



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 09:10 AM UTC

PDB ID : 7Z8I / pdb_00007z8i
EMDB ID : EMD-14552
Title : The barbed end complex of dynactin bound to BICDR1 and the cytoplasmic dynein tails (A2, B1, B2)
Authors : Chaaban, S.; Carter, A.P.
Deposited on : 2022-03-17
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation 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:

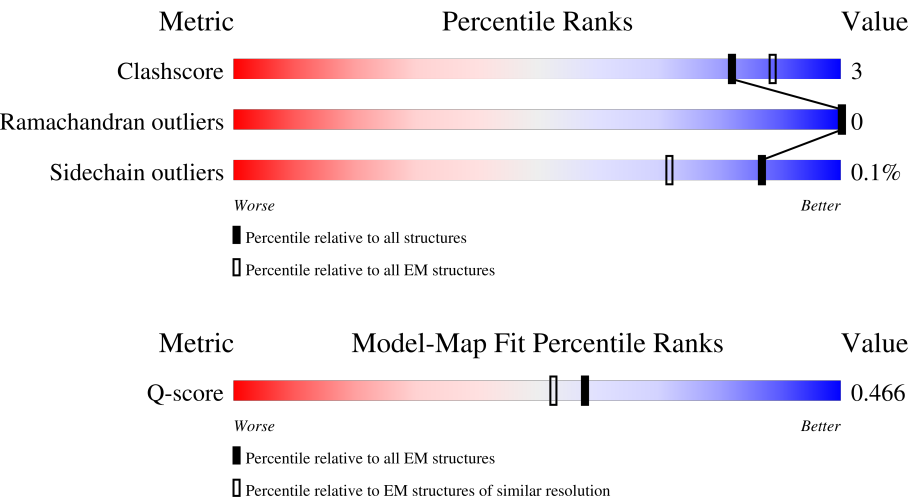
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.30 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.



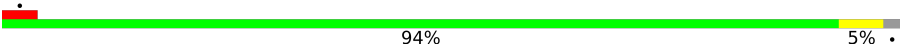
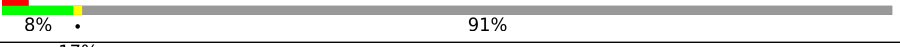
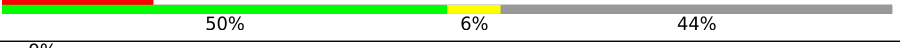
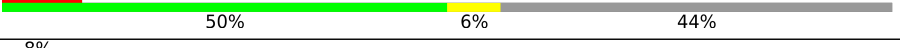
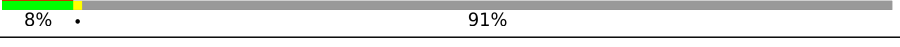
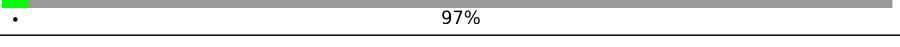
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	376	
1	B	376	
1	C	376	
1	D	376	

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Mol	Chain	Length	Quality of chain
1	E	376	 94% 5%
1	F	376	 10% 71% 26%
2	K	286	 20% 88% 9%
3	L	272	 9% 90% 9%
4	X	577	 13% 16% 84%
4	x	577	 13% 16% 84%
5	f	4646	 8% 14% 85%
5	m	4646	 12% 87%
5	n	4646	 8% 91%
6	h	638	 17% 50% 6% 44%
6	o	638	 9% 50% 6% 44%
7	j	492	 8% 8% 91%
7	r	492	 97%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 43425 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2944	1886	509	539	10		
1	B	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	C	375	Total	C	N	O	S	0	0
			2998	1918	514	556	10		
1	D	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	E	370	Total	C	N	O	S	0	0
			2944	1886	509	539	10		
1	F	279	Total	C	N	O	S	0	0
			2223	1429	385	400	9		

- Molecule 2 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	278	Total	C	N	O	S	0	0
			2264	1428	396	434	6		

- Molecule 3 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	269	Total	C	N	O	S	0	0
			2122	1323	370	418	11		

- Molecule 4 is a protein called BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	93	Total	C	N	O	S	0	0
			797	488	153	154	2		
4	x	93	Total	C	N	O	S	0	0
			797	488	153	154	2		

- Molecule 5 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	720	Total	C	N	O	S	0	0
			5943	3766	1074	1083	20		
5	m	602	Total	C	N	O	S	0	0
			4963	3148	900	900	15		
5	n	409	Total	C	N	O	S	0	0
			3387	2137	623	616	11		

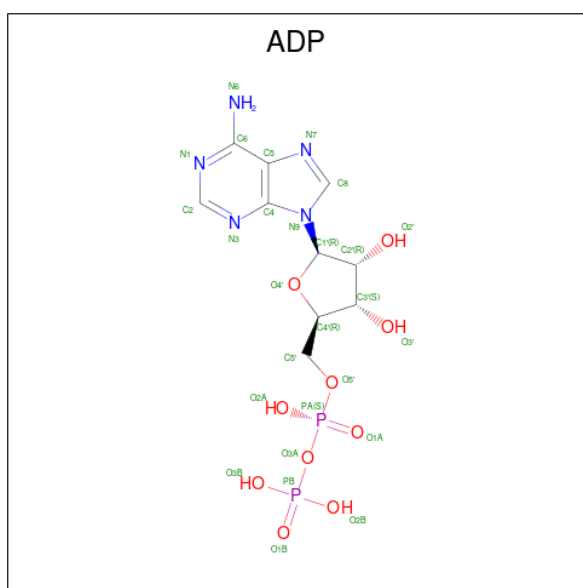
- Molecule 6 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		
6	o	358	Total	C	N	O	S	0	0
			2808	1771	490	532	15		

- Molecule 7 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	44	Total	C	N	O	S	0	0
			291	176	53	61	1		
7	r	14	Total	C	N	O		0	0
			56	28	14	14			

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



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

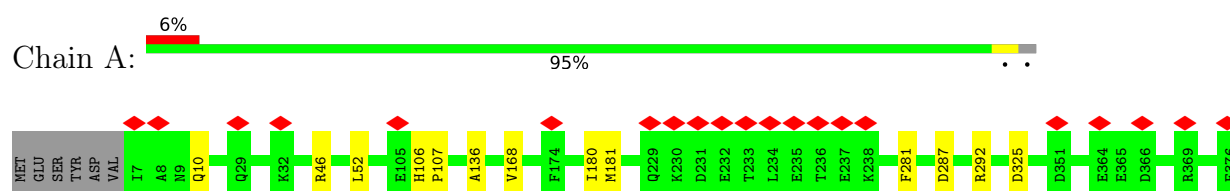
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Mg	0
			1	1	
9	B	1	Total	Mg	0
			1	1	
9	C	1	Total	Mg	0
			1	1	
9	D	1	Total	Mg	0
			1	1	
9	E	1	Total	Mg	0
			1	1	
9	F	1	Total	Mg	0
			1	1	

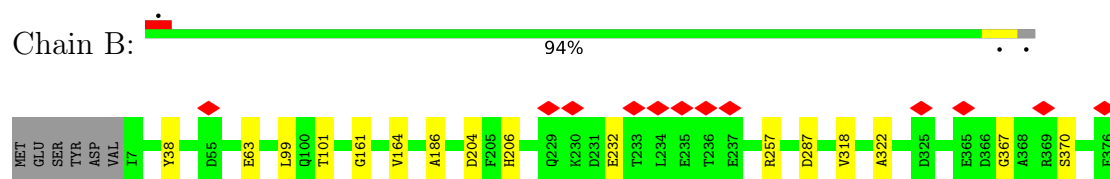
3 Residue-property plots [i](#)

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.

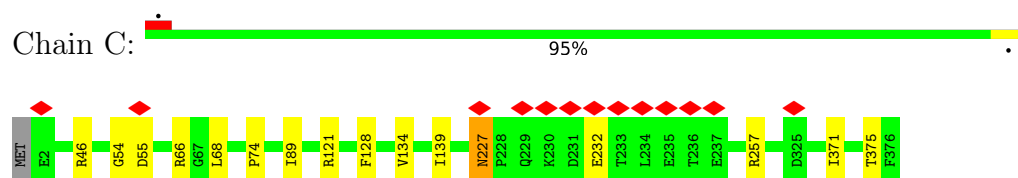
- Molecule 1: ARP1 actin related protein 1 homolog A



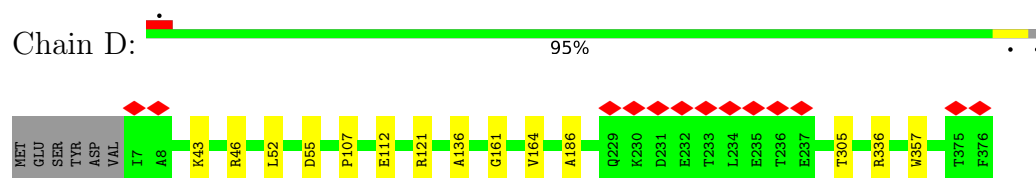
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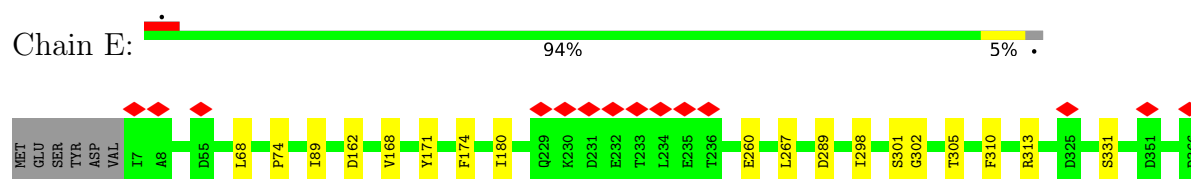
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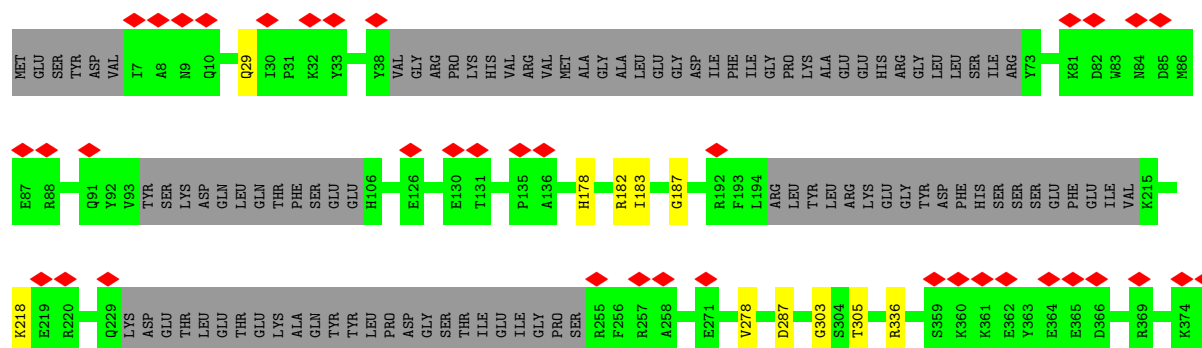


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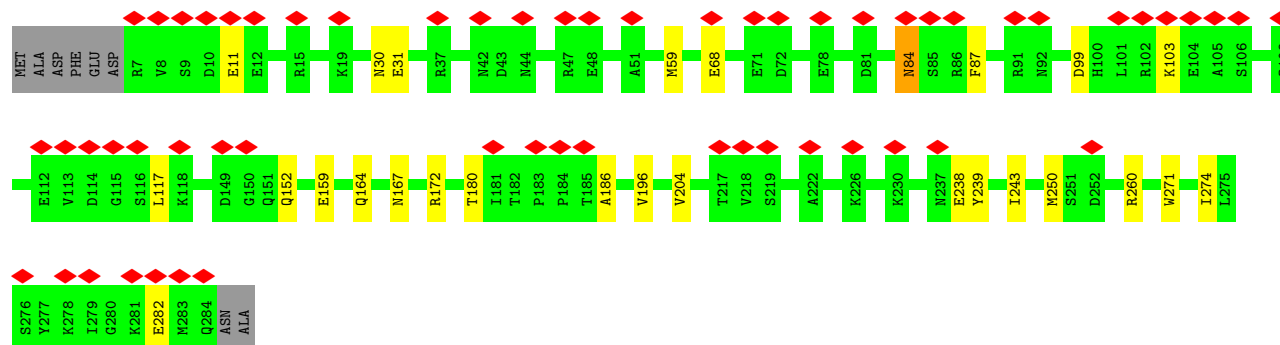
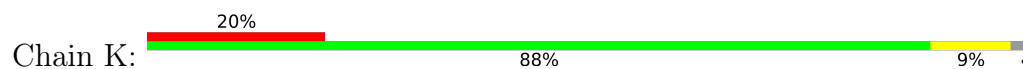




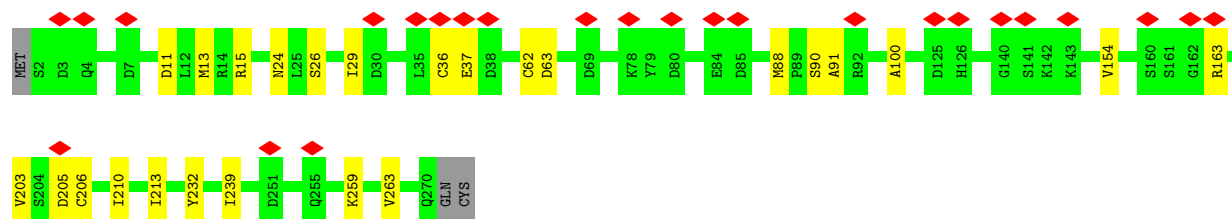
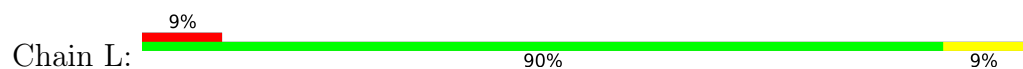
- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 2: Capping protein (Actin filament) muscle Z-line, alpha 1



- Molecule 3: F-actin capping protein beta subunit



- Molecule 4: BICD family-like cargo adapter 1



ALA	ALA	ALA	ALA	PHE	PRO	ARG	GLY	HIS	CYS	ALA	GLY	GLY	LEU	ALA	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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● Molecule 4: BICD family-like cargo adapter 1



THR	ASN	GLN	HIS	ILE	ILE	ARG	LEU	LEU	LEU	GLN	ALA	GLU	ILE	LYS	MET	LYS	THR	SER	ASP	ARG	GLU	GLU	HIS	GLN	ARG	LEU	THR	LEU	GLU	GLU	GLN	GLY	THR	ALA	ALA	ALA	LEU	VAL	PHE	PRO	GLY	GLY	PRO	GLY	GLY	LEU	ALA	GLU									
L184	E185	R186	Q187	Q188	L189	H190	L191	R192	GLU	ALA	ASP	ARG	VAL	GLN	GLU	GLN	ASN	GLN	GLN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	LEU	LEU	LEU	ASP	GLN	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU								
K121	A122	L123	L124	E125	R126	N127	Q128	D129	M130	S131	R132	Q133	Y134	E135	Q136	M137	H138	K139	E140	L141	T142	D143	K144	L145	E146	H147	L148	E149	Q150	E151	K152	H153	E154	R156	R157	R158	F159	E160	N161	R162	E167	G168	R169	V170	S171	E172	L173	E174	T175	D176	V177	K178	Q179	L180	Q181	D182	E183
LEU	ALA	LEU	LEU	ALA	ALA	GLY	GLU	SER	SER	PRO	GLY	HIS	PRO	GLN	ALA	GLU	PRO	SER	GLU	PRO	VAL	GLU	HIS	GLY	PRO	LEU	LEU	PRO	PRO	PRO	THR	GLN	ASP	P100	E101	L102	L103	S104	V105	I106	R107	Q108	K109	E110	K111	D112	L113	V114	L115	A116	A117	R118	L119	G120			

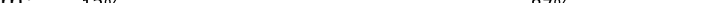






[illegible]

- Molecule 5: Cytoplasmic dynein 1 heavy chain 1

Chain m:  12% 87%

E783	L711	D570	VAL	+	SER	ALA
S784	G712	G573	ALA	D319	VAL	LEU
S785	G713	T574	GLN	R342	GLN	GLU
S786	S714	A575	ASN	R342	LYS	GLN
S787	G715		GLN	D351	ILE	ARG
S788	R716		GLY	D351	ALA	GLY
E789		E580	GLU	R354	GLU	LYS
S790	I717		VAL	R354	LEU	PHE
S791	T719	R583	PRO	V358	LEU	LEU
C792	I720	R587	PRO	D387	MET	ASP
E793		R593	GLN	D387	GLY	PRO
S794	SER		ASP	K394	LEU	SER
S795	THR	R596	MET	K394	HIS	GLN
S796	ARG		LYS	T398	LEU	LEU
E797	VAL	T601	VAL	R399	GLN	THR
S798	GLY	R602	ALA	K400	ASN	VAL
E803	ARG	R602	GLU	L401	LEU	GLU
S799	THR	E604	VAL	M402	GLU	ARG
T800	GLY	V612	LEU	H403	ILE	SER
I801	ASN		PHE	H403	PRO	GLN
S802	VAL		D513	E407	ASP	THR
L803	LEU	E617	A514		ILE	GLY
L804	K734		A515	V412	LEU	ASP
S805	L735	R622	D516	M413	PRO	VAL
S806	K736	F623	A517	E426	ILE	GLY
G807	K824	V625	N518	K429	H210	ASP
L808	S738	Q626	A519		M212	GLN
S809	F739		I520	D436	ILE	LYS
L740	L741	Q629	E521		A217	GLY
E811	P741		A526		K218	LEU
S812	E742	D640	E532	R441		GLU
Q813	I743	P643	V533	R442	Y221	LYS
A814			D534	E443	E222	ALA
L815	S747	T648	G535	E444	R223	PHE
S816	K754	V665	L536	M445	G224	TYR
A817	W755		D537	L446	E225	ASN
L818	L756		V538	K447	K226	GLU
S819		E574	S539	M448	P227	ILE
G819			K540			GLY
I820	R759	D685	E541	R451	G233	ILE
L821	F761	G686	E544	I452	D234	ALA
L822	L762	D687	A545	M453	K235	TYR
S823	A763				V236	GLY
W824	I764	R690	M550	R462	ASP	VAL
E825		M691	K551	L463	LEU	LYS
S826	A768		R552	V479	Q257	ASP
E827	H769	F699	Y553			ASN
K828	Q770	D700	D554	R482	D263	SER
L829	A771	D701	E555	V483	R264	LEU
D830	W772	R704	R556	L484	D265	PHE
	Q773			R485	P266	LYS
			R559	PRO	A267	ALA
		Q707	T562	GLN		THR
S833	F777	Q708		VAL	L299	ALA
Q834	A778	R709		THR		
S835	I779	S780		ALA		
L836	S780					
A837	L781					
S838	L782					









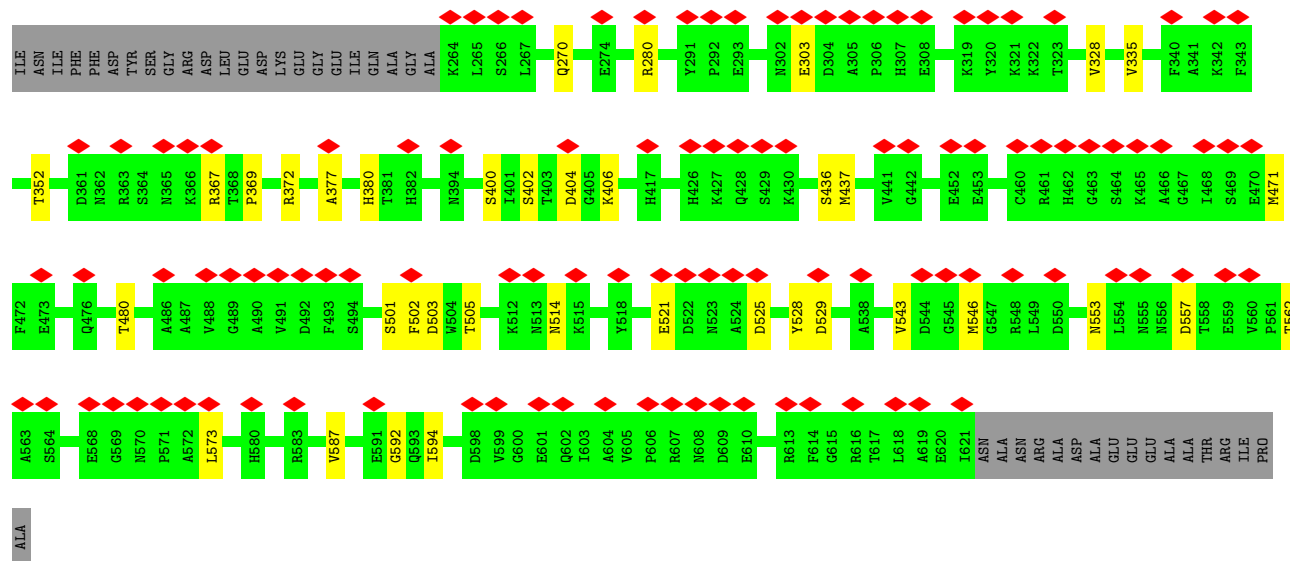






[illegible]

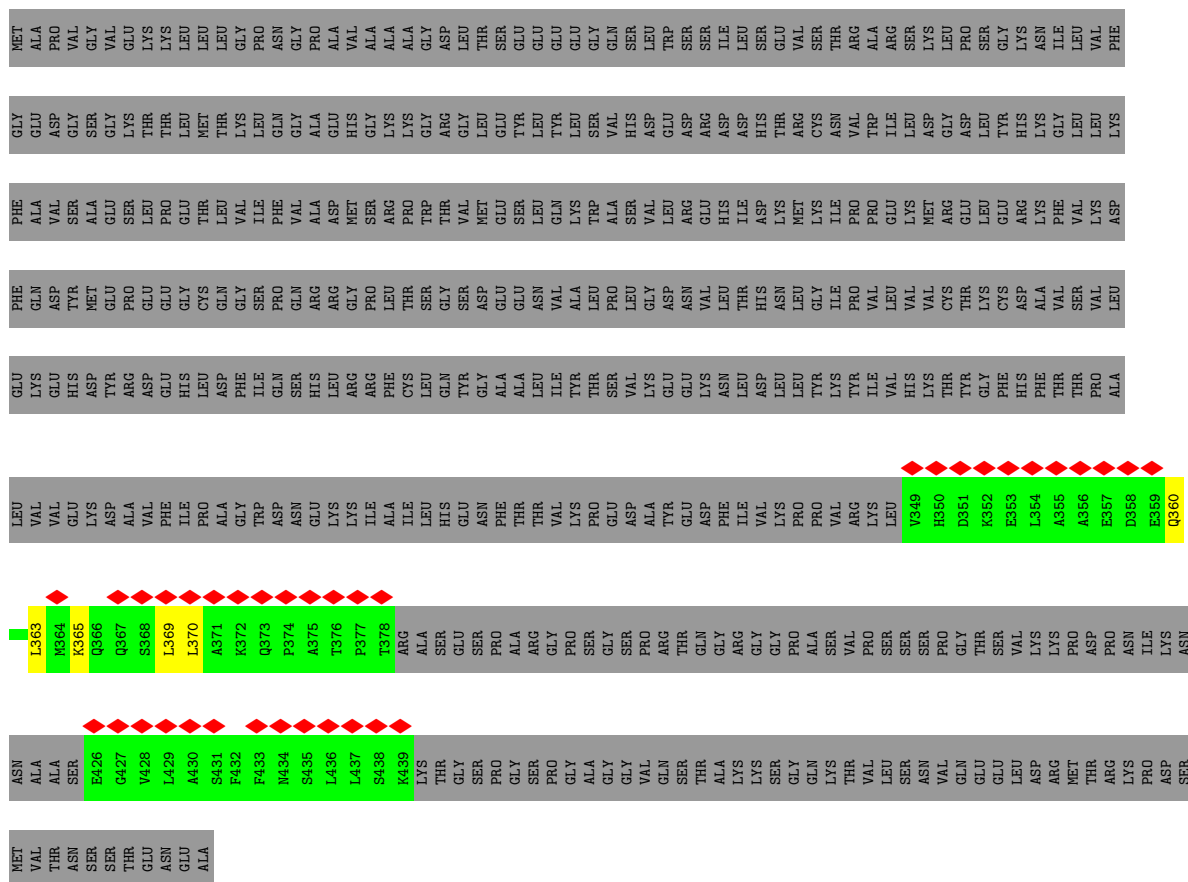
- Molecule 6: Cytoplasmic dynein 1 intermediate chain 2

[illegible]

- Molecule 6: Cytoplasmic dynein 1 intermediate chain 2

[illegible]

- Molecule 7: Cytoplasmic dynein 1 light intermediate chain 2



- Molecule 7: Cytoplasmic dynein 1 light intermediate chain 2



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179660	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.160	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0244	Depositor
Map size (Å)	955.776, 955.776, 955.776	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2445, 1.2445, 1.2445	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: 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	0.18	0/3013	0.38	0/4070
1	B	0.21	0/3025	0.40	0/4085
1	C	0.19	0/3068	0.37	0/4144
1	D	0.21	0/3025	0.41	0/4085
1	E	0.17	0/3013	0.36	0/4070
1	F	0.17	0/2272	0.39	0/3065
2	K	0.23	0/2316	0.50	0/3135
3	L	0.17	0/2156	0.38	0/2906
4	X	0.20	0/805	0.41	0/1072
4	x	0.23	0/805	0.49	0/1072
5	f	0.17	0/6045	0.38	0/8149
5	m	0.17	0/5048	0.37	0/6801
5	n	0.17	0/3442	0.38	0/4632
6	h	0.19	0/2887	0.40	0/3938
6	o	0.17	0/2887	0.36	0/3938
7	j	0.54	0/293	0.75	0/388
7	r	1.19	0/55	1.59	0/67
All	All	0.19	0/44155	0.40	0/59617

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2944	0	2938	7	0
1	B	2956	0	2950	8	0
1	C	2998	0	2983	13	0
1	D	2956	0	2950	8	0
1	E	2944	0	2938	12	0
1	F	2223	0	2233	8	0
2	K	2264	0	2186	18	0
3	L	2122	0	2113	14	0
4	X	797	0	797	4	0
4	x	797	0	797	4	0
5	f	5943	0	6059	39	0
5	m	4963	0	5069	30	0
5	n	3387	0	3444	21	0
6	h	2808	0	2673	21	0
6	o	2808	0	2673	24	0
7	j	291	0	251	5	0
7	r	56	0	15	0	0
8	A	27	0	12	0	0
8	B	27	0	12	0	0
8	C	27	0	12	0	0
8	D	27	0	12	0	0
8	E	27	0	12	1	0
8	F	27	0	12	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
All	All	43425	0	43141	218	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 3.

All (218) 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)
2:K:84:ASN:O	2:K:84:ASN:ND2	2.18	0.77
2:K:84:ASN:HD22	2:K:84:ASN:C	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:608:LEU:HD21	5:f:668:VAL:HG21	1.71	0.73
5:f:656:ARG:NH2	6:h:503:ASP:O	2.24	0.71
1:B:232:GLU:OE1	1:B:257:ARG:NH2	2.24	0.71
1:B:287:ASP:OD2	2:K:260:ARG:NH2	2.24	0.70
3:L:163:ARG:O	3:L:203:VAL:N	2.25	0.70
5:n:568:LEU:HD11	5:n:597:ILE:HG23	1.73	0.69
6:h:573:LEU:HD13	6:h:587:VAL:HG21	1.74	0.69
1:A:46:ARG:NH2	1:A:52:LEU:O	2.25	0.69
1:D:46:ARG:NH1	1:D:52:LEU:O	2.27	0.67
5:m:442:ARG:NH1	5:m:445:ASN:O	2.28	0.67
6:h:270:GLN:NE2	6:h:594:ILE:O	2.28	0.67
5:f:1012:LEU:O	5:f:1017:LYS:NZ	2.28	0.66
1:C:66:ARG:NH1	1:E:289:ASP:OD2	2.30	0.65
5:m:716:ARG:NH1	5:m:820:ILE:O	2.31	0.63
1:C:121:ARG:HD3	1:C:375:THR:HG21	1.81	0.62
5:f:476:LEU:HD23	5:f:557:ILE:HD12	1.82	0.61
5:n:479:VAL:HG13	5:n:590:ALA:HB2	1.83	0.61
1:C:227:ASN:O	1:C:227:ASN:ND2	2.33	0.61
6:h:380:HIS:HE2	6:h:400:SER:HG	1.49	0.61
5:n:591:LEU:HB3	5:n:597:ILE:HG21	1.82	0.61
6:h:328:VAL:O	6:h:367:ARG:NE	2.34	0.60
1:F:305:THR:O	1:F:336:ARG:NH1	2.33	0.60
6:o:549:LEU:HD12	6:o:587:VAL:HG11	1.83	0.60
5:f:581:MET:SD	5:f:611:ARG:NH2	2.74	0.60
5:f:576:LYS:O	5:f:611:ARG:NH1	2.34	0.60
4:X:137:MET:HE1	4:x:137:MET:HE1	1.84	0.60
5:m:629:GLN:N	5:m:629:GLN:OE1	2.36	0.59
2:K:159:GLU:OE2	2:K:172:ARG:NE	2.34	0.58
5:f:541:GLU:N	5:f:541:GLU:OE2	2.36	0.58
5:m:479:VAL:O	5:m:483:VAL:HG22	2.03	0.58
5:f:1013:THR:OG1	5:f:1016:GLU:OE1	2.20	0.58
5:n:374:ILE:HG23	5:n:434:LEU:HD22	1.86	0.57
2:K:11:GLU:N	2:K:11:GLU:OE1	2.37	0.57
5:m:394:LYS:O	5:m:398:THR:HG23	2.05	0.56
1:C:55:ASP:OD2	1:C:55:ASP:N	2.36	0.56
1:C:46:ARG:NH2	1:C:54:GLY:O	2.38	0.56
5:m:354:ARG:O	5:m:358:VAL:HG23	2.05	0.56
5:n:378:LEU:HD22	5:n:452:ILE:HD11	1.87	0.56
1:D:43:LYS:NZ	1:F:287:ASP:OD1	2.36	0.56
3:L:36:CYS:SG	3:L:37:GLU:N	2.78	0.56
1:B:204:ASP:OD1	1:B:206:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:870:ASP:OD1	5:f:873:THR:OG1	2.20	0.55
6:o:315:VAL:O	6:o:326:GLU:N	2.39	0.55
1:D:161:GLY:O	1:D:186:ALA:HB1	2.07	0.55
5:f:559:ARG:O	5:f:562:THR:OG1	2.23	0.55
1:F:187:GLY:O	1:F:218:LYS:NZ	2.39	0.54
1:B:161:GLY:O	1:B:186:ALA:HB1	2.08	0.54
5:m:526:ALA:HB2	5:m:556:ARG:HD2	1.89	0.54
5:f:592:PHE:O	5:f:598:ARG:NH2	2.40	0.54
5:m:483:VAL:HG23	5:m:484:LEU:CD2	2.38	0.54
2:K:239:TYR:CZ	2:K:243:ILE:HD11	2.43	0.53
5:n:315:SER:O	5:n:319:ASP:N	2.41	0.53
5:f:418:GLU:OE2	5:f:421:GLN:NE2	2.42	0.53
5:m:462:ARG:NH1	5:m:537:ASP:O	2.40	0.53
6:o:547:GLY:HA2	6:o:573:LEU:HD23	1.89	0.53
5:m:612:VAL:HG11	5:m:665:VAL:HG23	1.91	0.53
1:C:371:ILE:O	1:C:375:THR:OG1	2.25	0.53
6:o:424:LEU:HD12	6:o:468:ILE:HG13	1.90	0.53
6:h:525:ASP:OD2	6:h:546:MET:N	2.40	0.53
5:f:676:HIS:O	5:f:680:GLN:N	2.42	0.53
5:m:518:ASN:ND2	5:m:521:GLU:OE1	2.40	0.53
6:o:443:ASP:OD2	6:o:446:ASN:ND2	2.43	0.52
6:o:495:HIS:ND1	6:o:510:THR:HG23	2.24	0.52
3:L:11:ASP:OD1	3:L:15:ARG:NH1	2.42	0.52
4:X:141:LEU:HD22	4:x:141:LEU:HD13	1.90	0.52
3:L:62:CYS:SG	3:L:63:ASP:N	2.83	0.52
5:m:212:MET:SD	5:m:235:LYS:NZ	2.70	0.51
6:o:485:HIS:NE2	6:o:537:PRO:O	2.43	0.51
5:f:264:ARG:O	5:f:376:ARG:NH2	2.44	0.51
6:o:284:CYS:SG	6:o:285:LEU:N	2.83	0.51
1:E:68:LEU:HD23	1:E:68:LEU:O	2.10	0.51
2:K:117:LEU:HD21	2:K:152:GLN:HG2	1.92	0.51
3:L:26:SER:HA	3:L:29:ILE:HD12	1.91	0.51
6:o:501:SER:OG	6:o:502:PHE:N	2.44	0.51
5:f:658:LEU:HD21	5:f:690:ARG:HB2	1.92	0.50
1:E:301:SER:OG	1:E:302:GLY:N	2.45	0.50
3:L:154:VAL:HG11	3:L:213:ILE:HD13	1.93	0.50
6:h:369:PRO:O	6:h:372:ARG:NH2	2.44	0.50
1:F:182:ARG:C	1:F:183:ILE:HD13	2.37	0.50
6:h:303:GLU:OE2	6:h:303:GLU:N	2.43	0.50
6:o:510:THR:HG22	6:o:512:LYS:H	1.77	0.50
1:D:305:THR:O	1:D:336:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:335:VAL:HG22	6:h:352:THR:HG22	1.94	0.49
3:L:205:ASP:OD1	3:L:206:CYS:N	2.46	0.49
1:C:121:ARG:HG2	1:C:139:ILE:HD13	1.95	0.49
5:f:447:LYS:NZ	5:f:449:VAL:O	2.42	0.49
6:o:352:THR:OG1	6:o:356:GLN:O	2.29	0.49
6:h:557:ASP:N	6:h:557:ASP:OD1	2.46	0.49
4:X:137:MET:HE1	4:x:137:MET:CE	2.42	0.49
5:n:662:MET:SD	5:n:662:MET:N	2.85	0.49
5:f:315:SER:O	5:f:319:ASP:N	2.45	0.48
5:n:479:VAL:HG13	5:n:590:ALA:CB	2.43	0.48
1:C:232:GLU:OE2	1:C:257:ARG:NH1	2.47	0.48
1:D:107:PRO:HB3	1:D:136:ALA:HB3	1.96	0.48
3:L:100:ALA:HB2	3:L:210:ILE:HD12	1.96	0.48
6:o:576:VAL:HG23	6:o:587:VAL:HG12	1.95	0.48
5:f:900:VAL:HG11	5:f:1001:SER:HA	1.95	0.48
6:h:280:ARG:O	6:h:592:GLY:N	2.47	0.48
6:h:503:ASP:O	6:h:505:THR:HG23	2.13	0.48
1:B:38:TYR:OH	1:B:63:GLU:OE1	2.32	0.47
5:f:343:ASP:OD2	5:f:356:ALA:HB2	2.13	0.47
5:f:735:LEU:HB2	7:j:363:LEU:HD21	1.95	0.47
5:f:909:ARG:O	5:f:913:VAL:HG23	2.14	0.47
5:f:733:LEU:N	7:j:360:GLN:OE1	2.45	0.47
5:f:870:ASP:OD1	5:f:870:ASP:N	2.44	0.47
5:f:882:GLN:OE1	5:f:1000:GLN:N	2.43	0.47
6:h:553:ASN:N	6:h:562:THR:OG1	2.44	0.47
5:n:662:MET:HA	5:n:662:MET:HE3	1.96	0.47
1:C:68:LEU:HD13	1:E:171:TYR:HD2	1.80	0.47
7:j:365:LYS:O	7:j:369:LEU:HD23	2.15	0.47
5:m:526:ALA:HB1	5:m:553:TYR:HD1	1.80	0.47
1:C:139:ILE:O	1:C:375:THR:HG23	2.15	0.47
5:m:483:VAL:HG23	5:m:484:LEU:HD22	1.96	0.47
1:B:367:GLY:O	1:B:370:SER:OG	2.32	0.47
5:f:212:MET:O	5:f:216:VAL:HG23	2.14	0.47
6:h:471:MET:O	6:h:514:ASN:ND2	2.45	0.47
1:A:181:MET:HE2	1:A:281:PHE:HB2	1.97	0.46
1:F:29:GLN:OE1	1:F:29:GLN:N	2.49	0.46
6:h:505:THR:HG22	6:h:521:GLU:HG2	1.97	0.46
5:m:413:MET:HE1	5:m:463:LEU:HB3	1.96	0.46
6:o:557:ASP:N	6:o:557:ASP:OD1	2.49	0.46
2:K:204:VAL:HG21	3:L:232:TYR:HB3	1.97	0.46
3:L:90:SER:OG	3:L:91:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:609:ILE:HD11	5:f:669:LEU:HD11	1.97	0.46
5:f:697:GLU:OE1	5:f:697:GLU:N	2.45	0.46
5:n:541:GLU:OE1	5:n:541:GLU:N	2.40	0.46
6:h:529:ASP:OD1	6:h:543:VAL:HG22	2.15	0.46
1:D:136:ALA:HB1	1:D:357:TRP:CG	2.50	0.46
2:K:30:ASN:ND2	2:K:31:GLU:OE2	2.49	0.46
5:f:608:LEU:HD21	5:f:668:VAL:CG2	2.43	0.46
6:o:500:SER:OG	6:o:530:VAL:HG12	2.17	0.45
1:A:292:ARG:NH2	1:A:325:ASP:O	2.49	0.45
5:m:426:GLU:OE1	5:m:429:LYS:NZ	2.41	0.45
1:E:298:ILE:O	1:E:331:SER:N	2.46	0.45
2:K:196:VAL:HG13	3:L:239:ILE:HG21	1.97	0.45
5:n:378:LEU:CD2	5:n:452:ILE:HD11	2.46	0.45
5:n:483:VAL:HG12	5:n:484:LEU:HD22	1.98	0.45
6:h:436:SER:OG	6:h:437:MET:N	2.50	0.45
5:n:430:LEU:HD23	5:n:430:LEU:O	2.16	0.45
5:f:897:PRO:HA	5:f:900:VAL:HG12	1.98	0.45
5:m:233:GLY:O	5:m:236:VAL:HG22	2.17	0.45
1:D:55:ASP:OD1	1:D:55:ASP:N	2.50	0.45
5:f:876:GLU:OE1	5:f:880:ARG:NE	2.50	0.45
1:A:107:PRO:HB3	1:A:136:ALA:HB3	1.99	0.44
2:K:99:ASP:O	2:K:103:LYS:N	2.50	0.44
5:f:245:LEU:HD22	5:f:300:THR:HG23	2.00	0.44
2:K:59:MET:HE1	2:K:87:PHE:CZ	2.52	0.44
2:K:68:GLU:OE1	2:K:68:GLU:N	2.47	0.44
5:m:442:ARG:NH2	5:m:448:MET:HE2	2.32	0.44
5:f:469:PHE:CZ	5:f:530:VAL:HG11	2.53	0.44
1:B:318:VAL:O	1:B:322:ALA:N	2.48	0.44
2:K:164:GLN:OE1	2:K:167:ASN:ND2	2.51	0.44
1:E:267:LEU:O	1:F:178:HIS:NE2	2.51	0.43
2:K:180:THR:O	2:K:186:ALA:HB1	2.17	0.43
3:L:13:MET:HE1	3:L:24:ASN:HB3	2.00	0.43
5:m:413:MET:HE1	5:m:463:LEU:HD22	2.00	0.43
1:B:99:LEU:O	1:B:101:THR:HG23	2.18	0.43
4:X:141:LEU:HD21	4:x:141:LEU:HB3	2.01	0.43
6:h:402:SER:OG	6:h:404:ASP:OD1	2.21	0.43
5:m:601:ILE:HG23	5:m:604:TYR:HD2	1.83	0.43
3:L:259:LYS:O	3:L:263:VAL:HG12	2.18	0.43
5:f:820:ILE:CG2	7:j:370:LEU:HD21	2.49	0.43
5:m:401:LEU:HD21	5:m:412:VAL:HG11	2.00	0.43
6:o:478:PRO:C	6:o:501:SER:HG	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:o:505:THR:HG22	6:o:521:GLU:HG2	2.01	0.43
1:A:10:GLN:O	1:A:106:HIS:ND1	2.52	0.43
2:K:271:TRP:CE3	2:K:274:ILE:HD11	2.54	0.43
3:L:88:MET:HE2	3:L:88:MET:N	2.34	0.43
5:f:820:ILE:HG22	7:j:370:LEU:HD21	2.01	0.43
5:n:233:GLY:O	5:n:236:VAL:HG22	2.18	0.43
6:o:599:VAL:HG23	6:o:604:ALA:HB2	2.00	0.43
1:C:74:PRO:HG3	1:C:89:ILE:HD12	2.00	0.42
6:o:269:ARG:NH2	6:o:320:TYR:O	2.50	0.42
5:m:254:ARG:NH2	5:m:257:GLN:OE1	2.52	0.42
6:o:265:LEU:HD23	6:o:599:VAL:HG12	2.01	0.42
6:o:529:ASP:OD1	6:o:530:VAL:N	2.52	0.42
5:n:605:GLN:HG2	5:n:609:ILE:HD12	2.01	0.42
1:E:74:PRO:HG3	1:E:89:ILE:HD12	2.01	0.42
1:E:305:THR:HG22	1:E:310:PHE:CE2	2.54	0.42
5:n:476:LEU:HD13	5:n:594:ARG:NH1	2.34	0.42
5:m:707:GLN:HG2	5:m:764:ILE:HD11	2.01	0.42
6:o:599:VAL:CG2	6:o:604:ALA:HB2	2.49	0.42
5:f:413:MET:SD	5:f:413:MET:N	2.92	0.42
6:h:480:THR:OG1	6:h:528:TYR:O	2.36	0.42
5:m:583:ARG:NH1	6:o:518:TYR:OH	2.53	0.42
5:m:622:LYS:HE3	5:m:622:LYS:HB2	1.64	0.42
5:n:470:ARG:NH1	5:n:527:TYR:OH	2.53	0.42
1:A:287:ASP:OD1	1:A:287:ASP:N	2.52	0.41
1:E:168:VAL:HG13	1:E:180:ILE:CD1	2.51	0.41
1:E:260:GLU:OE1	1:E:313:ARG:NH2	2.53	0.41
5:f:529:ASN:O	5:f:552:ARG:NH2	2.53	0.41
6:h:377:ALA:O	6:h:406:LYS:NZ	2.41	0.41
5:m:580:GLU:OE1	5:m:580:GLU:N	2.50	0.41
5:n:378:LEU:HB3	5:n:452:ILE:HD11	2.02	0.41
1:C:128:PHE:O	1:C:134:VAL:HG22	2.20	0.41
5:m:559:ARG:O	5:m:562:THR:OG1	2.32	0.41
5:n:336:MET:N	5:n:336:MET:SD	2.94	0.41
1:A:168:VAL:HG13	1:A:180:ILE:CD1	2.50	0.41
6:h:501:SER:OG	6:h:502:PHE:N	2.53	0.41
1:F:183:ILE:HG12	1:F:278:VAL:HG21	2.02	0.41
5:m:227:PRO:HB2	5:m:299:LEU:HD22	2.03	0.41
1:E:162:ASP:OD1	8:E:800:ADP:O3'	2.30	0.41
2:K:250:MET:HE2	2:K:250:MET:HA	2.02	0.41
2:K:282:GLU:OE1	2:K:282:GLU:N	2.53	0.41
6:o:280:ARG:O	6:o:592:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:f:482:ARG:NH2	5:f:587:ARG:O	2.51	0.41
5:f:805:VAL:HG13	5:f:850:LEU:CD2	2.51	0.41
5:m:648:ILE:HG21	5:m:756:LEU:HD13	2.03	0.40
5:n:550:MET:O	5:n:550:MET:HE3	2.21	0.40
1:F:303:GLY:N	8:F:800:ADP:O2A	2.51	0.40
6:o:602:GLN:OE1	6:o:602:GLN:N	2.49	0.40
1:C:68:LEU:HD11	1:E:174:PHE:HB2	2.03	0.40
1:D:112:GLU:OE2	1:D:121:ARG:NH1	2.55	0.40
5:f:571:GLN:OE1	5:f:587:ARG:NH1	2.54	0.40
5:n:425:ASP:OD1	5:n:426:GLU:N	2.55	0.40
5:m:550:MET:HE2	5:m:550:MET:N	2.37	0.40

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	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	B	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
1	C	373/376 (99%)	362 (97%)	11 (3%)	0	100	100
1	D	368/376 (98%)	358 (97%)	10 (3%)	0	100	100
1	E	368/376 (98%)	355 (96%)	13 (4%)	0	100	100
1	F	269/376 (72%)	263 (98%)	6 (2%)	0	100	100
2	K	276/286 (96%)	264 (96%)	12 (4%)	0	100	100
3	L	267/272 (98%)	260 (97%)	7 (3%)	0	100	100
4	X	91/577 (16%)	91 (100%)	0	0	100	100
4	x	91/577 (16%)	91 (100%)	0	0	100	100
5	f	714/4646 (15%)	700 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	m	596/4646 (13%)	591 (99%)	5 (1%)	0	100	100
5	n	403/4646 (9%)	394 (98%)	9 (2%)	0	100	100
6	h	356/638 (56%)	347 (98%)	9 (2%)	0	100	100
6	o	356/638 (56%)	347 (98%)	9 (2%)	0	100	100
7	j	40/492 (8%)	39 (98%)	1 (2%)	0	100	100
7	r	12/492 (2%)	12 (100%)	0	0	100	100
All	All	5316/20166 (26%)	5192 (98%)	124 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	315/324 (97%)	315 (100%)	0	100	100
1	B	318/324 (98%)	317 (100%)	1 (0%)	86	86
1	C	323/324 (100%)	322 (100%)	1 (0%)	86	86
1	D	318/324 (98%)	317 (100%)	1 (0%)	86	86
1	E	315/324 (97%)	315 (100%)	0	100	100
1	F	239/324 (74%)	239 (100%)	0	100	100
2	K	247/254 (97%)	245 (99%)	2 (1%)	73	79
3	L	238/241 (99%)	238 (100%)	0	100	100
4	X	87/503 (17%)	87 (100%)	0	100	100
4	x	87/503 (17%)	87 (100%)	0	100	100
5	f	651/4125 (16%)	651 (100%)	0	100	100
5	m	539/4125 (13%)	539 (100%)	0	100	100
5	n	365/4125 (9%)	365 (100%)	0	100	100
6	h	309/557 (56%)	309 (100%)	0	100	100
6	o	309/557 (56%)	309 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	j	26/422 (6%)	26 (100%)	0	100	100
All	All	4686/17356 (27%)	4681 (100%)	5 (0%)	87	90

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

Mol	Chain	Res	Type
1	B	164	VAL
1	C	227	ASN
1	D	164	VAL
2	K	84	ASN
2	K	238	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	178	HIS
2	K	44	ASN
2	K	73	GLN
2	K	84	ASN
2	K	151	GLN
2	K	167	ASN
3	L	188	ASN
5	f	246	GLN
5	f	306	HIS
5	f	355	GLN
5	f	375	GLN
5	f	475	GLN
5	f	629	GLN
5	f	657	GLN
5	f	842	ASN
6	h	268	ASN
6	h	397	ASN
6	h	419	GLN
5	m	306	HIS
5	m	472	GLN
5	m	637	HIS
5	m	752	ASN
5	m	772	ASN
5	m	799	ASN
5	m	842	ASN
5	n	215	ASN

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Mol	Chain	Res	Type
5	n	375	GLN
5	n	465	GLN
6	o	371	GLN
6	o	419	GLN
6	o	462	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	E	800	9	28,29,29	1.36	4 (14%)	43,45,45	1.85	11 (25%)
8	ADP	B	800	9	28,29,29	1.35	4 (14%)	43,45,45	1.87	11 (25%)
8	ADP	C	800	9	28,29,29	1.36	5 (17%)	43,45,45	1.85	11 (25%)
8	ADP	A	800	9	28,29,29	1.38	5 (17%)	43,45,45	1.86	10 (23%)
8	ADP	F	800	9	28,29,29	1.37	4 (14%)	43,45,45	1.89	11 (25%)
8	ADP	D	800	9	28,29,29	1.35	4 (14%)	43,45,45	1.88	11 (25%)

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	E	800	9	-	3/16/32/32	0/3/3/3
8	ADP	B	800	9	-	0/16/32/32	0/3/3/3
8	ADP	C	800	9	-	3/16/32/32	0/3/3/3
8	ADP	A	800	9	-	0/16/32/32	0/3/3/3
8	ADP	F	800	9	-	4/16/32/32	0/3/3/3
8	ADP	D	800	9	-	3/16/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	800	ADP	C5-C4	4.49	1.47	1.39
8	A	800	ADP	C5-C4	4.45	1.47	1.39
8	E	800	ADP	C5-C4	4.43	1.47	1.39
8	C	800	ADP	C5-C4	4.42	1.47	1.39
8	B	800	ADP	C5-C4	4.42	1.47	1.39
8	D	800	ADP	C5-C4	4.40	1.46	1.39
8	A	800	ADP	C5-C6	2.66	1.48	1.41
8	F	800	ADP	C5-C6	2.57	1.48	1.41
8	D	800	ADP	C5-C6	2.56	1.48	1.41
8	C	800	ADP	C5-C6	2.55	1.48	1.41
8	B	800	ADP	C5-C6	2.54	1.48	1.41
8	E	800	ADP	C5-C6	2.53	1.48	1.41
8	C	800	ADP	C5-N7	-2.50	1.34	1.39
8	E	800	ADP	C5-N7	-2.46	1.34	1.39
8	F	800	ADP	C5-N7	-2.40	1.34	1.39
8	A	800	ADP	C5-N7	-2.38	1.34	1.39
8	B	800	ADP	C5-N7	-2.36	1.34	1.39
8	D	800	ADP	C5-N7	-2.35	1.34	1.39
8	A	800	ADP	C8-N7	2.32	1.36	1.31
8	F	800	ADP	C8-N7	2.30	1.36	1.31
8	C	800	ADP	C8-N7	2.28	1.36	1.31
8	B	800	ADP	C8-N7	2.28	1.36	1.31
8	D	800	ADP	C8-N7	2.26	1.36	1.31
8	E	800	ADP	C8-N7	2.25	1.36	1.31
8	A	800	ADP	C4-N9	-2.11	1.33	1.37
8	C	800	ADP	C4-N9	-2.09	1.33	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	800	ADP	C5-C4-N3	-5.81	118.72	126.72
8	D	800	ADP	C5-C4-N3	-5.74	118.81	126.72
8	E	800	ADP	C5-C4-N3	-5.72	118.84	126.72
8	B	800	ADP	C5-C4-N3	-5.71	118.85	126.72
8	A	800	ADP	C5-C4-N3	-5.68	118.89	126.72
8	C	800	ADP	C5-C4-N3	-5.66	118.93	126.72
8	F	800	ADP	N3-C4-N9	4.68	135.13	127.17
8	E	800	ADP	N3-C4-N9	4.62	135.02	127.17
8	B	800	ADP	N3-C4-N9	4.54	134.88	127.17
8	D	800	ADP	N3-C4-N9	4.53	134.88	127.17
8	C	800	ADP	N3-C4-N9	4.49	134.79	127.17
8	A	800	ADP	N3-C4-N9	4.39	134.63	127.17
8	D	800	ADP	C2-N3-C4	3.82	121.17	111.83
8	B	800	ADP	C2-N3-C4	3.79	121.09	111.83
8	A	800	ADP	C2-N3-C4	3.77	121.04	111.83
8	F	800	ADP	C2-N3-C4	3.77	121.03	111.83
8	E	800	ADP	C2-N3-C4	3.75	120.98	111.83
8	C	800	ADP	C2-N3-C4	3.71	120.89	111.83
8	D	800	ADP	N3-C2-N1	-3.66	123.04	128.58
8	A	800	ADP	C4-C5-N7	-3.60	106.47	110.58
8	B	800	ADP	N3-C2-N1	-3.58	123.16	128.58
8	F	800	ADP	N3-C2-N1	-3.55	123.22	128.58
8	E	800	ADP	N3-C2-N1	-3.52	123.25	128.58
8	D	800	ADP	C4-C5-N7	-3.50	106.58	110.58
8	A	800	ADP	N3-C2-N1	-3.49	123.31	128.58
8	C	800	ADP	N3-C2-N1	-3.48	123.31	128.58
8	F	800	ADP	C4-C5-N7	-3.48	106.61	110.58
8	B	800	ADP	C4-C5-N7	-3.45	106.64	110.58
8	C	800	ADP	C4-C5-N7	-3.40	106.69	110.58
8	E	800	ADP	C4-C5-N7	-3.39	106.70	110.58
8	F	800	ADP	C4-N9-C8	2.98	108.86	105.74
8	E	800	ADP	C4-N9-C8	2.94	108.83	105.74
8	B	800	ADP	C4-N9-C8	2.87	108.75	105.74
8	D	800	ADP	C4-N9-C8	2.87	108.75	105.74
8	C	800	ADP	C4-N9-C8	2.86	108.74	105.74
8	A	800	ADP	C4-N9-C8	2.84	108.72	105.74
8	F	800	ADP	C5-N7-C8	2.73	107.75	103.45
8	A	800	ADP	C5-N7-C8	2.73	107.74	103.45
8	D	800	ADP	C5-N7-C8	2.69	107.68	103.45
8	E	800	ADP	C5-N7-C8	2.67	107.65	103.45
8	B	800	ADP	C5-N7-C8	2.67	107.64	103.45
8	C	800	ADP	C5-N7-C8	2.64	107.59	103.45
8	F	800	ADP	C3'-C2'-C1'	2.48	106.15	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	800	ADP	C3'-C2'-C1'	2.39	105.98	101.46
8	A	800	ADP	N9-C8-N7	-2.36	110.59	113.94
8	F	800	ADP	N9-C8-N7	-2.33	110.63	113.94
8	C	800	ADP	C3'-C2'-C1'	2.31	105.84	101.46
8	E	800	ADP	N9-C8-N7	-2.30	110.67	113.94
8	D	800	ADP	N9-C8-N7	-2.29	110.68	113.94
8	C	800	ADP	N9-C8-N7	-2.29	110.69	113.94
8	D	800	ADP	C3'-C2'-C1'	2.28	105.78	101.46
8	B	800	ADP	N9-C8-N7	-2.28	110.70	113.94
8	E	800	ADP	C3'-C2'-C1'	2.26	105.73	101.46
8	A	800	ADP	C6-C5-N7	2.25	136.43	132.09
8	B	800	ADP	C6-C5-N7	2.17	136.27	132.09
8	D	800	ADP	C6-C5-N7	2.16	136.26	132.09
8	C	800	ADP	C6-C5-N7	2.10	136.14	132.09
8	A	800	ADP	C3'-C2'-C1'	2.09	105.42	101.46
8	C	800	ADP	C2-N1-C6	2.06	122.12	118.73
8	F	800	ADP	C2-N1-C6	2.05	122.10	118.73
8	E	800	ADP	C6-C5-N7	2.05	136.04	132.09
8	F	800	ADP	C6-C5-N7	2.05	136.03	132.09
8	D	800	ADP	C2-N1-C6	2.03	122.06	118.73
8	B	800	ADP	C2-N1-C6	2.03	122.06	118.73
8	E	800	ADP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

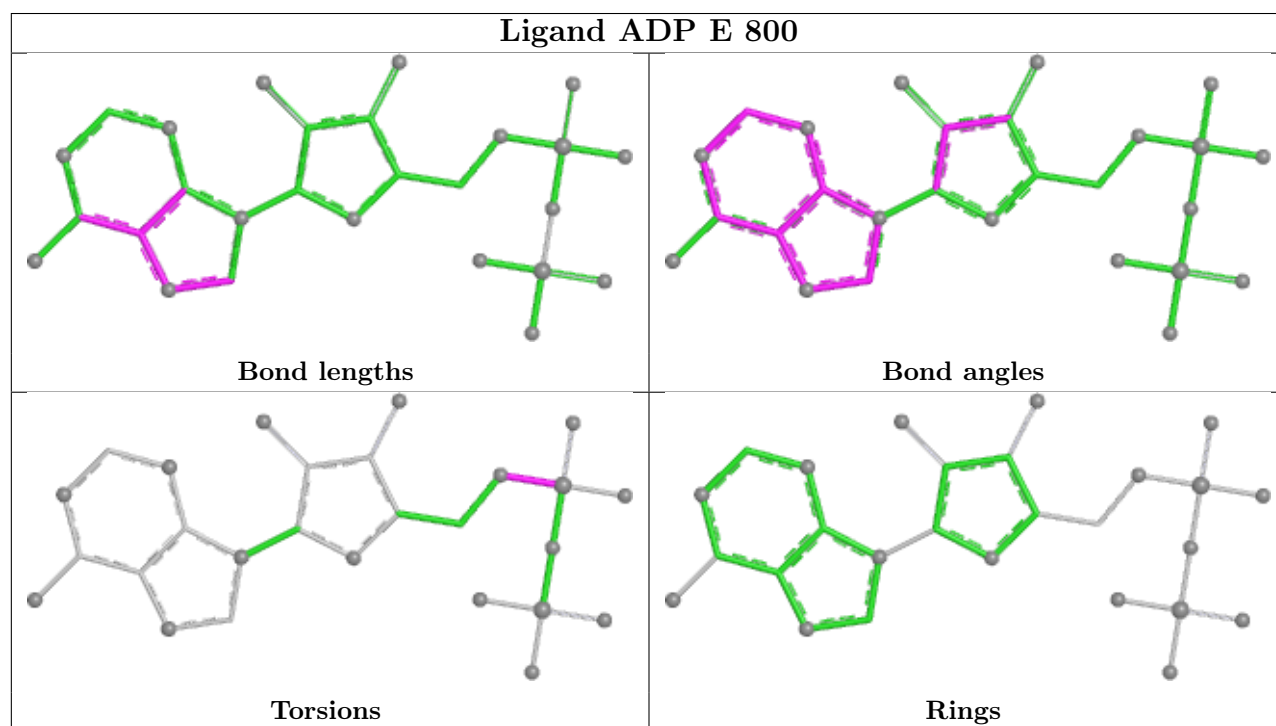
Mol	Chain	Res	Type	Atoms
8	C	800	ADP	C5'-O5'-PA-O1A
8	C	800	ADP	C5'-O5'-PA-O3A
8	D	800	ADP	C5'-O5'-PA-O1A
8	D	800	ADP	C5'-O5'-PA-O3A
8	E	800	ADP	C5'-O5'-PA-O1A
8	E	800	ADP	C5'-O5'-PA-O2A
8	E	800	ADP	C5'-O5'-PA-O3A
8	F	800	ADP	C5'-O5'-PA-O1A
8	F	800	ADP	C5'-O5'-PA-O2A
8	F	800	ADP	C5'-O5'-PA-O3A
8	C	800	ADP	C5'-O5'-PA-O2A
8	D	800	ADP	C5'-O5'-PA-O2A
8	F	800	ADP	PB-O3A-PA-O2A

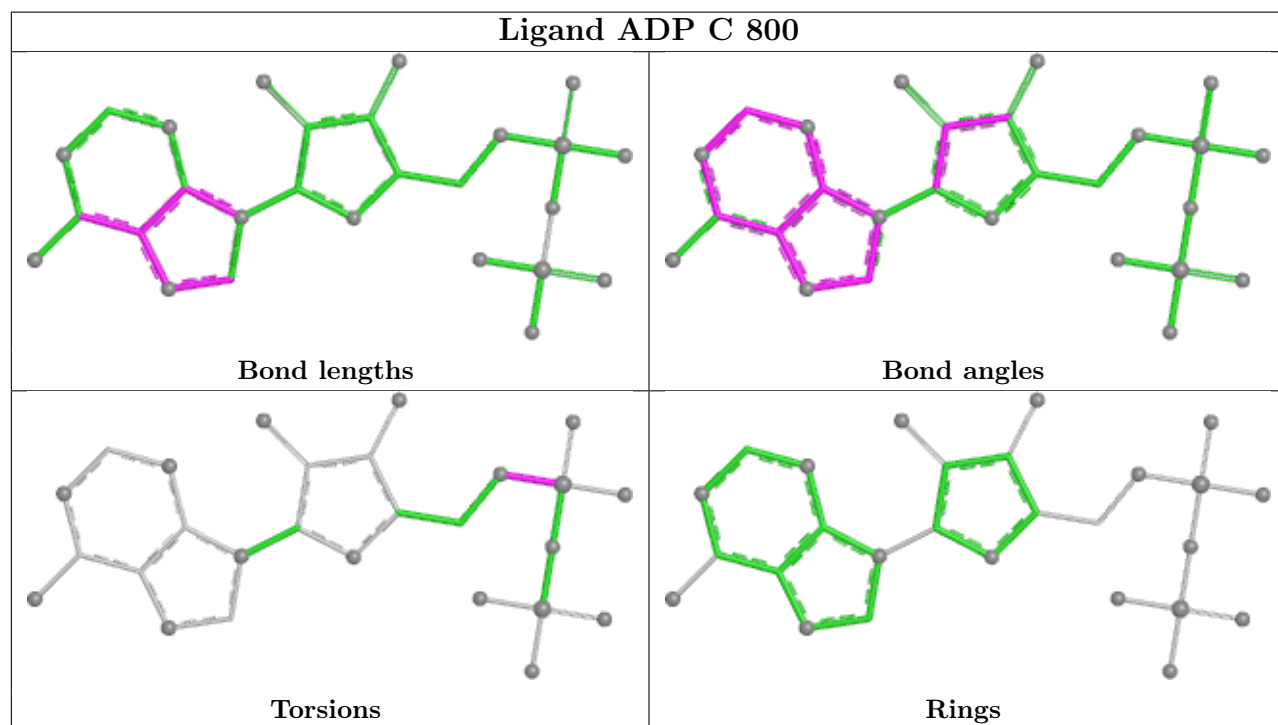
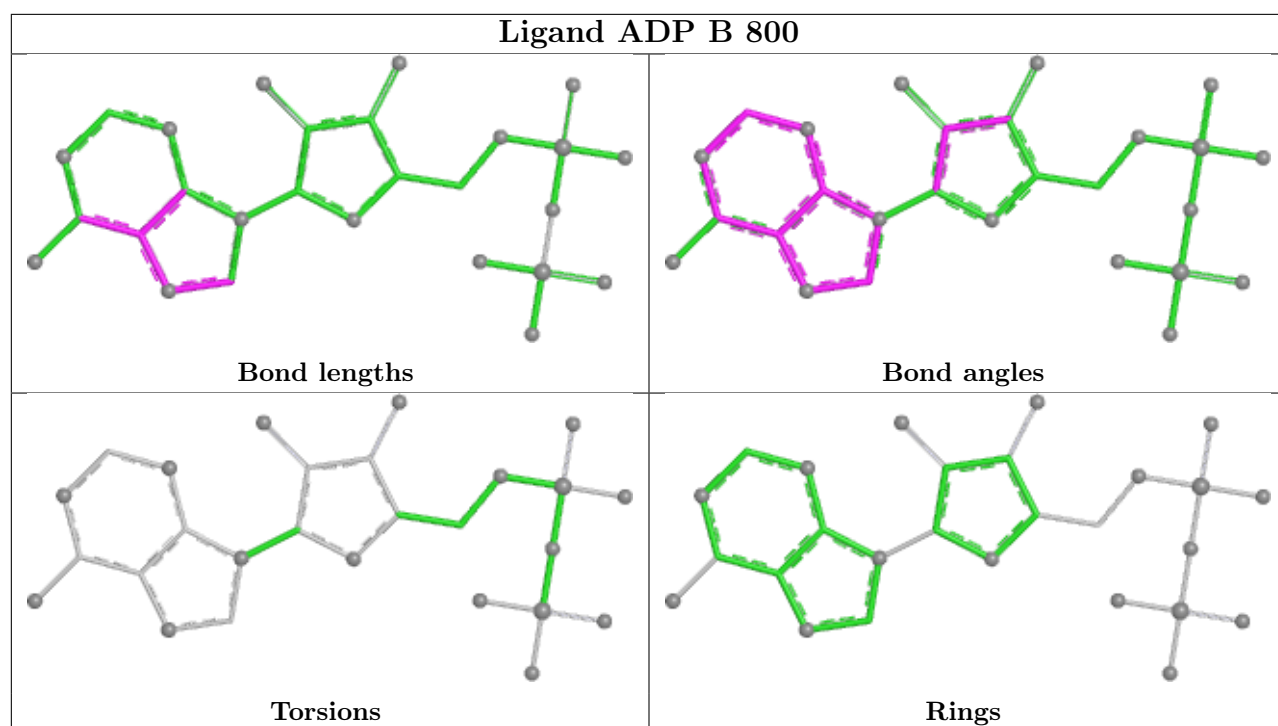
There are no ring outliers.

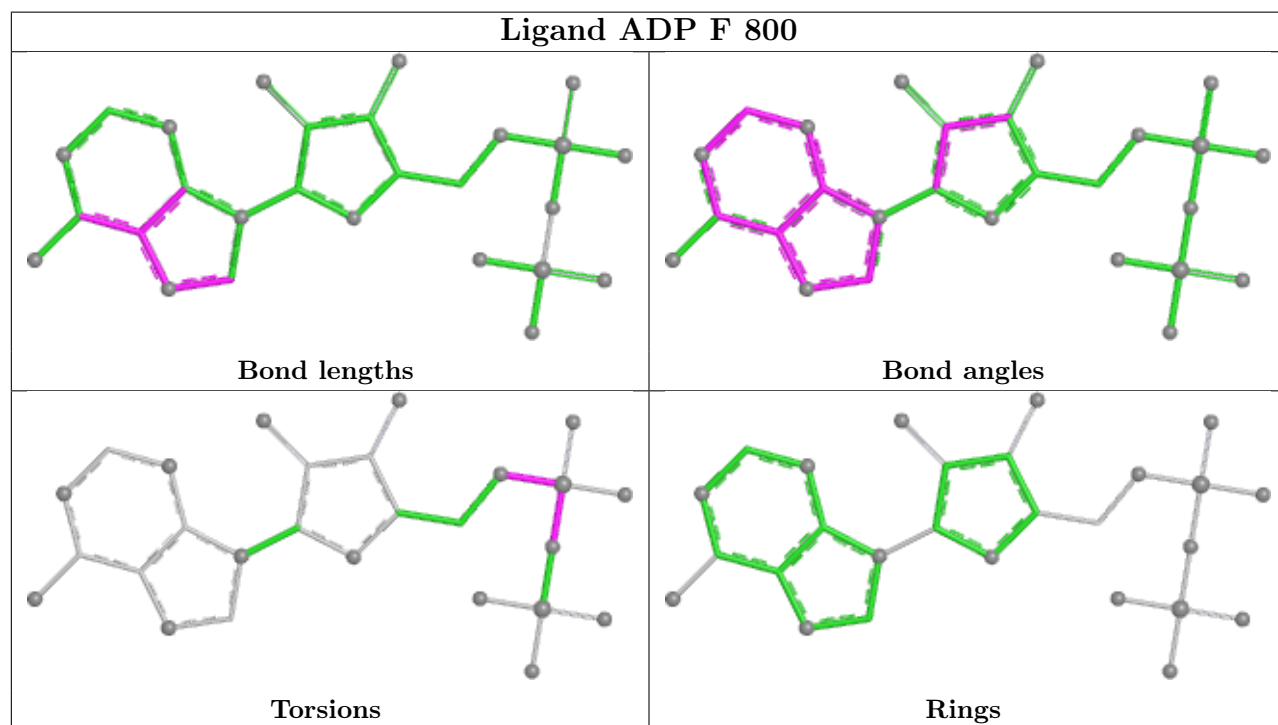
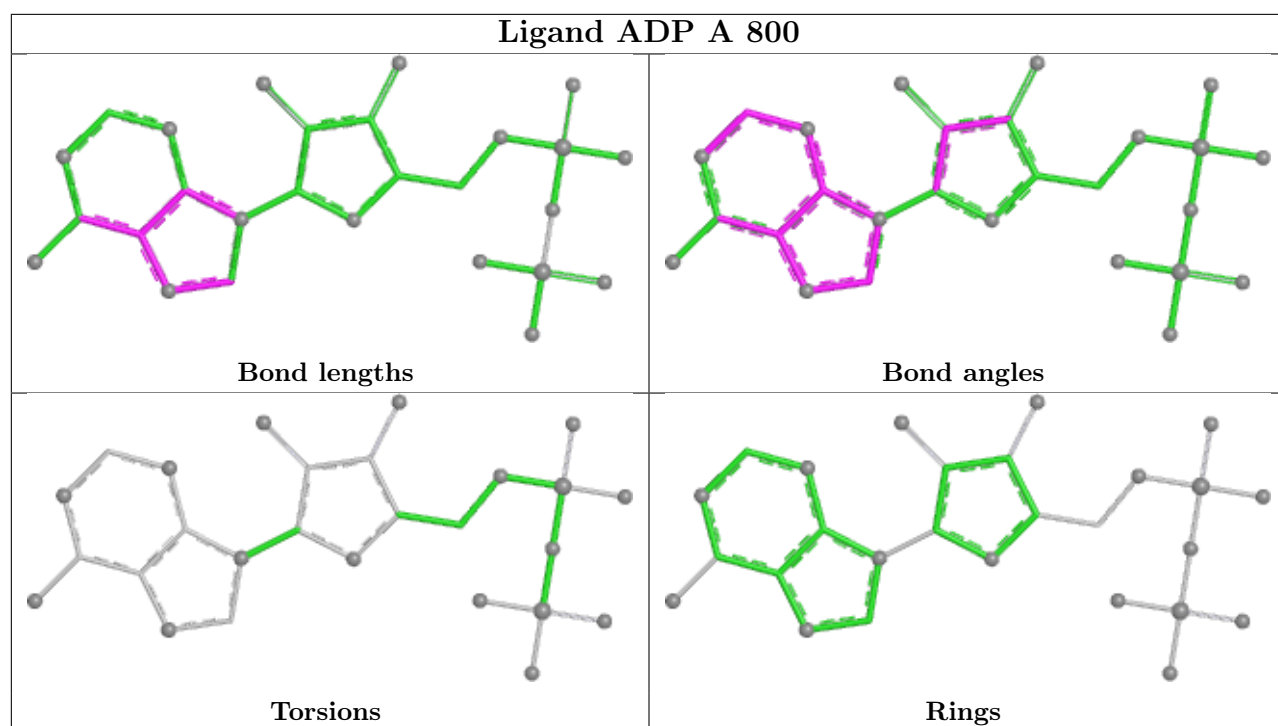
2 monomers are involved in 2 short contacts:

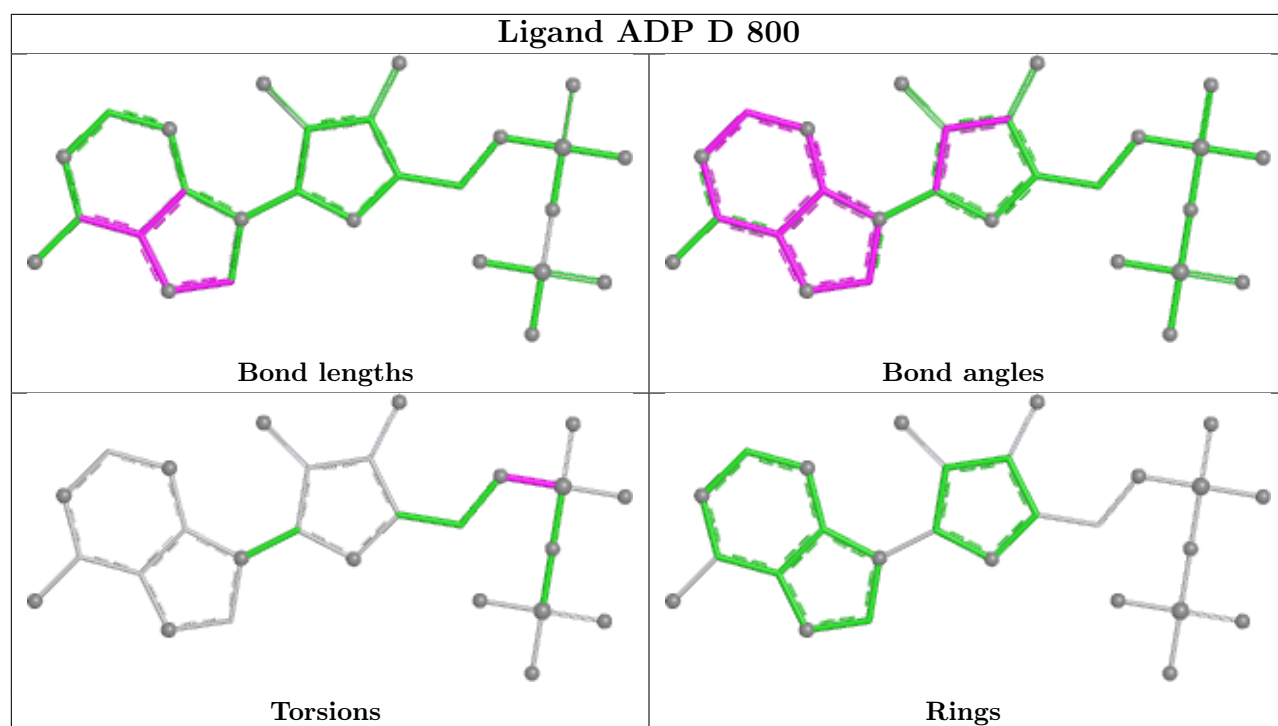
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	800	ADP	1	0
8	F	800	ADP	1	0

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](#)

There are no chain breaks in this entry.

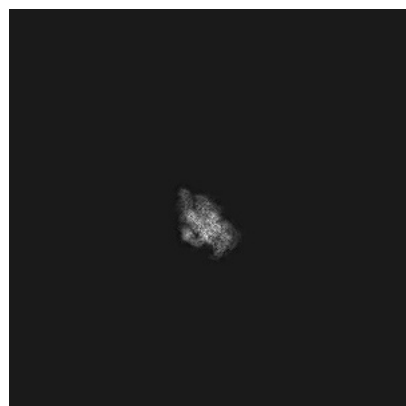
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14552. These allow visual inspection of the internal detail of the map and identification of artifacts.

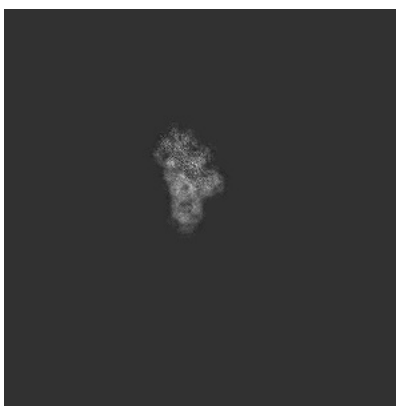
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

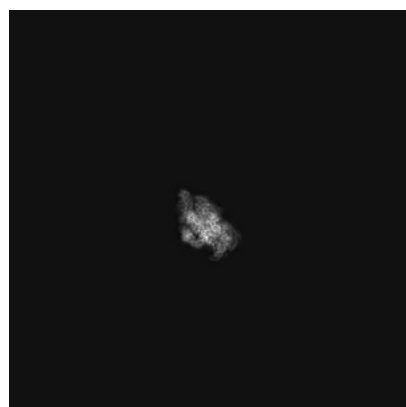


Y

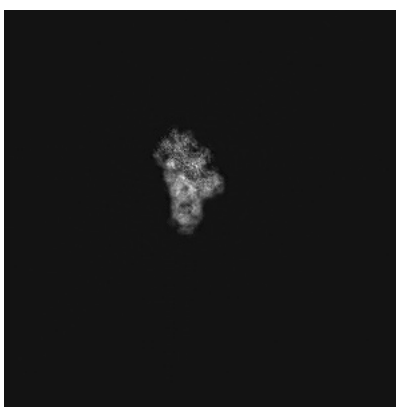


Z

6.1.2 Raw map



X



Y

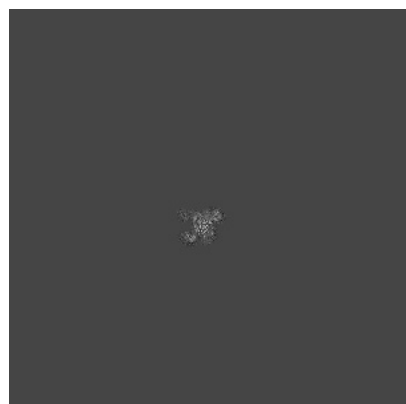


Z

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

6.2 Central slices [i](#)

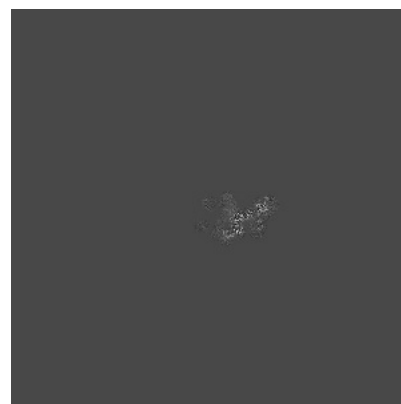
6.2.1 Primary map



X Index: 384

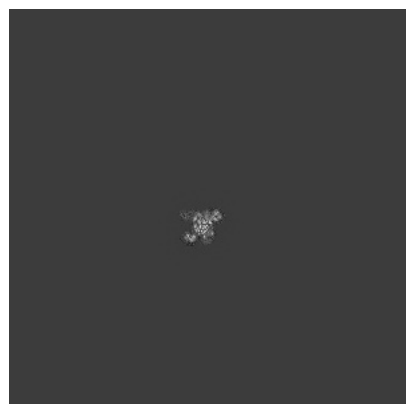


Y Index: 384



Z Index: 384

6.2.2 Raw map



X Index: 384



Y Index: 384

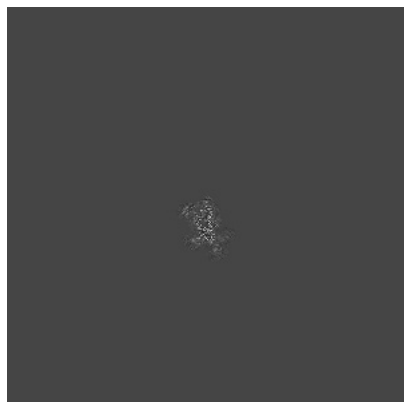


Z Index: 384

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: 478



Y Index: 388



Z Index: 349

6.3.2 Raw map



X Index: 440



Y Index: 388

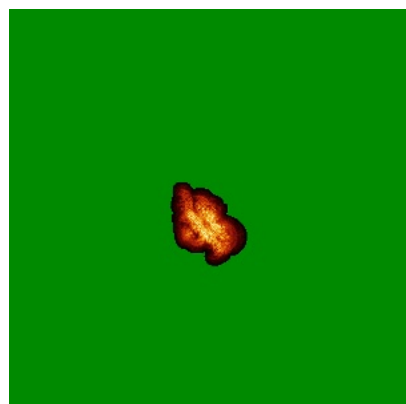


Z Index: 343

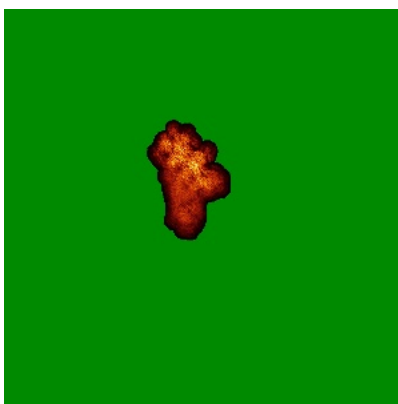
The images above show the largest variance slices of the map in three orthogonal directions.

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

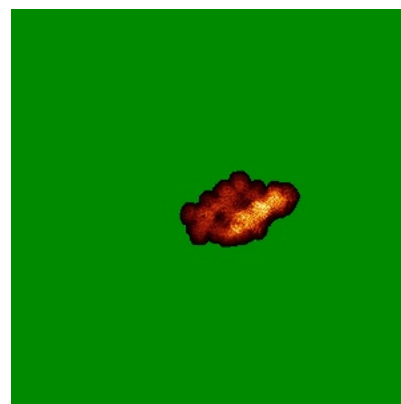
6.4.1 Primary map



X

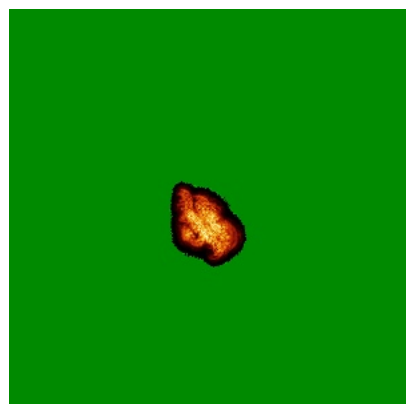


Y

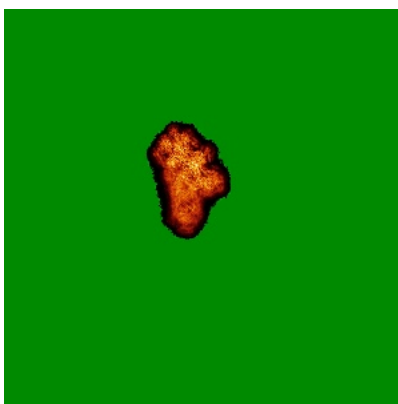


Z

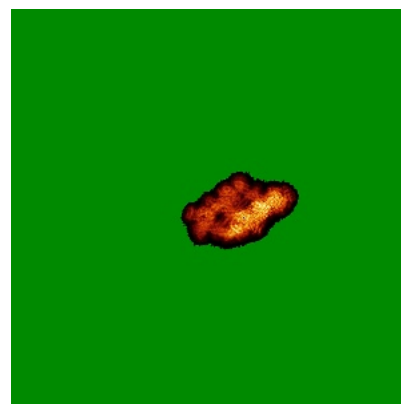
6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.0244. 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



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.

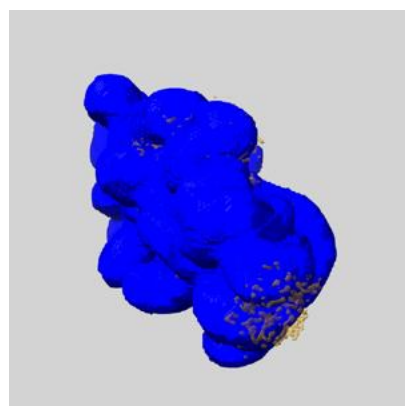
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

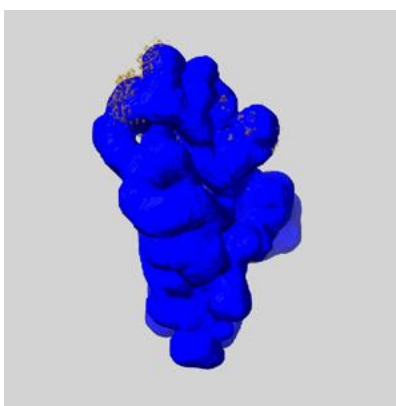
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

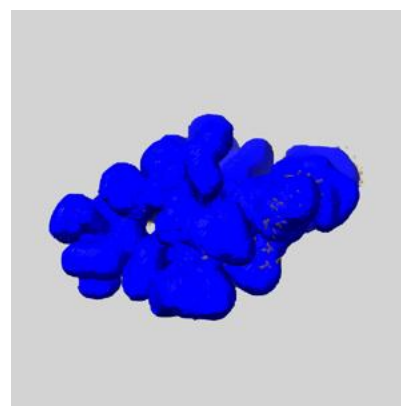
6.6.1 emd_14552_msk_1.map [i](#)



X



Y

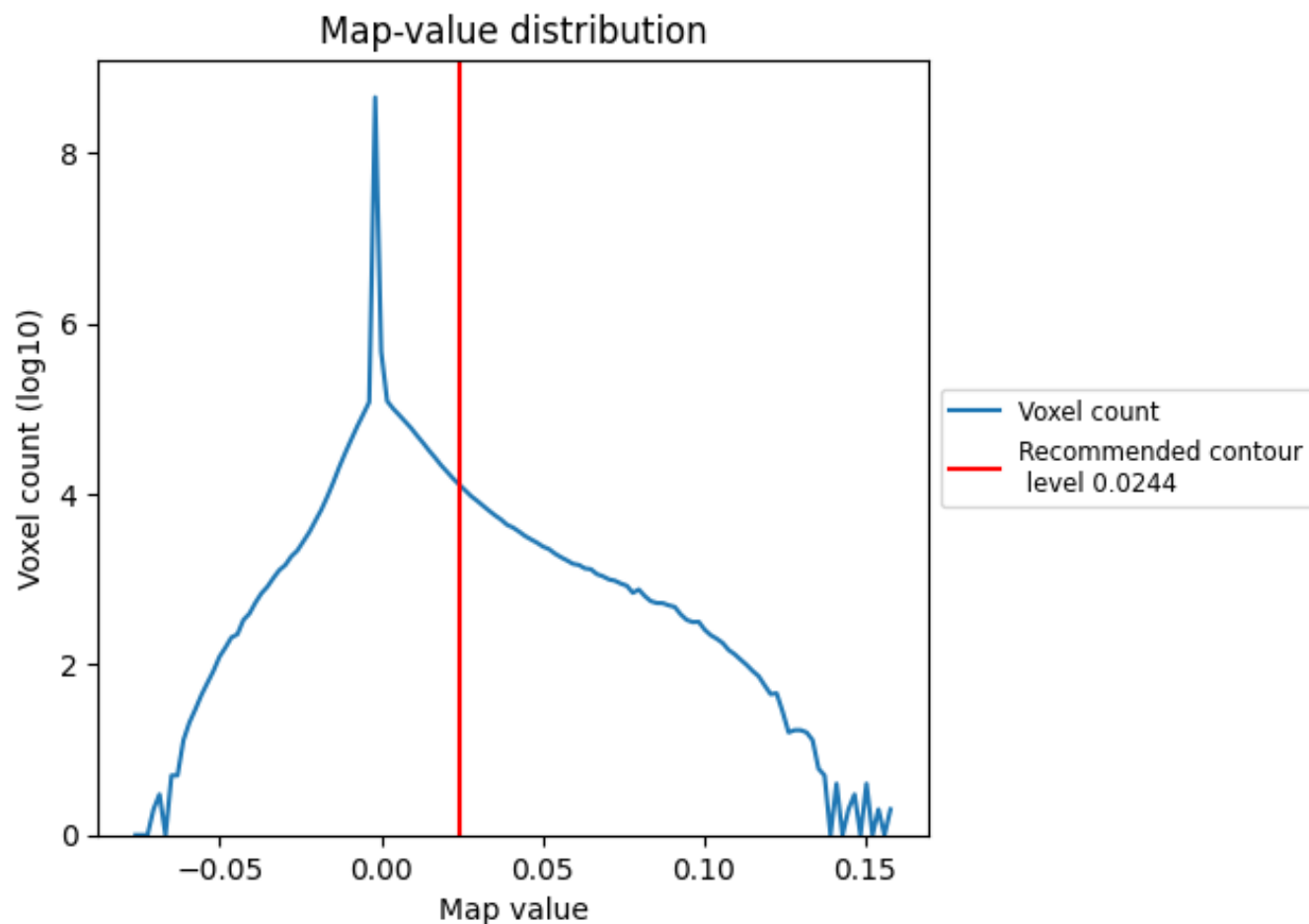


Z

7 Map analysis [i](#)

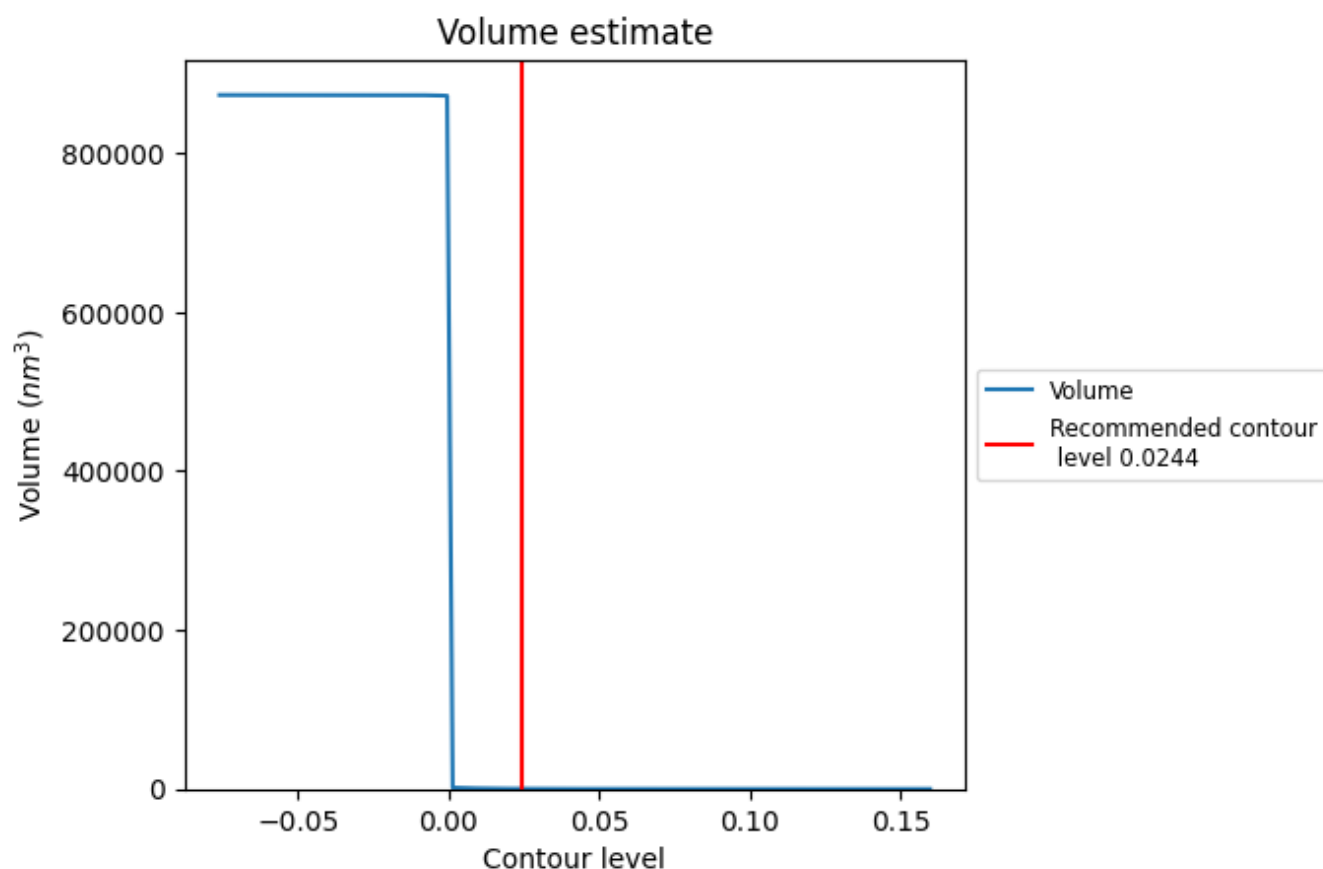
This section contains the results of statistical analysis of the map.

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.

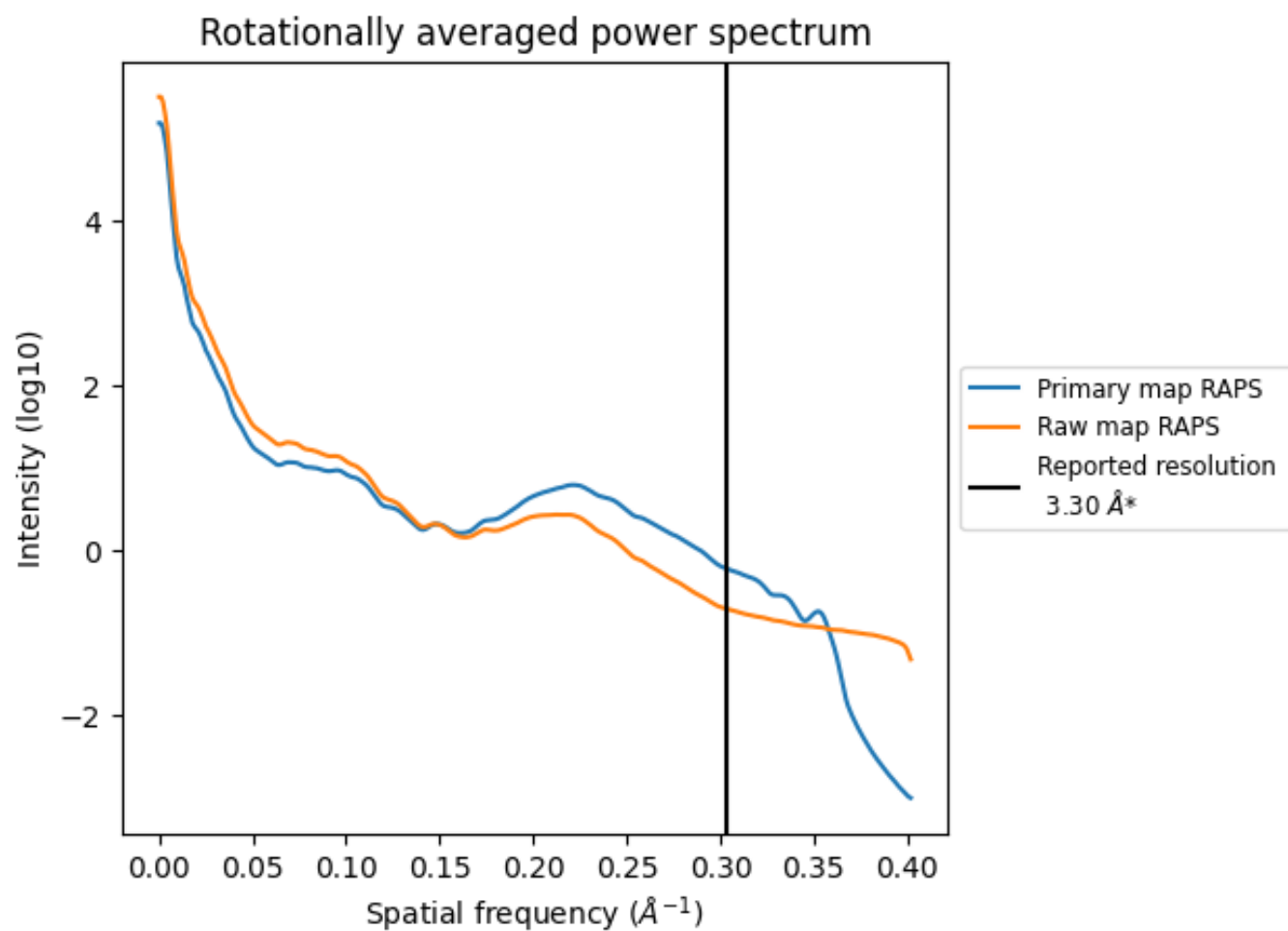
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm^3 ; this corresponds to an approximate mass of 201 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 ⓘ

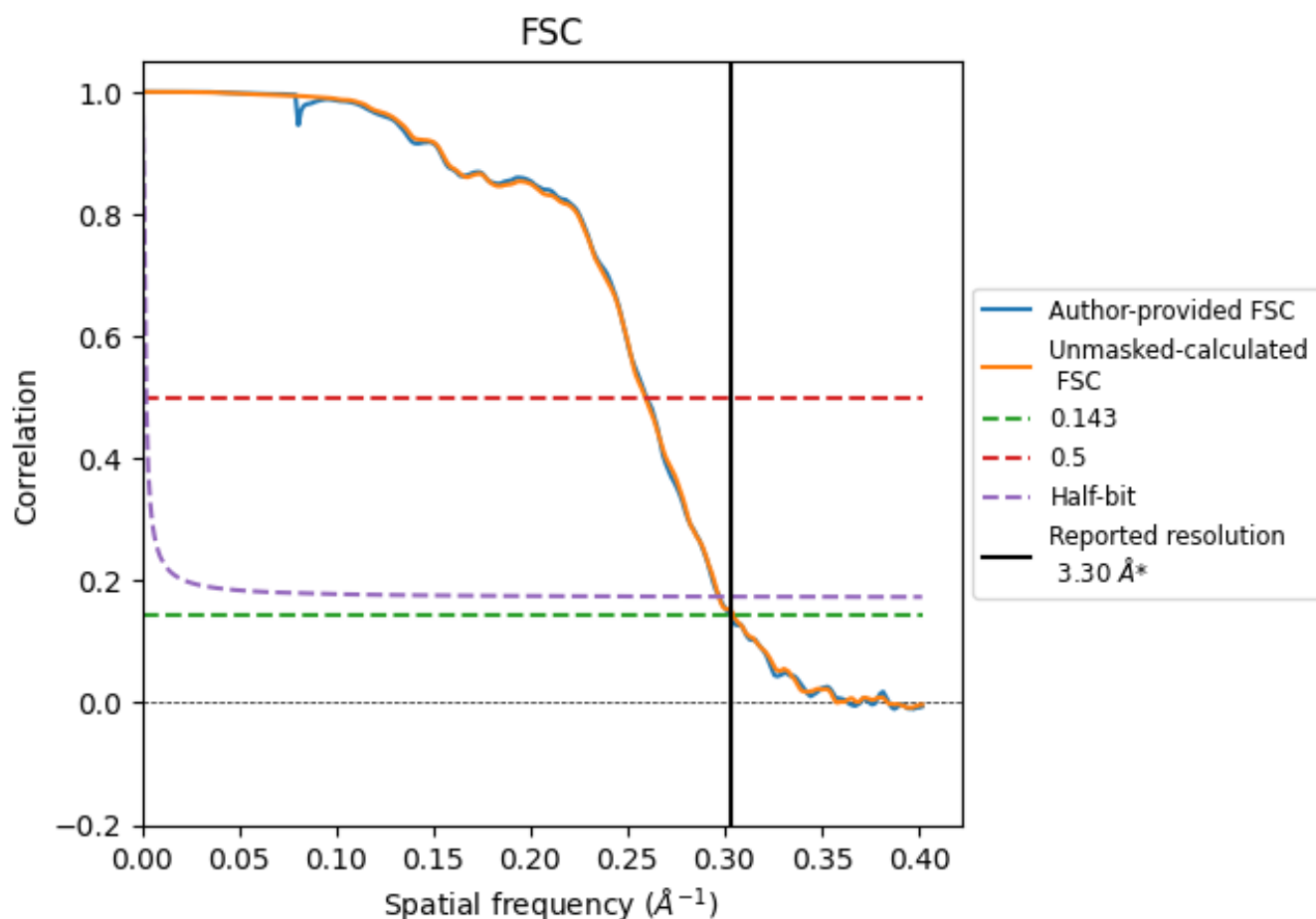


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

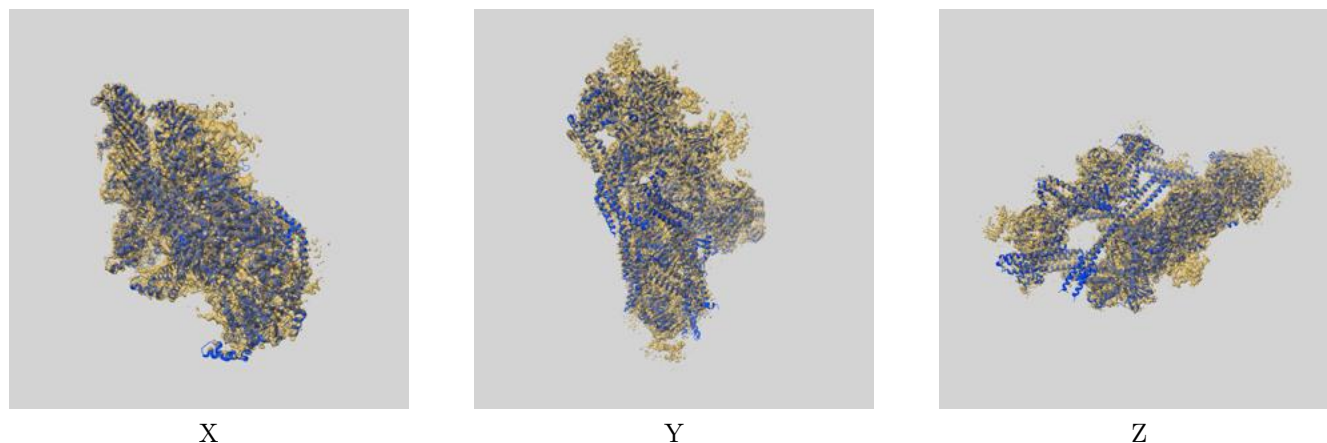
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.85	3.36
Unmasked-calculated*	3.28	3.86	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

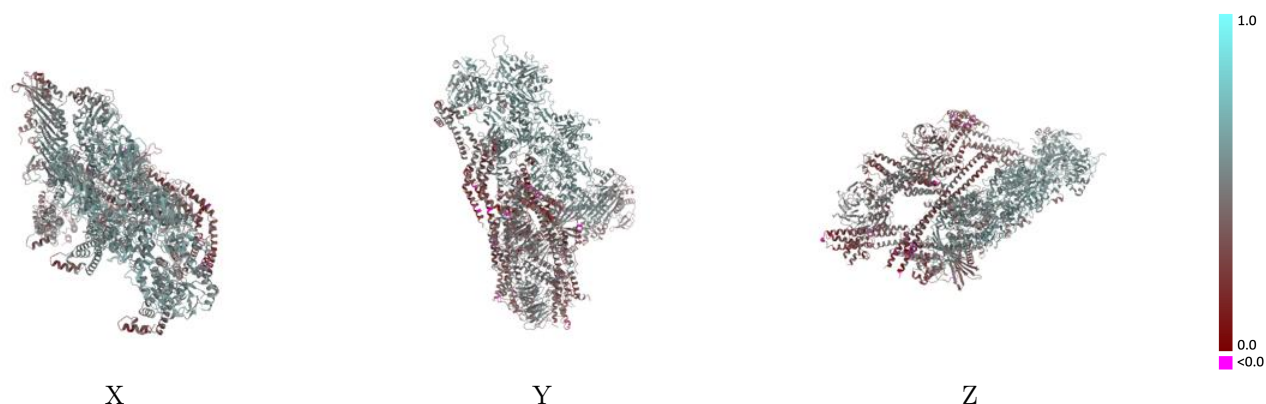
This section contains information regarding the fit between EMDB map EMD-14552 and PDB model 7Z8I. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



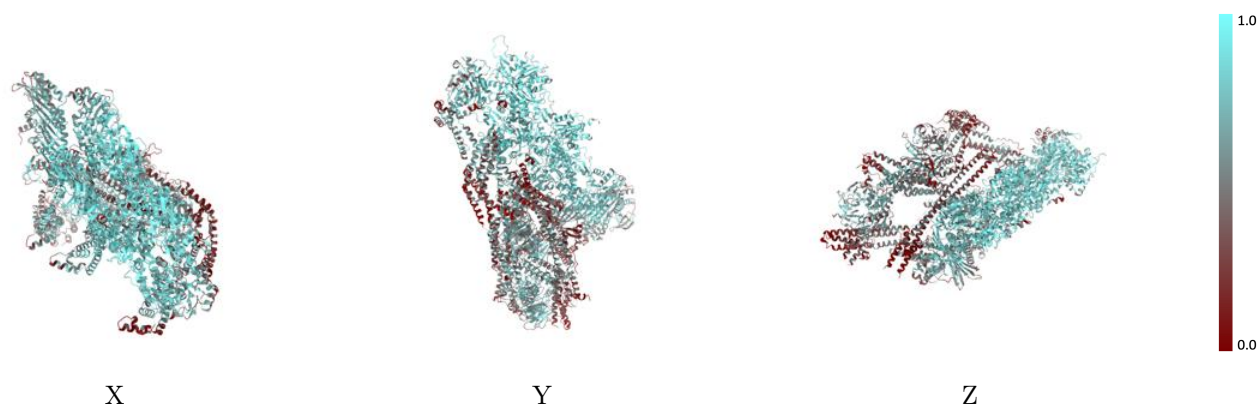
The images above show the 3D surface view of the map at the recommended contour level 0.0244 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



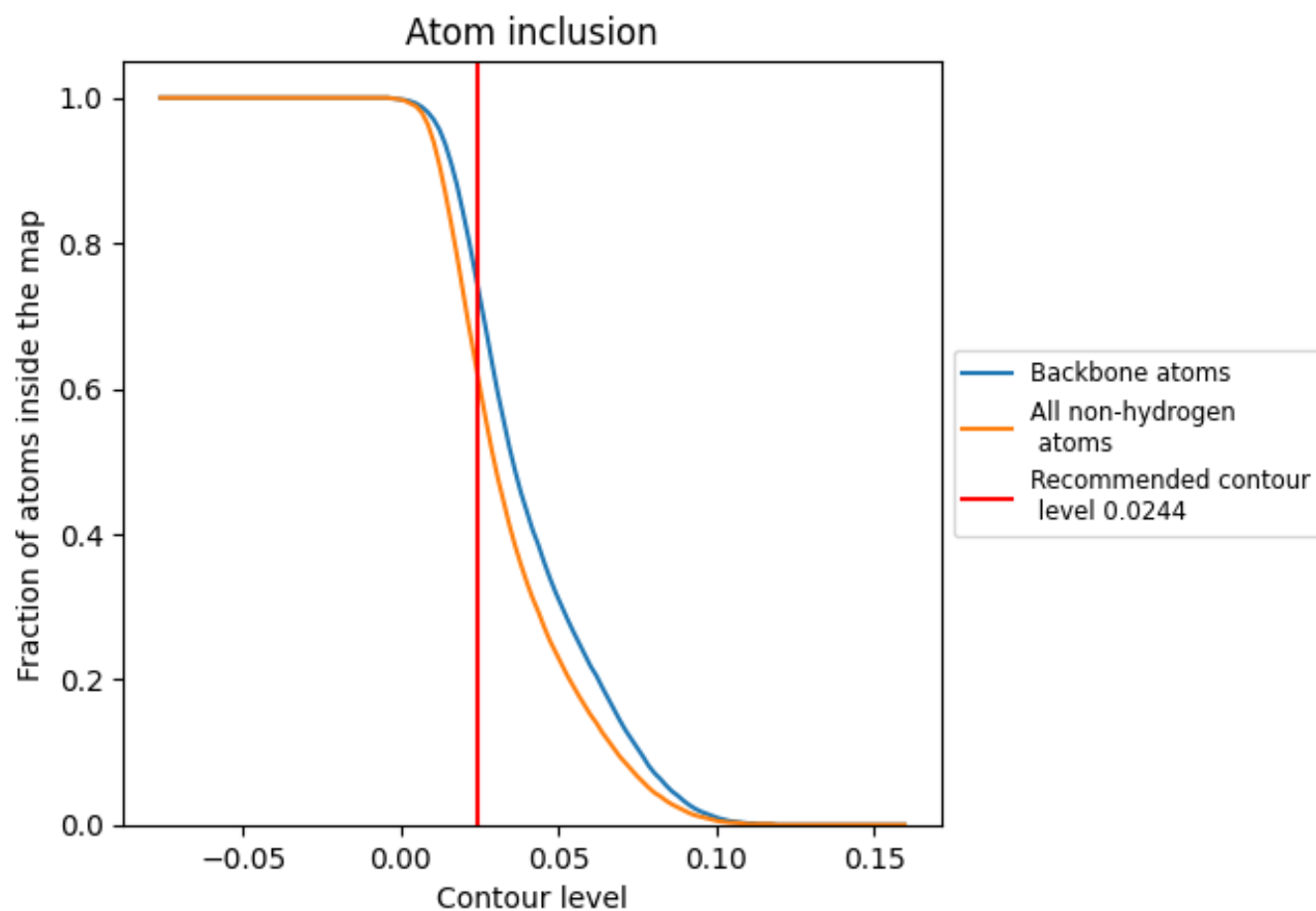
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0244).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.0244) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6180	 0.4660
A	 0.7690	 0.5260
B	 0.8420	 0.5740
C	 0.8330	 0.5680
D	 0.8400	 0.5680
E	 0.8140	 0.5580
F	 0.6940	 0.5430
K	 0.6070	 0.4370
L	 0.7070	 0.5050
X	 0.2520	 0.3140
f	 0.3780	 0.3520
h	 0.5100	 0.4130
j	 0.1550	 0.2620
m	 0.5450	 0.4330
n	 0.4780	 0.3890
o	 0.6160	 0.4620
r	 0.0180	 0.2060
x	 0.2350	 0.2950

