



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 03:55 AM UTC

PDB ID : 9NEI / pdb_00009nei
EMDB ID : EMD-49311
Title : GT-Shaker Class A
Authors : Tan, X.; Swartz, K.J.
Deposited on : 2025-02-19
Resolution : 2.97 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

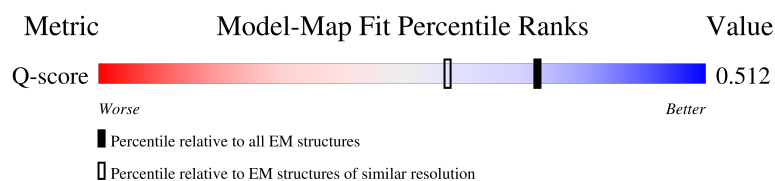
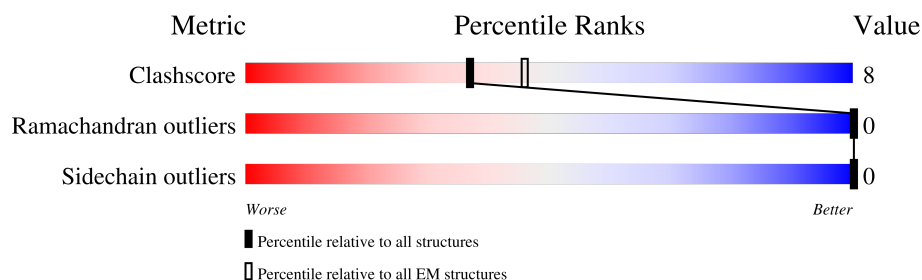
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 Å.

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



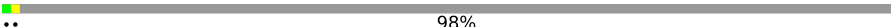
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13205 (2.47 - 3.47)

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	937	
1	B	937	
1	C	937	
1	D	937	

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Mol	Chain	Length	Quality of chain
1	G	937	 98%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7056 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 Potassium voltage-gated channel protein Shaker.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	210	Total	C	N	O	S	0	0
			1654	1119	255	273	7		
1	B	210	Total	C	N	O	S	0	0
			1648	1116	252	273	7		
1	C	210	Total	C	N	O	S	0	0
			1654	1119	255	273	7		
1	D	210	Total	C	N	O	S	0	0
			1647	1113	255	272	7		
1	G	15	Total	C	N	O	S	0	0
			98	61	15	21	1		

There are 1410 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-280	MET	-	initiating methionine	UNP P08510
A	-279	GLY	-	expression tag	UNP P08510
A	-278	SER	-	expression tag	UNP P08510
A	-277	SER	-	expression tag	UNP P08510
A	-276	HIS	-	expression tag	UNP P08510
A	-275	HIS	-	expression tag	UNP P08510
A	-274	HIS	-	expression tag	UNP P08510
A	-273	HIS	-	expression tag	UNP P08510
A	-272	HIS	-	expression tag	UNP P08510
A	-271	HIS	-	expression tag	UNP P08510
A	-270	HIS	-	expression tag	UNP P08510
A	-269	HIS	-	expression tag	UNP P08510
A	-268	GLY	-	expression tag	UNP P08510
A	-267	SER	-	expression tag	UNP P08510
A	-266	SER	-	expression tag	UNP P08510
A	-265	ARG	-	expression tag	UNP P08510
A	-264	VAL	-	expression tag	UNP P08510
A	-263	SER	-	expression tag	UNP P08510
A	-262	LYS	-	expression tag	UNP P08510
A	-261	GLY	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-260	GLU	-	expression tag	UNP P08510
A	-259	GLU	-	expression tag	UNP P08510
A	-258	LEU	-	expression tag	UNP P08510
A	-257	PHE	-	expression tag	UNP P08510
A	-256	THR	-	expression tag	UNP P08510
A	-255	GLY	-	expression tag	UNP P08510
A	-254	VAL	-	expression tag	UNP P08510
A	-253	VAL	-	expression tag	UNP P08510
A	-252	PRO	-	expression tag	UNP P08510
A	-251	ILE	-	expression tag	UNP P08510
A	-250	LEU	-	expression tag	UNP P08510
A	-249	VAL	-	expression tag	UNP P08510
A	-248	GLU	-	expression tag	UNP P08510
A	-247	LEU	-	expression tag	UNP P08510
A	-246	ASP	-	expression tag	UNP P08510
A	-245	GLY	-	expression tag	UNP P08510
A	-244	ASP	-	expression tag	UNP P08510
A	-243	VAL	-	expression tag	UNP P08510
A	-242	ASN	-	expression tag	UNP P08510
A	-241	GLY	-	expression tag	UNP P08510
A	-240	HIS	-	expression tag	UNP P08510
A	-239	LYS	-	expression tag	UNP P08510
A	-238	PHE	-	expression tag	UNP P08510
A	-237	SER	-	expression tag	UNP P08510
A	-236	VAL	-	expression tag	UNP P08510
A	-235	SER	-	expression tag	UNP P08510
A	-234	GLY	-	expression tag	UNP P08510
A	-233	GLU	-	expression tag	UNP P08510
A	-232	GLY	-	expression tag	UNP P08510
A	-231	GLU	-	expression tag	UNP P08510
A	-230	GLY	-	expression tag	UNP P08510
A	-229	ASP	-	expression tag	UNP P08510
A	-228	ALA	-	expression tag	UNP P08510
A	-227	THR	-	expression tag	UNP P08510
A	-226	TYR	-	expression tag	UNP P08510
A	-225	GLY	-	expression tag	UNP P08510
A	-224	LYS	-	expression tag	UNP P08510
A	-223	LEU	-	expression tag	UNP P08510
A	-222	THR	-	expression tag	UNP P08510
A	-221	LEU	-	expression tag	UNP P08510
A	-220	LYS	-	expression tag	UNP P08510
A	-219	LEU	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-218	ILE	-	expression tag	UNP P08510
A	-217	CYS	-	expression tag	UNP P08510
A	-216	THR	-	expression tag	UNP P08510
A	-215	THR	-	expression tag	UNP P08510
A	-214	GLY	-	expression tag	UNP P08510
A	-213	LYS	-	expression tag	UNP P08510
A	-212	LEU	-	expression tag	UNP P08510
A	-211	PRO	-	expression tag	UNP P08510
A	-210	VAL	-	expression tag	UNP P08510
A	-209	PRO	-	expression tag	UNP P08510
A	-208	TRP	-	expression tag	UNP P08510
A	-207	PRO	-	expression tag	UNP P08510
A	-206	THR	-	expression tag	UNP P08510
A	-205	LEU	-	expression tag	UNP P08510
A	-204	VAL	-	expression tag	UNP P08510
A	-203	THR	-	expression tag	UNP P08510
A	-202	THR	-	expression tag	UNP P08510
A	-201	LEU	-	expression tag	UNP P08510
A	-200	GLY	-	expression tag	UNP P08510
A	-199	TYR	-	expression tag	UNP P08510
A	-198	GLY	-	expression tag	UNP P08510
A	-197	LEU	-	expression tag	UNP P08510
A	-196	GLN	-	expression tag	UNP P08510
A	-195	CYS	-	expression tag	UNP P08510
A	-194	PHE	-	expression tag	UNP P08510
A	-193	ALA	-	expression tag	UNP P08510
A	-192	ARG	-	expression tag	UNP P08510
A	-191	TYR	-	expression tag	UNP P08510
A	-190	PRO	-	expression tag	UNP P08510
A	-189	ASP	-	expression tag	UNP P08510
A	-188	HIS	-	expression tag	UNP P08510
A	-187	MET	-	expression tag	UNP P08510
A	-186	LYS	-	expression tag	UNP P08510
A	-185	GLN	-	expression tag	UNP P08510
A	-184	HIS	-	expression tag	UNP P08510
A	-183	ASP	-	expression tag	UNP P08510
A	-182	PHE	-	expression tag	UNP P08510
A	-181	PHE	-	expression tag	UNP P08510
A	-180	LYS	-	expression tag	UNP P08510
A	-179	SER	-	expression tag	UNP P08510
A	-178	ALA	-	expression tag	UNP P08510
A	-177	MET	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-176	PRO	-	expression tag	UNP P08510
A	-175	GLU	-	expression tag	UNP P08510
A	-174	GLY	-	expression tag	UNP P08510
A	-173	TYR	-	expression tag	UNP P08510
A	-172	VAL	-	expression tag	UNP P08510
A	-171	GLN	-	expression tag	UNP P08510
A	-170	GLU	-	expression tag	UNP P08510
A	-169	ARG	-	expression tag	UNP P08510
A	-168	THR	-	expression tag	UNP P08510
A	-167	ILE	-	expression tag	UNP P08510
A	-166	PHE	-	expression tag	UNP P08510
A	-165	PHE	-	expression tag	UNP P08510
A	-164	LYS	-	expression tag	UNP P08510
A	-163	ASP	-	expression tag	UNP P08510
A	-162	ASP	-	expression tag	UNP P08510
A	-161	GLY	-	expression tag	UNP P08510
A	-160	ASN	-	expression tag	UNP P08510
A	-159	TYR	-	expression tag	UNP P08510
A	-158	LYS	-	expression tag	UNP P08510
A	-157	THR	-	expression tag	UNP P08510
A	-156	ARG	-	expression tag	UNP P08510
A	-155	ALA	-	expression tag	UNP P08510
A	-154	GLU	-	expression tag	UNP P08510
A	-153	VAL	-	expression tag	UNP P08510
A	-152	LYS	-	expression tag	UNP P08510
A	-151	PHE	-	expression tag	UNP P08510
A	-150	GLU	-	expression tag	UNP P08510
A	-149	GLY	-	expression tag	UNP P08510
A	-148	ASP	-	expression tag	UNP P08510
A	-147	THR	-	expression tag	UNP P08510
A	-146	LEU	-	expression tag	UNP P08510
A	-145	VAL	-	expression tag	UNP P08510
A	-144	ASN	-	expression tag	UNP P08510
A	-143	ARG	-	expression tag	UNP P08510
A	-142	ILE	-	expression tag	UNP P08510
A	-141	GLU	-	expression tag	UNP P08510
A	-140	LEU	-	expression tag	UNP P08510
A	-139	LYS	-	expression tag	UNP P08510
A	-138	GLY	-	expression tag	UNP P08510
A	-137	ILE	-	expression tag	UNP P08510
A	-136	ASP	-	expression tag	UNP P08510
A	-135	PHE	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-134	LYS	-	expression tag	UNP P08510
A	-133	GLU	-	expression tag	UNP P08510
A	-132	ASP	-	expression tag	UNP P08510
A	-131	GLY	-	expression tag	UNP P08510
A	-130	ASN	-	expression tag	UNP P08510
A	-129	ILE	-	expression tag	UNP P08510
A	-128	LEU	-	expression tag	UNP P08510
A	-127	GLY	-	expression tag	UNP P08510
A	-126	HIS	-	expression tag	UNP P08510
A	-125	LYS	-	expression tag	UNP P08510
A	-124	LEU	-	expression tag	UNP P08510
A	-123	GLU	-	expression tag	UNP P08510
A	-122	TYR	-	expression tag	UNP P08510
A	-121	ASN	-	expression tag	UNP P08510
A	-120	TYR	-	expression tag	UNP P08510
A	-119	ASN	-	expression tag	UNP P08510
A	-118	SER	-	expression tag	UNP P08510
A	-117	HIS	-	expression tag	UNP P08510
A	-116	ASN	-	expression tag	UNP P08510
A	-115	VAL	-	expression tag	UNP P08510
A	-114	TYR	-	expression tag	UNP P08510
A	-113	ILE	-	expression tag	UNP P08510
A	-112	THR	-	expression tag	UNP P08510
A	-111	ALA	-	expression tag	UNP P08510
A	-110	ASP	-	expression tag	UNP P08510
A	-109	LYS	-	expression tag	UNP P08510
A	-108	GLN	-	expression tag	UNP P08510
A	-107	LYS	-	expression tag	UNP P08510
A	-106	ASN	-	expression tag	UNP P08510
A	-105	GLY	-	expression tag	UNP P08510
A	-104	ILE	-	expression tag	UNP P08510
A	-103	LYS	-	expression tag	UNP P08510
A	-102	ALA	-	expression tag	UNP P08510
A	-101	ASN	-	expression tag	UNP P08510
A	-100	PHE	-	expression tag	UNP P08510
A	-99	LYS	-	expression tag	UNP P08510
A	-98	ILE	-	expression tag	UNP P08510
A	-97	ARG	-	expression tag	UNP P08510
A	-96	HIS	-	expression tag	UNP P08510
A	-95	ASN	-	expression tag	UNP P08510
A	-94	ILE	-	expression tag	UNP P08510
A	-93	GLU	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-92	ASP	-	expression tag	UNP P08510
A	-91	GLY	-	expression tag	UNP P08510
A	-90	GLY	-	expression tag	UNP P08510
A	-89	VAL	-	expression tag	UNP P08510
A	-88	GLN	-	expression tag	UNP P08510
A	-87	LEU	-	expression tag	UNP P08510
A	-86	ALA	-	expression tag	UNP P08510
A	-85	ASP	-	expression tag	UNP P08510
A	-84	HIS	-	expression tag	UNP P08510
A	-83	TYR	-	expression tag	UNP P08510
A	-82	GLN	-	expression tag	UNP P08510
A	-81	GLN	-	expression tag	UNP P08510
A	-80	ASN	-	expression tag	UNP P08510
A	-79	THR	-	expression tag	UNP P08510
A	-78	PRO	-	expression tag	UNP P08510
A	-77	ILE	-	expression tag	UNP P08510
A	-76	GLY	-	expression tag	UNP P08510
A	-75	ASP	-	expression tag	UNP P08510
A	-74	GLY	-	expression tag	UNP P08510
A	-73	PRO	-	expression tag	UNP P08510
A	-72	VAL	-	expression tag	UNP P08510
A	-71	LEU	-	expression tag	UNP P08510
A	-70	LEU	-	expression tag	UNP P08510
A	-69	PRO	-	expression tag	UNP P08510
A	-68	ASP	-	expression tag	UNP P08510
A	-67	ASN	-	expression tag	UNP P08510
A	-66	HIS	-	expression tag	UNP P08510
A	-65	TYR	-	expression tag	UNP P08510
A	-64	LEU	-	expression tag	UNP P08510
A	-63	SER	-	expression tag	UNP P08510
A	-62	TYR	-	expression tag	UNP P08510
A	-61	GLN	-	expression tag	UNP P08510
A	-60	SER	-	expression tag	UNP P08510
A	-59	LYS	-	expression tag	UNP P08510
A	-58	LEU	-	expression tag	UNP P08510
A	-57	SER	-	expression tag	UNP P08510
A	-56	LYS	-	expression tag	UNP P08510
A	-55	ASP	-	expression tag	UNP P08510
A	-54	PRO	-	expression tag	UNP P08510
A	-53	ASN	-	expression tag	UNP P08510
A	-52	GLU	-	expression tag	UNP P08510
A	-51	LYS	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-50	ARG	-	expression tag	UNP P08510
A	-49	ASP	-	expression tag	UNP P08510
A	-48	HIS	-	expression tag	UNP P08510
A	-47	MET	-	expression tag	UNP P08510
A	-46	VAL	-	expression tag	UNP P08510
A	-45	LEU	-	expression tag	UNP P08510
A	-44	LEU	-	expression tag	UNP P08510
A	-43	GLU	-	expression tag	UNP P08510
A	-42	PHE	-	expression tag	UNP P08510
A	-41	VAL	-	expression tag	UNP P08510
A	-40	THR	-	expression tag	UNP P08510
A	-39	ALA	-	expression tag	UNP P08510
A	-38	ALA	-	expression tag	UNP P08510
A	-37	GLY	-	expression tag	UNP P08510
A	-36	ILE	-	expression tag	UNP P08510
A	-35	THR	-	expression tag	UNP P08510
A	-34	LEU	-	expression tag	UNP P08510
A	-33	GLY	-	expression tag	UNP P08510
A	-32	MET	-	expression tag	UNP P08510
A	-31	ASP	-	expression tag	UNP P08510
A	-30	GLU	-	expression tag	UNP P08510
A	-29	LEU	-	expression tag	UNP P08510
A	-28	TYR	-	expression tag	UNP P08510
A	-27	LYS	-	expression tag	UNP P08510
A	-26	GLU	-	expression tag	UNP P08510
A	-25	ASN	-	expression tag	UNP P08510
A	-24	SER	-	expression tag	UNP P08510
A	-23	SER	-	expression tag	UNP P08510
A	-22	SER	-	expression tag	UNP P08510
A	-21	ASN	-	expression tag	UNP P08510
A	-20	ASN	-	expression tag	UNP P08510
A	-19	ASN	-	expression tag	UNP P08510
A	-18	ASN	-	expression tag	UNP P08510
A	-17	ASN	-	expression tag	UNP P08510
A	-16	ASN	-	expression tag	UNP P08510
A	-15	ASN	-	expression tag	UNP P08510
A	-14	ASN	-	expression tag	UNP P08510
A	-13	ASN	-	expression tag	UNP P08510
A	-12	ASN	-	expression tag	UNP P08510
A	-11	LEU	-	expression tag	UNP P08510
A	-10	GLY	-	expression tag	UNP P08510
A	-9	ILE	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLU	-	expression tag	UNP P08510
A	-7	GLU	-	expression tag	UNP P08510
A	-6	ASN	-	expression tag	UNP P08510
A	-5	LEU	-	expression tag	UNP P08510
A	-4	TYR	-	expression tag	UNP P08510
A	-3	PHE	-	expression tag	UNP P08510
A	-2	GLN	-	expression tag	UNP P08510
A	-1	GLY	-	expression tag	UNP P08510
A	0	THR	-	expression tag	UNP P08510
A	513	VAL	-	insertion	UNP P08510
B	-280	MET	-	initiating methionine	UNP P08510
B	-279	GLY	-	expression tag	UNP P08510
B	-278	SER	-	expression tag	UNP P08510
B	-277	SER	-	expression tag	UNP P08510
B	-276	HIS	-	expression tag	UNP P08510
B	-275	HIS	-	expression tag	UNP P08510
B	-274	HIS	-	expression tag	UNP P08510
B	-273	HIS	-	expression tag	UNP P08510
B	-272	HIS	-	expression tag	UNP P08510
B	-271	HIS	-	expression tag	UNP P08510
B	-270	HIS	-	expression tag	UNP P08510
B	-269	HIS	-	expression tag	UNP P08510
B	-268	GLY	-	expression tag	UNP P08510
B	-267	SER	-	expression tag	UNP P08510
B	-266	SER	-	expression tag	UNP P08510
B	-265	ARG	-	expression tag	UNP P08510
B	-264	VAL	-	expression tag	UNP P08510
B	-263	SER	-	expression tag	UNP P08510
B	-262	LYS	-	expression tag	UNP P08510
B	-261	GLY	-	expression tag	UNP P08510
B	-260	GLU	-	expression tag	UNP P08510
B	-259	GLU	-	expression tag	UNP P08510
B	-258	LEU	-	expression tag	UNP P08510
B	-257	PHE	-	expression tag	UNP P08510
B	-256	THR	-	expression tag	UNP P08510
B	-255	GLY	-	expression tag	UNP P08510
B	-254	VAL	-	expression tag	UNP P08510
B	-253	VAL	-	expression tag	UNP P08510
B	-252	PRO	-	expression tag	UNP P08510
B	-251	ILE	-	expression tag	UNP P08510
B	-250	LEU	-	expression tag	UNP P08510
B	-249	VAL	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-248	GLU	-	expression tag	UNP P08510
B	-247	LEU	-	expression tag	UNP P08510
B	-246	ASP	-	expression tag	UNP P08510
B	-245	GLY	-	expression tag	UNP P08510
B	-244	ASP	-	expression tag	UNP P08510
B	-243	VAL	-	expression tag	UNP P08510
B	-242	ASN	-	expression tag	UNP P08510
B	-241	GLY	-	expression tag	UNP P08510
B	-240	HIS	-	expression tag	UNP P08510
B	-239	LYS	-	expression tag	UNP P08510
B	-238	PHE	-	expression tag	UNP P08510
B	-237	SER	-	expression tag	UNP P08510
B	-236	VAL	-	expression tag	UNP P08510
B	-235	SER	-	expression tag	UNP P08510
B	-234	GLY	-	expression tag	UNP P08510
B	-233	GLU	-	expression tag	UNP P08510
B	-232	GLY	-	expression tag	UNP P08510
B	-231	GLU	-	expression tag	UNP P08510
B	-230	GLY	-	expression tag	UNP P08510
B	-229	ASP	-	expression tag	UNP P08510
B	-228	ALA	-	expression tag	UNP P08510
B	-227	THR	-	expression tag	UNP P08510
B	-226	TYR	-	expression tag	UNP P08510
B	-225	GLY	-	expression tag	UNP P08510
B	-224	LYS	-	expression tag	UNP P08510
B	-223	LEU	-	expression tag	UNP P08510
B	-222	THR	-	expression tag	UNP P08510
B	-221	LEU	-	expression tag	UNP P08510
B	-220	LYS	-	expression tag	UNP P08510
B	-219	LEU	-	expression tag	UNP P08510
B	-218	ILE	-	expression tag	UNP P08510
B	-217	CYS	-	expression tag	UNP P08510
B	-216	THR	-	expression tag	UNP P08510
B	-215	THR	-	expression tag	UNP P08510
B	-214	GLY	-	expression tag	UNP P08510
B	-213	LYS	-	expression tag	UNP P08510
B	-212	LEU	-	expression tag	UNP P08510
B	-211	PRO	-	expression tag	UNP P08510
B	-210	VAL	-	expression tag	UNP P08510
B	-209	PRO	-	expression tag	UNP P08510
B	-208	TRP	-	expression tag	UNP P08510
B	-207	PRO	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-206	THR	-	expression tag	UNP P08510
B	-205	LEU	-	expression tag	UNP P08510
B	-204	VAL	-	expression tag	UNP P08510
B	-203	THR	-	expression tag	UNP P08510
B	-202	THR	-	expression tag	UNP P08510
B	-201	LEU	-	expression tag	UNP P08510
B	-200	GLY	-	expression tag	UNP P08510
B	-199	TYR	-	expression tag	UNP P08510
B	-198	GLY	-	expression tag	UNP P08510
B	-197	LEU	-	expression tag	UNP P08510
B	-196	GLN	-	expression tag	UNP P08510
B	-195	CYS	-	expression tag	UNP P08510
B	-194	PHE	-	expression tag	UNP P08510
B	-193	ALA	-	expression tag	UNP P08510
B	-192	ARG	-	expression tag	UNP P08510
B	-191	TYR	-	expression tag	UNP P08510
B	-190	PRO	-	expression tag	UNP P08510
B	-189	ASP	-	expression tag	UNP P08510
B	-188	HIS	-	expression tag	UNP P08510
B	-187	MET	-	expression tag	UNP P08510
B	-186	LYS	-	expression tag	UNP P08510
B	-185	GLN	-	expression tag	UNP P08510
B	-184	HIS	-	expression tag	UNP P08510
B	-183	ASP	-	expression tag	UNP P08510
B	-182	PHE	-	expression tag	UNP P08510
B	-181	PHE	-	expression tag	UNP P08510
B	-180	LYS	-	expression tag	UNP P08510
B	-179	SER	-	expression tag	UNP P08510
B	-178	ALA	-	expression tag	UNP P08510
B	-177	MET	-	expression tag	UNP P08510
B	-176	PRO	-	expression tag	UNP P08510
B	-175	GLU	-	expression tag	UNP P08510
B	-174	GLY	-	expression tag	UNP P08510
B	-173	TYR	-	expression tag	UNP P08510
B	-172	VAL	-	expression tag	UNP P08510
B	-171	GLN	-	expression tag	UNP P08510
B	-170	GLU	-	expression tag	UNP P08510
B	-169	ARG	-	expression tag	UNP P08510
B	-168	THR	-	expression tag	UNP P08510
B	-167	ILE	-	expression tag	UNP P08510
B	-166	PHE	-	expression tag	UNP P08510
B	-165	PHE	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-164	LYS	-	expression tag	UNP P08510
B	-163	ASP	-	expression tag	UNP P08510
B	-162	ASP	-	expression tag	UNP P08510
B	-161	GLY	-	expression tag	UNP P08510
B	-160	ASN	-	expression tag	UNP P08510
B	-159	TYR	-	expression tag	UNP P08510
B	-158	LYS	-	expression tag	UNP P08510
B	-157	THR	-	expression tag	UNP P08510
B	-156	ARG	-	expression tag	UNP P08510
B	-155	ALA	-	expression tag	UNP P08510
B	-154	GLU	-	expression tag	UNP P08510
B	-153	VAL	-	expression tag	UNP P08510
B	-152	LYS	-	expression tag	UNP P08510
B	-151	PHE	-	expression tag	UNP P08510
B	-150	GLU	-	expression tag	UNP P08510
B	-149	GLY	-	expression tag	UNP P08510
B	-148	ASP	-	expression tag	UNP P08510
B	-147	THR	-	expression tag	UNP P08510
B	-146	LEU	-	expression tag	UNP P08510
B	-145	VAL	-	expression tag	UNP P08510
B	-144	ASN	-	expression tag	UNP P08510
B	-143	ARG	-	expression tag	UNP P08510
B	-142	ILE	-	expression tag	UNP P08510
B	-141	GLU	-	expression tag	UNP P08510
B	-140	LEU	-	expression tag	UNP P08510
B	-139	LYS	-	expression tag	UNP P08510
B	-138	GLY	-	expression tag	UNP P08510
B	-137	ILE	-	expression tag	UNP P08510
B	-136	ASP	-	expression tag	UNP P08510
B	-135	PHE	-	expression tag	UNP P08510
B	-134	LYS	-	expression tag	UNP P08510
B	-133	GLU	-	expression tag	UNP P08510
B	-132	ASP	-	expression tag	UNP P08510
B	-131	GLY	-	expression tag	UNP P08510
B	-130	ASN	-	expression tag	UNP P08510
B	-129	ILE	-	expression tag	UNP P08510
B	-128	LEU	-	expression tag	UNP P08510
B	-127	GLY	-	expression tag	UNP P08510
B	-126	HIS	-	expression tag	UNP P08510
B	-125	LYS	-	expression tag	UNP P08510
B	-124	LEU	-	expression tag	UNP P08510
B	-123	GLU	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-122	TYR	-	expression tag	UNP P08510
B	-121	ASN	-	expression tag	UNP P08510
B	-120	TYR	-	expression tag	UNP P08510
B	-119	ASN	-	expression tag	UNP P08510
B	-118	SER	-	expression tag	UNP P08510
B	-117	HIS	-	expression tag	UNP P08510
B	-116	ASN	-	expression tag	UNP P08510
B	-115	VAL	-	expression tag	UNP P08510
B	-114	TYR	-	expression tag	UNP P08510
B	-113	ILE	-	expression tag	UNP P08510
B	-112	THR	-	expression tag	UNP P08510
B	-111	ALA	-	expression tag	UNP P08510
B	-110	ASP	-	expression tag	UNP P08510
B	-109	LYS	-	expression tag	UNP P08510
B	-108	GLN	-	expression tag	UNP P08510
B	-107	LYS	-	expression tag	UNP P08510
B	-106	ASN	-	expression tag	UNP P08510
B	-105	GLY	-	expression tag	UNP P08510
B	-104	ILE	-	expression tag	UNP P08510
B	-103	LYS	-	expression tag	UNP P08510
B	-102	ALA	-	expression tag	UNP P08510
B	-101	ASN	-	expression tag	UNP P08510
B	-100	PHE	-	expression tag	UNP P08510
B	-99	LYS	-	expression tag	UNP P08510
B	-98	ILE	-	expression tag	UNP P08510
B	-97	ARG	-	expression tag	UNP P08510
B	-96	HIS	-	expression tag	UNP P08510
B	-95	ASN	-	expression tag	UNP P08510
B	-94	ILE	-	expression tag	UNP P08510
B	-93	GLU	-	expression tag	UNP P08510
B	-92	ASP	-	expression tag	UNP P08510
B	-91	GLY	-	expression tag	UNP P08510
B	-90	GLY	-	expression tag	UNP P08510
B	-89	VAL	-	expression tag	UNP P08510
B	-88	GLN	-	expression tag	UNP P08510
B	-87	LEU	-	expression tag	UNP P08510
B	-86	ALA	-	expression tag	UNP P08510
B	-85	ASP	-	expression tag	UNP P08510
B	-84	HIS	-	expression tag	UNP P08510
B	-83	TYR	-	expression tag	UNP P08510
B	-82	GLN	-	expression tag	UNP P08510
B	-81	GLN	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-80	ASN	-	expression tag	UNP P08510
B	-79	THR	-	expression tag	UNP P08510
B	-78	PRO	-	expression tag	UNP P08510
B	-77	ILE	-	expression tag	UNP P08510
B	-76	GLY	-	expression tag	UNP P08510
B	-75	ASP	-	expression tag	UNP P08510
B	-74	GLY	-	expression tag	UNP P08510
B	-73	PRO	-	expression tag	UNP P08510
B	-72	VAL	-	expression tag	UNP P08510
B	-71	LEU	-	expression tag	UNP P08510
B	-70	LEU	-	expression tag	UNP P08510
B	-69	PRO	-	expression tag	UNP P08510
B	-68	ASP	-	expression tag	UNP P08510
B	-67	ASN	-	expression tag	UNP P08510
B	-66	HIS	-	expression tag	UNP P08510
B	-65	TYR	-	expression tag	UNP P08510
B	-64	LEU	-	expression tag	UNP P08510
B	-63	SER	-	expression tag	UNP P08510
B	-62	TYR	-	expression tag	UNP P08510
B	-61	GLN	-	expression tag	UNP P08510
B	-60	SER	-	expression tag	UNP P08510
B	-59	LYS	-	expression tag	UNP P08510
B	-58	LEU	-	expression tag	UNP P08510
B	-57	SER	-	expression tag	UNP P08510
B	-56	LYS	-	expression tag	UNP P08510
B	-55	ASP	-	expression tag	UNP P08510
B	-54	PRO	-	expression tag	UNP P08510
B	-53	ASN	-	expression tag	UNP P08510
B	-52	GLU	-	expression tag	UNP P08510
B	-51	LYS	-	expression tag	UNP P08510
B	-50	ARG	-	expression tag	UNP P08510
B	-49	ASP	-	expression tag	UNP P08510
B	-48	HIS	-	expression tag	UNP P08510
B	-47	MET	-	expression tag	UNP P08510
B	-46	VAL	-	expression tag	UNP P08510
B	-45	LEU	-	expression tag	UNP P08510
B	-44	LEU	-	expression tag	UNP P08510
B	-43	GLU	-	expression tag	UNP P08510
B	-42	PHE	-	expression tag	UNP P08510
B	-41	VAL	-	expression tag	UNP P08510
B	-40	THR	-	expression tag	UNP P08510
B	-39	ALA	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	ALA	-	expression tag	UNP P08510
B	-37	GLY	-	expression tag	UNP P08510
B	-36	ILE	-	expression tag	UNP P08510
B	-35	THR	-	expression tag	UNP P08510
B	-34	LEU	-	expression tag	UNP P08510
B	-33	GLY	-	expression tag	UNP P08510
B	-32	MET	-	expression tag	UNP P08510
B	-31	ASP	-	expression tag	UNP P08510
B	-30	GLU	-	expression tag	UNP P08510
B	-29	LEU	-	expression tag	UNP P08510
B	-28	TYR	-	expression tag	UNP P08510
B	-27	LYS	-	expression tag	UNP P08510
B	-26	GLU	-	expression tag	UNP P08510
B	-25	ASN	-	expression tag	UNP P08510
B	-24	SER	-	expression tag	UNP P08510
B	-23	SER	-	expression tag	UNP P08510
B	-22	SER	-	expression tag	UNP P08510
B	-21	ASN	-	expression tag	UNP P08510
B	-20	ASN	-	expression tag	UNP P08510
B	-19	ASN	-	expression tag	UNP P08510
B	-18	ASN	-	expression tag	UNP P08510
B	-17	ASN	-	expression tag	UNP P08510
B	-16	ASN	-	expression tag	UNP P08510
B	-15	ASN	-	expression tag	UNP P08510
B	-14	ASN	-	expression tag	UNP P08510
B	-13	ASN	-	expression tag	UNP P08510
B	-12	ASN	-	expression tag	UNP P08510
B	-11	LEU	-	expression tag	UNP P08510
B	-10	GLY	-	expression tag	UNP P08510
B	-9	ILE	-	expression tag	UNP P08510
B	-8	GLU	-	expression tag	UNP P08510
B	-7	GLU	-	expression tag	UNP P08510
B	-6	ASN	-	expression tag	UNP P08510
B	-5	LEU	-	expression tag	UNP P08510
B	-4	TYR	-	expression tag	UNP P08510
B	-3	PHE	-	expression tag	UNP P08510
B	-2	GLN	-	expression tag	UNP P08510
B	-1	GLY	-	expression tag	UNP P08510
B	0	THR	-	expression tag	UNP P08510
B	513	VAL	-	insertion	UNP P08510
C	-280	MET	-	initiating methionine	UNP P08510
C	-279	GLY	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-278	SER	-	expression tag	UNP P08510
C	-277	SER	-	expression tag	UNP P08510
C	-276	HIS	-	expression tag	UNP P08510
C	-275	HIS	-	expression tag	UNP P08510
C	-274	HIS	-	expression tag	UNP P08510
C	-273	HIS	-	expression tag	UNP P08510
C	-272	HIS	-	expression tag	UNP P08510
C	-271	HIS	-	expression tag	UNP P08510
C	-270	HIS	-	expression tag	UNP P08510
C	-269	HIS	-	expression tag	UNP P08510
C	-268	GLY	-	expression tag	UNP P08510
C	-267	SER	-	expression tag	UNP P08510
C	-266	SER	-	expression tag	UNP P08510
C	-265	ARG	-	expression tag	UNP P08510
C	-264	VAL	-	expression tag	UNP P08510
C	-263	SER	-	expression tag	UNP P08510
C	-262	LYS	-	expression tag	UNP P08510
C	-261	GLY	-	expression tag	UNP P08510
C	-260	GLU	-	expression tag	UNP P08510
C	-259	GLU	-	expression tag	UNP P08510
C	-258	LEU	-	expression tag	UNP P08510
C	-257	PHE	-	expression tag	UNP P08510
C	-256	THR	-	expression tag	UNP P08510
C	-255	GLY	-	expression tag	UNP P08510
C	-254	VAL	-	expression tag	UNP P08510
C	-253	VAL	-	expression tag	UNP P08510
C	-252	PRO	-	expression tag	UNP P08510
C	-251	ILE	-	expression tag	UNP P08510
C	-250	LEU	-	expression tag	UNP P08510
C	-249	VAL	-	expression tag	UNP P08510
C	-248	GLU	-	expression tag	UNP P08510
C	-247	LEU	-	expression tag	UNP P08510
C	-246	ASP	-	expression tag	UNP P08510
C	-245	GLY	-	expression tag	UNP P08510
C	-244	ASP	-	expression tag	UNP P08510
C	-243	VAL	-	expression tag	UNP P08510
C	-242	ASN	-	expression tag	UNP P08510
C	-241	GLY	-	expression tag	UNP P08510
C	-240	HIS	-	expression tag	UNP P08510
C	-239	LYS	-	expression tag	UNP P08510
C	-238	PHE	-	expression tag	UNP P08510
C	-237	SER	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-236	VAL	-	expression tag	UNP P08510
C	-235	SER	-	expression tag	UNP P08510
C	-234	GLY	-	expression tag	UNP P08510
C	-233	GLU	-	expression tag	UNP P08510
C	-232	GLY	-	expression tag	UNP P08510
C	-231	GLU	-	expression tag	UNP P08510
C	-230	GLY	-	expression tag	UNP P08510
C	-229	ASP	-	expression tag	UNP P08510
C	-228	ALA	-	expression tag	UNP P08510
C	-227	THR	-	expression tag	UNP P08510
C	-226	TYR	-	expression tag	UNP P08510
C	-225	GLY	-	expression tag	UNP P08510
C	-224	LYS	-	expression tag	UNP P08510
C	-223	LEU	-	expression tag	UNP P08510
C	-222	THR	-	expression tag	UNP P08510
C	-221	LEU	-	expression tag	UNP P08510
C	-220	LYS	-	expression tag	UNP P08510
C	-219	LEU	-	expression tag	UNP P08510
C	-218	ILE	-	expression tag	UNP P08510
C	-217	CYS	-	expression tag	UNP P08510
C	-216	THR	-	expression tag	UNP P08510
C	-215	THR	-	expression tag	UNP P08510
C	-214	GLY	-	expression tag	UNP P08510
C	-213	LYS	-	expression tag	UNP P08510
C	-212	LEU	-	expression tag	UNP P08510
C	-211	PRO	-	expression tag	UNP P08510
C	-210	VAL	-	expression tag	UNP P08510
C	-209	PRO	-	expression tag	UNP P08510
C	-208	TRP	-	expression tag	UNP P08510
C	-207	PRO	-	expression tag	UNP P08510
C	-206	THR	-	expression tag	UNP P08510
C	-205	LEU	-	expression tag	UNP P08510
C	-204	VAL	-	expression tag	UNP P08510
C	-203	THR	-	expression tag	UNP P08510
C	-202	THR	-	expression tag	UNP P08510
C	-201	LEU	-	expression tag	UNP P08510
C	-200	GLY	-	expression tag	UNP P08510
C	-199	TYR	-	expression tag	UNP P08510
C	-198	GLY	-	expression tag	UNP P08510
C	-197	LEU	-	expression tag	UNP P08510
C	-196	GLN	-	expression tag	UNP P08510
C	-195	CYS	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-194	PHE	-	expression tag	UNP P08510
C	-193	ALA	-	expression tag	UNP P08510
C	-192	ARG	-	expression tag	UNP P08510
C	-191	TYR	-	expression tag	UNP P08510
C	-190	PRO	-	expression tag	UNP P08510
C	-189	ASP	-	expression tag	UNP P08510
C	-188	HIS	-	expression tag	UNP P08510
C	-187	MET	-	expression tag	UNP P08510
C	-186	LYS	-	expression tag	UNP P08510
C	-185	GLN	-	expression tag	UNP P08510
C	-184	HIS	-	expression tag	UNP P08510
C	-183	ASP	-	expression tag	UNP P08510
C	-182	PHE	-	expression tag	UNP P08510
C	-181	PHE	-	expression tag	UNP P08510
C	-180	LYS	-	expression tag	UNP P08510
C	-179	SER	-	expression tag	UNP P08510
C	-178	ALA	-	expression tag	UNP P08510
C	-177	MET	-	expression tag	UNP P08510
C	-176	PRO	-	expression tag	UNP P08510
C	-175	GLU	-	expression tag	UNP P08510
C	-174	GLY	-	expression tag	UNP P08510
C	-173	TYR	-	expression tag	UNP P08510
C	-172	VAL	-	expression tag	UNP P08510
C	-171	GLN	-	expression tag	UNP P08510
C	-170	GLU	-	expression tag	UNP P08510
C	-169	ARG	-	expression tag	UNP P08510
C	-168	THR	-	expression tag	UNP P08510
C	-167	ILE	-	expression tag	UNP P08510
C	-166	PHE	-	expression tag	UNP P08510
C	-165	PHE	-	expression tag	UNP P08510
C	-164	LYS	-	expression tag	UNP P08510
C	-163	ASP	-	expression tag	UNP P08510
C	-162	ASP	-	expression tag	UNP P08510
C	-161	GLY	-	expression tag	UNP P08510
C	-160	ASN	-	expression tag	UNP P08510
C	-159	TYR	-	expression tag	UNP P08510
C	-158	LYS	-	expression tag	UNP P08510
C	-157	THR	-	expression tag	UNP P08510
C	-156	ARG	-	expression tag	UNP P08510
C	-155	ALA	-	expression tag	UNP P08510
C	-154	GLU	-	expression tag	UNP P08510
C	-153	VAL	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-152	LYS	-	expression tag	UNP P08510
C	-151	PHE	-	expression tag	UNP P08510
C	-150	GLU	-	expression tag	UNP P08510
C	-149	GLY	-	expression tag	UNP P08510
C	-148	ASP	-	expression tag	UNP P08510
C	-147	THR	-	expression tag	UNP P08510
C	-146	LEU	-	expression tag	UNP P08510
C	-145	VAL	-	expression tag	UNP P08510
C	-144	ASN	-	expression tag	UNP P08510
C	-143	ARG	-	expression tag	UNP P08510
C	-142	ILE	-	expression tag	UNP P08510
C	-141	GLU	-	expression tag	UNP P08510
C	-140	LEU	-	expression tag	UNP P08510
C	-139	LYS	-	expression tag	UNP P08510
C	-138	GLY	-	expression tag	UNP P08510
C	-137	ILE	-	expression tag	UNP P08510
C	-136	ASP	-	expression tag	UNP P08510
C	-135	PHE	-	expression tag	UNP P08510
C	-134	LYS	-	expression tag	UNP P08510
C	-133	GLU	-	expression tag	UNP P08510
C	-132	ASP	-	expression tag	UNP P08510
C	-131	GLY	-	expression tag	UNP P08510
C	-130	ASN	-	expression tag	UNP P08510
C	-129	ILE	-	expression tag	UNP P08510
C	-128	LEU	-	expression tag	UNP P08510
C	-127	GLY	-	expression tag	UNP P08510
C	-126	HIS	-	expression tag	UNP P08510
C	-125	LYS	-	expression tag	UNP P08510
C	-124	LEU	-	expression tag	UNP P08510
C	-123	GLU	-	expression tag	UNP P08510
C	-122	TYR	-	expression tag	UNP P08510
C	-121	ASN	-	expression tag	UNP P08510
C	-120	TYR	-	expression tag	UNP P08510
C	-119	ASN	-	expression tag	UNP P08510
C	-118	SER	-	expression tag	UNP P08510
C	-117	HIS	-	expression tag	UNP P08510
C	-116	ASN	-	expression tag	UNP P08510
C	-115	VAL	-	expression tag	UNP P08510
C	-114	TYR	-	expression tag	UNP P08510
C	-113	ILE	-	expression tag	UNP P08510
C	-112	THR	-	expression tag	UNP P08510
C	-111	ALA	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-110	ASP	-	expression tag	UNP P08510
C	-109	LYS	-	expression tag	UNP P08510
C	-108	GLN	-	expression tag	UNP P08510
C	-107	LYS	-	expression tag	UNP P08510
C	-106	ASN	-	expression tag	UNP P08510
C	-105	GLY	-	expression tag	UNP P08510
C	-104	ILE	-	expression tag	UNP P08510
C	-103	LYS	-	expression tag	UNP P08510
C	-102	ALA	-	expression tag	UNP P08510
C	-101	ASN	-	expression tag	UNP P08510
C	-100	PHE	-	expression tag	UNP P08510
C	-99	LYS	-	expression tag	UNP P08510
C	-98	ILE	-	expression tag	UNP P08510
C	-97	ARG	-	expression tag	UNP P08510
C	-96	HIS	-	expression tag	UNP P08510
C	-95	ASN	-	expression tag	UNP P08510
C	-94	ILE	-	expression tag	UNP P08510
C	-93	GLU	-	expression tag	UNP P08510
C	-92	ASP	-	expression tag	UNP P08510
C	-91	GLY	-	expression tag	UNP P08510
C	-90	GLY	-	expression tag	UNP P08510
C	-89	VAL	-	expression tag	UNP P08510
C	-88	GLN	-	expression tag	UNP P08510
C	-87	LEU	-	expression tag	UNP P08510
C	-86	ALA	-	expression tag	UNP P08510
C	-85	ASP	-	expression tag	UNP P08510
C	-84	HIS	-	expression tag	UNP P08510
C	-83	TYR	-	expression tag	UNP P08510
C	-82	GLN	-	expression tag	UNP P08510
C	-81	GLN	-	expression tag	UNP P08510
C	-80	ASN	-	expression tag	UNP P08510
C	-79	THR	-	expression tag	UNP P08510
C	-78	PRO	-	expression tag	UNP P08510
C	-77	ILE	-	expression tag	UNP P08510
C	-76	GLY	-	expression tag	UNP P08510
C	-75	ASP	-	expression tag	UNP P08510
C	-74	GLY	-	expression tag	UNP P08510
C	-73	PRO	-	expression tag	UNP P08510
C	-72	VAL	-	expression tag	UNP P08510
C	-71	LEU	-	expression tag	UNP P08510
C	-70	LEU	-	expression tag	UNP P08510
C	-69	PRO	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-68	ASP	-	expression tag	UNP P08510
C	-67	ASN	-	expression tag	UNP P08510
C	-66	HIS	-	expression tag	UNP P08510
C	-65	TYR	-	expression tag	UNP P08510
C	-64	LEU	-	expression tag	UNP P08510
C	-63	SER	-	expression tag	UNP P08510
C	-62	TYR	-	expression tag	UNP P08510
C	-61	GLN	-	expression tag	UNP P08510
C	-60	SER	-	expression tag	UNP P08510
C	-59	LYS	-	expression tag	UNP P08510
C	-58	LEU	-	expression tag	UNP P08510
C	-57	SER	-	expression tag	UNP P08510
C	-56	LYS	-	expression tag	UNP P08510
C	-55	ASP	-	expression tag	UNP P08510
C	-54	PRO	-	expression tag	UNP P08510
C	-53	ASN	-	expression tag	UNP P08510
C	-52	GLU	-	expression tag	UNP P08510
C	-51	LYS	-	expression tag	UNP P08510
C	-50	ARG	-	expression tag	UNP P08510
C	-49	ASP	-	expression tag	UNP P08510
C	-48	HIS	-	expression tag	UNP P08510
C	-47	MET	-	expression tag	UNP P08510
C	-46	VAL	-	expression tag	UNP P08510
C	-45	LEU	-	expression tag	UNP P08510
C	-44	LEU	-	expression tag	UNP P08510
C	-43	GLU	-	expression tag	UNP P08510
C	-42	PHE	-	expression tag	UNP P08510
C	-41	VAL	-	expression tag	UNP P08510
C	-40	THR	-	expression tag	UNP P08510
C	-39	ALA	-	expression tag	UNP P08510
C	-38	ALA	-	expression tag	UNP P08510
C	-37	GLY	-	expression tag	UNP P08510
C	-36	ILE	-	expression tag	UNP P08510
C	-35	THR	-	expression tag	UNP P08510
C	-34	LEU	-	expression tag	UNP P08510
C	-33	GLY	-	expression tag	UNP P08510
C	-32	MET	-	expression tag	UNP P08510
C	-31	ASP	-	expression tag	UNP P08510
C	-30	GLU	-	expression tag	UNP P08510
C	-29	LEU	-	expression tag	UNP P08510
C	-28	TYR	-	expression tag	UNP P08510
C	-27	LYS	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-26	GLU	-	expression tag	UNP P08510
C	-25	ASN	-	expression tag	UNP P08510
C	-24	SER	-	expression tag	UNP P08510
C	-23	SER	-	expression tag	UNP P08510
C	-22	SER	-	expression tag	UNP P08510
C	-21	ASN	-	expression tag	UNP P08510
C	-20	ASN	-	expression tag	UNP P08510
C	-19	ASN	-	expression tag	UNP P08510
C	-18	ASN	-	expression tag	UNP P08510
C	-17	ASN	-	expression tag	UNP P08510
C	-16	ASN	-	expression tag	UNP P08510
C	-15	ASN	-	expression tag	UNP P08510
C	-14	ASN	-	expression tag	UNP P08510
C	-13	ASN	-	expression tag	UNP P08510
C	-12	ASN	-	expression tag	UNP P08510
C	-11	LEU	-	expression tag	UNP P08510
C	-10	GLY	-	expression tag	UNP P08510
C	-9	ILE	-	expression tag	UNP P08510
C	-8	GLU	-	expression tag	UNP P08510
C	-7	GLU	-	expression tag	UNP P08510
C	-6	ASN	-	expression tag	UNP P08510
C	-5	LEU	-	expression tag	UNP P08510
C	-4	TYR	-	expression tag	UNP P08510
C	-3	PHE	-	expression tag	UNP P08510
C	-2	GLN	-	expression tag	UNP P08510
C	-1	GLY	-	expression tag	UNP P08510
C	0	THR	-	expression tag	UNP P08510
C	513	VAL	-	insertion	UNP P08510
D	-280	MET	-	initiating methionine	UNP P08510
D	-279	GLY	-	expression tag	UNP P08510
D	-278	SER	-	expression tag	UNP P08510
D	-277	SER	-	expression tag	UNP P08510
D	-276	HIS	-	expression tag	UNP P08510
D	-275	HIS	-	expression tag	UNP P08510
D	-274	HIS	-	expression tag	UNP P08510
D	-273	HIS	-	expression tag	UNP P08510
D	-272	HIS	-	expression tag	UNP P08510
D	-271	HIS	-	expression tag	UNP P08510
D	-270	HIS	-	expression tag	UNP P08510
D	-269	HIS	-	expression tag	UNP P08510
D	-268	GLY	-	expression tag	UNP P08510
D	-267	SER	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-266	SER	-	expression tag	UNP P08510
D	-265	ARG	-	expression tag	UNP P08510
D	-264	VAL	-	expression tag	UNP P08510
D	-263	SER	-	expression tag	UNP P08510
D	-262	LYS	-	expression tag	UNP P08510
D	-261	GLY	-	expression tag	UNP P08510
D	-260	GLU	-	expression tag	UNP P08510
D	-259	GLU	-	expression tag	UNP P08510
D	-258	LEU	-	expression tag	UNP P08510
D	-257	PHE	-	expression tag	UNP P08510
D	-256	THR	-	expression tag	UNP P08510
D	-255	GLY	-	expression tag	UNP P08510
D	-254	VAL	-	expression tag	UNP P08510
D	-253	VAL	-	expression tag	UNP P08510
D	-252	PRO	-	expression tag	UNP P08510
D	-251	ILE	-	expression tag	UNP P08510
D	-250	LEU	-	expression tag	UNP P08510
D	-249	VAL	-	expression tag	UNP P08510
D	-248	GLU	-	expression tag	UNP P08510
D	-247	LEU	-	expression tag	UNP P08510
D	-246	ASP	-	expression tag	UNP P08510
D	-245	GLY	-	expression tag	UNP P08510
D	-244	ASP	-	expression tag	UNP P08510
D	-243	VAL	-	expression tag	UNP P08510
D	-242	ASN	-	expression tag	UNP P08510
D	-241	GLY	-	expression tag	UNP P08510
D	-240	HIS	-	expression tag	UNP P08510
D	-239	LYS	-	expression tag	UNP P08510
D	-238	PHE	-	expression tag	UNP P08510
D	-237	SER	-	expression tag	UNP P08510
D	-236	VAL	-	expression tag	UNP P08510
D	-235	SER	-	expression tag	UNP P08510
D	-234	GLY	-	expression tag	UNP P08510
D	-233	GLU	-	expression tag	UNP P08510
D	-232	GLY	-	expression tag	UNP P08510
D	-231	GLU	-	expression tag	UNP P08510
D	-230	GLY	-	expression tag	UNP P08510
D	-229	ASP	-	expression tag	UNP P08510
D	-228	ALA	-	expression tag	UNP P08510
D	-227	THR	-	expression tag	UNP P08510
D	-226	TYR	-	expression tag	UNP P08510
D	-225	GLY	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-224	LYS	-	expression tag	UNP P08510
D	-223	LEU	-	expression tag	UNP P08510
D	-222	THR	-	expression tag	UNP P08510
D	-221	LEU	-	expression tag	UNP P08510
D	-220	LYS	-	expression tag	UNP P08510
D	-219	LEU	-	expression tag	UNP P08510
D	-218	ILE	-	expression tag	UNP P08510
D	-217	CYS	-	expression tag	UNP P08510
D	-216	THR	-	expression tag	UNP P08510
D	-215	THR	-	expression tag	UNP P08510
D	-214	GLY	-	expression tag	UNP P08510
D	-213	LYS	-	expression tag	UNP P08510
D	-212	LEU	-	expression tag	UNP P08510
D	-211	PRO	-	expression tag	UNP P08510
D	-210	VAL	-	expression tag	UNP P08510
D	-209	PRO	-	expression tag	UNP P08510
D	-208	TRP	-	expression tag	UNP P08510
D	-207	PRO	-	expression tag	UNP P08510
D	-206	THR	-	expression tag	UNP P08510
D	-205	LEU	-	expression tag	UNP P08510
D	-204	VAL	-	expression tag	UNP P08510
D	-203	THR	-	expression tag	UNP P08510
D	-202	THR	-	expression tag	UNP P08510
D	-201	LEU	-	expression tag	UNP P08510
D	-200	GLY	-	expression tag	UNP P08510
D	-199	TYR	-	expression tag	UNP P08510
D	-198	GLY	-	expression tag	UNP P08510
D	-197	LEU	-	expression tag	UNP P08510
D	-196	GLN	-	expression tag	UNP P08510
D	-195	CYS	-	expression tag	UNP P08510
D	-194	PHE	-	expression tag	UNP P08510
D	-193	ALA	-	expression tag	UNP P08510
D	-192	ARG	-	expression tag	UNP P08510
D	-191	TYR	-	expression tag	UNP P08510
D	-190	PRO	-	expression tag	UNP P08510
D	-189	ASP	-	expression tag	UNP P08510
D	-188	HIS	-	expression tag	UNP P08510
D	-187	MET	-	expression tag	UNP P08510
D	-186	LYS	-	expression tag	UNP P08510
D	-185	GLN	-	expression tag	UNP P08510
D	-184	HIS	-	expression tag	UNP P08510
D	-183	ASP	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-182	PHE	-	expression tag	UNP P08510
D	-181	PHE	-	expression tag	UNP P08510
D	-180	LYS	-	expression tag	UNP P08510
D	-179	SER	-	expression tag	UNP P08510
D	-178	ALA	-	expression tag	UNP P08510
D	-177	MET	-	expression tag	UNP P08510
D	-176	PRO	-	expression tag	UNP P08510
D	-175	GLU	-	expression tag	UNP P08510
D	-174	GLY	-	expression tag	UNP P08510
D	-173	TYR	-	expression tag	UNP P08510
D	-172	VAL	-	expression tag	UNP P08510
D	-171	GLN	-	expression tag	UNP P08510
D	-170	GLU	-	expression tag	UNP P08510
D	-169	ARG	-	expression tag	UNP P08510
D	-168	THR	-	expression tag	UNP P08510
D	-167	ILE	-	expression tag	UNP P08510
D	-166	PHE	-	expression tag	UNP P08510
D	-165	PHE	-	expression tag	UNP P08510
D	-164	LYS	-	expression tag	UNP P08510
D	-163	ASP	-	expression tag	UNP P08510
D	-162	ASP	-	expression tag	UNP P08510
D	-161	GLY	-	expression tag	UNP P08510
D	-160	ASN	-	expression tag	UNP P08510
D	-159	TYR	-	expression tag	UNP P08510
D	-158	LYS	-	expression tag	UNP P08510
D	-157	THR	-	expression tag	UNP P08510
D	-156	ARG	-	expression tag	UNP P08510
D	-155	ALA	-	expression tag	UNP P08510
D	-154	GLU	-	expression tag	UNP P08510
D	-153	VAL	-	expression tag	UNP P08510
D	-152	LYS	-	expression tag	UNP P08510
D	-151	PHE	-	expression tag	UNP P08510
D	-150	GLU	-	expression tag	UNP P08510
D	-149	GLY	-	expression tag	UNP P08510
D	-148	ASP	-	expression tag	UNP P08510
D	-147	THR	-	expression tag	UNP P08510
D	-146	LEU	-	expression tag	UNP P08510
D	-145	VAL	-	expression tag	UNP P08510
D	-144	ASN	-	expression tag	UNP P08510
D	-143	ARG	-	expression tag	UNP P08510
D	-142	ILE	-	expression tag	UNP P08510
D	-141	GLU	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-140	LEU	-	expression tag	UNP P08510
D	-139	LYS	-	expression tag	UNP P08510
D	-138	GLY	-	expression tag	UNP P08510
D	-137	ILE	-	expression tag	UNP P08510
D	-136	ASP	-	expression tag	UNP P08510
D	-135	PHE	-	expression tag	UNP P08510
D	-134	LYS	-	expression tag	UNP P08510
D	-133	GLU	-	expression tag	UNP P08510
D	-132	ASP	-	expression tag	UNP P08510
D	-131	GLY	-	expression tag	UNP P08510
D	-130	ASN	-	expression tag	UNP P08510
D	-129	ILE	-	expression tag	UNP P08510
D	-128	LEU	-	expression tag	UNP P08510
D	-127	GLY	-	expression tag	UNP P08510
D	-126	HIS	-	expression tag	UNP P08510
D	-125	LYS	-	expression tag	UNP P08510
D	-124	LEU	-	expression tag	UNP P08510
D	-123	GLU	-	expression tag	UNP P08510
D	-122	TYR	-	expression tag	UNP P08510
D	-121	ASN	-	expression tag	UNP P08510
D	-120	TYR	-	expression tag	UNP P08510
D	-119	ASN	-	expression tag	UNP P08510
D	-118	SER	-	expression tag	UNP P08510
D	-117	HIS	-	expression tag	UNP P08510
D	-116	ASN	-	expression tag	UNP P08510
D	-115	VAL	-	expression tag	UNP P08510
D	-114	TYR	-	expression tag	UNP P08510
D	-113	ILE	-	expression tag	UNP P08510
D	-112	THR	-	expression tag	UNP P08510
D	-111	ALA	-	expression tag	UNP P08510
D	-110	ASP	-	expression tag	UNP P08510
D	-109	LYS	-	expression tag	UNP P08510
D	-108	GLN	-	expression tag	UNP P08510
D	-107	LYS	-	expression tag	UNP P08510
D	-106	ASN	-	expression tag	UNP P08510
D	-105	GLY	-	expression tag	UNP P08510
D	-104	ILE	-	expression tag	UNP P08510
D	-103	LYS	-	expression tag	UNP P08510
D	-102	ALA	-	expression tag	UNP P08510
D	-101	ASN	-	expression tag	UNP P08510
D	-100	PHE	-	expression tag	UNP P08510
D	-99	LYS	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-98	ILE	-	expression tag	UNP P08510
D	-97	ARG	-	expression tag	UNP P08510
D	-96	HIS	-	expression tag	UNP P08510
D	-95	ASN	-	expression tag	UNP P08510
D	-94	ILE	-	expression tag	UNP P08510
D	-93	GLU	-	expression tag	UNP P08510
D	-92	ASP	-	expression tag	UNP P08510
D	-91	GLY	-	expression tag	UNP P08510
D	-90	GLY	-	expression tag	UNP P08510
D	-89	VAL	-	expression tag	UNP P08510
D	-88	GLN	-	expression tag	UNP P08510
D	-87	LEU	-	expression tag	UNP P08510
D	-86	ALA	-	expression tag	UNP P08510
D	-85	ASP	-	expression tag	UNP P08510
D	-84	HIS	-	expression tag	UNP P08510
D	-83	TYR	-	expression tag	UNP P08510
D	-82	GLN	-	expression tag	UNP P08510
D	-81	GLN	-	expression tag	UNP P08510
D	-80	ASN	-	expression tag	UNP P08510
D	-79	THR	-	expression tag	UNP P08510
D	-78	PRO	-	expression tag	UNP P08510
D	-77	ILE	-	expression tag	UNP P08510
D	-76	GLY	-	expression tag	UNP P08510
D	-75	ASP	-	expression tag	UNP P08510
D	-74	GLY	-	expression tag	UNP P08510
D	-73	PRO	-	expression tag	UNP P08510
D	-72	VAL	-	expression tag	UNP P08510
D	-71	LEU	-	expression tag	UNP P08510
D	-70	LEU	-	expression tag	UNP P08510
D	-69	PRO	-	expression tag	UNP P08510
D	-68	ASP	-	expression tag	UNP P08510
D	-67	ASN	-	expression tag	UNP P08510
D	-66	HIS	-	expression tag	UNP P08510
D	-65	TYR	-	expression tag	UNP P08510
D	-64	LEU	-	expression tag	UNP P08510
D	-63	SER	-	expression tag	UNP P08510
D	-62	TYR	-	expression tag	UNP P08510
D	-61	GLN	-	expression tag	UNP P08510
D	-60	SER	-	expression tag	UNP P08510
D	-59	LYS	-	expression tag	UNP P08510
D	-58	LEU	-	expression tag	UNP P08510
D	-57	SER	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-56	LYS	-	expression tag	UNP P08510
D	-55	ASP	-	expression tag	UNP P08510
D	-54	PRO	-	expression tag	UNP P08510
D	-53	ASN	-	expression tag	UNP P08510
D	-52	GLU	-	expression tag	UNP P08510
D	-51	LYS	-	expression tag	UNP P08510
D	-50	ARG	-	expression tag	UNP P08510
D	-49	ASP	-	expression tag	UNP P08510
D	-48	HIS	-	expression tag	UNP P08510
D	-47	MET	-	expression tag	UNP P08510
D	-46	VAL	-	expression tag	UNP P08510
D	-45	LEU	-	expression tag	UNP P08510
D	-44	LEU	-	expression tag	UNP P08510
D	-43	GLU	-	expression tag	UNP P08510
D	-42	PHE	-	expression tag	UNP P08510
D	-41	VAL	-	expression tag	UNP P08510
D	-40	THR	-	expression tag	UNP P08510
D	-39	ALA	-	expression tag	UNP P08510
D	-38	ALA	-	expression tag	UNP P08510
D	-37	GLY	-	expression tag	UNP P08510
D	-36	ILE	-	expression tag	UNP P08510
D	-35	THR	-	expression tag	UNP P08510
D	-34	LEU	-	expression tag	UNP P08510
D	-33	GLY	-	expression tag	UNP P08510
D	-32	MET	-	expression tag	UNP P08510
D	-31	ASP	-	expression tag	UNP P08510
D	-30	GLU	-	expression tag	UNP P08510
D	-29	LEU	-	expression tag	UNP P08510
D	-28	TYR	-	expression tag	UNP P08510
D	-27	LYS	-	expression tag	UNP P08510
D	-26	GLU	-	expression tag	UNP P08510
D	-25	ASN	-	expression tag	UNP P08510
D	-24	SER	-	expression tag	UNP P08510
D	-23	SER	-	expression tag	UNP P08510
D	-22	SER	-	expression tag	UNP P08510
D	-21	ASN	-	expression tag	UNP P08510
D	-20	ASN	-	expression tag	UNP P08510
D	-19	ASN	-	expression tag	UNP P08510
D	-18	ASN	-	expression tag	UNP P08510
D	-17	ASN	-	expression tag	UNP P08510
D	-16	ASN	-	expression tag	UNP P08510
D	-15	ASN	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	ASN	-	expression tag	UNP P08510
D	-13	ASN	-	expression tag	UNP P08510
D	-12	ASN	-	expression tag	UNP P08510
D	-11	LEU	-	expression tag	UNP P08510
D	-10	GLY	-	expression tag	UNP P08510
D	-9	ILE	-	expression tag	UNP P08510
D	-8	GLU	-	expression tag	UNP P08510
D	-7	GLU	-	expression tag	UNP P08510
D	-6	ASN	-	expression tag	UNP P08510
D	-5	LEU	-	expression tag	UNP P08510
D	-4	TYR	-	expression tag	UNP P08510
D	-3	PHE	-	expression tag	UNP P08510
D	-2	GLN	-	expression tag	UNP P08510
D	-1	GLY	-	expression tag	UNP P08510
D	0	THR	-	expression tag	UNP P08510
D	513	VAL	-	insertion	UNP P08510
G	-278	MET	-	initiating methionine	UNP P08510
G	-277	GLY	-	expression tag	UNP P08510
G	-276	SER	-	expression tag	UNP P08510
G	-275	SER	-	expression tag	UNP P08510
G	-274	HIS	-	expression tag	UNP P08510
G	-273	HIS	-	expression tag	UNP P08510
G	-272	HIS	-	expression tag	UNP P08510
G	-271	HIS	-	expression tag	UNP P08510
G	-270	HIS	-	expression tag	UNP P08510
G	-269	HIS	-	expression tag	UNP P08510
G	-268	HIS	-	expression tag	UNP P08510
G	-267	HIS	-	expression tag	UNP P08510
G	-266	GLY	-	expression tag	UNP P08510
G	-265	SER	-	expression tag	UNP P08510
G	-264	SER	-	expression tag	UNP P08510
G	-263	ARG	-	expression tag	UNP P08510
G	-262	VAL	-	expression tag	UNP P08510
G	-261	SER	-	expression tag	UNP P08510
G	-260	LYS	-	expression tag	UNP P08510
G	-259	GLY	-	expression tag	UNP P08510
G	-258	GLU	-	expression tag	UNP P08510
G	-257	GLU	-	expression tag	UNP P08510
G	-256	LEU	-	expression tag	UNP P08510
G	-255	PHE	-	expression tag	UNP P08510
G	-254	THR	-	expression tag	UNP P08510
G	-253	GLY	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-252	VAL	-	expression tag	UNP P08510
G	-251	VAL	-	expression tag	UNP P08510
G	-250	PRO	-	expression tag	UNP P08510
G	-249	ILE	-	expression tag	UNP P08510
G	-248	LEU	-	expression tag	UNP P08510
G	-247	VAL	-	expression tag	UNP P08510
G	-246	GLU	-	expression tag	UNP P08510
G	-245	LEU	-	expression tag	UNP P08510
G	-244	ASP	-	expression tag	UNP P08510
G	-243	GLY	-	expression tag	UNP P08510
G	-242	ASP	-	expression tag	UNP P08510
G	-241	VAL	-	expression tag	UNP P08510
G	-240	ASN	-	expression tag	UNP P08510
G	-239	GLY	-	expression tag	UNP P08510
G	-238	HIS	-	expression tag	UNP P08510
G	-237	LYS	-	expression tag	UNP P08510
G	-236	PHE	-	expression tag	UNP P08510
G	-235	SER	-	expression tag	UNP P08510
G	-234	VAL	-	expression tag	UNP P08510
G	-233	SER	-	expression tag	UNP P08510
G	-232	GLY	-	expression tag	UNP P08510
G	-231	GLU	-	expression tag	UNP P08510
G	-230	GLY	-	expression tag	UNP P08510
G	-229	GLU	-	expression tag	UNP P08510
G	-228	GLY	-	expression tag	UNP P08510
G	-227	ASP	-	expression tag	UNP P08510
G	-226	ALA	-	expression tag	UNP P08510
G	-225	THR	-	expression tag	UNP P08510
G	-224	TYR	-	expression tag	UNP P08510
G	-223	GLY	-	expression tag	UNP P08510
G	-222	LYS	-	expression tag	UNP P08510
G	-221	LEU	-	expression tag	UNP P08510
G	-220	THR	-	expression tag	UNP P08510
G	-219	LEU	-	expression tag	UNP P08510
G	-218	LYS	-	expression tag	UNP P08510
G	-217	LEU	-	expression tag	UNP P08510
G	-216	ILE	-	expression tag	UNP P08510
G	-215	CYS	-	expression tag	UNP P08510
G	-214	THR	-	expression tag	UNP P08510
G	-213	THR	-	expression tag	UNP P08510
G	-212	GLY	-	expression tag	UNP P08510
G	-211	LYS	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-210	LEU	-	expression tag	UNP P08510
G	-209	PRO	-	expression tag	UNP P08510
G	-208	VAL	-	expression tag	UNP P08510
G	-207	PRO	-	expression tag	UNP P08510
G	-206	TRP	-	expression tag	UNP P08510
G	-205	PRO	-	expression tag	UNP P08510
G	-204	THR	-	expression tag	UNP P08510
G	-203	LEU	-	expression tag	UNP P08510
G	-202	VAL	-	expression tag	UNP P08510
G	-201	THR	-	expression tag	UNP P08510
G	-200	THR	-	expression tag	UNP P08510
G	-199	LEU	-	expression tag	UNP P08510
G	-198	GLY	-	expression tag	UNP P08510
G	-197	TYR	-	expression tag	UNP P08510
G	-196	GLY	-	expression tag	UNP P08510
G	-195	LEU	-	expression tag	UNP P08510
G	-194	GLN	-	expression tag	UNP P08510
G	-193	CYS	-	expression tag	UNP P08510
G	-192	PHE	-	expression tag	UNP P08510
G	-191	ALA	-	expression tag	UNP P08510
G	-190	ARG	-	expression tag	UNP P08510
G	-189	TYR	-	expression tag	UNP P08510
G	-188	PRO	-	expression tag	UNP P08510
G	-187	ASP	-	expression tag	UNP P08510
G	-186	HIS	-	expression tag	UNP P08510
G	-185	MET	-	expression tag	UNP P08510
G	-184	LYS	-	expression tag	UNP P08510
G	-183	GLN	-	expression tag	UNP P08510
G	-182	HIS	-	expression tag	UNP P08510
G	-181	ASP	-	expression tag	UNP P08510
G	-180	PHE	-	expression tag	UNP P08510
G	-179	PHE	-	expression tag	UNP P08510
G	-178	LYS	-	expression tag	UNP P08510
G	-177	SER	-	expression tag	UNP P08510
G	-176	ALA	-	expression tag	UNP P08510
G	-175	MET	-	expression tag	UNP P08510
G	-174	PRO	-	expression tag	UNP P08510
G	-173	GLU	-	expression tag	UNP P08510
G	-172	GLY	-	expression tag	UNP P08510
G	-171	TYR	-	expression tag	UNP P08510
G	-170	VAL	-	expression tag	UNP P08510
G	-169	GLN	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-168	GLU	-	expression tag	UNP P08510
G	-167	ARG	-	expression tag	UNP P08510
G	-166	THR	-	expression tag	UNP P08510
G	-165	ILE	-	expression tag	UNP P08510
G	-164	PHE	-	expression tag	UNP P08510
G	-163	PHE	-	expression tag	UNP P08510
G	-162	LYS	-	expression tag	UNP P08510
G	-161	ASP	-	expression tag	UNP P08510
G	-160	ASP	-	expression tag	UNP P08510
G	-159	GLY	-	expression tag	UNP P08510
G	-158	ASN	-	expression tag	UNP P08510
G	-157	TYR	-	expression tag	UNP P08510
G	-156	LYS	-	expression tag	UNP P08510
G	-155	THR	-	expression tag	UNP P08510
G	-154	ARG	-	expression tag	UNP P08510
G	-153	ALA	-	expression tag	UNP P08510
G	-152	GLU	-	expression tag	UNP P08510
G	-151	VAL	-	expression tag	UNP P08510
G	-150	LYS	-	expression tag	UNP P08510
G	-149	PHE	-	expression tag	UNP P08510
G	-148	GLU	-	expression tag	UNP P08510
G	-147	GLY	-	expression tag	UNP P08510
G	-146	ASP	-	expression tag	UNP P08510
G	-145	THR	-	expression tag	UNP P08510
G	-144	LEU	-	expression tag	UNP P08510
G	-143	VAL	-	expression tag	UNP P08510
G	-142	ASN	-	expression tag	UNP P08510
G	-141	ARG	-	expression tag	UNP P08510
G	-140	ILE	-	expression tag	UNP P08510
G	-139	GLU	-	expression tag	UNP P08510
G	-138	LEU	-	expression tag	UNP P08510
G	-137	LYS	-	expression tag	UNP P08510
G	-136	GLY	-	expression tag	UNP P08510
G	-135	ILE	-	expression tag	UNP P08510
G	-134	ASP	-	expression tag	UNP P08510
G	-133	PHE	-	expression tag	UNP P08510
G	-132	LYS	-	expression tag	UNP P08510
G	-131	GLU	-	expression tag	UNP P08510
G	-130	ASP	-	expression tag	UNP P08510
G	-129	GLY	-	expression tag	UNP P08510
G	-128	ASN	-	expression tag	UNP P08510
G	-127	ILE	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-126	LEU	-	expression tag	UNP P08510
G	-125	GLY	-	expression tag	UNP P08510
G	-124	HIS	-	expression tag	UNP P08510
G	-123	LYS	-	expression tag	UNP P08510
G	-122	LEU	-	expression tag	UNP P08510
G	-121	GLU	-	expression tag	UNP P08510
G	-120	TYR	-	expression tag	UNP P08510
G	-119	ASN	-	expression tag	UNP P08510
G	-118	TYR	-	expression tag	UNP P08510
G	-117	ASN	-	expression tag	UNP P08510
G	-116	SER	-	expression tag	UNP P08510
G	-115	HIS	-	expression tag	UNP P08510
G	-114	ASN	-	expression tag	UNP P08510
G	-113	VAL	-	expression tag	UNP P08510
G	-112	TYR	-	expression tag	UNP P08510
G	-111	ILE	-	expression tag	UNP P08510
G	-110	THR	-	expression tag	UNP P08510
G	-109	ALA	-	expression tag	UNP P08510
G	-108	ASP	-	expression tag	UNP P08510
G	-107	LYS	-	expression tag	UNP P08510
G	-106	GLN	-	expression tag	UNP P08510
G	-105	LYS	-	expression tag	UNP P08510
G	-104	ASN	-	expression tag	UNP P08510
G	-103	GLY	-	expression tag	UNP P08510
G	-102	ILE	-	expression tag	UNP P08510
G	-101	LYS	-	expression tag	UNP P08510
G	-100	ALA	-	expression tag	UNP P08510
G	-99	ASN	-	expression tag	UNP P08510
G	-98	PHE	-	expression tag	UNP P08510
G	-97	LYS	-	expression tag	UNP P08510
G	-96	ILE	-	expression tag	UNP P08510
G	-95	ARG	-	expression tag	UNP P08510
G	-94	HIS	-	expression tag	UNP P08510
G	-93	ASN	-	expression tag	UNP P08510
G	-92	ILE	-	expression tag	UNP P08510
G	-91	GLU	-	expression tag	UNP P08510
G	-90	ASP	-	expression tag	UNP P08510
G	-89	GLY	-	expression tag	UNP P08510
G	-88	GLY	-	expression tag	UNP P08510
G	-87	VAL	-	expression tag	UNP P08510
G	-86	GLN	-	expression tag	UNP P08510
G	-85	LEU	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-84	ALA	-	expression tag	UNP P08510
G	-83	ASP	-	expression tag	UNP P08510
G	-82	HIS	-	expression tag	UNP P08510
G	-81	TYR	-	expression tag	UNP P08510
G	-80	GLN	-	expression tag	UNP P08510
G	-79	GLN	-	expression tag	UNP P08510
G	-78	ASN	-	expression tag	UNP P08510
G	-77	THR	-	expression tag	UNP P08510
G	-76	PRO	-	expression tag	UNP P08510
G	-75	ILE	-	expression tag	UNP P08510
G	-74	GLY	-	expression tag	UNP P08510
G	-73	ASP	-	expression tag	UNP P08510
G	-72	GLY	-	expression tag	UNP P08510
G	-71	PRO	-	expression tag	UNP P08510
G	-70	VAL	-	expression tag	UNP P08510
G	-69	LEU	-	expression tag	UNP P08510
G	-68	LEU	-	expression tag	UNP P08510
G	-67	PRO	-	expression tag	UNP P08510
G	-66	ASP	-	expression tag	UNP P08510
G	-65	ASN	-	expression tag	UNP P08510
G	-64	HIS	-	expression tag	UNP P08510
G	-63	TYR	-	expression tag	UNP P08510
G	-62	LEU	-	expression tag	UNP P08510
G	-61	SER	-	expression tag	UNP P08510
G	-60	TYR	-	expression tag	UNP P08510
G	-59	GLN	-	expression tag	UNP P08510
G	-58	SER	-	expression tag	UNP P08510
G	-57	LYS	-	expression tag	UNP P08510
G	-56	LEU	-	expression tag	UNP P08510
G	-55	SER	-	expression tag	UNP P08510
G	-54	LYS	-	expression tag	UNP P08510
G	-53	ASP	-	expression tag	UNP P08510
G	-52	PRO	-	expression tag	UNP P08510
G	-51	ASN	-	expression tag	UNP P08510
G	-50	GLU	-	expression tag	UNP P08510
G	-49	LYS	-	expression tag	UNP P08510
G	-48	ARG	-	expression tag	UNP P08510
G	-47	ASP	-	expression tag	UNP P08510
G	-46	HIS	-	expression tag	UNP P08510
G	-45	MET	-	expression tag	UNP P08510
G	-44	VAL	-	expression tag	UNP P08510
G	-43	LEU	-	expression tag	UNP P08510

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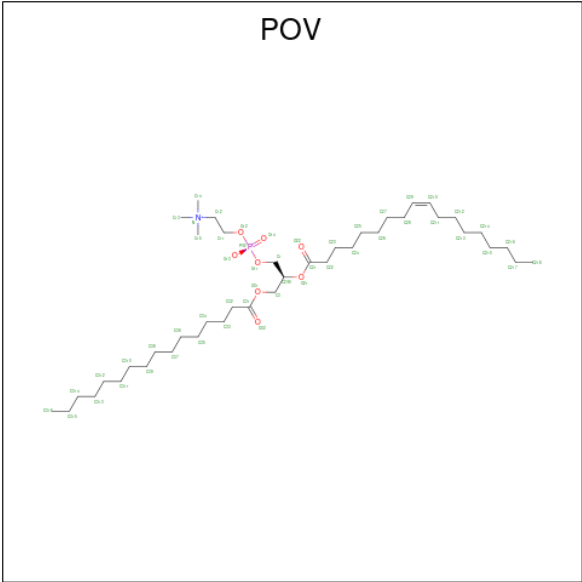
Chain	Residue	Modelled	Actual	Comment	Reference
G	-42	LEU	-	expression tag	UNP P08510
G	-41	GLU	-	expression tag	UNP P08510
G	-40	PHE	-	expression tag	UNP P08510
G	-39	VAL	-	expression tag	UNP P08510
G	-38	THR	-	expression tag	UNP P08510
G	-37	ALA	-	expression tag	UNP P08510
G	-36	ALA	-	expression tag	UNP P08510
G	-35	GLY	-	expression tag	UNP P08510
G	-34	ILE	-	expression tag	UNP P08510
G	-33	THR	-	expression tag	UNP P08510
G	-32	LEU	-	expression tag	UNP P08510
G	-31	GLY	-	expression tag	UNP P08510
G	-30	MET	-	expression tag	UNP P08510
G	-29	ASP	-	expression tag	UNP P08510
G	-28	GLU	-	expression tag	UNP P08510
G	-27	LEU	-	expression tag	UNP P08510
G	-26	TYR	-	expression tag	UNP P08510
G	-25	LYS	-	expression tag	UNP P08510
G	-24	GLU	-	expression tag	UNP P08510
G	-23	ASN	-	expression tag	UNP P08510
G	-22	SER	-	expression tag	UNP P08510
G	-21	SER	-	expression tag	UNP P08510
G	-20	SER	-	expression tag	UNP P08510
G	-19	ASN	-	expression tag	UNP P08510
G	-18	ASN	-	expression tag	UNP P08510
G	-17	ASN	-	expression tag	UNP P08510
G	-16	ASN	-	expression tag	UNP P08510
G	-15	ASN	-	expression tag	UNP P08510
G	-14	ASN	-	expression tag	UNP P08510
G	-13	ASN	-	expression tag	UNP P08510
G	-12	ASN	-	expression tag	UNP P08510
G	-11	ASN	-	expression tag	UNP P08510
G	-10	ASN	-	expression tag	UNP P08510
G	-9	LEU	-	expression tag	UNP P08510
G	-8	GLY	-	expression tag	UNP P08510
G	-7	ILE	-	expression tag	UNP P08510
G	-6	GLU	-	expression tag	UNP P08510
G	-5	GLU	-	expression tag	UNP P08510
G	-4	ASN	-	expression tag	UNP P08510
G	-3	LEU	-	expression tag	UNP P08510
G	-2	TYR	-	expression tag	UNP P08510
G	-1	PHE	-	expression tag	UNP P08510

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLN	-	expression tag	UNP P08510
G	1	GLY	-	expression tag	UNP P08510
G	2	THR	-	expression tag	UNP P08510
G	515	VAL	-	insertion	UNP P08510

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			11	9	2	
2	A	1	Total	C	O	0
			21	17	4	
2	A	1	Total	C		0
			6	6		
2	A	1	Total	C		0
			8	8		
2	A	1	Total	C		0
			12	12		
2	A	1	Total	C		0
			10	10		
2	A	1	Total	C	O	0
			13	11	2	
2	B	1	Total	C	O	0
			21	17	4	
2	B	1	Total	C		0
			6	6		

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Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C 8 8	0
2	B	1	Total C 12 12	0
2	B	1	Total C O 13 11 2	0
2	B	1	Total C 10 10	0
2	B	1	Total C 7 7	0
2	B	1	Total C O 13 11 2	0
2	B	1	Total C O 11 9 2	0
2	C	1	Total C 7 7	0
2	C	1	Total C O 21 17 4	0
2	C	1	Total C 6 6	0
2	C	1	Total C 8 8	0
2	C	1	Total C 12 12	0
2	C	1	Total C O 13 11 2	0
2	C	1	Total C 10 10	0
2	C	1	Total C 7 7	0
2	C	1	Total C O 11 9 2	0
2	D	1	Total C O 11 9 2	0
2	D	1	Total C O 21 17 4	0
2	D	1	Total C 6 6	0
2	D	1	Total C 8 8	0
2	D	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	C	0
			10	10	
2	D	1	Total	C	0
			7	7	

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	K	0
			1	1	
3	B	1	Total	K	0
			1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	O	0
			1	1	

- Molecule 1: Potassium voltage-gated channel protein Shaker

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141882	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.199	Depositor
Minimum map value	-0.645	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	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: POV, K

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	0.31	0/1695	0.49	0/2307
1	B	0.19	0/1689	0.35	0/2300
1	C	0.18	0/1695	0.35	0/2307
1	D	0.18	0/1687	0.35	0/2296
1	G	0.23	0/98	0.77	0/131
All	All	0.22	0/6864	0.40	0/9341

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	1654	0	1706	26	0
1	B	1648	0	1695	29	0
1	C	1654	0	1706	32	0
1	D	1647	0	1698	29	0
1	G	98	0	95	8	0
2	A	81	0	107	0	0
2	B	101	0	133	1	0
2	C	95	0	127	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	75	0	101	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	7056	0	7368	109	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 8.

The worst 5 of 109 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:A:403:LEU:HD21	1:A:470:ILE:CD1	2.02	0.90
1:A:403:LEU:HD21	1:A:470:ILE:HD13	1.61	0.81
1:G:1:GLY:HA3	1:G:4:ALA:HB3	1.69	0.75
1:A:403:LEU:HD21	1:A:470:ILE:HD11	1.73	0.70
1:C:448:MET:HE3	1:C:451:VAL:HG21	1.74	0.68

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	202/937 (22%)	196 (97%)	6 (3%)	0	100	100
1	B	202/937 (22%)	200 (99%)	2 (1%)	0	100	100
1	C	202/937 (22%)	199 (98%)	3 (2%)	0	100	100
1	D	202/937 (22%)	199 (98%)	3 (2%)	0	100	100
1	G	13/937 (1%)	10 (77%)	3 (23%)	0	100	100
All	All	821/4685 (18%)	804 (98%)	17 (2%)	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	179/822 (22%)	179 (100%)	0	100	100
1	B	178/822 (22%)	178 (100%)	0	100	100
1	C	179/822 (22%)	179 (100%)	0	100	100
1	D	178/822 (22%)	178 (100%)	0	100	100
1	G	8/822 (1%)	8 (100%)	0	100	100
All	All	722/4110 (18%)	722 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	313	ASN
1	D	480	ASN
1	D	482	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

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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
2	POV	D	702	-	20,20,51	1.51	3 (15%)	22,22,59	1.43	2 (9%)
2	POV	D	703	-	5,5,51	0.65	0	4,4,59	0.61	0
2	POV	C	702	-	20,20,51	1.51	3 (15%)	22,22,59	1.45	3 (13%)
2	POV	B	702	-	20,20,51	1.51	3 (15%)	22,22,59	1.49	3 (13%)
2	POV	C	701	-	6,6,51	0.73	0	5,5,59	0.69	0
2	POV	D	705	-	11,11,51	0.77	0	10,10,59	0.83	0
2	POV	D	707	-	6,6,51	0.73	0	5,5,59	0.69	0
2	POV	A	702	-	20,20,51	1.51	3 (15%)	22,22,59	1.43	2 (9%)
2	POV	C	704	-	7,7,51	0.81	0	6,6,59	0.75	0
2	POV	B	705	-	11,11,51	0.77	0	10,10,59	0.83	0
2	POV	B	704	-	7,7,51	0.81	0	6,6,59	0.75	0
2	POV	C	703	-	5,5,51	0.65	0	4,4,59	0.62	0
2	POV	B	703	-	5,5,51	0.64	0	4,4,59	0.63	0
2	POV	C	707	-	9,9,51	0.78	0	8,8,59	0.81	0
2	POV	B	710	-	10,10,51	1.50	1 (10%)	10,10,59	1.11	1 (10%)
2	POV	A	705	-	11,11,51	0.77	0	10,10,59	0.82	0
2	POV	B	706	-	12,12,51	1.40	2 (16%)	12,12,59	1.23	1 (8%)
2	POV	B	707	-	9,9,51	0.79	0	8,8,59	0.81	0
2	POV	A	704	-	7,7,51	0.81	0	6,6,59	0.76	0
2	POV	A	706	-	9,9,51	0.78	0	8,8,59	0.82	0
2	POV	C	708	-	6,6,51	0.72	0	5,5,59	0.71	0
2	POV	A	707	-	12,12,51	1.41	2 (16%)	12,12,59	1.22	0
2	POV	A	701	-	10,10,51	1.49	1 (10%)	10,10,59	1.08	1 (10%)
2	POV	C	705	-	11,11,51	0.76	0	10,10,59	0.83	0
2	POV	C	709	-	10,10,51	1.49	1 (10%)	10,10,59	1.11	1 (10%)
2	POV	D	704	-	7,7,51	0.81	0	6,6,59	0.75	0
2	POV	D	706	-	9,9,51	0.77	0	8,8,59	0.84	0
2	POV	A	703	-	5,5,51	0.65	0	4,4,59	0.63	0
2	POV	D	701	-	10,10,51	1.49	1 (10%)	10,10,59	1.11	1 (10%)
2	POV	B	708	-	6,6,51	0.73	0	5,5,59	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	POV	B	709	-	12,12,51	1.41	2 (16%)	12,12,59	1.24	0
2	POV	C	706	-	12,12,51	1.41	2 (16%)	12,12,59	1.24	1 (8%)

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	POV	D	702	-	-	13/21/21/55	-
2	POV	D	703	-	-	3/3/3/55	-
2	POV	C	702	-	-	13/21/21/55	-
2	POV	B	702	-	-	11/21/21/55	-
2	POV	C	701	-	-	3/4/4/55	-
2	POV	D	705	-	-	3/9/9/55	-
2	POV	D	707	-	-	3/4/4/55	-
2	POV	A	702	-	-	12/21/21/55	-
2	POV	C	704	-	-	2/5/5/55	-
2	POV	B	705	-	-	4/9/9/55	-
2	POV	B	704	-	-	3/5/5/55	-
2	POV	C	703	-	-	2/3/3/55	-
2	POV	B	703	-	-	3/3/3/55	-
2	POV	C	707	-	-	1/7/7/55	-
2	POV	B	710	-	-	6/9/9/55	-
2	POV	A	705	-	-	4/9/9/55	-
2	POV	B	706	-	-	5/10/10/55	-
2	POV	B	707	-	-	2/7/7/55	-
2	POV	A	704	-	-	2/5/5/55	-
2	POV	A	706	-	-	3/7/7/55	-
2	POV	C	708	-	-	3/4/4/55	-
2	POV	A	707	-	-	4/10/10/55	-
2	POV	A	701	-	-	6/9/9/55	-
2	POV	C	705	-	-	4/9/9/55	-
2	POV	C	709	-	-	5/9/9/55	-
2	POV	D	704	-	-	2/5/5/55	-
2	POV	D	706	-	-	3/7/7/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	703	-	-	3/3/3/55	-
2	POV	D	701	-	-	7/9/9/55	-
2	POV	B	708	-	-	3/4/4/55	-
2	POV	B	709	-	-	6/10/10/55	-
2	POV	C	706	-	-	4/10/10/55	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	POV	O31-C31	3.90	1.44	1.33
2	C	702	POV	O31-C31	3.87	1.44	1.33
2	B	702	POV	O31-C31	3.86	1.44	1.33
2	D	702	POV	O31-C31	3.86	1.44	1.33
2	D	701	POV	O31-C31	3.74	1.44	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	702	POV	O21-C21-C22	3.68	119.45	111.48
2	C	702	POV	O21-C21-C22	3.68	119.44	111.48
2	B	702	POV	O21-C21-C22	3.67	119.42	111.48
2	D	702	POV	O21-C21-C22	3.64	119.35	111.48
2	A	702	POV	O31-C31-C32	2.92	120.73	111.83

There are no chirality outliers.

5 of 148 torsion outliers are listed below:

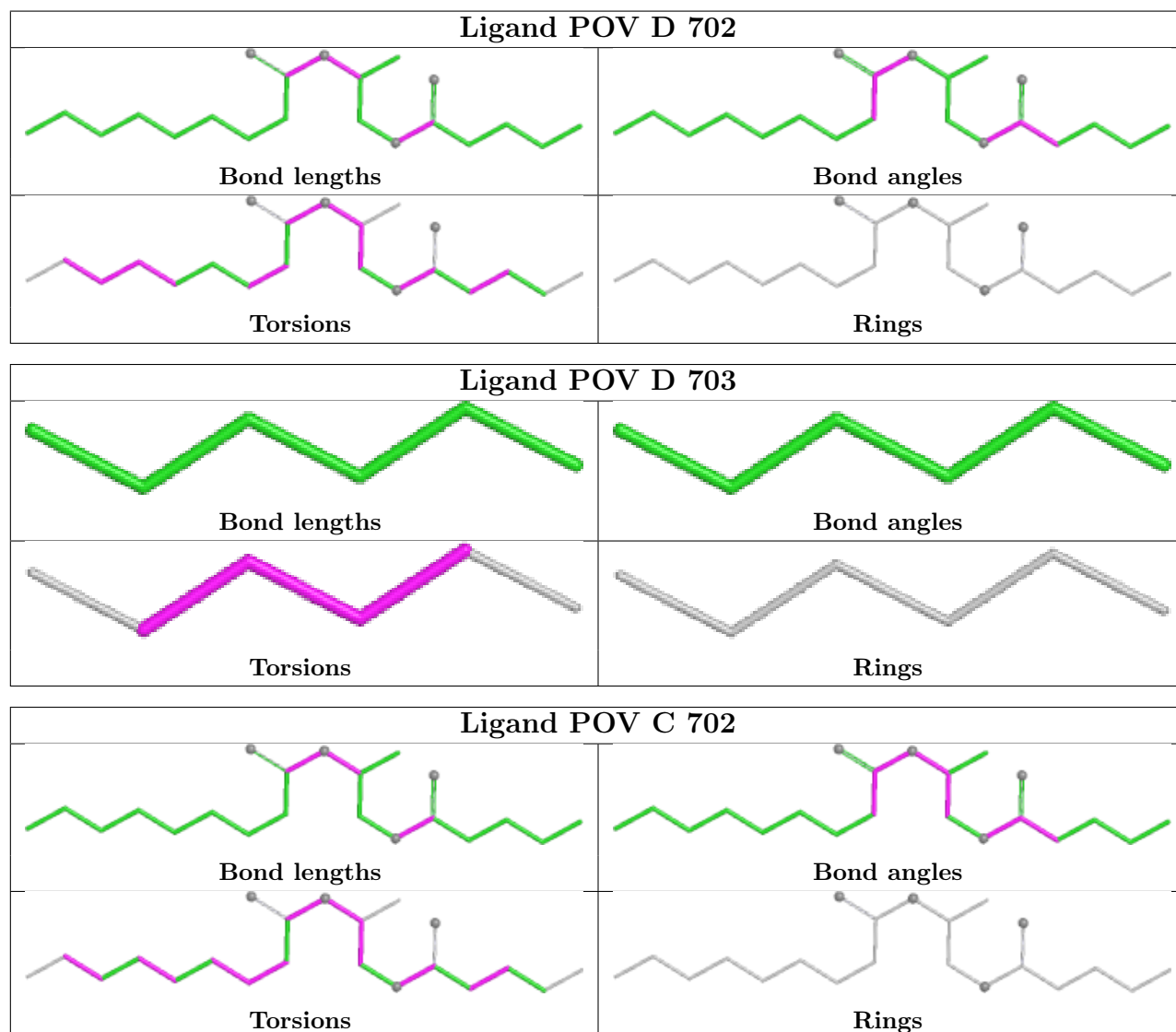
Mol	Chain	Res	Type	Atoms
2	A	702	POV	C1-C2-O21-C21
2	B	702	POV	O21-C2-C3-O31
2	B	702	POV	C1-C2-O21-C21
2	B	702	POV	C3-C2-O21-C21
2	C	702	POV	O21-C2-C3-O31

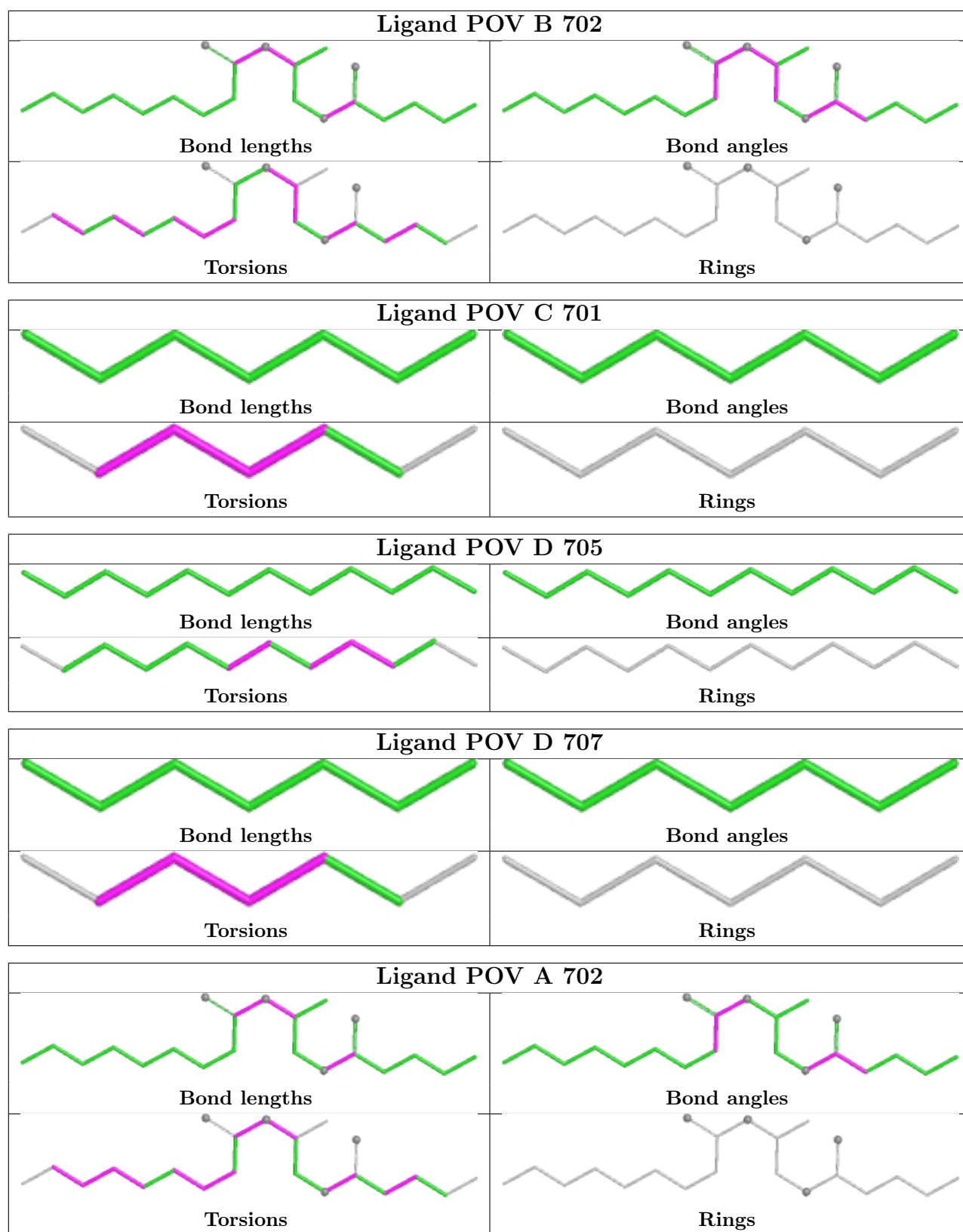
There are no ring outliers.

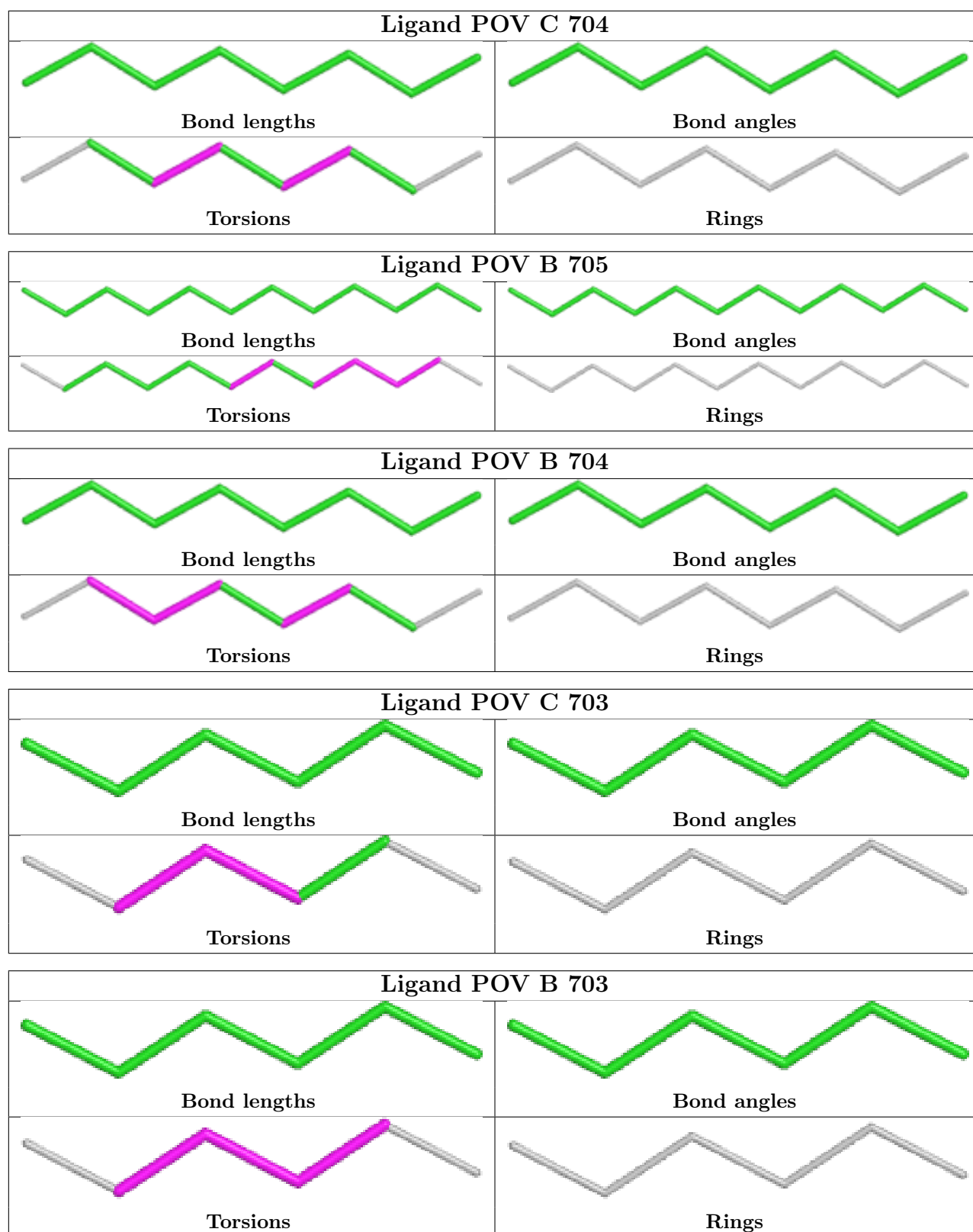
2 monomers are involved in 2 short contacts:

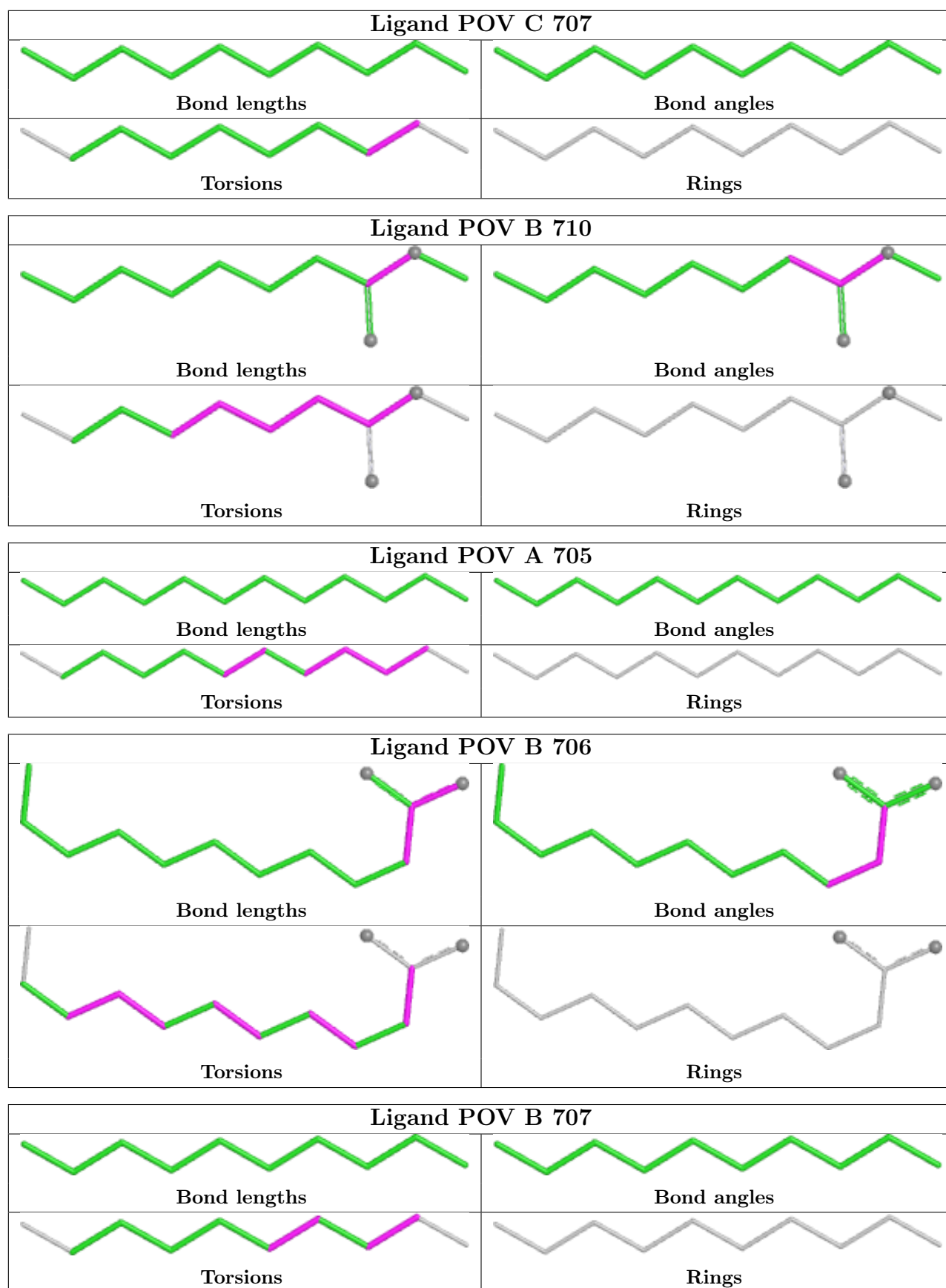
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	709	POV	1	0
2	B	709	POV	1	0

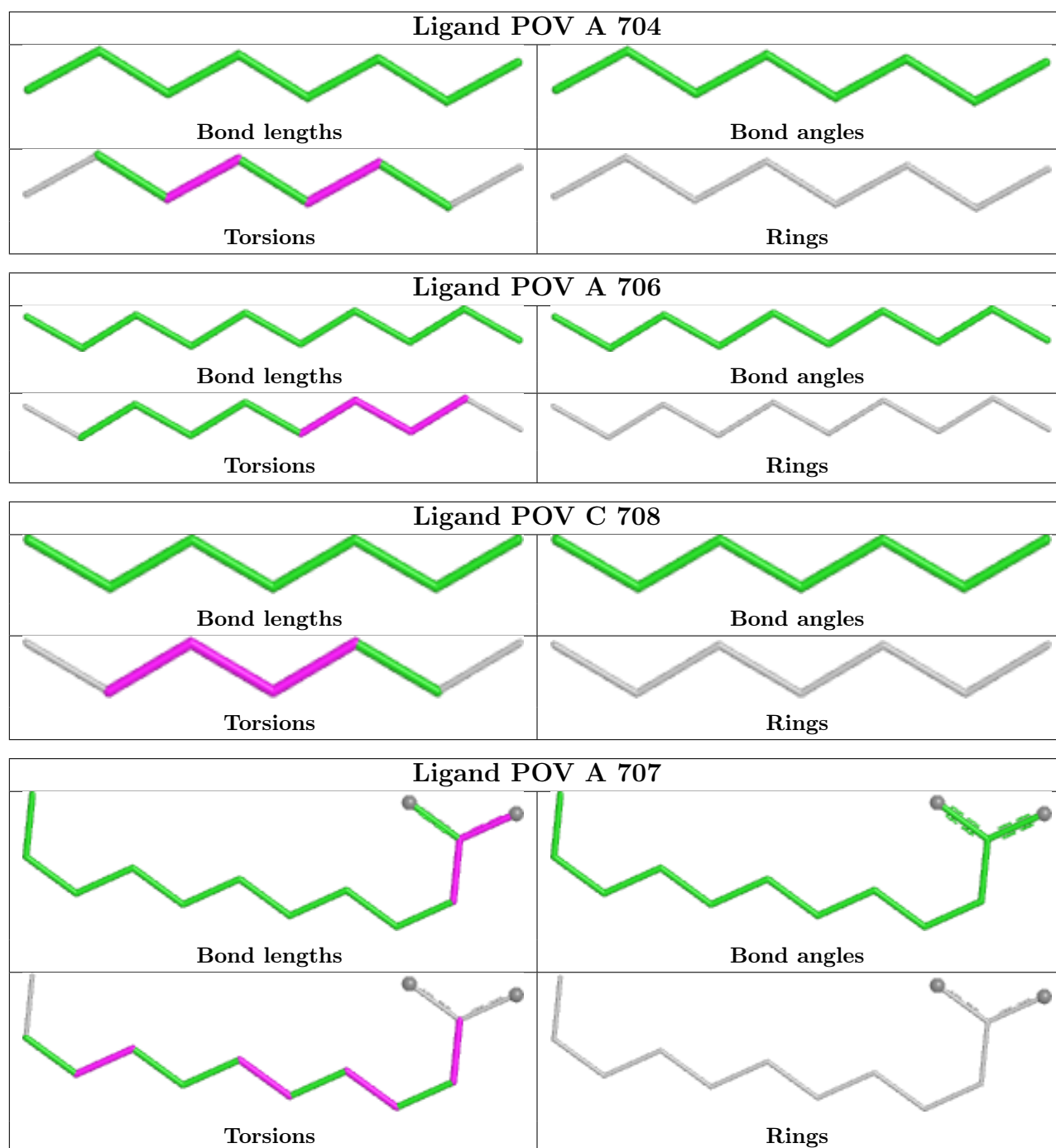
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

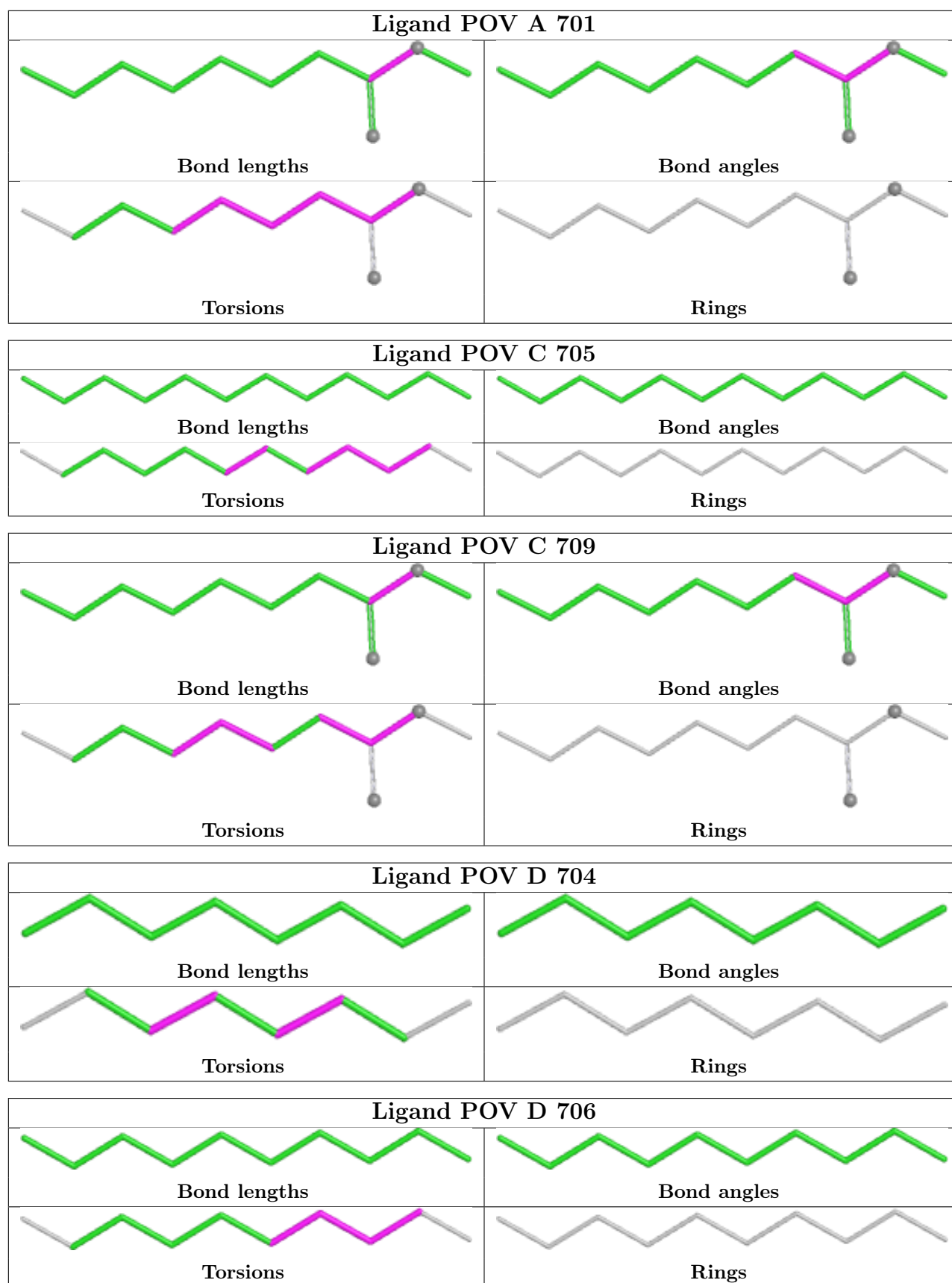


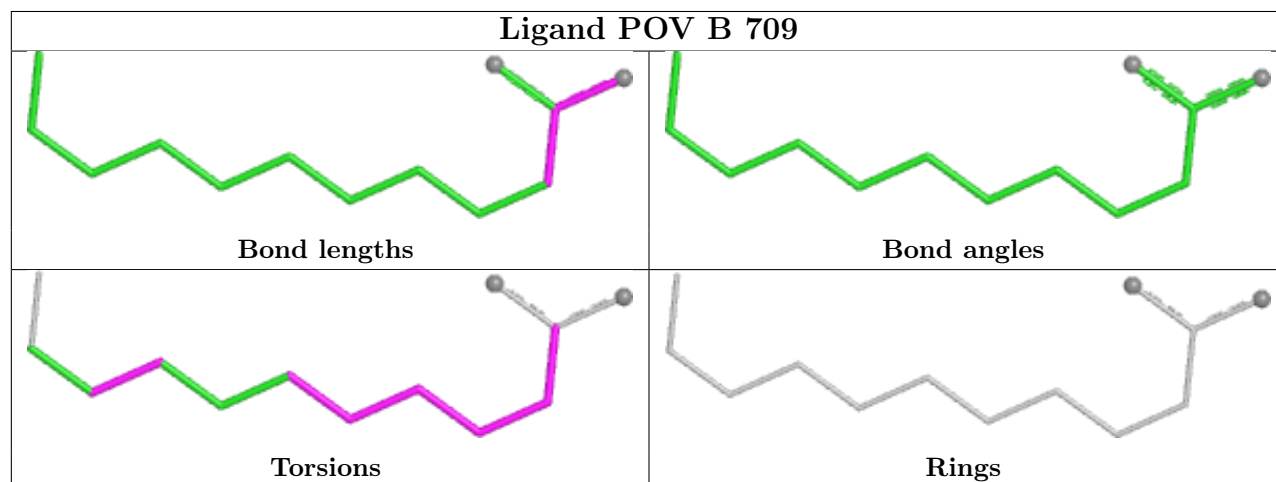
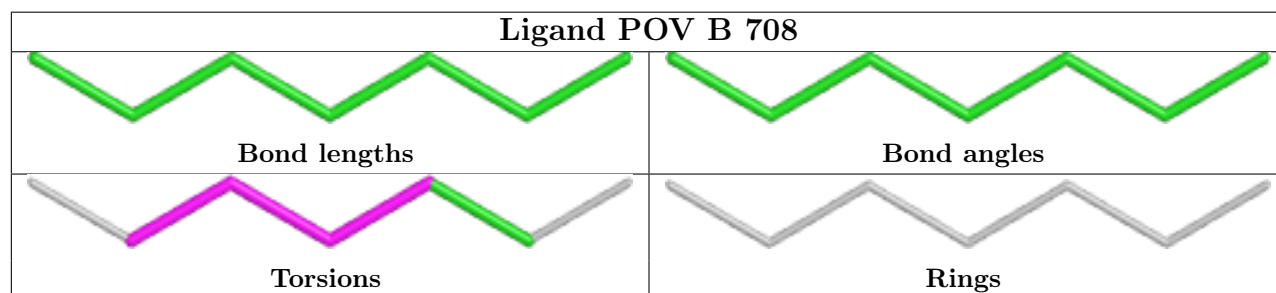
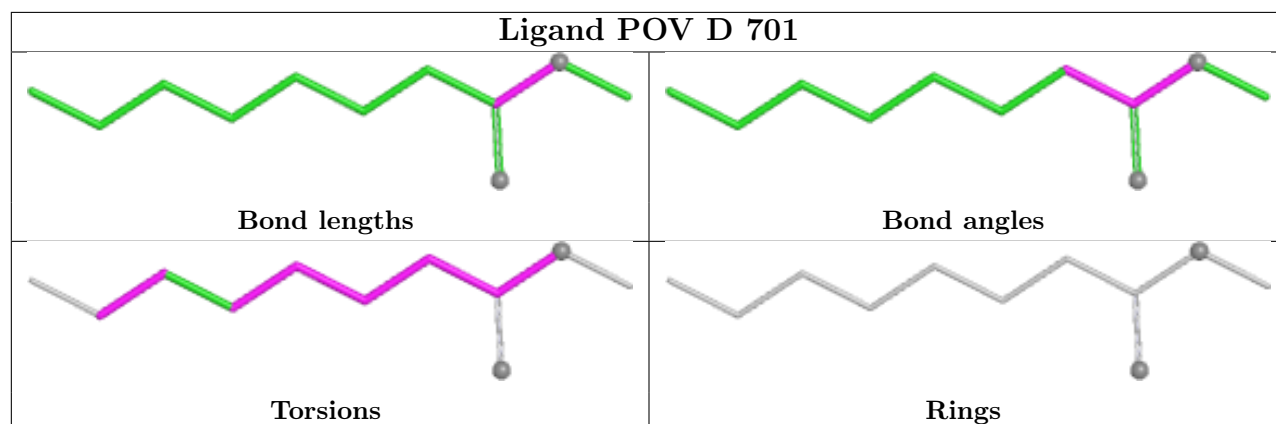
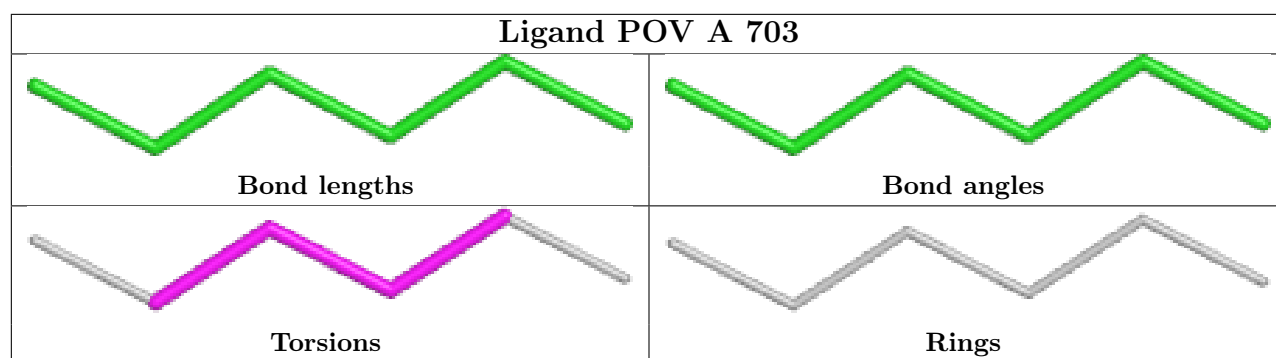


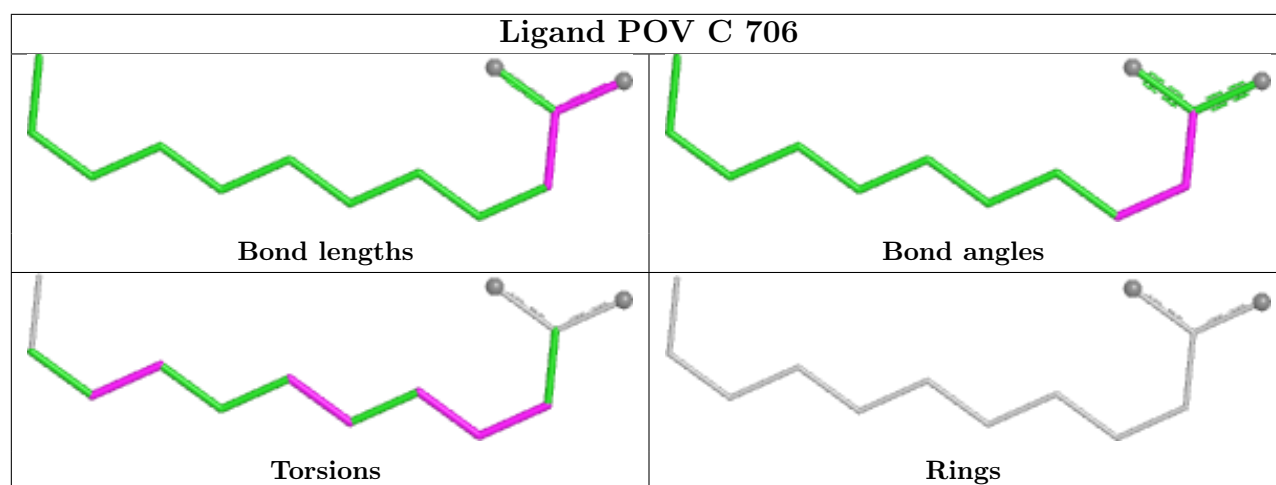












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

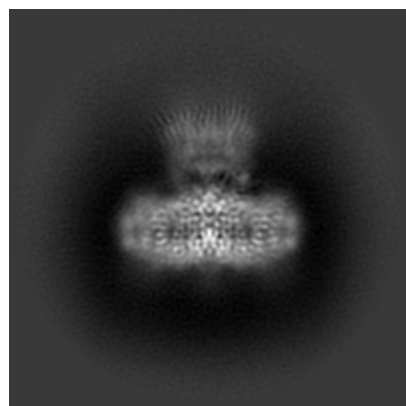
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49311. These allow visual inspection of the internal detail of the map and identification of artifacts.

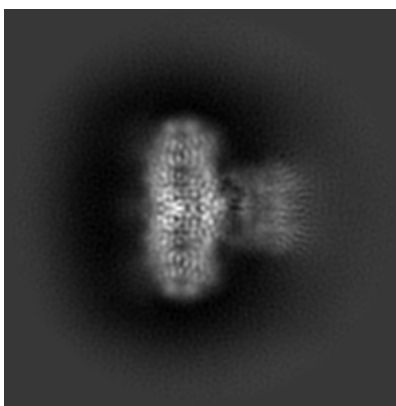
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

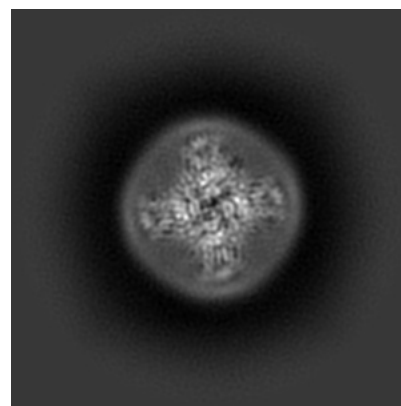
6.1.1 Primary map



X

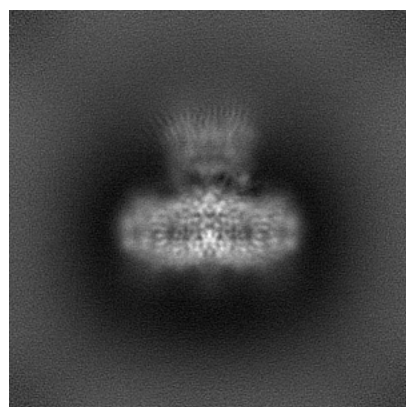


Y

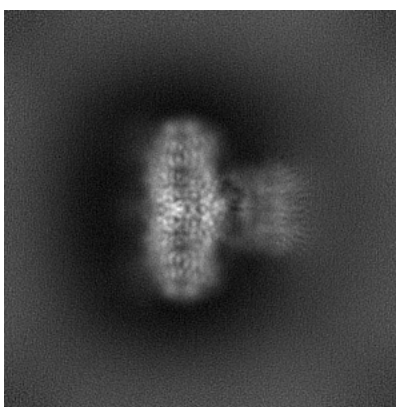


Z

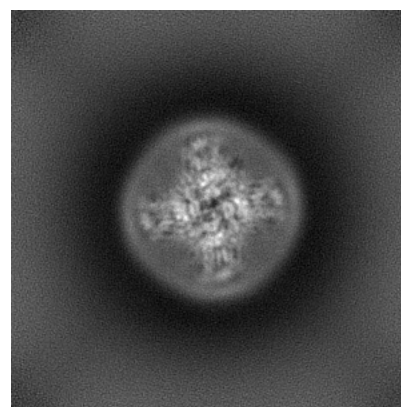
6.1.2 Raw map



X



Y

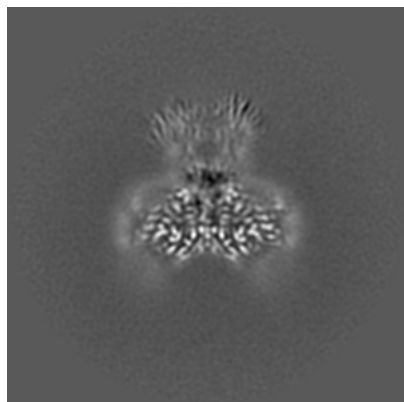


Z

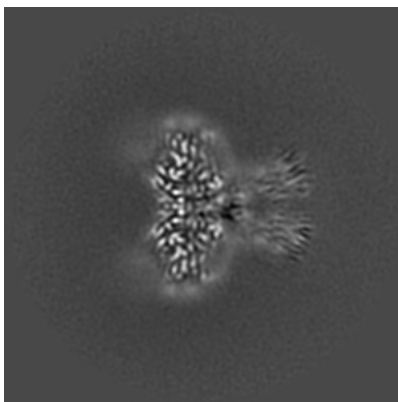
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

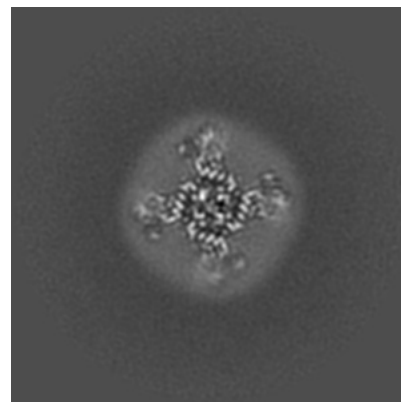
6.2.1 Primary map



X Index: 150

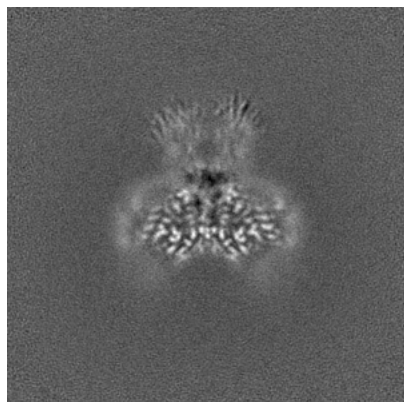


Y Index: 150

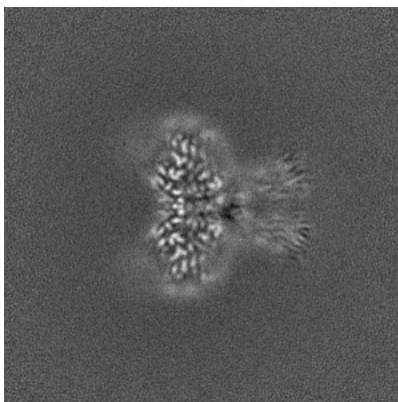


Z Index: 150

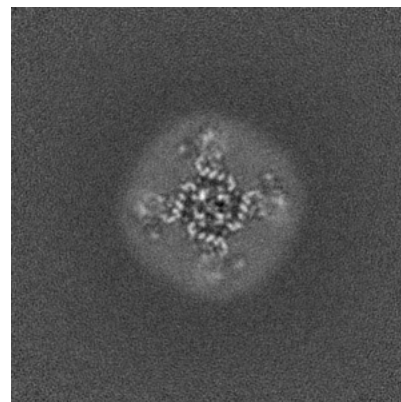
6.2.2 Raw map



X Index: 150



Y Index: 150

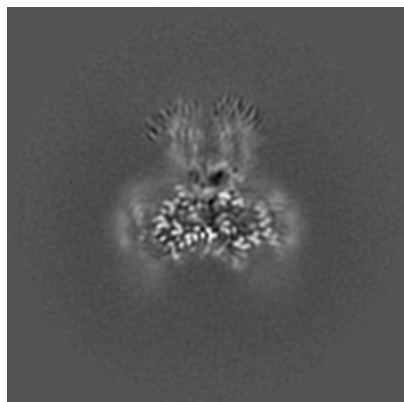


Z Index: 150

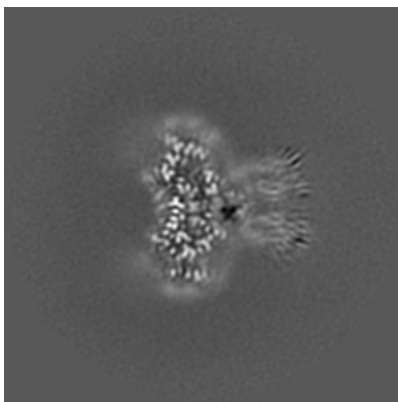
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

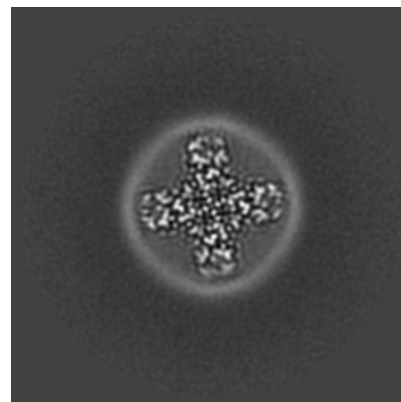
6.3.1 Primary map



X Index: 154

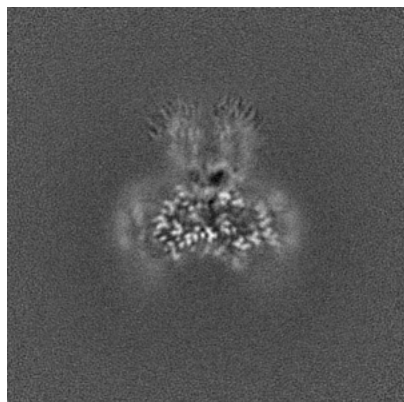


Y Index: 146

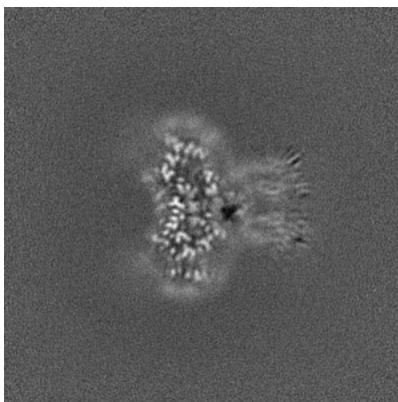


Z Index: 125

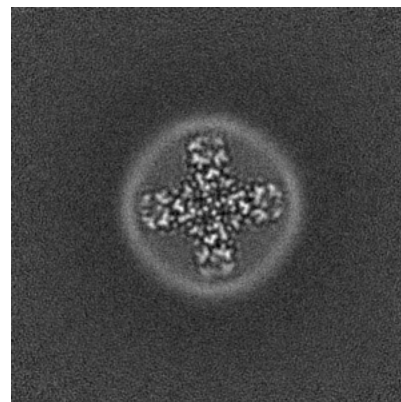
6.3.2 Raw map



X Index: 154



Y Index: 146

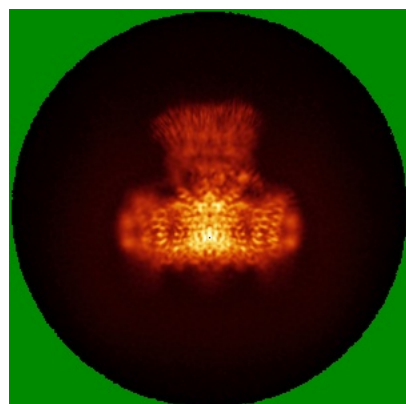


Z Index: 125

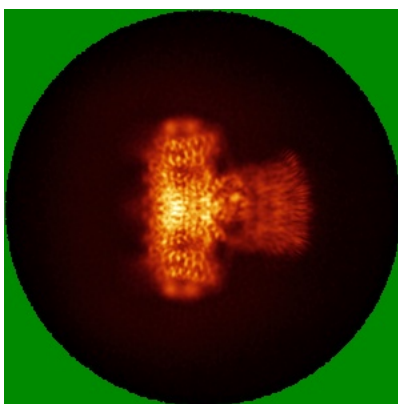
The images above show the largest variance slices of the map in three orthogonal directions.

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

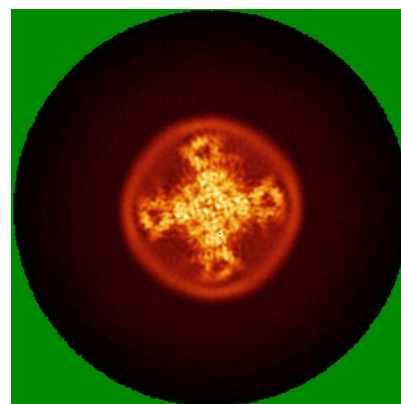
6.4.1 Primary map



X

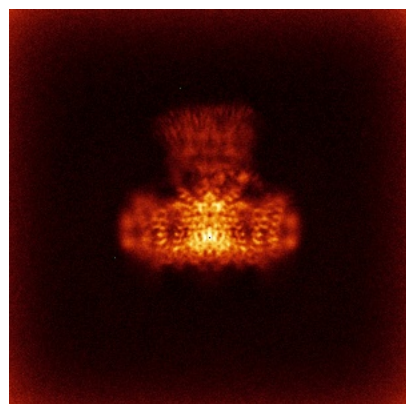


Y

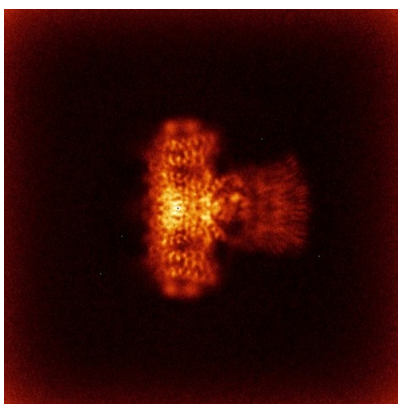


Z

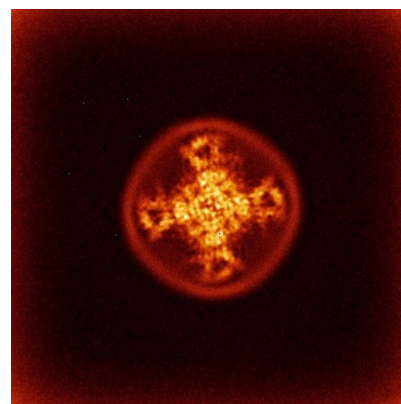
6.4.2 Raw map



X



Y

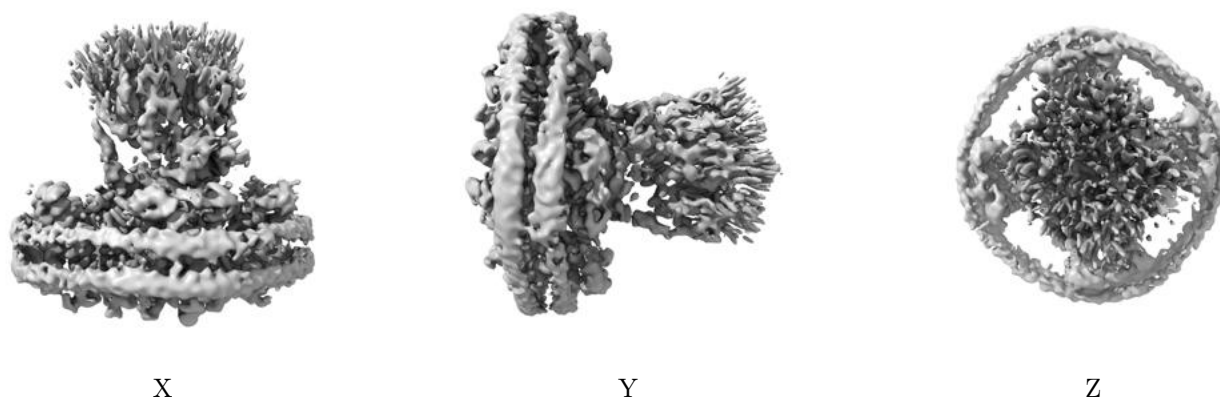


Z

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

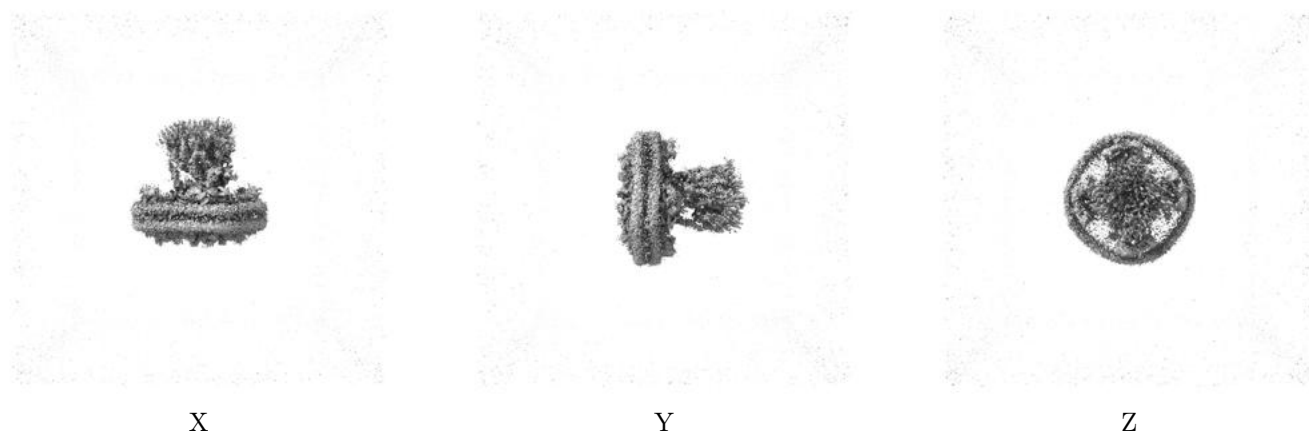
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

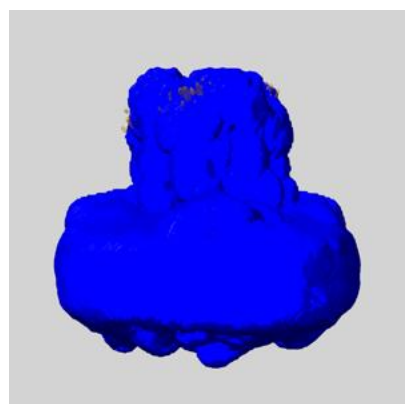
6.6 Mask visualisation [i](#)

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

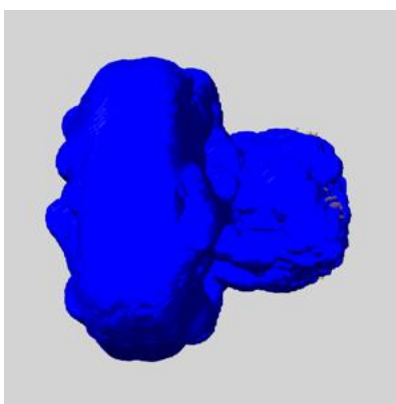
A mask typically either:

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

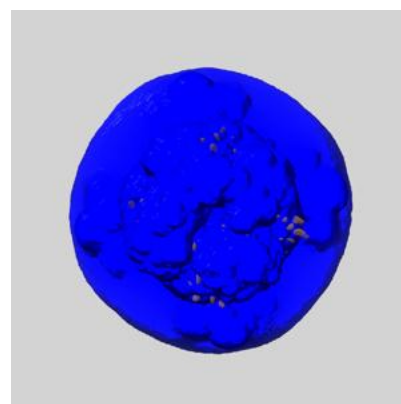
6.6.1 emd_49311_msk_1.map [i](#)



X



Y

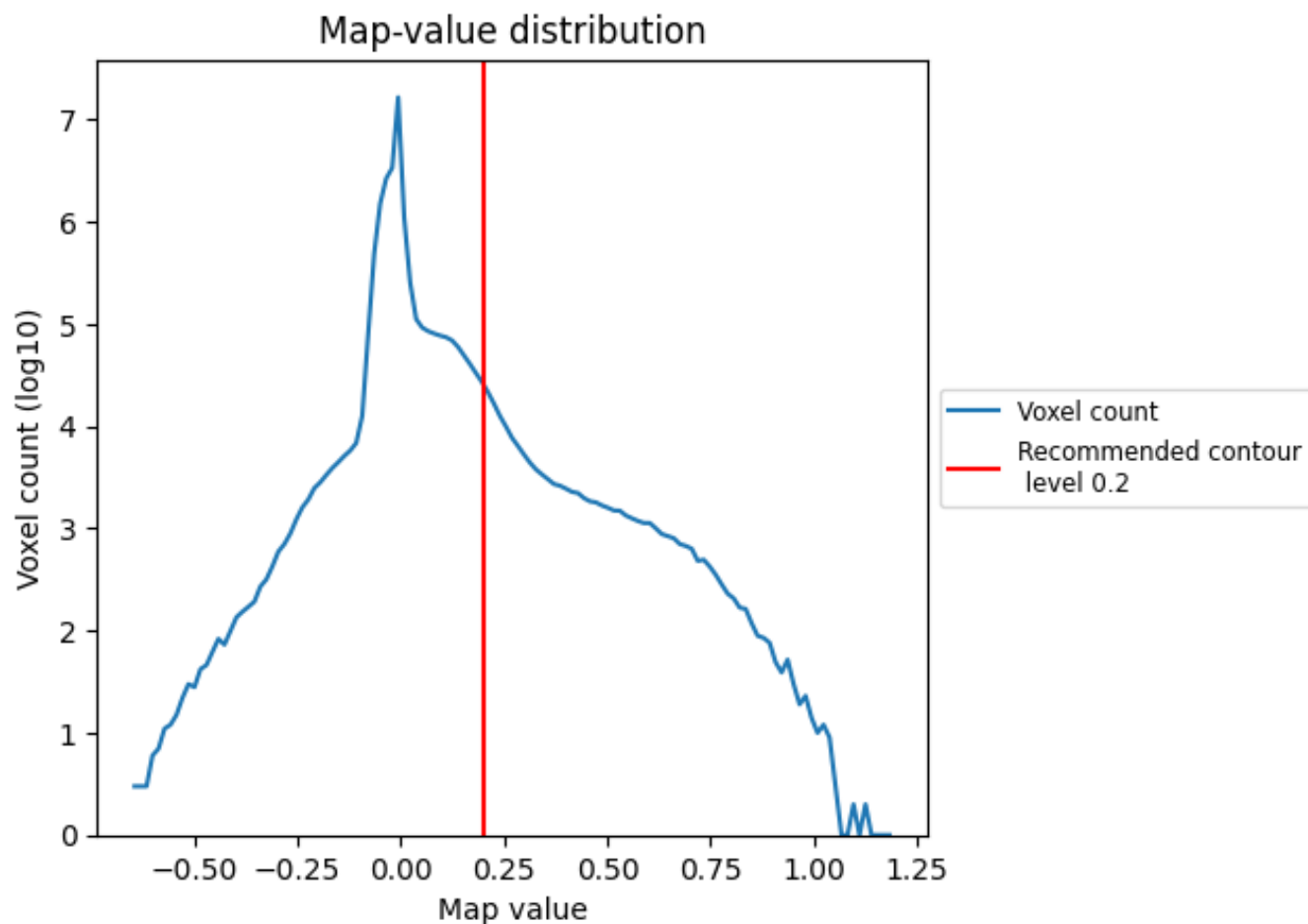


Z

7 Map analysis [i](#)

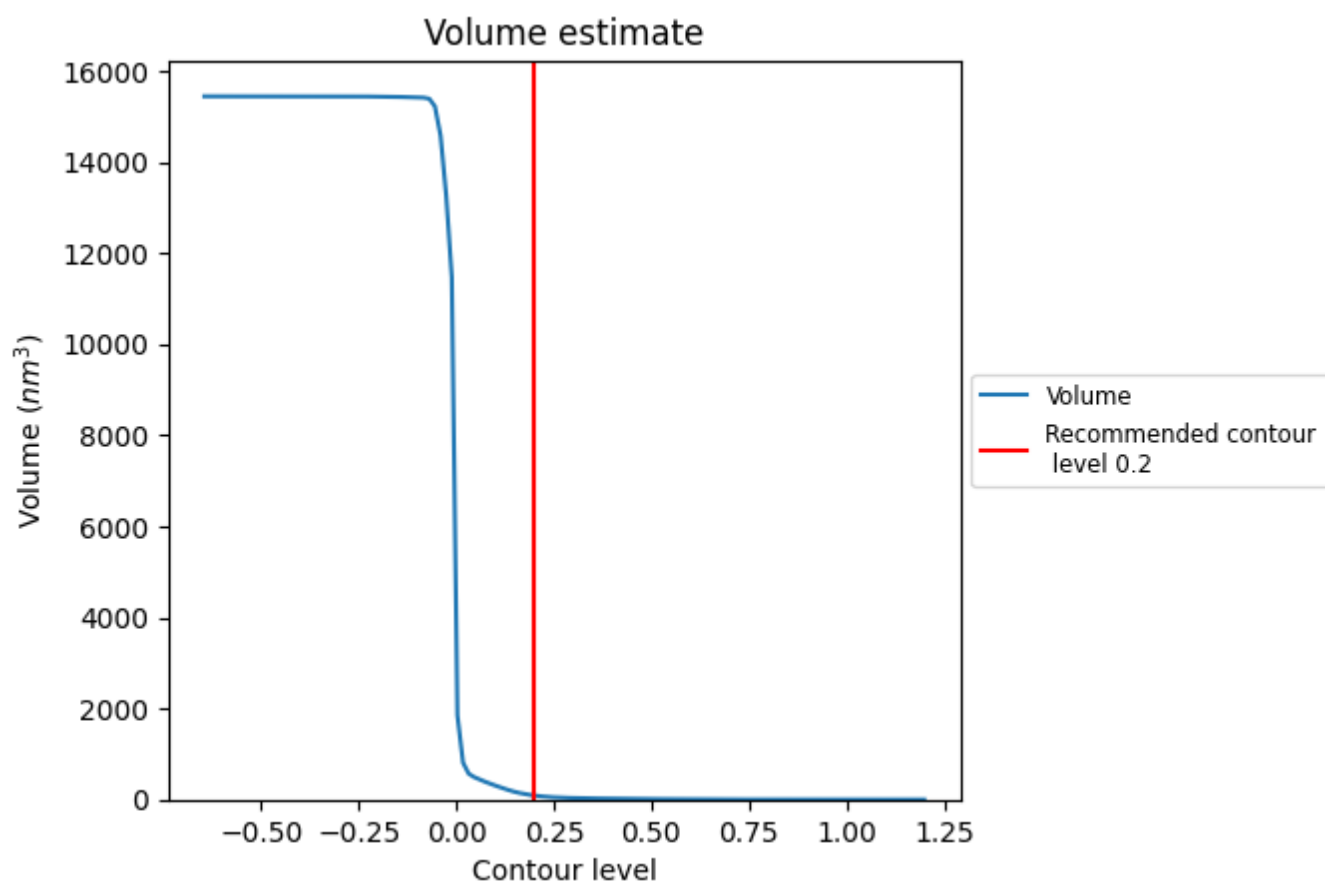
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

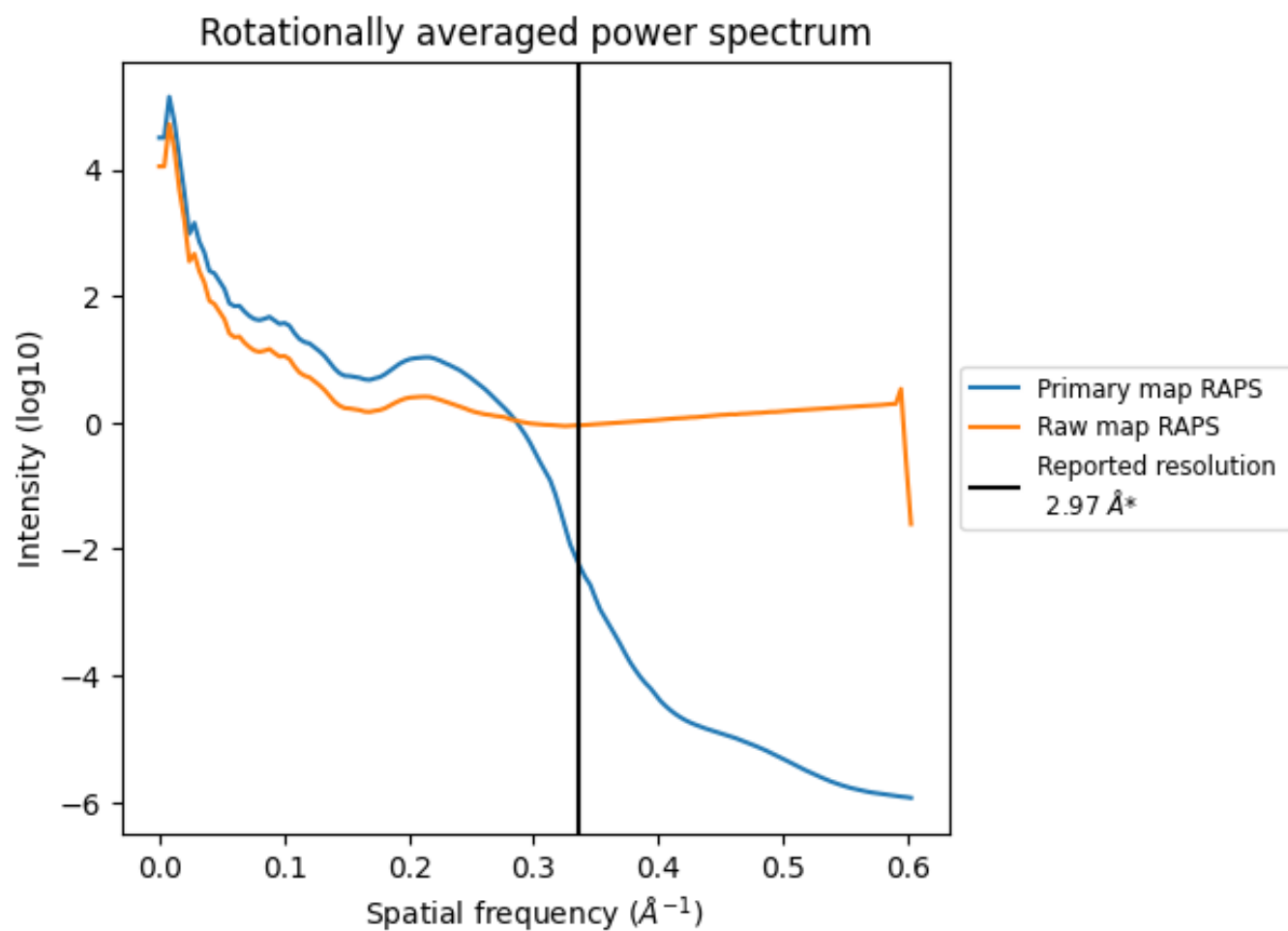
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 80 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 ⓘ

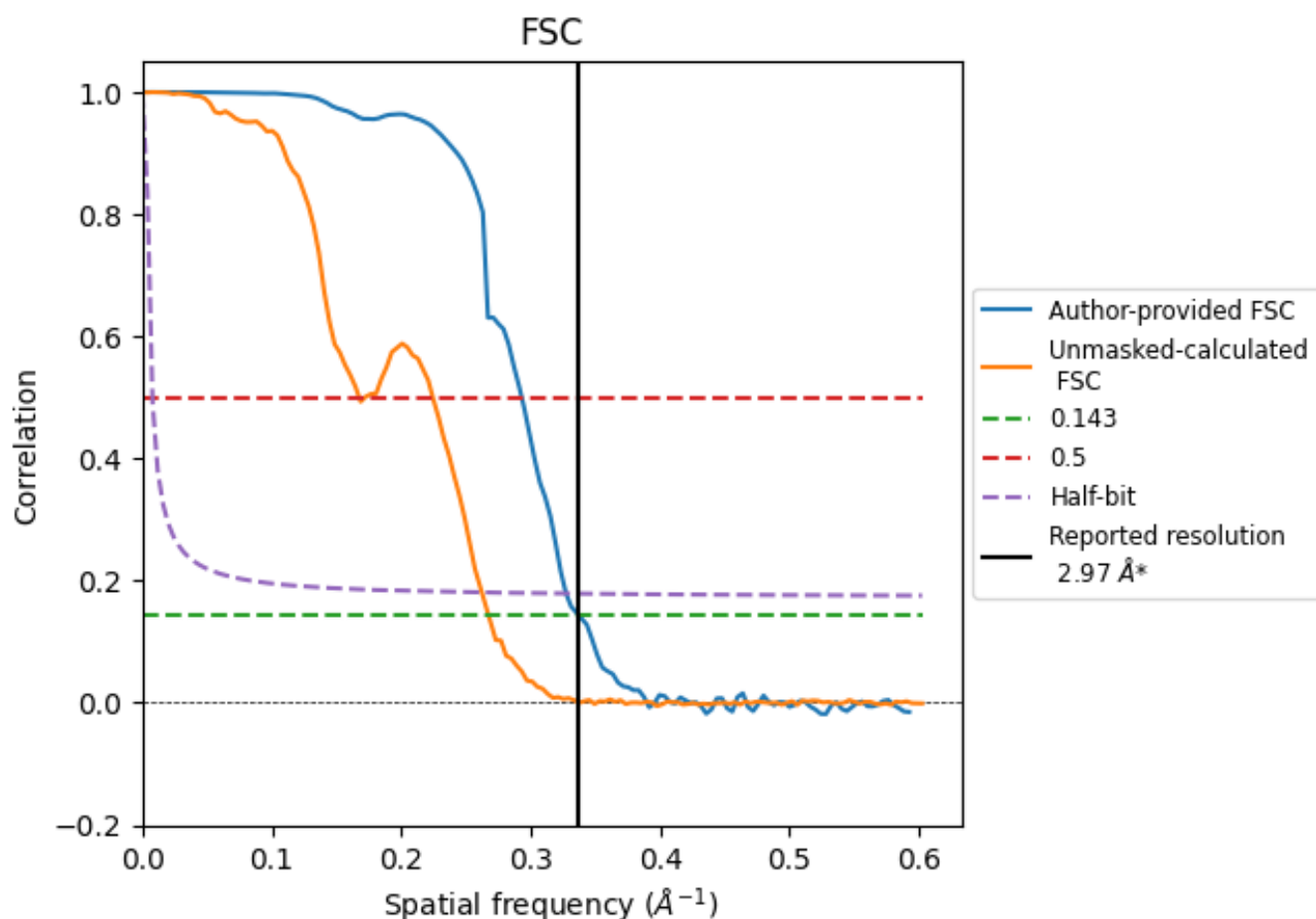


*Reported resolution corresponds to spatial frequency of 0.337 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.337 \AA^{-1}

8.2 Resolution estimates [i](#)

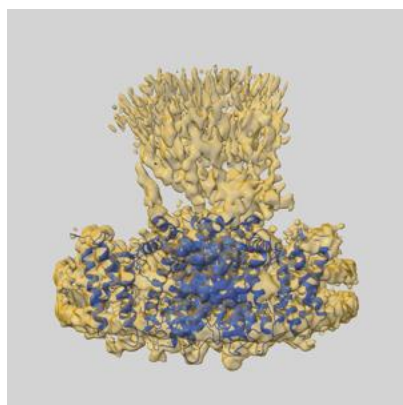
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.41	3.05
Unmasked-calculated*	3.74	5.97	3.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.97 by more than 10 %

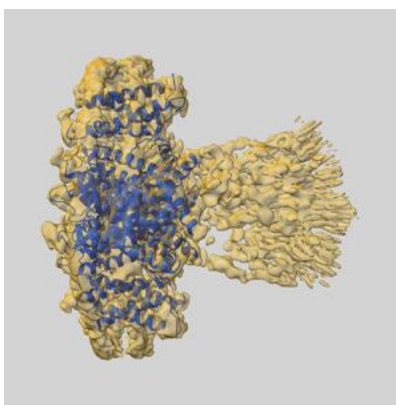
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49311 and PDB model 9NEI. Per-residue inclusion information can be found in section [3](#) on page [41](#).

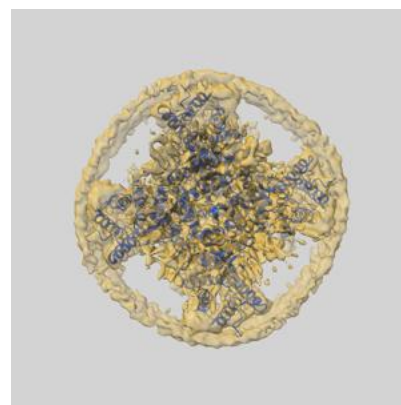
9.1 Map-model overlay [i](#)



X



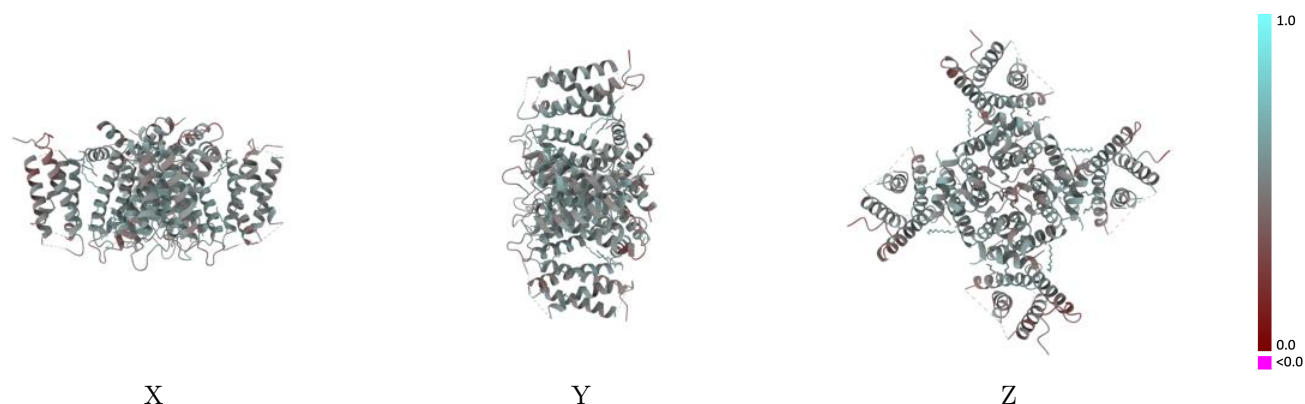
Y



Z

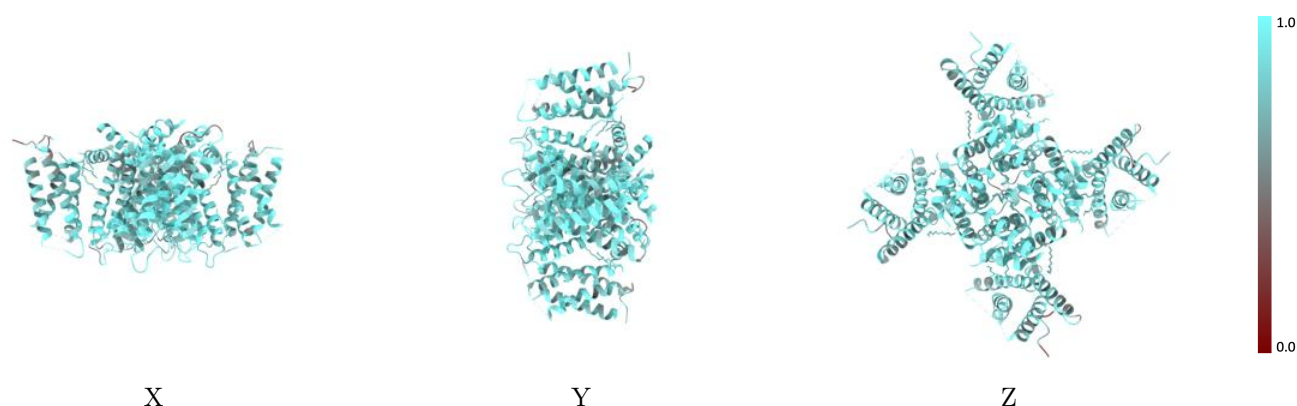
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



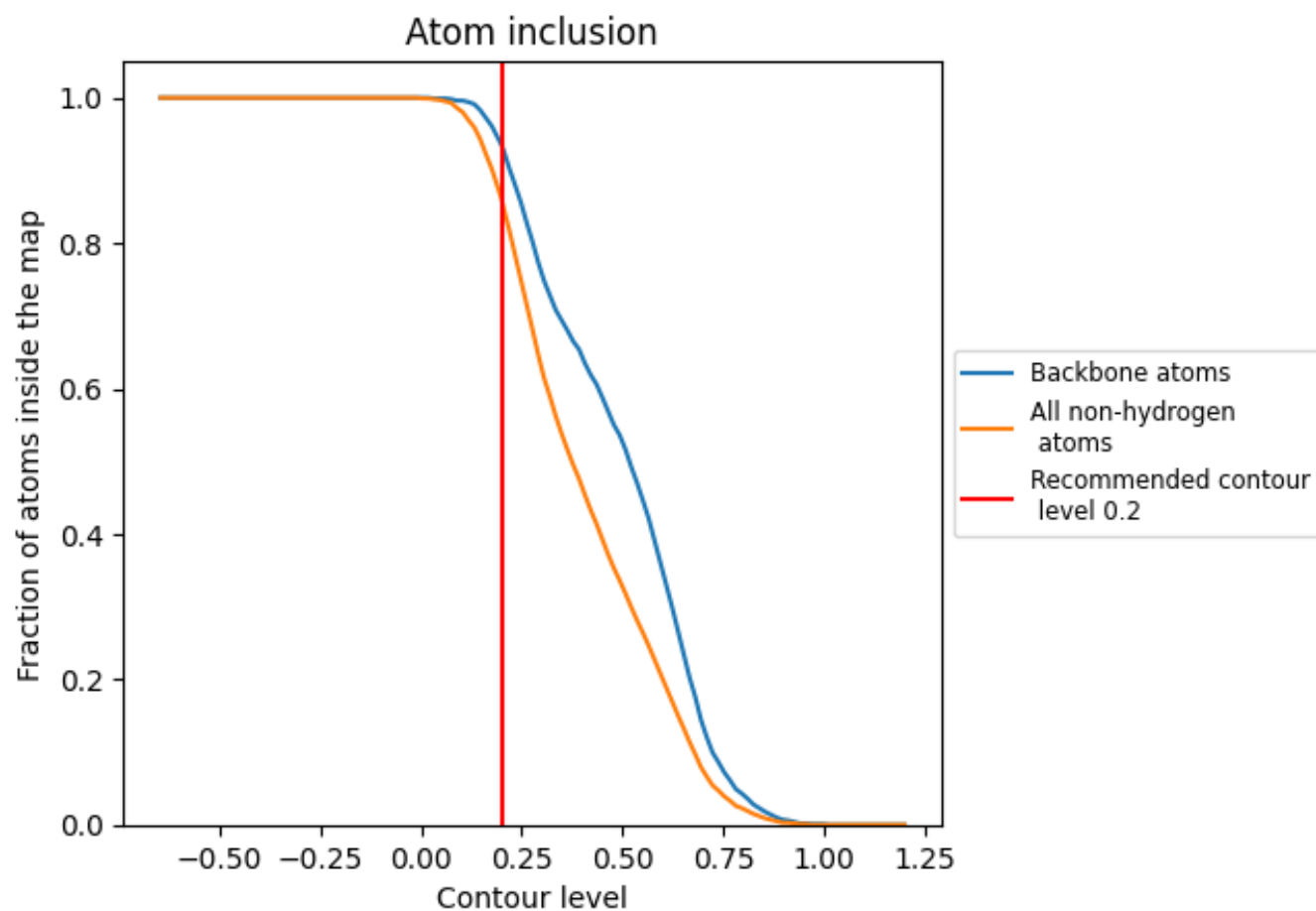
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 86% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8610	<div></div> 0.5120
A	<div></div> 0.8750	<div></div> 0.5180
B	<div></div> 0.8640	<div></div> 0.5190
C	<div></div> 0.8680	<div></div> 0.5180
D	<div></div> 0.8390	<div></div> 0.5000
G	<div></div> 0.8040	<div></div> 0.3940

