



## wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 11:13 am GMT

PDB ID : 6SC2  
EMDB ID : EMD-4303  
Title : Structure of the dynein-2 complex; IFT-train bound model  
Authors : Toropova, K.; Zalyte, R.; Mukhopadhyay, A.G.; Mladenov, M.; Carter, A.P.;  
Roberts, A.J.  
Deposited on : 2019-07-23  
Resolution : 3.90 Å(reported)

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

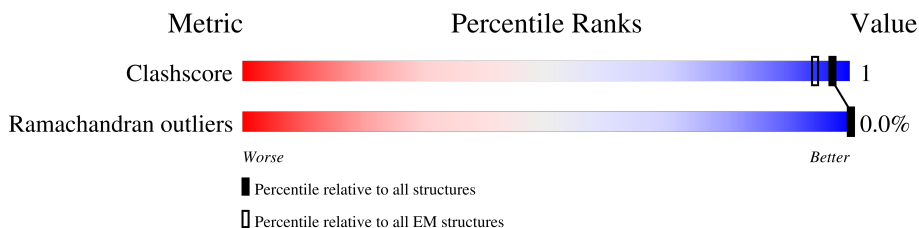
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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

Mol	Chain	Length	Quality of chain
1	A	4513	15% 86% 13%
2	B	4513	17% 86% 13%
3	C	1066	8% 46% 54%
4	D	564	8% 79% 21%
5	E	351	87% 11%
5	F	351	23% 88% 12%
6	G	96	97%
6	H	96	9% 97%
7	I	89	96%

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Mol	Chain	Length	Quality of chain
7	J	89	 96% ..
7	K	89	 6% 96% ..
7	L	89	 96% ..
7	M	89	 96% ..
7	N	89	 8% 96% ..

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50276 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 O6-alkylguanine-DNA alkyltransferase mutant,DYNC2H1 variant protein,O6-alkylguanine-DNA alkyltransferase mutant,Cytoplasmic dynein 2 heavy chain 1,DYNC2H1 variant protein,DYNC2H1 variant protein,DYNC2H1 variant protein.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
1	A	3914	19386	11558	3914	3914	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-205	GLY	-	expression tag	UNP E5BBQ0
A	-176	ARG	GLU	conflict	UNP E5BBQ0
A	-27	PRO	-	linker	UNP E5BBQ0
A	-26	GLY	-	linker	UNP E5BBQ0
A	-25	LEU	-	linker	UNP E5BBQ0
A	-24	GLY	-	linker	UNP E5BBQ0
A	-23	GLY	-	linker	UNP E5BBQ0
A	-22	SER	-	linker	UNP E5BBQ0
A	-21	LEU	-	linker	UNP E5BBQ0
A	-20	GLU	-	linker	UNP E5BBQ0
A	-19	VAL	-	linker	UNP E5BBQ0
A	-18	LEU	-	linker	UNP E5BBQ0
A	-17	PHE	-	linker	UNP E5BBQ0
A	-16	GLN	-	linker	UNP E5BBQ0
A	-15	GLY	-	linker	UNP E5BBQ0
A	-14	PRO	-	linker	UNP E5BBQ0
A	-13	ASP	-	linker	UNP E5BBQ0
A	-12	TYR	-	linker	UNP E5BBQ0
A	-11	ASP	-	linker	UNP E5BBQ0
A	-10	ILE	-	linker	UNP E5BBQ0
A	-9	PRO	-	linker	UNP E5BBQ0
A	-8	THR	-	linker	UNP E5BBQ0
A	-7	THR	-	linker	UNP E5BBQ0
A	-6	LEU	-	linker	UNP E5BBQ0
A	-5	GLU	-	linker	UNP E5BBQ0
A	-4	VAL	-	linker	UNP E5BBQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	LEU	-	linker	UNP E5BBQ0
A	-2	PHE	-	linker	UNP E5BBQ0
A	-1	GLN	-	linker	UNP E5BBQ0
A	0	GLY	-	linker	UNP E5BBQ0
A	1	PRO	-	linker	UNP E5BBQ0

- Molecule 2 is a protein called O6-alkylguanine-DNA alkyltransferase mutant,DYNC2H1 variant protein,O6-alkylguanine-DNA alkyltransferase mutant,Cytoplasmic dynein 2 heavy chain 1,DYNC2H1 variant protein,DYNC2H1 variant protein,DYNC2H1 variant protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	3930	19466	11606	3930	3930	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-205	GLY	-	expression tag	UNP E5BBQ0
B	-176	ARG	GLU	conflict	UNP E5BBQ0
B	-27	PRO	-	linker	UNP E5BBQ0
B	-26	GLY	-	linker	UNP E5BBQ0
B	-25	LEU	-	linker	UNP E5BBQ0
B	-24	GLY	-	linker	UNP E5BBQ0
B	-23	GLY	-	linker	UNP E5BBQ0
B	-22	SER	-	linker	UNP E5BBQ0
B	-21	LEU	-	linker	UNP E5BBQ0
B	-20	GLU	-	linker	UNP E5BBQ0
B	-19	VAL	-	linker	UNP E5BBQ0
B	-18	LEU	-	linker	UNP E5BBQ0
B	-17	PHE	-	linker	UNP E5BBQ0
B	-16	GLN	-	linker	UNP E5BBQ0
B	-15	GLY	-	linker	UNP E5BBQ0
B	-14	PRO	-	linker	UNP E5BBQ0
B	-13	ASP	-	linker	UNP E5BBQ0
B	-12	TYR	-	linker	UNP E5BBQ0
B	-11	ASP	-	linker	UNP E5BBQ0
B	-10	ILE	-	linker	UNP E5BBQ0
B	-9	PRO	-	linker	UNP E5BBQ0
B	-8	THR	-	linker	UNP E5BBQ0
B	-7	THR	-	linker	UNP E5BBQ0
B	-6	LEU	-	linker	UNP E5BBQ0
B	-5	GLU	-	linker	UNP E5BBQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	VAL	-	linker	UNP E5BBQ0
B	-3	LEU	-	linker	UNP E5BBQ0
B	-2	PHE	-	linker	UNP E5BBQ0
B	-1	GLN	-	linker	UNP E5BBQ0
B	0	GLY	-	linker	UNP E5BBQ0
B	1	PRO	-	linker	UNP E5BBQ0

- Molecule 3 is a protein called WD repeat-containing protein 60.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	494	2443	1455	494	494	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	225	LYS	ASN	conflict	UNP Q8WVS4
C	292	PHE	SER	conflict	UNP Q8WVS4

- Molecule 4 is a protein called WD repeat-containing protein 34.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	446	2201	1309	446	446	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	537	TRP	-	expression tag	UNP Q96EX3
D	538	SER	-	expression tag	UNP Q96EX3
D	539	HIS	-	expression tag	UNP Q96EX3
D	540	PRO	-	expression tag	UNP Q96EX3
D	541	GLN	-	expression tag	UNP Q96EX3
D	542	PHE	-	expression tag	UNP Q96EX3
D	543	GLU	-	expression tag	UNP Q96EX3
D	544	LYS	-	expression tag	UNP Q96EX3
D	545	GLY	-	expression tag	UNP Q96EX3
D	546	SER	-	expression tag	UNP Q96EX3
D	547	ALA	-	expression tag	UNP Q96EX3
D	548	GLY	-	expression tag	UNP Q96EX3
D	549	SER	-	expression tag	UNP Q96EX3
D	550	ALA	-	expression tag	UNP Q96EX3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	551	ALA	-	expression tag	UNP Q96EX3
D	552	GLY	-	expression tag	UNP Q96EX3
D	553	SER	-	expression tag	UNP Q96EX3
D	554	GLY	-	expression tag	UNP Q96EX3
D	555	ALA	-	expression tag	UNP Q96EX3
D	556	GLY	-	expression tag	UNP Q96EX3
D	557	TRP	-	expression tag	UNP Q96EX3
D	558	SER	-	expression tag	UNP Q96EX3
D	559	HIS	-	expression tag	UNP Q96EX3
D	560	PRO	-	expression tag	UNP Q96EX3
D	561	GLN	-	expression tag	UNP Q96EX3
D	562	PHE	-	expression tag	UNP Q96EX3
D	563	GLU	-	expression tag	UNP Q96EX3
D	564	LYS	-	expression tag	UNP Q96EX3

- Molecule 5 is a protein called Cytoplasmic dynein 2 light intermediate chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	312	Total	C	N	O	0	0
			1542	918	312	312		
5	F	310	Total	C	N	O	0	0
			1532	912	310	310		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	93	Total	C	N	O	0	0
			462	276	93	93		
6	H	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 7 is a protein called Dynein light chain 1, cytoplasmic.

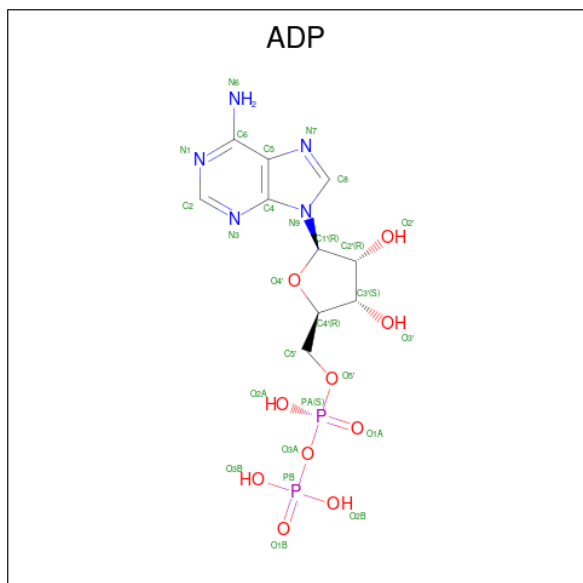
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	86	Total	C	N	O	0	0
			426	254	86	86		
7	J	86	Total	C	N	O	0	0
			426	254	86	86		
7	K	86	Total	C	N	O	0	0
			426	254	86	86		
7	L	86	Total	C	N	O	0	0
			426	254	86	86		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	M	86	Total 426	C 254	N 86	O 86	0	0
7	N	86	Total 426	C 254	N 86	O 86	0	0

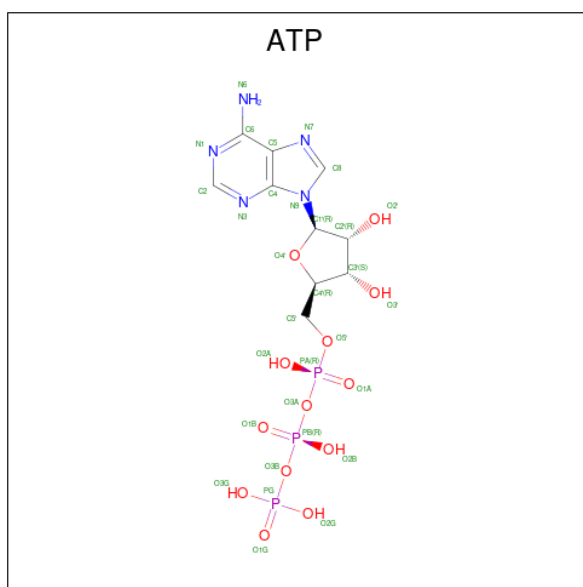
- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	Total 81	C 30	N 15	O 30	P 6	0
8	A	1	Total 81	C 30	N 15	O 30	P 6	0
8	A	1	Total 81	C 30	N 15	O 30	P 6	0
8	B	1	Total 81	C 30	N 15	O 30	P 6	0
8	B	1	Total 81	C 30	N 15	O 30	P 6	0
8	B	1	Total 81	C 30	N 15	O 30	P 6	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





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

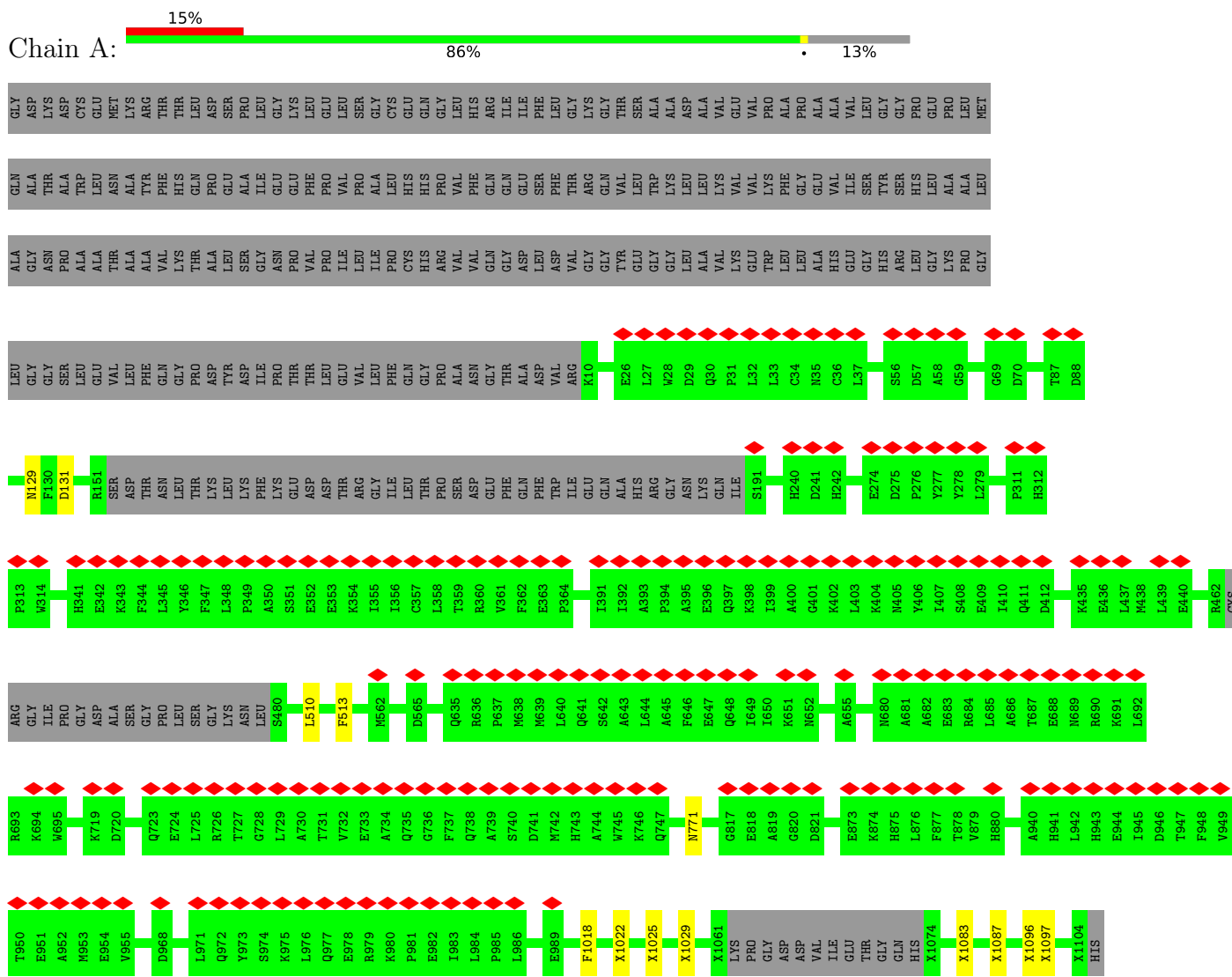
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	A	1	1	1	0
10	B	1	1	1	0

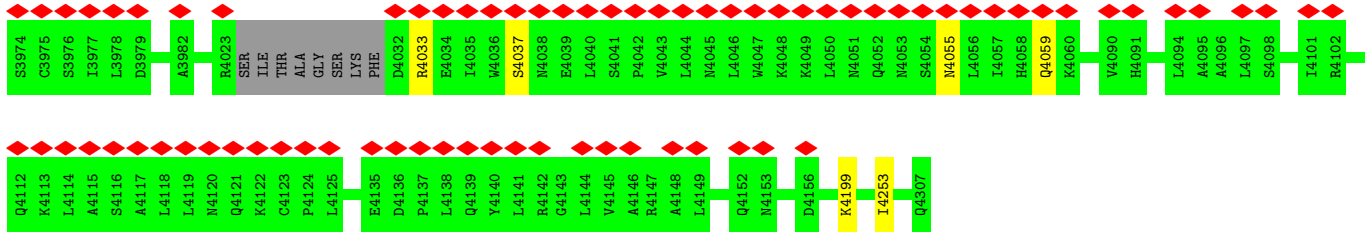
### 3 Residue-property plots [i](#)

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.

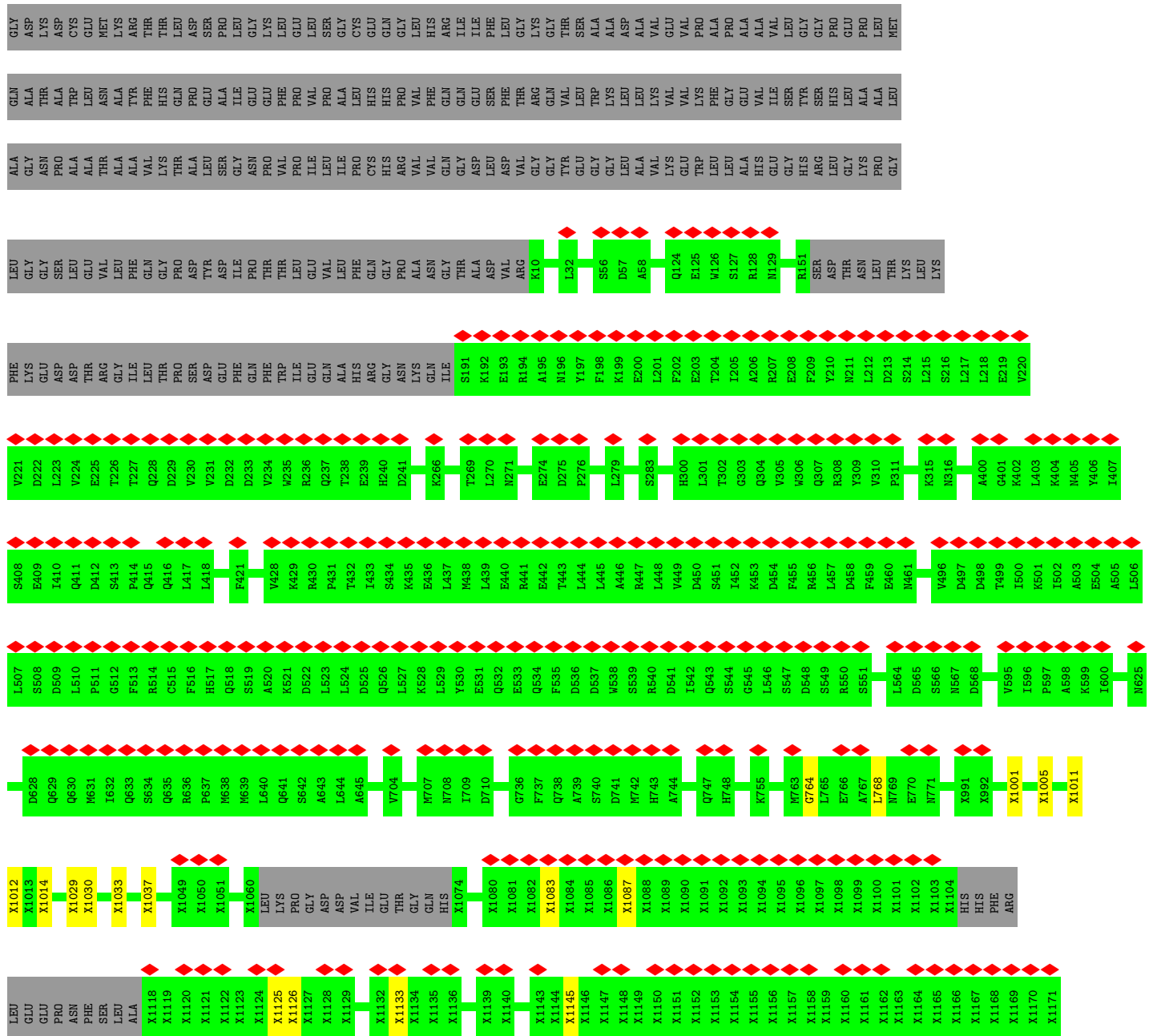
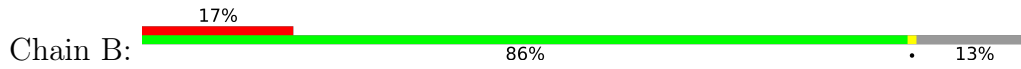
- Molecule 1: O6-alkylguanine-DNA alkyltransferase mutant,DYNC2H1 variant protein,O6-alkylguanine-DNA alkyltransferase mutant,Cytoplasmic dynein 2 heavy chain 1,DYNC2H1 variant protein,DYNC2H1 variant protein,DYNC2H1 variant protein







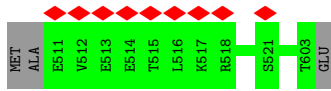
• Molecule 2: O6-alkylguanine-DNA alkyltransferase mutant, DYNC2H1 variant protein, O6-alkylguanine-DNA alkyltransferase mutant, Cytoplasmic dynein 2 heavy chain 1, DYNC2H1 variant protein, DYNC2H1 variant protein, DYNC2H1 variant protein



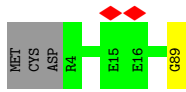




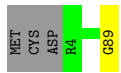




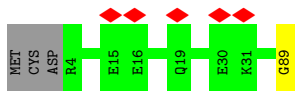
• Molecule 7: Dynein light chain 1, cytoplasmic



• Molecule 7: Dynein light chain 1, cytoplasmic



• Molecule 7: Dynein light chain 1, cytoplasmic



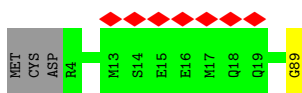
• Molecule 7: Dynein light chain 1, cytoplasmic



• Molecule 7: Dynein light chain 1, cytoplasmic



• Molecule 7: Dynein light chain 1, cytoplasmic





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	57265	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.809	Depositor
Minimum map value	-2.662	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.503	Depositor
Recommended contour level	0.414	Depositor
Map size (Å)	466.29, 621.72003, 763.02	wwPDB
Map dimensions	33, 44, 54	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	14.13, 14.130001, 14.13	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: ATP, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.30	0/18221	0.50	2/25383 (0.0%)
2	B	0.29	0/17832	0.50	1/24840 (0.0%)
3	C	0.31	0/2437	0.53	0/3386
4	D	0.31	0/2198	0.55	0/3055
5	E	0.29	0/1538	0.50	0/2136
5	F	0.29	0/1528	0.50	0/2122
6	G	0.31	0/461	0.48	0/642
6	H	0.31	0/461	0.48	0/642
7	I	0.88	1/425 (0.2%)	0.75	1/591 (0.2%)
7	J	0.96	1/425 (0.2%)	0.77	1/591 (0.2%)
7	K	0.88	1/425 (0.2%)	0.75	1/591 (0.2%)
7	L	0.96	2/425 (0.5%)	0.77	1/591 (0.2%)
7	M	0.88	1/425 (0.2%)	0.75	1/591 (0.2%)
7	N	0.96	2/425 (0.5%)	0.76	1/591 (0.2%)
All	All	0.36	8/47226 (0.0%)	0.52	9/65752 (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	5
2	B	0	5
5	E	0	1
5	F	0	1
All	All	0	12

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	89	GLY	C-O	9.47	1.38	1.23
7	N	89	GLY	C-O	9.44	1.38	1.23
7	J	89	GLY	C-O	9.39	1.38	1.23
7	M	89	GLY	C-O	9.22	1.38	1.23
7	I	89	GLY	C-O	9.21	1.38	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	89	GLY	CA-C-O	7.64	134.35	120.60
7	L	89	GLY	CA-C-O	7.62	134.32	120.60
7	N	89	GLY	CA-C-O	7.53	134.16	120.60
1	A	1803	LYS	C-N-CA	5.43	135.28	121.70
2	B	1803	LYS	C-N-CA	5.41	135.23	121.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1133	UNK	Mainchain
1	A	1592	LEU	Peptide
1	A	2462	SER	Peptide
1	A	2565	LEU	Peptide
1	A	3584	PHE	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19386	0	8241	18	0
2	B	19466	0	8167	17	0
3	C	2443	0	1071	3	0
4	D	2201	0	1005	2	0
5	E	1542	0	672	3	0
5	F	1532	0	668	0	0
6	G	462	0	192	0	0
6	H	462	0	192	0	0
7	I	426	0	195	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	426	0	195	0	0
7	K	426	0	195	0	0
7	L	426	0	195	0	0
7	M	426	0	195	0	0
7	N	426	0	195	0	0
8	A	81	0	36	0	0
8	B	81	0	36	0	0
9	A	31	0	12	1	0
9	B	31	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
All	All	50276	0	21474	43	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 1.

The worst 5 of 43 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)
3:C:555:TRP:O	3:C:565:VAL:CB	2.08	1.00
2:B:1145:UNK:CB	2:B:1231:UNK:CB	2.40	0.99
2:B:1145:UNK:CA	2:B:1231:UNK:CB	2.62	0.76
1:A:1018:PHE:O	1:A:1022:UNK:CB	2.39	0.71
3:C:555:TRP:C	3:C:565:VAL:CB	2.60	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	3665/4513 (81%)	3426 (94%)	239 (6%)	0	<b>100</b> <b>100</b>

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	3589/4513 (80%)	3350 (93%)	239 (7%)	0	100	100
3	C	482/1066 (45%)	463 (96%)	19 (4%)	0	100	100
4	D	440/564 (78%)	402 (91%)	37 (8%)	1 (0%)	47	79
5	E	304/351 (87%)	282 (93%)	21 (7%)	1 (0%)	41	75
5	F	302/351 (86%)	287 (95%)	15 (5%)	0	100	100
6	G	91/96 (95%)	87 (96%)	4 (4%)	0	100	100
6	H	91/96 (95%)	89 (98%)	2 (2%)	0	100	100
7	I	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
7	J	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
7	K	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
7	L	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
7	M	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
7	N	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
All	All	9468/12084 (78%)	8875 (94%)	591 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	495	THR
5	E	93	LEU

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 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	4405	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
9	ATP	A	4402	10	26,33,33	0.89	1 (3%)	31,52,52	1.70	5 (16%)
8	ADP	A	4401	-	24,29,29	0.92	1 (4%)	29,45,45	1.40	3 (10%)
8	ADP	B	4405	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	5 (17%)
8	ADP	B	4404	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
8	ADP	B	4401	-	24,29,29	0.92	1 (4%)	29,45,45	1.41	4 (13%)
8	ADP	A	4404	-	24,29,29	0.93	1 (4%)	29,45,45	1.47	4 (13%)
9	ATP	B	4402	10	26,33,33	0.89	1 (3%)	31,52,52	1.70	5 (16%)

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	4405	-	-	1/12/32/32	0/3/3/3
9	ATP	A	4402	10	-	1/18/38/38	0/3/3/3
8	ADP	A	4401	-	-	0/12/32/32	0/3/3/3
8	ADP	B	4405	-	-	0/12/32/32	0/3/3/3
8	ADP	B	4404	-	-	3/12/32/32	0/3/3/3
8	ADP	B	4401	-	-	0/12/32/32	0/3/3/3
8	ADP	A	4404	-	-	3/12/32/32	0/3/3/3
9	ATP	B	4402	10	-	1/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4405	ADP	C5-C4	2.20	1.46	1.40
8	B	4405	ADP	C5-C4	2.16	1.46	1.40
8	B	4404	ADP	C5-C4	2.14	1.46	1.40
9	A	4402	ATP	C5-C4	2.13	1.46	1.40
9	B	4402	ATP	C5-C4	2.13	1.46	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	4402	ATP	PA-O3A-PB	-4.78	116.41	132.83
9	B	4402	ATP	PA-O3A-PB	-4.78	116.43	132.83
9	B	4402	ATP	PB-O3B-PG	-4.09	118.80	132.83
9	A	4402	ATP	PB-O3B-PG	-4.07	118.85	132.83
8	B	4404	ADP	C3'-C2'-C1'	3.70	106.55	100.98

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4404	ADP	C5'-O5'-PA-O3A
8	B	4404	ADP	C5'-O5'-PA-O2A
8	B	4404	ADP	C5'-O5'-PA-O3A
9	A	4402	ATP	C5'-O5'-PA-O3A
9	B	4402	ATP	C5'-O5'-PA-O3A

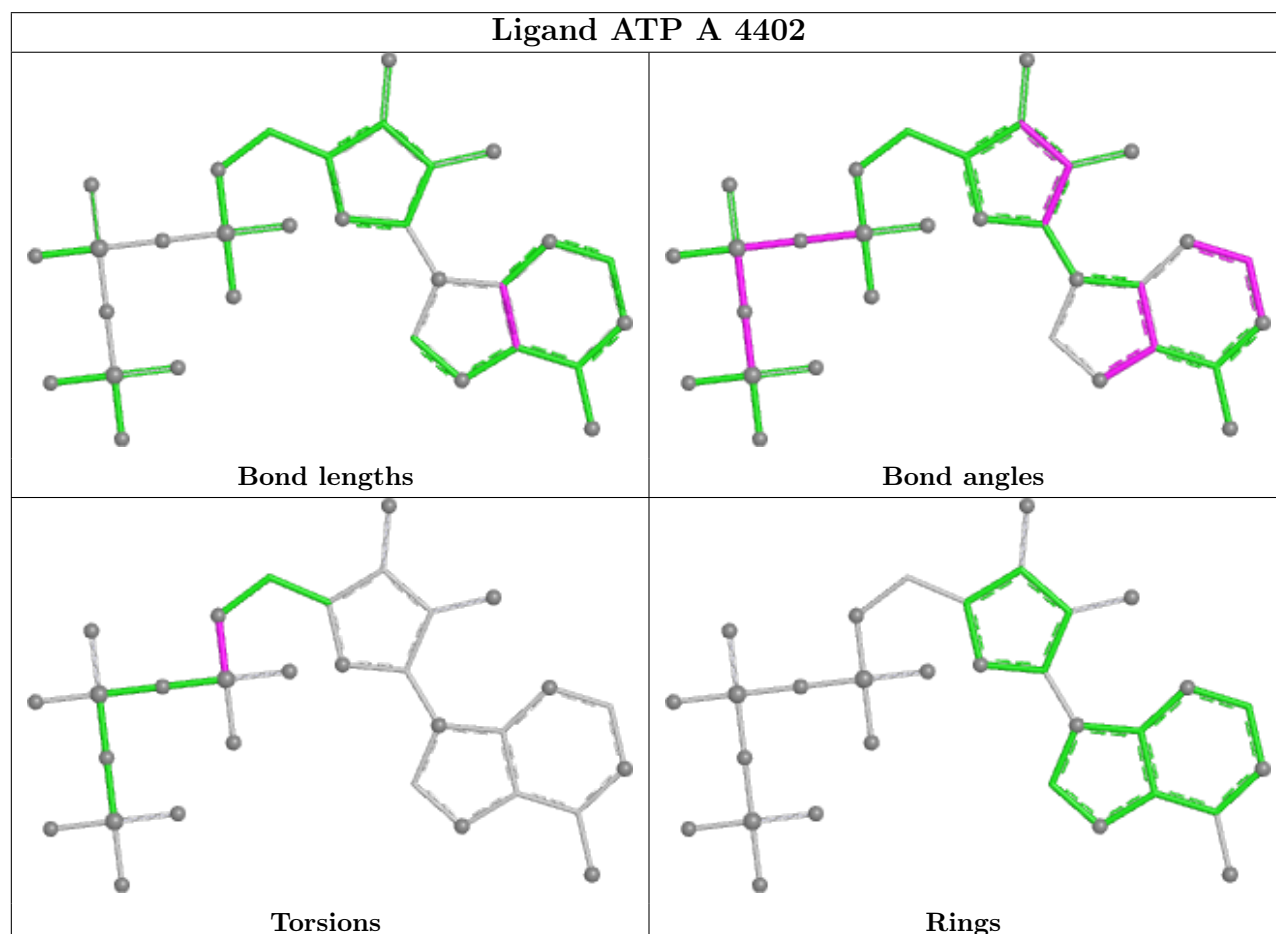
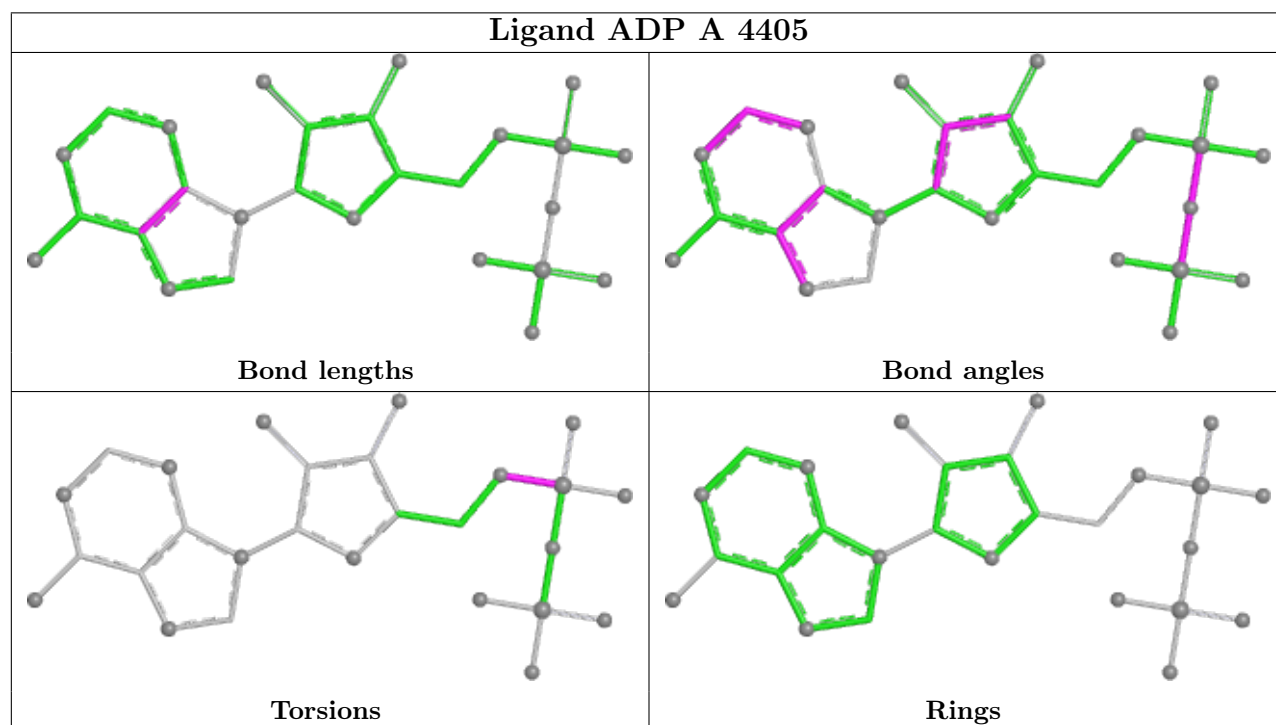
There are no ring outliers.

1 monomer is involved in 1 short contact:

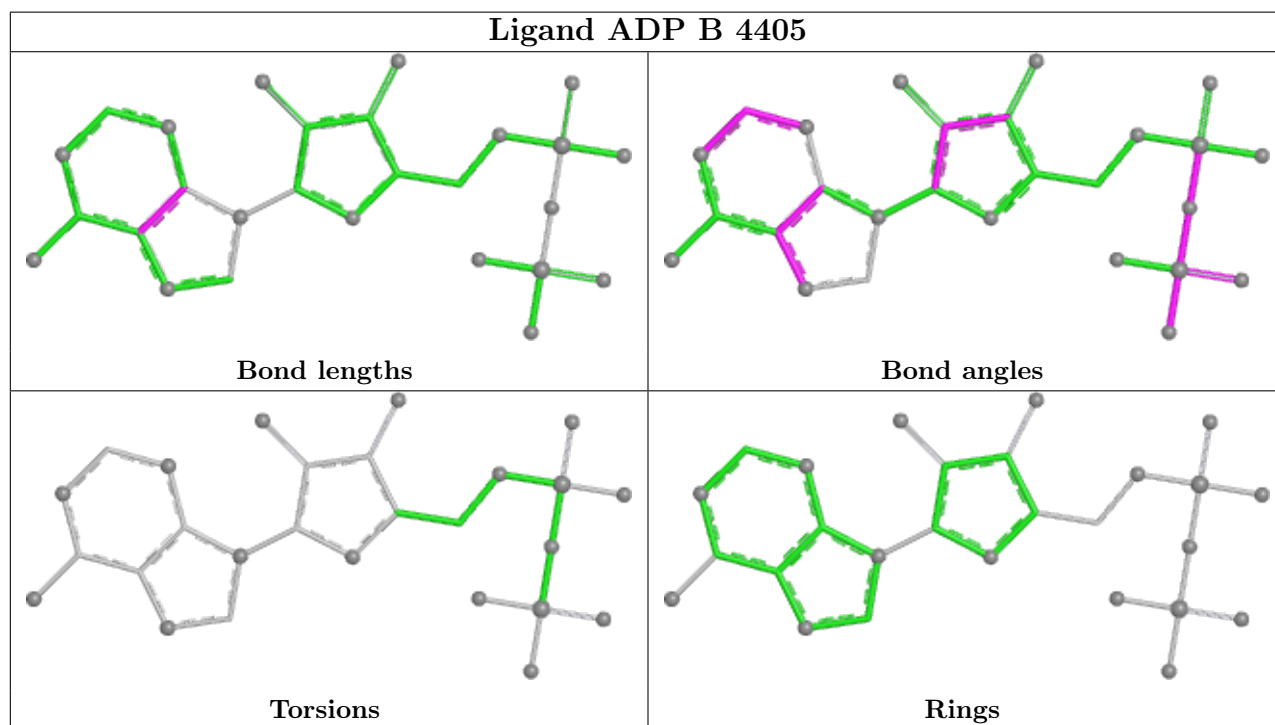
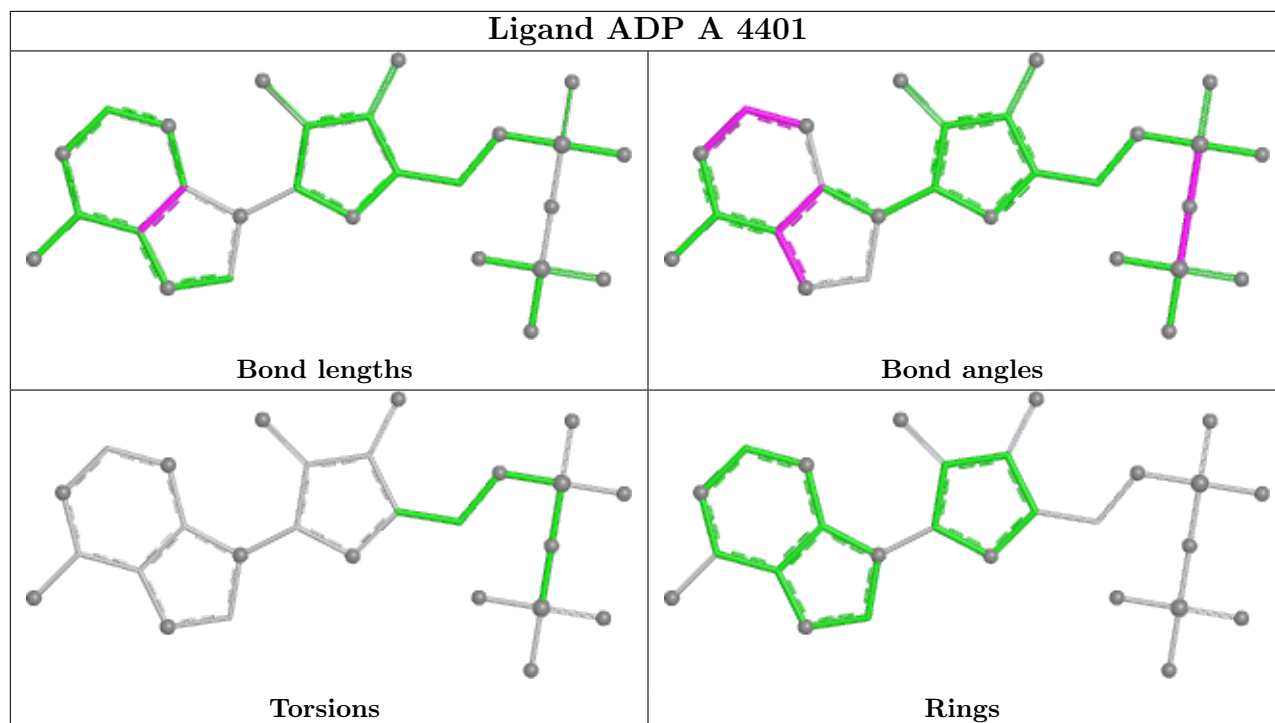
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	4402	ATP	1	0

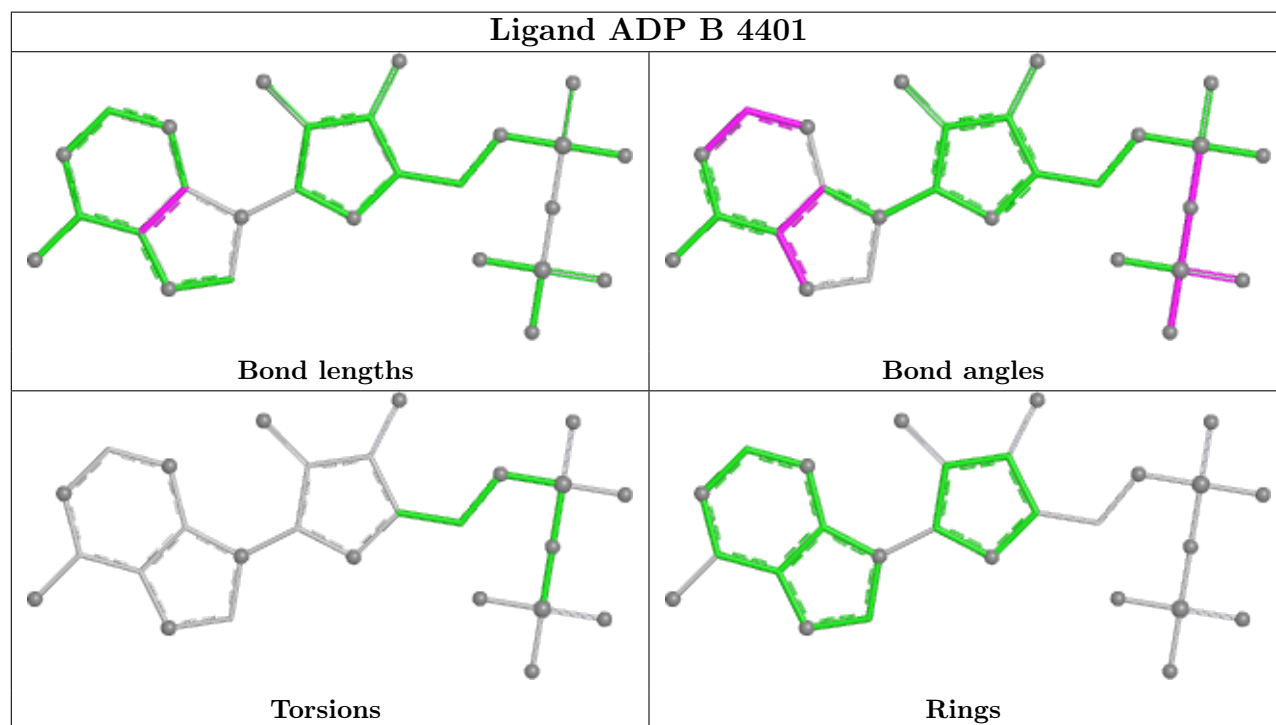
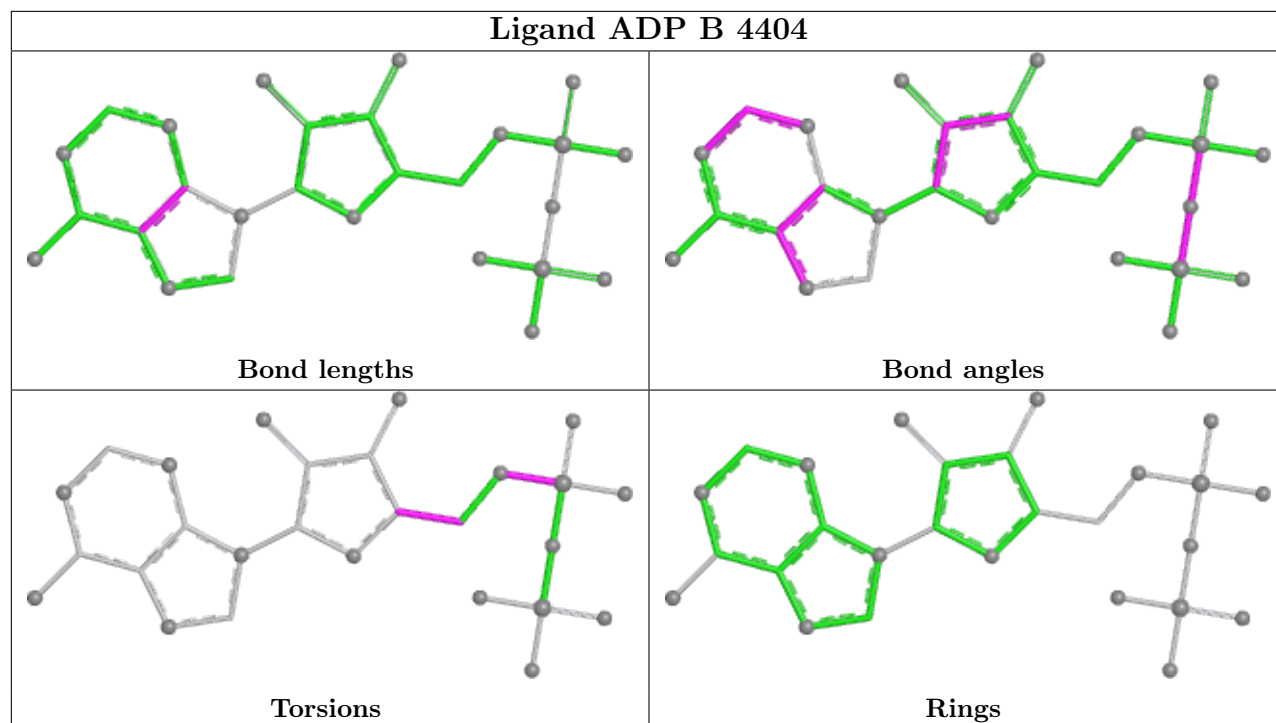
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

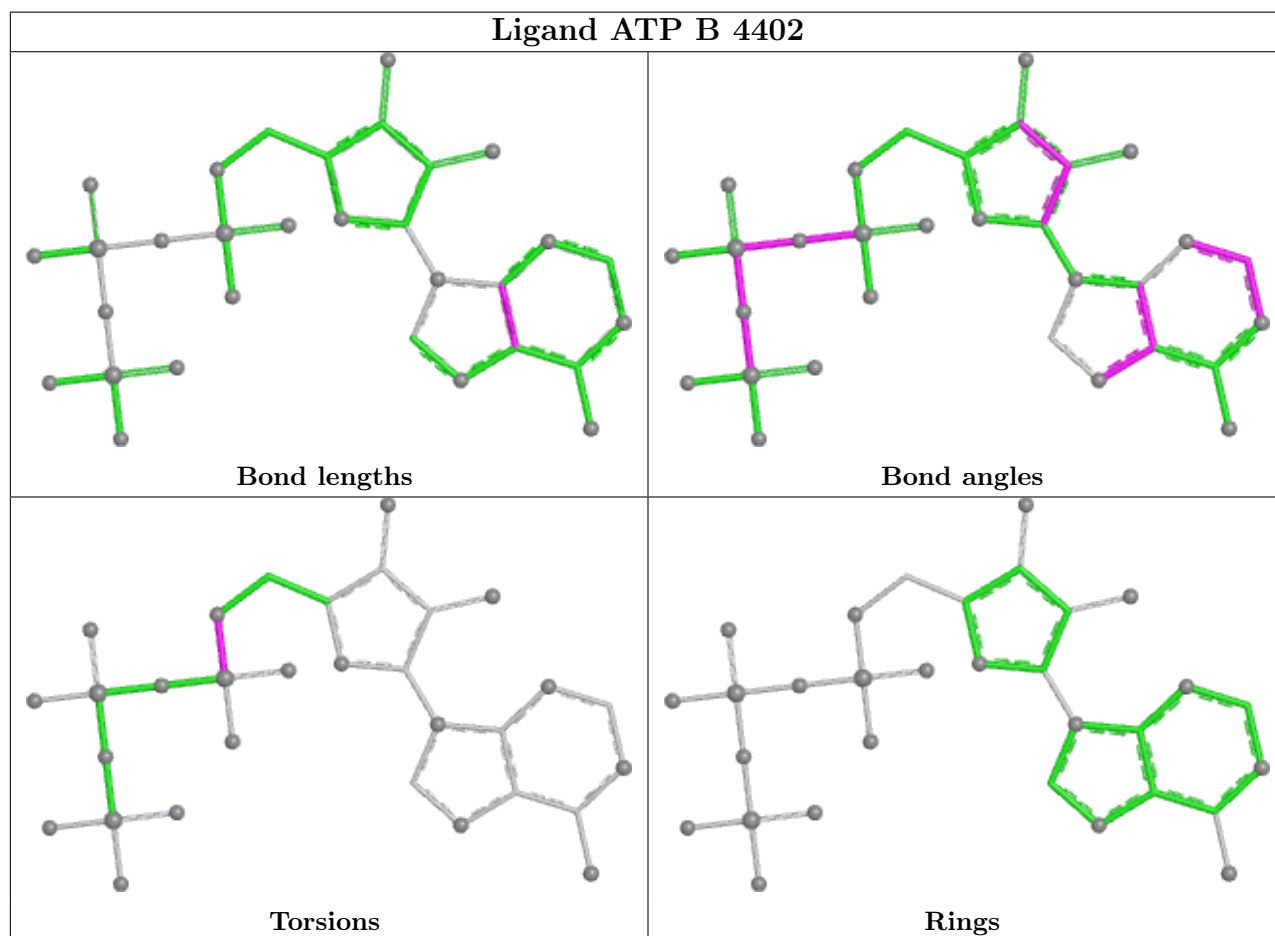
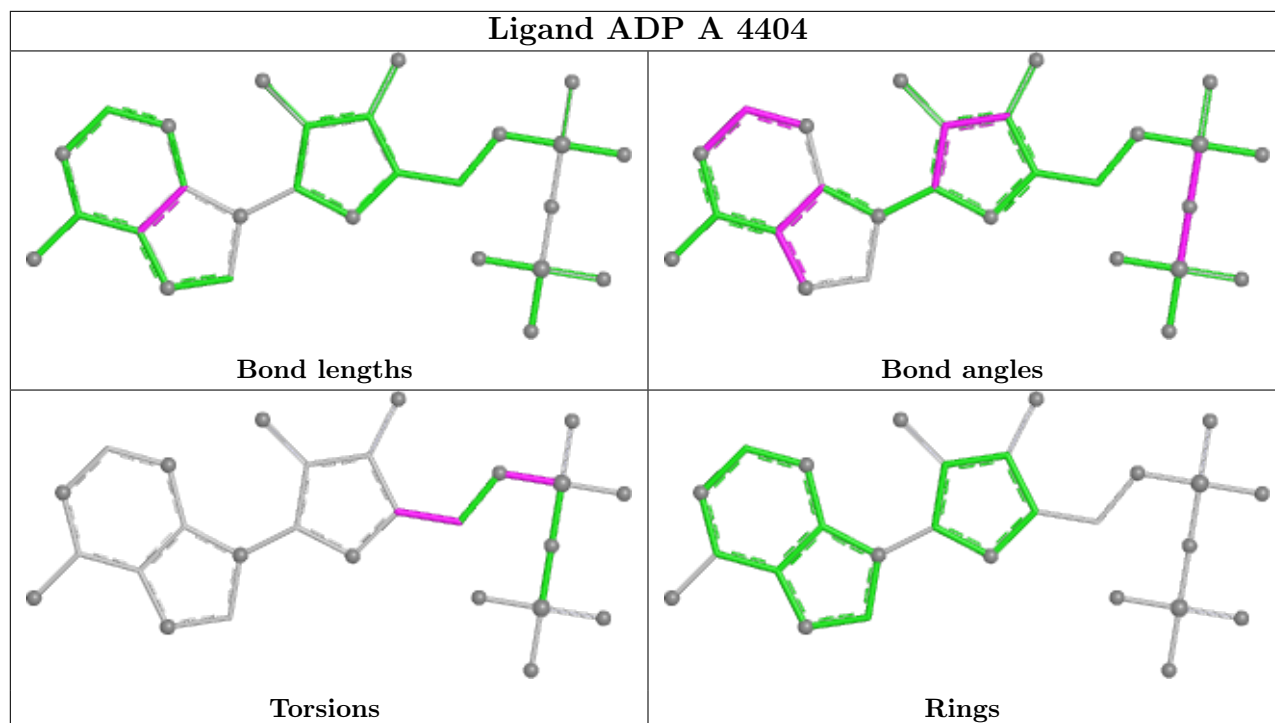
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

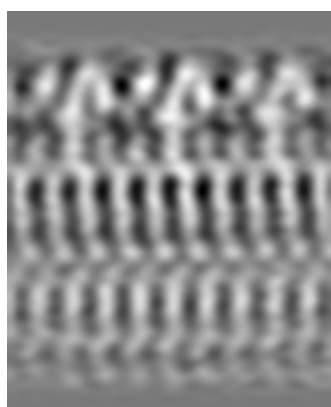
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4303. 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

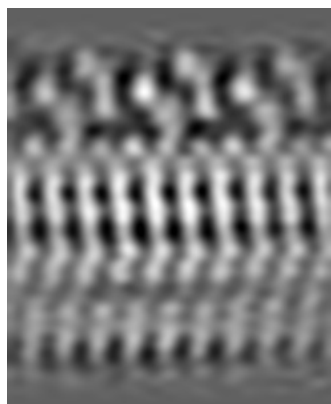


Z

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

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

#### 6.2.1 Primary map



X Index: 16



Y Index: 22

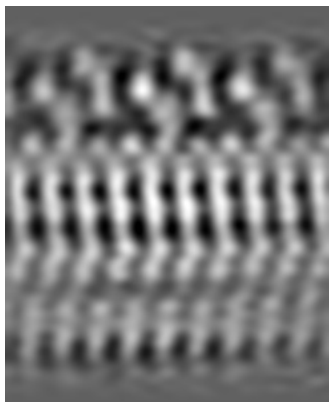


Z Index: 27

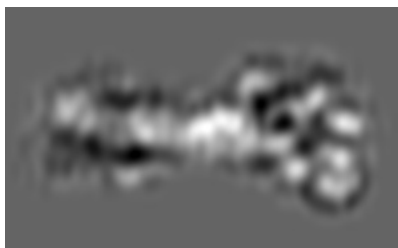
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 16



Y Index: 24

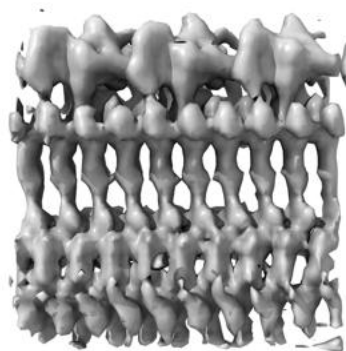


Z Index: 41

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.414. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

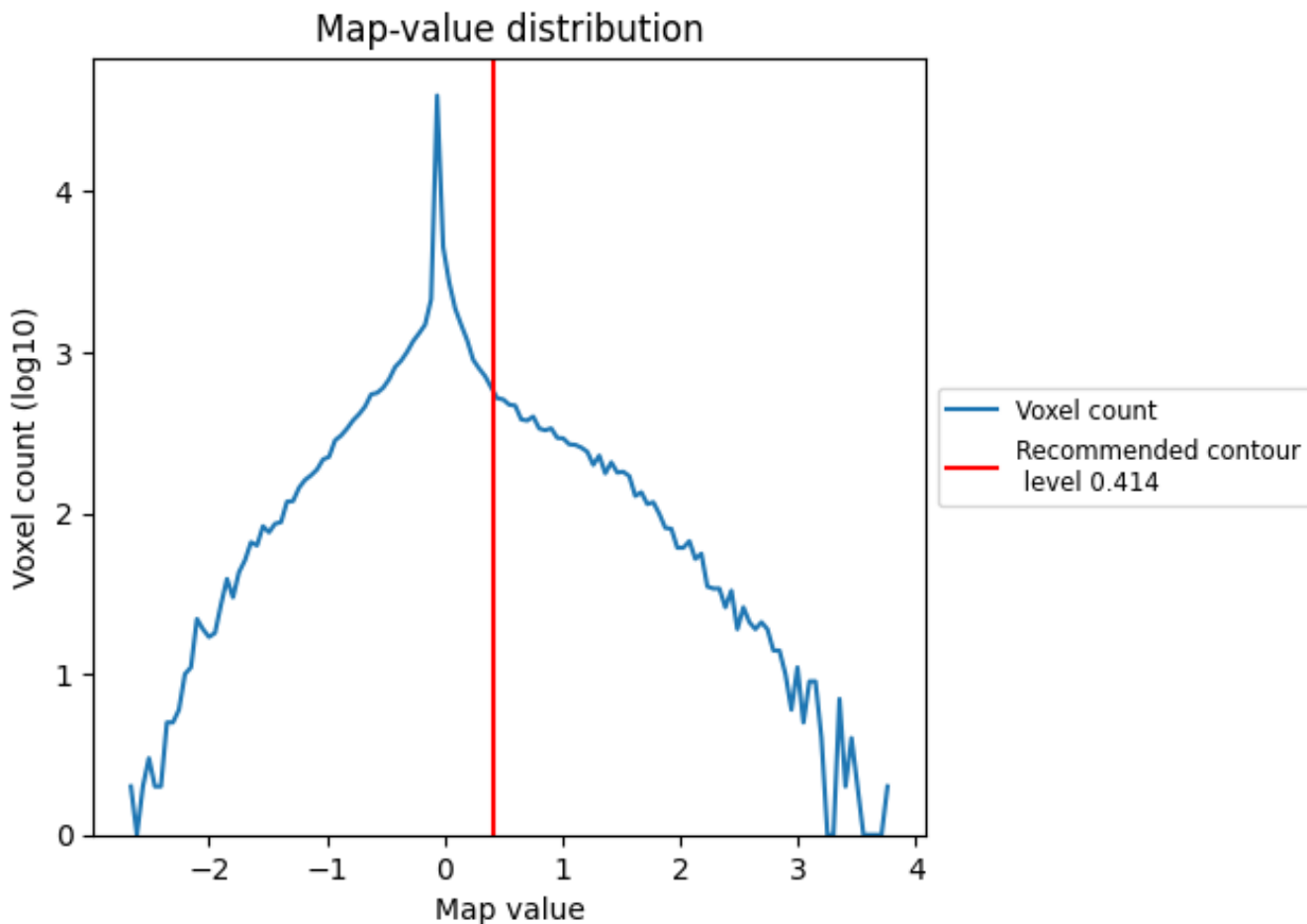
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

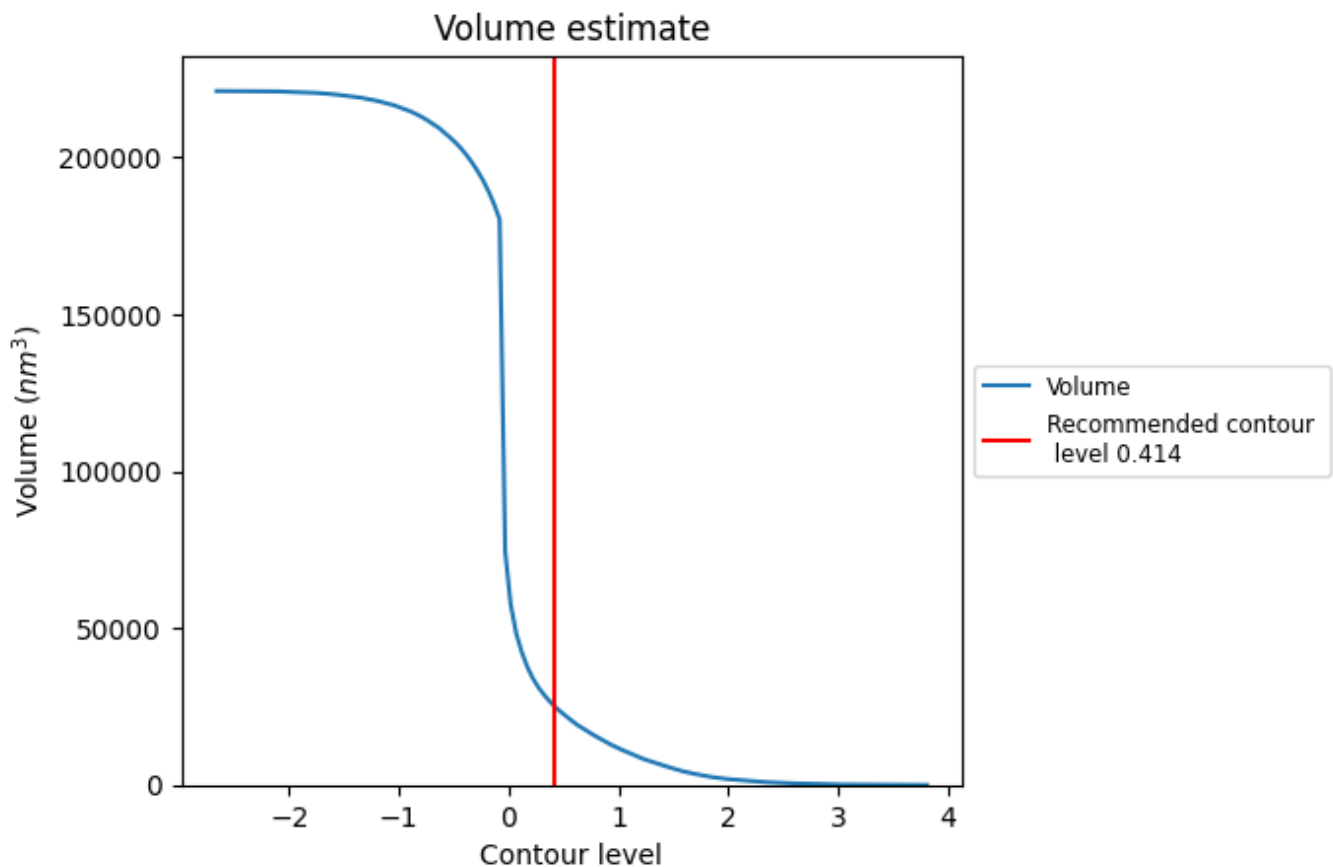
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 25157  $\text{nm}^3$ ; this corresponds to an approximate mass of 22725 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum [\(i\)](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

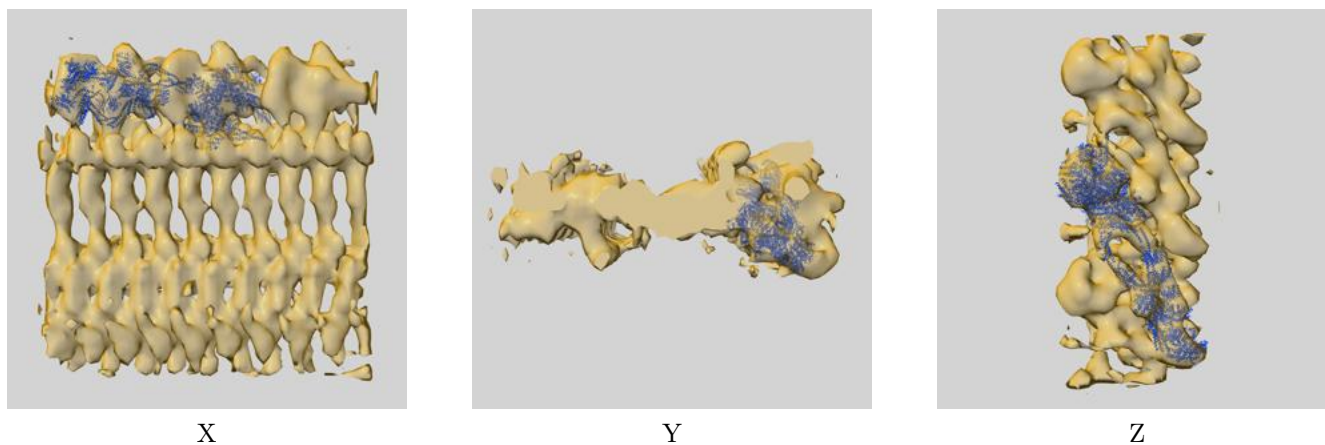
## 8 Fourier-Shell correlation

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

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

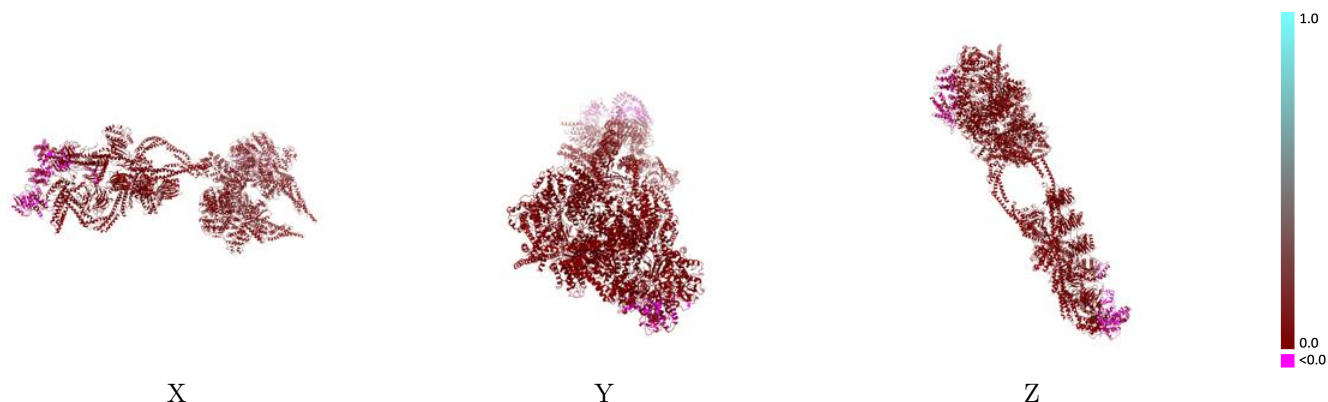
This section contains information regarding the fit between EMDB map EMD-4303 and PDB model 6SC2. Per-residue inclusion information can be found in section 3 on page 10.

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



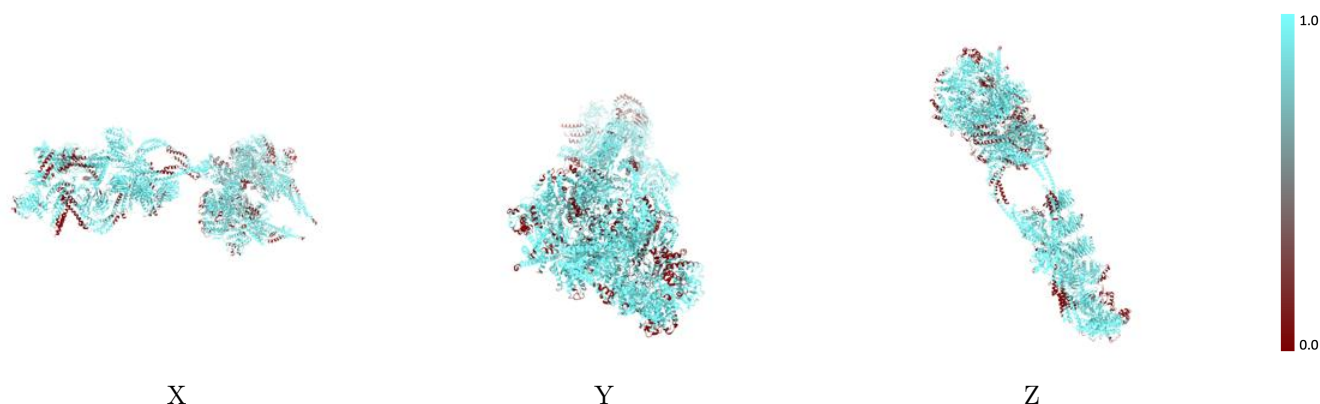
The images above show the 3D surface view of the map at the recommended contour level 0.414 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



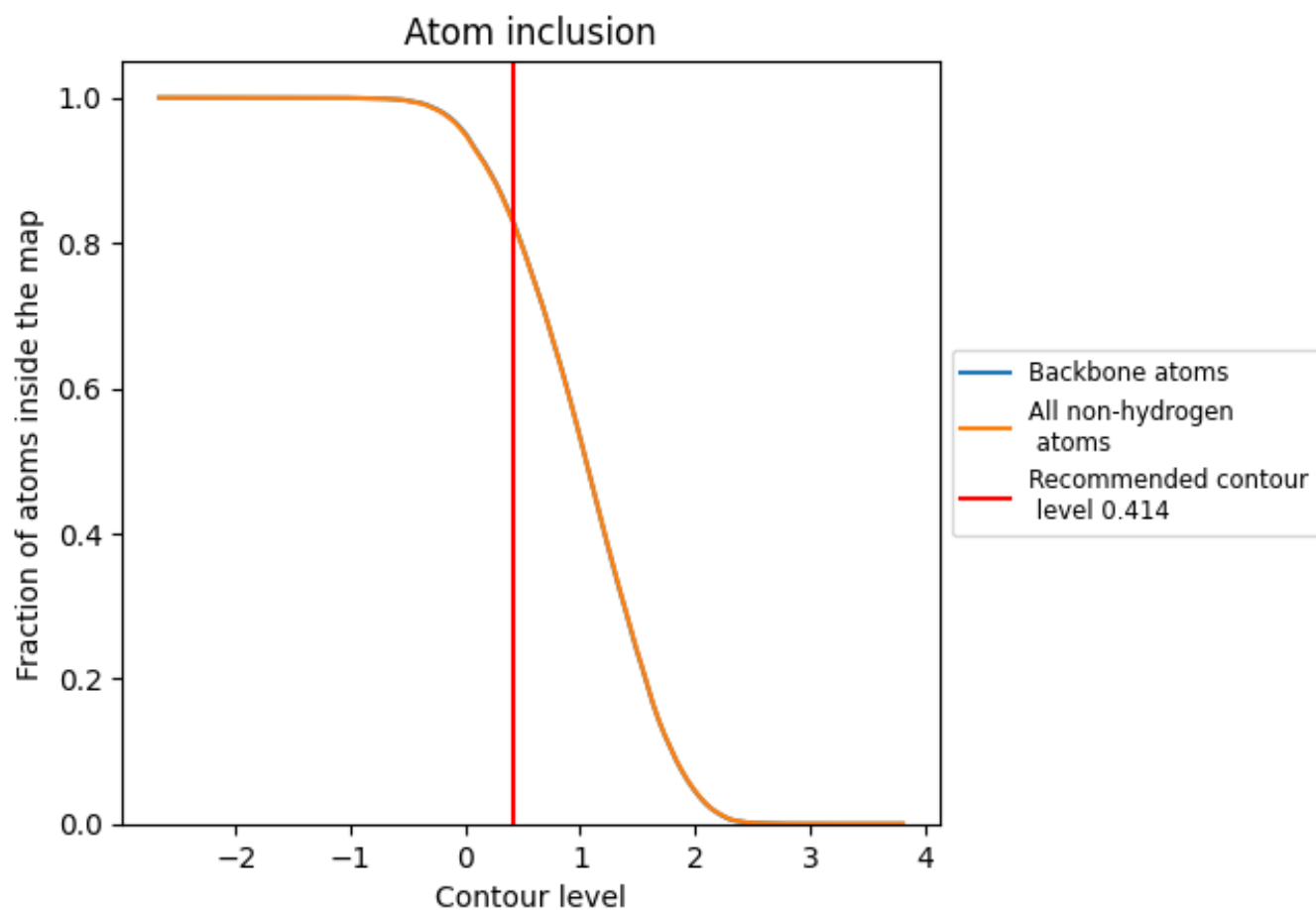
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.414).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.414) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8295	 0.0020
A	 0.8231	 0.0030
B	 0.8000	 0.0010
C	 0.8346	 -0.0030
D	 0.8887	 0.0010
E	 0.9831	 0.0000
F	 0.7409	 0.0000
G	 0.9762	 0.0000
H	 0.8983	 0.0060
I	 0.9765	 0.0000
J	 0.9930	 0.0000
K	 0.9343	 0.0000
L	 1.0000	 0.0000
M	 0.9977	 0.0000
N	 0.9202	 0.0000

