



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 07:49 PM EDT

PDB ID : 6BCQ
EMDB ID : EMD-7085
Title : cryo-EM structure of TRPM4 in ATP bound state with long coiled coil at 3.3 angstrom resolution
Authors : Guo, J.; She, J.; Chen, Q.; Bai, X.; Jiang, Y.
Deposited on : 2017-10-20
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

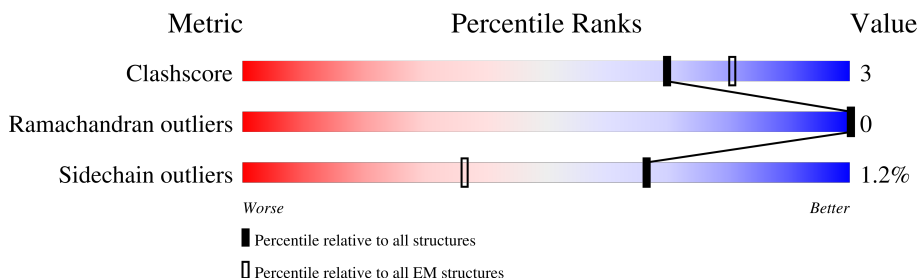
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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 ≥ 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	1254	<div> <div>35%</div> <div>71%</div> <div>7%</div> <div>22%</div> </div>
1	B	1254	<div> <div>35%</div> <div>72%</div> <div>7%</div> <div>22%</div> </div>
1	C	1254	<div> <div>36%</div> <div>72%</div> <div>7%</div> <div>22%</div> </div>
1	D	1254	<div> <div>35%</div> <div>71%</div> <div>7%</div> <div>22%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31048 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 Transient receptor potential cation channel subfamily M member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	983	Total	C	N	O	S	0	0
			7731	4976	1353	1367	35		
1	A	983	Total	C	N	O	S	0	0
			7731	4976	1353	1367	35		
1	C	983	Total	C	N	O	S	0	0
			7731	4976	1353	1367	35		
1	D	983	Total	C	N	O	S	0	0
			7731	4976	1353	1367	35		

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1214	ARG	-	expression tag	UNP Q7TN37
B	1215	ASN	-	expression tag	UNP Q7TN37
B	1216	SER	-	expression tag	UNP Q7TN37
B	1217	LYS	-	expression tag	UNP Q7TN37
B	1218	ALA	-	expression tag	UNP Q7TN37
B	1219	TYR	-	expression tag	UNP Q7TN37
B	1220	VAL	-	expression tag	UNP Q7TN37
B	1221	ASP	-	expression tag	UNP Q7TN37
B	1222	GLU	-	expression tag	UNP Q7TN37
B	1223	LEU	-	expression tag	UNP Q7TN37
B	1224	THR	-	expression tag	UNP Q7TN37
B	1225	SER	-	expression tag	UNP Q7TN37
B	1226	ARG	-	expression tag	UNP Q7TN37
B	1227	GLY	-	expression tag	UNP Q7TN37
B	1228	ARG	-	expression tag	UNP Q7TN37
B	1229	LEU	-	expression tag	UNP Q7TN37
B	1230	GLU	-	expression tag	UNP Q7TN37
B	1231	VAL	-	expression tag	UNP Q7TN37
B	1232	LEU	-	expression tag	UNP Q7TN37
B	1233	PHE	-	expression tag	UNP Q7TN37
B	1234	GLN	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1235	GLY	-	expression tag	UNP Q7TN37
B	1236	PRO	-	expression tag	UNP Q7TN37
B	1237	ASP	-	expression tag	UNP Q7TN37
B	1238	TYR	-	expression tag	UNP Q7TN37
B	1239	LYS	-	expression tag	UNP Q7TN37
B	1240	ASP	-	expression tag	UNP Q7TN37
B	1241	ASP	-	expression tag	UNP Q7TN37
B	1242	ASP	-	expression tag	UNP Q7TN37
B	1243	ASP	-	expression tag	UNP Q7TN37
B	1244	LYS	-	expression tag	UNP Q7TN37
B	1245	HIS	-	expression tag	UNP Q7TN37
B	1246	HIS	-	expression tag	UNP Q7TN37
B	1247	HIS	-	expression tag	UNP Q7TN37
B	1248	HIS	-	expression tag	UNP Q7TN37
B	1249	HIS	-	expression tag	UNP Q7TN37
B	1250	HIS	-	expression tag	UNP Q7TN37
B	1251	HIS	-	expression tag	UNP Q7TN37
B	1252	HIS	-	expression tag	UNP Q7TN37
B	1253	HIS	-	expression tag	UNP Q7TN37
B	1254	HIS	-	expression tag	UNP Q7TN37
A	1214	ARG	-	expression tag	UNP Q7TN37
A	1215	ASN	-	expression tag	UNP Q7TN37
A	1216	SER	-	expression tag	UNP Q7TN37
A	1217	LYS	-	expression tag	UNP Q7TN37
A	1218	ALA	-	expression tag	UNP Q7TN37
A	1219	TYR	-	expression tag	UNP Q7TN37
A	1220	VAL	-	expression tag	UNP Q7TN37
A	1221	ASP	-	expression tag	UNP Q7TN37
A	1222	GLU	-	expression tag	UNP Q7TN37
A	1223	LEU	-	expression tag	UNP Q7TN37
A	1224	THR	-	expression tag	UNP Q7TN37
A	1225	SER	-	expression tag	UNP Q7TN37
A	1226	ARG	-	expression tag	UNP Q7TN37
A	1227	GLY	-	expression tag	UNP Q7TN37
A	1228	ARG	-	expression tag	UNP Q7TN37
A	1229	LEU	-	expression tag	UNP Q7TN37
A	1230	GLU	-	expression tag	UNP Q7TN37
A	1231	VAL	-	expression tag	UNP Q7TN37
A	1232	LEU	-	expression tag	UNP Q7TN37
A	1233	PHE	-	expression tag	UNP Q7TN37
A	1234	GLN	-	expression tag	UNP Q7TN37
A	1235	GLY	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	PRO	-	expression tag	UNP Q7TN37
A	1237	ASP	-	expression tag	UNP Q7TN37
A	1238	TYR	-	expression tag	UNP Q7TN37
A	1239	LYS	-	expression tag	UNP Q7TN37
A	1240	ASP	-	expression tag	UNP Q7TN37
A	1241	ASP	-	expression tag	UNP Q7TN37
A	1242	ASP	-	expression tag	UNP Q7TN37
A	1243	ASP	-	expression tag	UNP Q7TN37
A	1244	LYS	-	expression tag	UNP Q7TN37
A	1245	HIS	-	expression tag	UNP Q7TN37
A	1246	HIS	-	expression tag	UNP Q7TN37
A	1247	HIS	-	expression tag	UNP Q7TN37
A	1248	HIS	-	expression tag	UNP Q7TN37
A	1249	HIS	-	expression tag	UNP Q7TN37
A	1250	HIS	-	expression tag	UNP Q7TN37
A	1251	HIS	-	expression tag	UNP Q7TN37
A	1252	HIS	-	expression tag	UNP Q7TN37
A	1253	HIS	-	expression tag	UNP Q7TN37
A	1254	HIS	-	expression tag	UNP Q7TN37
C	1214	ARG	-	expression tag	UNP Q7TN37
C	1215	ASN	-	expression tag	UNP Q7TN37
C	1216	SER	-	expression tag	UNP Q7TN37
C	1217	LYS	-	expression tag	UNP Q7TN37
C	1218	ALA	-	expression tag	UNP Q7TN37
C	1219	TYR	-	expression tag	UNP Q7TN37
C	1220	VAL	-	expression tag	UNP Q7TN37
C	1221	ASP	-	expression tag	UNP Q7TN37
C	1222	GLU	-	expression tag	UNP Q7TN37
C	1223	LEU	-	expression tag	UNP Q7TN37
C	1224	THR	-	expression tag	UNP Q7TN37
C	1225	SER	-	expression tag	UNP Q7TN37
C	1226	ARG	-	expression tag	UNP Q7TN37
C	1227	GLY	-	expression tag	UNP Q7TN37
C	1228	ARG	-	expression tag	UNP Q7TN37
C	1229	LEU	-	expression tag	UNP Q7TN37
C	1230	GLU	-	expression tag	UNP Q7TN37
C	1231	VAL	-	expression tag	UNP Q7TN37
C	1232	LEU	-	expression tag	UNP Q7TN37
C	1233	PHE	-	expression tag	UNP Q7TN37
C	1234	GLN	-	expression tag	UNP Q7TN37
C	1235	GLY	-	expression tag	UNP Q7TN37
C	1236	PRO	-	expression tag	UNP Q7TN37

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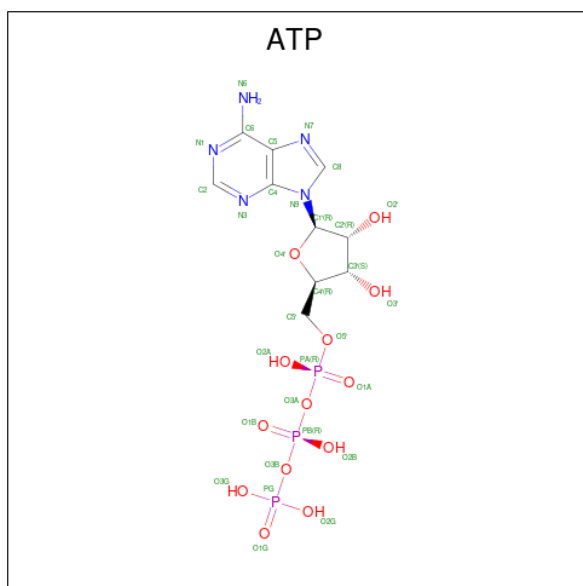
Chain	Residue	Modelled	Actual	Comment	Reference
C	1237	ASP	-	expression tag	UNP Q7TN37
C	1238	TYR	-	expression tag	UNP Q7TN37
C	1239	LYS	-	expression tag	UNP Q7TN37
C	1240	ASP	-	expression tag	UNP Q7TN37
C	1241	ASP	-	expression tag	UNP Q7TN37
C	1242	ASP	-	expression tag	UNP Q7TN37
C	1243	ASP	-	expression tag	UNP Q7TN37
C	1244	LYS	-	expression tag	UNP Q7TN37
C	1245	HIS	-	expression tag	UNP Q7TN37
C	1246	HIS	-	expression tag	UNP Q7TN37
C	1247	HIS	-	expression tag	UNP Q7TN37
C	1248	HIS	-	expression tag	UNP Q7TN37
C	1249	HIS	-	expression tag	UNP Q7TN37
C	1250	HIS	-	expression tag	UNP Q7TN37
C	1251	HIS	-	expression tag	UNP Q7TN37
C	1252	HIS	-	expression tag	UNP Q7TN37
C	1253	HIS	-	expression tag	UNP Q7TN37
C	1254	HIS	-	expression tag	UNP Q7TN37
D	1214	ARG	-	expression tag	UNP Q7TN37
D	1215	ASN	-	expression tag	UNP Q7TN37
D	1216	SER	-	expression tag	UNP Q7TN37
D	1217	LYS	-	expression tag	UNP Q7TN37
D	1218	ALA	-	expression tag	UNP Q7TN37
D	1219	TYR	-	expression tag	UNP Q7TN37
D	1220	VAL	-	expression tag	UNP Q7TN37
D	1221	ASP	-	expression tag	UNP Q7TN37
D	1222	GLU	-	expression tag	UNP Q7TN37
D	1223	LEU	-	expression tag	UNP Q7TN37
D	1224	THR	-	expression tag	UNP Q7TN37
D	1225	SER	-	expression tag	UNP Q7TN37
D	1226	ARG	-	expression tag	UNP Q7TN37
D	1227	GLY	-	expression tag	UNP Q7TN37
D	1228	ARG	-	expression tag	UNP Q7TN37
D	1229	LEU	-	expression tag	UNP Q7TN37
D	1230	GLU	-	expression tag	UNP Q7TN37
D	1231	VAL	-	expression tag	UNP Q7TN37
D	1232	LEU	-	expression tag	UNP Q7TN37
D	1233	PHE	-	expression tag	UNP Q7TN37
D	1234	GLN	-	expression tag	UNP Q7TN37
D	1235	GLY	-	expression tag	UNP Q7TN37
D	1236	PRO	-	expression tag	UNP Q7TN37
D	1237	ASP	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1238	TYR	-	expression tag	UNP Q7TN37
D	1239	LYS	-	expression tag	UNP Q7TN37
D	1240	ASP	-	expression tag	UNP Q7TN37
D	1241	ASP	-	expression tag	UNP Q7TN37
D	1242	ASP	-	expression tag	UNP Q7TN37
D	1243	ASP	-	expression tag	UNP Q7TN37
D	1244	LYS	-	expression tag	UNP Q7TN37
D	1245	HIS	-	expression tag	UNP Q7TN37
D	1246	HIS	-	expression tag	UNP Q7TN37
D	1247	HIS	-	expression tag	UNP Q7TN37
D	1248	HIS	-	expression tag	UNP Q7TN37
D	1249	HIS	-	expression tag	UNP Q7TN37
D	1250	HIS	-	expression tag	UNP Q7TN37
D	1251	HIS	-	expression tag	UNP Q7TN37
D	1252	HIS	-	expression tag	UNP Q7TN37
D	1253	HIS	-	expression tag	UNP Q7TN37
D	1254	HIS	-	expression tag	UNP Q7TN37

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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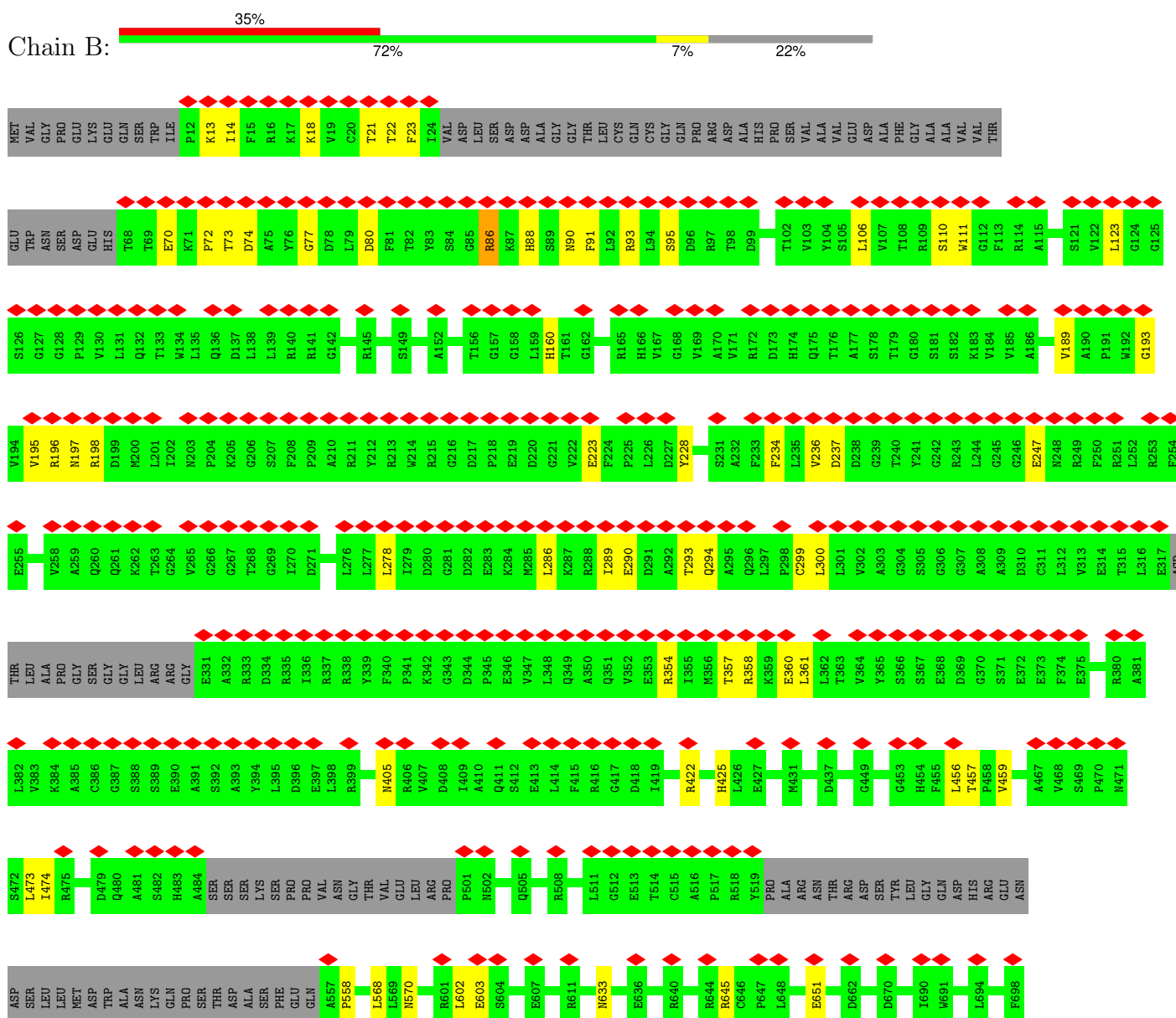
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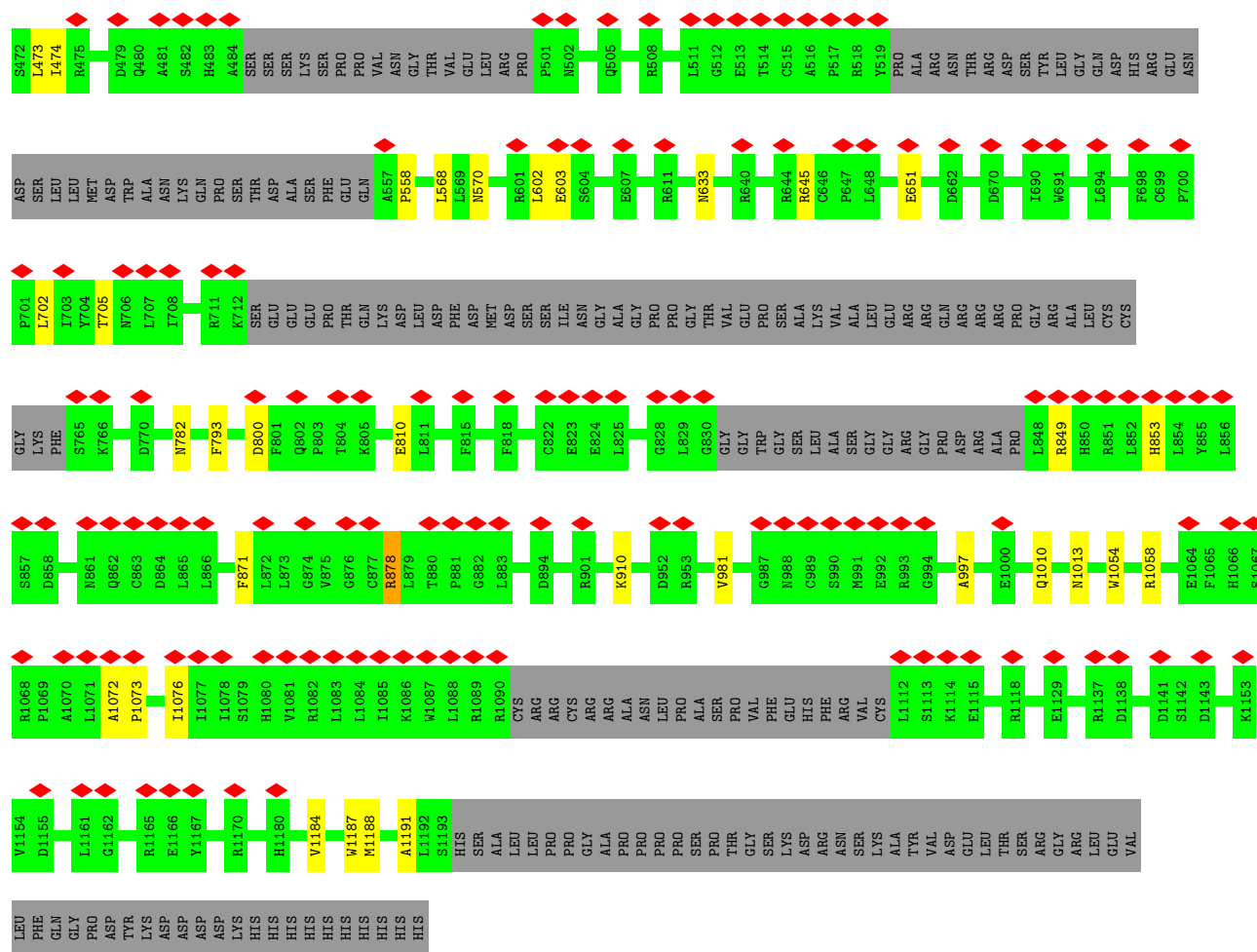
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots

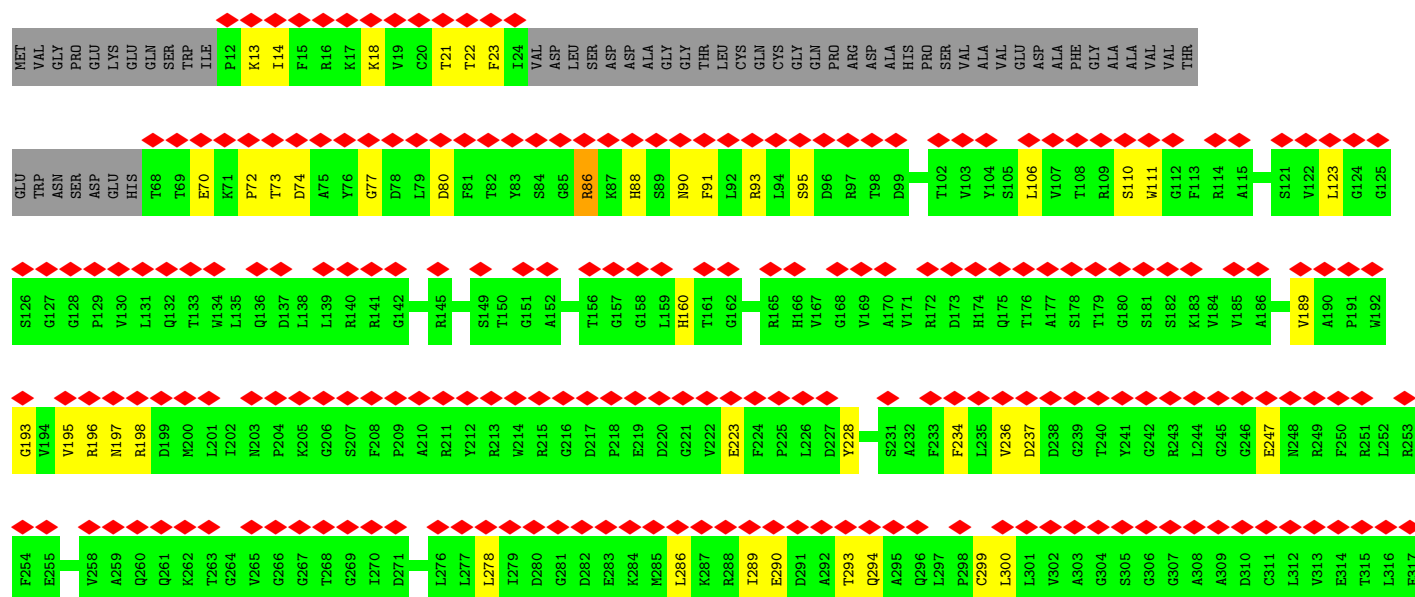
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily M member 4





- Molecule 1: Transient receptor potential cation channel subfamily M member 4



LEU	V1154	H1068	Y855	CYS	G699	ASP	S472	L382	THR	E255	V194
PHE	D1155	P1069	L856	CYS	P700	SER	L473	V383	LEU	V258	V195
GLN	L1161	A1070	S857	LEU	P701	LEU	I474	K384	ALA	A259	R196
PRO	G1162	A1072	D858	PHE	L702	MET	R475	C385	PRO	Q261	R197
ASP	R1165	P1073	N861	ASP	I703	ASP	D479	C386	SER	Q262	R198
TYR	E1166	I1076	Q862	TRP	Y704	TRP	Q480	G387	GLY	K263	D199
LYS	Y1167	I1077	C863	ALA	W706	ALA	A481	S388	GLY	L201	M200
ASP	Y1167	I1078	D864	ASN	L707	LYS	S482	S389	LEU	G264	L202
ASP	R1170	S1079	L865	GLN	I708	GLN	H483	E390	ARG	V265	N203
LYS	H1180	H1080	L866	PRO	R711	PRO	A484	A391	GLY	G266	P204
HIS	H1180	V1081	L866	SER	K712	SER	SER	S392	E331	G267	P204
HIS	V1184	D800	F871	THR	SER	THR	SER	A393	R333	G268	K206
HIS	V1184	F801	L872	ALA	GLU	ALA	SER	Y394	R333	G269	G207
HIS	W1187	Q802	L873	PHE	GLU	SER	LYS	L395	D334	I270	F208
HIS	M1188	L1083	G874	GLU	GLU	PRO	PRO	D396	R335	D271	P209
HIS	A1191	P803	V875	GLN	THR	VAL	VAL	E397	I336	L276	A210
HIS	S1193	T804	G876	ASP	GLN	ASN	GLY	L398	R337	L277	R211
HIS	S1193	K805	C877	P558	LYS	THR	THR	R399	R338	L278	Y212
HIS	S1193	E810	B878	L568	ASP	VAL	VAL	N405	F340	I279	R213
SER	SER	L811	L879	L569	LEU	GLU	GLU	R406	P341	D280	W214
LEU	LEU	T880	F815	N570	ASP	LEU	LEU	V407	K342	G281	R215
PRO	PRO	P881	F818	R601	ASP	ARG	ARG	D408	G343	G282	G216
PRO	PRO	G882	L883	L602	ASP	PRO	P501	I409	D344	E283	D217
GLY	GLY	C822	C822	E603	ASP	ASN	N502	A410	F345	K284	P218
ALA	ALA	E823	E824	S604	SER	ILE	Q505	S412	E346	M285	E219
ASN	ASN	E824	L825	E607	GLY	ASN	R508	E413	V347	L286	D220
LEU	LEU	R901	E945	R611	ALA	GLY	R508	L414	L348	K287	G221
PRO	PRO	E945	D952	N633	GLY	ALA	L511	F415	Q349	R288	V222
PRO	PRO	R953	R953	E636	GLY	PRO	G512	R416	A350	I289	E223
VAL	VAL	V981	V981	R640	THR	VAL	T514	G417	Q351	P225	F224
PHE	PHE	G987	G987	R644	GLU	GLU	C515	D418	V352	D291	L226
HIS	HIS	N988	N988	R645	PRO	PRO	A516	I419	E353	A292	D227
ARG	ARG	C989	C989	R646	ALA	ALA	P517	R422	R354	Q294	Y228
ARG	ARG	S990	S990	P647	LYS	LYS	R518	H425	I355	A295	S231
CYS	CYS	M991	M991	L648	VAL	VAL	Y519	L425	M356	Q296	A232
L1112	L1112	E992	E992	E651	ALA	LEU	PRO	E427	T357	L297	F233
S1113	S1113	R993	R993	E651	LEU	LEU	ALA	M431	R358	P298	F234
K1114	K1114	G994	G994	D662	GLY	GLY	ASN	D437	K359	C299	L235
E1115	E1115	A997	A997	D670	ARG	ARG	THR	L362	L361	L300	V236
R1118	R1118	E1000	E1000	D670	ARG	ARG	ASP	V364	T363	L301	D237
E1129	E1129	Q1010	Q1010	D670	ARG	ARG	ASP	Y365	V302	V302	D238
R1137	R1137	N1013	N1013	D670	ARG	ARG	ASP	S366	A303	G304	G239
D1138	D1138	R1068	R1068	D670	ARG	ARG	ASP	H453	G304	S305	T240
D1141	D1141	E1064	E1064	D670	GLY	GLY	THR	H454	G306	S305	Y241
S1142	S1142	F1065	F1065	D670	ALA	ALA	ASP	F455	G307	G306	G242
K1153	K1153	H1066	H1066	D670	ALA	ALA	ASP	L456	G307	G307	R243
		S1067	S1067	D670	LEU	LEU	ASN	T457	G370	A308	L244
				D670	ASP	ASP	GLY	V459	E372	A309	G245
				D670	ASP	ASP	GLY	A467	E373	D310	E247
				D670	ASP	ASP	GLY	V468	E374	C311	N248
				D670	ASP	ASP	GLY	S469	E375	L312	R249
				D670	ASP	ASP	GLY	P470	E375	V313	F250
				D670	ASP	ASP	GLY	N471	E375	L252	R251
				D670	ASP	ASP	GLY		E375	L316	R253
				D670	ASP	ASP	GLY		E375	E317	F254
				D670	ASP	ASP	GLY		E375	ASP	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	14646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The CTF correction was performed during the map refinement in Relion.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	276.06003, 276.06003, 276.06003	wwPDB
Map dimensions	258, 258, 258	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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	0.37	0/7903	0.54	0/10719
1	B	0.37	0/7903	0.54	0/10719
1	C	0.37	0/7903	0.54	0/10719
1	D	0.37	0/7903	0.54	0/10719
All	All	0.37	0/31612	0.54	0/42876

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	7731	0	7732	55	0
1	B	7731	0	7732	52	0
1	C	7731	0	7732	52	0
1	D	7731	0	7732	54	0
2	A	31	0	12	2	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	2	0
All	All	31048	0	30976	212	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.

The worst 5 of 212 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:C:86:ARG:HD3	1:C:228:TYR:CD2	2.13	0.82
1:B:86:ARG:HD3	1:B:228:TYR:CD2	2.17	0.80
1:D:86:ARG:HD3	1:D:228:TYR:CD2	2.15	0.80
1:A:86:ARG:HD3	1:A:228:TYR:CD2	2.17	0.79
1:D:160:HIS:HD2	2:D:2000:ATP:C2	2.06	0.73

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	967/1254 (77%)	914 (94%)	53 (6%)	0	100	100
1	B	967/1254 (77%)	913 (94%)	54 (6%)	0	100	100
1	C	967/1254 (77%)	913 (94%)	54 (6%)	0	100	100
1	D	967/1254 (77%)	914 (94%)	53 (6%)	0	100	100
All	All	3868/5016 (77%)	3654 (94%)	214 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	811/1063 (76%)	801 (99%)	10 (1%)	67	79
1	B	811/1063 (76%)	801 (99%)	10 (1%)	67	79
1	C	811/1063 (76%)	801 (99%)	10 (1%)	67	79
1	D	811/1063 (76%)	801 (99%)	10 (1%)	67	79
All	All	3244/4252 (76%)	3204 (99%)	40 (1%)	66	79

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	878	ARG
1	D	570	ASN
1	C	1058	ARG
1	D	93	ARG
1	D	782	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	633	ASN
1	D	405	ASN
1	C	782	ASN
1	C	1013	ASN
1	D	570	ASN

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

4 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	C	2000	-	28,33,33	1.02	2 (7%)	34,52,52	1.12	2 (5%)
2	ATP	B	2000	-	28,33,33	1.03	2 (7%)	34,52,52	1.14	2 (5%)
2	ATP	D	2000	-	28,33,33	1.01	2 (7%)	34,52,52	1.13	2 (5%)
2	ATP	A	2000	-	28,33,33	1.03	2 (7%)	34,52,52	1.13	2 (5%)

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	C	2000	-	-	0/18/38/38	0/3/3/3
2	ATP	B	2000	-	-	0/18/38/38	0/3/3/3
2	ATP	D	2000	-	-	0/18/38/38	0/3/3/3
2	ATP	A	2000	-	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	ATP	PA-O3A	2.44	1.62	1.59
2	C	2000	ATP	PA-O3A	2.40	1.62	1.59
2	B	2000	ATP	PA-O3A	2.39	1.62	1.59
2	D	2000	ATP	PA-O3A	2.34	1.62	1.59
2	C	2000	ATP	PB-O3A	2.24	1.61	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	ATP	N3-C2-N1	-3.22	124.30	128.67
2	D	2000	ATP	N3-C2-N1	-3.16	124.38	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	ATP	N3-C2-N1	-3.14	124.41	128.67
2	C	2000	ATP	N3-C2-N1	-3.06	124.52	128.67
2	D	2000	ATP	C4-C5-N7	-2.35	106.86	109.34

There are no chirality outliers.

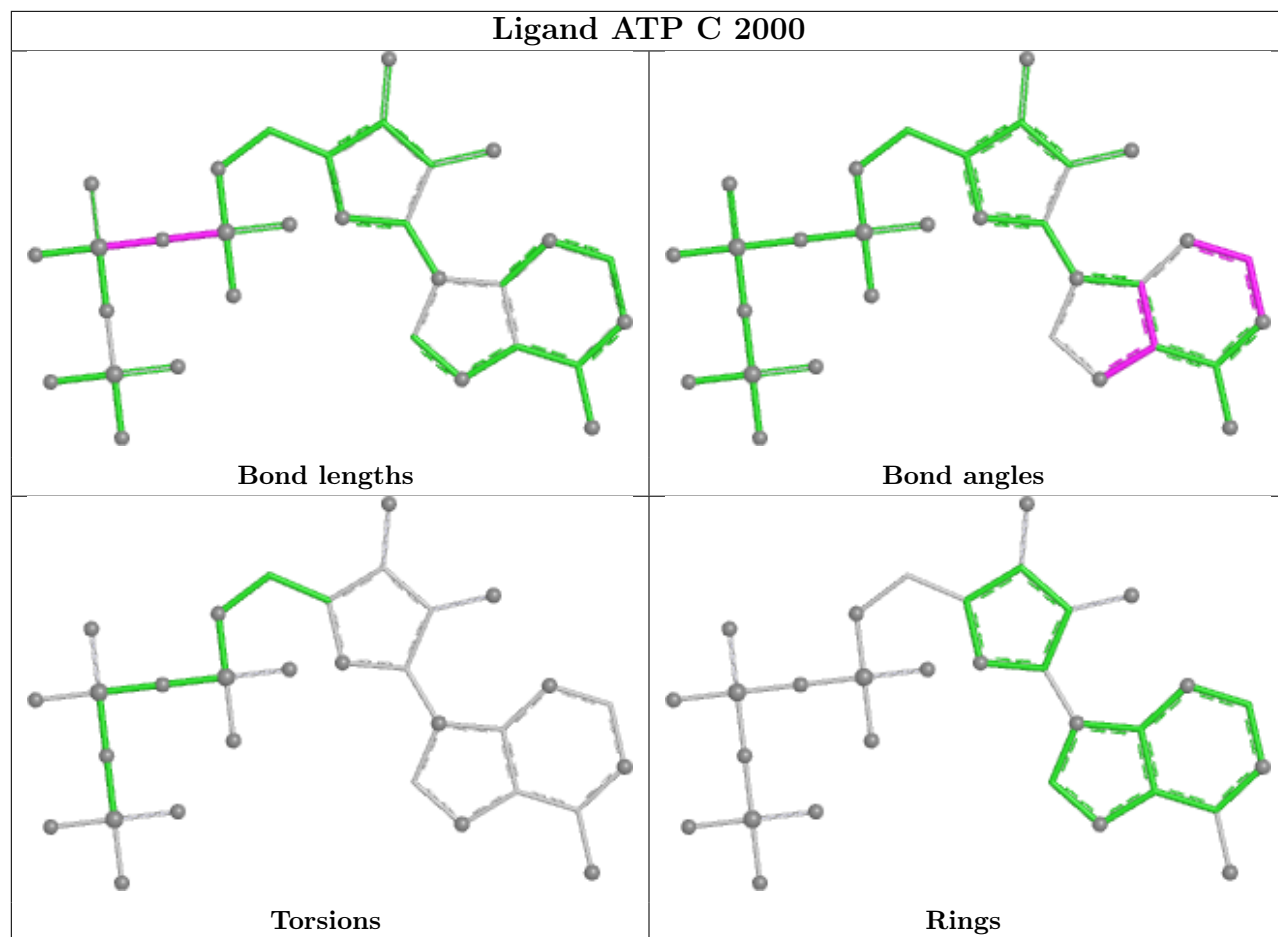
There are no torsion outliers.

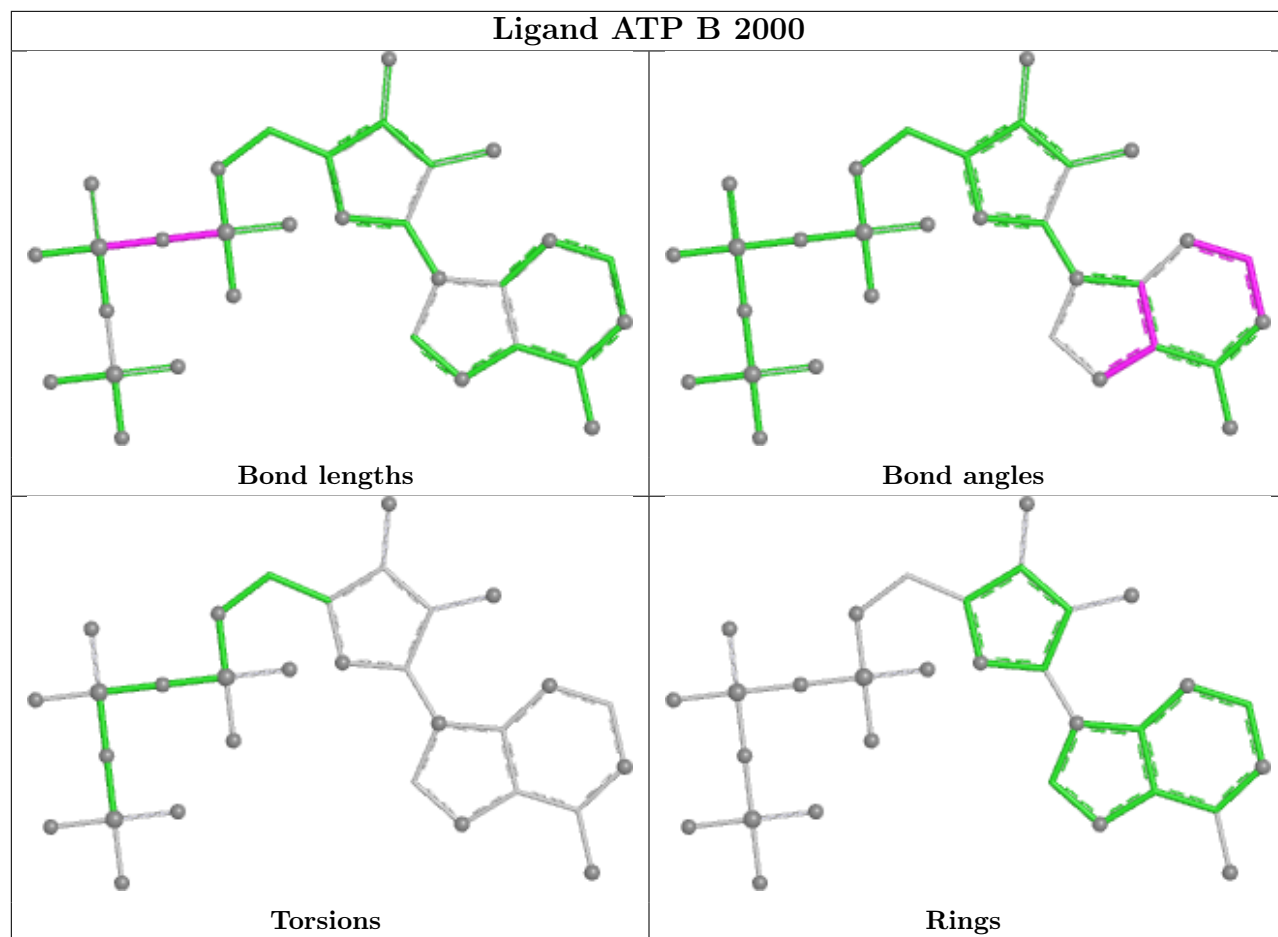
There are no ring outliers.

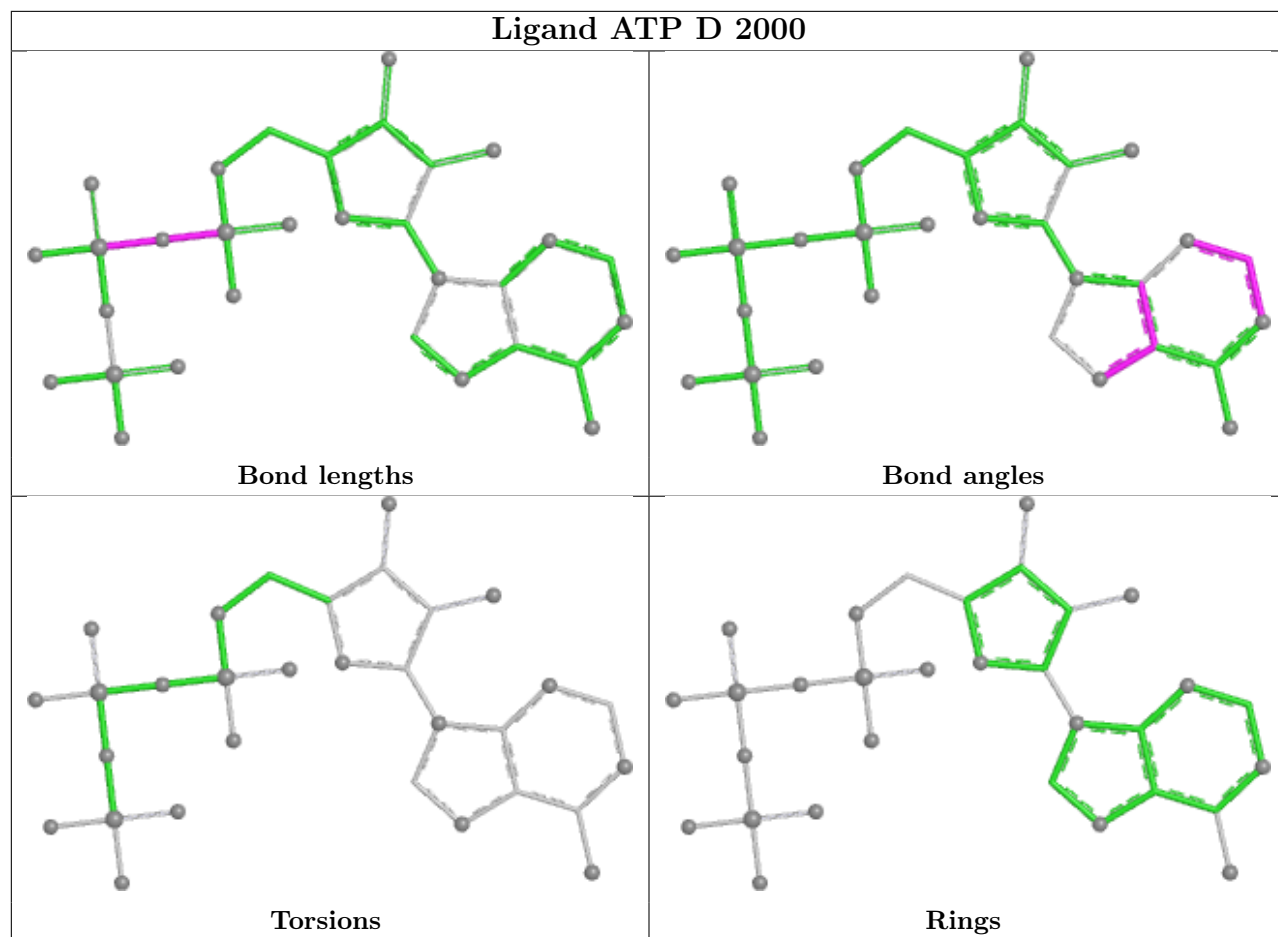
4 monomers are involved in 6 short contacts:

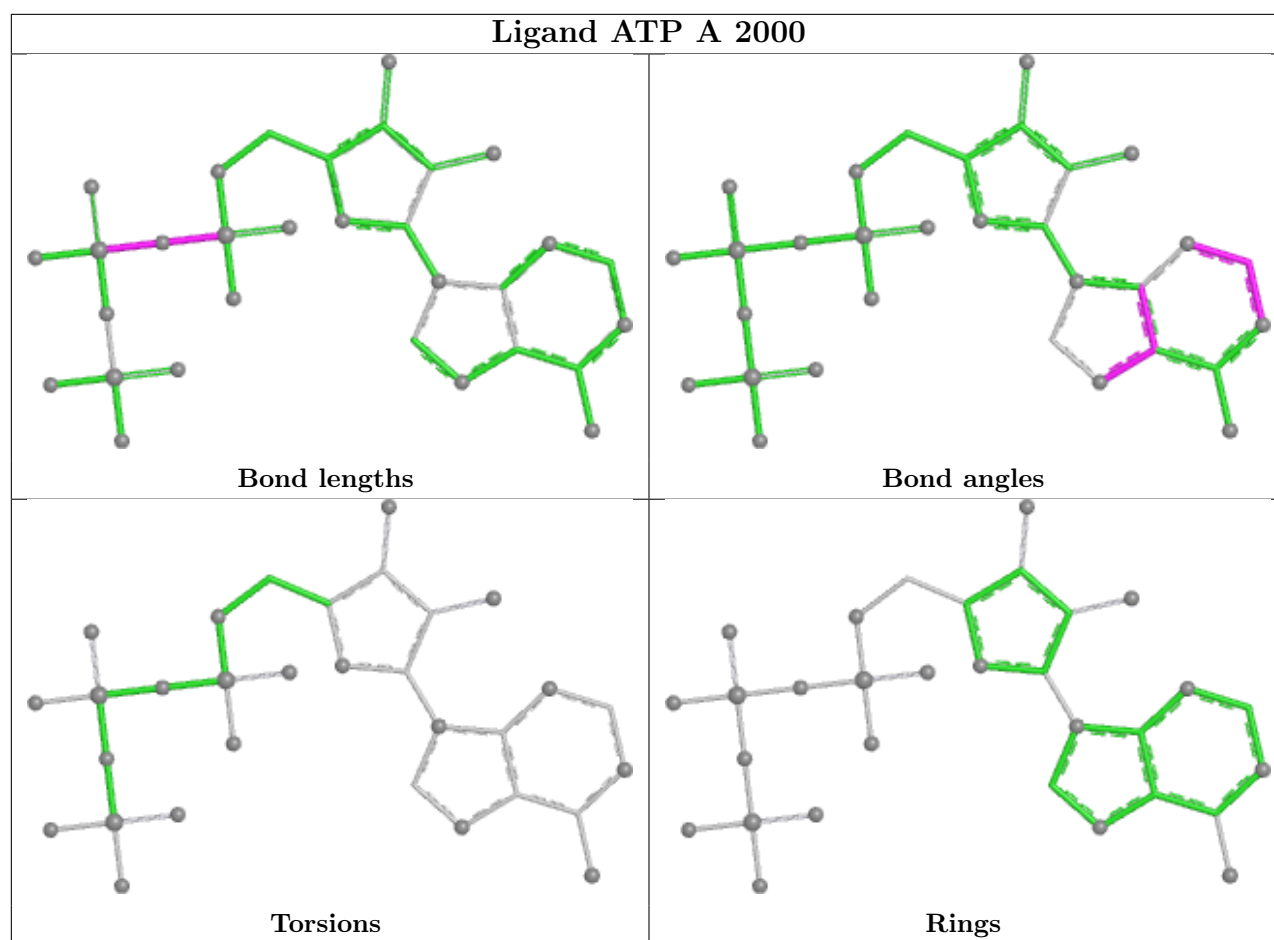
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	ATP	1	0
2	B	2000	ATP	1	0
2	D	2000	ATP	2	0
2	A	2000	ATP	2	0

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.

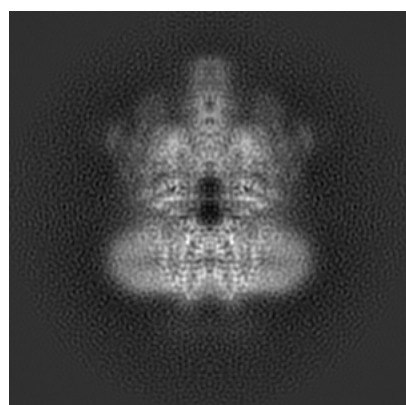
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7085. These allow visual inspection of the internal detail of the map and identification of artifacts.

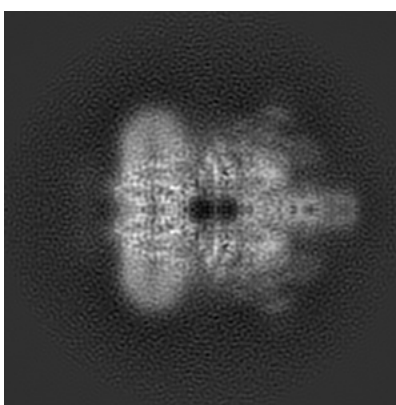
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

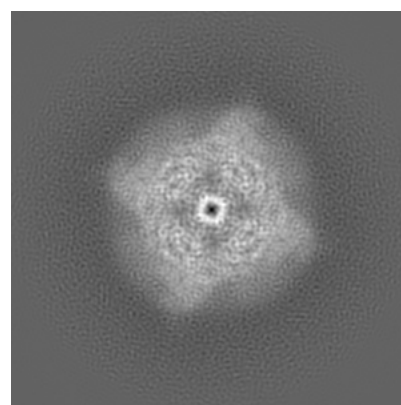
6.1.1 Primary map



X



Y



Z

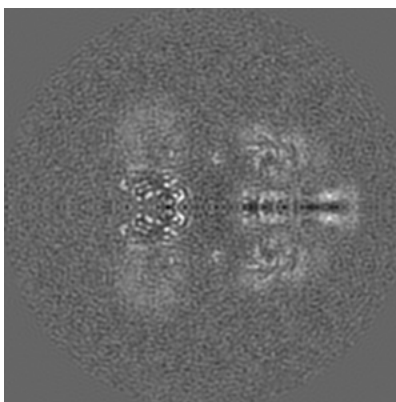
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

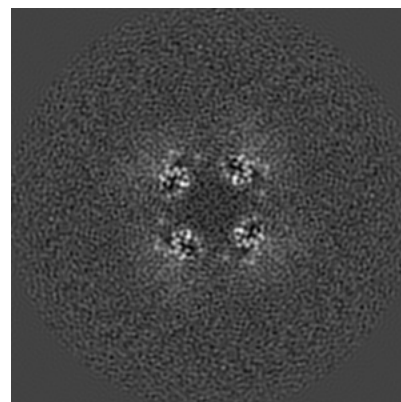
6.2.1 Primary map



X Index: 129



Y Index: 129

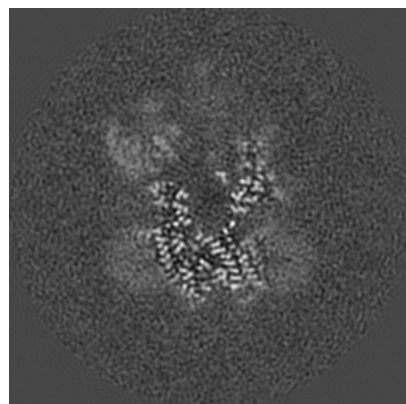


Z Index: 129

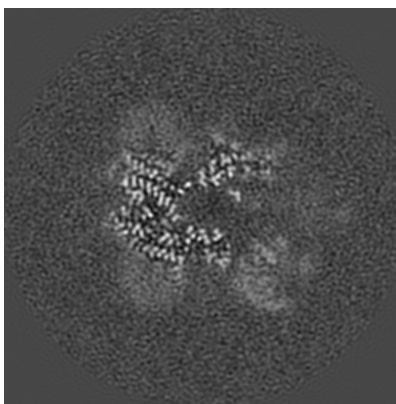
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

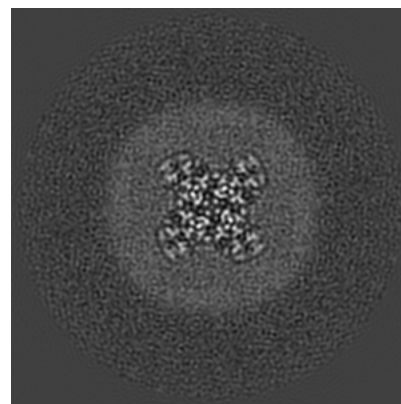
6.3.1 Primary map



X Index: 113



Y Index: 145

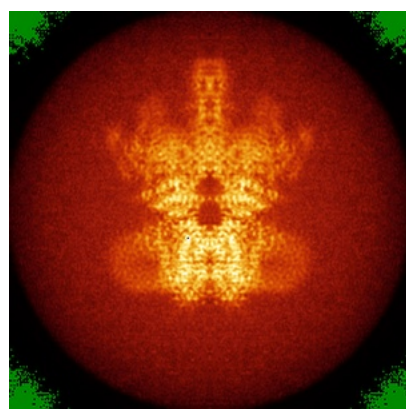


Z Index: 89

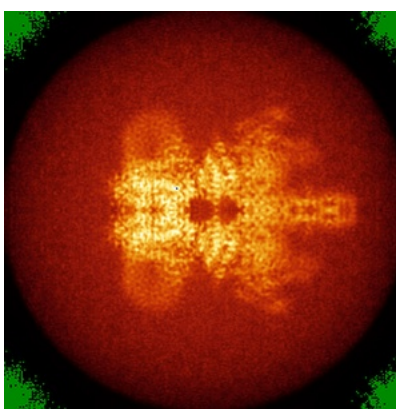
The images above show the largest variance slices of the map in three orthogonal directions.

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

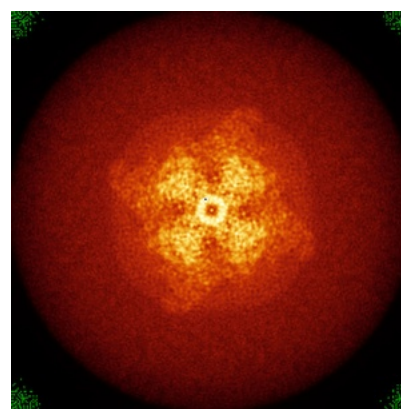
6.4.1 Primary map



X



Y

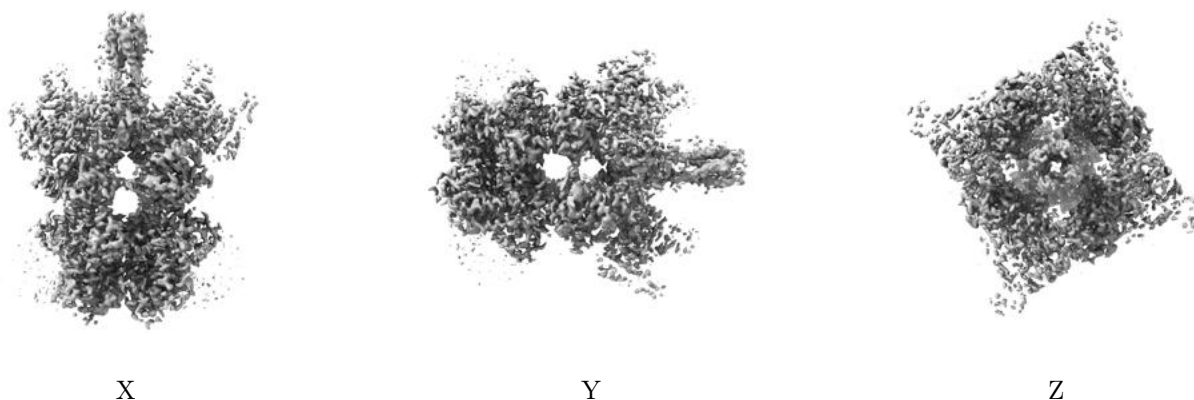


Z

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

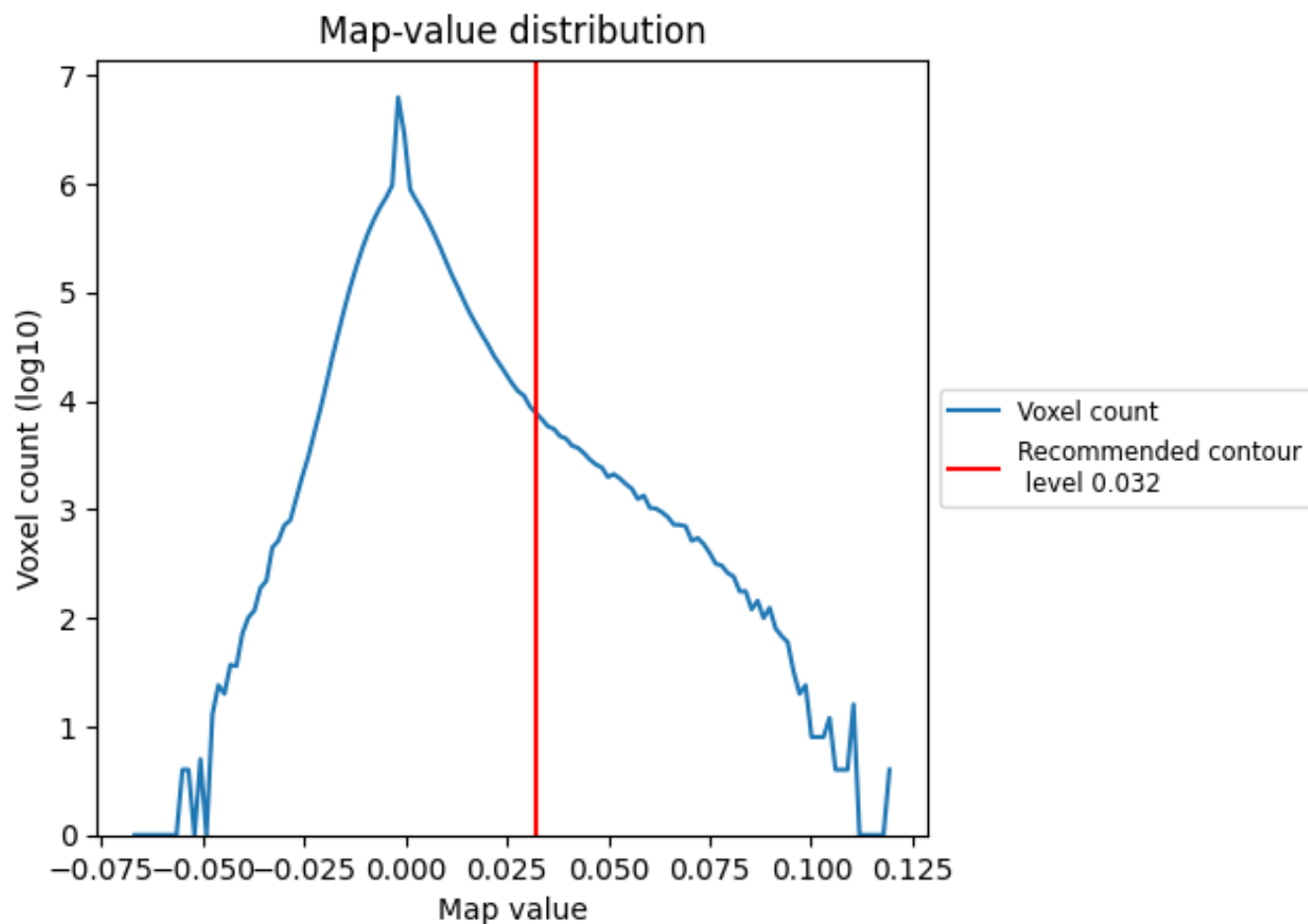
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

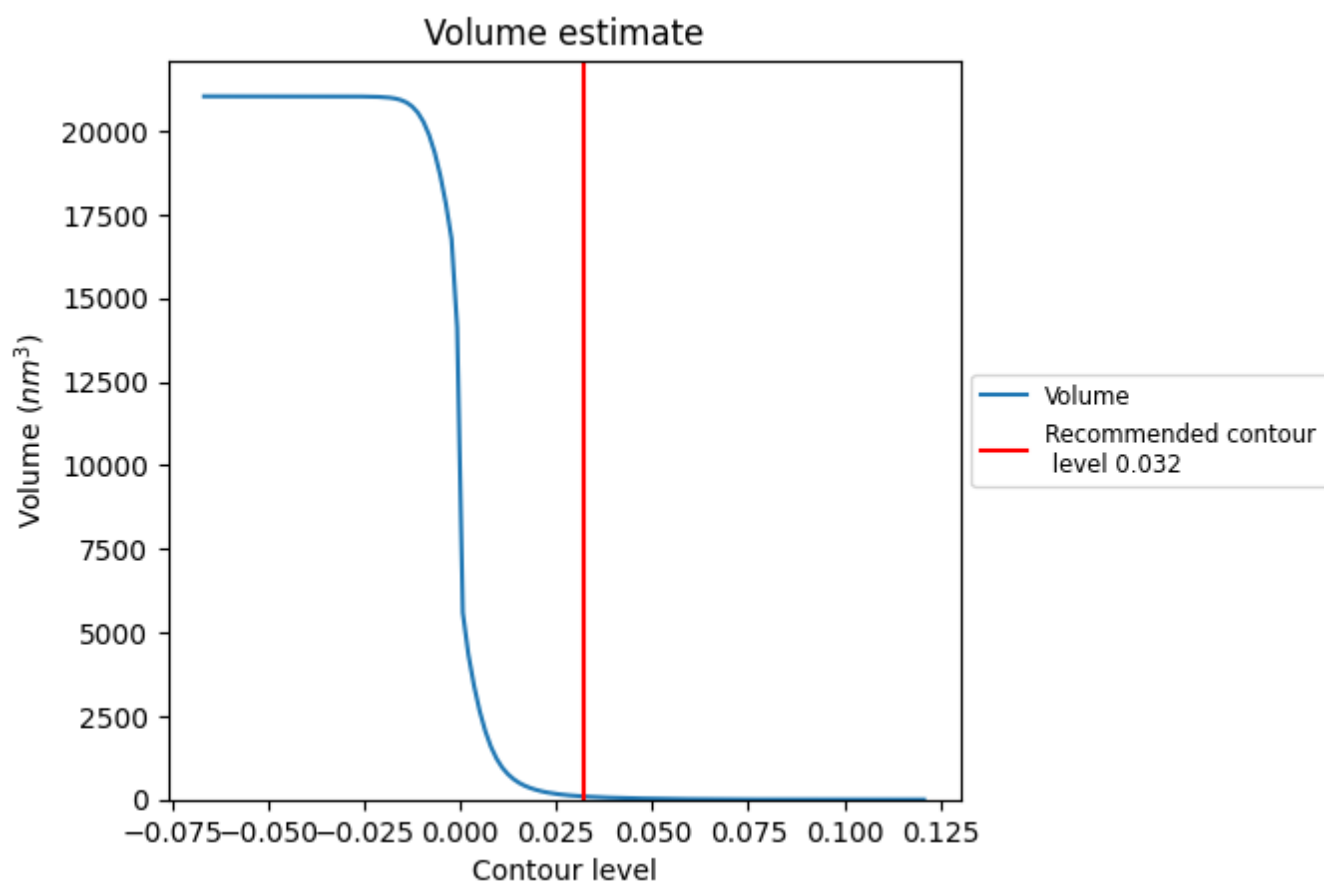
This section contains the results of statistical analysis of the map.

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.

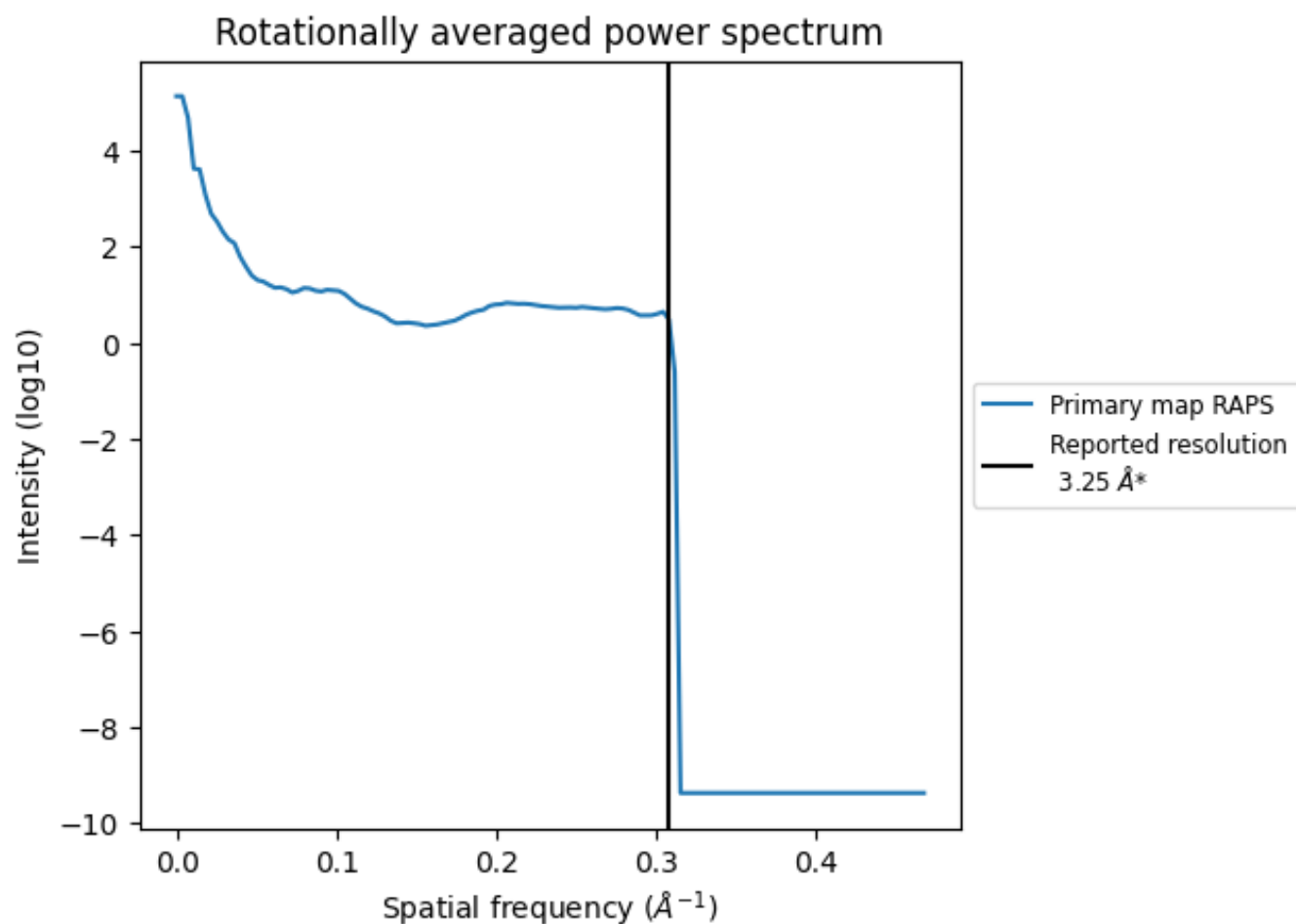
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; this corresponds to an approximate mass of 85 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 0.308 Å⁻¹

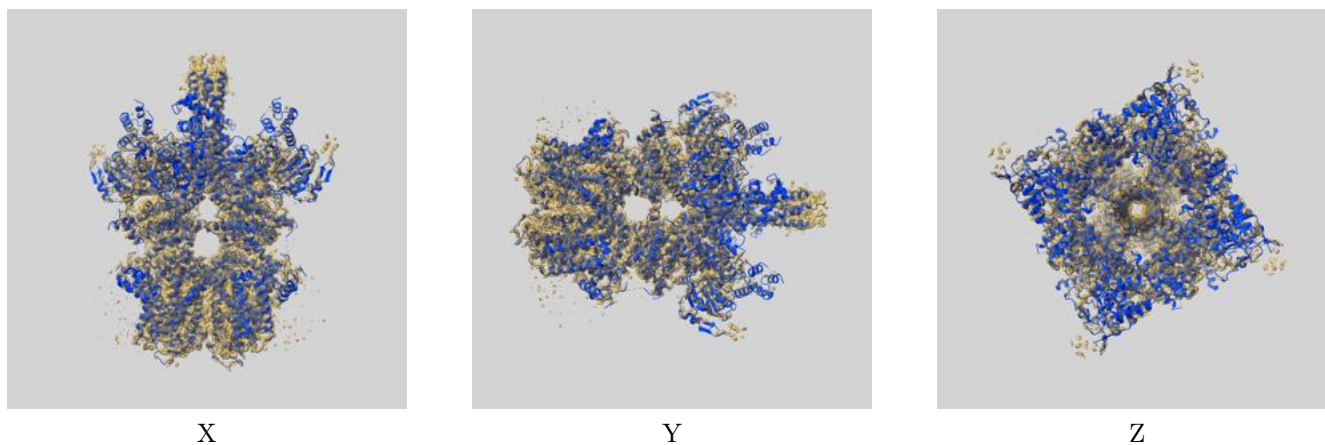
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

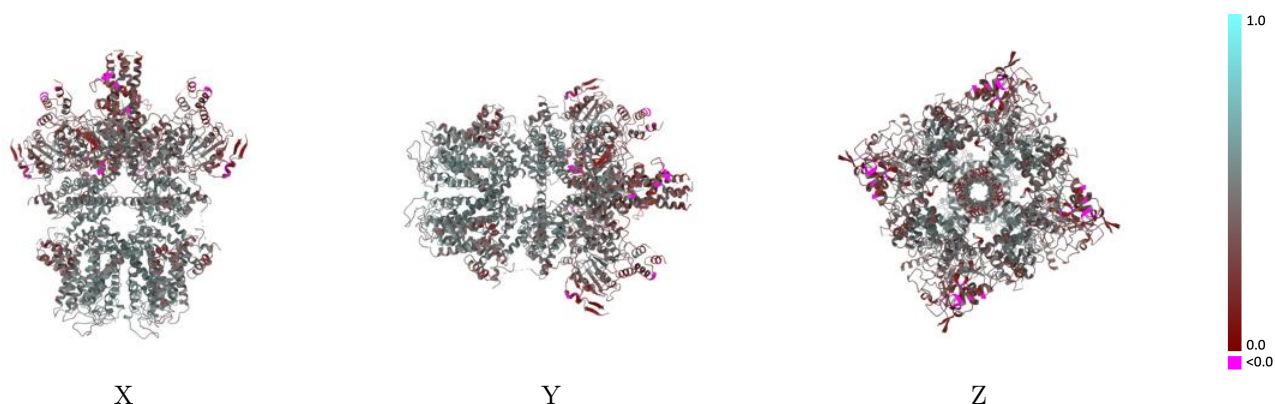
This section contains information regarding the fit between EMDB map EMD-7085 and PDB model 6BCQ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



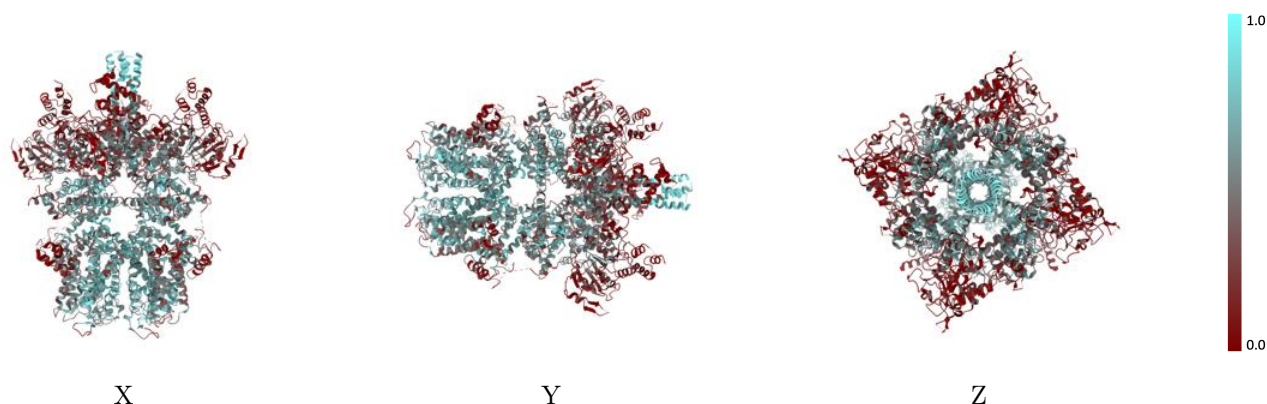
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



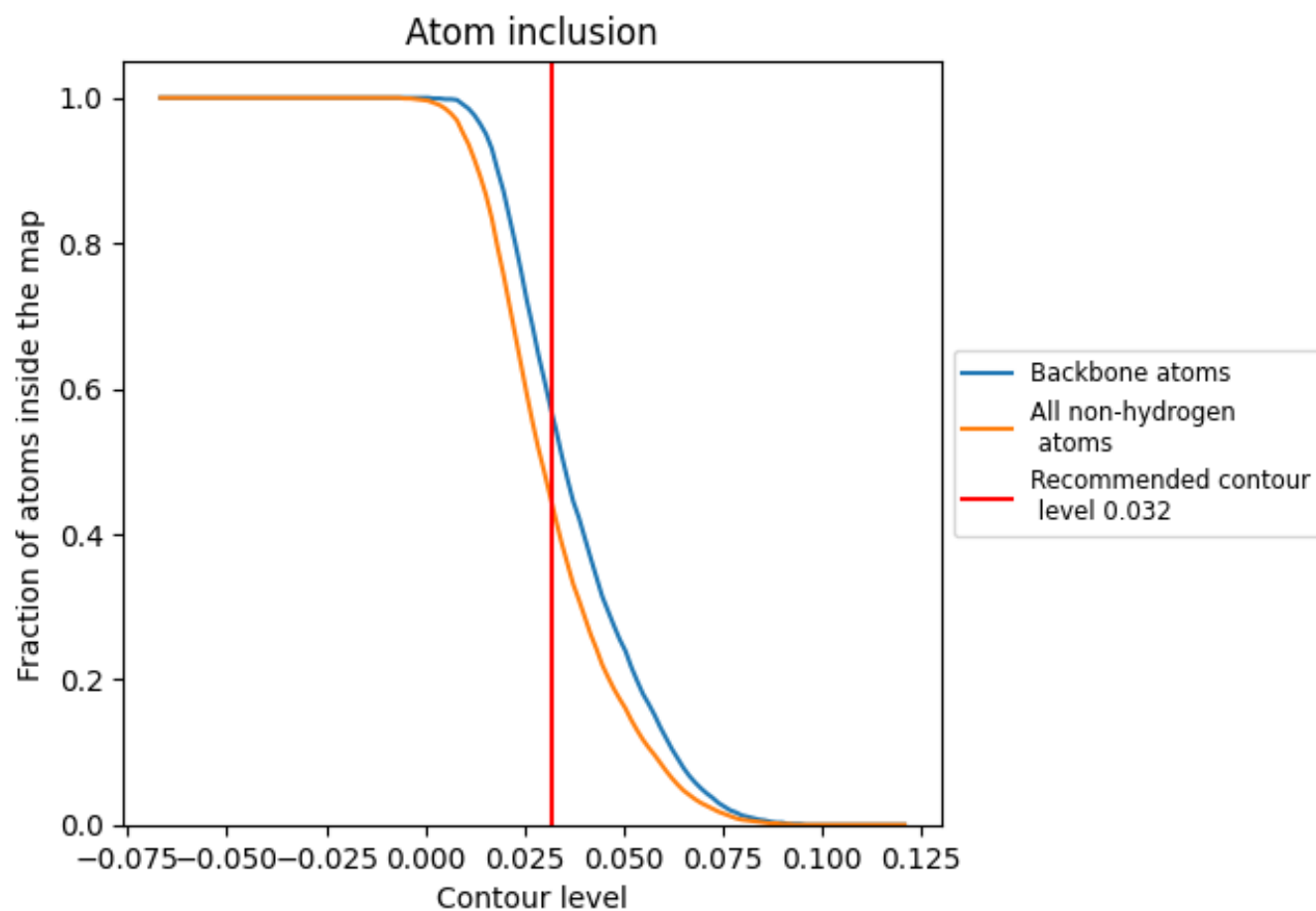
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 44% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4400	<div></div> 0.4330
A	<div></div> 0.4410	<div></div> 0.4330
B	<div></div> 0.4410	<div></div> 0.4330
C	<div></div> 0.4390	<div></div> 0.4330
D	<div></div> 0.4400	<div></div> 0.4330

