wwPDB EM Validation Summary Report

Sep 28, 2024 – 03:56 PM EDT

PDB ID	:	7SX3
EMDB ID	:	EMD-25492
Title	:	Human NALCN-FAM155A-UNC79-UNC80 channelosome with CaM bound, conformation 1/2
Authors	:	Kschonsak, M.; Chua, H.C.; Weidling, C.; Chakouri, N.; Noland, C.L.; Schott, K.; Chang, T.; Tam, C.; Patel, N.; Arthur, C.P.; Leitner, A.; Ben-Johny, M.; Ciferri, C.; Pless, S.A.; Payandeh, J.
Deposited on	:	2021-11-22
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

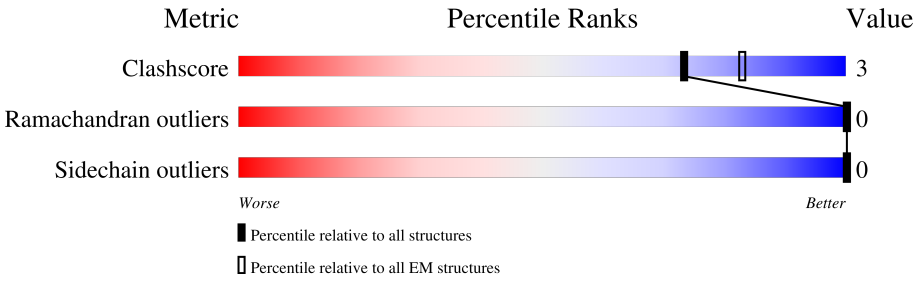
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2042	63% 5% 32%
2	B	483	30% 68%
3	C	149	46% 67% 9% 23%
4	D	2561	51% 45%
5	E	3283	45% 51%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 37959 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 Sodium leak channel non-selective protein,Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1386	Total	C	N	O	S	0	0
			11344	7478	1870	1906	90		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1739	GLY	-	linker	UNP Q8IZF0
A	1740	GLY	-	linker	UNP Q8IZF0
A	1741	SER	-	linker	UNP Q8IZF0
A	1742	LEU	-	linker	UNP Q8IZF0
A	1743	VAL	-	linker	UNP Q8IZF0
A	1744	PRO	-	linker	UNP Q8IZF0
A	1745	ARG	-	linker	UNP Q8IZF0
A	1746	GLY	-	linker	UNP Q8IZF0
A	1747	SER	-	linker	UNP Q8IZF0
A	1748	SER	-	linker	UNP Q8IZF0
A	1749	GLY	-	linker	UNP Q8IZF0
A	1750	GLU	-	linker	UNP Q8IZF0
A	1751	ASN	-	linker	UNP Q8IZF0
A	1752	LEU	-	linker	UNP Q8IZF0
A	1753	TYR	-	linker	UNP Q8IZF0
A	1754	PHE	-	linker	UNP Q8IZF0
A	1755	GLN	-	linker	UNP Q8IZF0
A	1756	GLY	-	linker	UNP Q8IZF0
A	1757	SER	-	linker	UNP Q8IZF0
A	1758	SER	-	linker	UNP Q8IZF0
A	1759	GLY	-	linker	UNP Q8IZF0
A	1966	LYS	ALA	conflict	UNP A0A7G8ZY66
A	2001	GLY	-	expression tag	UNP A0A7G8ZY66
A	2002	ASP	-	expression tag	UNP A0A7G8ZY66
A	2003	TYR	-	expression tag	UNP A0A7G8ZY66
A	2004	LYS	-	expression tag	UNP A0A7G8ZY66
A	2005	ASP	-	expression tag	UNP A0A7G8ZY66

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2006	ASP	-	expression tag	UNP A0A7G8ZY66
A	2007	ASP	-	expression tag	UNP A0A7G8ZY66
A	2008	ASP	-	expression tag	UNP A0A7G8ZY66
A	2009	LYS	-	expression tag	UNP A0A7G8ZY66
A	2010	GLY	-	expression tag	UNP A0A7G8ZY66
A	2011	SER	-	expression tag	UNP A0A7G8ZY66
A	2012	GLY	-	expression tag	UNP A0A7G8ZY66
A	2013	SER	-	expression tag	UNP A0A7G8ZY66
A	2014	ALA	-	expression tag	UNP A0A7G8ZY66
A	2015	TRP	-	expression tag	UNP A0A7G8ZY66
A	2016	SER	-	expression tag	UNP A0A7G8ZY66
A	2017	HIS	-	expression tag	UNP A0A7G8ZY66
A	2018	PRO	-	expression tag	UNP A0A7G8ZY66
A	2019	GLN	-	expression tag	UNP A0A7G8ZY66
A	2020	PHE	-	expression tag	UNP A0A7G8ZY66
A	2021	GLU	-	expression tag	UNP A0A7G8ZY66
A	2022	LYS	-	expression tag	UNP A0A7G8ZY66
A	2023	GLY	-	expression tag	UNP A0A7G8ZY66
A	2024	GLY	-	expression tag	UNP A0A7G8ZY66
A	2025	GLY	-	expression tag	UNP A0A7G8ZY66
A	2026	SER	-	expression tag	UNP A0A7G8ZY66
A	2027	GLY	-	expression tag	UNP A0A7G8ZY66
A	2028	GLY	-	expression tag	UNP A0A7G8ZY66
A	2029	GLY	-	expression tag	UNP A0A7G8ZY66
A	2030	SER	-	expression tag	UNP A0A7G8ZY66
A	2031	GLY	-	expression tag	UNP A0A7G8ZY66
A	2032	GLY	-	expression tag	UNP A0A7G8ZY66
A	2033	SER	-	expression tag	UNP A0A7G8ZY66
A	2034	ALA	-	expression tag	UNP A0A7G8ZY66
A	2035	TRP	-	expression tag	UNP A0A7G8ZY66
A	2036	SER	-	expression tag	UNP A0A7G8ZY66
A	2037	HIS	-	expression tag	UNP A0A7G8ZY66
A	2038	PRO	-	expression tag	UNP A0A7G8ZY66
A	2039	GLN	-	expression tag	UNP A0A7G8ZY66
A	2040	PHE	-	expression tag	UNP A0A7G8ZY66
A	2041	GLU	-	expression tag	UNP A0A7G8ZY66
A	2042	LYS	-	expression tag	UNP A0A7G8ZY66

- Molecule 2 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	153	Total	C	N	O	S	0	0
			1256	801	193	246	16		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	459	GLY	-	expression tag	UNP B1AL88
B	460	GLY	-	expression tag	UNP B1AL88
B	461	SER	-	expression tag	UNP B1AL88
B	462	GLY	-	expression tag	UNP B1AL88
B	463	GLY	-	expression tag	UNP B1AL88
B	464	SER	-	expression tag	UNP B1AL88
B	465	ASP	-	expression tag	UNP B1AL88
B	466	TYR	-	expression tag	UNP B1AL88
B	467	LYS	-	expression tag	UNP B1AL88
B	468	ASP	-	expression tag	UNP B1AL88
B	469	ASP	-	expression tag	UNP B1AL88
B	470	ASP	-	expression tag	UNP B1AL88
B	471	ASP	-	expression tag	UNP B1AL88
B	472	LYS	-	expression tag	UNP B1AL88
B	473	GLY	-	expression tag	UNP B1AL88
B	474	ASN	-	expression tag	UNP B1AL88
B	475	SER	-	expression tag	UNP B1AL88
B	476	ASP	-	expression tag	UNP B1AL88
B	477	TYR	-	expression tag	UNP B1AL88
B	478	LYS	-	expression tag	UNP B1AL88
B	479	ASP	-	expression tag	UNP B1AL88
B	480	ASP	-	expression tag	UNP B1AL88
B	481	ASP	-	expression tag	UNP B1AL88
B	482	ASP	-	expression tag	UNP B1AL88
B	483	LYS	-	expression tag	UNP B1AL88

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	114	Total	C	N	O	S	0	0
			926	579	149	189	9		

- Molecule 4 is a protein called UNC79,Protein unc-79 homolog,Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1418	Total	C	N	O	S	0	0
			11107	7213	1845	1953	96		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2636	GLY	-	expression tag	UNP Q9P2D8
D	2637	GLY	-	expression tag	UNP Q9P2D8
D	2638	SER	-	expression tag	UNP Q9P2D8
D	2639	GLY	-	expression tag	UNP Q9P2D8
D	2640	GLY	-	expression tag	UNP Q9P2D8
D	2641	SER	-	expression tag	UNP Q9P2D8
D	2642	ASP	-	expression tag	UNP Q9P2D8
D	2643	TYR	-	expression tag	UNP Q9P2D8
D	2644	LYS	-	expression tag	UNP Q9P2D8
D	2645	ASP	-	expression tag	UNP Q9P2D8
D	2646	ASP	-	expression tag	UNP Q9P2D8
D	2647	ASP	-	expression tag	UNP Q9P2D8
D	2648	ASP	-	expression tag	UNP Q9P2D8
D	2649	LYS	-	expression tag	UNP Q9P2D8
D	2650	GLY	-	expression tag	UNP Q9P2D8
D	2651	ASN	-	expression tag	UNP Q9P2D8
D	2652	SER	-	expression tag	UNP Q9P2D8
D	2653	ASP	-	expression tag	UNP Q9P2D8
D	2654	TYR	-	expression tag	UNP Q9P2D8
D	2655	LYS	-	expression tag	UNP Q9P2D8
D	2656	ASP	-	expression tag	UNP Q9P2D8
D	2657	ASP	-	expression tag	UNP Q9P2D8
D	2658	ASP	-	expression tag	UNP Q9P2D8
D	2659	ASP	-	expression tag	UNP Q9P2D8
D	2660	LYS	-	expression tag	UNP Q9P2D8

- Molecule 5 is a protein called Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1611	Total	C	N	O	S	0	0
			12977	8412	2202	2270	93		

There are 25 discrepancies between the modelled and reference sequences:

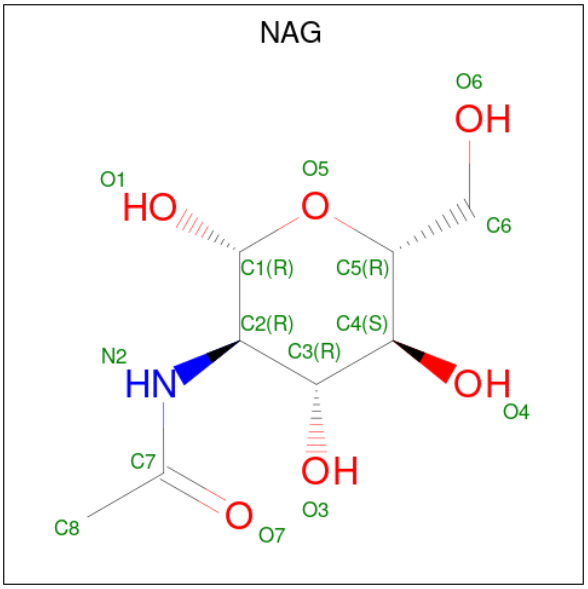
Chain	Residue	Modelled	Actual	Comment	Reference
E	3259	GLY	-	expression tag	UNP Q8N2C7
E	3260	GLY	-	expression tag	UNP Q8N2C7
E	3261	SER	-	expression tag	UNP Q8N2C7
E	3262	GLY	-	expression tag	UNP Q8N2C7
E	3263	GLY	-	expression tag	UNP Q8N2C7
E	3264	SER	-	expression tag	UNP Q8N2C7
E	3265	ASP	-	expression tag	UNP Q8N2C7
E	3266	TYR	-	expression tag	UNP Q8N2C7

Continued on next page...

Continued from previous page...

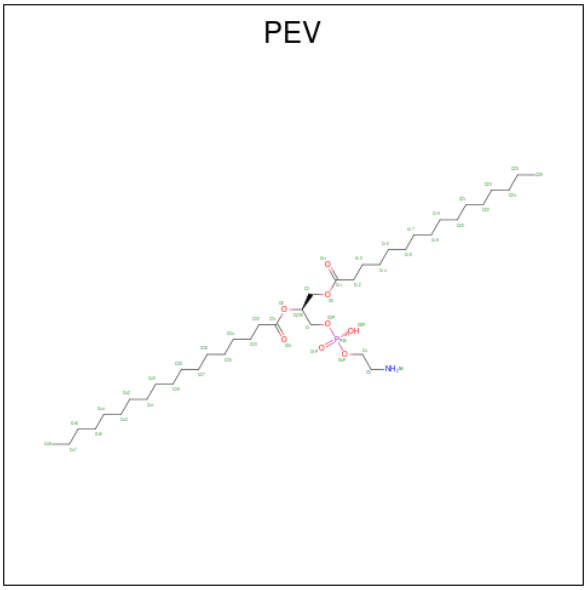
Chain	Residue	Modelled	Actual	Comment	Reference
E	3267	LYS	-	expression tag	UNP Q8N2C7
E	3268	ASP	-	expression tag	UNP Q8N2C7
E	3269	ASP	-	expression tag	UNP Q8N2C7
E	3270	ASP	-	expression tag	UNP Q8N2C7
E	3271	ASP	-	expression tag	UNP Q8N2C7
E	3272	LYS	-	expression tag	UNP Q8N2C7
E	3273	GLY	-	expression tag	UNP Q8N2C7
E	3274	ASN	-	expression tag	UNP Q8N2C7
E	3275	SER	-	expression tag	UNP Q8N2C7
E	3276	ASP	-	expression tag	UNP Q8N2C7
E	3277	TYR	-	expression tag	UNP Q8N2C7
E	3278	LYS	-	expression tag	UNP Q8N2C7
E	3279	ASP	-	expression tag	UNP Q8N2C7
E	3280	ASP	-	expression tag	UNP Q8N2C7
E	3281	ASP	-	expression tag	UNP Q8N2C7
E	3282	ASP	-	expression tag	UNP Q8N2C7
E	3283	LYS	-	expression tag	UNP Q8N2C7

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



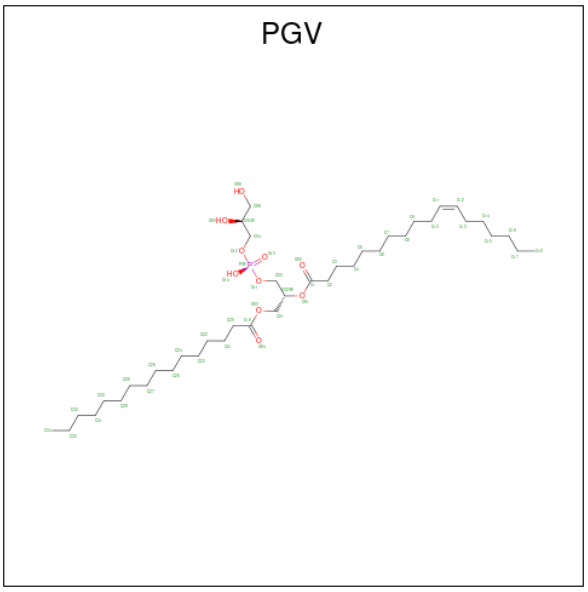
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



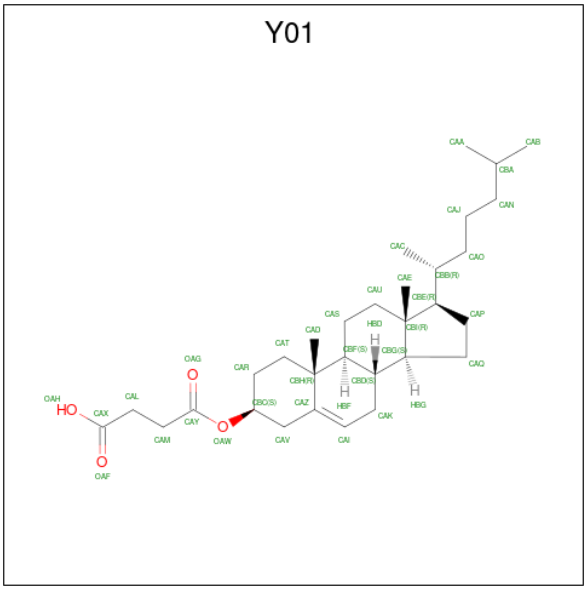
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
7	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
7	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	A	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 8 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	P	0
			31	22	8	1	
8	A	1	Total	C	O	P	0
			43	34	8	1	

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			35	31	4	
9	A	1	Total	C	O	0
			35	31	4	

Continued on next page...

Continued from previous page...

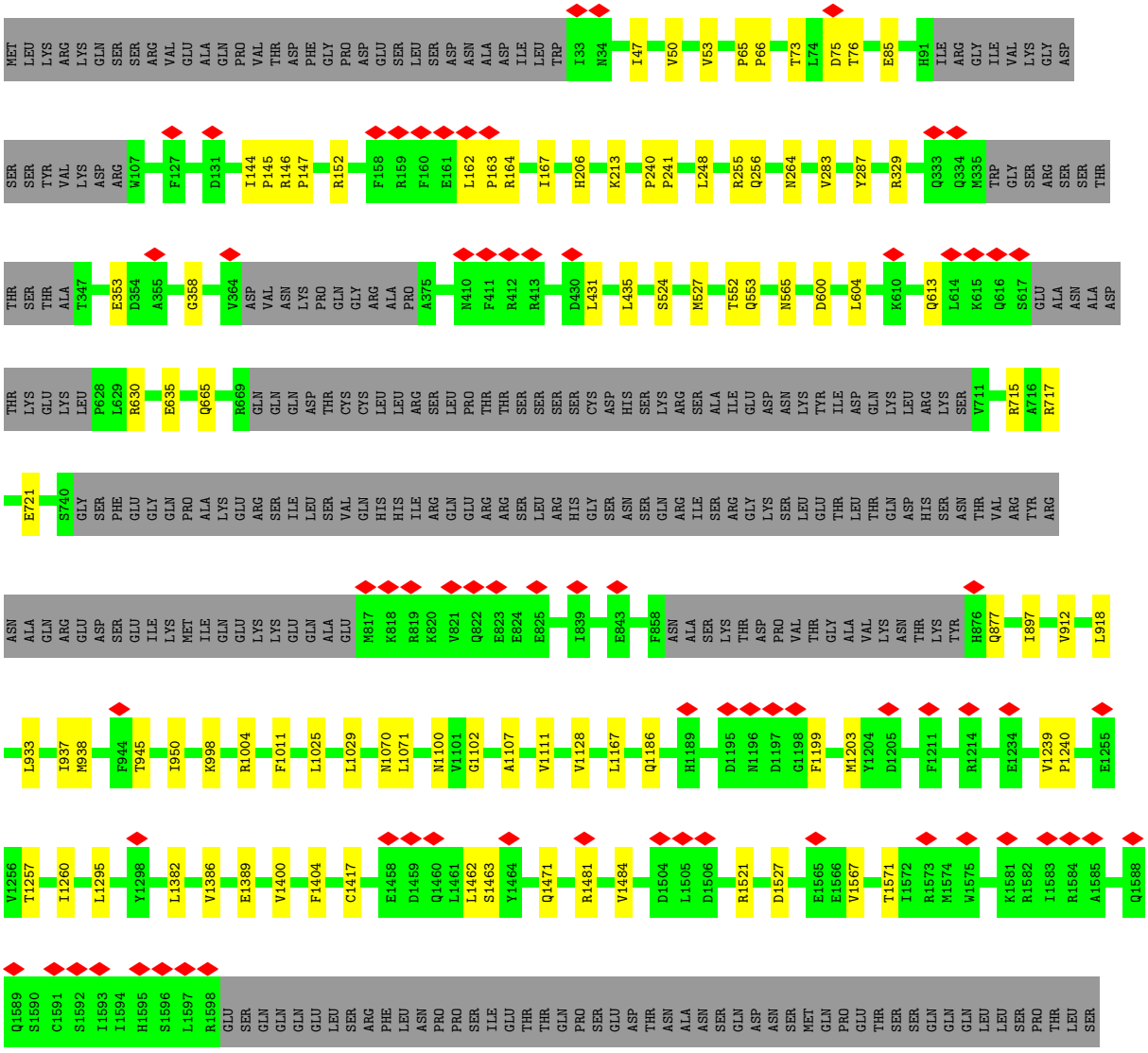
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			35	31	4	

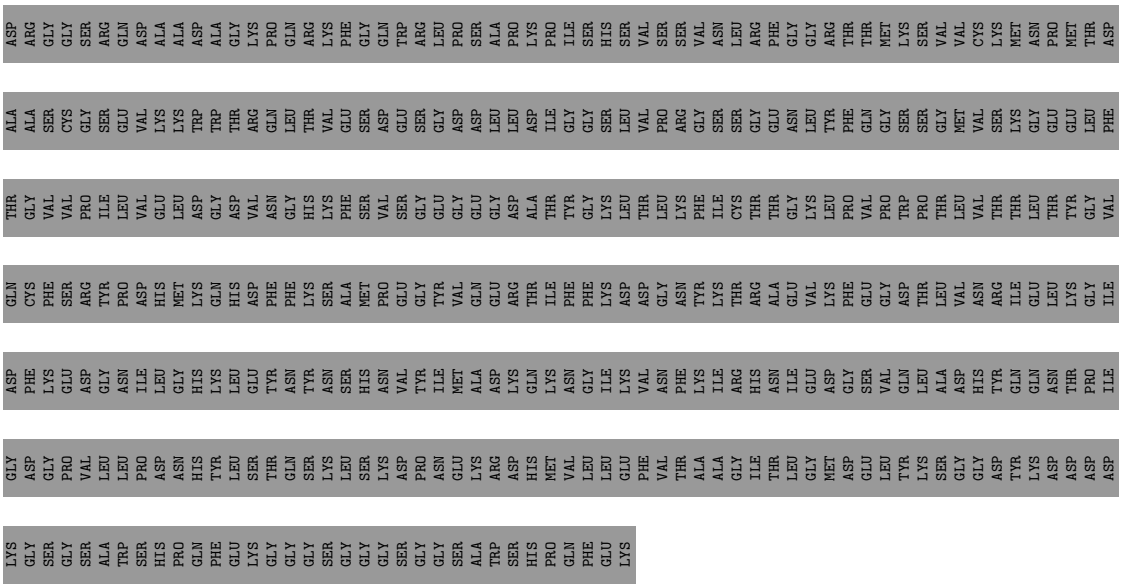
3 Residue-property plots (i)

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

• Molecule 1: Sodium leak channel non-selective protein,Enhanced green fluorescent protein

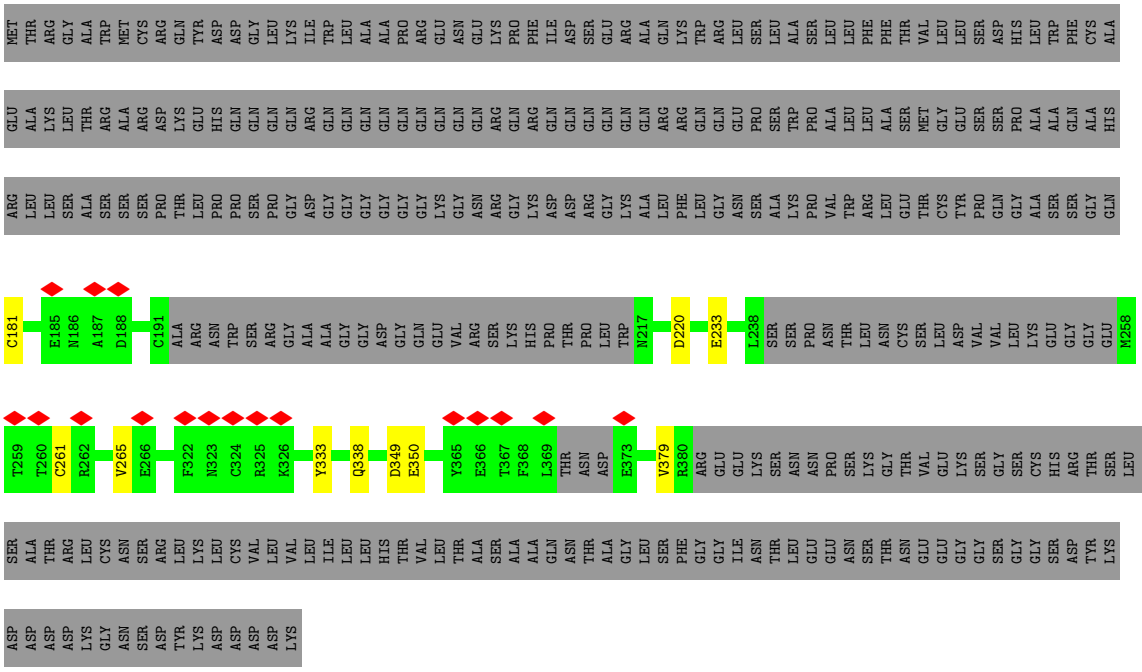
Chain A:





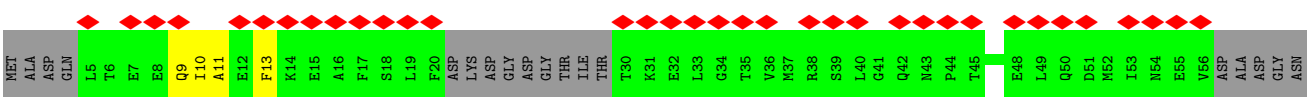
• Molecule 2: Transmembrane protein FAM155A

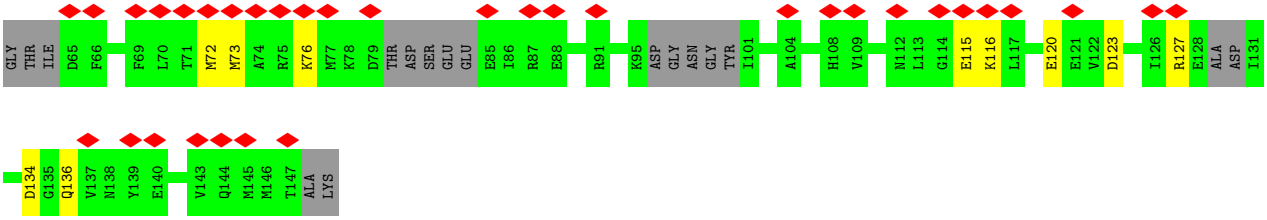
Chain B:



• Molecule 3: Calmodulin-1

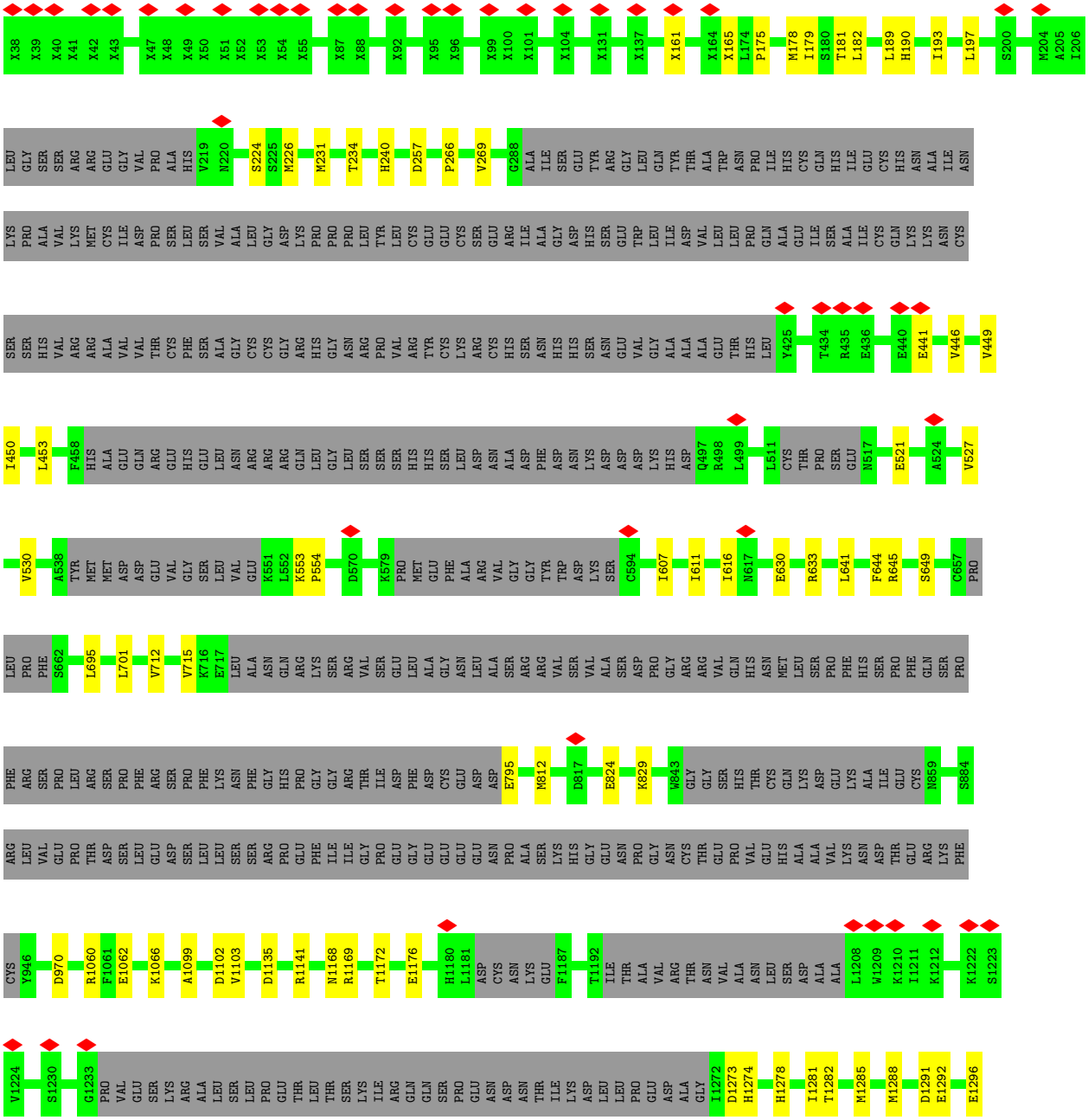
Chain C:

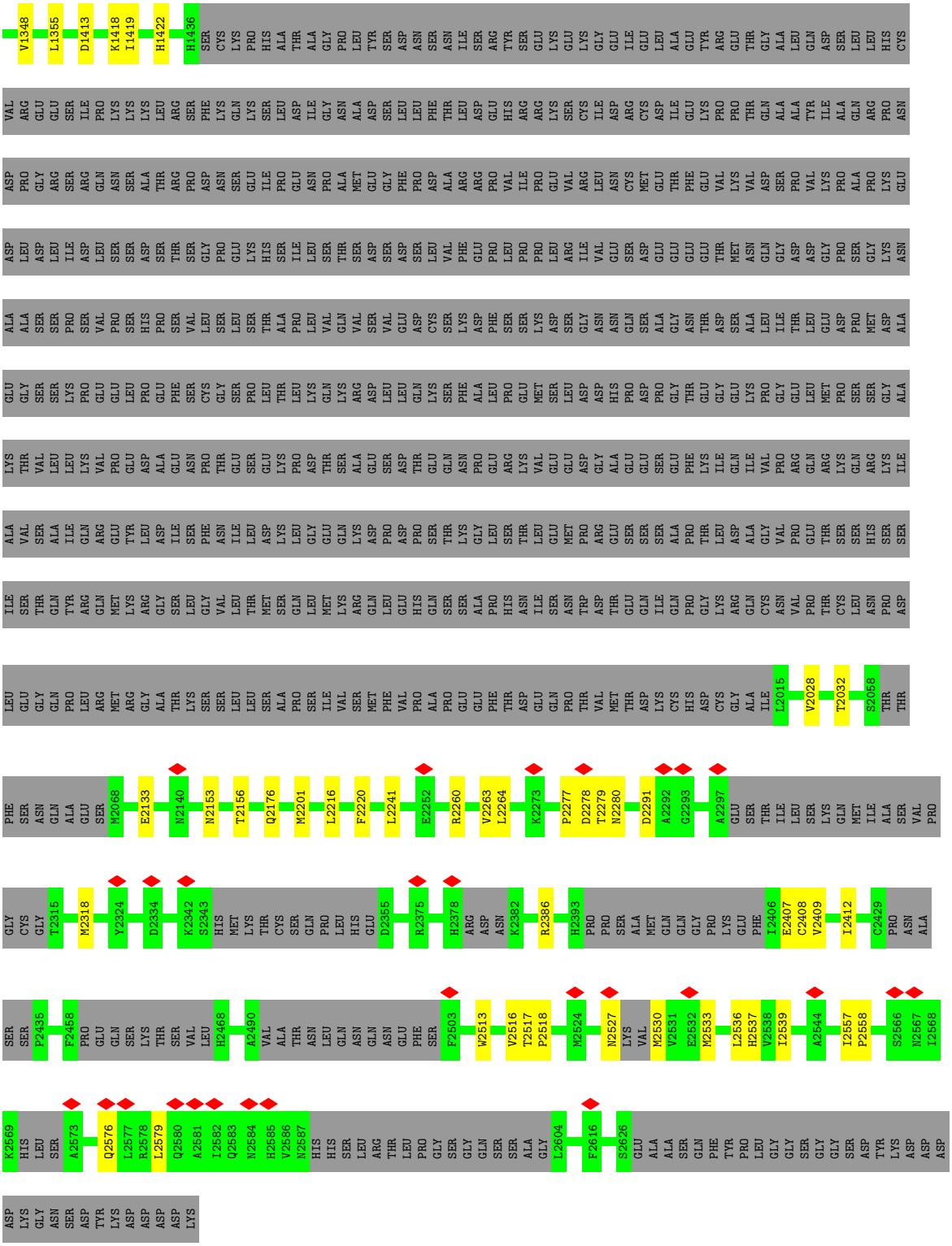




• Molecule 4: UNC79,Protein unc-79 homolog,Protein unc-79 homolog

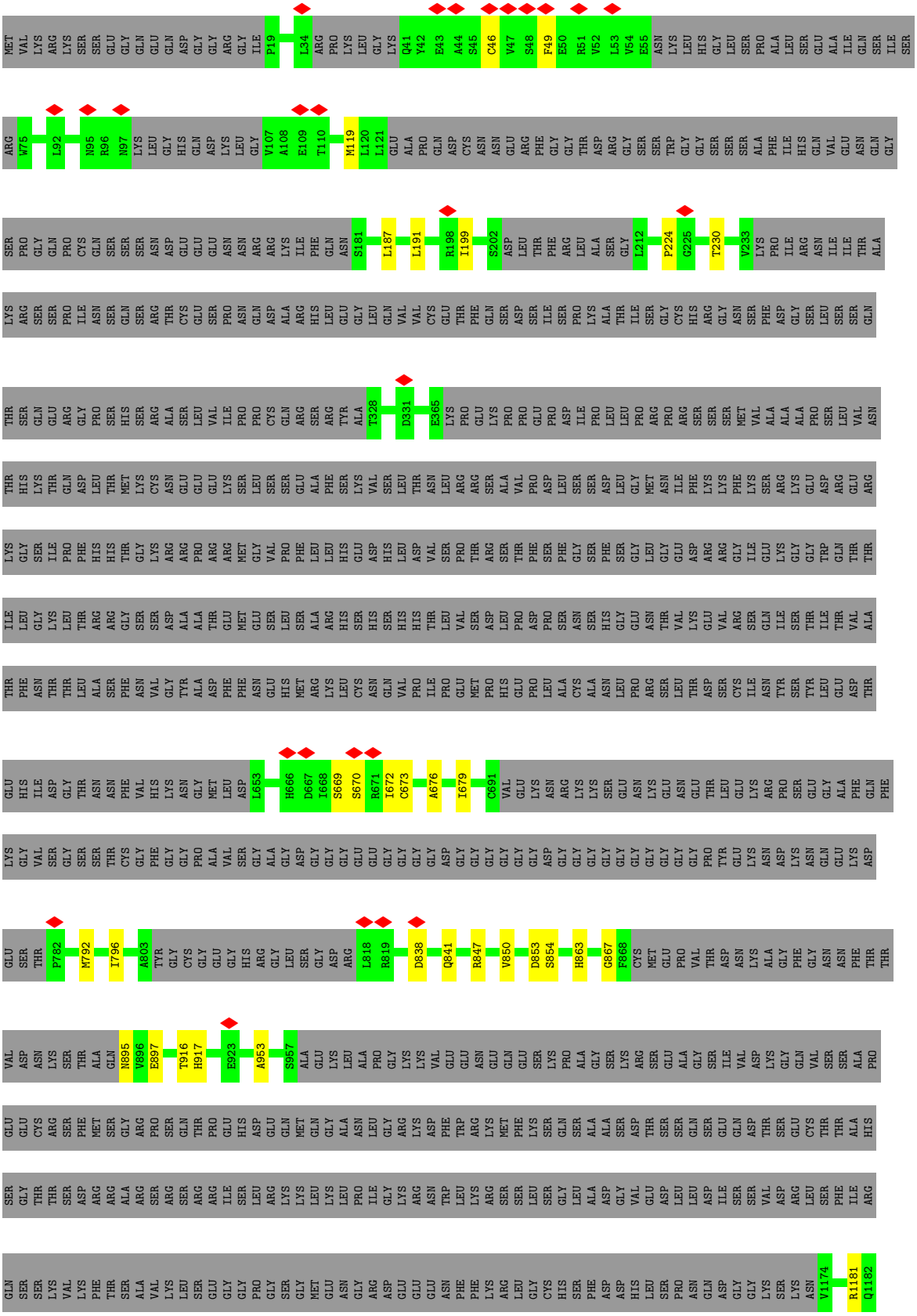
Chain D:

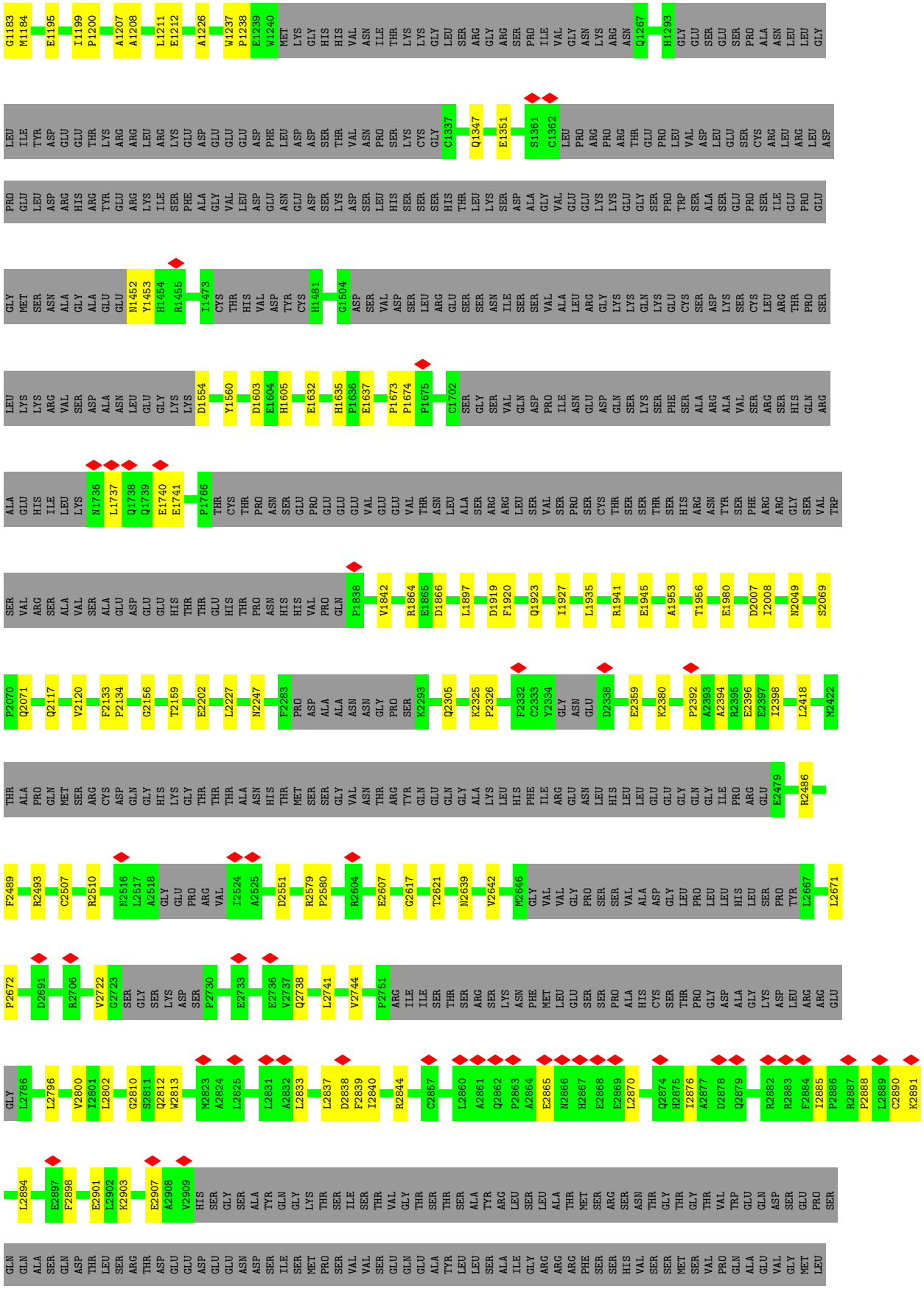




• Molecule 5: Protein unc-80 homolog

Chain E:


MET VAL LYS ARG LYS SER SER GLU GLY GLN GLU GLN ASP GLY GLY ARG GLY ILE P19 L34 ARG PRO LYS LEU GLY LYS Q41 Y42 E43 A44 S45 C46 V47 S48 F49 E50 R51 V52 L53 V54 E55 ASN LYS LEU HIS GLY LEU SER PRO ALA LEU SER GLU ALA ILE GLN SER ILE
ARG W75 L92 N95 R96 N97 LYS LEU GLY HIS GLN ASP LYS LEU GLY V107 A108 E109 T110 M119 L120 L121 GLU GLY ALA PRO GLN ASP CYS ASN ASN GLU ARG PHE GLY GLY THR ASP ARG GLY SER TRP GLY GLY SER SER SER ALA PHE ILE HIS GLN VAL GLU ASN GLN GLY
SER PRO GLY GLN PRO CYS GLN SER SER SER ASN ASP GLU GLU GLU ASN ASN ARG ARG LYS ILE PHE GLN ASN S181 L187 L191 R196 I199 S202 ASP LEU THR PHE ARG LEU ALA SER GLY L212 P224 G225 T230 V233 LYS PRO ILE ARG ASN ILE ILE THR ALA
LYS ARG SER SER PRO ILE ASN SER GLN SER ARG THR CYS GLU SER PRO ASN GLN ASP ALA ARG HIS LEU GLU GLY LEU GLN VAL VAL CYS GLU THR PHE GLN SER ASP SER ILE SER PRO LYS ALA THR ILE SER GLY CYS HIS ARG GLY ASN SER PHE ASP GLY SER LEU SER SER GLN
THR SER GLN GLU ARG GLY PRO SER HIS SER ARG ALA SER LEU VAL ILE PRO PRO CYS GLN ARG SER ARG TYR ALA T328 D331 E365 LYS PRO GLU LYS PRO PRO GLU PRO ASP ILE PRO LEU LEU PRO ARG PRO ARG SER SER SER MET VAL ALA ALA ALA PRO SER LEU VAL ASN
THR HIS LYS THR GLN ASP LEU THR MET LYS CYS ASN GLU GLU GLU LYS SER LEU SER SER GLU ALA PHE SER LYS VAL SER LEU THR ASN LEU ARG ARG SER ALA VAL PRO ASP LEU SER SER ASP LEU GLY MET ASN ILE PHE LYS LYS PHE LYS SER ARG LYS GLU ASP ARG GLU ARG
LYS GLY SER ILE PRO PHE HIS HIS THR GLY LYS ARG ARG PRO ARG ARG MET GLY VAL PRO PHE LEU LEU HIS GLU ASP HIS LEU ASP VAL SER PRO THR ARG SER THR PHE SER PHE GLY SER PHE SER GLY LEU GLY GLU ASP ARG ARG GLY ILE GLU LYS GLY GLY TRP GLN THR THR
ILE LEU GLY LYS LEU THR ARG ARG GLY SER SER ASP ALA ALA THR GLU MET GLU SER LEU SER ALA ARG HIS SER HIS SER HIS HIS THR LEU VAL SER ASP PRO LEU PRO ASP PRO PRO SER ASN SER HIS GLY GLU ASN THR VAL LYS GLU VAL ARG SER GLN ILE SER THR ILE THR VAL ALA
THR PHE ASN THR THR LEU ALA SER PHE ASN VAL GLY TYR ALA ASP PHE PHE ASN GLU HIS MET ARG LYS LEU CYS ASN GLN VAL PRO ILE PRO GLU MET PRO HIS GLU PRO LEU ALA CYS ALA ASN LEU PRO ARG SER LEU THR ASP SER CYS ILE ASN TYR SER TYR LEU GLU ASP THR
GLU HIS ILE ASP GLY THR ASN ASN PHE VAL HIS LYS ASN GLY MET LEU ASP L653 H666 D667 I668 S669 S670 R671 I672 C673 A676 I679 C691 VAL GLU LYS ASN ARG LYS LYS SER GLU ASN LYS GLU ASN GLU THR LEU GLU LYS ARG PRO SER GLU GLY GLY ALA PHE GLN PHE
LYS GLY VAL SER GLY SER SER THR CYS GLY PHE GLY GLY PRO ALA VAL SER GLY ALA GLY ASP GLY GLY GLU GLU GLY GLY ASP GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY PRO TYR GLU LYS ASN ASP LYS ASN GLN GLU LYS ASP
GLU SER THR P782 M792 I796 A803 TYR GLY CYS GLY GLU GLY HIS ARG GLY LEU SER GLY ASP ARG L818 R819 D838 Q841 R847 V850 D853 S854 H863 G867 F868 CYS MET GLU PRO VAL THR ASP ASN LYS ALA GLY PHE GLY ASN ASN PHE THR THR
VAL ASP ASN LYS SER THR ALA GLN N895 V896 E897 T916 H917 E923 A953 S957 ALA GLU LYS LEU ALA PRO GLY LYS LYS VAL GLU GLU ASN GLU GLN GLU SER LYS PRO ALA GLY SER LYS ARG SER GLU ALA GLY SER ILE ILE VAL ASP LYS GLY GLN VAL SER SER ALA PRO
GLU GLU CYS ARG SER PHE MET SER GLY ARG PRO SER GLN THR PRO GLU HIS ASP GLU GLN MET GLN GLY ALA LEU GLY ARG LYS ASP PHE TRP ARG LYS MET PHE LYS SER GLN SER ALA ALA SER ASP THR SER SER GLN SER GLU GLN ASP THR SER GLU CYS THR THR ALA HIS
SER GLY THR THR SER ASP ARG ALA ARG SER ARG SER ARG ARG ILE SER LEU ARG LYS LYS LEU LYS LEU PRO ILE GLY LYS ARG ASN TRP LEU LYS ARG SER SER LEU SER GLY LEU ALA ASP GLY VAL GLU ASP LEU LEU LEU ASP ILE SER SER VAL ASP ARG LEU SER PHE ILE ARG
GLN SER SER LYS VAL LYS PHE THR SER ALA VAL LYS LEU SER GLU GLY GLY PRO GLY SER GLY MET GLN GLU GLU ASN GLY ARG ASP GLU GLU GLU GLU ASN PHE PHE PHE LYS ARG LEU GLY CYS HIS SER PHE ASP ASP HIS LEU SER PRO ASN GLN ASP GLY GLY LYS SER LYS ASN V1174 R1181 Q1182



PRO SER GLN SER GLU PRO ASN VAL LEU ASP ASP SER GLN GLY LEU ALA ALA GLU GLY SER LEU SER ARG VAL ALA SER ILE GLN SER GLU PRO GLY GLN GLN GLN ASN LEU LEU VAL GLN GLN PRO LEU GLY ARG LYS ARG GLY LEU ARG GLN LEU ARG ARG PRO LEU LEU SER ARG GLN LYS

THR GLN THR GLU PRO ARG ASN ARG GLN GLY ALA ARG LEU SER THR THR ARG ARG SER ILE GLN PRO LYS THR LYS PRO SER ALA ASP GLN LYS ARG SER VAL THR PHE ILE GLU ALA GLN PRO GLU PRO ALA ALA ALA PRO THR ASP ALA LEU PRO ALA THR GLY GLN LEU GLN LEU GLY CYS

SER PRO ALA PRO SER ARG LYS PRO GLU ALA MET ASP GLU PRO VAL LEU THR SER SER PRO ALA ILE VAL VAL ALA ASP LEU HIS SER VAL SER PRO LYS GLN SER GLU ASN PHE PRO THR GLU GLU GLY GLU LYS GLU GLU ASP THR GLU ALA GLN GLY ALA THR ALA HIS SER PRO LEU

SER ALA GLN LEU SER ASP PRO ASP ASP PHE THR GLY LEU GLU THR SER SER LEU LEU GLN HIS GLY ASP THR VAL LEU HIS ILE SER GLU GLU ASN GLY MET GLU ASN PRO LEU LEU SER SER GLN PHE THR PHE THR PRO THR GLU LEU GLY LYS THR ASP ALA VAL LEU ASP GLU SER

HIS VAL GLY GLY SER GLY GLY SER ASP TYR LYS ASP ASP ASP LYS GLY ASN SER ASP TYR LYS ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; selected micrographs with a CTF fit of 10.0 A or better	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64.009	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	68.237	Depositor
Minimum map value	-6.453	Depositor
Average map value	1.978	Depositor
Map value standard deviation	1.683	Depositor
Recommended contour level	7.9	Depositor
Map size (Å)	469.28, 469.28, 469.28	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1732, 1.1732, 1.1732	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, PGV, TYS, Y01, NAG

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	0.25	0/11612	0.48	0/15717
2	B	0.29	0/1286	0.47	0/1740
3	C	0.26	0/932	0.53	0/1240
4	D	0.24	0/10967	0.45	0/14850
5	E	0.25	0/13267	0.47	0/17989
All	All	0.25	0/38064	0.47	0/51536

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

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	11344	0	11588	65	0
2	B	1256	0	1150	6	0
3	C	926	0	892	12	0
4	D	11107	0	11071	71	0
5	E	12977	0	13225	83	0
6	A	28	0	26	0	0
7	A	142	0	176	6	0
8	A	74	0	96	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	105	0	147	1	0
All	All	37959	0	38371	237	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 237 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:717:ARG:NH1	4:D:970:ASP:OD1	2.21	0.73
1:A:998:LYS:O	1:A:1004:ARG:NH1	2.23	0.72
5:E:2394:ALA:O	5:E:2398:ILE:HD12	1.92	0.68
1:A:85:GLU:OE2	1:A:152:ARG:NH2	2.26	0.68
5:E:2486:ARG:NE	5:E:2551:ASP:OD2	2.26	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	1369/2042 (67%)	1327 (97%)	42 (3%)	0	100	100
2	B	145/483 (30%)	137 (94%)	8 (6%)	0	100	100
3	C	102/149 (68%)	97 (95%)	5 (5%)	0	100	100
4	D	1292/2561 (50%)	1262 (98%)	30 (2%)	0	100	100
5	E	1559/3283 (48%)	1520 (98%)	39 (2%)	0	100	100
All	All	4467/8518 (52%)	4343 (97%)	124 (3%)	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	1251/1822 (69%)	1251 (100%)	0	100	100
2	B	144/417 (34%)	144 (100%)	0	100	100
3	C	102/127 (80%)	102 (100%)	0	100	100
4	D	1211/2219 (55%)	1211 (100%)	0	100	100
5	E	1442/2873 (50%)	1442 (100%)	0	100	100
All	All	4150/7458 (56%)	4150 (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. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TYS	A	287	1	15,16,17	1.61	3 (20%)	15,22,24	0.67	0

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
1	TYS	A	287	1	-	5/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	TYS	O1-S	4.29	1.63	1.45
1	A	287	TYS	OH-CZ	-3.17	1.37	1.42
1	A	287	TYS	OH-S	-2.36	1.53	1.58

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	287	TYS	CE2-CZ-OH-S
1	A	287	TYS	CA-CB-CG-CD2
1	A	287	TYS	CA-CB-CG-CD1
1	A	287	TYS	CE1-CZ-OH-S
1	A	287	TYS	CZ-OH-S-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	2102	1	14,14,15	0.19	0	17,19,21	0.43	0
9	Y01	A	2109	-	38,38,38	1.39	5 (13%)	57,57,57	1.98	9 (15%)
9	Y01	A	2110	-	38,38,38	1.24	4 (10%)	57,57,57	1.98	10 (17%)
9	Y01	A	2111	-	38,38,38	1.25	4 (10%)	57,57,57	1.97	11 (19%)
6	NAG	A	2101	-	14,14,15	0.21	0	17,19,21	0.42	0
7	PEV	A	2104	-	39,39,48	1.19	3 (7%)	42,44,53	1.11	2 (4%)
7	PEV	A	2105	-	33,33,48	1.24	3 (9%)	36,38,53	1.15	2 (5%)
8	PGV	A	2108	-	42,42,50	1.03	5 (11%)	45,47,56	1.14	2 (4%)
7	PEV	A	2106	-	30,30,48	1.29	3 (10%)	33,35,53	1.19	2 (6%)
7	PEV	A	2103	-	36,36,48	1.21	3 (8%)	39,41,53	1.08	2 (5%)
8	PGV	A	2107	-	30,30,50	1.11	2 (6%)	32,35,56	1.11	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	2102	1	-	0/6/23/26	0/1/1/1
9	Y01	A	2109	-	-	9/19/77/77	0/4/4/4
9	Y01	A	2110	-	-	9/19/77/77	0/4/4/4
9	Y01	A	2111	-	-	8/19/77/77	0/4/4/4
6	NAG	A	2101	-	-	2/6/23/26	0/1/1/1
7	PEV	A	2104	-	-	19/43/43/52	-
7	PEV	A	2105	-	-	15/37/37/52	-
8	PGV	A	2108	-	-	19/44/44/55	-
7	PEV	A	2106	-	-	15/34/34/52	-
7	PEV	A	2103	-	-	20/40/40/52	-
8	PGV	A	2107	-	-	13/33/33/55	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2109	Y01	CAK-CAI	-4.50	1.41	1.50
9	A	2110	Y01	CAK-CAI	-4.44	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2111	Y01	CAK-CAI	-4.40	1.41	1.50
8	A	2107	PGV	O01-C02	-3.93	1.40	1.47
7	A	2105	PEV	O3-C11	3.20	1.42	1.33

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2110	Y01	CAV-CAZ-CBH	7.92	126.56	116.42
9	A	2109	Y01	CAV-CAZ-CBH	7.77	126.37	116.42
9	A	2111	Y01	CAV-CAZ-CBH	7.59	126.14	116.42
9	A	2111	Y01	OAW-CAY-OAG	-5.30	111.32	123.70
9	A	2109	Y01	CAV-CAZ-CAI	-5.27	113.43	120.57

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2103	PEV	C4-O4P-P-O3P
7	A	2103	PEV	C4-O4P-P-O1P
7	A	2103	PEV	C4-O4P-P-O2P
7	A	2103	PEV	C5-C4-O4P-P
7	A	2103	PEV	O4P-C4-C5-N6

There are no ring outliers.

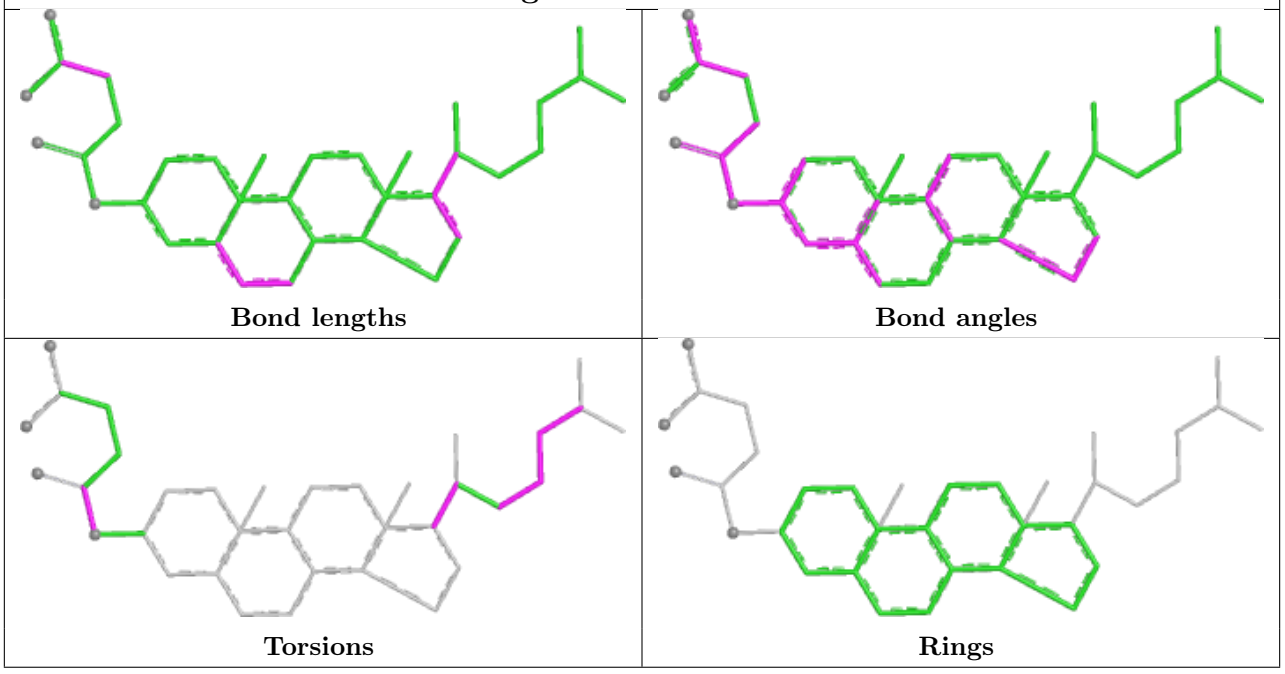
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2111	Y01	1	0
7	A	2105	PEV	2	0
7	A	2106	PEV	2	0
7	A	2103	PEV	2	0

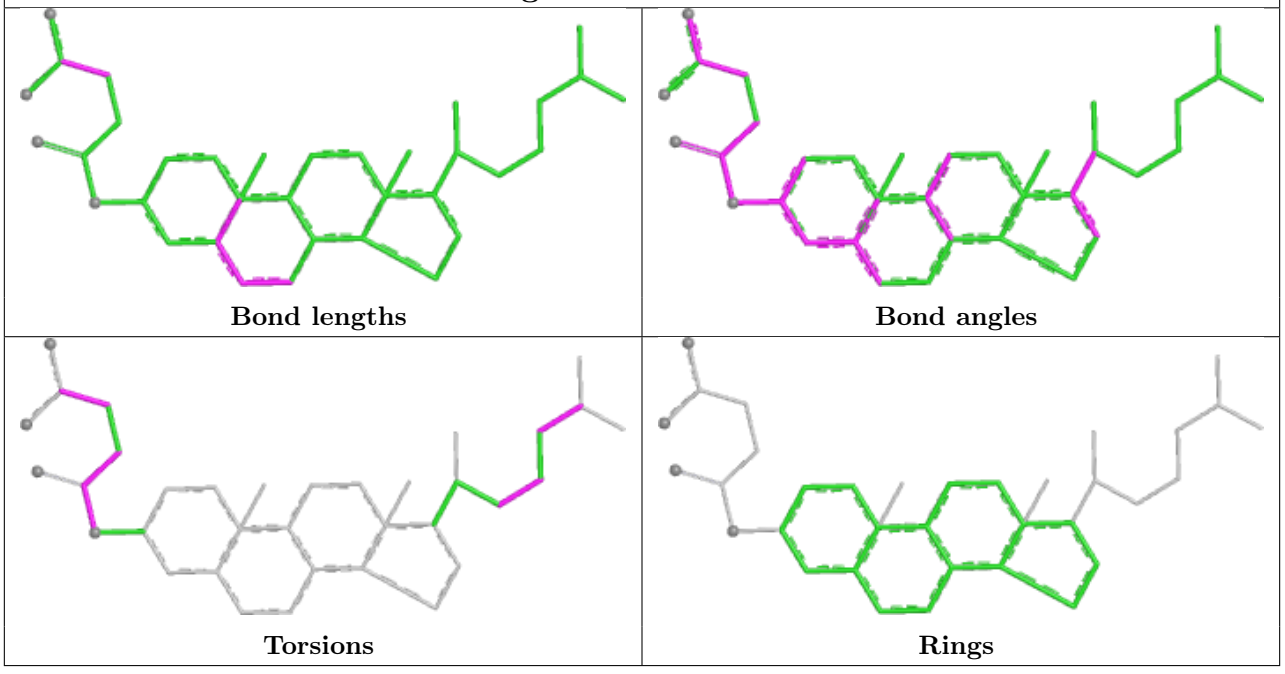
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

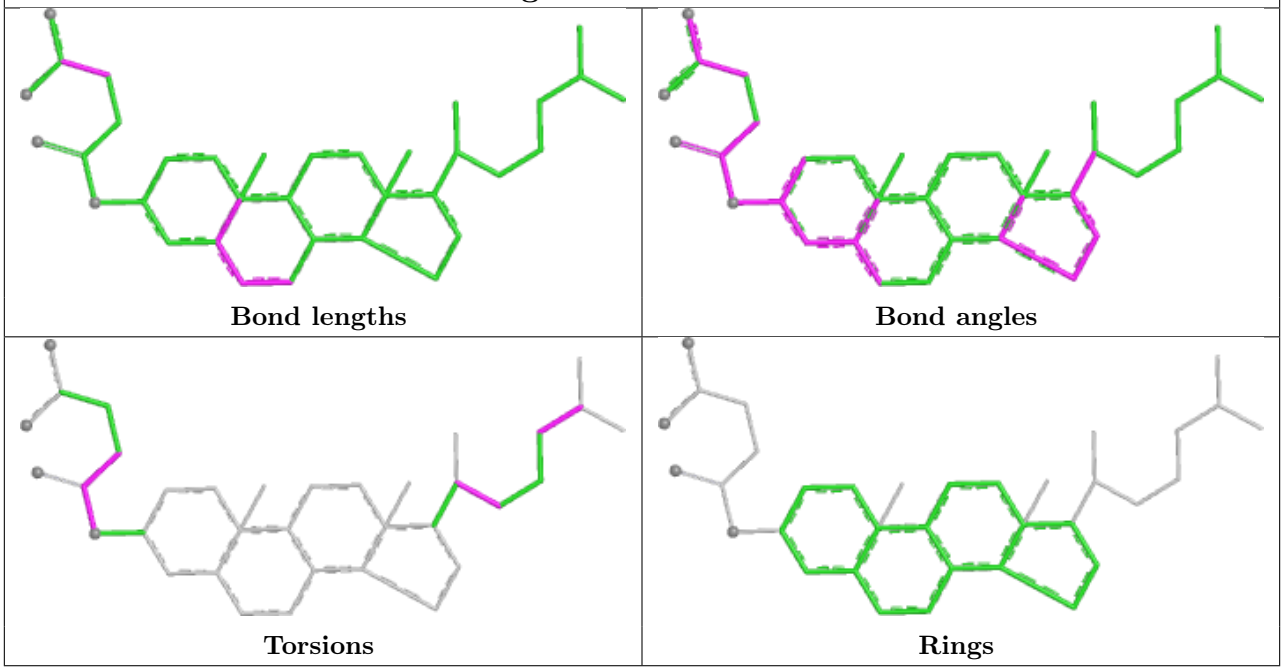
Ligand Y01 A 2109



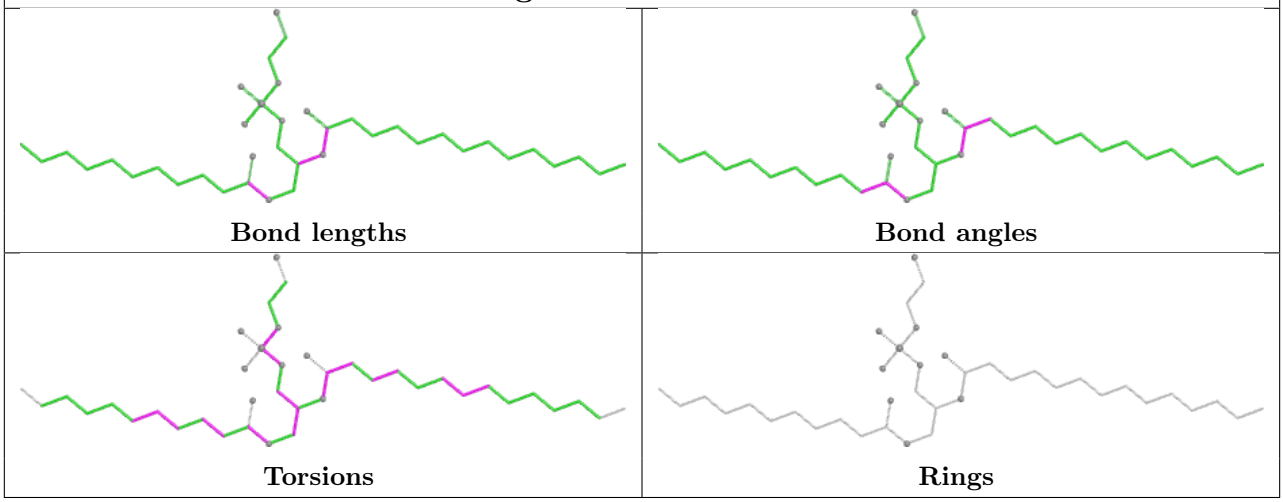
Ligand Y01 A 2110



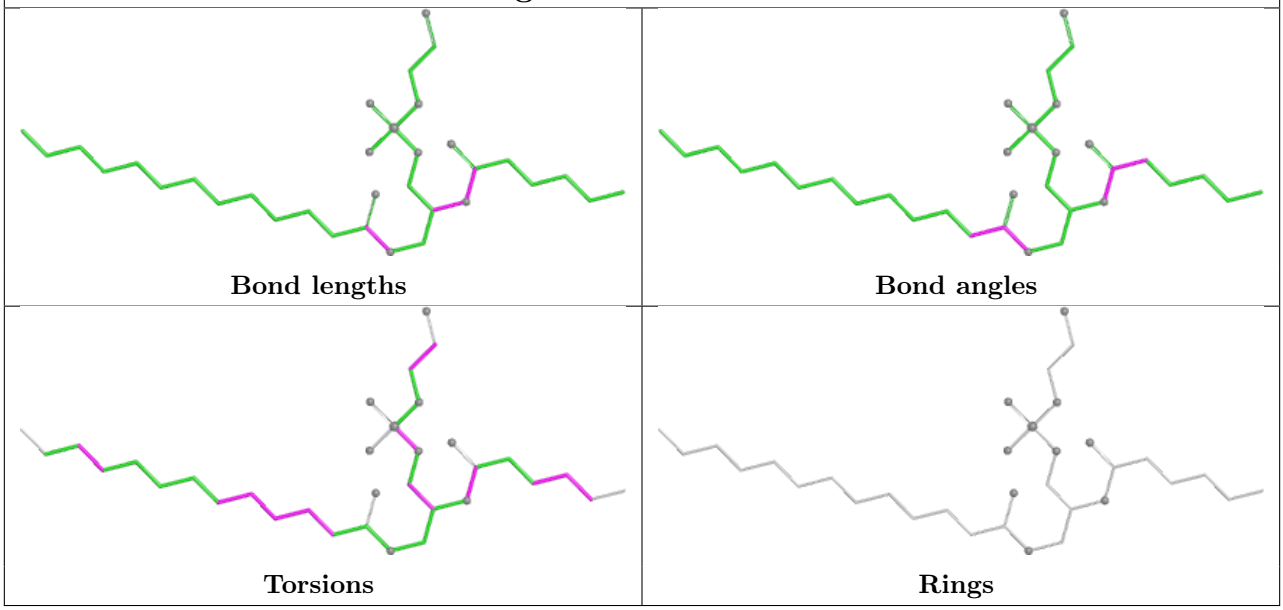
Ligand Y01 A 2111



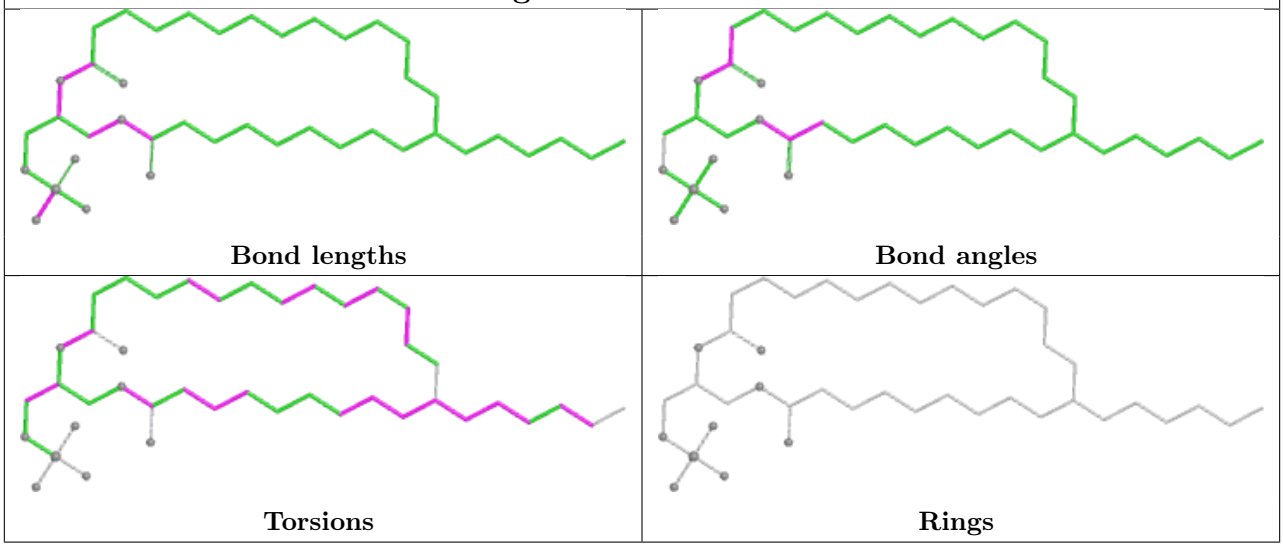
Ligand PEV A 2104



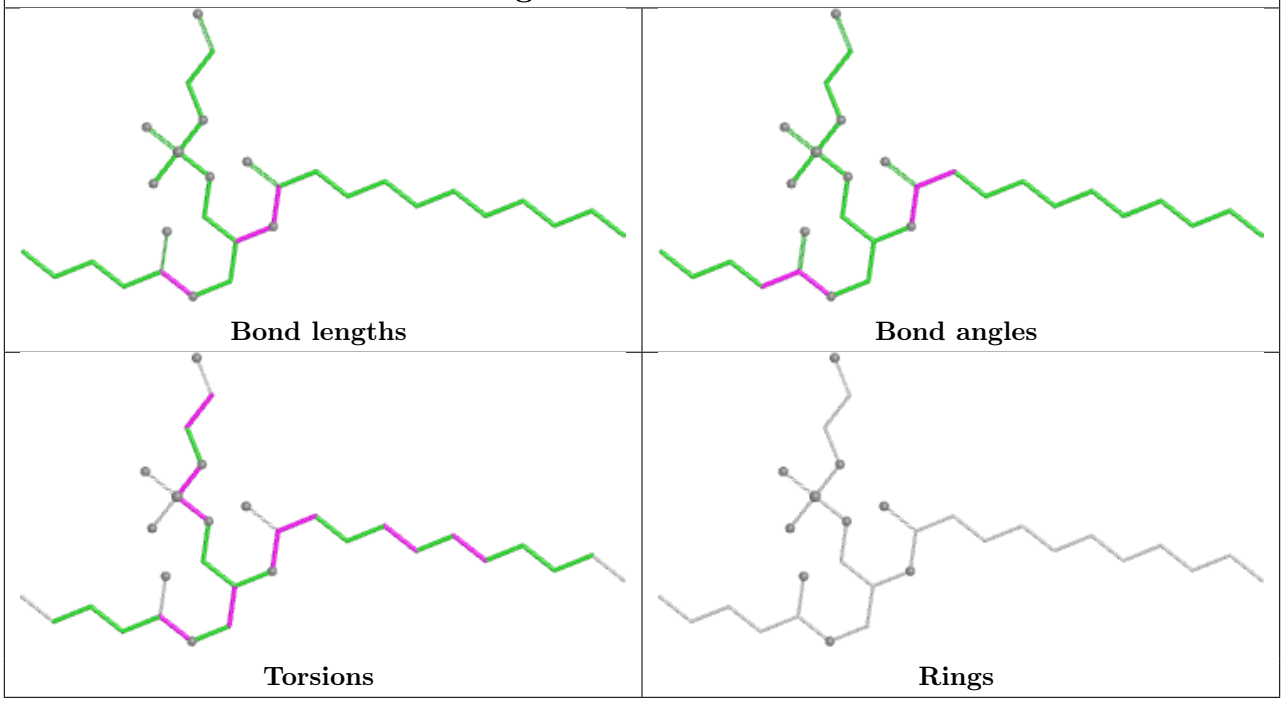
Ligand PEV A 2105



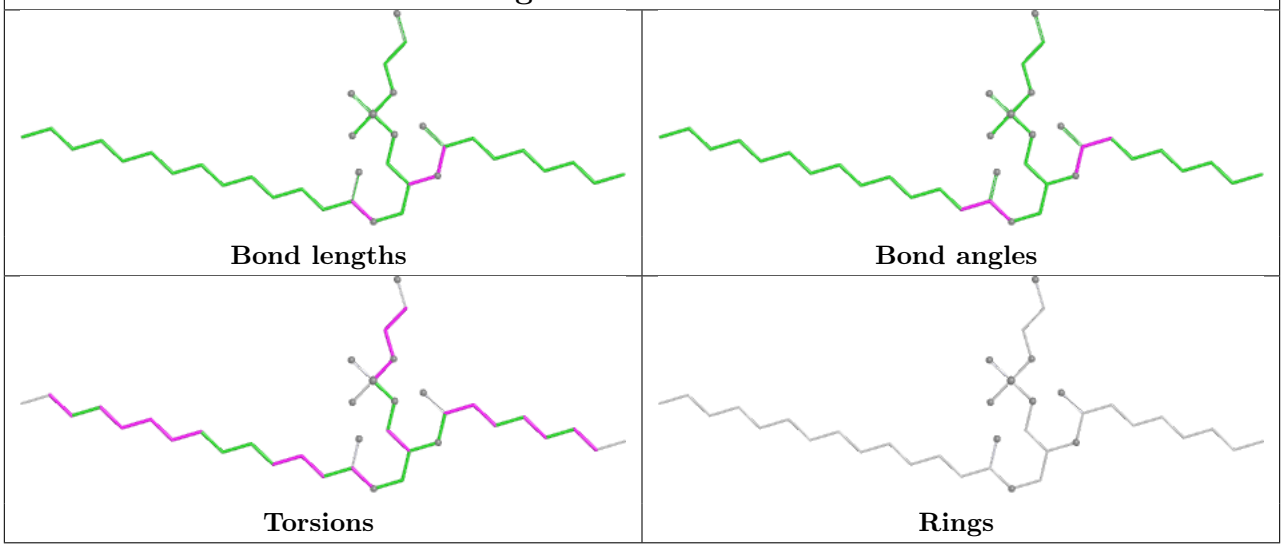
Ligand PGV A 2108



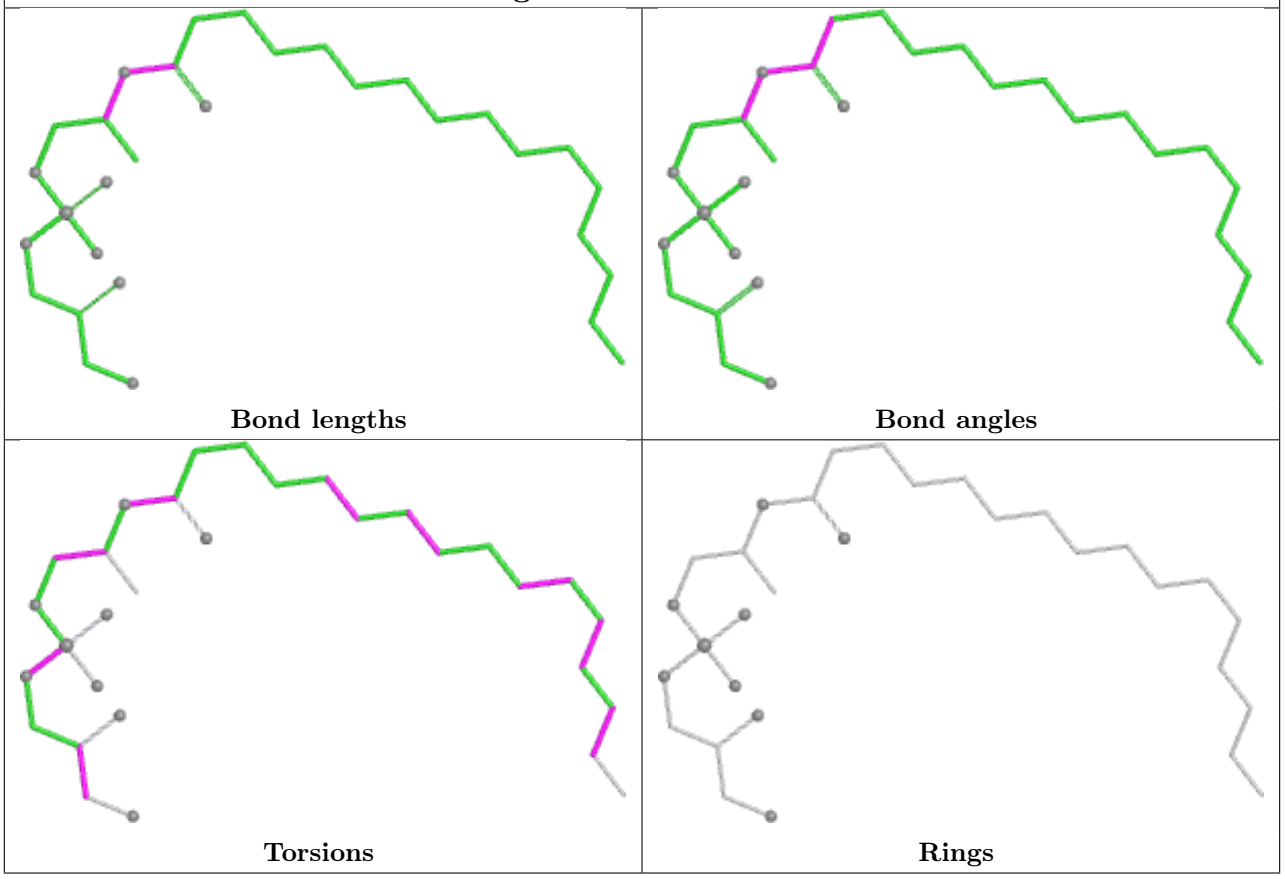
Ligand PEV A 2106



Ligand PEV A 2103



Ligand PGV A 2107



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	105:UNK	C	127:UNK	N	15.40
1	D	165:UNK	C	174:LEU	N	12.02
1	D	55:UNK	C	85:UNK	N	9.92
1	D	142:UNK	C	147:UNK	N	8.53

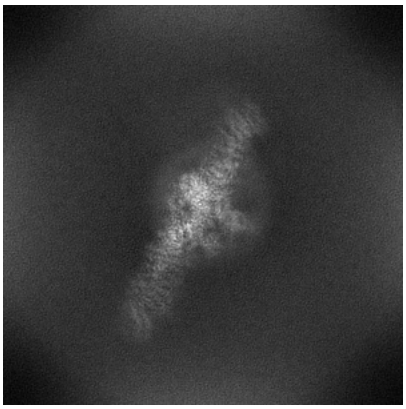
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25492. These allow visual inspection of the internal detail of the map and identification of artifacts.

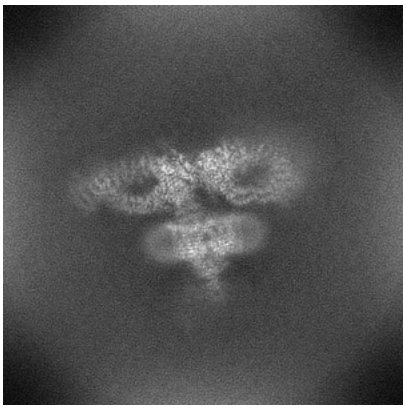
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

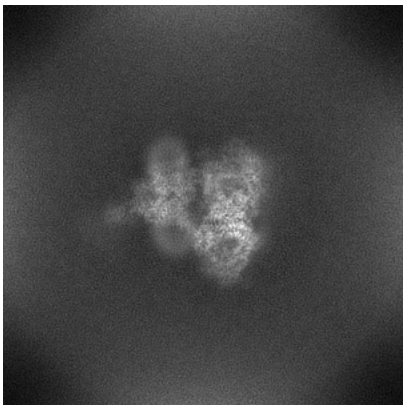
6.1.1 Primary map



X

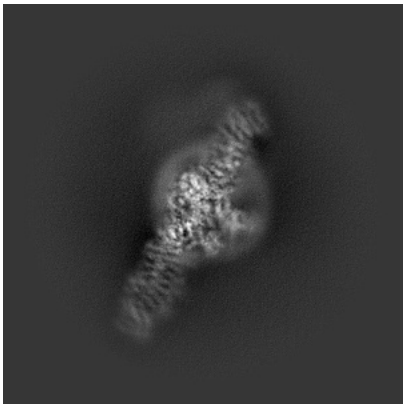


Y

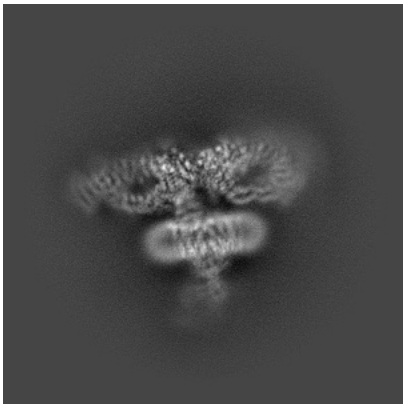


Z

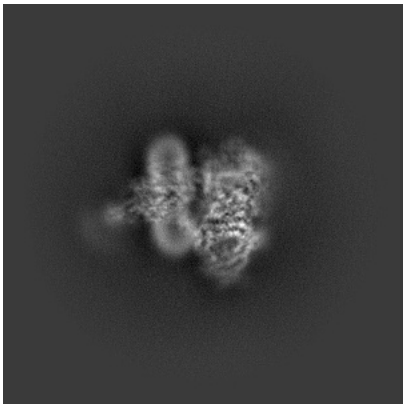
6.1.2 Raw map



X



Y

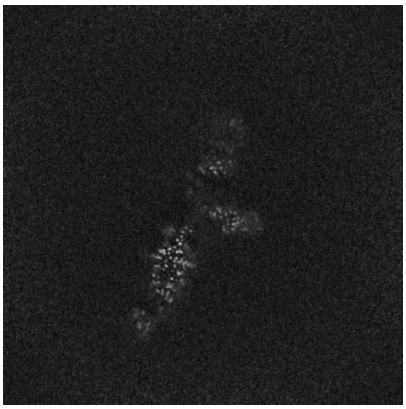


Z

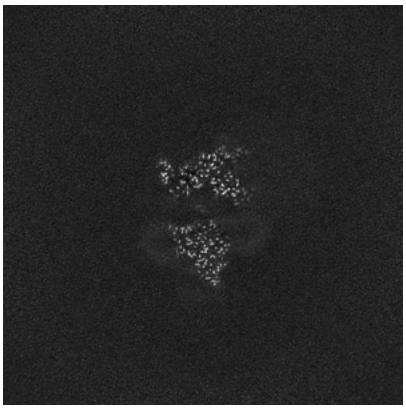
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

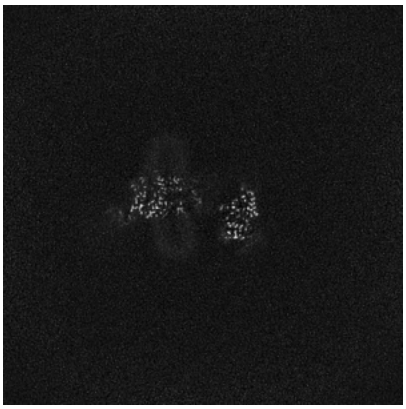
6.2.1 Primary map



X Index: 200

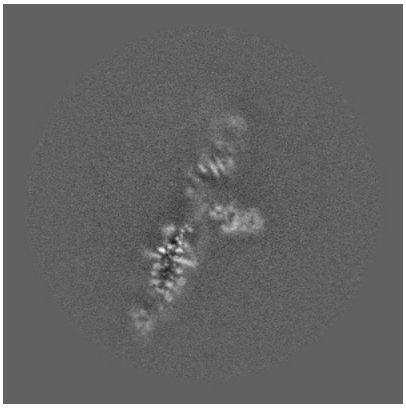


Y Index: 200

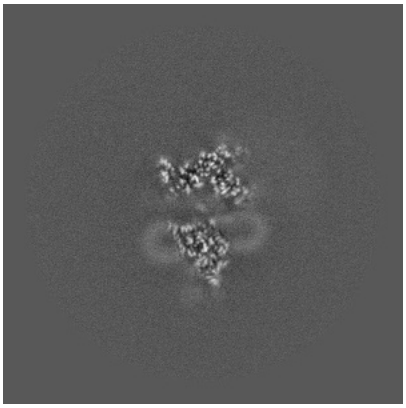


Z Index: 200

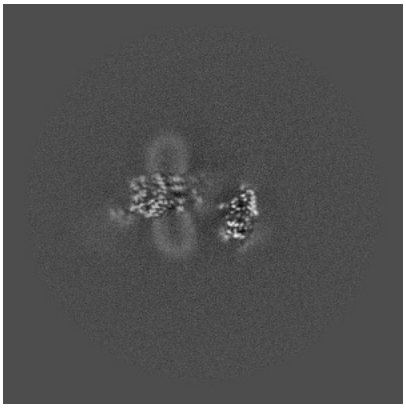
6.2.2 Raw map



X Index: 200



Y Index: 200

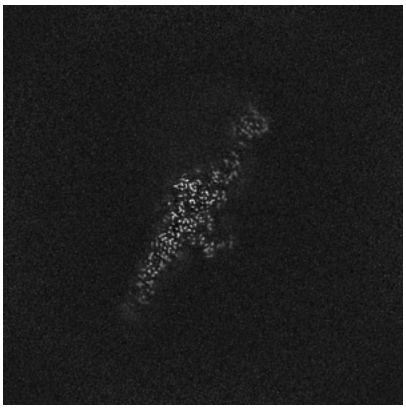


Z Index: 200

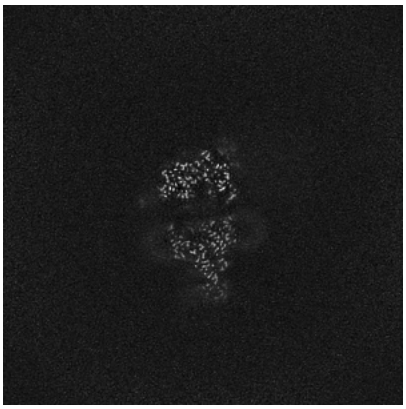
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

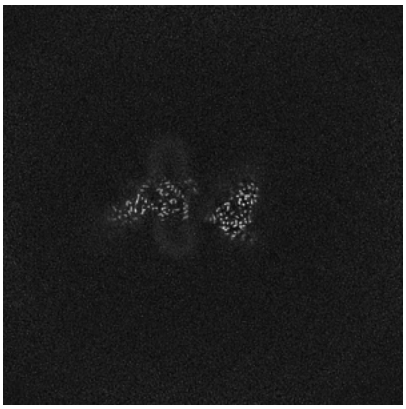
6.3.1 Primary map



X Index: 238

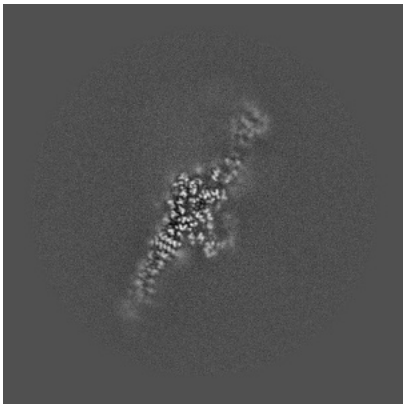


Y Index: 192

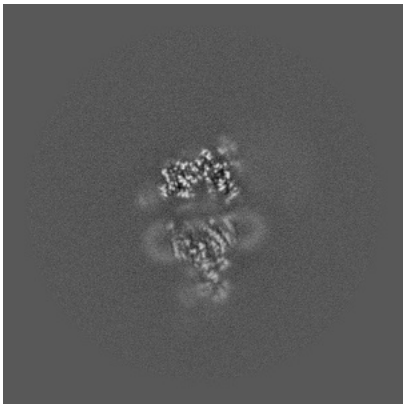


Z Index: 209

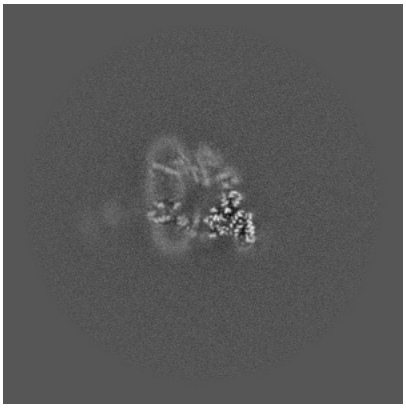
6.3.2 Raw map



X Index: 237



Y Index: 192

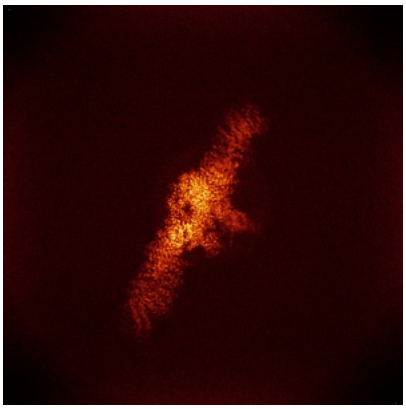


Z Index: 178

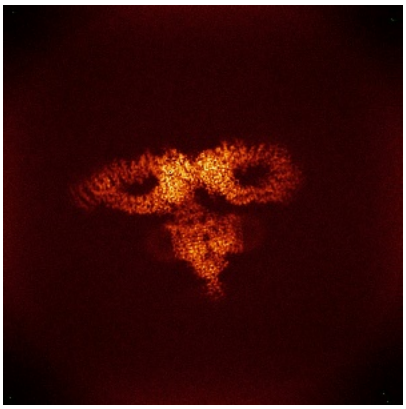
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

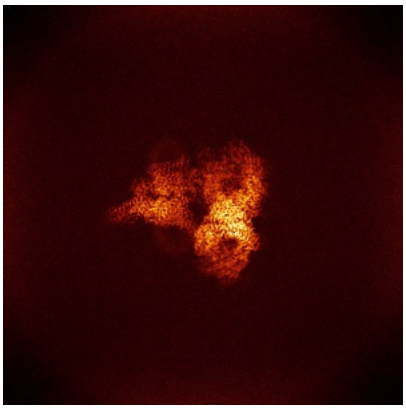
6.4.1 Primary map



X

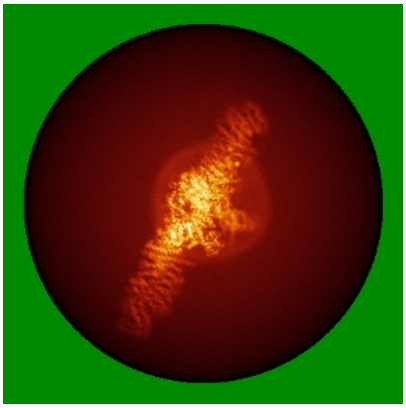


Y

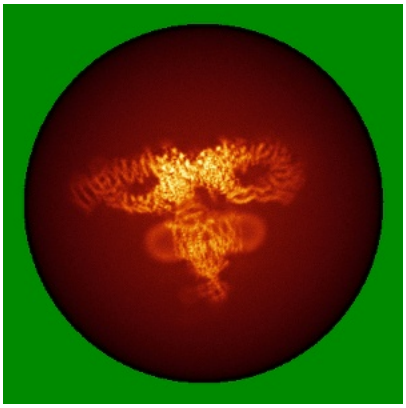


Z

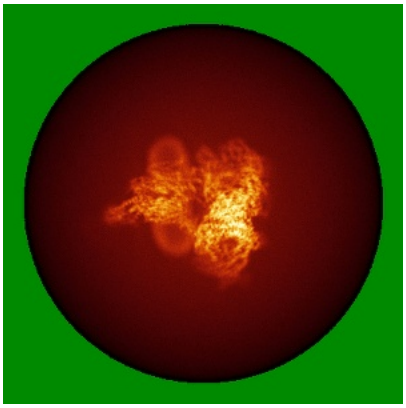
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.9. 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

X Y Z

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.

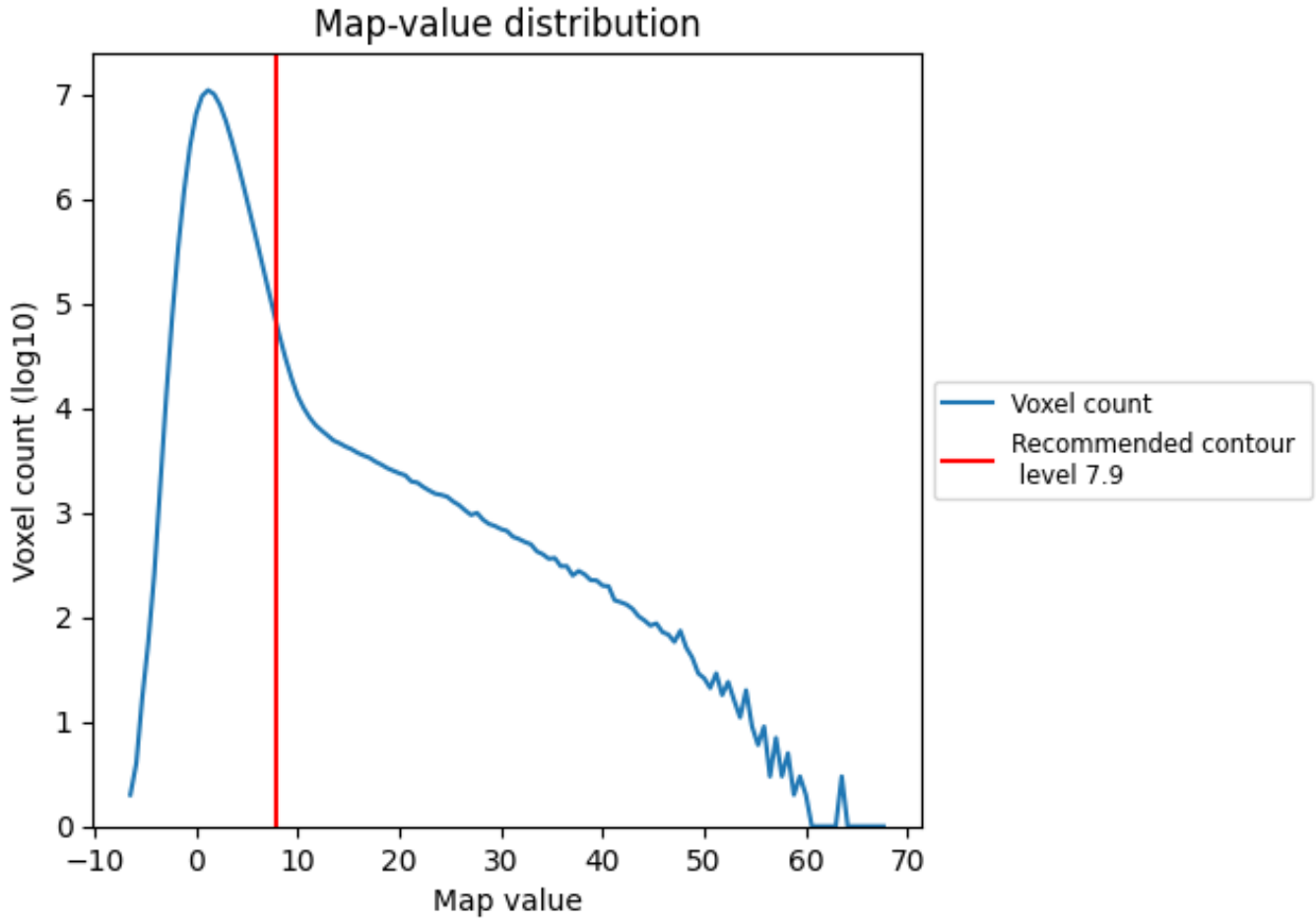
6.6 Mask visualisation (i)

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

7 Map analysis

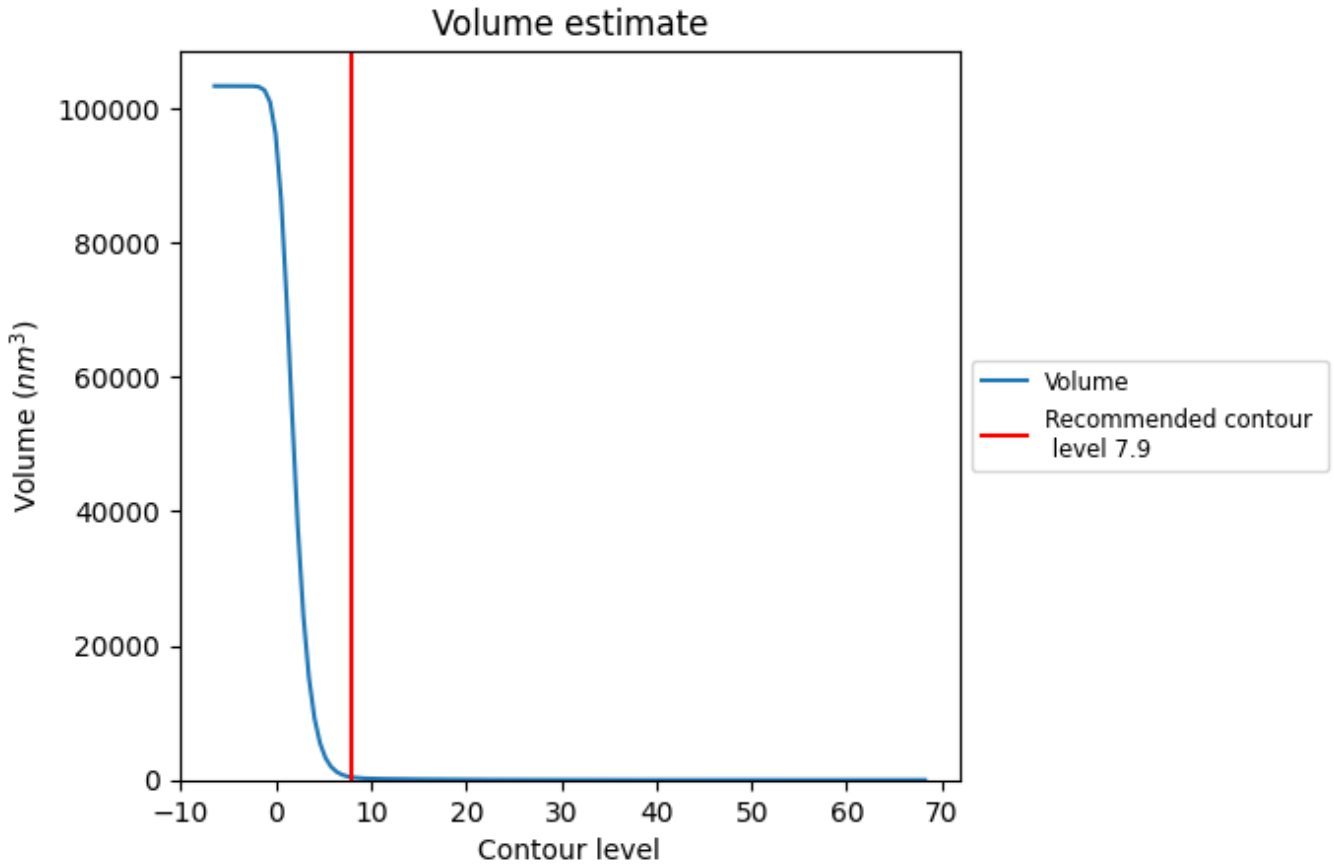
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

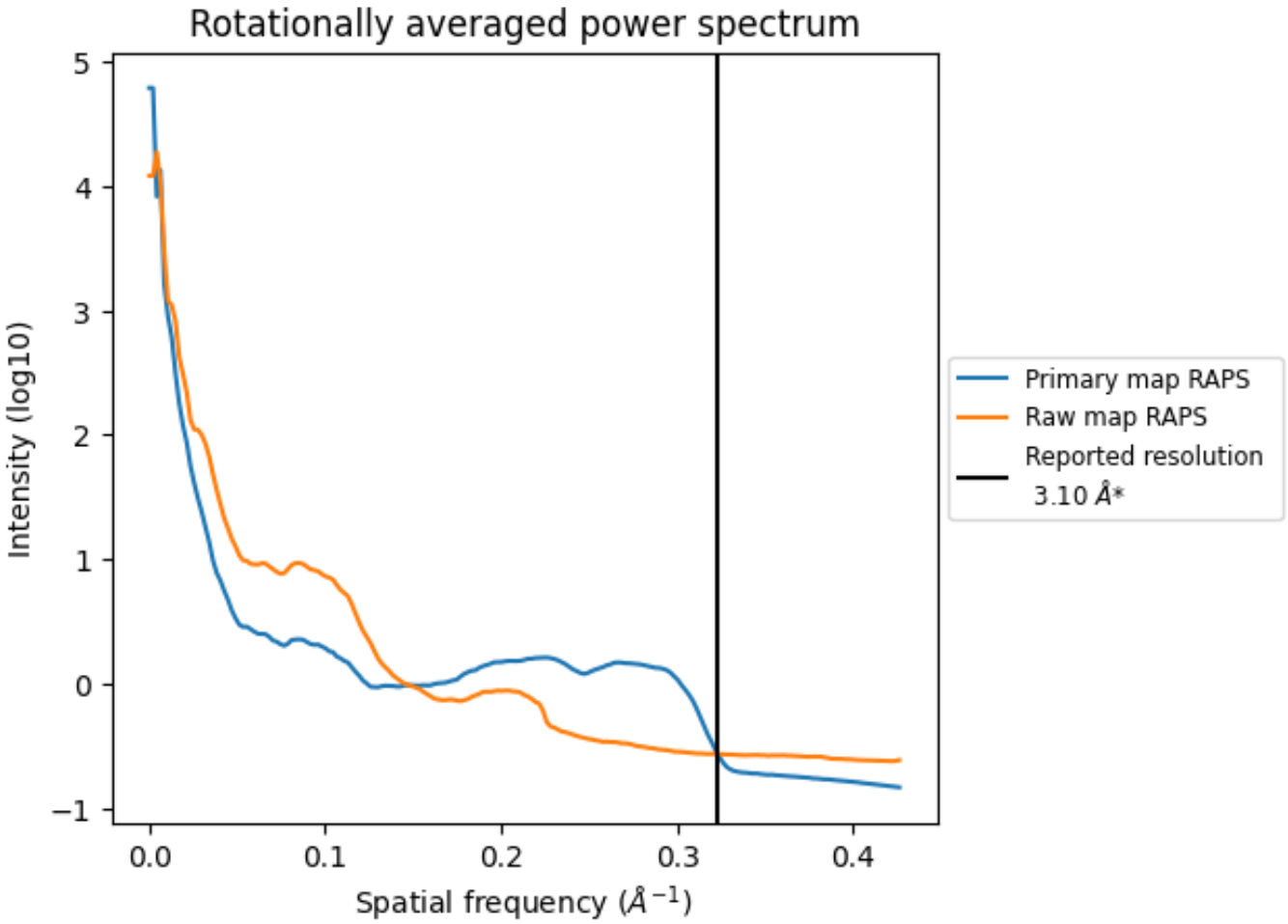
7.2 Volume estimate (i)



The volume at the recommended contour level is 430 nm^3; this corresponds to an approximate mass of 389 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

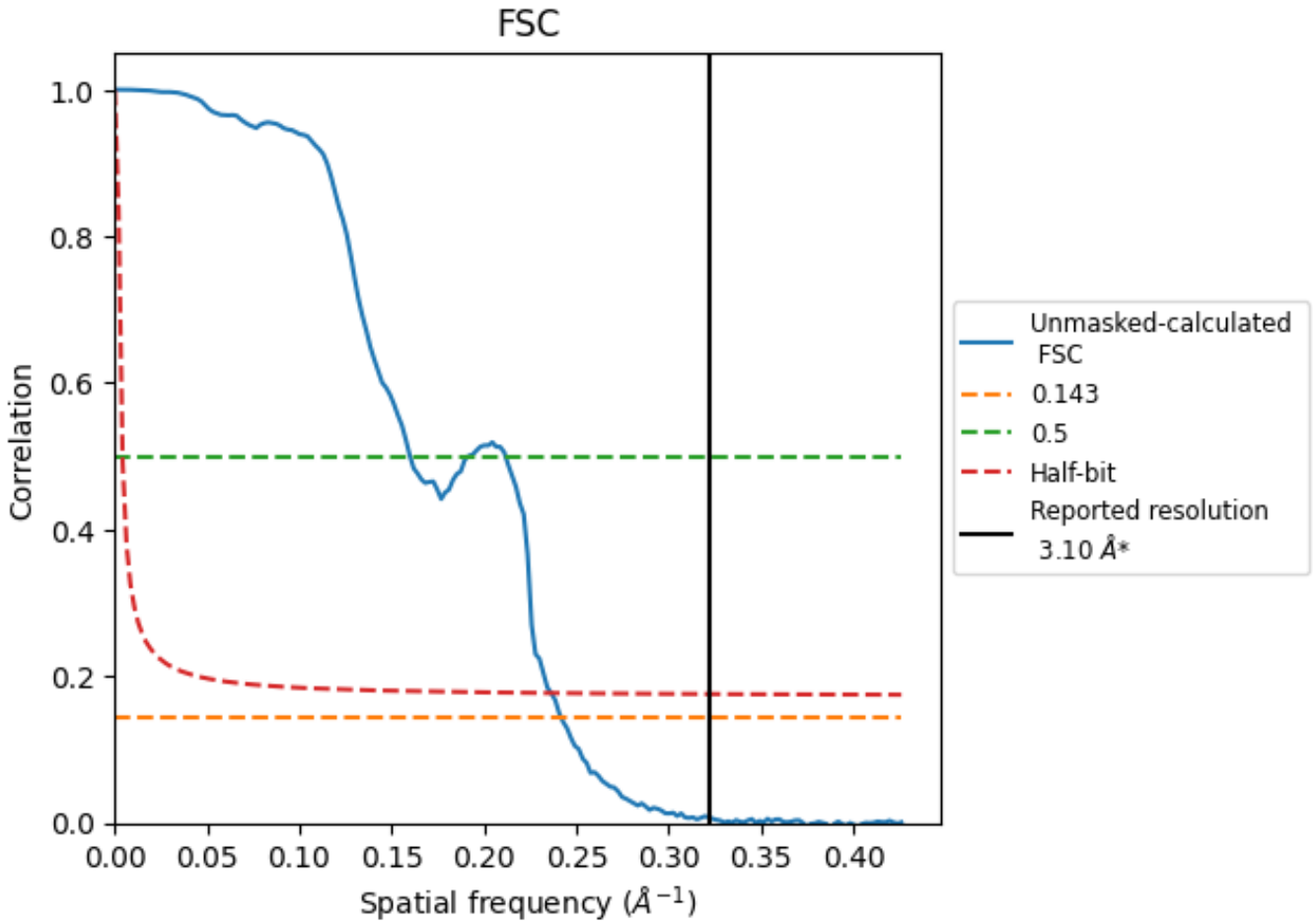


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

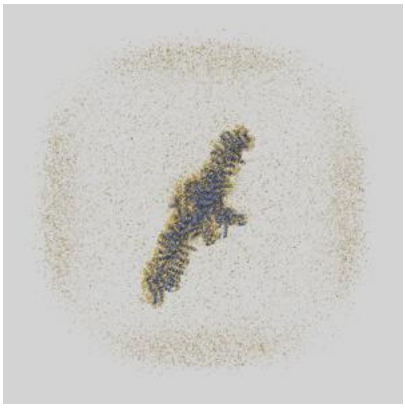
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	6.25	4.23

*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 4.13 differs from the reported value 3.1 by more than 10 %

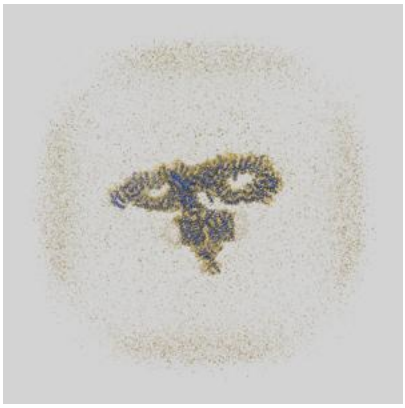
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25492 and PDB model 7SX3. Per-residue inclusion information can be found in section 3 on page 11.

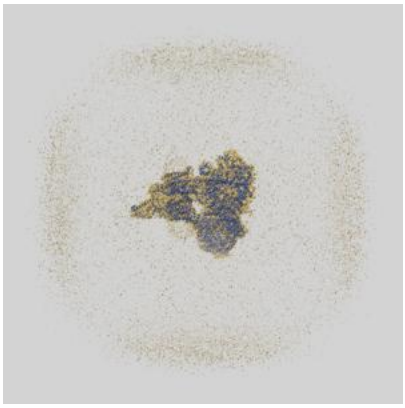
9.1 Map-model overlay



X



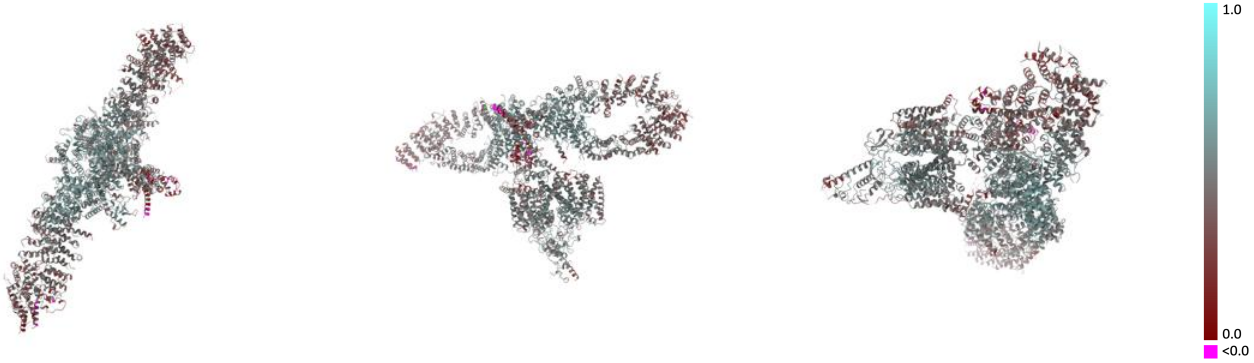
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.9 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.

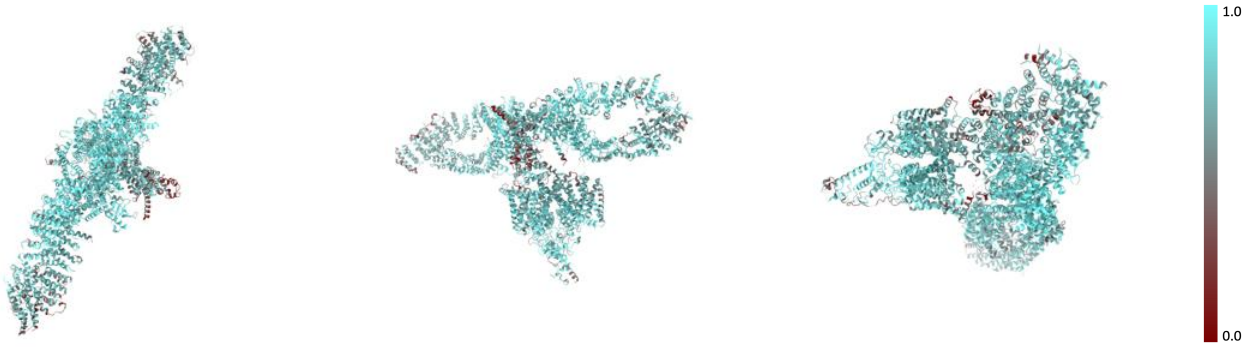
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

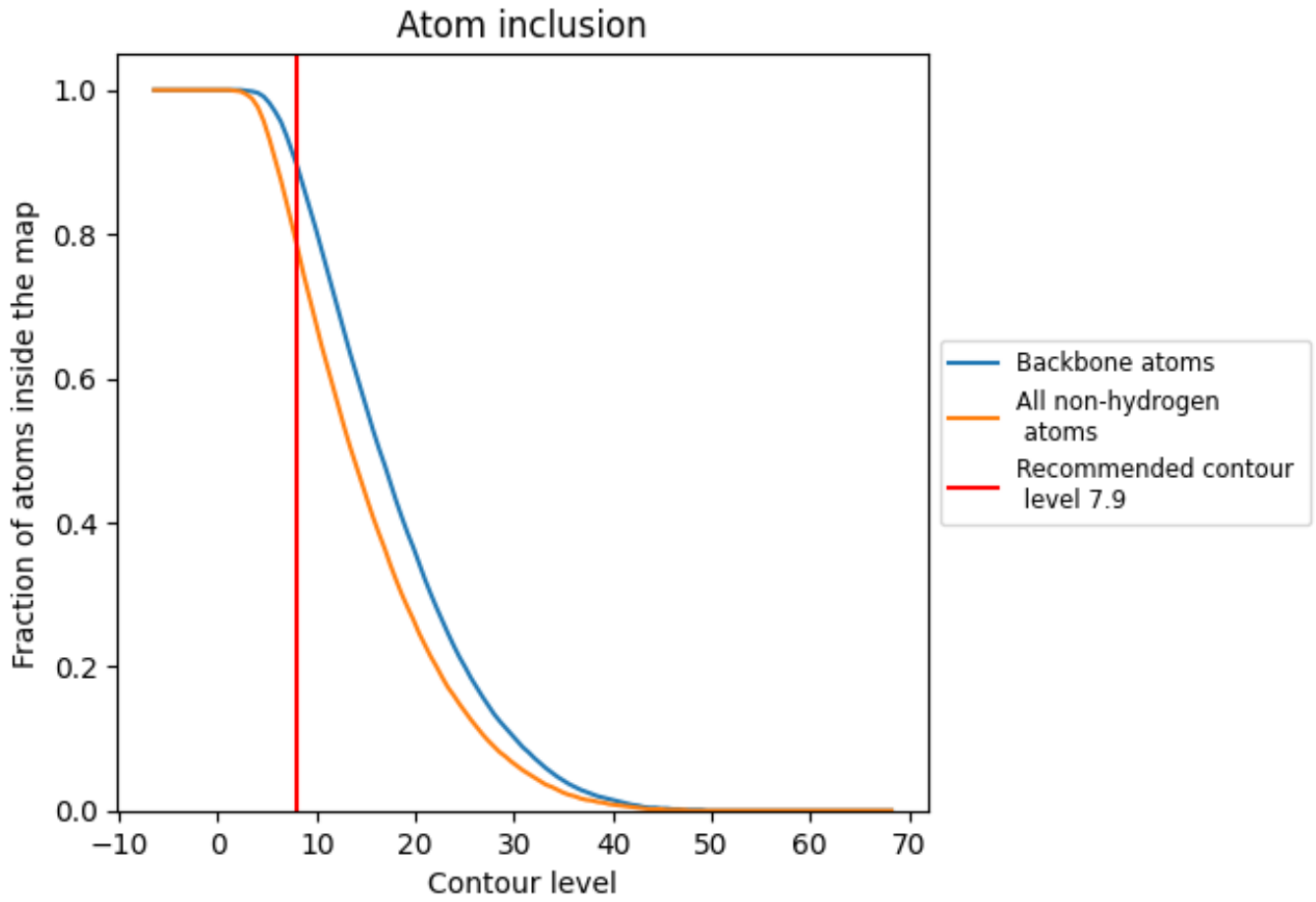
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (7.9).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (7.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.4700
A	0.7700	0.4810
B	0.7460	0.4640
C	0.3450	0.2430
D	0.8100	0.4700
E	0.8250	0.4770