



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 03:42 PM JST

PDB ID : 6JBJ  
EMDB ID : EMD-9791  
Title : Cryo-EM structure of human lysosomal cobalamin exporter ABCD4  
Authors : Xu, D.; Feng, Z.; Hou, W.T.; Jiang, Y.L.; Wang, L.; Sun, L.F.; Zhou, C.Z.;  
Chen, Y.  
Deposited on : 2019-01-25  
Resolution : 3.60 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](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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

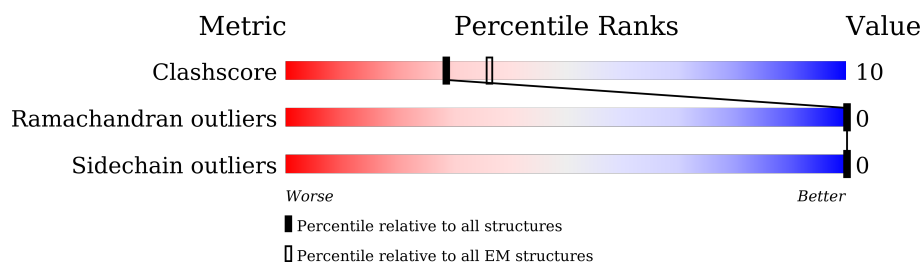
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	648	<div> <div>87%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>13%</div> </div> </div>
1	B	648	<div> <div>87%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9166 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 ATP-binding cassette sub-family D member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	565	Total	C	N	O	S	0	0
			4552	2947	762	823	20		
1	B	565	Total	C	N	O	S	0	0
			4552	2947	762	823	20		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-41	MET	-	expression tag	UNP O14678
A	-40	ALA	-	expression tag	UNP O14678
A	-39	SER	-	expression tag	UNP O14678
A	-38	TRP	-	expression tag	UNP O14678
A	-37	SER	-	expression tag	UNP O14678
A	-36	HIS	-	expression tag	UNP O14678
A	-35	PRO	-	expression tag	UNP O14678
A	-34	GLN	-	expression tag	UNP O14678
A	-33	PHE	-	expression tag	UNP O14678
A	-32	GLU	-	expression tag	UNP O14678
A	-31	LYS	-	expression tag	UNP O14678
A	-30	GLY	-	expression tag	UNP O14678
A	-29	GLY	-	expression tag	UNP O14678
A	-28	GLY	-	expression tag	UNP O14678
A	-27	ALA	-	expression tag	UNP O14678
A	-26	ARG	-	expression tag	UNP O14678
A	-25	GLY	-	expression tag	UNP O14678
A	-24	GLY	-	expression tag	UNP O14678
A	-23	SER	-	expression tag	UNP O14678
A	-22	GLY	-	expression tag	UNP O14678
A	-21	GLY	-	expression tag	UNP O14678
A	-20	GLY	-	expression tag	UNP O14678
A	-19	SER	-	expression tag	UNP O14678
A	-18	TRP	-	expression tag	UNP O14678
A	-17	SER	-	expression tag	UNP O14678
A	-16	HIS	-	expression tag	UNP O14678

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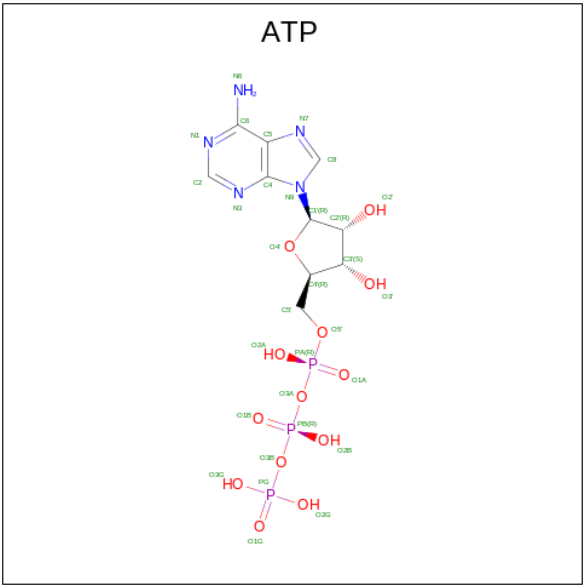
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	PRO	-	expression tag	UNP O14678
A	-14	GLN	-	expression tag	UNP O14678
A	-13	PHE	-	expression tag	UNP O14678
A	-12	GLU	-	expression tag	UNP O14678
A	-11	LYS	-	expression tag	UNP O14678
A	-10	GLY	-	expression tag	UNP O14678
A	-9	PHE	-	expression tag	UNP O14678
A	-8	ASP	-	expression tag	UNP O14678
A	-7	TYR	-	expression tag	UNP O14678
A	-6	LYS	-	expression tag	UNP O14678
A	-5	ASP	-	expression tag	UNP O14678
A	-4	ASP	-	expression tag	UNP O14678
A	-3	ASP	-	expression tag	UNP O14678
A	-2	ASP	-	expression tag	UNP O14678
A	-1	LYS	-	expression tag	UNP O14678
A	0	GLY	-	expression tag	UNP O14678
A	1	THR	-	expression tag	UNP O14678
A	549	GLN	GLU	engineered mutation	UNP O14678
B	-41	MET	-	expression tag	UNP O14678
B	-40	ALA	-	expression tag	UNP O14678
B	-39	SER	-	expression tag	UNP O14678
B	-38	TRP	-	expression tag	UNP O14678
B	-37	SER	-	expression tag	UNP O14678
B	-36	HIS	-	expression tag	UNP O14678
B	-35	PRO	-	expression tag	UNP O14678
B	-34	GLN	-	expression tag	UNP O14678
B	-33	PHE	-	expression tag	UNP O14678
B	-32	GLU	-	expression tag	UNP O14678
B	-31	LYS	-	expression tag	UNP O14678
B	-30	GLY	-	expression tag	UNP O14678
B	-29	GLY	-	expression tag	UNP O14678
B	-28	GLY	-	expression tag	UNP O14678
B	-27	ALA	-	expression tag	UNP O14678
B	-26	ARG	-	expression tag	UNP O14678
B	-25	GLY	-	expression tag	UNP O14678
B	-24	GLY	-	expression tag	UNP O14678
B	-23	SER	-	expression tag	UNP O14678
B	-22	GLY	-	expression tag	UNP O14678
B	-21	GLY	-	expression tag	UNP O14678
B	-20	GLY	-	expression tag	UNP O14678
B	-19	SER	-	expression tag	UNP O14678
B	-18	TRP	-	expression tag	UNP O14678

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP O14678
B	-16	HIS	-	expression tag	UNP O14678
B	-15	PRO	-	expression tag	UNP O14678
B	-14	GLN	-	expression tag	UNP O14678
B	-13	PHE	-	expression tag	UNP O14678
B	-12	GLU	-	expression tag	UNP O14678
B	-11	LYS	-	expression tag	UNP O14678
B	-10	GLY	-	expression tag	UNP O14678
B	-9	PHE	-	expression tag	UNP O14678
B	-8	ASP	-	expression tag	UNP O14678
B	-7	TYR	-	expression tag	UNP O14678
B	-6	LYS	-	expression tag	UNP O14678
B	-5	ASP	-	expression tag	UNP O14678
B	-4	ASP	-	expression tag	UNP O14678
B	-3	ASP	-	expression tag	UNP O14678
B	-2	ASP	-	expression tag	UNP O14678
B	-1	LYS	-	expression tag	UNP O14678
B	0	GLY	-	expression tag	UNP O14678
B	1	THR	-	expression tag	UNP O14678
B	549	GLN	GLU	engineered mutation	UNP O14678

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

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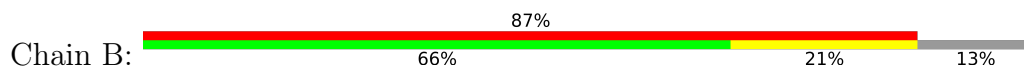
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	31	10	5	13	3	0



L499	A500	G501	L502	S503	N504	L505	V506	A507	R508	T509	E510	G511	L512	D513	Q514	Q515	V516	D517	W518	N519	W520	Y521	D522	V523	L524	S525	P526	G527	E528	M529	Q530	R531	L532	S533	F534	A535	R536	L537	F538	Y539	Q541	P542	K543	Y544	A545	V546	L547	D548	Q549	A550	T551	S552	A553	L554	T555	E556	E557	V558
E559	S560	E561	L562	Y563	R564	L565	G566	Q567	Q568	L569	G570	M571	T572	F573	I574	S575	V576	G577	H578	R579	Q580	S581	L582	E583	K584	F585	H586	S587	L588	V589	L590	K591	L592	C593	G594	G595	R596	R597	W598	E599	L600	M601	R602	I603	K604	VAL	GLU											

- Molecule 1: ATP-binding cassette sub-family D member 4



MET	ALA	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	ALA	ARG	GLY	GLY	SER	TRP	SER	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	THR	ALA	VAL	ALA	GLY	PRO	GLY	ALA	GLY	ALA	R13	P14	R15	L16	D17	L18															
Q19	F20	L21	Q22	R23	F24	L25	Q26	L27	L28	K29	V30	L31	F32	P33	S34	W35	S36	S37	Q38	N39	A40	L41	M42	F43	L44	T45	L46	L47	C48	L49	T50	L51	L52	E53	Q54	F55	V56	I57	F58	L59	Q59	V60	G61	L62	I63	P64	S65	Q66	Y67	F68	G69	V70	L71	G72	N73	K74	D75	L76	E77	G78
F79	K80	T81	L82	T83	F84	L85	A86	V87	M88	L89	I90	V91	L92	N93	S94	T95	L96	K97	S98	F99	D100	Q101	F102	T103	C104	N105	L106	L107	Y108	V109	S110	W111	R112	K113	D114	L115	T116	E117	H118	L119	H120	R121	L122	Y123	F124	L125	G126	R127	A128	Y129	I130	T131	L132	N133	V134	L135	R136	D137	D138	
I139	D140	M141	P142	D143	Q144	R145	I146	S147	Q148	D149	V150	E151	R152	F153	C154	R155	Q156	L157	S158	S159	M160	A161	S162	K163	L164	I165	I166	S167	P168	F169	T170	W171	V172	Y173	Y174	T175	Y176	Q177	C178	F179	Q180	S181	T182	G183	W184	L185	G186	P187	V188	S189	I190	F191	G192	Y193	F194	L195	L196	G197	T198	
V199	V200	N201	K202	T203	L204	M205	G206	P207	I208	V209	M210	K211	L212	V213	H214	Q215	E216	K217	L218	E219	G220	D221	F222	R223	F224	K225	H226	M227	Q228	I229	R230	V231	N232	A233	E234	P235	A236	A237	F238	Y239	R240	A241	G242	H243	V244	E245	H246	M247	R248	T249	D250	R251	R252	L253	Q254	R255	L256	L257	Q258	
T259	Q260	R261	E262	L263	M264	S265	K266	E267	L268	W269	L270	Y271	L272	G273	I274	N275	T276	F277	D278	Y279	L280	G281	S282	L283	L284	S285	Y286	V287	V288	L289	A290	I291	P292	L293	F294	S295	G296	V297	Y298	G299	D300	L301	S302	P303	A304	E305	L306	S307	T308	L309	V310	S311	K312	N313	A314	F315	V316	C317	I318	
Y319	L320	I321	S322	C323	F324	T325	Q326	L327	I328	D329	L330	S331	T332	T333	L334	S335	D336	V337	A338	G339	Y340	T341	H342	R343	I344	G345	Q346	L347	R348	E349	T350	L351	L352	D353	M354	S355	L356	L357	SER	GLN	ASP	CYS	ILE	LEU	GLY	SER	TRP	GLY	LEU	ASP	THR	PRO	PRO	GLY	TRP	PRO				
ALA	ALA	GLU	PRO	ALA	D384	T385	A386	F387	L388	L389	E390	R391	V392	S393	I394	S395	A396	P397	S398	S399	D400	K401	P402	L403	I404	K405	D406	L407	S408	L409	K410	I411	S412	E413	G414	Q415	S416	L417	L418	I419	T420	G421	M422	T423	G424	T425	G426	K427	T428	S429	L430	L431	R432	V433	L434	G435	G436	L437	W438	
T439	S440	T441	R442	G443	S444	V445	Q446	M447	L448	T449	D450	F451	G452	P453	H454	G455	V456	L457	F458	L459	P460	Q461	K462	P463	F464	F465	T466	D467	G468	T469	L470	R471	E472	Q473	V474	I475	Y476	P477	L478	K479	E480	V481	Y482	P483	D484	S485	G486	S487	A488	D489	D490	E491	R492	I493	L494	R495	F496	L497	E498	
L499	A500	G501	L502	S503	N504	L505	V506	A507	R508	T509	E510	G511	L512	D513	Q514	Q515	V516	D517	W518	N519	W520	Y521	D522	V523	L524	S525	P526	G527	E528	M529	Q530	R531	L532	S533	F534	A535	R536	L537	F538	Y539	L540	Q541	P542	K543	Y544	A545	V546	L547	D548	Q549	A550	T551	S552	A553	L554	T555	E556	E557	V558	
E559	S560	E561	L562	Y563	R564	L565	G566	Q567	Q568	L569	G570	M571	T572	F573	I574	S575	V576	G577	H578	R579	Q580	S581	L582	E583	K584	F585	H586	S587	L588	V589	L590	K591	L592	C593	G594	G595	R596	R597	W598	E599	L600	M601	R602	I603	K604	VAL	GLU													



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276557	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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

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	0.39	0/4651	0.59	1/6299 (0.0%)
1	B	0.39	0/4651	0.59	1/6299 (0.0%)
All	All	0.39	0/9302	0.59	2/12598 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	502	LEU	CA-CB-CG	5.33	127.56	115.30

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	4552	0	4618	107	0
1	B	4552	0	4618	112	0
2	A	31	0	12	2	0
2	B	31	0	12	2	0
All	All	9166	0	9260	192	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 10.

All (192) 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:461:GLN:HE22	1:B:549:GLN:HE21	1.08	0.93
1:A:461:GLN:HE22	1:A:549:GLN:HE21	1.08	0.91
1:A:426:GLY:HA2	2:A:701:ATP:O2A	1.82	0.80
1:B:426:GLY:HA2	2:B:701:ATP:O2A	1.82	0.78
1:A:139:ILE:HG13	1:A:350:THR:HG21	1.70	0.74
1:B:385:THR:HA	1:B:411:ILE:O	1.87	0.74
1:A:385:THR:HA	1:A:411:ILE:O	1.87	0.73
1:B:139:ILE:HG13	1:B:350:THR:HG21	1.70	0.73
1:B:461:GLN:HE22	1:B:549:GLN:NE2	1.87	0.71
1:A:112:ARG:HD3	1:B:260:GLN:HE22	1.60	0.67
1:A:386:ALA:HB3	1:A:411:ILE:HB	1.78	0.65
1:B:386:ALA:HB3	1:B:411:ILE:HB	1.78	0.65
1:A:461:GLN:HE22	1:A:549:GLN:NE2	1.87	0.64
1:A:145:ARG:HD3	1:A:347:LEU:HB2	1.81	0.61
1:B:145:ARG:HD3	1:B:347:LEU:HB2	1.81	0.61
1:A:260:GLN:HE22	1:B:112:ARG:HD3	1.65	0.61
1:B:423:THR:O	2:B:701:ATP:O1B	2.21	0.59
1:B:129:TYR:O	1:B:133:ASN:ND2	2.35	0.59
1:A:422:ASN:O	1:A:427:LYS:NZ	2.35	0.59
1:A:423:THR:O	2:A:701:ATP:O1B	2.21	0.59
1:A:129:TYR:O	1:A:133:ASN:ND2	2.35	0.58
1:A:117:GLU:OE2	1:B:254:GLN:NE2	2.36	0.58
1:B:525:SER:O	1:B:529:MET:N	2.35	0.58
1:A:525:SER:O	1:A:529:MET:N	2.35	0.57
1:A:301:LEU:HB2	1:A:305:GLU:H	1.70	0.57
1:A:67:TYR:CZ	1:B:286:TYR:HB3	2.40	0.57
1:A:419:ILE:HB	1:A:576:VAL:HG22	1.88	0.55
1:B:301:LEU:HB2	1:B:305:GLU:H	1.70	0.55
1:A:213:VAL:HG13	1:A:343:ARG:HD3	1.88	0.55
1:B:419:ILE:HB	1:B:576:VAL:HG22	1.88	0.55
1:B:422:ASN:O	1:B:427:LYS:NZ	2.35	0.55
1:B:213:VAL:HG13	1:B:343:ARG:HD3	1.88	0.54
1:A:36:SER:HA	1:A:41:LEU:HD13	1.89	0.54
1:A:147:SER:OG	1:A:148:GLN:N	2.41	0.54
1:B:36:SER:HA	1:B:41:LEU:HD13	1.89	0.53
1:A:49:LEU:HD21	1:A:99:PHE:HB3	1.90	0.53
1:A:143:ASP:N	1:A:143:ASP:OD1	2.42	0.53
1:B:209:VAL:HG13	1:B:339:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD22	1:A:339:GLY:HA3	1.91	0.53
1:B:147:SER:OG	1:B:148:GLN:N	2.41	0.53
1:A:144:GLN:OE1	1:A:343:ARG:NH2	2.39	0.52
1:A:209:VAL:HG13	1:A:339:GLY:HA2	1.90	0.52
1:B:60:VAL:HA	1:B:63:ILE:HG12	1.92	0.52
1:B:392:VAL:H	1:B:407:LEU:H	1.58	0.52
1:A:230:ARG:NH1	1:B:140:ASP:O	2.39	0.52
1:A:392:VAL:H	1:A:407:LEU:H	1.58	0.52
1:B:212:LEU:HD22	1:B:339:GLY:HA3	1.91	0.52
1:B:501:GLY:HA3	1:B:531:ARG:HH21	1.75	0.52
1:B:49:LEU:HD21	1:B:99:PHE:HB3	1.90	0.52
1:A:474:VAL:HG21	1:A:493:ILE:HG12	1.92	0.52
1:A:404:ILE:HA	1:A:596:GLY:HA2	1.92	0.52
1:B:469:THR:HG23	1:B:472:GLU:H	1.74	0.52
1:B:582:LEU:O	1:B:586:HIS:ND1	2.40	0.52
1:A:140:ASP:O	1:B:230:ARG:NH1	2.42	0.51
1:A:526:PRO:CG	1:B:461:GLN:HG2	2.41	0.51
1:B:474:VAL:HG21	1:B:493:ILE:HG12	1.92	0.51
1:A:286:TYR:HB3	1:B:67:TYR:CZ	2.45	0.51
1:A:501:GLY:HA3	1:A:531:ARG:HH21	1.75	0.51
1:A:469:THR:HG23	1:A:472:GLU:H	1.74	0.51
1:B:143:ASP:N	1:B:143:ASP:OD1	2.42	0.51
1:A:60:VAL:HA	1:A:63:ILE:HG12	1.91	0.51
1:A:582:LEU:O	1:A:586:HIS:ND1	2.40	0.51
1:A:248:ARG:NH1	1:B:467:ASP:O	2.45	0.50
1:A:467:ASP:O	1:B:248:ARG:NH1	2.44	0.50
1:A:254:GLN:NE2	1:B:117:GLU:OE2	2.45	0.50
1:B:404:ILE:HA	1:B:596:GLY:HA2	1.92	0.50
1:B:461:GLN:NE2	1:B:549:GLN:HG2	2.27	0.50
1:A:385:THR:O	1:A:448:LEU:HB2	2.12	0.50
1:A:461:GLN:NE2	1:A:549:GLN:HG2	2.27	0.50
1:B:385:THR:O	1:B:448:LEU:HB2	2.12	0.49
1:A:130:TYR:HA	1:B:233:ALA:HB1	1.95	0.49
1:A:90:ILE:HG21	1:B:280:LEU:HB2	1.95	0.49
1:A:467:ASP:N	1:A:467:ASP:OD1	2.46	0.49
1:A:461:GLN:HG2	1:B:526:PRO:CG	2.43	0.48
1:A:461:GLN:OE1	1:A:549:GLN:HB2	2.14	0.48
1:B:140:ASP:OD1	1:B:145:ARG:NH1	2.41	0.48
1:A:205:MET:HG2	1:A:335:SER:HB3	1.96	0.48
1:B:141:ASN:ND2	1:B:221:ASP:OD1	2.46	0.48
1:A:233:ALA:HB1	1:B:130:TYR:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLN:O	1:B:536:ARG:NH2	2.47	0.48
1:A:301:LEU:HD22	1:A:304:ALA:HB3	1.96	0.48
1:B:140:ASP:OD1	1:B:140:ASP:N	2.42	0.48
1:B:39:ASN:ND2	1:B:114:ASP:OD2	2.44	0.47
1:B:412:SER:O	1:B:544:TYR:HE1	1.97	0.47
1:B:144:GLN:OE1	1:B:343:ARG:NH2	2.39	0.47
1:B:386:ALA:HB2	1:B:544:TYR:CD1	2.49	0.47
1:B:301:LEU:HD22	1:B:304:ALA:HB3	1.96	0.47
1:A:141:ASN:ND2	1:A:221:ASP:OD1	2.46	0.47
1:B:205:MET:HG2	1:B:335:SER:HB3	1.96	0.47
1:A:386:ALA:HB2	1:A:544:TYR:CD1	2.49	0.47
1:A:412:SER:O	1:A:544:TYR:HE1	1.97	0.47
1:B:412:SER:OG	1:B:413:GLU:N	2.48	0.47
1:B:489:ASP:N	1:B:489:ASP:OD1	2.45	0.47
1:A:412:SER:OG	1:A:413:GLU:N	2.48	0.47
1:B:461:GLN:OE1	1:B:549:GLN:HB2	2.14	0.47
1:B:467:ASP:OD1	1:B:467:ASP:N	2.46	0.46
1:A:489:ASP:N	1:A:489:ASP:OD1	2.45	0.46
1:A:551:THR:OG1	1:A:552:SER:N	2.48	0.46
1:A:244:VAL:HG22	1:B:479:LYS:HB3	1.97	0.46
1:A:502:LEU:HD12	1:A:505:LEU:HD13	1.98	0.46
1:A:526:PRO:HG3	1:B:461:GLN:HG2	1.97	0.46
1:A:289:ILE:HG21	1:A:310:VAL:HG12	1.98	0.46
1:B:151:GLU:OE1	1:B:155:ARG:NH2	2.48	0.46
1:A:395:SER:HB2	1:A:402:PRO:HA	1.97	0.46
1:B:395:SER:HB2	1:B:402:PRO:HA	1.98	0.46
1:A:28:LEU:HD22	1:A:31:LEU:HD12	1.98	0.46
1:A:140:ASP:N	1:A:140:ASP:OD1	2.42	0.46
1:A:473:GLN:O	1:A:536:ARG:NH2	2.47	0.46
1:A:459:LEU:HB2	1:A:547:LEU:HA	1.99	0.45
1:B:428:THR:HA	1:B:431:LEU:HD13	1.98	0.45
1:B:551:THR:OG1	1:B:552:SER:N	2.48	0.45
1:A:257:LEU:HD12	1:B:109:VAL:HG13	1.98	0.45
1:A:151:GLU:OE1	1:A:155:ARG:NH2	2.48	0.45
1:A:461:GLN:HG2	1:B:526:PRO:HG3	1.99	0.45
1:B:413:GLU:N	1:B:544:TYR:OH	2.49	0.45
1:A:138:ASP:OD1	1:A:138:ASP:N	2.50	0.45
1:A:428:THR:HA	1:A:431:LEU:HD13	1.97	0.45
1:A:559:GLU:OE1	1:A:579:ARG:NE	2.50	0.45
1:B:502:LEU:HD12	1:B:505:LEU:HD13	1.98	0.45
1:B:417:LEU:HD22	1:B:588:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LEU:HB2	1:B:547:LEU:HA	1.99	0.45
1:B:559:GLU:OE1	1:B:579:ARG:NE	2.50	0.45
1:A:413:GLU:N	1:A:544:TYR:OH	2.49	0.45
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.86	0.45
1:A:39:ASN:ND2	1:A:114:ASP:OD2	2.44	0.44
1:A:386:ALA:N	1:A:411:ILE:O	2.50	0.44
1:A:119:LEU:HD11	1:A:344:ILE:HG23	1.99	0.44
1:B:138:ASP:N	1:B:138:ASP:OD1	2.50	0.44
1:B:289:ILE:HG21	1:B:310:VAL:HG12	1.98	0.44
1:A:399:SER:OG	1:A:400:ASP:N	2.51	0.44
1:B:28:LEU:HD22	1:B:31:LEU:HD12	1.98	0.44
1:B:119:LEU:HD11	1:B:344:ILE:HG23	1.99	0.44
1:B:412:SER:C	1:B:544:TYR:OH	2.56	0.44
1:A:25:LEU:O	1:A:29:LYS:N	2.51	0.44
1:A:145:ARG:HA	1:A:149:ASP:HB2	2.00	0.44
1:A:417:LEU:HD22	1:A:588:LEU:HD12	1.99	0.44
1:B:50:THR:HG23	1:B:166:ILE:HD13	2.00	0.44
1:B:225:LYS:HA	1:B:225:LYS:HD2	1.89	0.44
1:A:50:THR:HG23	1:A:166:ILE:HD13	2.00	0.43
1:A:412:SER:C	1:A:544:TYR:OH	2.56	0.43
1:B:25:LEU:O	1:B:29:LYS:N	2.50	0.43
1:A:389:LEU:HB2	1:A:409:LEU:HB3	2.00	0.43
1:A:131:THR:HG22	1:A:135:LEU:HD12	2.01	0.43
1:B:386:ALA:N	1:B:411:ILE:O	2.50	0.43
1:A:352:LEU:O	1:A:355:SER:OG	2.32	0.43
1:A:526:PRO:O	1:A:552:SER:OG	2.32	0.43
1:B:399:SER:OG	1:B:400:ASP:N	2.51	0.43
1:A:134:VAL:HG23	1:A:135:LEU:HG	2.01	0.43
1:A:555:THR:HB	1:A:579:ARG:HH21	1.83	0.43
1:B:277:PHE:HE2	1:B:325:THR:HA	1.84	0.43
1:A:279:TYR:HB3	1:B:90:ILE:HD12	2.00	0.42
1:B:253:LEU:HG	1:B:257:LEU:HD23	2.02	0.42
1:A:277:PHE:HE2	1:A:325:THR:HA	1.84	0.42
1:A:524:LEU:HB3	1:A:525:SER:H	1.69	0.42
1:B:131:THR:HG22	1:B:135:LEU:HD12	2.01	0.42
1:A:90:ILE:HD12	1:B:279:TYR:HB3	2.02	0.42
1:B:145:ARG:HA	1:B:149:ASP:HB2	2.00	0.42
1:B:555:THR:HB	1:B:579:ARG:HH21	1.83	0.42
1:A:112:ARG:HH11	1:B:260:GLN:HE22	1.67	0.42
1:B:134:VAL:HG23	1:B:135:LEU:HG	2.01	0.42
1:A:140:ASP:OD1	1:A:145:ARG:NH1	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:VAL:HA	1:A:561:GLU:HB3	2.02	0.42
1:B:251:ARG:HE	1:B:251:ARG:HB2	1.62	0.42
1:B:459:LEU:HD23	1:B:459:LEU:HA	1.91	0.42
1:B:525:SER:HB3	1:B:528:GLU:HG2	2.02	0.42
1:B:558:VAL:HA	1:B:561:GLU:HB3	2.02	0.42
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.88	0.42
1:A:223:ARG:HG3	1:B:227:MET:HE1	2.02	0.42
1:A:253:LEU:HG	1:A:257:LEU:HD23	2.02	0.42
1:A:525:SER:HB3	1:A:528:GLU:HG2	2.02	0.42
1:B:389:LEU:HB2	1:B:409:LEU:HB3	2.00	0.42
1:A:109:VAL:HG13	1:B:257:LEU:HD12	2.02	0.41
1:A:587:SER:OG	1:A:588:LEU:N	2.53	0.41
1:A:72:GLY:HA2	1:B:306:LEU:HB3	2.02	0.41
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.94	0.41
1:B:587:SER:OG	1:B:588:LEU:N	2.53	0.41
1:A:526:PRO:HG2	1:B:461:GLN:HG2	2.01	0.41
1:B:394:ILE:O	1:B:403:LEU:N	2.53	0.41
1:A:57:ILE:HA	1:A:60:VAL:HG12	2.03	0.41
1:B:152:ARG:HB3	1:B:340:TYR:CE2	2.56	0.41
1:B:600:LEU:HA	1:B:600:LEU:HD23	1.81	0.41
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.88	0.41
1:A:522:ASP:OD1	1:A:523:VAL:HG23	2.21	0.41
1:A:604:LYS:HA	1:A:604:LYS:HD3	1.87	0.41
1:B:90:ILE:HD13	1:B:90:ILE:HA	1.91	0.41
1:B:118:HIS:HA	1:B:121:ARG:HH21	1.86	0.41
1:B:522:ASP:OD1	1:B:523:VAL:HG23	2.21	0.41
1:A:118:HIS:HA	1:A:121:ARG:HH21	1.86	0.40
1:A:218:LEU:HD12	1:A:259:THR:HG21	2.03	0.40
1:A:280:LEU:HB2	1:B:90:ILE:HG21	2.03	0.40
1:B:31:LEU:O	1:B:39:ASN:ND2	2.41	0.40
1:B:385:THR:CA	1:B:411:ILE:O	2.65	0.40

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	561/648 (87%)	510 (91%)	51 (9%)	0	100	100
1	B	561/648 (87%)	510 (91%)	51 (9%)	0	100	100
All	All	1122/1296 (87%)	1020 (91%)	102 (9%)	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	506/563 (90%)	506 (100%)	0	100	100
1	B	506/563 (90%)	506 (100%)	0	100	100
All	All	1012/1126 (90%)	1012 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	GLN
1	B	549	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ATP	B	701	-	26,33,33	0.65	0	31,52,52	0.73	1 (3%)
2	ATP	A	701	-	26,33,33	0.65	0	31,52,52	0.72	1 (3%)

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
2	ATP	B	701	-	-	8/18/38/38	0/3/3/3
2	ATP	A	701	-	-	8/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ATP	C5-C6-N6	2.29	123.83	120.35
2	A	701	ATP	C5-C6-N6	2.27	123.80	120.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	O4'-C4'-C5'-O5'

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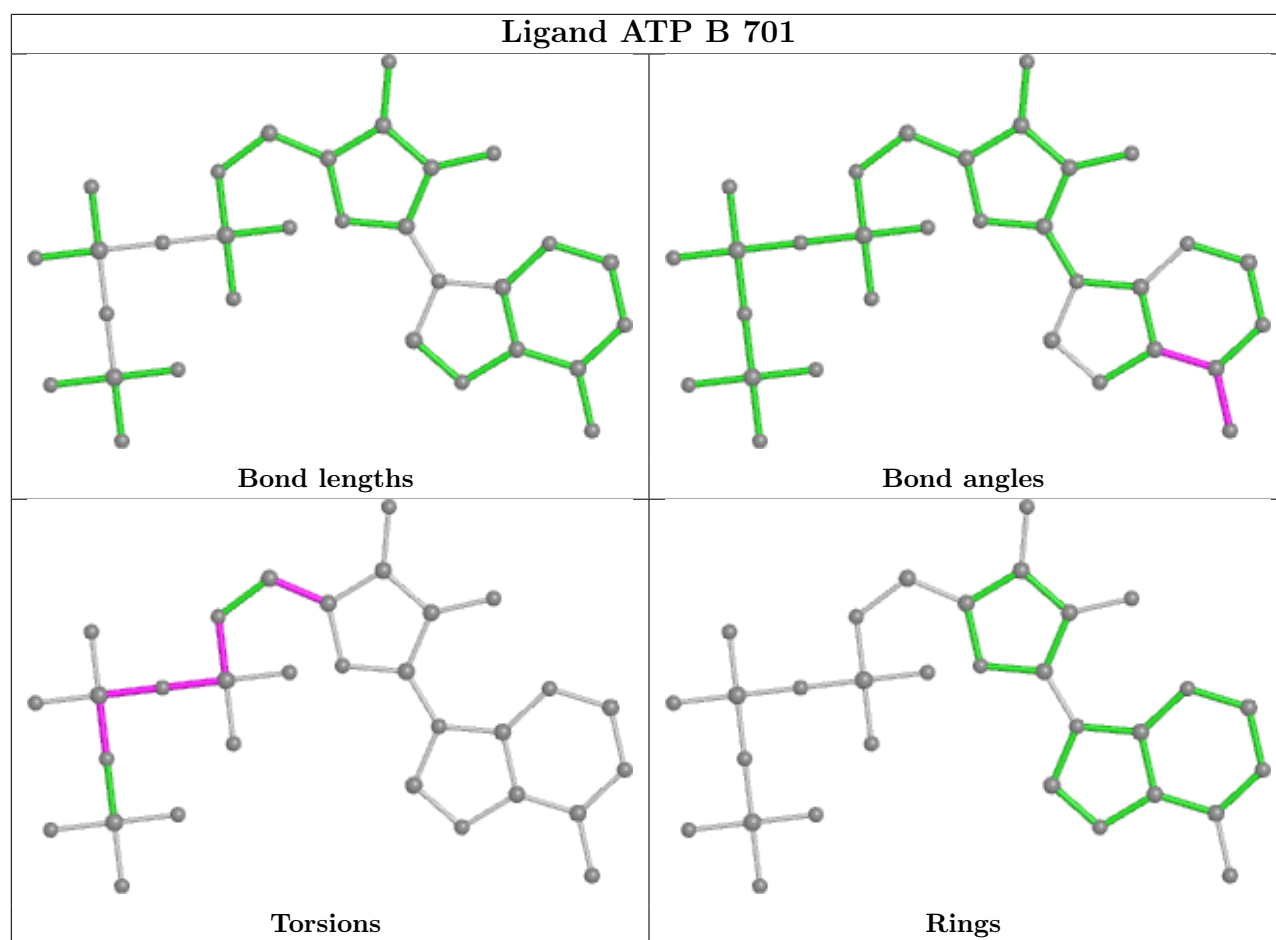
Mol	Chain	Res	Type	Atoms
2	B	701	ATP	O4'-C4'-C5'-O5'
2	A	701	ATP	PA-O3A-PB-O1B
2	A	701	ATP	PB-O3A-PA-O1A
2	B	701	ATP	PA-O3A-PB-O1B
2	B	701	ATP	PB-O3A-PA-O1A
2	A	701	ATP	PG-O3B-PB-O1B
2	B	701	ATP	PG-O3B-PB-O1B
2	A	701	ATP	PA-O3A-PB-O2B
2	A	701	ATP	PB-O3A-PA-O2A
2	B	701	ATP	PA-O3A-PB-O2B
2	B	701	ATP	PB-O3A-PA-O2A
2	A	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O1A
2	A	701	ATP	C3'-C4'-C5'-O5'
2	B	701	ATP	C3'-C4'-C5'-O5'

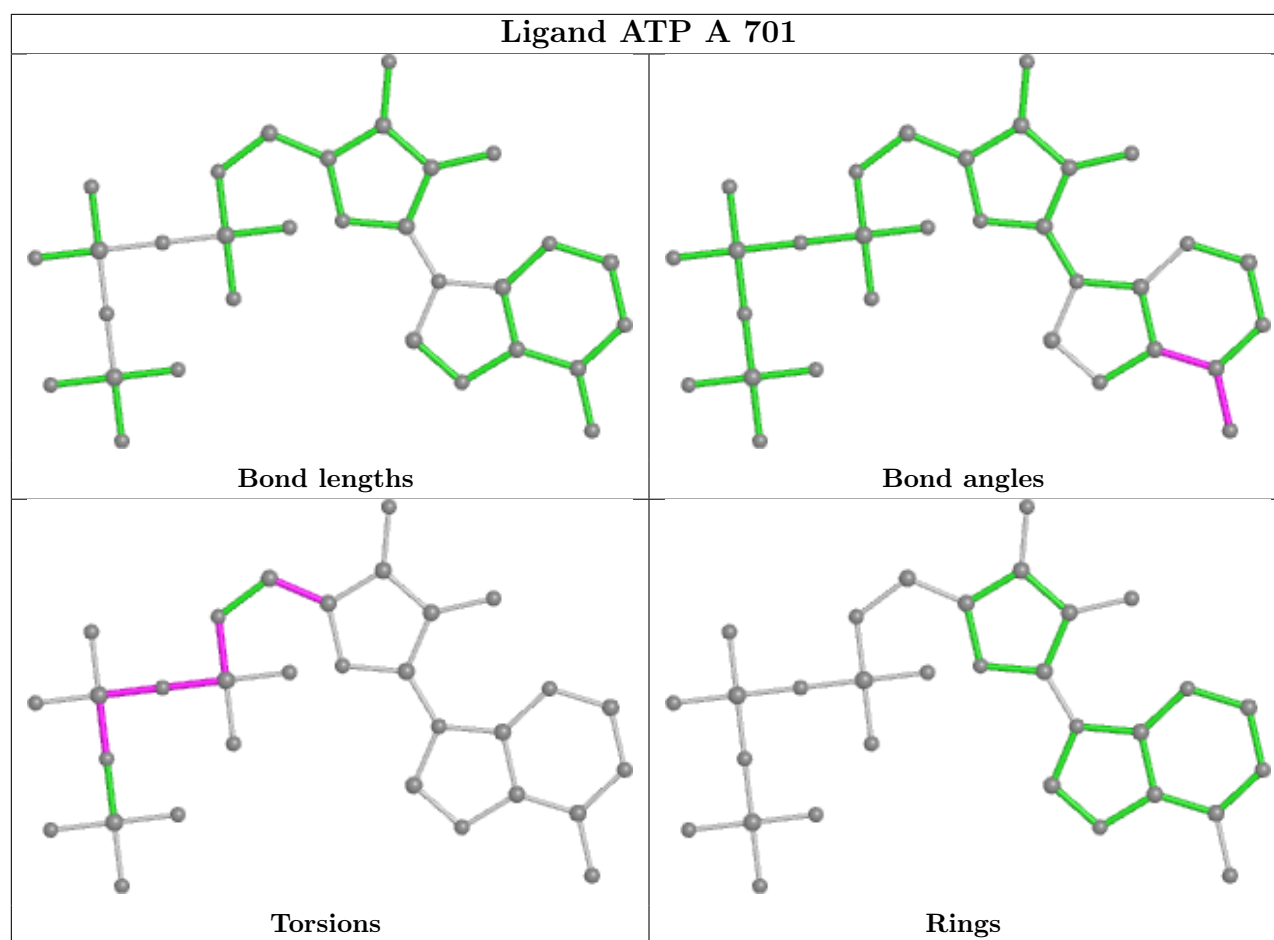
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ATP	2	0
2	A	701	ATP	2	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.

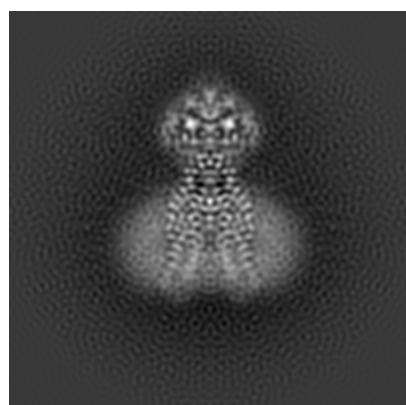
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9791. These allow visual inspection of the internal detail of the map and identification of artifacts.

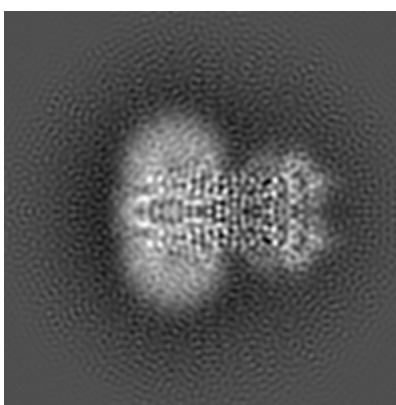
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

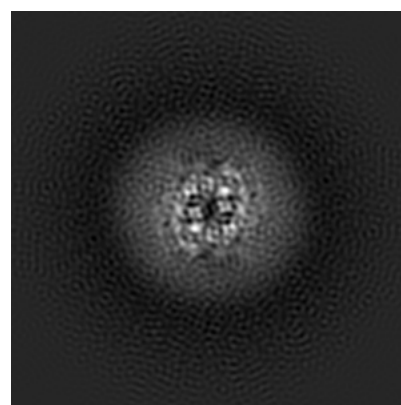
#### 6.1.1 Primary map



X



Y

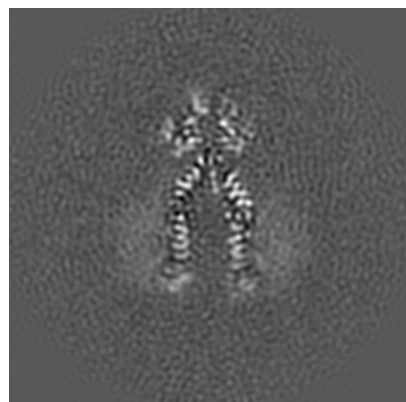


Z

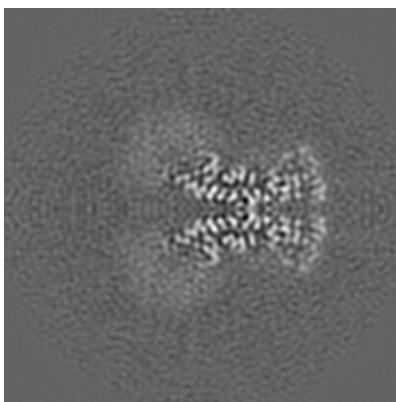
The images above show the map projected in three orthogonal directions.

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

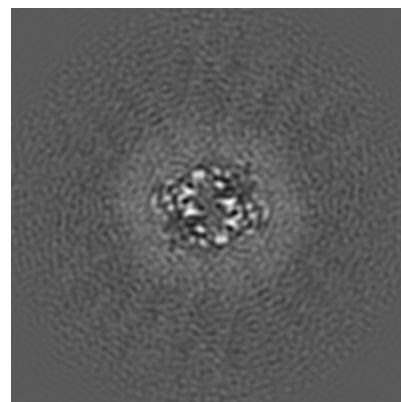
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

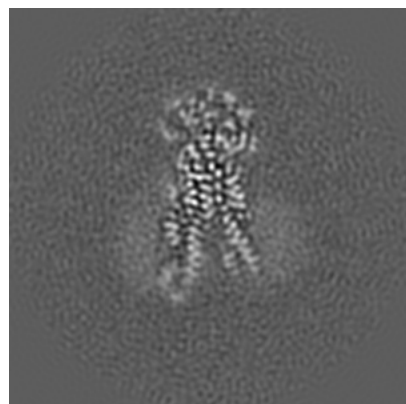


Z Index: 100

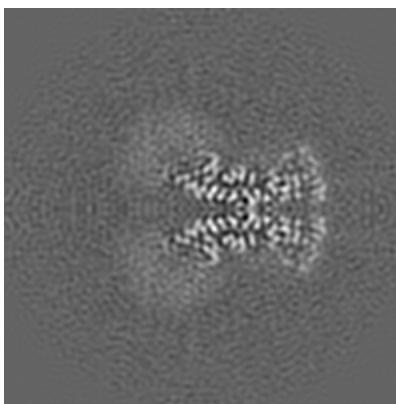
The images above show central slices of the map in three orthogonal directions.

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

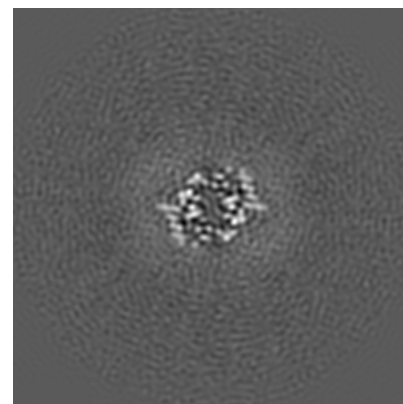
### 6.3.1 Primary map



X Index: 91



Y Index: 100



Z Index: 105

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

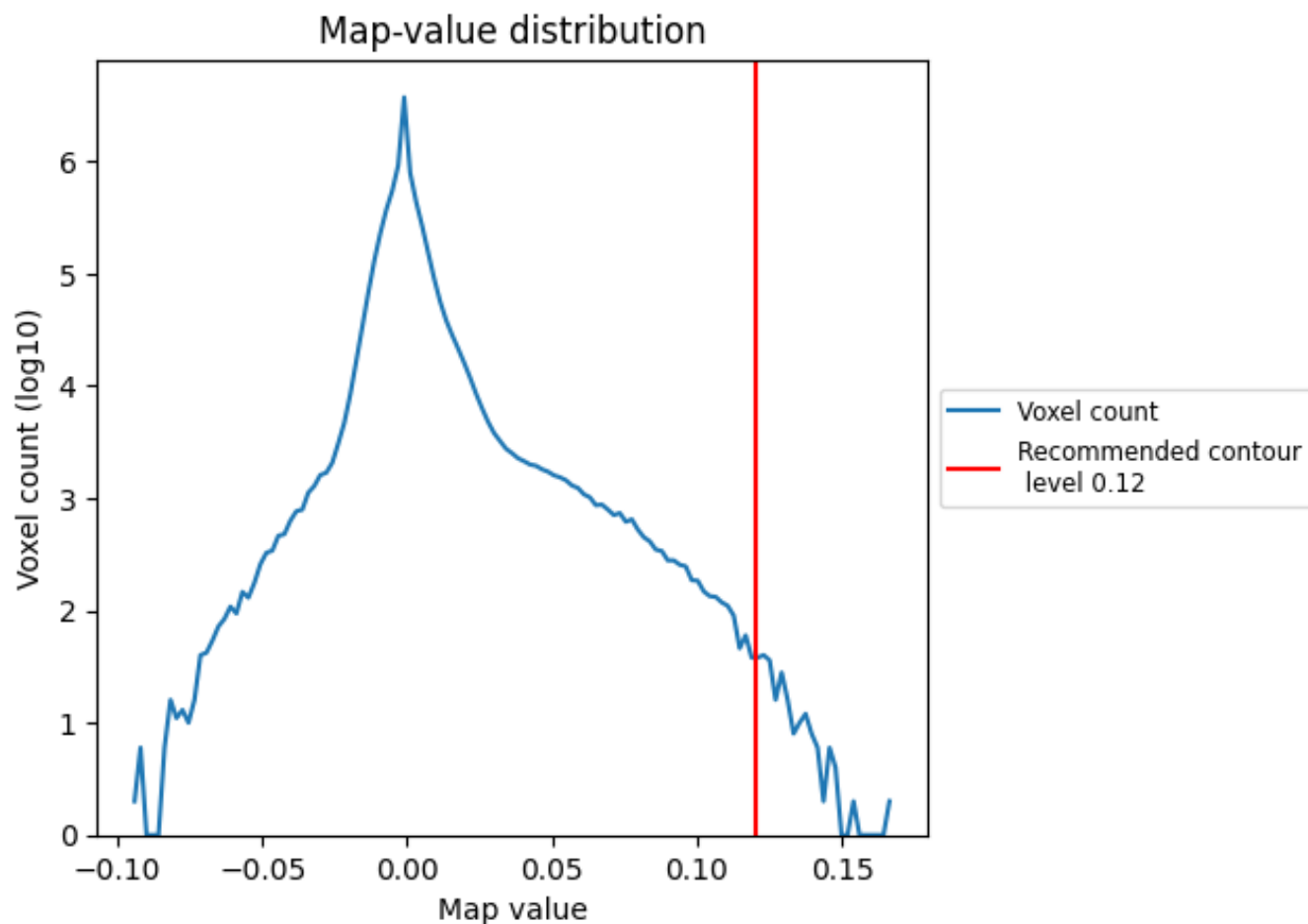
## 6.5 Mask visualisation

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.

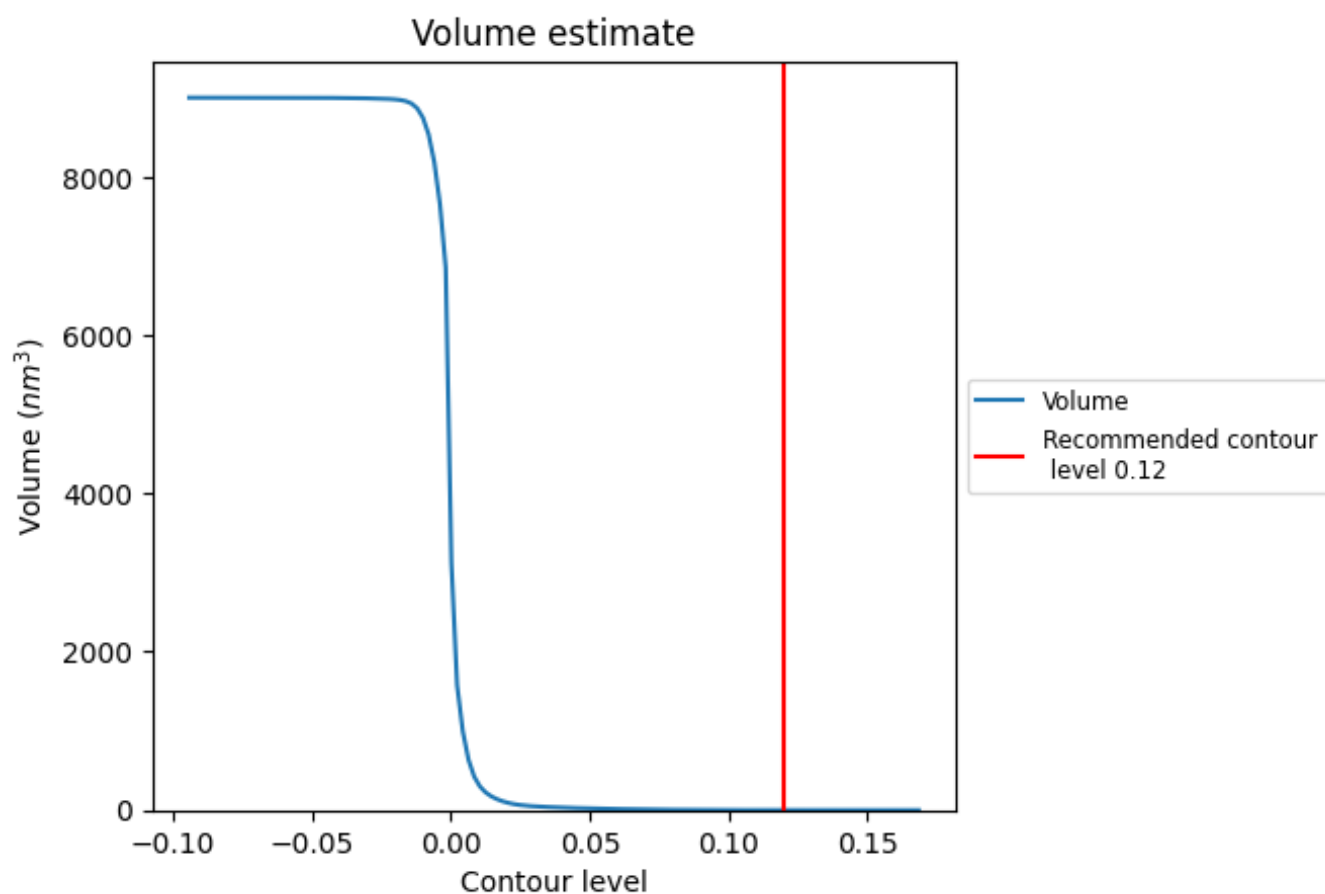
### 7.1 Map-value distribution [i](#)



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.



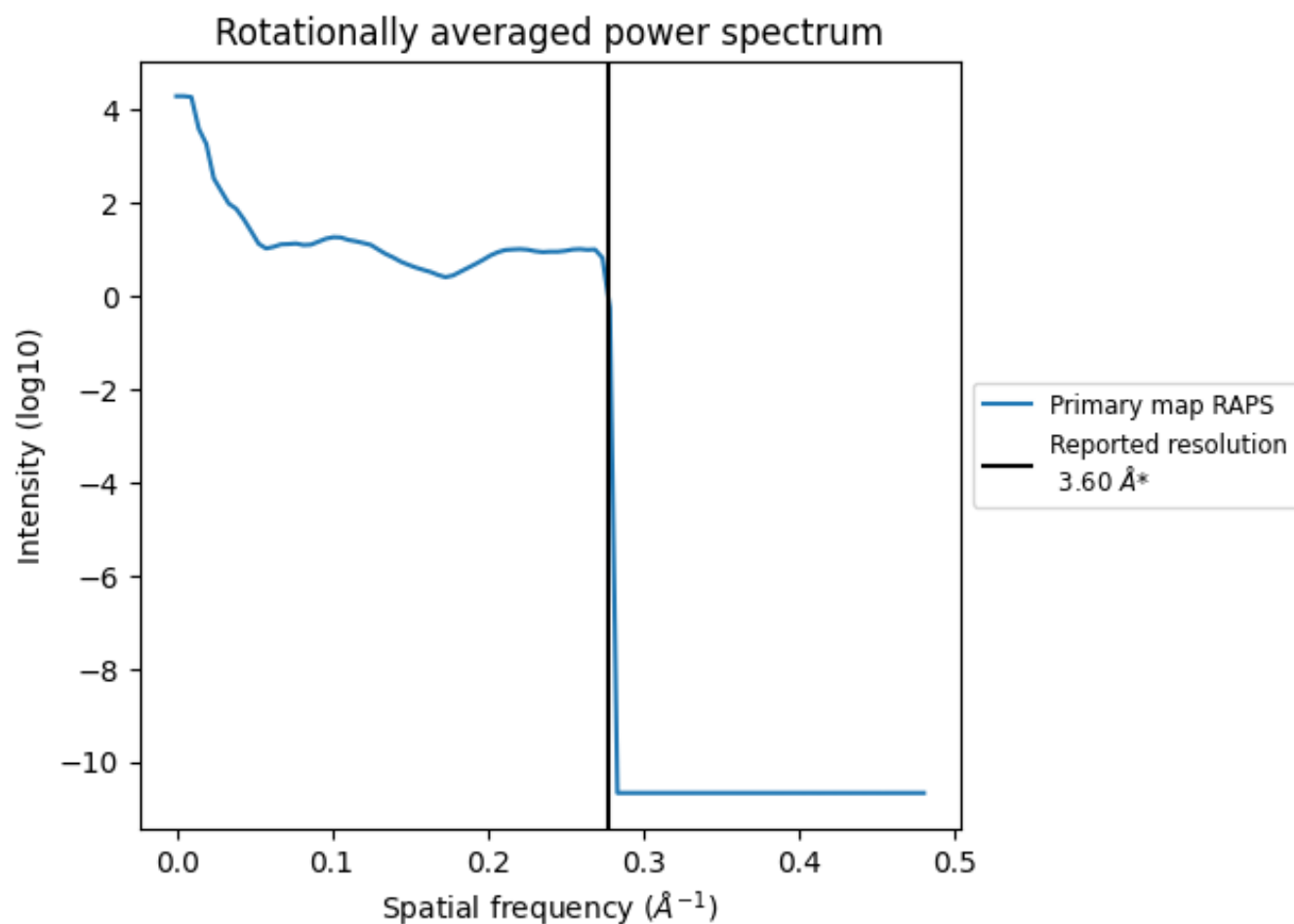
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 0 nm<sup>3</sup>; this corresponds to an approximate mass of 0 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 0.278 Å<sup>-1</sup>

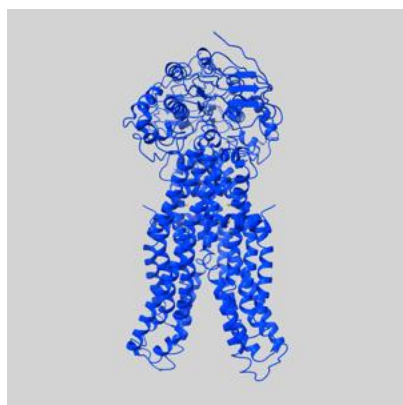
## 8 Fourier-Shell correlation ⓘ

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

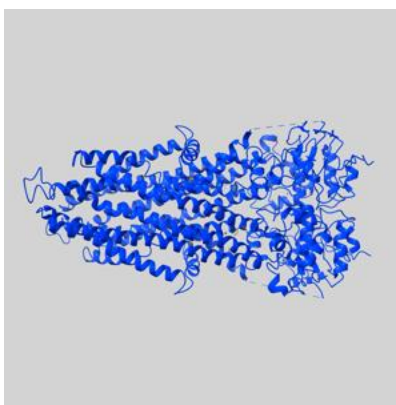
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9791 and PDB model 6JBJ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

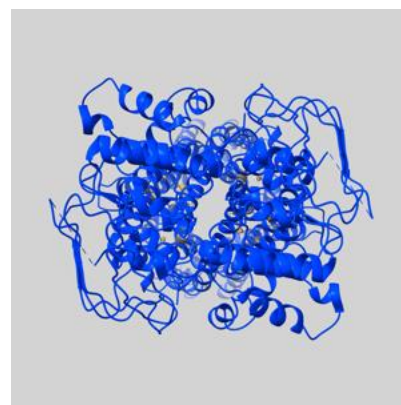
### 9.1 Map-model overlay [i](#)



X



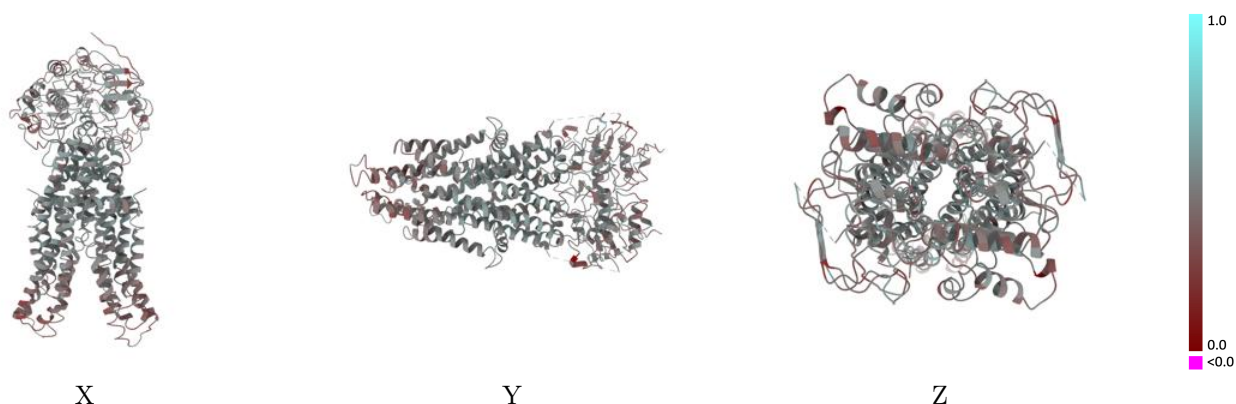
Y



Z

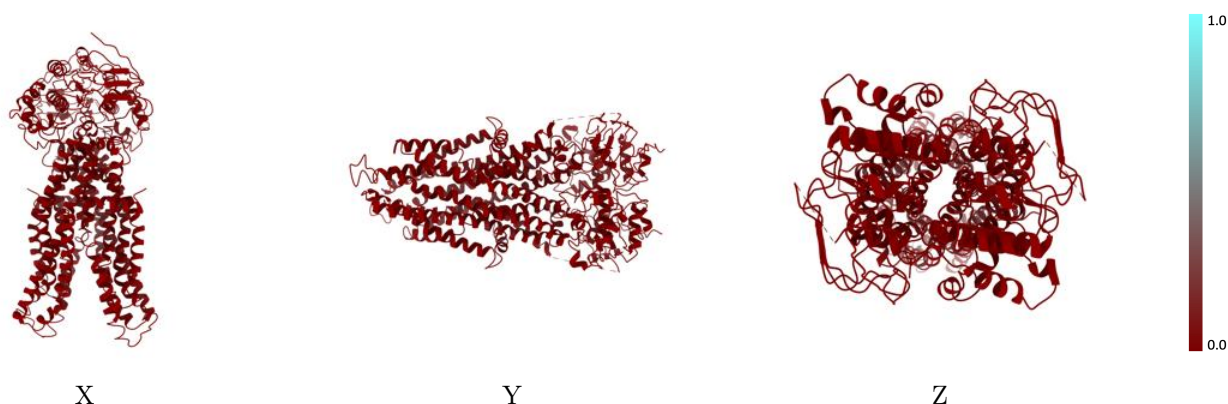
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



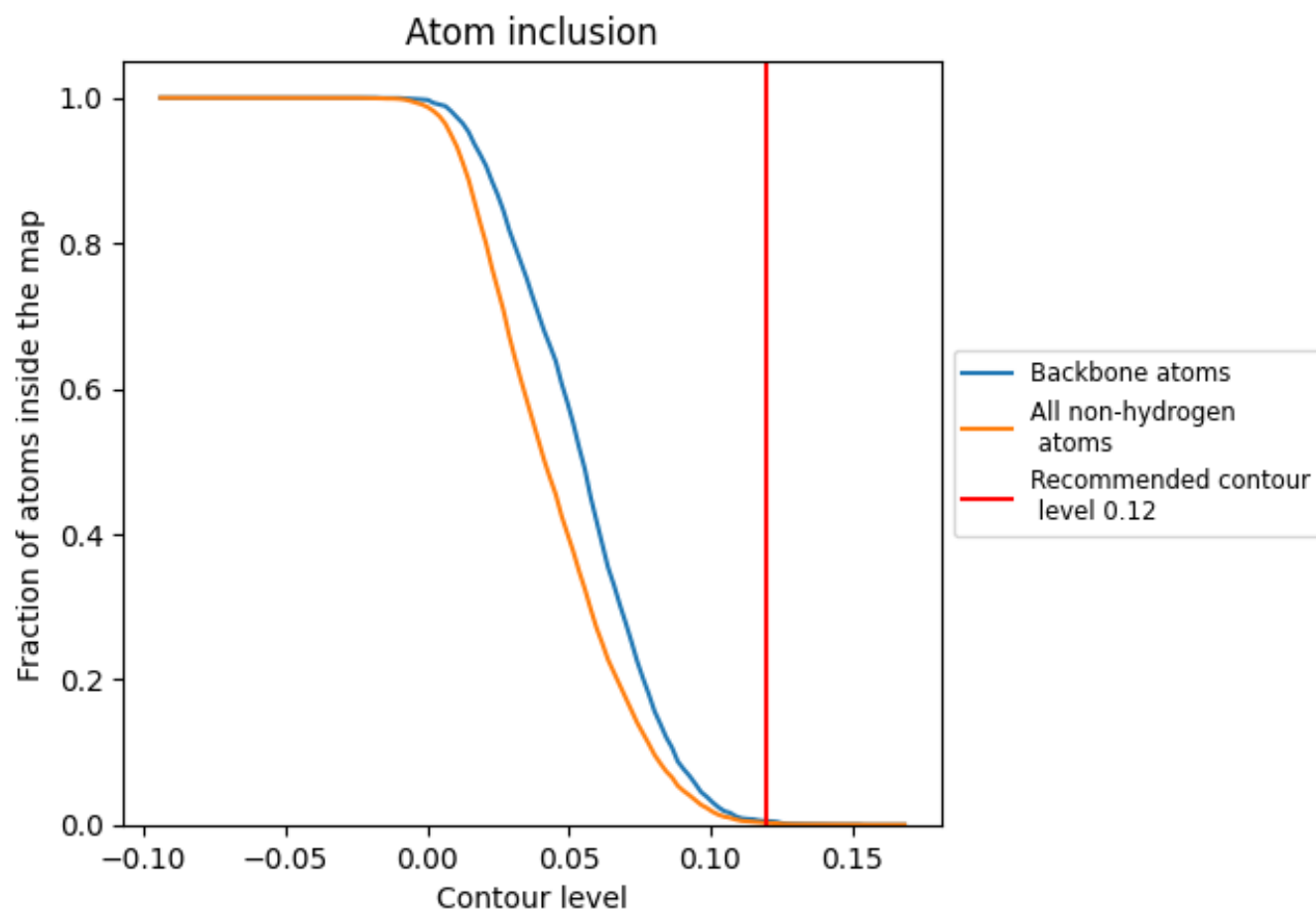
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.0025	<div><div></div></div> 0.4580
A	<div><div></div></div> 0.0025	<div><div></div></div> 0.4570
B	<div><div></div></div> 0.0025	<div><div></div></div> 0.4580

