



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 09:40 AM EST

PDB ID : 7K5B  
EMDB ID : EMD-22679  
Title : Structure of outer-arm dynein bound to microtubule doublet in microtubule binding state 2 (MTBS-2)  
Authors : Rao, Q.; Zhang, K.  
Deposited on : 2020-09-16  
Resolution : 4.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

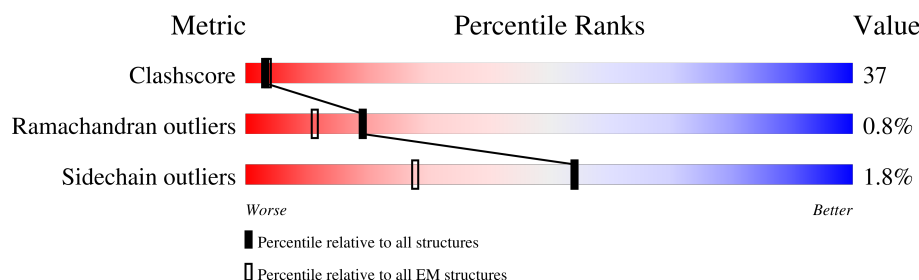
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

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




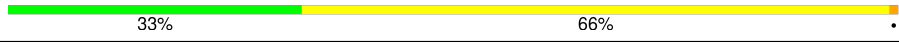
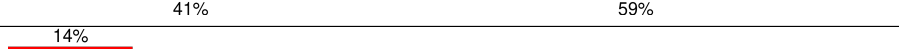




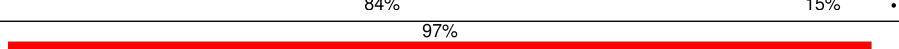

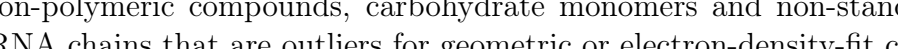
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4615	
2	B	4588	
3	C	3947	
4	D	595	
5	E	557	
6	F	128	
7	G	151	
8	H	91	

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Mol	Chain	Length	Quality of chain
9	I	106	
10	J	95	
11	K	90	
12	L	111	
13	M	87	
14	N	114	
15	O	120	
16	P	112	
17	Q	192	
18	R	150	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	ADP	A	4701	-	-	X	-
19	ADP	A	4901	-	-	X	-
19	ADP	B	5501	-	-	X	-
19	ADP	C	4702	-	-	X	-
20	ATP	A	4801	-	-	X	-
20	ATP	B	5601	-	-	X	-
21	MG	A	5002	-	-	X	-

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 119573 atoms, of which 156 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 Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4453	Total	C	N	O	S	0	0
			33975	21575	5802	6440	158		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3238	ASN	ASP	conflict	UNP Q22A67

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4524	Total	C	N	O	S	0	0
			34751	22080	5950	6571	150		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	ALA	GLN	conflict	UNP I7M9J2
B	1287	ALA	LEU	conflict	UNP I7M9J2
B	3977	ALA	SER	conflict	UNP I7M9J2

- Molecule 3 is a protein called gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	3947	Total	C	N	O	S	0	0
			30427	19395	5159	5724	149		

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	579	Total	C	N	O	S	0	0
			4680	2975	791	883	31		

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	555	Total	C	N	O	S	0	0
			4440	2798	762	858	22		

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	128	Total	C	N	O	S	0	0
			996	625	176	193	2		

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1024	636	184	203	1		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	106	Total	C	N	O	S	0	0
			827	526	134	161	6		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	95	Total	C	N	O	S	0	0
			807	527	135	140	5		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			754	489	124	137	4		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	111	Total	C	N	O	S	0	0
			855	555	145	152	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	87	Total	C	N	O	S	0	0
			735	477	123	130	5		

- Molecule 14 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	N	O	S	0	0
			852	542	142	165	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	92	ALA	ASN	conflict	UNP A4VEB3

- Molecule 15 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	120	Total	C	N	O	S	0	0
			994	639	173	179	3		

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	109	Total	C	N	O	0	0
			541	323	109	109		

- Molecule 17 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	192	Total	C	N	O	0	0
			1006	610	203	193		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ALA	SER	conflict	UNP Q1HGH9

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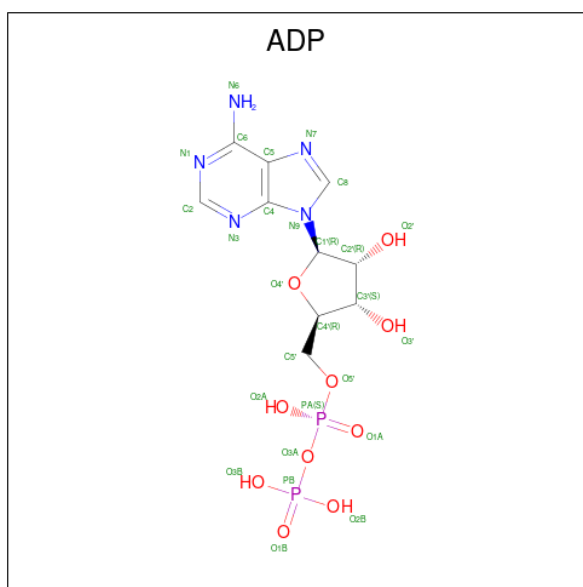
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Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	MET	TYR	conflict	UNP Q1HGH9

- Molecule 18 is a protein called Dynein light chain 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	150	Total	C	H	N	O	0	0
			895	439	156	150	150		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

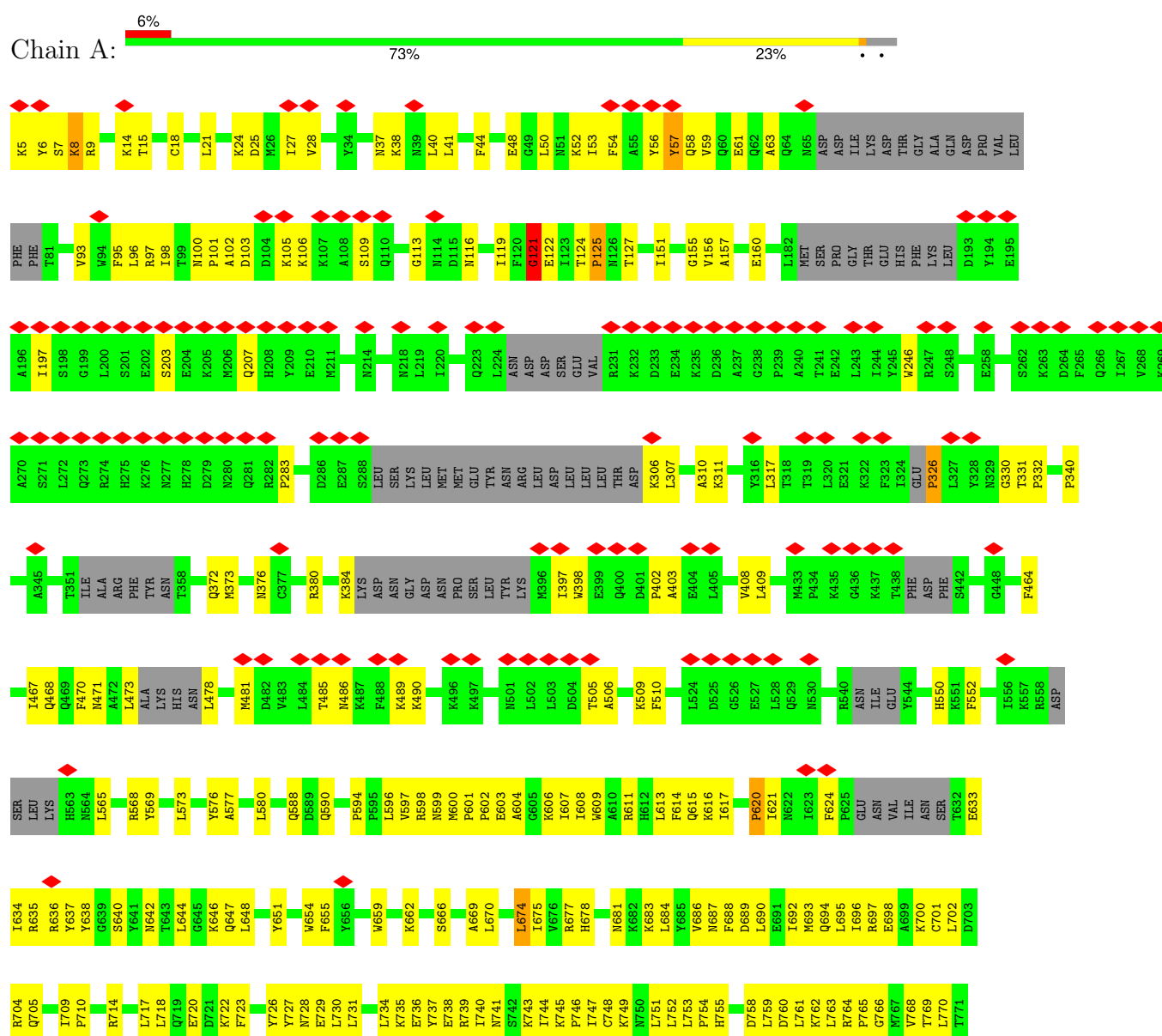
Mol	Chain	Residues	Atoms	AltConf
21	A	3	Total Mg 3 3	0
21	B	3	Total Mg 3 3	0
21	C	3	Total Mg 3 3	0



### 3 Residue-property plots

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

- Molecule 1: Dynein heavy chain, outer arm protein





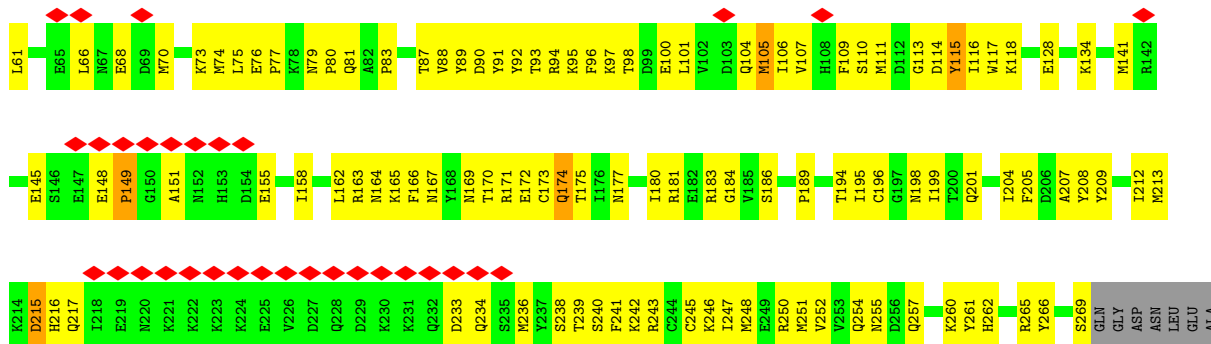
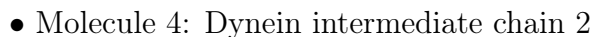
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V4121	D3854	K3622	S3455	I3346	D3283	K3216	L3121	L2951	E2772	S2488	L2298	S2084
V4126	A3855	K3627	C3457	K3349	M3284	D3219	I3124	R2956	K2776	A2489	R2311	D2089
I4130	A3879	C3627	T3485	P3351	F3286	V3291	Q3126	L2960	C2786	G2496	R2316	R2095
S4138	E3895	A3630	R3488	K3352	K3287	E3222	E3127	I2963	V2783	T2497	R2316	G2096
I4155	L3896	E3637	L3488	R3353	K3288	E3222	T3128	I2963	I2794	A2498	E2319	G2096
P4180	D3898	L3638	F3493	Q3354	K3289	K3224	I3131	I2963	N2795	T2499	Y2330	L2097
GLN	I3900	K3641	D3496	V3356	L3290	A3226	E3140	M2372	E2796	T2500	F2336	L2098
PRD	S3903	F3647	I3500	E3360	F3293	P3229	E3141	I2976	D2797	D2511	F2336	I2101
ASN	N3914	T3648	A3378	L3377	L3230	D3231	Q3144	F2987	D2797	K2514	Q2340	K2106
SER	Q3651	Q3651	Q3379	A3378	I3232	I3232	L3145	R2982	I2799	M2515	S2341	E2117
I4185	I3380	I3380	I3380	I3380	K3234	K3234	N3146	R2982	I2800	K2553	V2357	I2120
S4190	D3532	L3654	P3533	Y3383	I3298	Y3235	E3147	L2999	E2801	N2564	T3380	F2121
V4194	Q3534	N3684	Q3534	I3384	N3299	I3236	A3148	C3000	E2802	F2566	T3380	E2122
I4209	G3535	L3691	G3535	K3386	E3300	K3237	T3149	L3018	E2803	V2567	L2363	I2141
D4209	Q3536	L3696	Q3537	L3387	E3301	M3237	E3162	C3022	A2804	Q2573	C2367	I2142
V4240	P3538	L3696	G3538	K3388	I3302	N3238	S3163	W3026	K2836	L2576	V2372	I2155
D4241	Q3539	S3702	K3389	D3389	I3306	L3240	K3164	T3041	L2839	L2576	V2372	G2162
GLY	W3540	S3702	V3390	V3390	E3307	V3242	K3165	F3042	V2840	M2602	F2386	K2163
GLY	I3541	L3706	I3541	E3396	I3310	F3243	Q3179	F3046	L2850	I2608	S2390	S2164
Q4245	K3544	L3707	L3544	E3396	Q3112	F3244	Q3179	L3049	G2863	N2611	L2411	L2170
P4252	L3545	D3709	S3546	N3399	S3313	I3251	Q3179	L3059	V2866	T2621	I2418	T2171
Y4265	S3546	T3710	S3546	E3402	E3314	Q3252	Q3179	M3060	G2870	R2624	Q2420	T2175
P4270	I3549	L3711	I3549	A3406	D3315	E3254	Q3179	L3067	S2871	K2663	K2421	T2183
T4287	R3553	L3712	R3553	K3410	W3316	E3255	E3185	H3067	G2870	L2668	E2426	M2196
G4313	C3554	V3715	C3554	K3410	I3322	R3257	Q3186	R3083	S2875	L2668	T2426	E2202
E4317	H3560	L3716	H3560	S3421	T3323	F3258	I3187	F3092	L2876	W2676	V2428	I2203
Q4321	P3561	N3718	P3561	L3422	K3324	K3260	S3188	F3092	T2877	N2696	F2429	S2204
L4331	L3568	T3719	L3568	L3422	A3328	K3261	K3191	Y3095	D2901	R2697	D2430	D2205
N4336	E3573	V3726	E3573	E3425	A3329	E3262	E3195	F3095	D2901	E2697	D2436	D2206
E4339	T3577	R3748	T3577	W3429	A3330	G3263	E3193	Y3099	D2905	L2699	C2443	V2211
E4342	I3583	P3749	I3583	I3436	I3332	K3264	A3194	K3100	I2906	I2723	W2448	V2220
L4347	E3584	T3752	E3584	K3440	L3333	V3266	R3196	T3101	K2907	L2723	V2448	N2220
L4368	N3585	R3753	N3585	R3441	K3334	L3267	R3196	Y3103	T2921	L2727	P2450	L2224
V4382	V3587	S3755	V3587	K3442	W3335	F3268	E3105	F3104	F2922	F2728	P2450	P2451
	D3592	L3803	D3592	L3443	A3338	L3269	K3106	F3105	M2924	L2745	Q2452	Q2452
	P3593	T3824	P3593	V3444	I3339	K3270	K3106	K3106	T2925	V2746	S2453	T2227
	K3604	K3833	K3604	N3446	Y3340	E3271	L3110	L3110	L2935	V2746	T2463	G2259
		T3837		V3447	E3341	S3272	E3114	E3114	L2935	V2746	T2463	G2259
				S3446	K3344	Y3273	E3211	E3211	T2938	V2746	T2463	G2259
				S3450	K3345	D3274	A3211	A3211	T2938	V2746	T2463	G2259
				T3451	K3345	E3275	A3211	A3211	T2938	V2746	T2463	G2259
				A3452	K3346	S3276	A3211	A3211	T2938	V2746	T2463	G2259
				F3453	K3346	G3277	A3211	A3211	T2938	V2746	T2463	G2259
						I3276	A3211	A3211	T2938	V2746	T2463	G2259
						Q3279	A3211	A3211	T2938	V2746	T2463	G2259



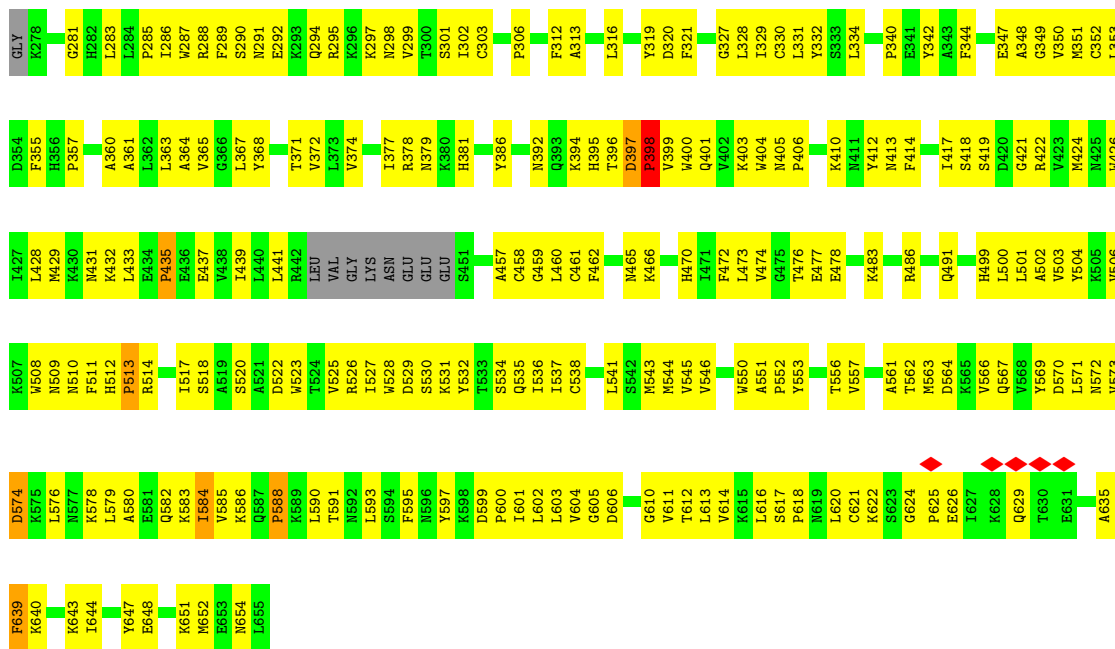
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N2462	K2470	C2479	E2488	N2492	T2493	V2494	D2503	V2512	A2513	T2514	L2515	H2516	R2519	T2526	R2531	A2540	G2543	K2544	T2545	A2546	V2560	S2568	S2569	L2574	Q2577	K2586	N2591	V2592	T2601	M2609	P2610	Y2615	G2616	T2617	Q2618	S2619	P2620	I2621	Q2622														
W2260	D2264	L2267	D2268	P2269	E2270	W2271	R2300	L2301	L2302	F2303	E2304	L2308	R2309	W2310	A2311	E2326	N2332	P2333	Y2334	M2335	E2352	D2363	D2364	V2365	A2366	L2382	D2383	P2395	L2409	D2410	A2411	L2412	L2413	L2417	P2418	D2427	L2432	F2436	L2441	G2445													
L2040	G2044	R2049	L2058	L2066	K2070	L2083	E2084	Q2085	T2116	D2117	D2118	I2121	D2128	L2129	F2130	T2150	T2151	M2155	V2176	R2177	P2185	S2188	G2189	K2190	T2191	C2192	N2203	E2206	D2207	N2214	T2219	F2231	V2237	V2240	M2248	Y2252																	
K1758	N1770	L1771	I1772	E1783	W1784	W1785	K1786	I1787	I1788	T1792	I1793	R1798	I1806	S1819	W1825	I1856	W1857	F1860	Y1863	I1868	K1912	V1922	M1923	W1924	F1925	M1936	G1942	Q1945	S1946	G1947	M1956	V1966	A2009	G2010	R2011	E2023	N2038	W2039															
L1599	K1602	K1603	K1604	S1605	F1606	R1607	K1608	F1609	Y1610	F1611	L1612	L1617	L1618	L1621	S1622	M1623	A1627	P1628	L1634	C1637	F1638	L1641	A1650	M1662	D1666	G1680	A1681	V1682	H1684	L1687	K1705	A1708	W1711	D1715	Q1728	L1731	T1734																
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K1436	E1437	A1438	K1439	E1440	K1441	K1442	L1443	L1444	K1445	N1446	I1447	E1448	Q1449	W1450	Q1454	V1455	F1456	E1457	F1458	T1459	E1460	Y1461	K1462	E1463	T1464	K1465	F1467	S1469	L1470	D1471	M1472	M1473	M1474	L1477	H1480	L1484	M1485	G1486	M1487	K1488	S1489	Q1490	G1491	K1492	Y1493	V1494	E1495	Y1498	D1499	R1500	V1501	E1502	
L1333	K1334	A1335	D1336	I1337	L1338	L1339	D1340	T1341	N1342	K1343	T1344	L1345	G1346	T1347	Q1348	F1349	K1350	N1351	L1352	P1353	K1354	R1357	K1360	T1374	V1375	L1376	P1377	L1378	A1381	M1387	L1395	S1409	F1410	Y1411	F1412	E1413	D1414	L1420	Y1423	E1424	V1427	E1428	E1429	I1430	V1431	D1432	V1433	A1434	Q1435				
V1146	I1147	S1148	L1149	V1150	K1151	D1152	E1153	P1155	R1156	I1160	I1161	L1162	M1163	M1164	K1165	E1166	M1167	K1170	L1171	K1172	K1173	H1174	N1175	V1176	P1177	I1178	T1179	E1180	T1183	D1184	D1185	P1186	I1190	D1191	M1192	N1196	F1197	I1198	E1199	I1200	Y1201	G1202	R1203	V1204	F1205	K1206	V1207	K1208	A1209	D1210	I1211	P1213	
N1079	L1080	Q1081	P1082	M1083	K1084	L1087	V1091	W1094	Y1098	T1099	D1100	F1101	L1102	G1103	N1104	Q1105	F1106	R1107	T1108	Q1109	Q1110	K1111	N1112	L1113	D1114	F1115	I1116	I1117	E1118	K1119	T1120	K1121	D1122	G1123	I1124	K1125	N1127	P1128	A1129	D1130	H1131	E1132	H1135	L1136	K1137	K1138	L1139	L1140	M1141	S1142	V1143	M1144	K1145
N1010	GLU	ASN	GLU	PRO	LYS	ASP	GLU	ASP	GLY	LYS	GLY	ASP	ASP	GLU	GLY	ASN	THR	GLN	LYS	ASN	PRO	LEU	LEU	LYS	GLY	CYS	ARG	ALA	LYS	ILE	PRO	N1046	L1049	F1050	D1051	I1054	T1055	H1056	L1057	K1058	Q1061	I1067	K1068	T1069	P1070	E1071	W1075	L1076	R1077	I1078			



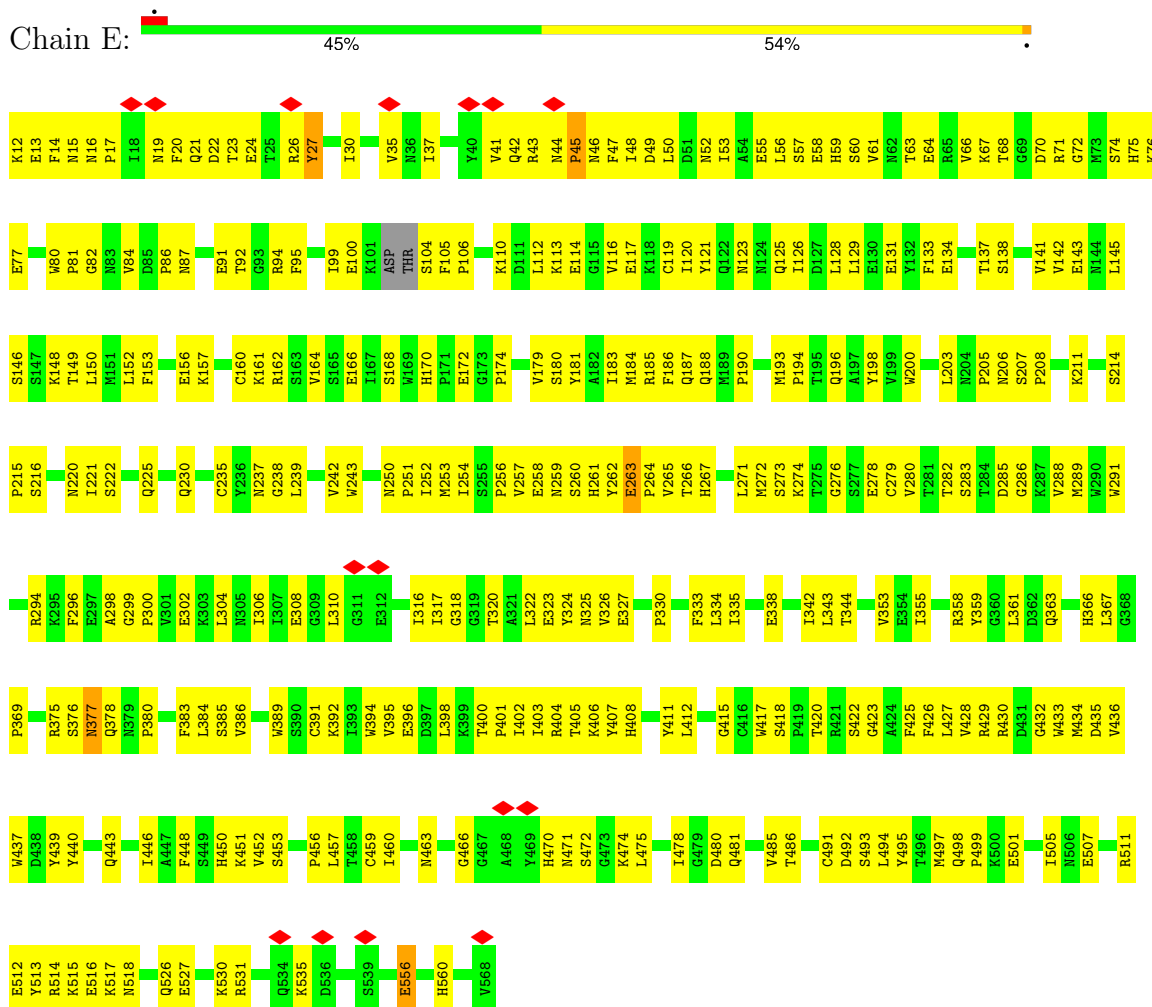




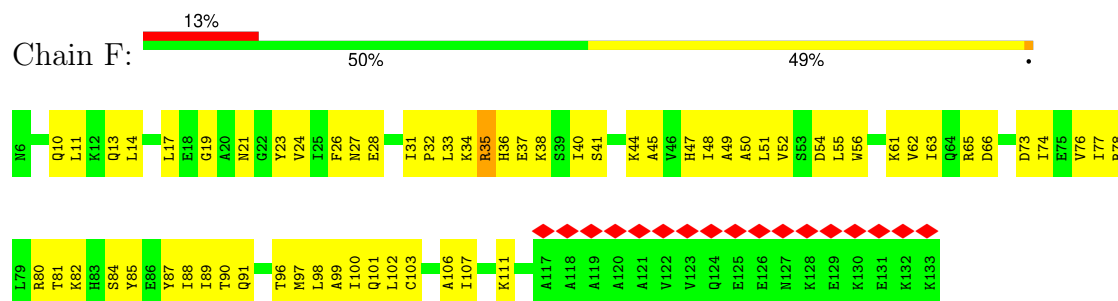




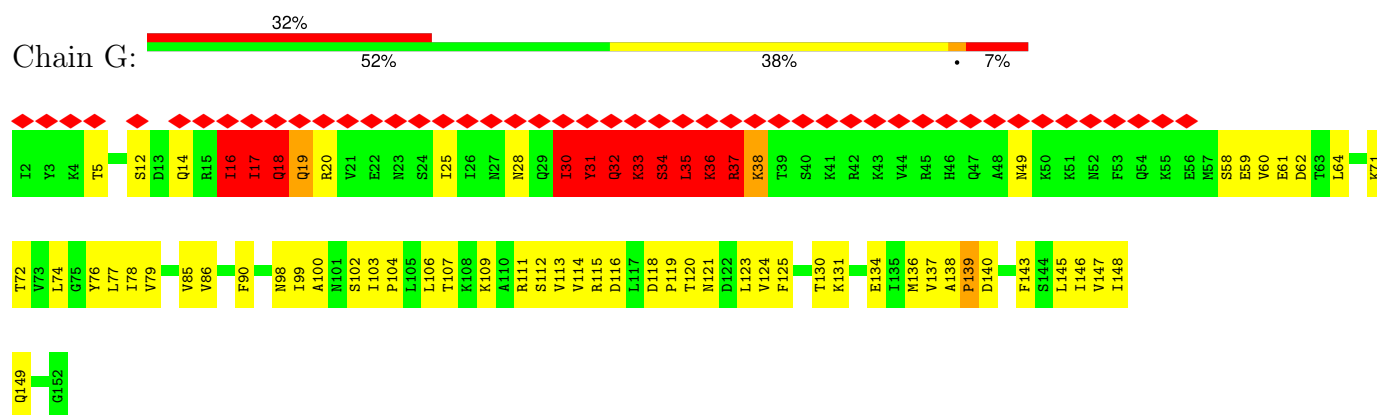
- Molecule 5: Flagellar outer dynein arm intermediate protein, putative



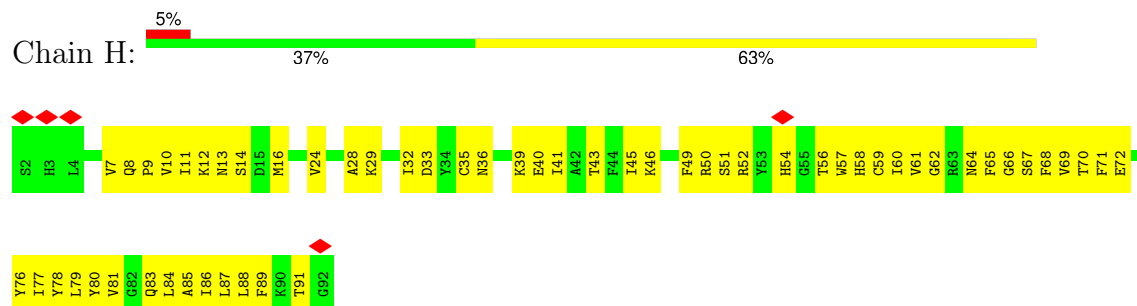
- Molecule 6: Dynein light chain roadblock-type 2 protein



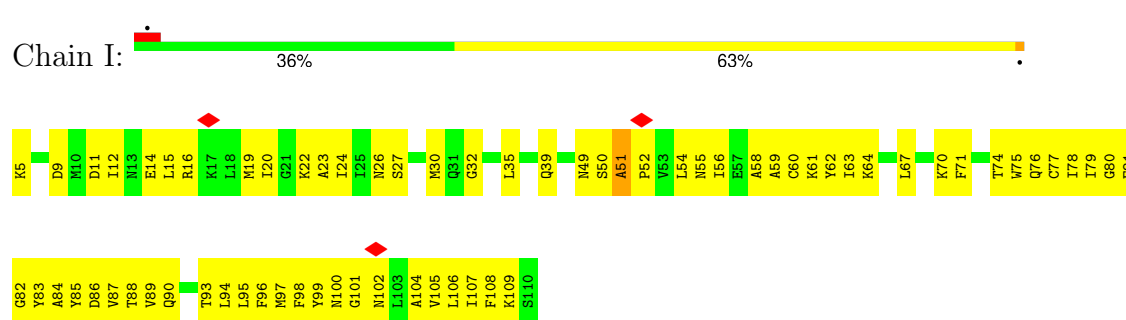
- Molecule 7: Dynein light chain roadblock-type 2 protein



- Molecule 8: Dynein light chain

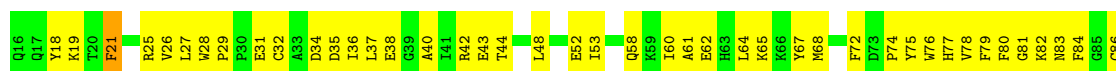


- Molecule 9: Dynein light chain



- Molecule 10: Dynein light chain





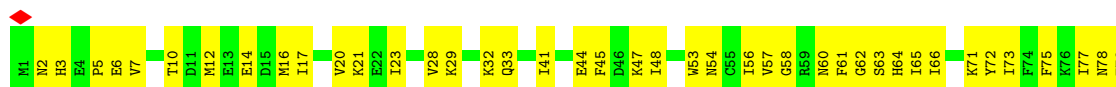
• Molecule 11: Dynein light chain



• Molecule 12: Dynein light chain



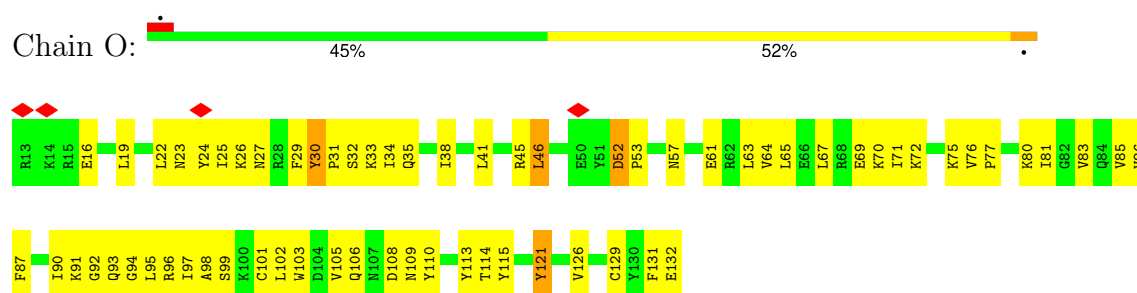
• Molecule 13: Dynein light chain



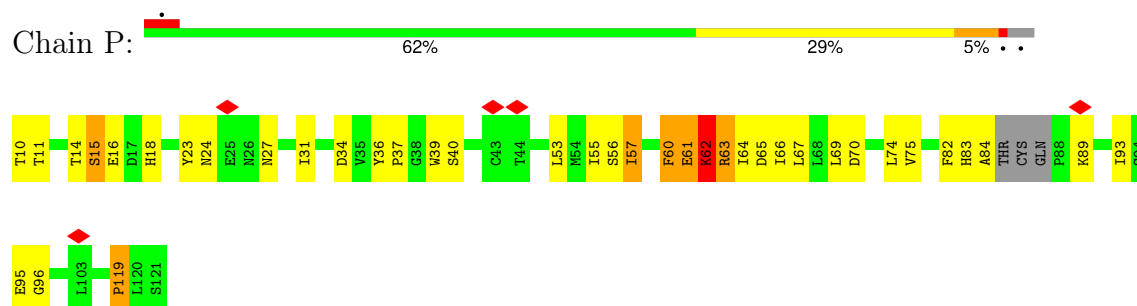
• Molecule 14: Dynein light chain tctex-type 1 protein



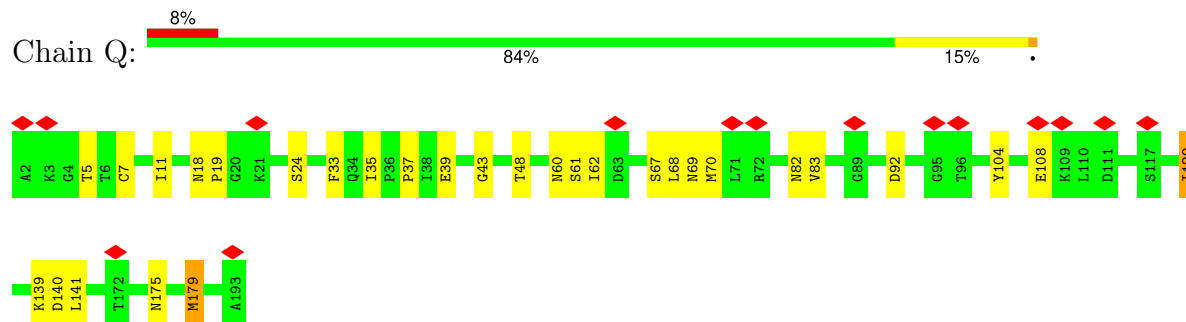
• Molecule 15: Dynein light chain 2A



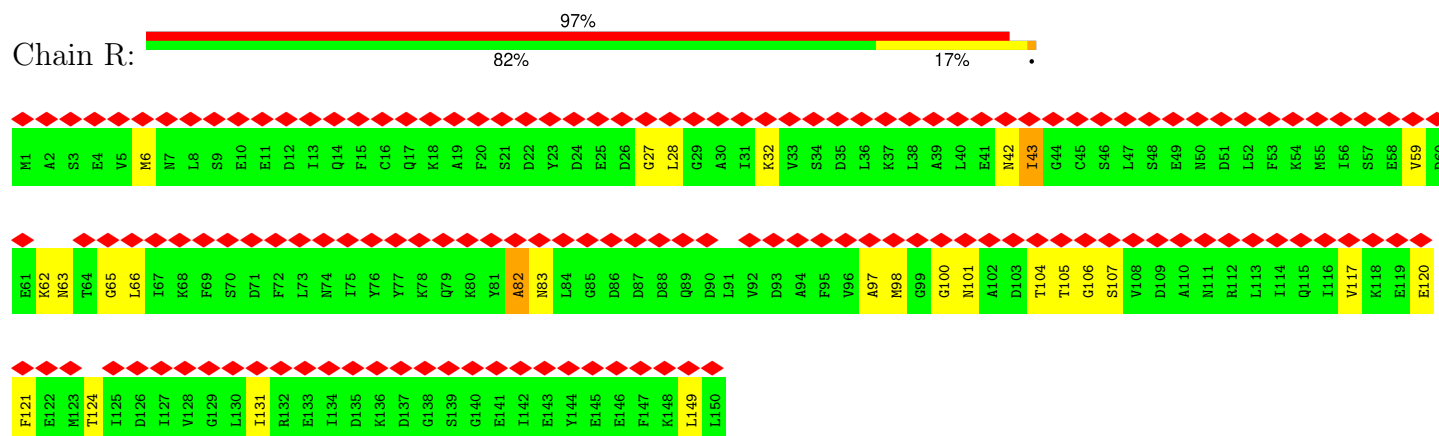
• Molecule 16: Thioredoxin



• Molecule 17: Dynein light chain 1



• Molecule 18: Dynein light chain 4A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.594	Depositor
Minimum map value	0.000	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.189	Depositor
Recommended contour level	0.7	Depositor
Map size ( $\text{\AA}$ )	527.86786, 493.20984, 462.55084	wwPDB
Map dimensions	396, 370, 347	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3329996, 1.3329996, 1.3329996	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.71	7/34544 (0.0%)	0.81	27/46728 (0.1%)
2	B	0.72	7/35358 (0.0%)	0.82	36/47850 (0.1%)
3	C	0.67	2/31033 (0.0%)	0.77	24/42007 (0.1%)
4	D	0.63	1/4789 (0.0%)	0.74	6/6477 (0.1%)
5	E	0.61	0/4540	0.64	0/6136
6	F	0.57	0/1008	0.58	0/1355
7	G	0.63	0/1030	0.98	11/1403 (0.8%)
8	H	0.63	0/767	0.61	0/1031
9	I	0.65	0/838	0.59	0/1131
10	J	0.61	0/832	0.65	0/1119
11	K	0.62	0/776	0.60	0/1038
12	L	0.60	0/872	0.61	0/1176
13	M	0.61	0/752	0.61	0/1006
14	N	0.66	0/864	0.67	0/1175
15	O	0.64	0/1012	0.64	0/1358
16	P	1.92	3/538 (0.6%)	1.60	15/746 (2.0%)
17	Q	0.33	0/1009	0.59	3/1392 (0.2%)
18	R	0.83	1/738 (0.1%)	0.95	2/1025 (0.2%)
All	All	0.70	21/121300 (0.0%)	0.79	124/164153 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	11
3	C	0	1
4	D	0	1
7	G	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	2
All	All	0	31

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1067	PRO	N-CD	51.30	2.19	1.47
2	B	59	THR	C-N	-39.10	0.44	1.34
16	P	62	LYS	C-N	-30.53	0.63	1.34
16	P	15	SER	C-N	20.51	1.81	1.34
1	A	1649	ALA	C-N	-17.37	0.94	1.34

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1171	ILE	CA-C-N	-49.31	8.71	117.20
1	A	1171	ILE	C-N-CA	-46.87	4.53	121.70
2	B	59	THR	O-C-N	-39.33	59.78	122.70
2	B	49	PHE	O-C-N	-27.89	78.07	122.70
3	C	467	THR	N-CA-CB	23.73	155.38	110.30

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1171	ILE	Mainchain,Peptide
1	A	121	GLY	Mainchain
1	A	1649	ALA	Mainchain
2	B	25	GLN	Peptide
2	B	49	PHE	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33975	0	32379	2211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	34751	0	33289	2334	0
3	C	30427	0	29352	1238	0
4	D	4680	0	4511	1070	0
5	E	4440	0	4311	909	0
6	F	996	0	1019	263	0
7	G	1024	0	883	189	0
8	H	750	0	734	219	0
9	I	827	0	826	293	0
10	J	807	0	772	268	0
11	K	754	0	716	122	0
12	L	855	0	854	211	0
13	M	735	0	738	192	0
14	N	852	0	799	201	0
15	O	994	0	1017	311	0
16	P	541	0	217	56	0
17	Q	1006	0	512	51	0
18	R	739	156	339	45	0
19	A	54	0	23	31	0
19	B	54	0	24	18	0
19	C	54	0	22	32	0
20	A	31	0	12	10	0
20	B	31	0	12	43	0
20	C	31	0	12	2	0
21	A	3	0	0	2	0
21	B	3	0	0	0	0
21	C	3	0	0	0	0
All	All	119417	156	113373	8535	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 37.

The worst 5 of 8535 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)
10:J:86:CYS:SG	11:K:61:VAL:HG22	1.24	1.72
1:A:3235:TYR:CE2	1:A:3269:LEU:HD13	1.25	1.71
3:C:196:PRO:HA	3:C:239:TRP:CZ2	1.23	1.67
2:B:3118:TYR:CE2	2:B:3452:LEU:HA	1.25	1.64
4:D:170:THR:CG2	13:M:66:ILE:CG1	1.74	1.64

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	4391/4615 (95%)	4176 (95%)	190 (4%)	25 (1%)	22	60
2	B	4498/4588 (98%)	4258 (95%)	203 (4%)	37 (1%)	16	54
3	C	3923/3947 (99%)	3698 (94%)	202 (5%)	23 (1%)	22	60
4	D	569/595 (96%)	546 (96%)	16 (3%)	7 (1%)	11	44
5	E	551/557 (99%)	531 (96%)	18 (3%)	2 (0%)	30	68
6	F	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
7	G	147/151 (97%)	134 (91%)	7 (5%)	6 (4%)	2	18
8	H	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
9	I	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	13	49
10	J	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
11	K	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
12	L	109/111 (98%)	104 (95%)	4 (4%)	1 (1%)	14	51
13	M	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
14	N	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
15	O	118/120 (98%)	112 (95%)	4 (3%)	2 (2%)	7	36
16	P	103/112 (92%)	90 (87%)	7 (7%)	6 (6%)	1	15
17	Q	190/192 (99%)	174 (92%)	13 (7%)	3 (2%)	8	37
18	R	148/150 (99%)	121 (82%)	19 (13%)	8 (5%)	1	16
All	All	15444/15849 (97%)	14615 (95%)	708 (5%)	121 (1%)	19	54

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PRO
1	A	125	PRO
1	A	127	THR
1	A	151	ILE

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Mol	Chain	Res	Type
1	A	1171	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3430/4191 (82%)	3358 (98%)	72 (2%)	48	67
2	B	3525/4135 (85%)	3447 (98%)	78 (2%)	47	65
3	C	3139/3505 (90%)	3091 (98%)	48 (2%)	60	75
4	D	511/545 (94%)	507 (99%)	4 (1%)	79	84
5	E	488/496 (98%)	484 (99%)	4 (1%)	79	84
6	F	105/105 (100%)	104 (99%)	1 (1%)	73	81
7	G	86/141 (61%)	86 (100%)	0	100	100
8	H	82/82 (100%)	82 (100%)	0	100	100
9	I	91/91 (100%)	91 (100%)	0	100	100
10	J	82/82 (100%)	81 (99%)	1 (1%)	67	79
11	K	80/80 (100%)	80 (100%)	0	100	100
12	L	90/99 (91%)	90 (100%)	0	100	100
13	M	78/78 (100%)	78 (100%)	0	100	100
14	N	84/101 (83%)	84 (100%)	0	100	100
15	O	108/108 (100%)	106 (98%)	2 (2%)	52	69
17	Q	11/176 (6%)	11 (100%)	0	100	100
All	All	11990/14015 (86%)	11780 (98%)	210 (2%)	54	71

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3077	SER
2	B	4464	TYR
4	D	174	GLN
2	B	3269	LEU

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Mol	Chain	Res	Type
2	B	3800	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	105	ASN
3	C	2951	ASN
14	N	89	GLN
3	C	213	GLN
3	C	1888	GLN

### 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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z  > 2$
20	ATP	C	4201	21	28,33,33	0.69	0	34,52,52	0.90	2 (5%)
19	ADP	A	4701	21	24,29,29	0.85	0	29,45,45	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	ATP	B	5601	21	28,33,33	0.75	0	34,52,52	0.78	1 (2%)
19	ADP	C	4702	21	24,29,29	0.75	1 (4%)	29,45,45	1.25	3 (10%)
19	ADP	A	4901	21	24,29,29	0.88	1 (4%)	29,45,45	1.23	3 (10%)
19	ADP	B	5602	21	24,29,29	0.73	0	29,45,45	0.74	1 (3%)
19	ADP	B	5501	21	24,29,29	0.74	0	29,45,45	0.83	1 (3%)
20	ATP	A	4801	21	28,33,33	0.87	0	34,52,52	1.12	2 (5%)
19	ADP	C	4703	21	24,29,29	0.72	0	29,45,45	1.04	2 (6%)

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
20	ATP	C	4201	21	-	1/18/38/38	0/3/3/3
19	ADP	A	4701	21	-	8/12/32/32	0/3/3/3
20	ATP	B	5601	21	-	1/18/38/38	0/3/3/3
19	ADP	C	4702	21	-	5/12/32/32	0/3/3/3
19	ADP	A	4901	21	-	6/12/32/32	0/3/3/3
19	ADP	B	5602	21	-	1/12/32/32	0/3/3/3
19	ADP	B	5501	21	-	1/12/32/32	0/3/3/3
20	ATP	A	4801	21	-	3/18/38/38	0/3/3/3
19	ADP	C	4703	21	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	4901	ADP	O4'-C1'	2.03	1.43	1.40
19	C	4702	ADP	C8-N7	-2.02	1.31	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	4702	ADP	C4'-O4'-C1'	-4.32	105.97	109.92
20	A	4801	ATP	N3-C2-N1	-3.77	123.56	128.67
19	C	4703	ADP	C4'-O4'-C1'	-3.64	106.59	109.92
19	A	4901	ADP	N3-C2-N1	-3.49	123.94	128.67
19	A	4701	ADP	N3-C2-N1	-3.46	123.98	128.67

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

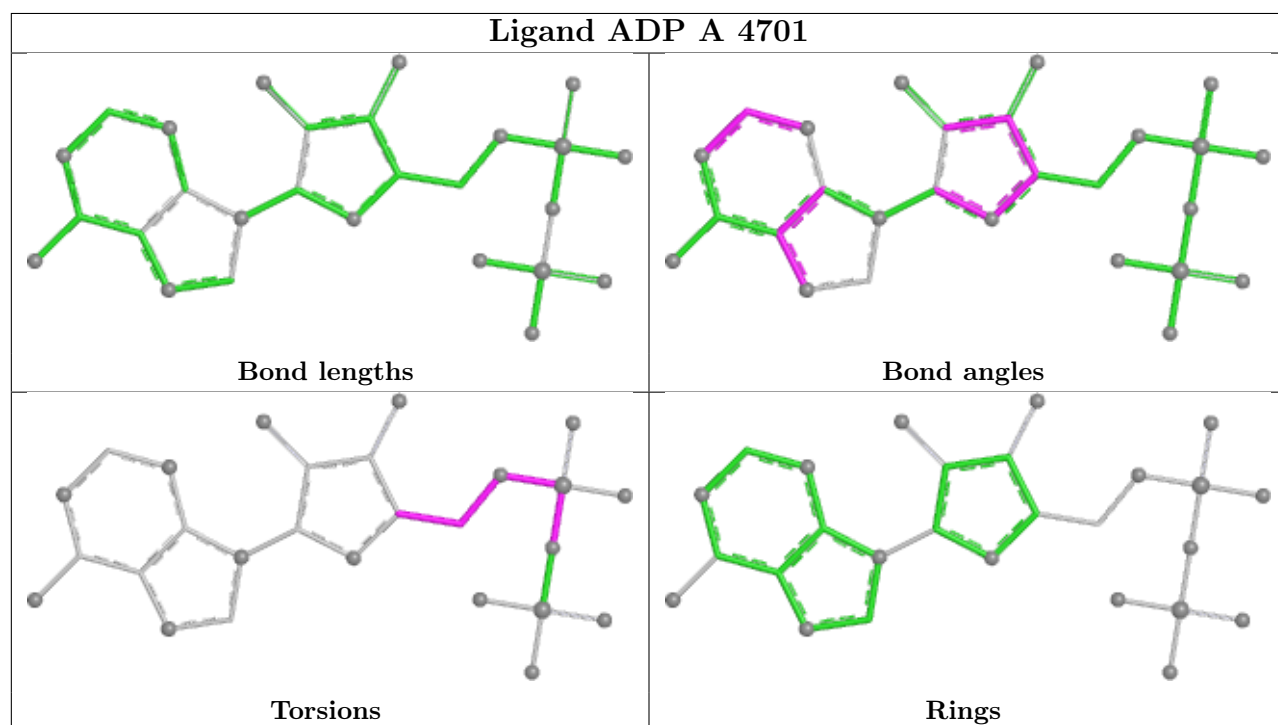
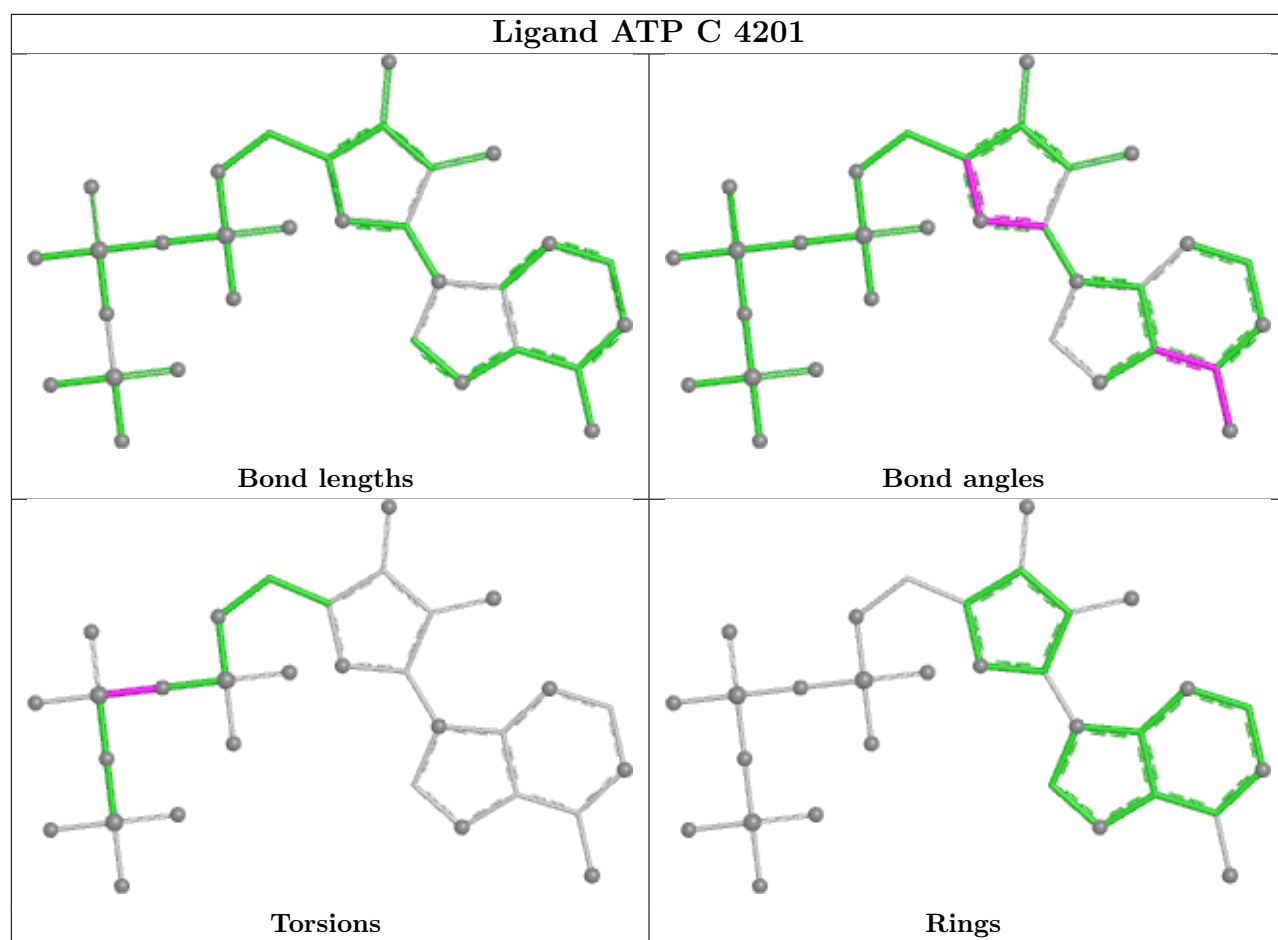
Mol	Chain	Res	Type	Atoms
19	A	4701	ADP	PB-O3A-PA-O5'
19	A	4701	ADP	C5'-O5'-PA-O1A
19	A	4701	ADP	C5'-O5'-PA-O2A
19	A	4701	ADP	C5'-O5'-PA-O3A
19	A	4901	ADP	PB-O3A-PA-O5'

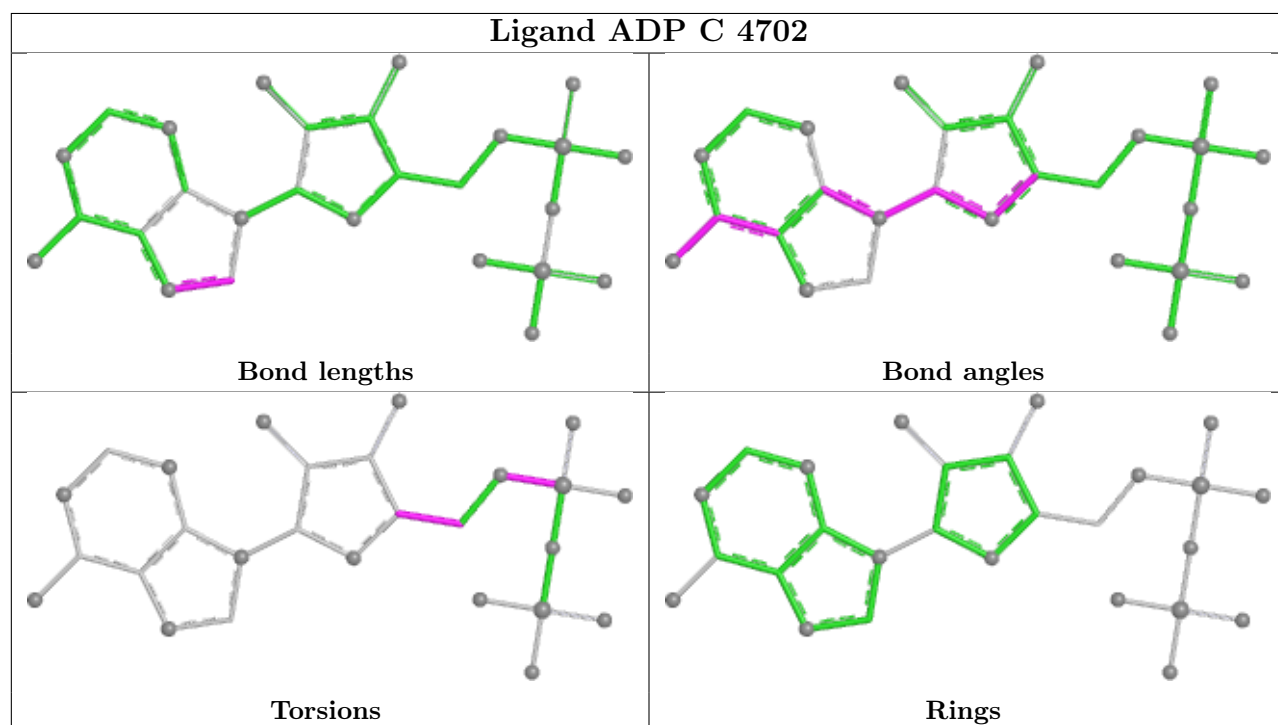
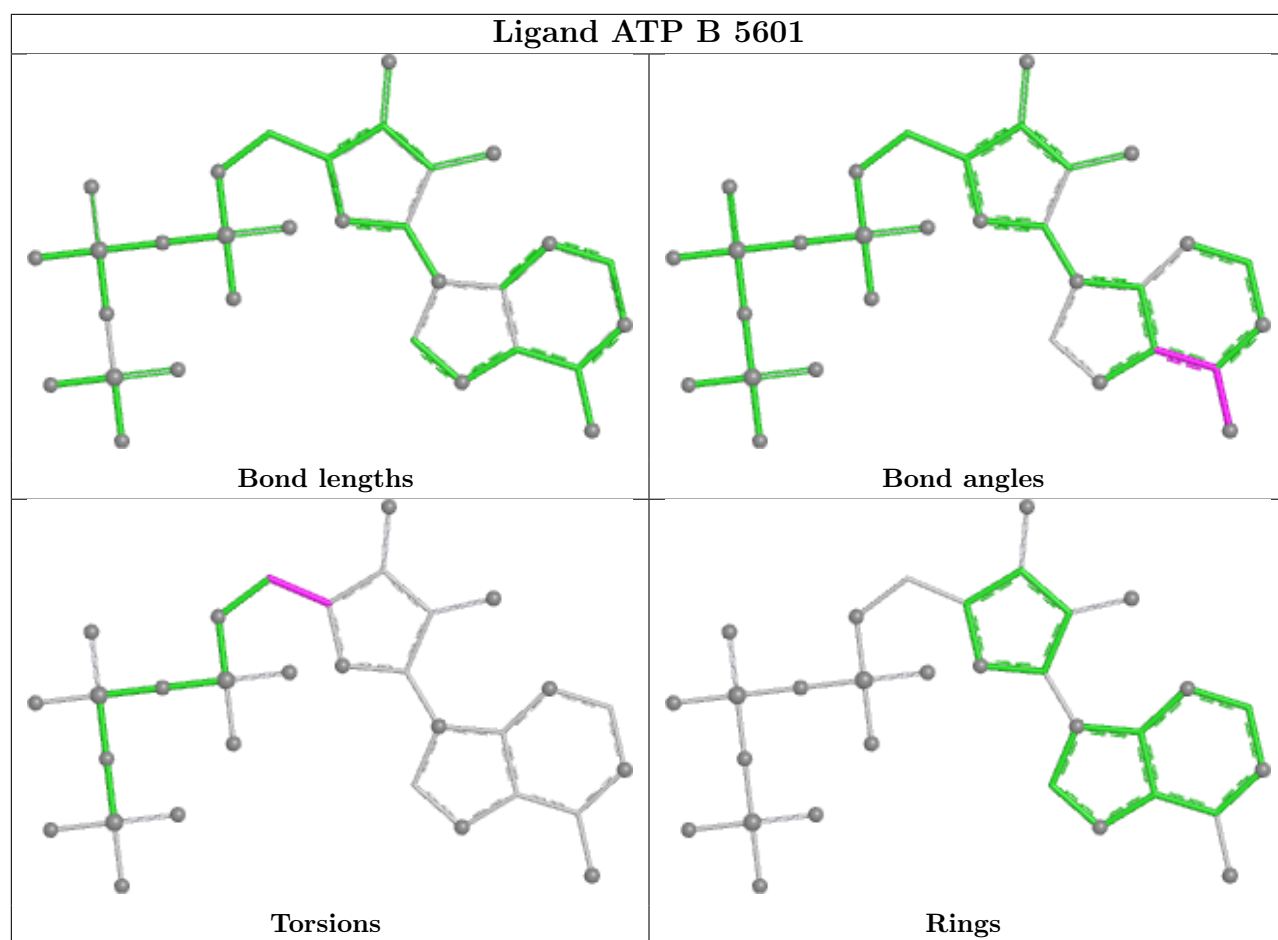
There are no ring outliers.

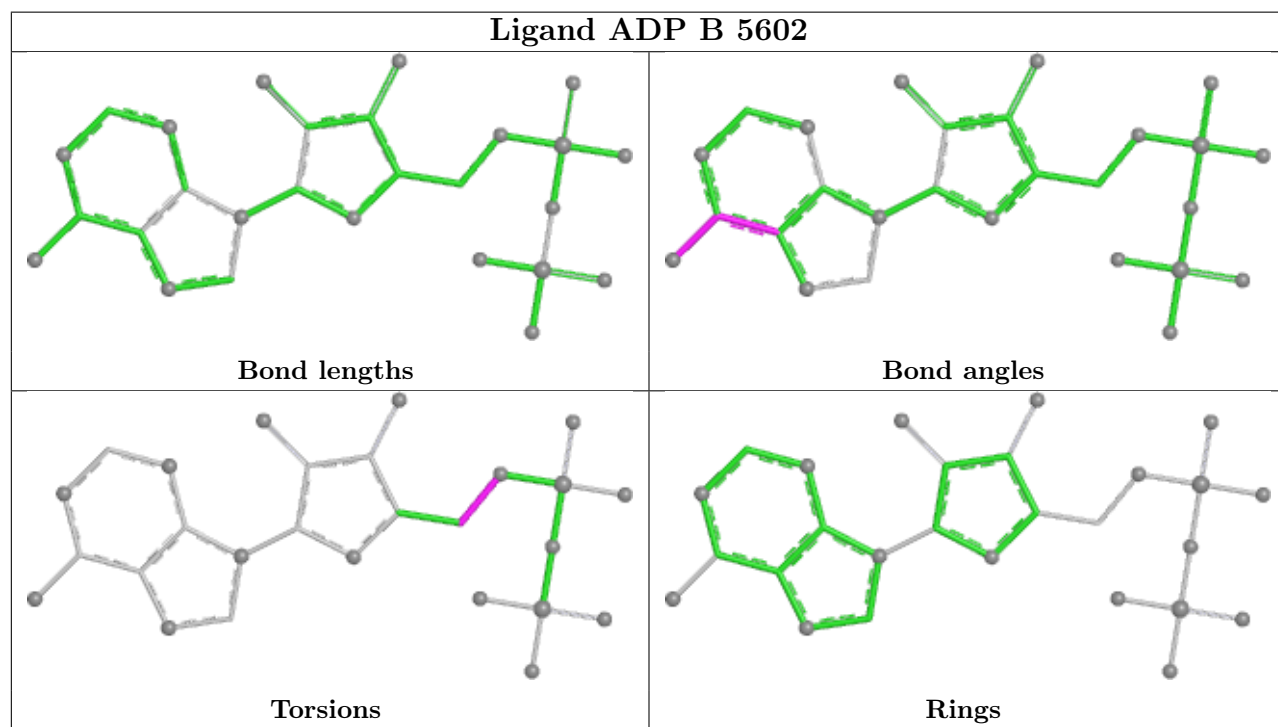
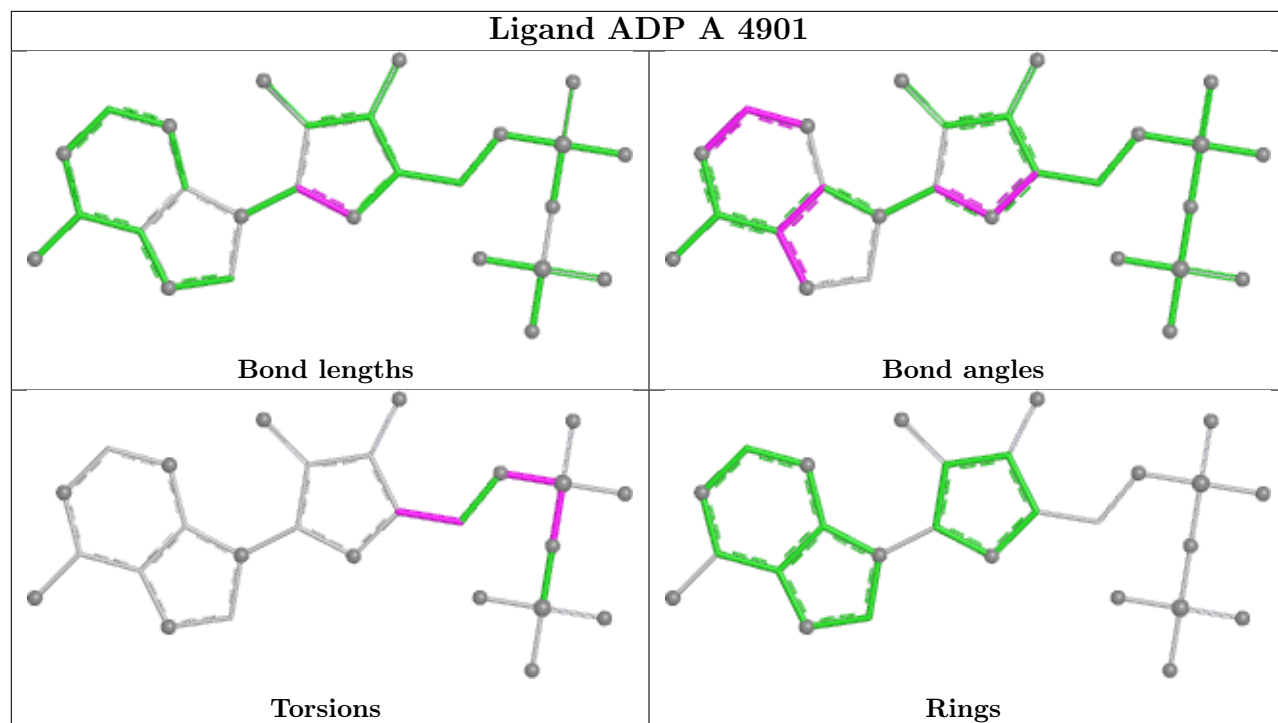
9 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	4201	ATP	2	0
19	A	4701	ADP	12	0
20	B	5601	ATP	43	0
19	C	4702	ADP	25	0
19	A	4901	ADP	19	0
19	B	5602	ADP	2	0
19	B	5501	ADP	16	0
20	A	4801	ATP	10	0
19	C	4703	ADP	7	0

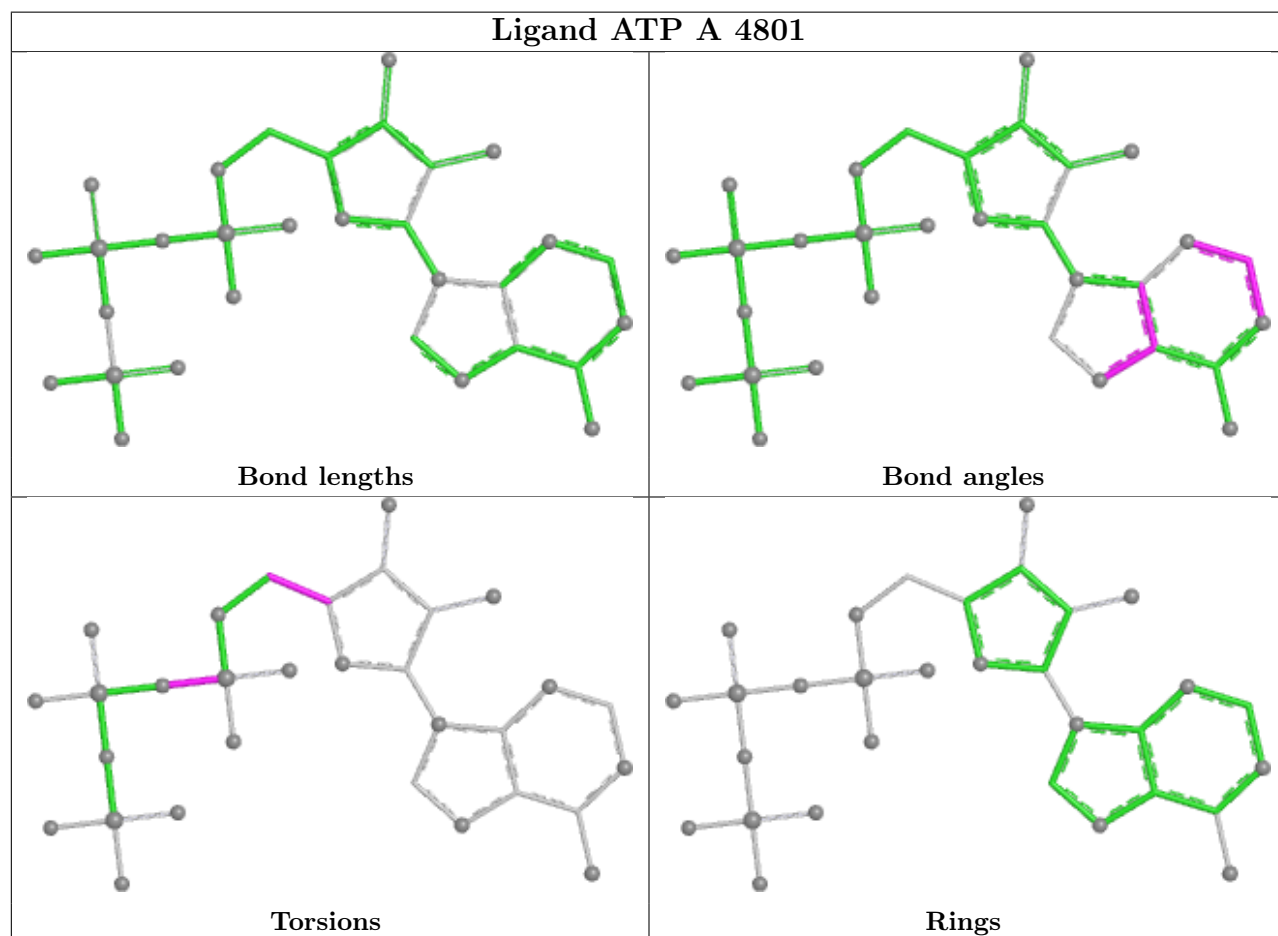
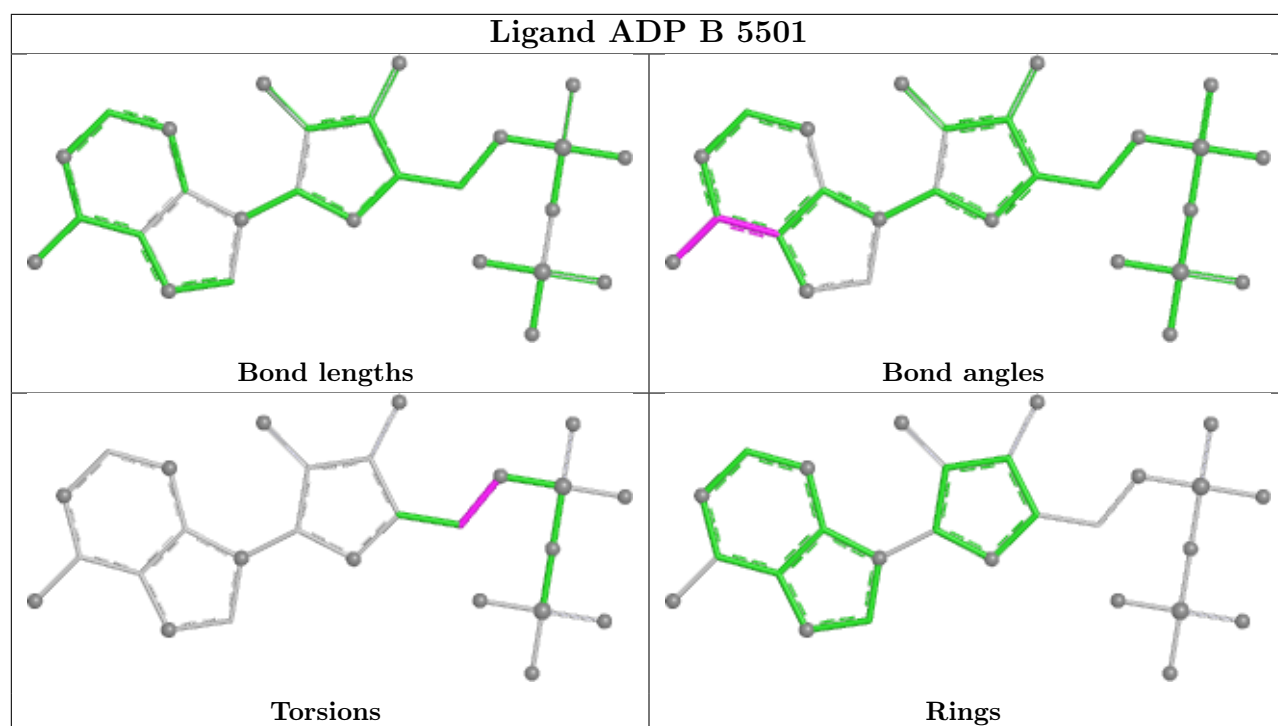
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

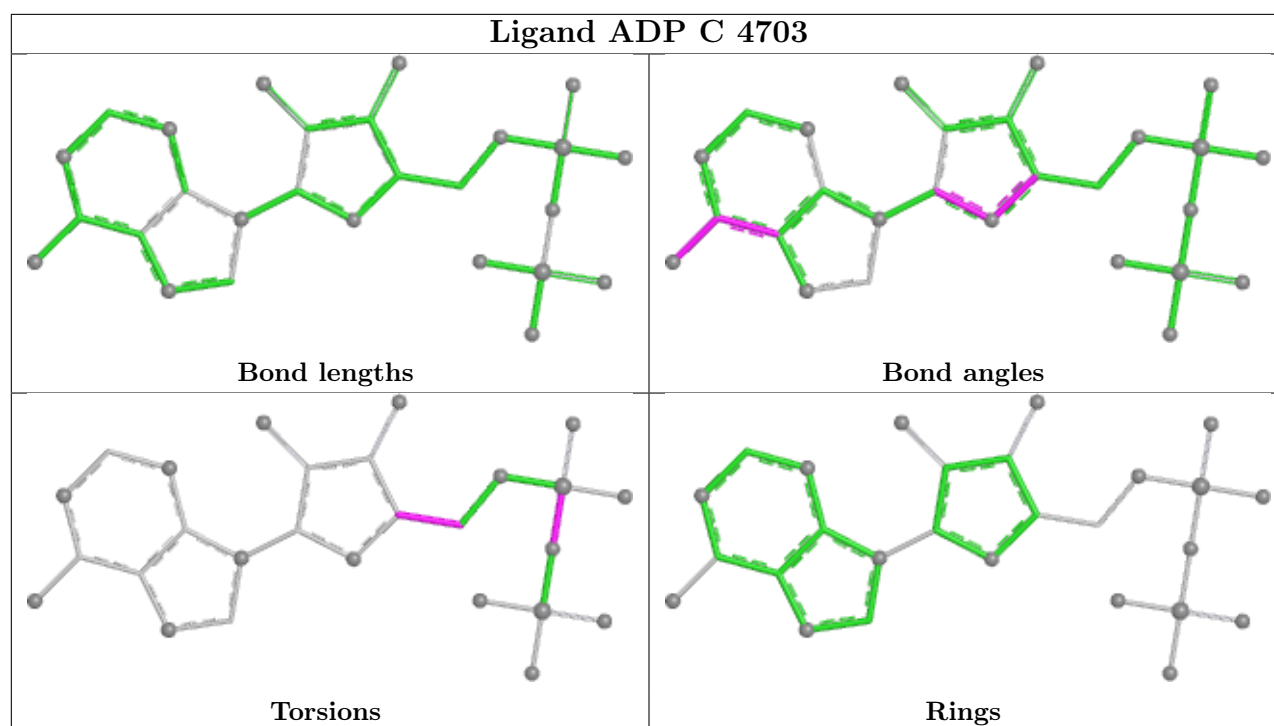












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	12
3	C	11
2	B	11
16	P	4
4	D	2
7	G	1
18	R	1

The worst 5 of 42 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3277:MET	C	3380:MET	N	42.67
1	A	1235:PRO	C	1246:MET	N	14.08
1	C	809:ARG	C	818:ILE	N	13.93
1	C	449:TYR	C	452:ASN	N	13.33

*Continued on next page...*

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	665:ILE	C	670:SER	N	11.69

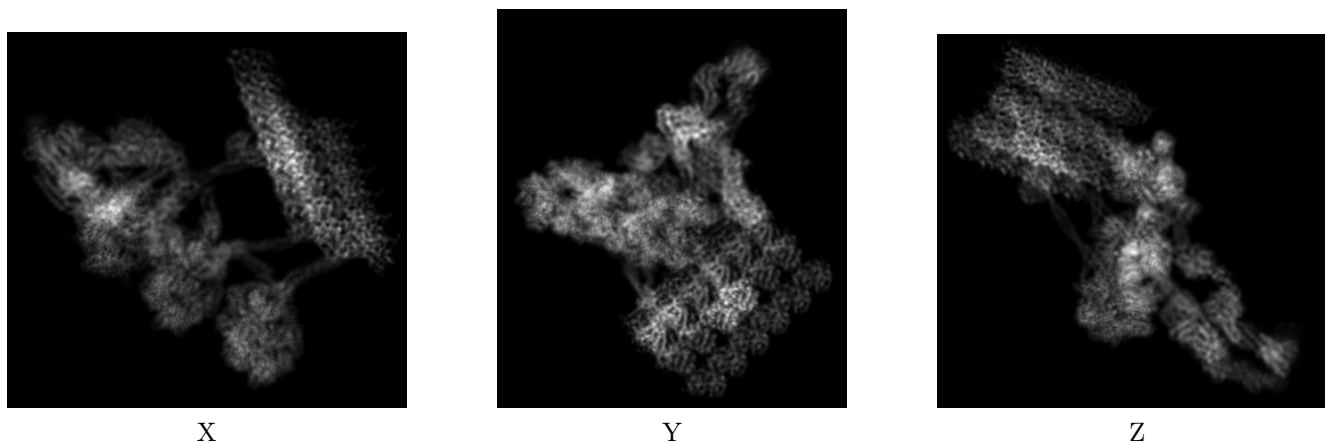
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22679. 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](#)

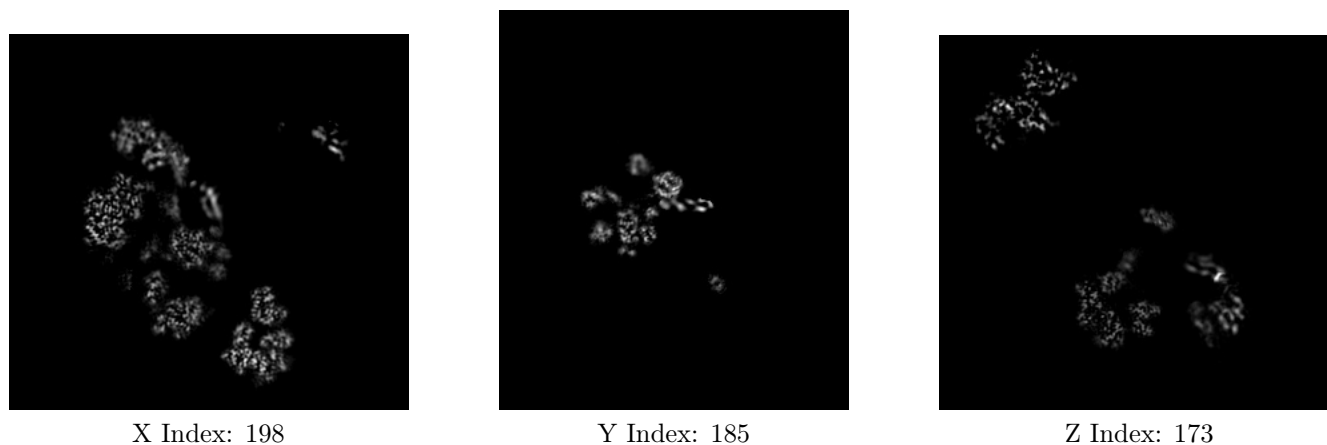
#### 6.1.1 Primary map



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

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

#### 6.2.1 Primary map



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: 97



Y Index: 249

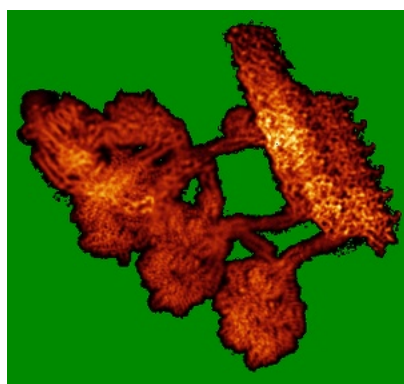


Z Index: 228

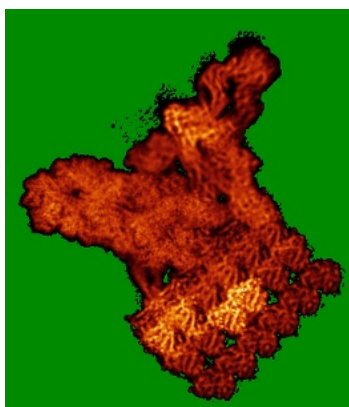
The images above show the largest variance slices of the map in three orthogonal directions.

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

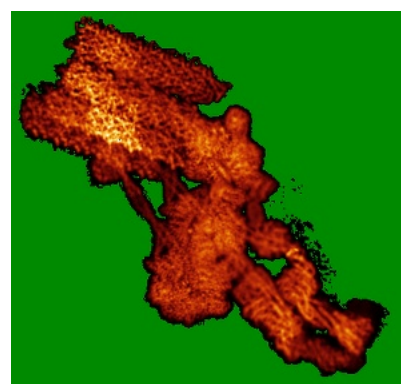
### 6.4.1 Primary map



X



Y

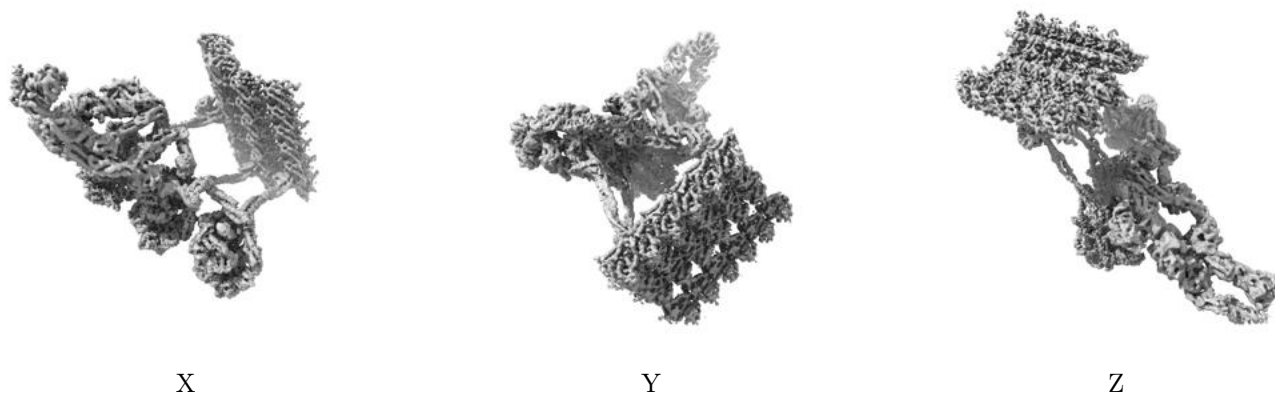


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

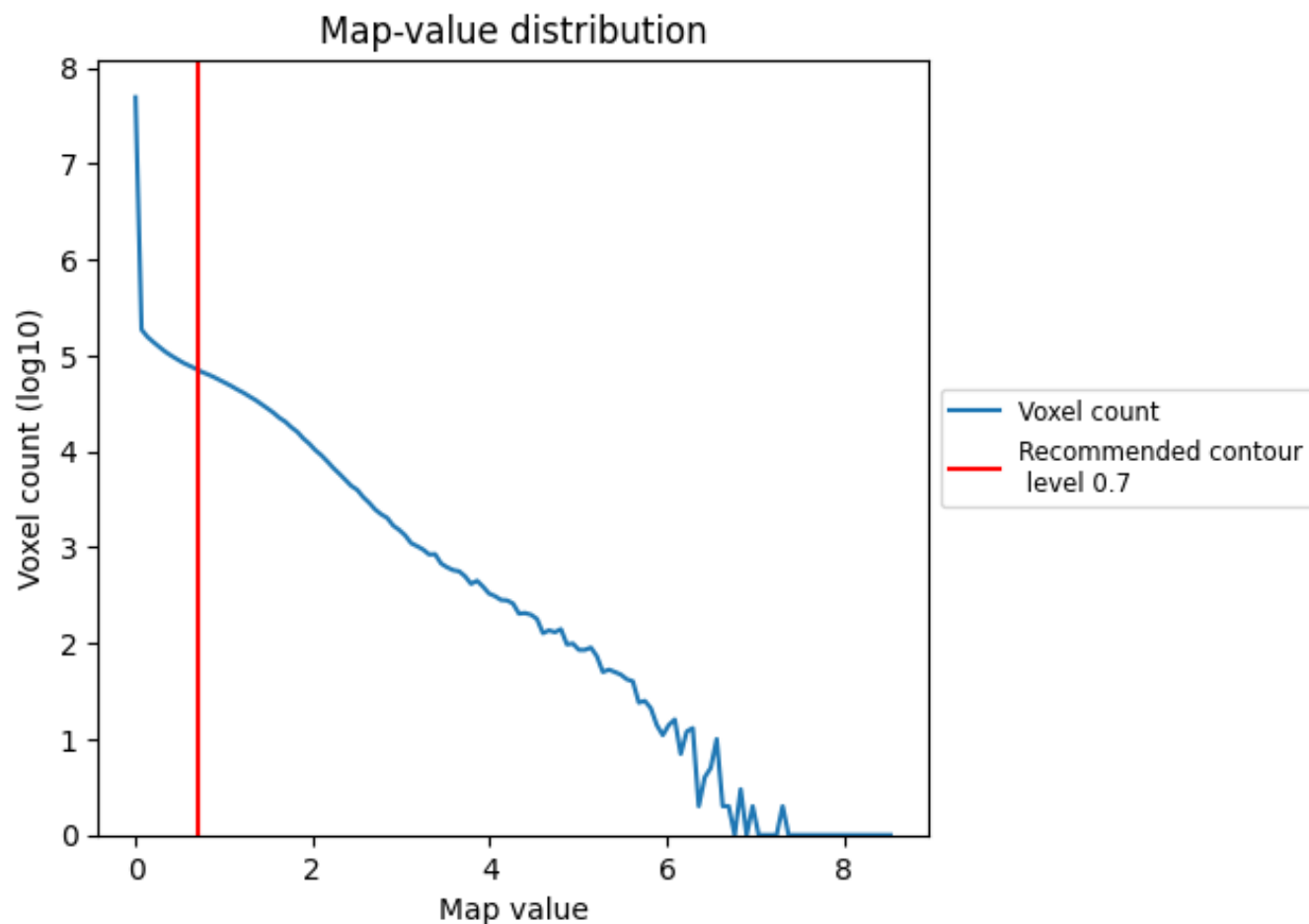
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

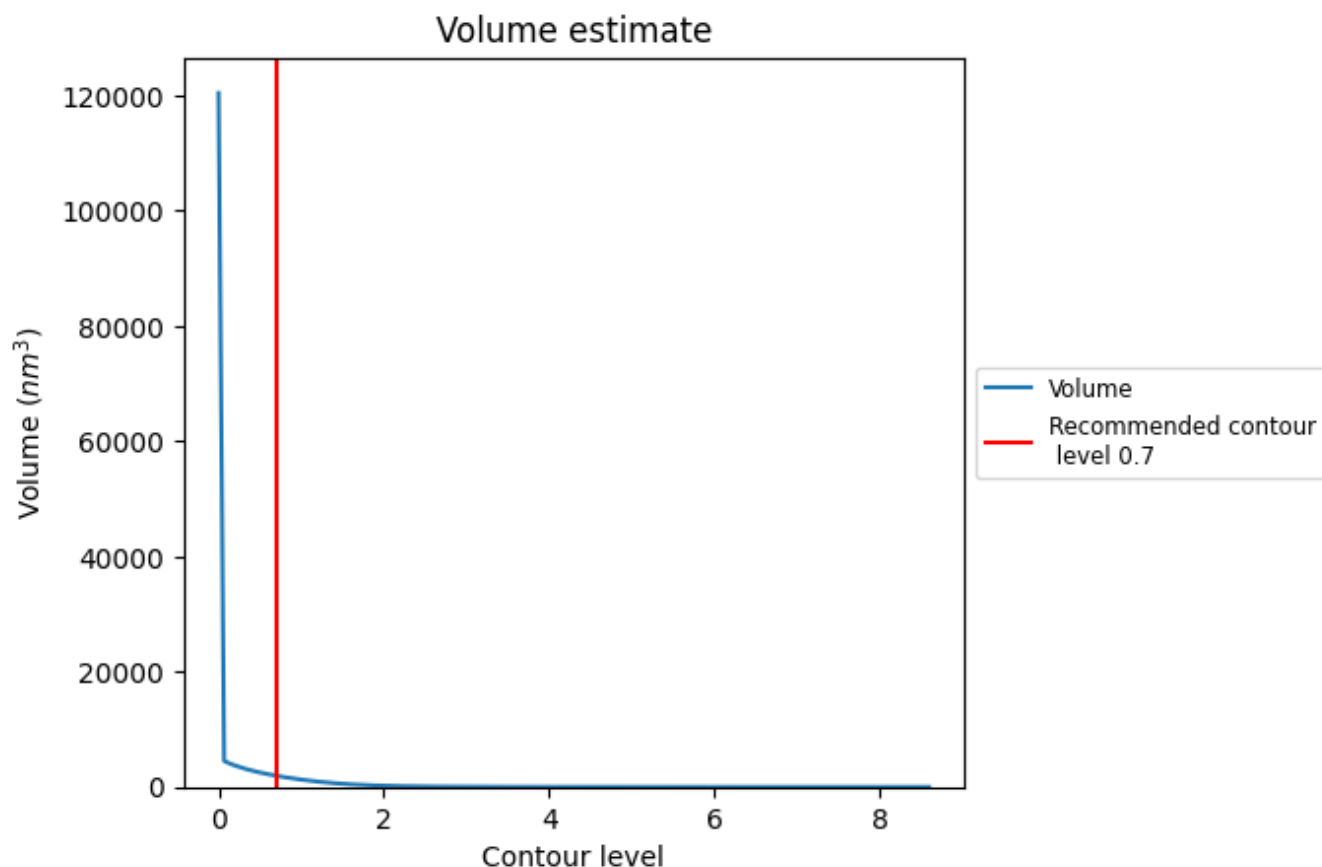
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1940 nm<sup>3</sup>; this corresponds to an approximate mass of 1753 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.



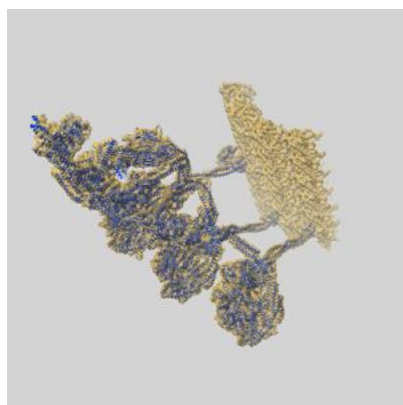
## 8 Fourier-Shell correlation

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

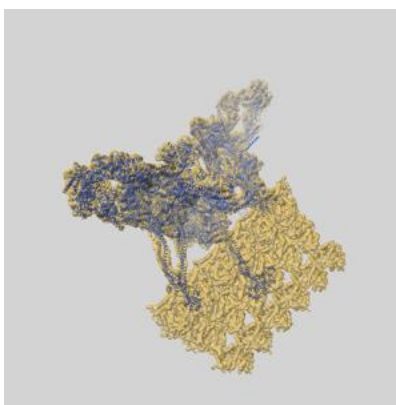
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22679 and PDB model 7K5B. Per-residue inclusion information can be found in section [3](#) on page [9](#).

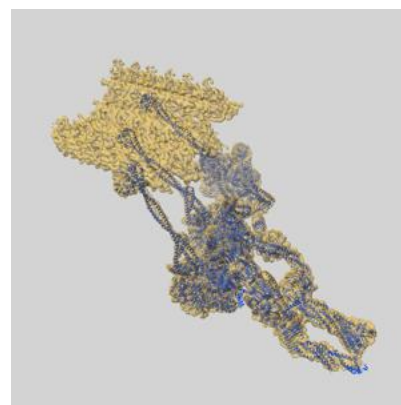
### 9.1 Map-model overlay [i](#)



X



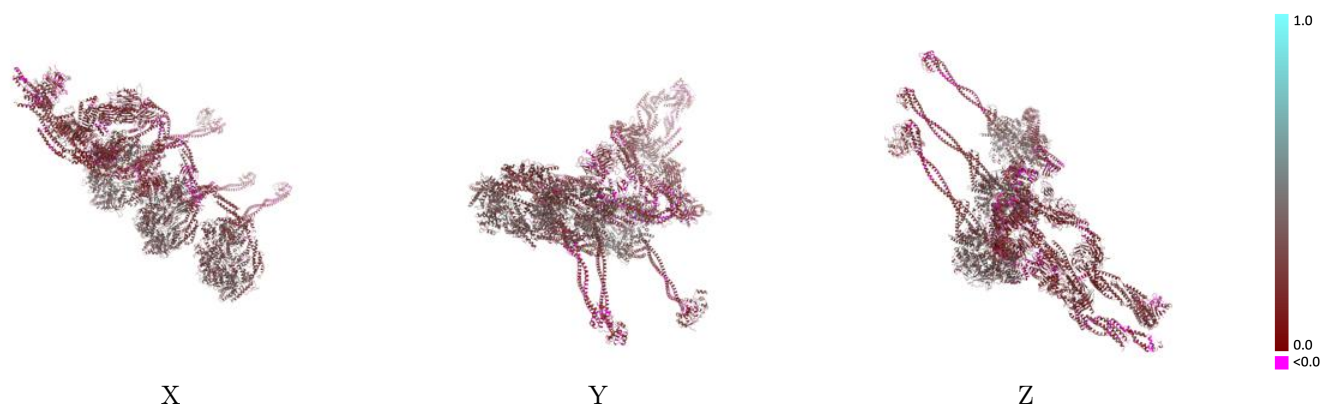
Y



Z

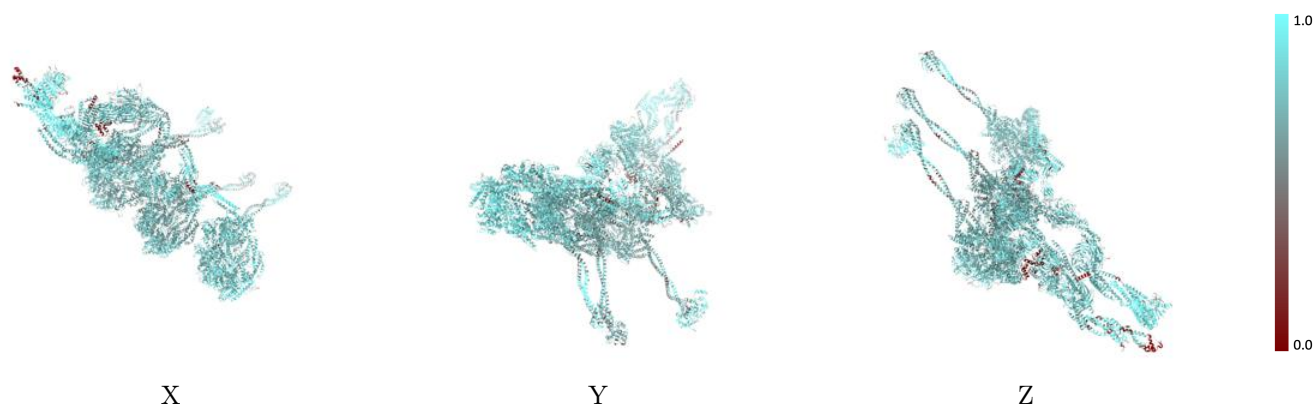
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



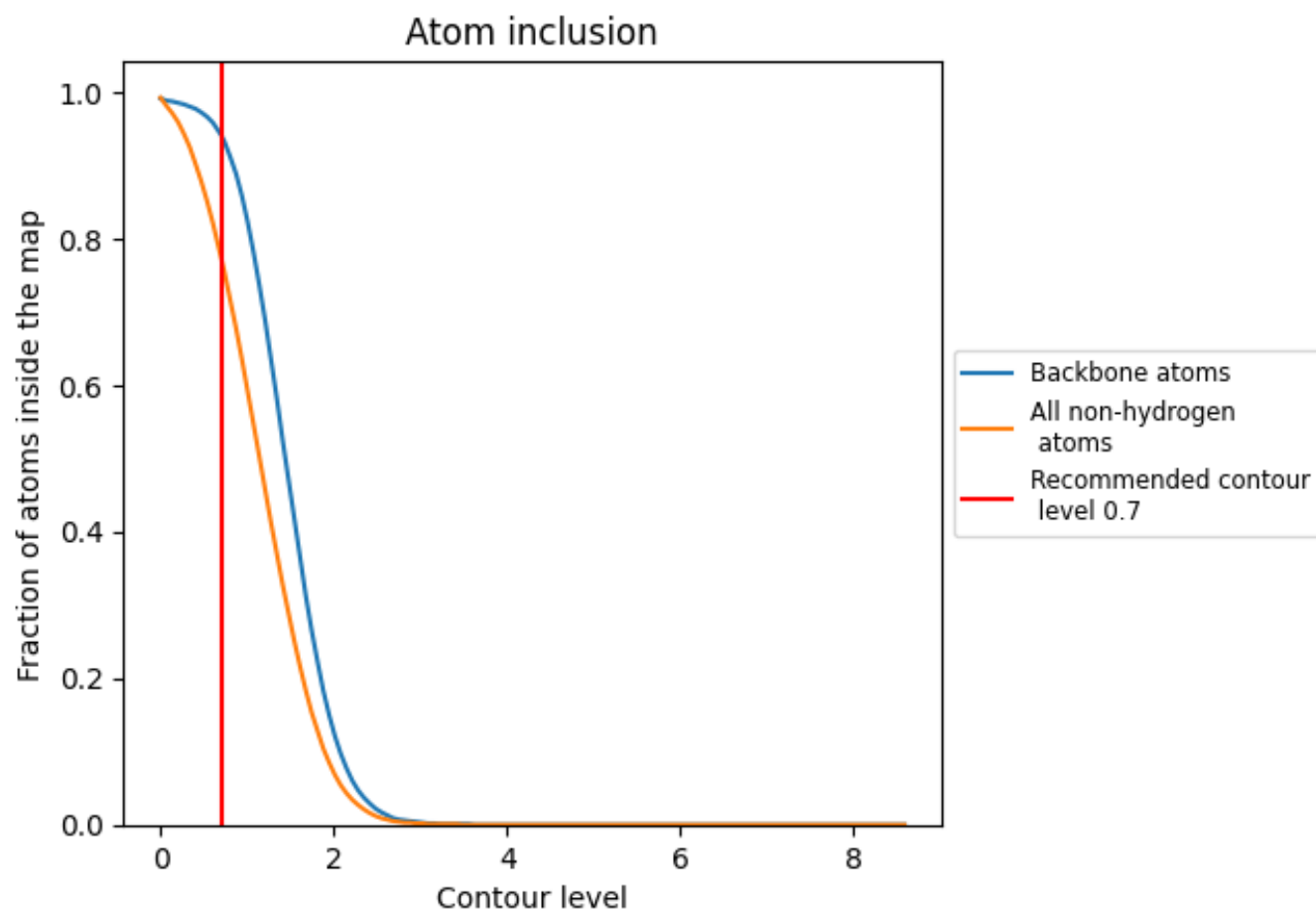
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 77% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.2640
A	 0.7590	 0.2830
B	 0.7570	 0.2730
C	 0.8180	 0.2860
D	 0.8030	 0.2060
E	 0.8280	 0.2060
F	 0.7010	 0.1850
G	 0.6180	 0.1440
H	 0.7740	 0.1860
I	 0.8050	 0.1730
J	 0.7950	 0.1850
K	 0.8070	 0.1780
L	 0.6570	 0.1780
M	 0.7680	 0.1590
N	 0.7670	 0.1640
O	 0.7500	 0.1440
P	 0.8910	 0.1510
Q	 0.8490	 0.2450
R	 0.0270	 -0.0320

