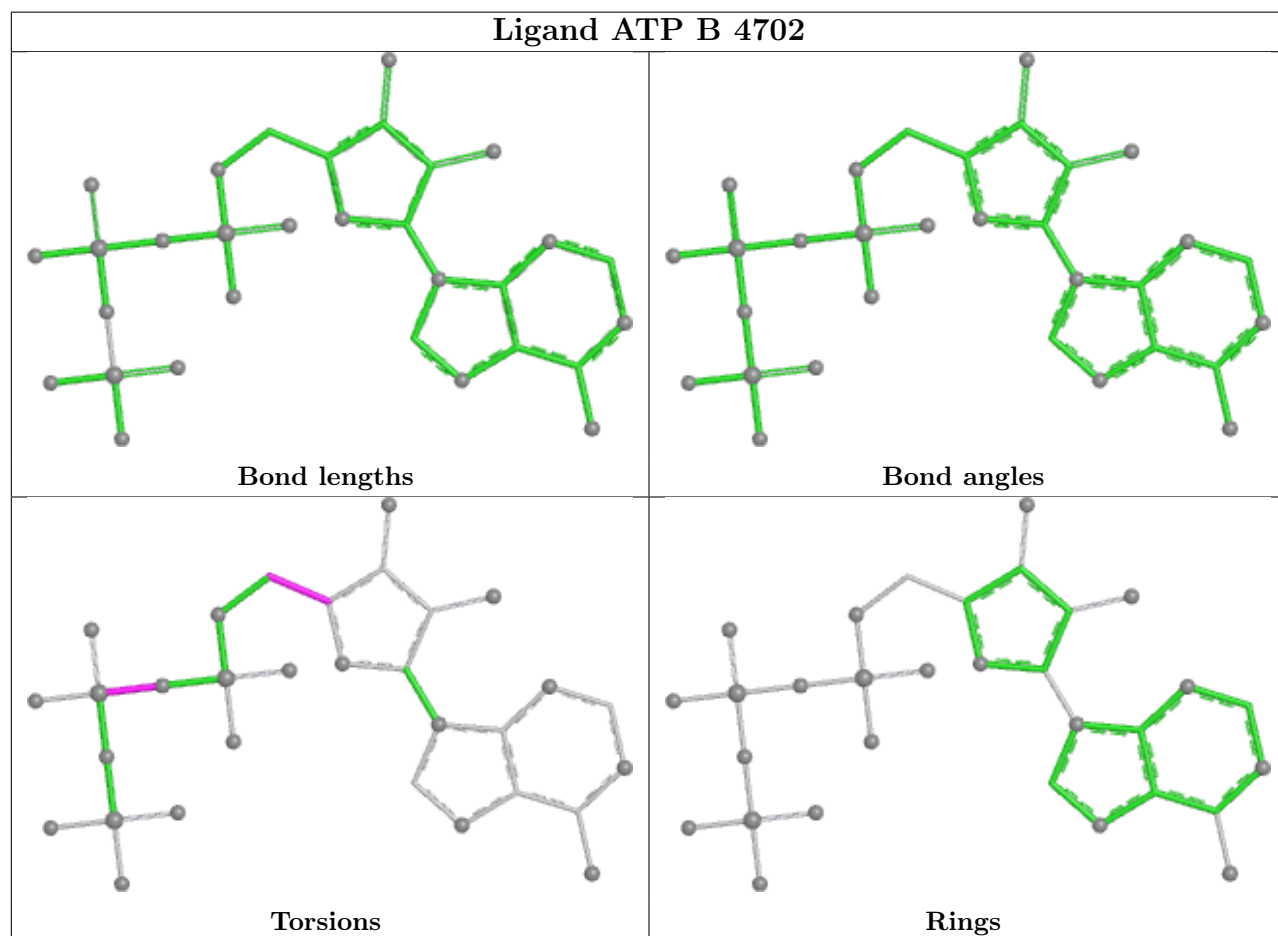
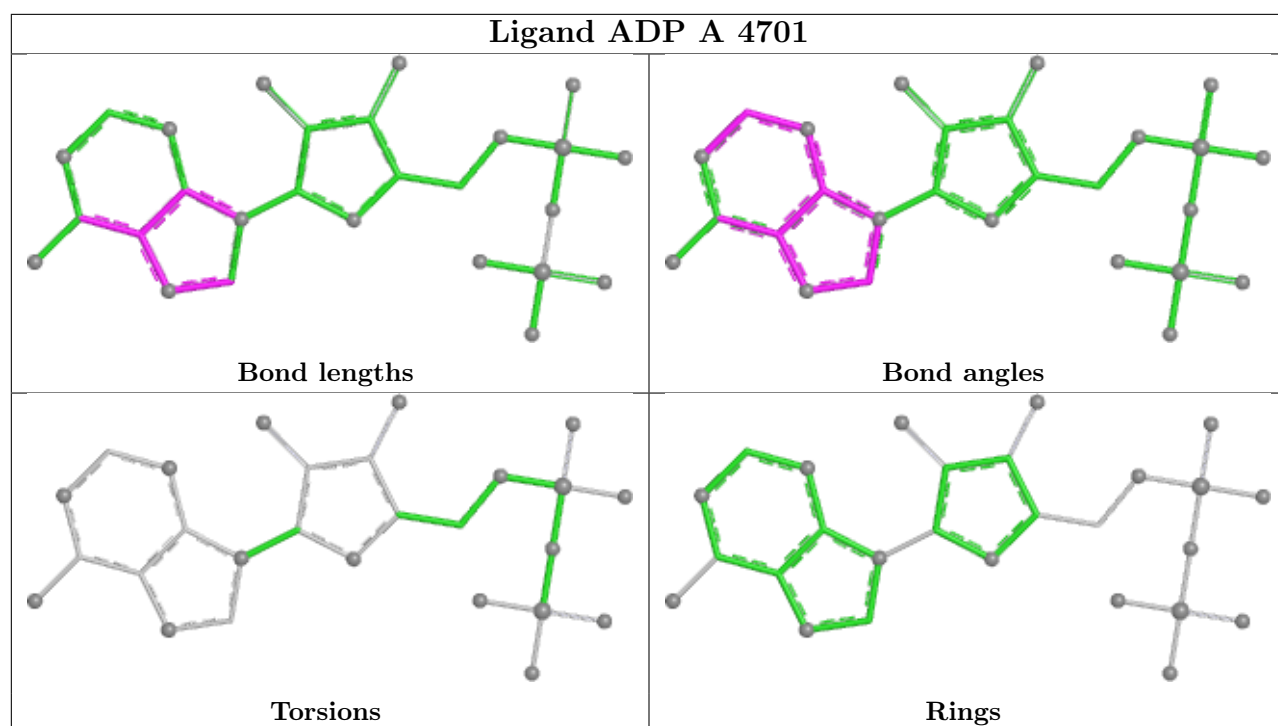
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4701	ADP	1	0
9	B	4702	ATP	2	0
8	B	4704	ADP	1	0

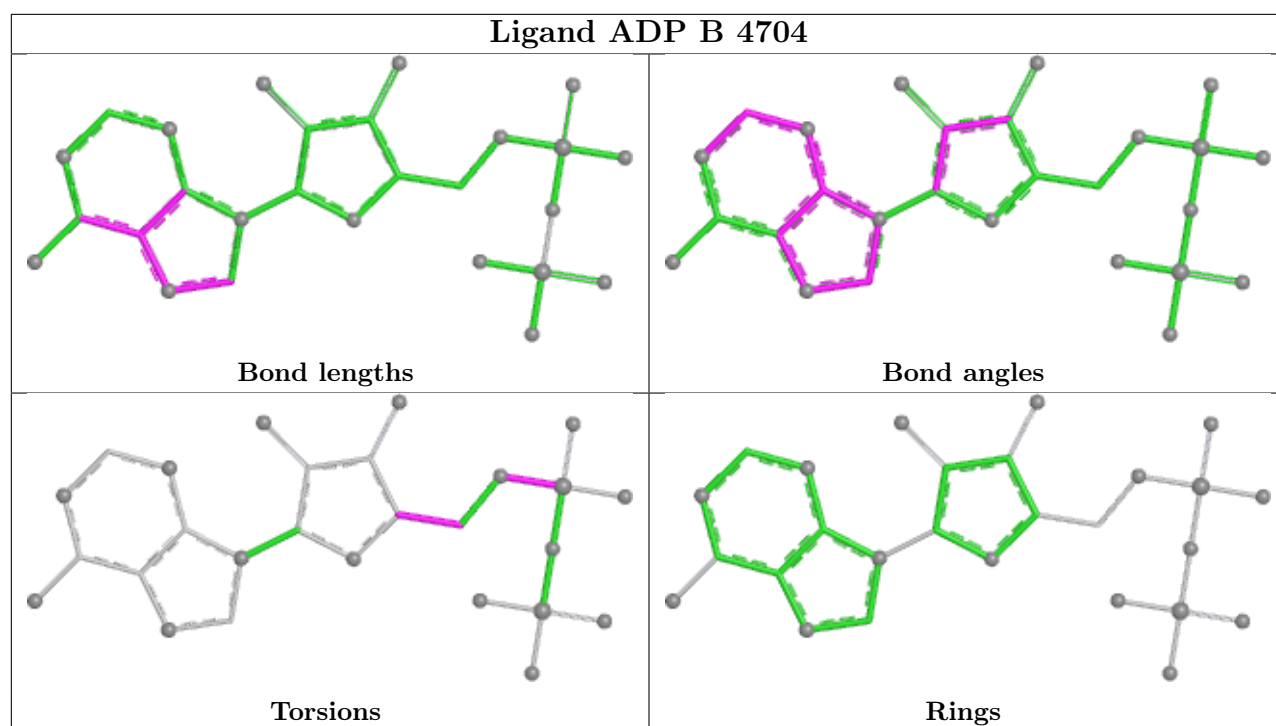
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1394:MET	C	1395:LYS	N	8.64
1	A	1394:MET	C	1395:LYS	N	5.37

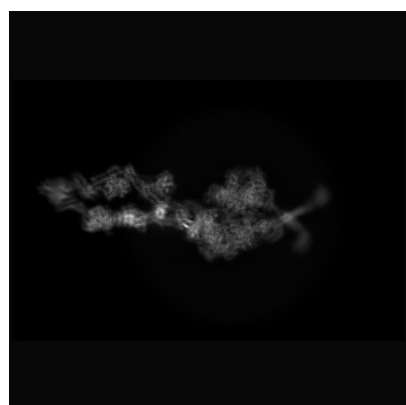
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47382. These allow visual inspection of the internal detail of the map and identification of artifacts.

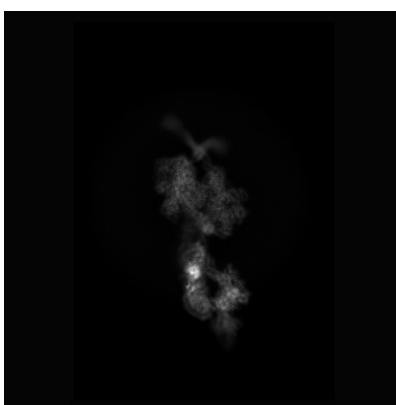
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

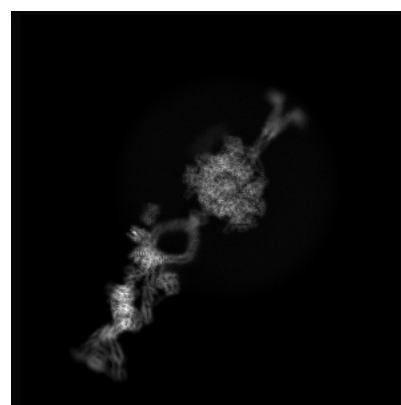
6.1.1 Primary map



X



Y

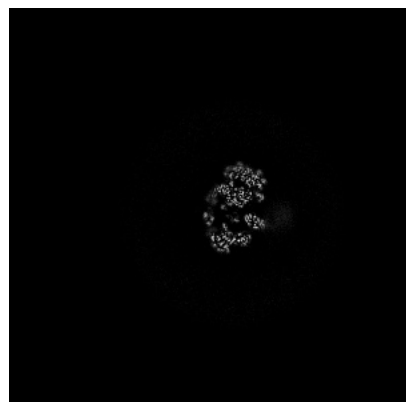


Z

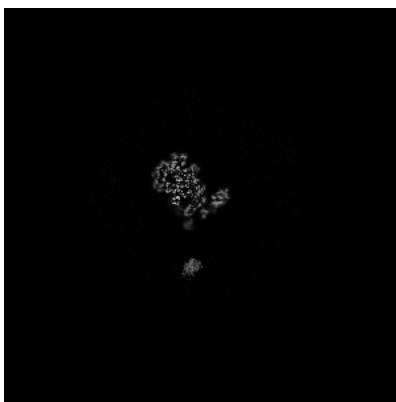
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210

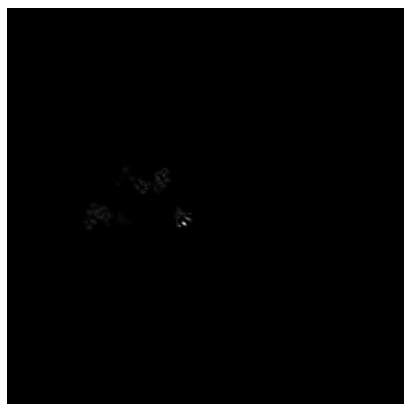


Z Index: 210

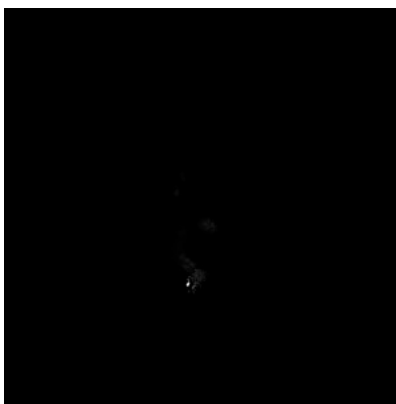
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 130



Y Index: 186

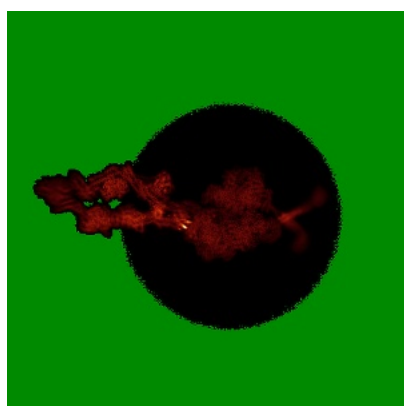


Z Index: 198

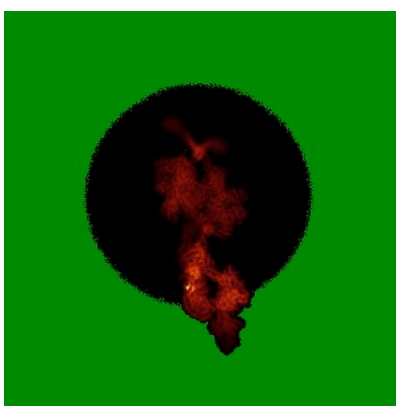
The images above show the largest variance slices of the map in three orthogonal directions.

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

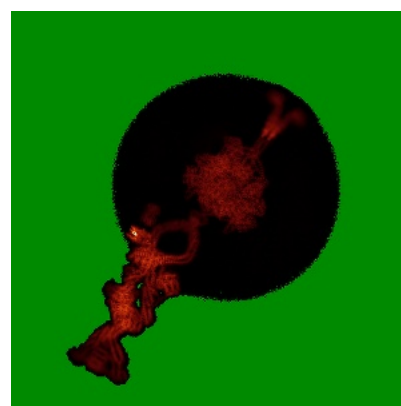
6.4.1 Primary map



X



Y

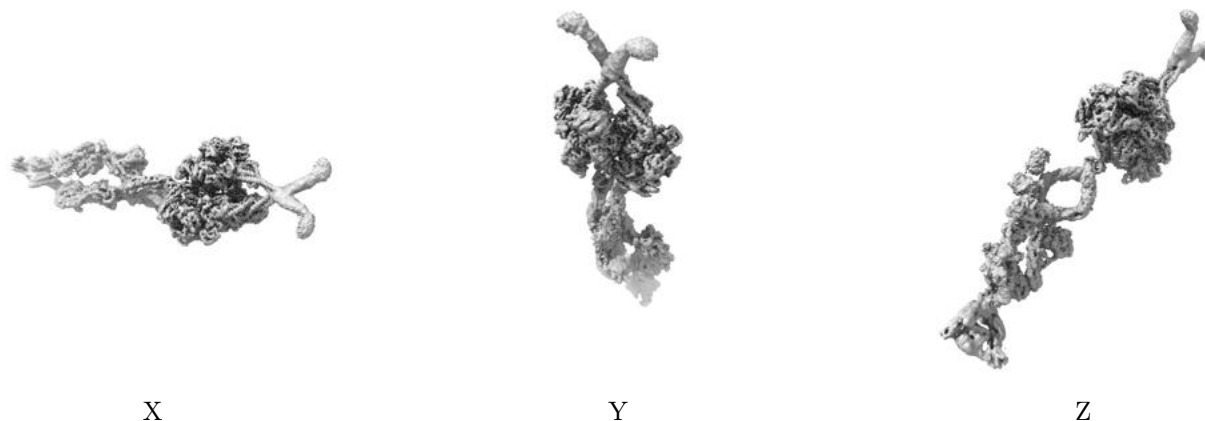


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

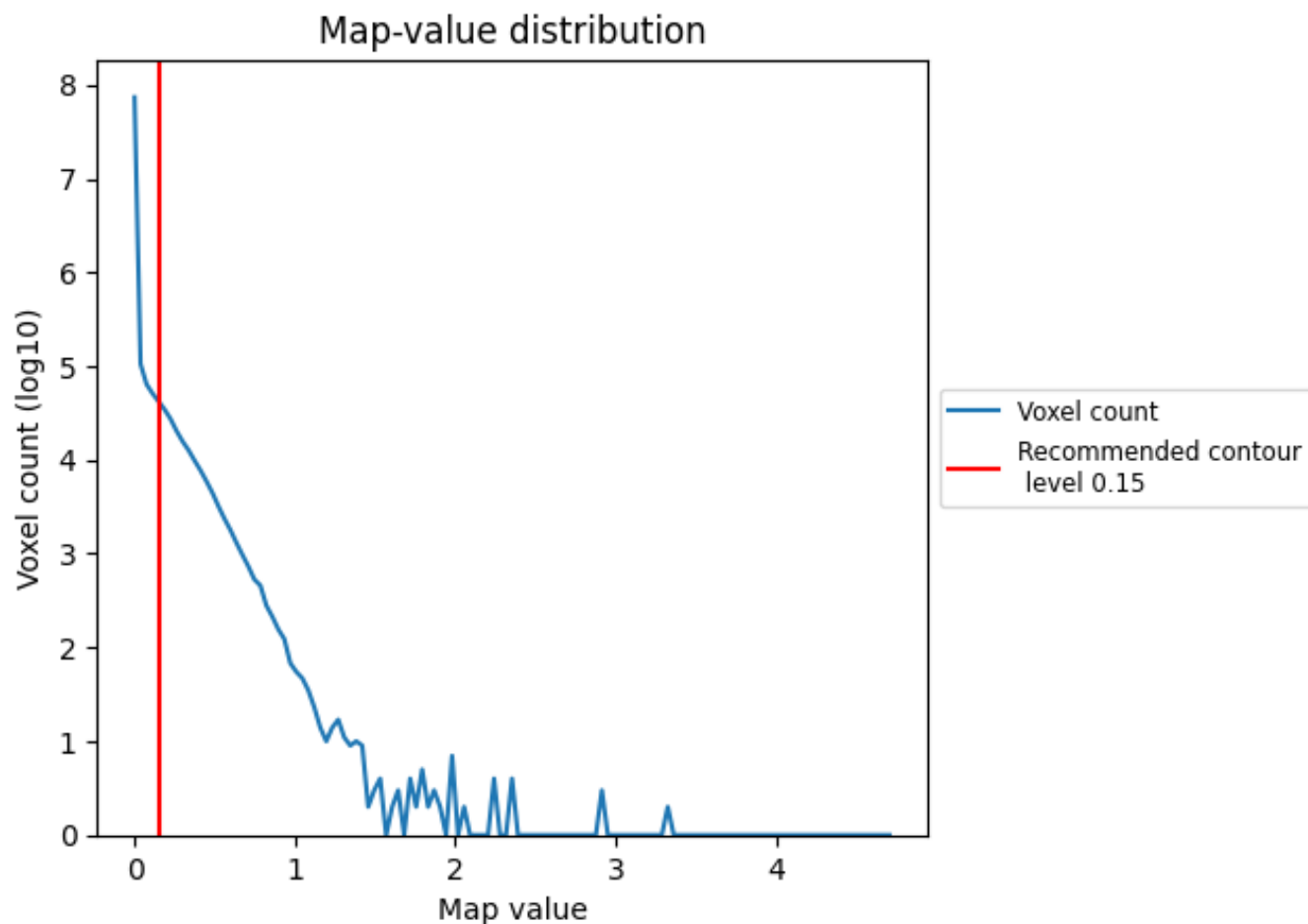
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

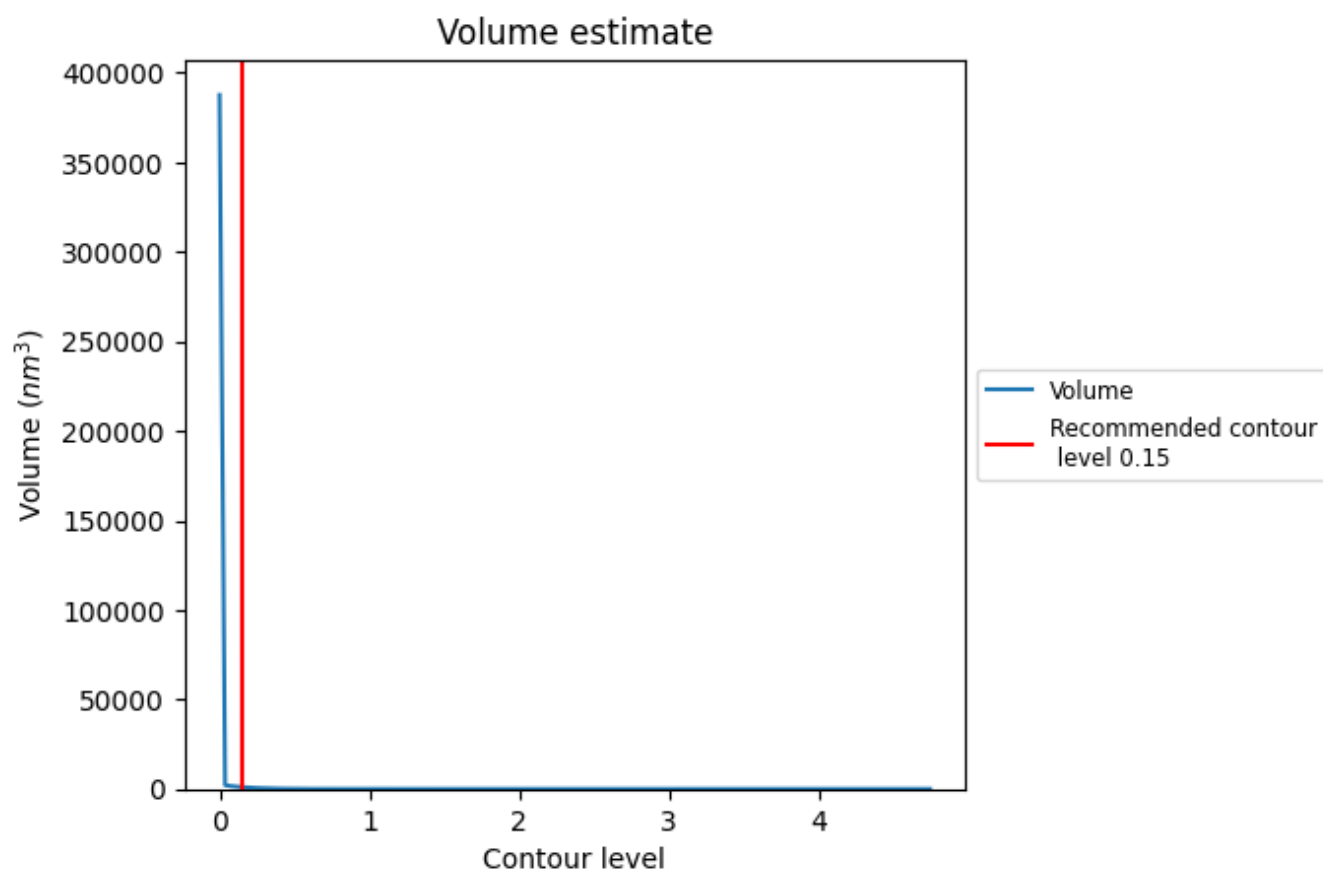
This section contains the results of statistical analysis of the map.

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.

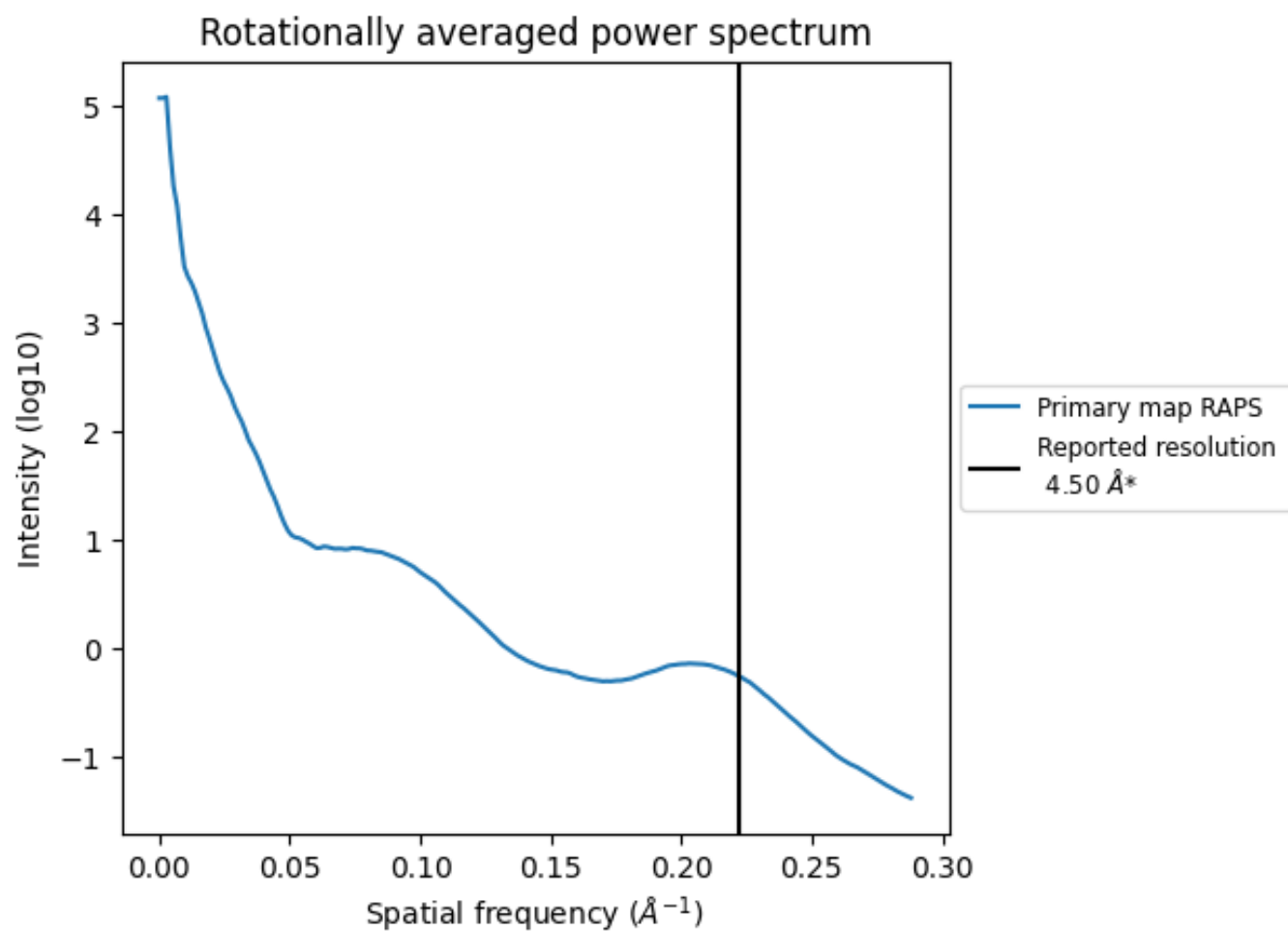
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1011 nm^3 ; this corresponds to an approximate mass of 913 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 0.222 \AA^{-1}

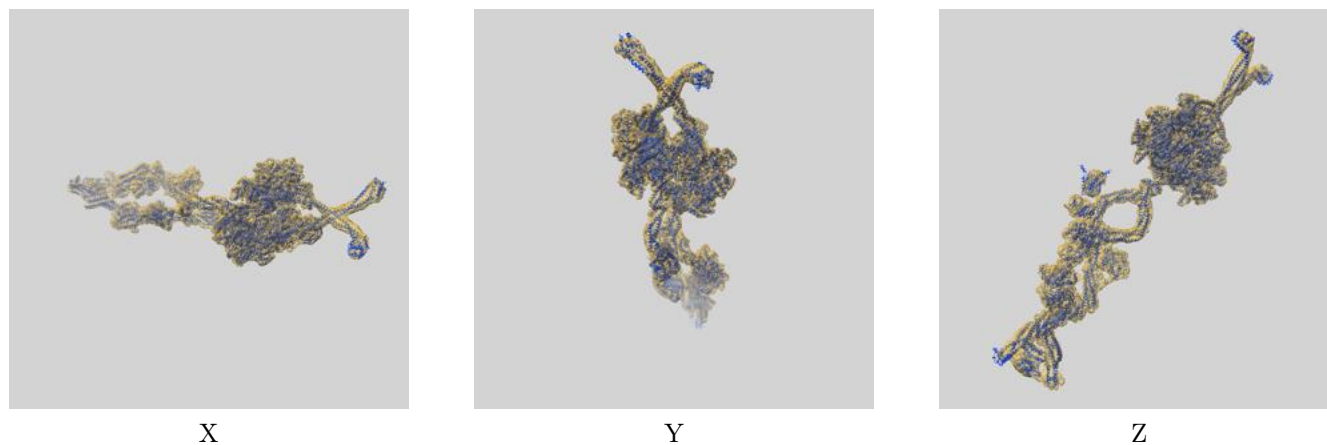
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47382 and PDB model 9E13. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



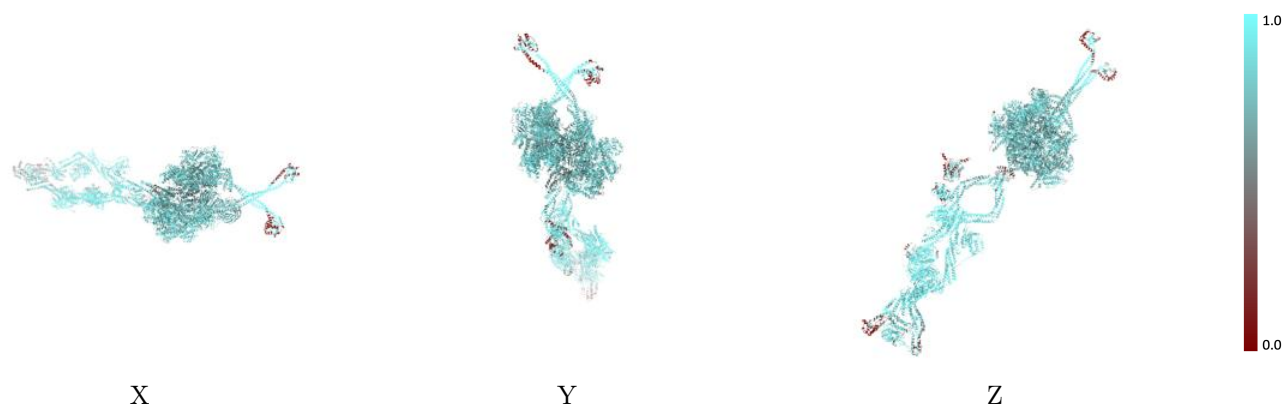
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



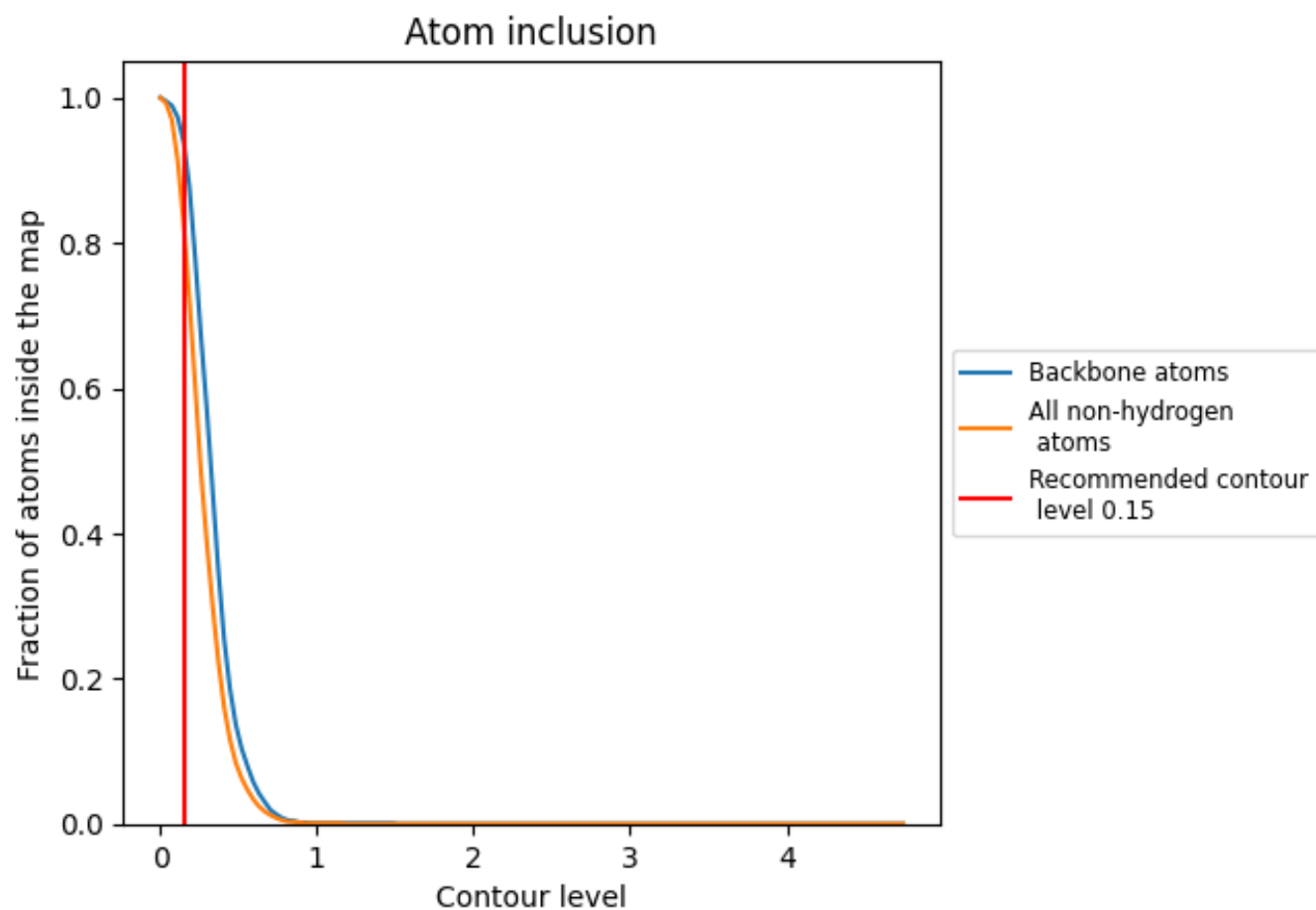
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.3450
A	 0.8020	 0.3540
B	 0.8320	 0.3620
C	 0.9310	 0.3560
D	 0.9320	 0.2890
E	 0.9490	 0.3300
F	 0.9530	 0.3150
G	 0.7640	 0.1010
H	 0.8580	 0.1450
I	 0.7760	 0.1040
J	 0.8010	 0.0940
K	 0.3960	 0.0350
L	 0.5500	 0.0770
O	 0.8570	 0.4980
P	 0.7510	 0.3890

