



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:37 PM UTC

PDB ID : 7SX3 / pdb_00007sx3
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 Full wwPDB EM Validation 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

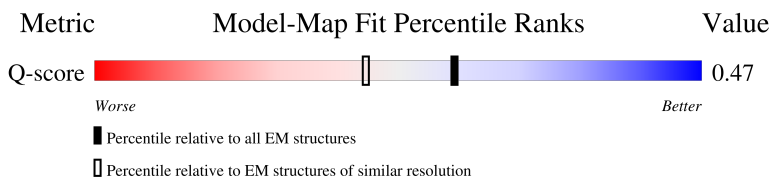
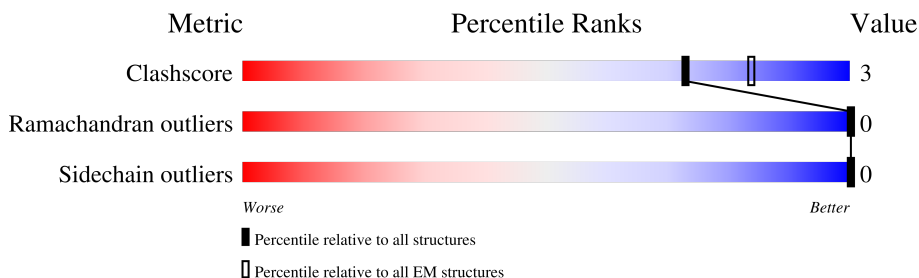
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	2042	
2	B	483	
3	C	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	2561	51% 5% 45%
5	E	3283	45% 51%

2 Entry composition

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	
			1256	801	193	246	16	
							0	0

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:

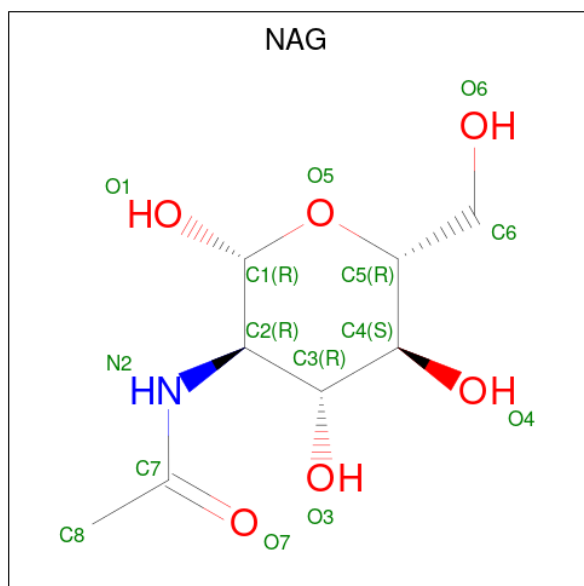
Chain	Residue	Modelled	Actual	Comment	Reference
E	3259	GLY	-	expression tag	UNP Q8N2C7
E	3260	GLY	-	expression tag	UNP Q8N2C7
E	3261	SER	-	expression tag	UNP Q8N2C7
E	3262	GLY	-	expression tag	UNP Q8N2C7
E	3263	GLY	-	expression tag	UNP Q8N2C7
E	3264	SER	-	expression tag	UNP Q8N2C7
E	3265	ASP	-	expression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

Continued on next page...

Continued from previous page...

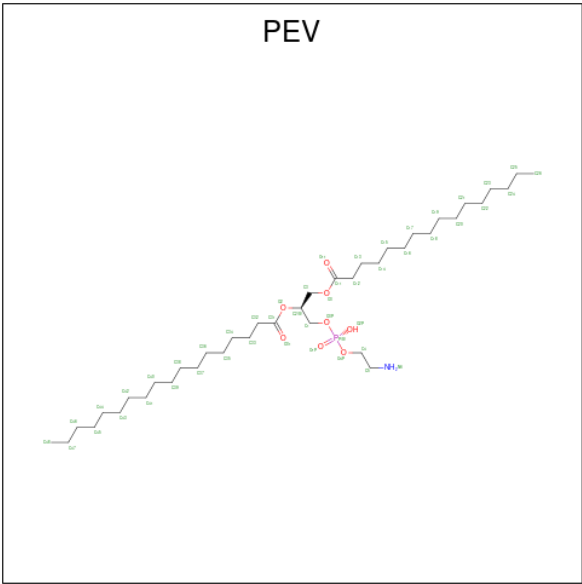
Chain	Residue	Modelled	Actual	Comment	Reference
E	3267	LYS	-	expression tag	UNP Q8N2C7
E	3268	ASP	-	expression tag	UNP Q8N2C7
E	3269	ASP	-	expression tag	UNP Q8N2C7
E	3270	ASP	-	expression tag	UNP Q8N2C7
E	3271	ASP	-	expression tag	UNP Q8N2C7
E	3272	LYS	-	expression tag	UNP Q8N2C7
E	3273	GLY	-	expression 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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



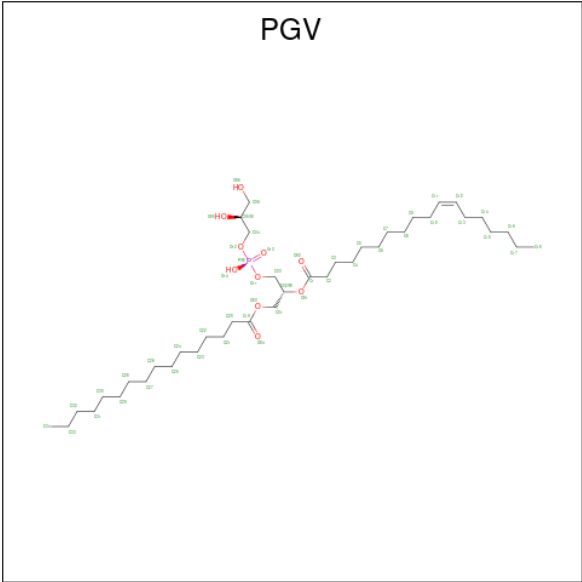
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is (1S)-2-{{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PEV) (formula: C₃₉H₇₈NO₈P).



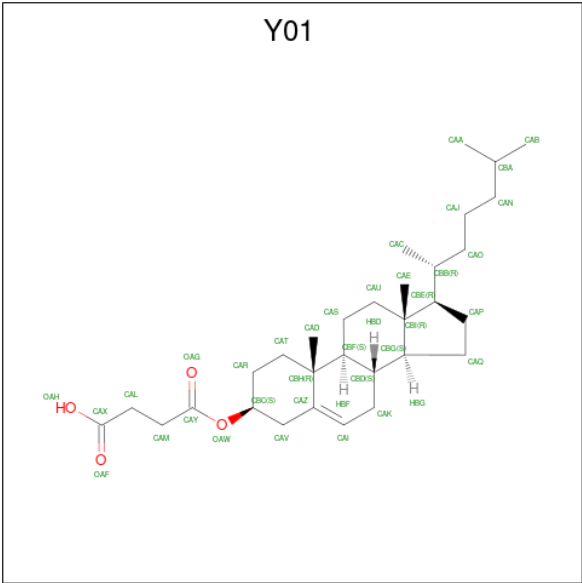
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
7	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
7	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	A	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 8 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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 (CCD ID: Y01) (formula: C₃₁H₅₀O₄).



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		

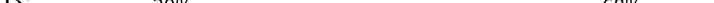
Continued on next page...

Continued from previous page...

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

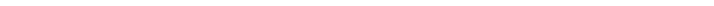
ASP	GLU	GLY	PHE	PRO	PHE	PRO	PHE	PRO	GLU	THR	THR	PRO
GLU	GLY	VAL	GLY	VAL	GLU	VAL	GLY	VAL	GLN	THR	GLY	GLU
LEU	VAL	GLN	ASP	TRP	TRP	TRP	GLY	SER	SER	LYS	MET	THR
TYR	LYS	LEU	THR	PRO	THR	THR	THR	SER	SER	GLY	VAL	SER
SER	GLY	ALA	LEU	THR	LEU	THR	GLY	GLY	GLY	VAL	VAL	GLN
GLY	GLY	ASP	VAL	LEU	VAL	LEU	MET	VAL	VAL	CYS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

- Molecule 2: Transmembrane protein FAM155A

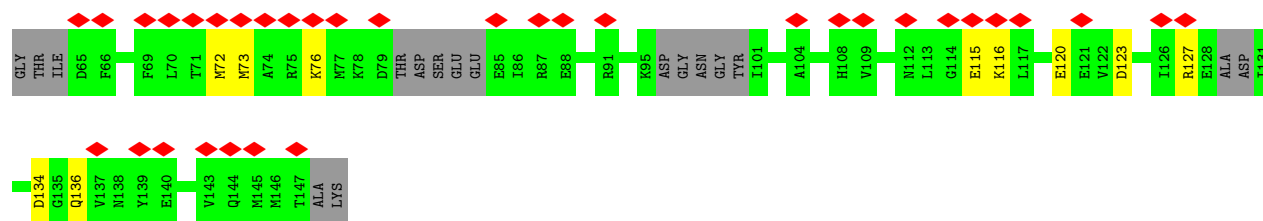
Chain B:  29% 68%

TYR	VAL	T259	C181	GLU	MET
LYS	SER	T260	E185	ALA	THR
ASP	SER	R261	N186	LEU	ARG
ASP	ALA	R262	A187	LEU	GLY
ASP	THR		D188	THR	ALA
ASP	ARG			ARG	TRP
LYS	LEU	V265		SER	ALA
GLY	CYS	E266		SER	MET
ASN	ASN		C191	ASP	CYS
SER	SER		ALA	THR	ARG
ASP	ARG	F322	ARG	LEU	GLN
TYR	LEU	N323	ASN	GLU	TYR
LYS	LYS	C324	TRP	HIS	ASP
ASP	LEU	R325	SER	GLN	ASP
ASP	CYS	K326	ARG	PRO	LEU
ASP	VAL		GLY	GLN	GLY
ASP	LEU		ALA	ASP	LYS
LYS	VAL	Y333	ALA	GLY	ILE
	LEU		GLY	GLN	TRP
	ILE	Q338	GLY	GLN	LEU
	LEU	D347	ASP	GLN	ALA
	LEU	N348	GLY	GLN	ALA
	HIS	D349	GLN	GLN	PRO
	THR	E350	GLU	LYS	ARG
	VAL		VAL	GLN	GLU
	LEU		ARG	GLN	ASN
	THR	Y365	SER	ASN	GLU
	ALA	E366	LYS	ARG	GLY
	SER	T367	HIS	GLN	LYS
	ALA	F368	PRO	ASP	PHE
	ALA	L369	THR	GLN	ILE
	GLN		PRO	ASP	ASP
	ASN	THR	LEU	GLN	SER
	THR	ASN	TRP	GLY	GLU
	ALA	E373	N217	LYS	ARG
	GLY		D220	ALA	ALA
	LEU			LEU	GLN
	SER	V379	E233	ARG	LYS
	PHE	R380	L238	LEU	TRP
	GLY	ARG	SER	GLY	LEU
	GLY	GLU	ASN	ASN	SER
	ILE	GLU	ALA	ALA	LEU
	ASN	LYS	SER	LYS	ALA
	THR	SER	PRO	PRO	SER
	LEU	ASN	ASN	VAL	LEU
	GLU	ASN	THR	TRP	LEU
	GLU	PRO	LEU	ARG	PHE
	ASN	SER	ASN	LEU	THR
	SER	LYS	CYS	GLU	VAL
	THR	GLY	SER	THR	LEU
	ASN	THR	LEU	CYS	THR
	GLU	VAL	ASP	TYR	LEU
	GLU	GLU	VAL	PRO	SER
	GLY	LYS	VAL	GLN	ASP
	GLY	SER	LEU	GLY	HIS
	SER	GLY	LYS	ALA	LEU
	GLY	SER	GLU	SER	THR
	GLY	CYS	GLY	SER	PHE
	SER	HIS	GLY	GLN	CYS
	ASP	ARG	GLU	GLN	ALA
		THR		HIS	ALA
		SER		LEU	

- Molecule 3: Calmodulin-1

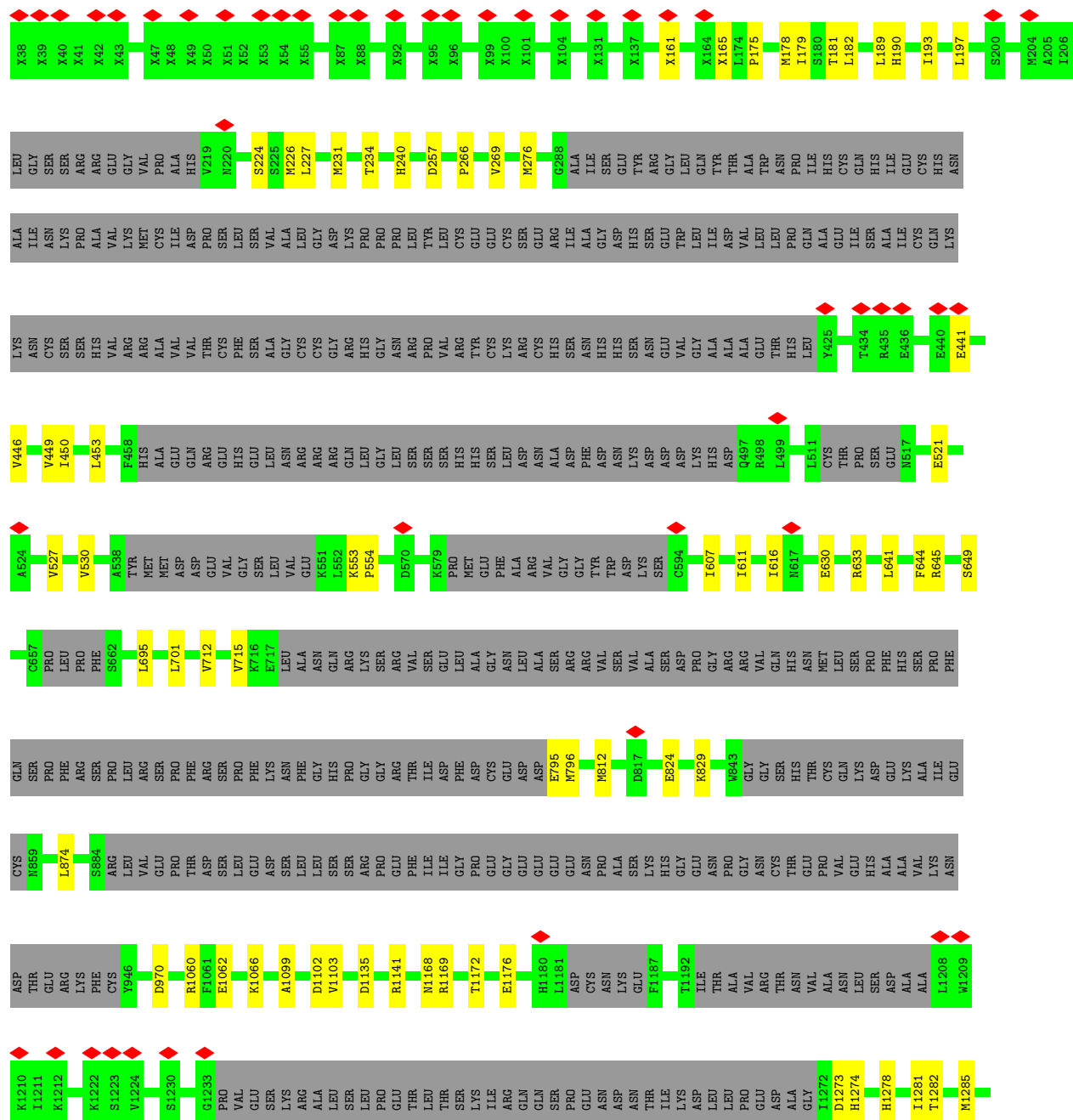
Chain C:  46% 66% 10% 23%

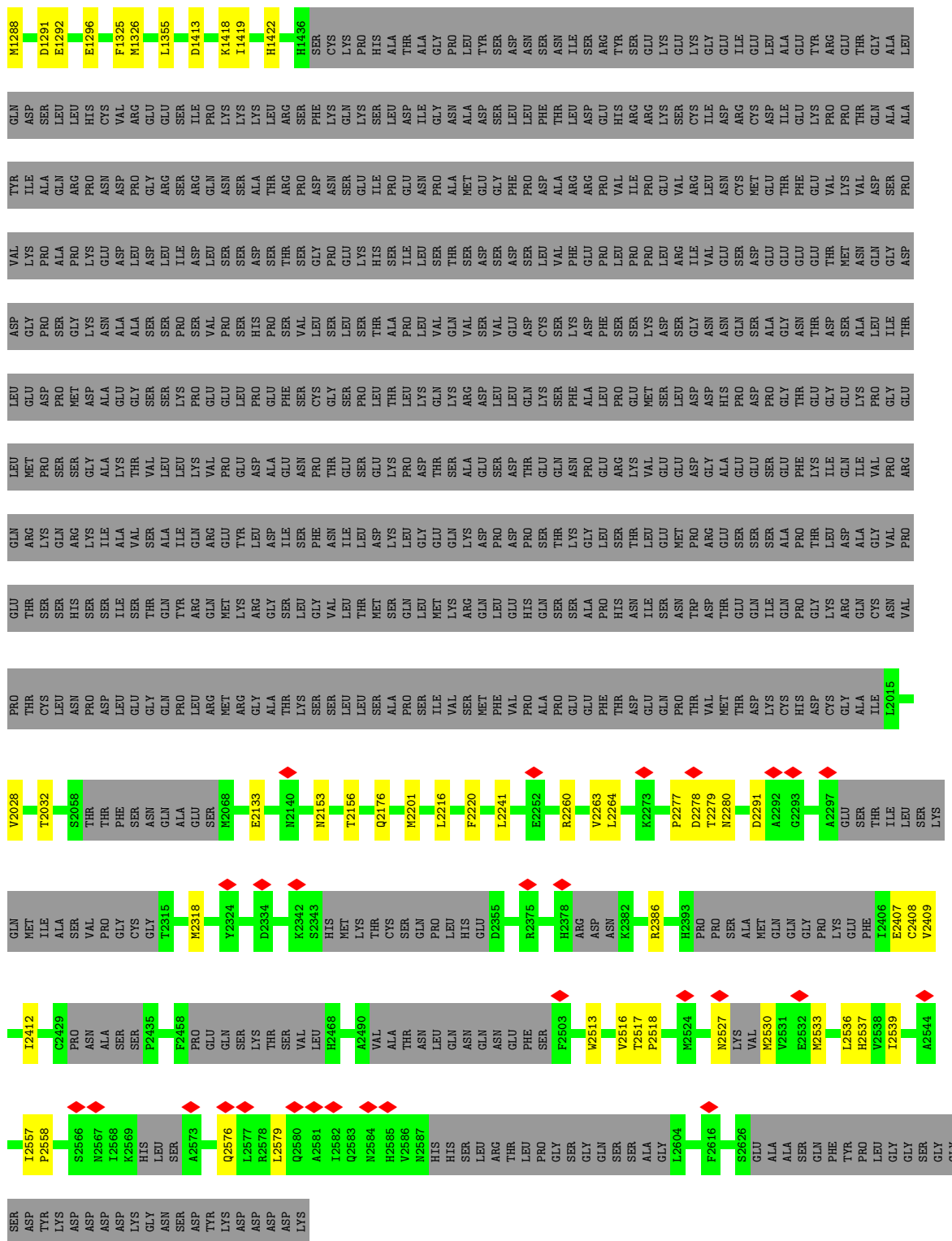
MET	L5
ALA	T6
ASP	E7
GLN	E8
	Q9
	I10
	A11
	E12
	F13
	K14
	E15
	A16
	F17
	S18
	L19
	F20
ASP	
LYS	
ASP	
GLY	
ASP	
GLY	
THR	
ILE	
LEU	
THR	
	T30
	K31
	E32
	L33
	G34
	T35
	V36
	M37
	R38
	S39
	L40
	G41
	Q42
	N43
	P44
	T45
	E48
	L49
	Q50
	D51
	M52
	I53
	N54
	E55
	V56
ASP	
ALA	
ASP	
GLY	



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

Chain D: 51% 5% 45%





- Molecule 5: Protein unc-80 homolog









4 Experimental information

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 Å or better	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/11612	0.30	0/15717
2	B	0.17	0/1286	0.35	0/1740
3	C	0.13	0/932	0.37	0/1240
4	D	0.11	0/10967	0.30	0/14850
5	E	0.11	0/13267	0.28	0/17989
All	All	0.12	0/38064	0.30	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 [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	11344	0	11588	70	0
2	B	1256	0	1150	7	0
3	C	926	0	892	13	0
4	D	11107	0	11071	75	0
5	E	12977	0	13225	85	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	250	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.

All (250) 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
4:D:1141:ARG:NH2	4:D:1176:GLU:OE2	2.28	0.66
5:E:2838:ASP:OD1	5:E:2839:PHE:N	2.29	0.66
5:E:895:ASN:ND2	5:E:897:GLU:OE2	2.29	0.65
1:A:206:HIS:CE1	1:A:248:LEU:HD12	2.33	0.64
4:D:224:SER:N	4:D:257:ASP:OD1	2.31	0.63
5:E:2418:LEU:O	5:E:2493:ARG:NH2	2.32	0.62
4:D:824:GLU:O	4:D:829:LYS:NZ	2.34	0.61
4:D:2291:ASP:OD2	4:D:2318:MET:N	2.35	0.60
5:E:2069:SER:O	5:E:2071:GLN:NE2	2.35	0.60
3:C:116:LYS:O	3:C:116:LYS:HD3	2.02	0.60
5:E:1737:LEU:O	5:E:1740:GLU:N	2.35	0.60
1:A:721:GLU:OE1	1:A:721:GLU:N	2.33	0.60
4:D:1135:ASP:OD1	4:D:1169:ARG:NH1	2.35	0.60
5:E:224:PRO:O	5:E:230:THR:OG1	2.20	0.60
5:E:2325:LYS:HE3	5:E:2325:LYS:HA	1.83	0.60
5:E:2738:GLN:OE1	5:E:2812:GLN:NE2	2.35	0.59
1:A:1100:ASN:OD1	1:A:1102:GLY:N	2.35	0.58
3:C:123:ASP:OD2	3:C:127:ARG:NH2	2.37	0.58
4:D:2216:LEU:HB3	4:D:2220:PHE:CE2	2.39	0.58
1:A:255:ARG:NH2	1:A:264:ASN:OD1	2.37	0.58
4:D:616:ILE:O	4:D:616:ILE:HG13	2.04	0.56
5:E:1181:ARG:NH2	5:E:1554:ASP:OD1	2.39	0.56
5:E:1919:ASP:OD1	5:E:1920:PHE:N	2.38	0.56
2:B:233:GLU:OE1	2:B:233:GLU:N	2.39	0.55
2:B:349:ASP:OD1	2:B:350:GLU:N	2.40	0.55
4:D:2201:MET:HG3	4:D:2220:PHE:CD1	2.41	0.55
1:A:897:ILE:HD12	7:A:2105:PEV:H212	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:GLN:NE2	1:A:1167:LEU:O	2.38	0.54
5:E:1977:MET:HE3	5:E:1977:MET:HA	1.89	0.54
5:E:1953:ALA:O	5:E:1956:THR:OG1	2.25	0.54
5:E:2840:ILE:O	5:E:2844:ARG:N	2.40	0.54
1:A:256:GLN:NE2	1:A:565:ASN:OD1	2.39	0.54
4:D:234:THR:O	4:D:240:HIS:NE2	2.41	0.54
1:A:1521:ARG:HG2	1:A:1521:ARG:HH11	1.73	0.54
4:D:190:HIS:O	4:D:193:ILE:HG22	2.08	0.53
5:E:2903:LYS:O	5:E:2907:GLU:OE1	2.27	0.53
4:D:226:MET:HA	4:D:226:MET:HE2	1.89	0.53
5:E:1945:GLU:OE2	5:E:2049:ASN:ND2	2.41	0.53
4:D:266:PRO:O	4:D:269:VAL:HG12	2.09	0.53
1:A:913:MET:HE1	1:A:976:VAL:CG2	2.40	0.52
1:A:1070:ASN:OD1	1:A:1071:LEU:N	2.43	0.52
5:E:1864:ARG:NH2	5:E:1866:ASP:OD2	2.42	0.52
4:D:553:LYS:N	4:D:554:PRO:CD	2.73	0.52
4:D:1296:GLU:N	4:D:1296:GLU:OE1	2.43	0.52
1:A:1011:PHE:HE1	7:A:2103:PEV:H202	1.73	0.51
1:A:630:ARG:NH2	1:A:945:THR:O	2.43	0.51
1:A:950:ILE:HG23	1:A:950:ILE:O	2.11	0.50
3:C:13:PHE:HZ	3:C:73:MET:SD	2.34	0.50
1:A:715:ARG:NH1	1:A:715:ARG:HB2	2.27	0.50
4:D:2533:MET:SD	4:D:2537:HIS:NE2	2.85	0.50
5:E:1347:GLN:O	5:E:1351:GLU:OE1	2.30	0.50
5:E:2202:GLU:OE1	5:E:2247:ASN:ND2	2.45	0.50
5:E:1923:GLN:O	5:E:1927:ILE:HD12	2.12	0.50
5:E:863:HIS:O	5:E:867:GLY:N	2.45	0.49
1:A:73:THR:O	1:A:76:THR:HG22	2.12	0.49
5:E:2489:PHE:O	5:E:2493:ARG:NH1	2.45	0.49
2:B:333:TYR:OH	2:B:379:VAL:HG22	2.12	0.49
1:A:1481:ARG:CG	1:A:1481:ARG:O	2.61	0.49
1:A:600:ASP:OD1	1:A:600:ASP:O	2.30	0.48
1:A:329:ARG:NH2	1:A:604:LEU:O	2.45	0.48
1:A:1382:LEU:O	1:A:1386:VAL:HG23	2.12	0.48
4:D:2133:GLU:OE2	4:D:2176:GLN:NE2	2.45	0.48
1:A:53:VAL:HB	1:A:146:ARG:HE	1.77	0.48
1:A:213:LYS:HE3	1:A:213:LYS:HA	1.95	0.48
1:A:552:THR:O	1:A:553:GLN:HB2	2.13	0.48
7:A:2106:PEV:C34	7:A:2106:PEV:H122	2.43	0.48
3:C:9:GLN:HB2	3:C:13:PHE:HE2	1.77	0.48
4:D:2028:VAL:O	4:D:2032:THR:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2639:ASN:O	5:E:2642:VAL:HG22	2.14	0.48
4:D:441:GLU:OE1	4:D:441:GLU:N	2.45	0.48
4:D:449:VAL:O	4:D:453:LEU:HD13	2.13	0.48
2:B:181:CYS:N	2:B:220:ASP:OD1	2.47	0.48
5:E:1212:GLU:HA	5:E:1212:GLU:OE1	2.14	0.48
5:E:1452:ASN:OD1	5:E:1453:TYR:N	2.42	0.48
4:D:2278:ASP:OD1	4:D:2279:THR:N	2.46	0.47
4:D:2386:ARG:HG3	4:D:2386:ARG:HH11	1.78	0.47
4:D:1418:LYS:O	4:D:1422:HIS:ND1	2.44	0.47
4:D:2260:ARG:HA	4:D:2263:VAL:HG12	1.96	0.47
5:E:1208:ALA:HA	5:E:1211:LEU:HD13	1.96	0.47
5:E:1635:HIS:ND1	5:E:1637:GLU:OE1	2.47	0.47
3:C:10:ILE:HG23	3:C:11:ALA:N	2.30	0.47
1:A:208:VAL:CG2	1:A:246:MET:HE3	2.45	0.47
5:E:1347:GLN:NE2	5:E:1351:GLU:OE2	2.47	0.47
4:D:161:UNK:O	4:D:165:UNK:N	2.48	0.47
4:D:179:ILE:HG13	4:D:197:LEU:HD21	1.96	0.47
5:E:1237:TRP:HB3	5:E:1238:PRO:HD2	1.97	0.47
1:A:1025:LEU:O	1:A:1029:LEU:HD23	2.14	0.47
4:D:795:GLU:N	4:D:795:GLU:OE1	2.48	0.47
5:E:46:CYS:HA	5:E:49:PHE:HB3	1.97	0.46
1:A:1404:PHE:CE1	2:B:338:GLN:OE1	2.68	0.46
1:A:913:MET:HE2	1:A:973:PRO:O	2.16	0.46
1:A:1107:ALA:O	1:A:1111:VAL:HG23	2.15	0.46
4:D:1060:ARG:NH1	4:D:1102:ASP:OD2	2.48	0.46
5:E:670:SER:HA	5:E:673:CYS:SG	2.56	0.46
5:E:853:ASP:OD1	5:E:854:SER:N	2.49	0.46
5:E:1195:GLU:HA	5:E:1195:GLU:OE1	2.16	0.46
5:E:1199:ILE:HB	5:E:1200:PRO:CD	2.46	0.46
5:E:1737:LEU:O	5:E:1741:GLU:OE1	2.34	0.46
1:A:75:ASP:OD1	1:A:146:ARG:NH1	2.48	0.46
4:D:2201:MET:SD	4:D:2241:LEU:HD21	2.56	0.46
5:E:669:SER:H	5:E:672:ILE:HB	1.80	0.46
4:D:712:VAL:O	4:D:715:VAL:HG12	2.16	0.46
4:D:231:MET:HB2	4:D:269:VAL:HG23	1.98	0.46
1:A:206:HIS:ND1	1:A:248:LEU:HD12	2.30	0.46
1:A:665:GLN:NE2	5:E:2227:LEU:O	2.49	0.46
1:A:1186:GLN:O	1:A:1471:GLN:NE2	2.48	0.46
5:E:838:ASP:HB3	5:E:841:GLN:HB3	1.98	0.46
5:E:2722:VAL:HG12	5:E:2722:VAL:O	2.16	0.46
4:D:521:GLU:H	4:D:521:GLU:CD	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:PRO:O	4:D:179:ILE:HD12	2.17	0.45
4:D:182:LEU:HD22	4:D:190:HIS:CE1	2.52	0.45
5:E:2876:ILE:HD12	5:E:2876:ILE:H	1.81	0.45
1:A:715:ARG:HB2	1:A:715:ARG:HH11	1.82	0.45
1:A:1511:LEU:HD21	1:A:1515:MET:HE3	1.97	0.45
4:D:2277:PRO:HG2	4:D:2280:ASN:OD1	2.17	0.45
5:E:2865:GLU:O	5:E:2870:LEU:HD13	2.16	0.45
1:A:50:VAL:HA	1:A:53:VAL:HG12	1.99	0.45
3:C:72:MET:O	3:C:76:LYS:HG3	2.16	0.45
4:D:644:PHE:O	4:D:645:ARG:C	2.60	0.45
4:D:824:GLU:OE1	4:D:824:GLU:HA	2.17	0.45
1:A:431:LEU:HD12	1:A:435:LEU:HD23	1.98	0.45
5:E:1941:ARG:NH2	5:E:1980:GLU:OE1	2.48	0.45
1:A:1400:VAL:HG13	1:A:1417:CYS:HB2	1.99	0.45
3:C:115:GLU:OE1	3:C:115:GLU:N	2.44	0.45
4:D:1413:ASP:N	4:D:1413:ASP:OD1	2.50	0.45
9:A:2111:Y01:HAC1	9:A:2111:Y01:HAE2	1.99	0.45
4:D:2527:ASN:HB3	4:D:2530:MET:HE2	1.99	0.45
1:A:1481:ARG:O	1:A:1481:ARG:HG2	2.16	0.45
4:D:1102:ASP:OD1	4:D:1103:VAL:N	2.50	0.45
4:D:2557:ILE:N	4:D:2558:PRO:HD2	2.32	0.45
5:E:1207:ALA:O	5:E:1211:LEU:CD1	2.64	0.45
5:E:2359:GLU:OE1	5:E:2359:GLU:HA	2.17	0.45
4:D:2409:VAL:O	4:D:2412:ILE:HG22	2.17	0.44
5:E:1603:ASP:OD1	5:E:1605:HIS:N	2.50	0.44
7:A:2106:PEV:H122	7:A:2106:PEV:H341	1.99	0.44
3:C:52:MET:HG2	3:C:73:MET:HE2	1.98	0.44
1:A:1567:VAL:O	1:A:1571:THR:HG23	2.17	0.44
4:D:607:ILE:O	4:D:611:ILE:HG12	2.18	0.44
1:A:65:PRO:N	1:A:66:PRO:CD	2.81	0.44
1:A:329:ARG:NH1	1:A:600:ASP:OD1	2.51	0.44
5:E:953:ALA:HB2	5:E:1183:GLY:HA3	2.00	0.44
1:A:146:ARG:N	1:A:147:PRO:CD	2.81	0.44
1:A:1011:PHE:HZ	7:A:2103:PEV:H211	1.82	0.44
3:C:9:GLN:HB2	3:C:13:PHE:CE2	2.51	0.44
1:A:162:LEU:HB2	1:A:163:PRO:HD2	2.00	0.44
4:D:178:MET:O	4:D:181:THR:HG22	2.18	0.44
5:E:187:LEU:O	5:E:191:LEU:HD12	2.18	0.44
4:D:179:ILE:HG21	4:D:226:MET:SD	2.58	0.44
5:E:2838:ASP:OD1	5:E:2838:ASP:C	2.60	0.44
4:D:2153:ASN:O	4:D:2156:THR:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2536:LEU:O	4:D:2539:ILE:HG22	2.18	0.43
1:A:1239:VAL:HB	1:A:1240:PRO:HD3	2.00	0.43
3:C:120:GLU:OE1	3:C:120:GLU:N	2.41	0.43
5:E:1632:GLU:O	5:E:1635:HIS:HB2	2.18	0.43
5:E:2507:CYS:O	5:E:2510:ARG:N	2.51	0.43
4:D:1062:GLU:OE2	4:D:1066:LYS:NZ	2.51	0.43
4:D:2407:GLU:HG2	4:D:2408:CYS:N	2.34	0.43
1:A:206:HIS:ND1	1:A:248:LEU:CD1	2.82	0.43
4:D:1419:ILE:H	4:D:1419:ILE:HD12	1.83	0.43
5:E:2133:PHE:HB3	5:E:2134:PRO:HD3	1.99	0.43
5:E:2833:LEU:O	5:E:2837:LEU:HD23	2.18	0.43
4:D:645:ARG:O	4:D:649:SER:N	2.51	0.43
5:E:1226:ALA:HB1	5:E:1351:GLU:OE1	2.19	0.43
4:D:1288:MET:HG3	4:D:1355:LEU:HD21	2.00	0.43
5:E:1842:VAL:O	5:E:1842:VAL:HG13	2.18	0.43
1:A:635:GLU:OE1	1:A:635:GLU:N	2.50	0.43
3:C:10:ILE:CG2	3:C:11:ALA:N	2.82	0.43
4:D:2260:ARG:O	4:D:2264:LEU:HD23	2.19	0.43
1:A:877:GLN:OE1	1:A:877:GLN:HA	2.18	0.43
1:A:1257:THR:HA	1:A:1260:ILE:HG22	2.00	0.43
4:D:189:LEU:O	4:D:189:LEU:HD12	2.17	0.43
4:D:2576:GLN:HA	4:D:2579:LEU:HD12	2.00	0.43
5:E:2617:GLY:O	5:E:2621:THR:HG23	2.19	0.43
1:A:1295:LEU:HD23	1:A:1295:LEU:O	2.19	0.43
4:D:179:ILE:HB	4:D:226:MET:HE1	2.01	0.43
4:D:630:GLU:OE2	4:D:633:ARG:NH2	2.50	0.43
4:D:1168:ASN:O	4:D:1172:THR:HG23	2.19	0.43
5:E:199:ILE:HG23	5:E:199:ILE:O	2.18	0.43
5:E:2007:ASP:OD1	5:E:2008:ILE:N	2.51	0.42
1:A:937:ILE:HG13	1:A:938:MET:N	2.34	0.42
1:A:162:LEU:O	1:A:164:ARG:N	2.52	0.42
1:A:167:ILE:HD12	1:A:167:ILE:H	1.85	0.42
5:E:2890:CYS:SG	5:E:2891:LYS:N	2.92	0.42
4:D:446:VAL:O	4:D:450:ILE:HG13	2.19	0.42
1:A:240:PRO:HB2	1:A:241:PRO:HD2	2.02	0.42
1:A:162:LEU:HB2	1:A:163:PRO:CD	2.49	0.42
1:A:912:VAL:HG23	1:A:918:LEU:HB2	2.00	0.42
1:A:47:ILE:O	1:A:50:VAL:HG12	2.19	0.42
3:C:13:PHE:CZ	3:C:73:MET:SD	3.13	0.42
4:D:1278:HIS:O	4:D:1282:THR:HG23	2.19	0.42
4:D:812:MET:HE1	4:D:874:LEU:HD23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1273:ASP:OD1	4:D:1274:HIS:N	2.51	0.42
4:D:701:LEU:HD11	4:D:812:MET:HG2	2.02	0.42
4:D:1099:ALA:O	4:D:1102:ASP:HB2	2.20	0.42
4:D:1291:ASP:OD1	4:D:1292:GLU:N	2.46	0.42
5:E:2885:ILE:O	5:E:2885:ILE:HG13	2.19	0.42
1:A:1462:LEU:HD23	1:A:1463:SER:O	2.19	0.41
4:D:796:MET:HA	4:D:796:MET:HE2	2.02	0.41
5:E:2392:PRO:O	5:E:2396:GLU:HG2	2.20	0.41
5:E:2888:PRO:HG2	5:E:2894:LEU:HD21	2.02	0.41
5:E:1351:GLU:OE2	5:E:1560:TYR:OH	2.39	0.41
1:A:1128:VAL:HG12	1:A:1128:VAL:O	2.20	0.41
5:E:676:ALA:O	5:E:679:ILE:HG22	2.20	0.41
5:E:953:ALA:CB	5:E:1184:MET:CE	2.98	0.41
5:E:2579:ARG:N	5:E:2580:PRO:HD2	2.35	0.41
5:E:2802:LEU:HD11	5:E:2813:TRP:HZ3	1.85	0.41
1:A:144:ILE:N	1:A:145:PRO:CD	2.83	0.41
4:D:2513:TRP:HA	4:D:2516:VAL:HG12	2.03	0.41
4:D:2517:THR:N	4:D:2518:PRO:HD2	2.35	0.41
1:A:381:MET:HE1	1:A:435:LEU:O	2.20	0.41
4:D:1281:ILE:O	4:D:1285:MET:HG2	2.20	0.41
5:E:2305:GLN:OE1	5:E:2380:LYS:NZ	2.40	0.41
5:E:2325:LYS:N	5:E:2326:PRO:HD2	2.35	0.41
5:E:2796:LEU:HD11	5:E:2901:GLU:OE2	2.20	0.41
5:E:792:MET:O	5:E:796:ILE:HG12	2.21	0.41
5:E:1897:LEU:HD23	5:E:1935:LEU:HD11	2.03	0.41
1:A:897:ILE:CD1	7:A:2105:PEV:H212	2.51	0.41
2:B:347:ASP:C	2:B:347:ASP:OD1	2.64	0.41
4:D:227:LEU:HG	4:D:231:MET:HE1	2.03	0.41
5:E:1673:PRO:HA	5:E:1674:PRO:HD3	1.97	0.41
5:E:2156:GLY:O	5:E:2159:THR:HG22	2.20	0.41
5:E:2008:ILE:HG13	5:E:2008:ILE:O	2.20	0.41
5:E:2810:GLY:HA2	5:E:2813:TRP:CE2	2.56	0.41
1:A:283:VAL:HG22	1:A:1389:GLU:OE1	2.21	0.41
2:B:261:CYS:O	2:B:265:VAL:HG23	2.21	0.41
4:D:527:VAL:HA	4:D:530:VAL:HG12	2.02	0.41
4:D:641:LEU:HD23	4:D:695:LEU:HD21	2.02	0.41
5:E:847:ARG:O	5:E:850:VAL:HG12	2.21	0.41
5:E:2630:PHE:CD1	5:E:2630:PHE:C	2.99	0.41
5:E:2800:VAL:HG22	5:E:2898:PHE:CD2	2.56	0.41
5:E:2117:GLN:O	5:E:2120:VAL:HG12	2.21	0.41
5:E:2607:GLU:OE1	5:E:2607:GLU:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:LEU:O	1:A:937:ILE:HG23	2.21	0.40
5:E:1637:GLU:OE1	5:E:1637:GLU:N	2.54	0.40
1:A:523:ILE:HG22	1:A:527:MET:HE2	2.02	0.40
4:D:2201:MET:SD	4:D:2241:LEU:CD2	3.10	0.40
5:E:2741:LEU:HA	5:E:2744:VAL:HG12	2.03	0.40
1:A:1484:VAL:HG22	1:A:1527:ASP:HB2	2.04	0.40
4:D:240:HIS:HB2	4:D:276:MET:HE3	2.03	0.40
1:A:353:GLU:OE1	1:A:358:GLY:HA3	2.21	0.40
1:A:1199:PHE:O	1:A:1203:MET:HG2	2.21	0.40
3:C:134:ASP:OD1	3:C:136:GLN:N	2.46	0.40
5:E:2671:LEU:N	5:E:2672:PRO:HD2	2.36	0.40
4:D:1325:PHE:C	4:D:1326:MET:HE2	2.47	0.40
5:E:916:THR:HG23	5:E:917:HIS:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	135	GLN
1	A	736	GLN
1	A	829	ASN
1	A	1037	GLN
1	A	1162	ASN
1	A	1189	HIS
1	A	1291	HIS
1	A	1318	HIS
1	A	1365	ASN
1	A	1570	GLN
4	D	190	HIS
4	D	220	ASN
4	D	535	HIS
4	D	690	HIS
4	D	859	ASN
4	D	1049	ASN
4	D	1053	ASN
4	D	1083	HIS
4	D	1279	GLN
4	D	1365	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	1434	GLN
4	D	2087	HIS
4	D	2100	GLN
4	D	2367	GLN
4	D	2393	HIS
4	D	2576	GLN
5	E	349	GLN
5	E	786	HIS
5	E	826	ASN
5	E	828	GLN
5	E	1267	GLN
5	E	1470	GLN
5	E	1657	GLN
5	E	2515	GLN
5	E	2542	HIS
5	E	2633	HIS
5	E	2879	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
7	PEV	A	2106	-	30,30,48	1.29	3 (10%)	33,35,53	1.19	2 (6%)
7	PEV	A	2105	-	33,33,48	1.24	3 (9%)	36,38,53	1.15	2 (5%)
7	PEV	A	2104	-	39,39,48	1.19	3 (7%)	42,44,53	1.11	2 (4%)
9	Y01	A	2111	-	38,38,38	1.25	4 (10%)	57,57,57	1.97	11 (19%)
8	PGV	A	2107	-	30,30,50	1.11	2 (6%)	32,35,56	1.11	2 (6%)
8	PGV	A	2108	-	42,42,50	1.03	5 (11%)	45,47,56	1.14	2 (4%)
6	NAG	A	2101	-	14,14,15	0.21	0	17,19,21	0.42	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%)
7	PEV	A	2103	-	36,36,48	1.21	3 (8%)	39,41,53	1.08	2 (5%)
6	NAG	A	2102	1	14,14,15	0.19	0	17,19,21	0.43	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
7	PEV	A	2106	-	-	15/34/34/52	-
7	PEV	A	2105	-	-	15/37/37/52	-
7	PEV	A	2104	-	-	19/43/43/52	-
9	Y01	A	2111	-	-	8/19/77/77	0/4/4/4
8	PGV	A	2107	-	-	13/33/33/55	-
8	PGV	A	2108	-	-	19/44/44/55	-
6	NAG	A	2101	-	-	2/6/23/26	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
7	PEV	A	2103	-	-	20/40/40/52	-
6	NAG	A	2102	1	-	0/6/23/26	0/1/1/1

All (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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2106	PEV	O3-C11	3.14	1.42	1.33
7	A	2103	PEV	O3-C11	3.10	1.42	1.33
7	A	2104	PEV	O3-C11	3.09	1.42	1.33
7	A	2103	PEV	O2-C31	2.93	1.42	1.34
7	A	2104	PEV	O2-C31	2.93	1.42	1.34
7	A	2106	PEV	O2-C31	2.89	1.42	1.34
7	A	2105	PEV	O2-C31	2.88	1.42	1.34
8	A	2108	PGV	P-O12	2.81	1.65	1.54
9	A	2111	Y01	CAI-CAZ	2.78	1.38	1.33
9	A	2109	Y01	CAI-CAZ	2.75	1.38	1.33
9	A	2110	Y01	CAI-CAZ	2.75	1.38	1.33
8	A	2108	PGV	O01-C02	-2.69	1.40	1.46
7	A	2105	PEV	O2-C2	-2.61	1.40	1.46
7	A	2103	PEV	O2-C2	-2.58	1.40	1.46
7	A	2106	PEV	O2-C2	-2.56	1.40	1.46
7	A	2104	PEV	O2-C2	-2.54	1.40	1.46
9	A	2109	Y01	CAP-CBE	2.42	1.59	1.54
8	A	2108	PGV	O03-C19	2.41	1.40	1.33
8	A	2107	PGV	O01-C1	2.27	1.40	1.34
9	A	2111	Y01	CBH-CAZ	-2.24	1.48	1.52
9	A	2109	Y01	CBB-CBE	2.23	1.58	1.54
8	A	2108	PGV	O01-C1	2.23	1.40	1.34
8	A	2108	PGV	O03-C01	-2.22	1.40	1.45
9	A	2111	Y01	CAL-CAX	2.20	1.55	1.50
9	A	2110	Y01	CBH-CAZ	-2.14	1.48	1.52
9	A	2109	Y01	CAL-CAX	2.10	1.55	1.50
9	A	2110	Y01	CAL-CAX	2.01	1.55	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
9	A	2109	Y01	OAW-CAY-CAM	5.25	122.85	111.48
9	A	2111	Y01	OAW-CAY-CAM	5.23	122.80	111.48
9	A	2110	Y01	OAW-CAY-OAG	-5.15	111.67	123.70
9	A	2109	Y01	OAW-CAY-OAG	-5.14	111.69	123.70
9	A	2110	Y01	CAV-CAZ-CAI	-5.11	113.64	120.57
9	A	2110	Y01	OAW-CAY-CAM	5.03	122.36	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2111	Y01	CAV-CAZ-CAI	-4.90	113.93	120.57
7	A	2104	PEV	O2-C31-C32	4.13	120.42	111.48
7	A	2106	PEV	O2-C31-C32	4.09	120.33	111.48
8	A	2107	PGV	O01-C1-C2	3.99	120.12	111.48
8	A	2108	PGV	O01-C1-C2	3.94	120.01	111.48
7	A	2105	PEV	O2-C31-C32	3.92	119.95	111.48
7	A	2103	PEV	O2-C31-C32	3.77	119.64	111.48
9	A	2111	Y01	OAW-CBC-CAV	-2.93	102.00	108.04
9	A	2110	Y01	OAW-CBC-CAV	-2.86	102.15	108.04
9	A	2109	Y01	OAW-CBC-CAV	-2.85	102.17	108.04
7	A	2106	PEV	O3-C11-C12	2.76	120.26	111.83
7	A	2104	PEV	O3-C11-C12	2.74	120.18	111.83
7	A	2105	PEV	O3-C11-C12	2.64	119.88	111.83
7	A	2103	PEV	O3-C11-C12	2.57	119.68	111.83
8	A	2108	PGV	O03-C19-C20	2.57	119.66	111.83
9	A	2110	Y01	OAW-CBC-CAR	2.46	114.19	108.37
9	A	2109	Y01	OAW-CBC-CAR	2.38	114.00	108.37
9	A	2109	Y01	CAS-CBF-CBD	-2.36	108.48	111.78
9	A	2109	Y01	CAP-CAQ-CBG	-2.30	100.65	105.14
9	A	2111	Y01	CAP-CAQ-CBG	-2.20	100.85	105.14
9	A	2110	Y01	OAF-CAX-CAL	-2.19	116.15	123.09
9	A	2111	Y01	OAW-CBC-CAR	2.16	113.46	108.37
9	A	2109	Y01	OAF-CAX-CAL	-2.15	116.26	123.09
9	A	2110	Y01	CBH-CAZ-CAI	-2.14	119.80	122.93
9	A	2111	Y01	CAP-CBE-CBB	-2.09	109.01	112.18
8	A	2107	PGV	C02-O01-C1	-2.08	114.78	117.78
9	A	2111	Y01	OAF-CAX-CAL	-2.08	116.50	123.09
9	A	2110	Y01	CAP-CBE-CBB	-2.07	109.05	112.18
9	A	2111	Y01	CBH-CAZ-CAI	-2.05	119.93	122.93
9	A	2110	Y01	CAS-CBF-CBD	-2.04	108.93	111.78
9	A	2111	Y01	CAQ-CBG-CBI	-2.01	101.47	103.84

There are no chirality outliers.

All (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
7	A	2104	PEV	C1-O3P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2104	PEV	C1-O3P-P-O2P
7	A	2104	PEV	C1-O3P-P-O4P
7	A	2105	PEV	C32-C31-O2-C2
7	A	2105	PEV	C1-O3P-P-O1P
7	A	2105	PEV	C1-O3P-P-O2P
7	A	2105	PEV	C1-O3P-P-O4P
7	A	2105	PEV	O4P-C4-C5-N6
7	A	2106	PEV	C1-O3P-P-O2P
7	A	2106	PEV	C1-O3P-P-O4P
7	A	2106	PEV	C4-O4P-P-O3P
7	A	2106	PEV	O4P-C4-C5-N6
8	A	2107	PGV	C04-O12-P-O11
8	A	2107	PGV	C04-O12-P-O14
8	A	2107	PGV	C01-C02-C03-O11
8	A	2108	PGV	C2-C1-O01-C02
9	A	2111	Y01	OAG-CAY-OAW-CBC
7	A	2104	PEV	O11-C11-O3-C3
7	A	2106	PEV	O11-C11-O3-C3
7	A	2104	PEV	C12-C11-O3-C3
9	A	2111	Y01	CAM-CAY-OAW-CBC
7	A	2106	PEV	C12-C11-O3-C3
8	A	2108	PGV	C20-C19-O03-C01
7	A	2105	PEV	O31-C31-O2-C2
8	A	2108	PGV	O02-C1-O01-C02
8	A	2108	PGV	O04-C19-O03-C01
7	A	2103	PEV	C12-C11-O3-C3
6	A	2101	NAG	O5-C5-C6-O6
9	A	2109	Y01	CAO-CBB-CBE-CBI
8	A	2108	PGV	C19-C20-C21-C22
7	A	2103	PEV	O11-C11-O3-C3
9	A	2109	Y01	CAC-CBB-CBE-CBI
9	A	2109	Y01	CAN-CAJ-CAO-CBB
7	A	2104	PEV	C32-C31-O2-C2
9	A	2109	Y01	CAC-CBB-CBE-CAP
7	A	2104	PEV	O31-C31-O2-C2
8	A	2107	PGV	C04-C05-C06-O06
9	A	2110	Y01	CAJ-CAN-CBA-CAA
9	A	2111	Y01	CAJ-CAO-CBB-CBE
9	A	2110	Y01	CAM-CAY-OAW-CBC
7	A	2104	PEV	C36-C37-C38-C39
7	A	2104	PEV	C14-C15-C16-C17
8	A	2108	PGV	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	2107	PGV	C2-C1-O01-C02
7	A	2103	PEV	C12-C13-C14-C15
7	A	2103	PEV	C17-C18-C19-C20
9	A	2111	Y01	CAJ-CAO-CBB-CAC
8	A	2107	PGV	O02-C1-O01-C02
9	A	2110	Y01	CAJ-CAN-CBA-CAB
8	A	2108	PGV	C26-C27-C28-C29
8	A	2108	PGV	C24-C25-C26-C27
7	A	2106	PEV	C32-C31-O2-C2
9	A	2109	Y01	CAM-CAY-OAW-CBC
8	A	2108	PGV	C31-C32-C33-C34
9	A	2109	Y01	OAG-CAY-OAW-CBC
9	A	2110	Y01	OAG-CAY-OAW-CBC
8	A	2107	PGV	C6-C7-C8-C9
7	A	2105	PEV	C12-C13-C14-C15
9	A	2109	Y01	CAJ-CAN-CBA-CAB
9	A	2111	Y01	CAJ-CAN-CBA-CAB
8	A	2108	PGV	C11-C12-C13-C14
8	A	2107	PGV	C4-C5-C6-C7
8	A	2107	PGV	O05-C05-C06-O06
7	A	2106	PEV	C33-C34-C35-C36
7	A	2105	PEV	C19-C20-C21-C22
7	A	2104	PEV	C13-C14-C15-C16
7	A	2104	PEV	O2-C2-C3-O3
8	A	2108	PGV	C20-C21-C22-C23
7	A	2106	PEV	O31-C31-O2-C2
7	A	2105	PEV	C13-C14-C15-C16
8	A	2108	PGV	C4-C5-C6-C7
7	A	2104	PEV	C11-C12-C13-C14
7	A	2103	PEV	O3P-C1-C2-C3
7	A	2106	PEV	C1-C2-C3-O3
7	A	2103	PEV	C19-C20-C21-C22
8	A	2107	PGV	O01-C02-C03-O11
8	A	2108	PGV	O01-C02-C03-O11
6	A	2101	NAG	C4-C5-C6-O6
9	A	2109	Y01	CAO-CAJ-CAN-CBA
7	A	2106	PEV	O2-C2-C3-O3
7	A	2103	PEV	C18-C19-C20-C21
7	A	2105	PEV	C33-C34-C35-C36
8	A	2108	PGV	C01-C02-C03-O11
9	A	2109	Y01	CAJ-CAN-CBA-CAA
9	A	2111	Y01	CAJ-CAN-CBA-CAA

Continued on next page...

Continued from previous page...

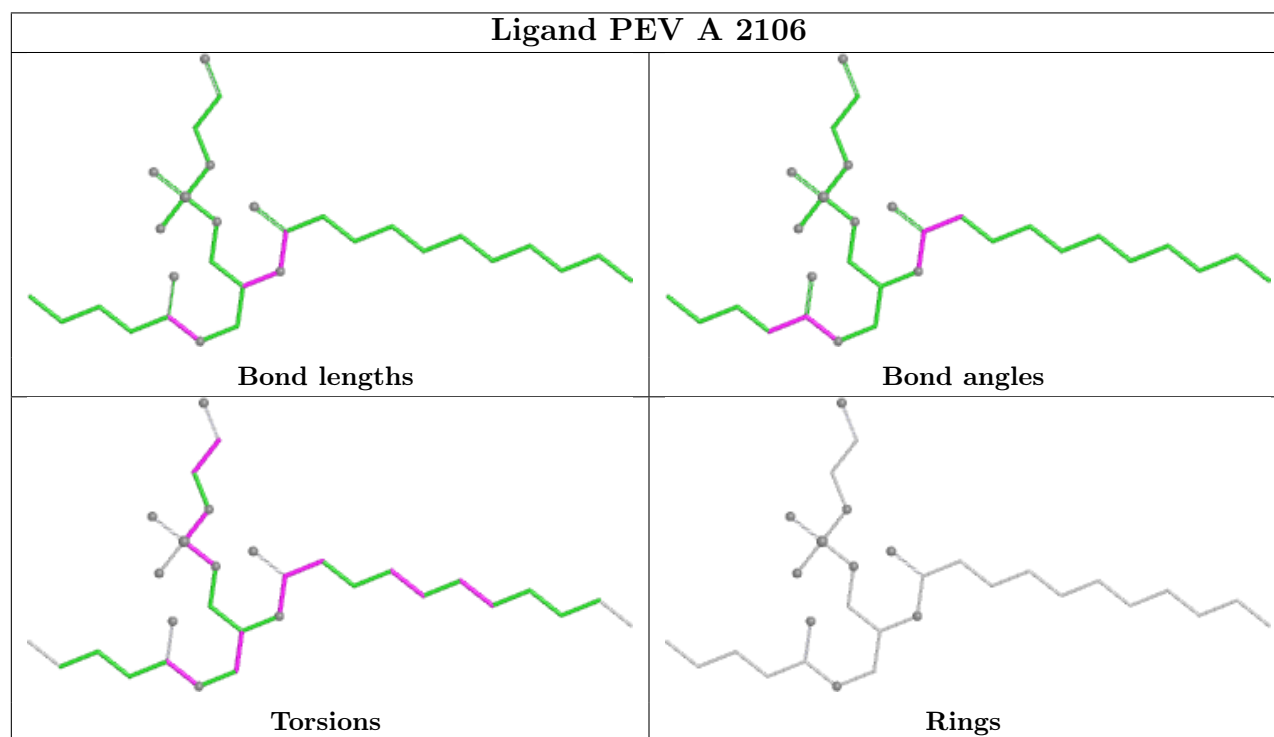
Mol	Chain	Res	Type	Atoms
8	A	2108	PGV	C28-C29-C30-C31
7	A	2103	PEV	O3P-C1-C2-O2
7	A	2104	PEV	C35-C36-C37-C38
7	A	2106	PEV	C35-C36-C37-C38
8	A	2108	PGV	C27-C28-C29-C30
7	A	2105	PEV	O3P-C1-C2-C3
8	A	2107	PGV	C13-C14-C15-C16
7	A	2104	PEV	O3P-C1-C2-O2
7	A	2104	PEV	C4-O4P-P-O3P
7	A	2106	PEV	C4-O4P-P-O2P
7	A	2103	PEV	C11-C12-C13-C14
7	A	2105	PEV	C11-C12-C13-C14
7	A	2105	PEV	O3P-C1-C2-O2
7	A	2104	PEV	C1-C2-C3-O3
7	A	2104	PEV	C32-C33-C34-C35
8	A	2108	PGV	C9-C10-C11-C12
9	A	2110	Y01	CAN-CAJ-CAO-CBB
9	A	2110	Y01	CAM-CAL-CAX-OAF
8	A	2108	PGV	C7-C8-C9-C10
9	A	2110	Y01	CAM-CAL-CAX-OAH
7	A	2105	PEV	C14-C15-C16-C17
7	A	2104	PEV	O3P-C1-C2-C3
7	A	2103	PEV	C35-C36-C37-C38
8	A	2107	PGV	C9-C10-C11-C12
7	A	2103	PEV	C33-C34-C35-C36
8	A	2108	PGV	C29-C30-C31-C32
7	A	2105	PEV	C32-C33-C34-C35
7	A	2106	PEV	O2-C31-C32-C33
8	A	2107	PGV	C11-C12-C13-C14
7	A	2103	PEV	C21-C22-C23-C24
7	A	2103	PEV	C16-C17-C18-C19
9	A	2111	Y01	CAL-CAM-CAY-OAW
9	A	2110	Y01	CAL-CAM-CAY-OAW
7	A	2103	PEV	C31-C32-C33-C34
7	A	2106	PEV	O31-C31-C32-C33
7	A	2103	PEV	O2-C31-C32-C33
9	A	2110	Y01	CAL-CAM-CAY-OAG
9	A	2111	Y01	CAL-CAM-CAY-OAG
7	A	2104	PEV	O2-C31-C32-C33

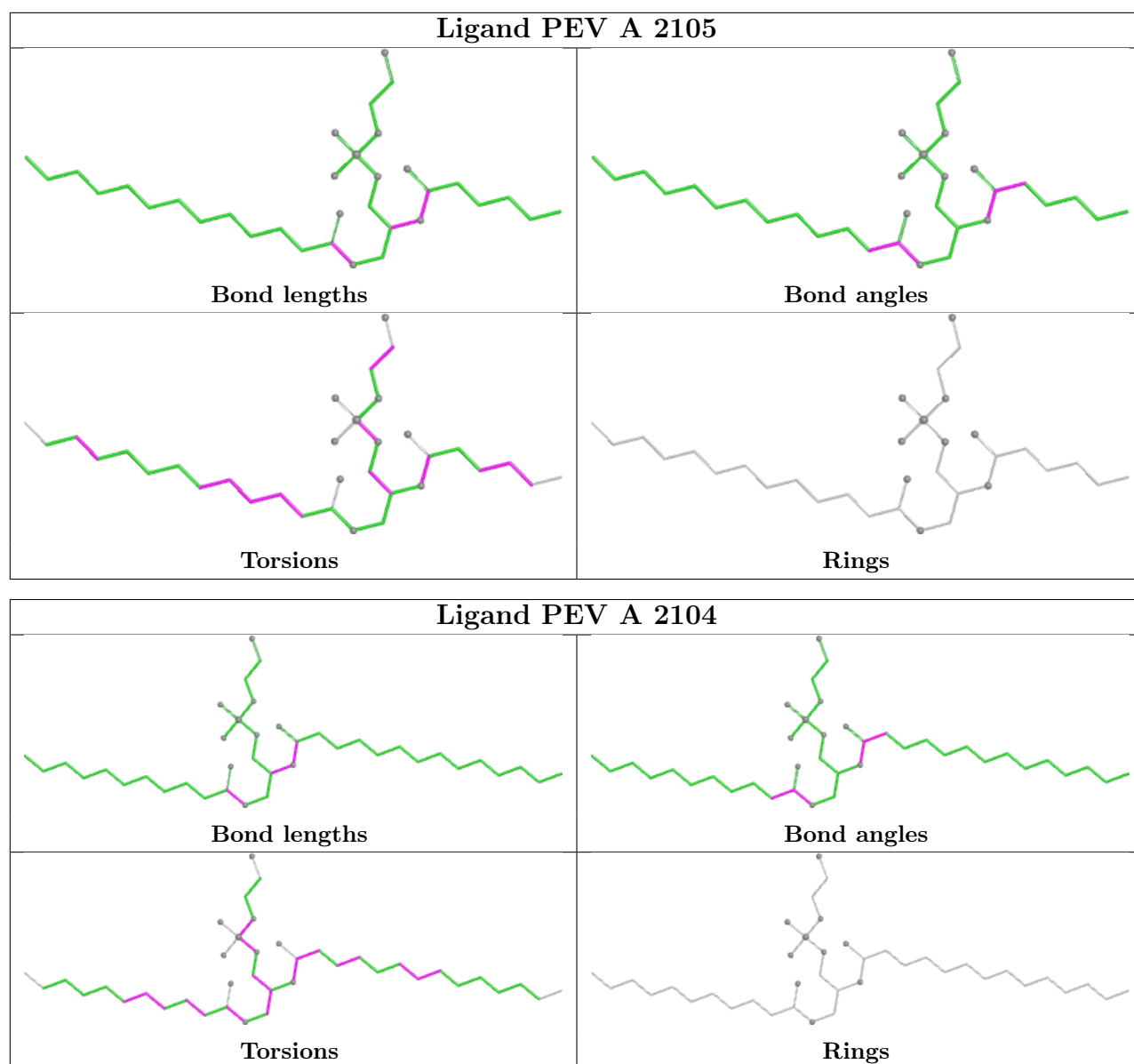
There are no ring outliers.

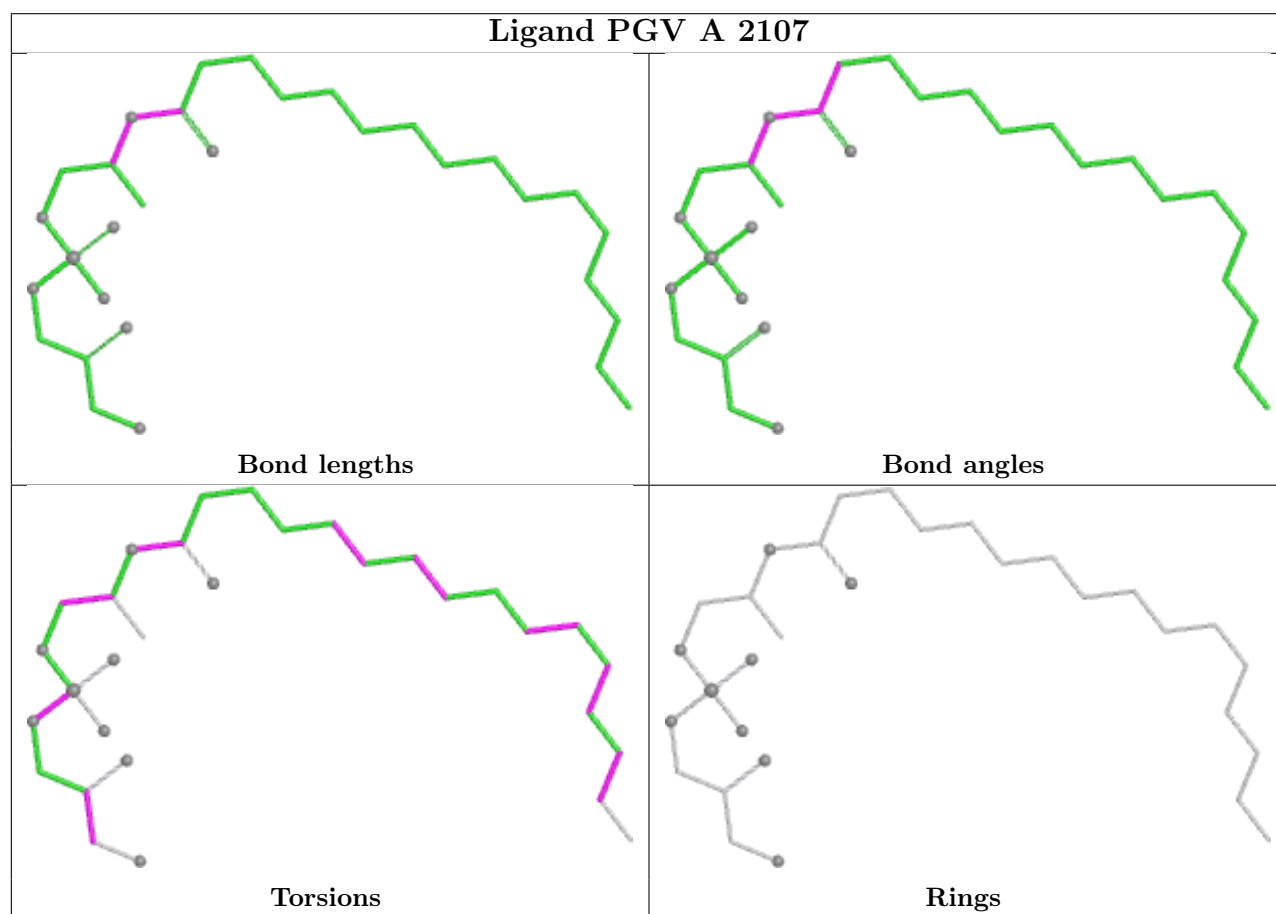
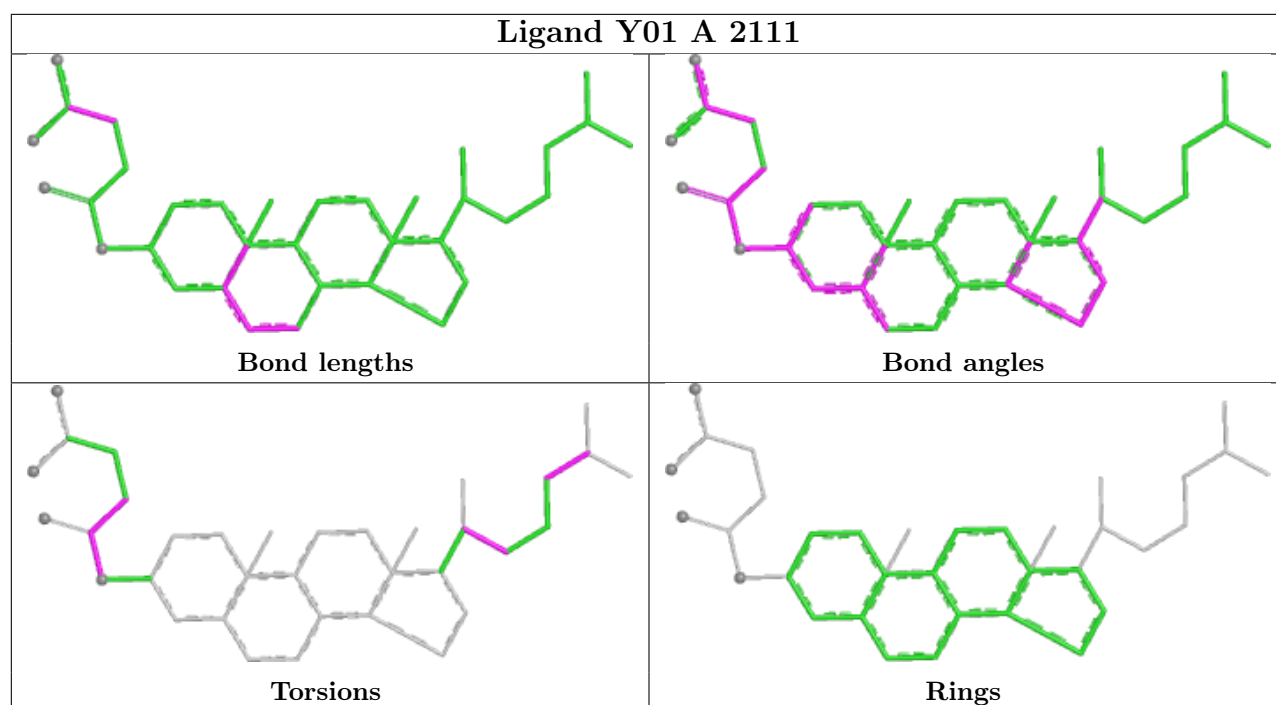
4 monomers are involved in 7 short contacts:

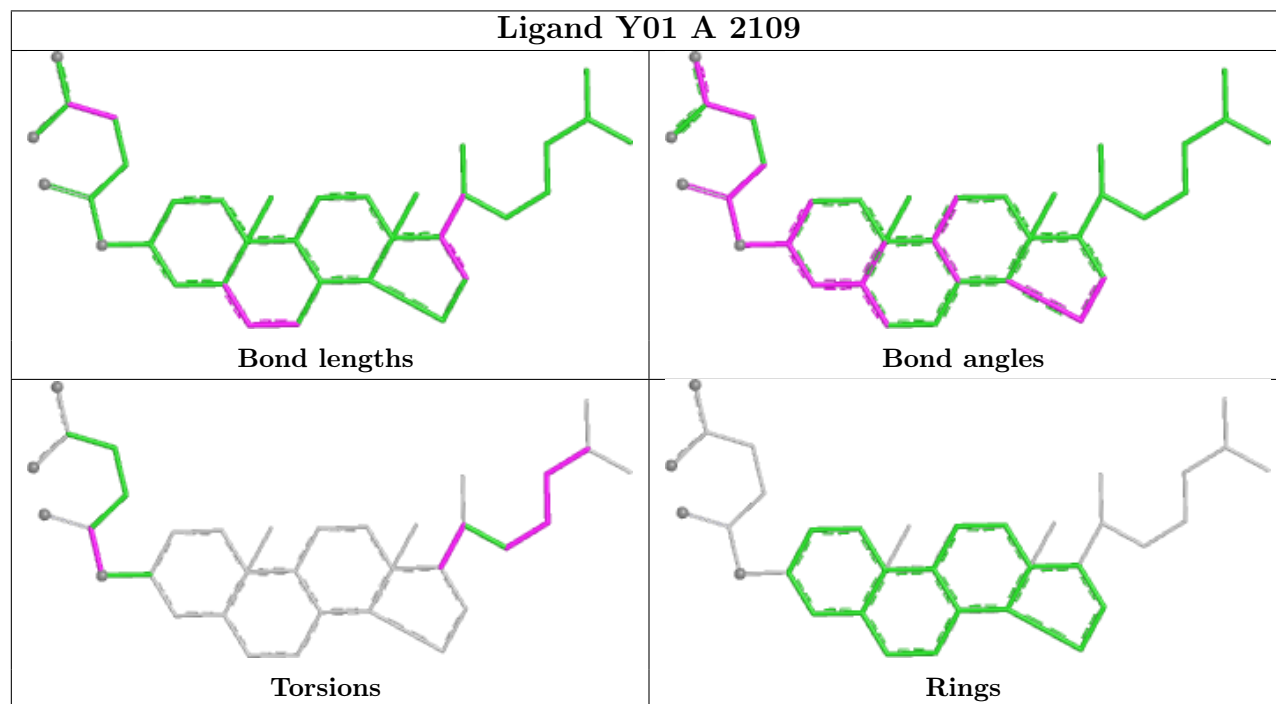
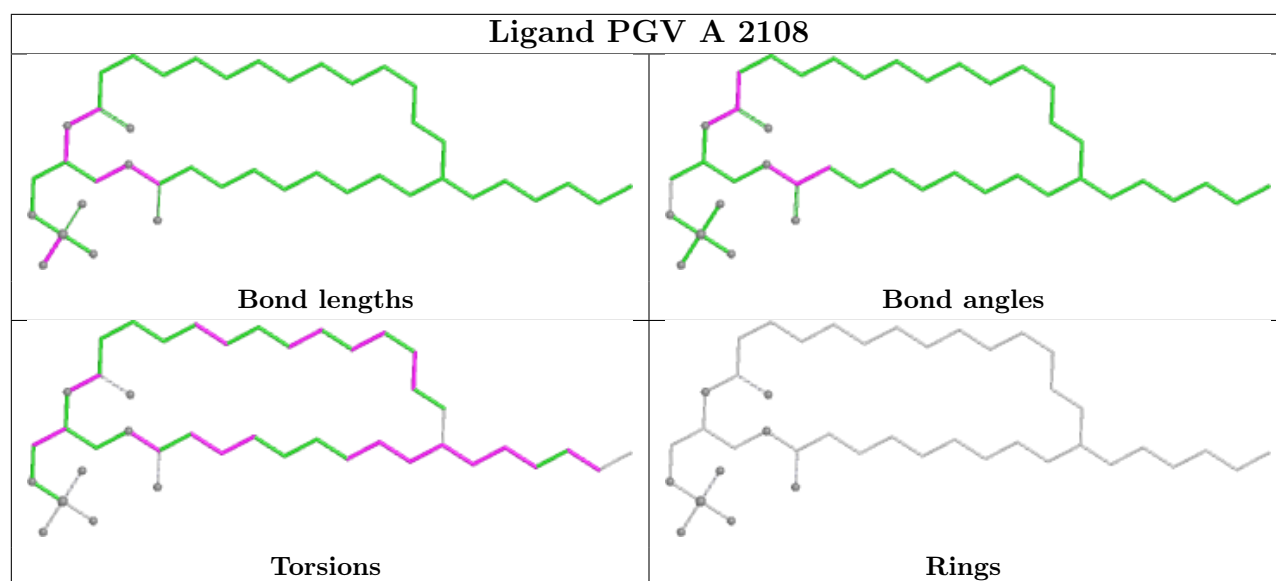
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2106	PEV	2	0
7	A	2105	PEV	2	0
9	A	2111	Y01	1	0
7	A	2103	PEV	2	0

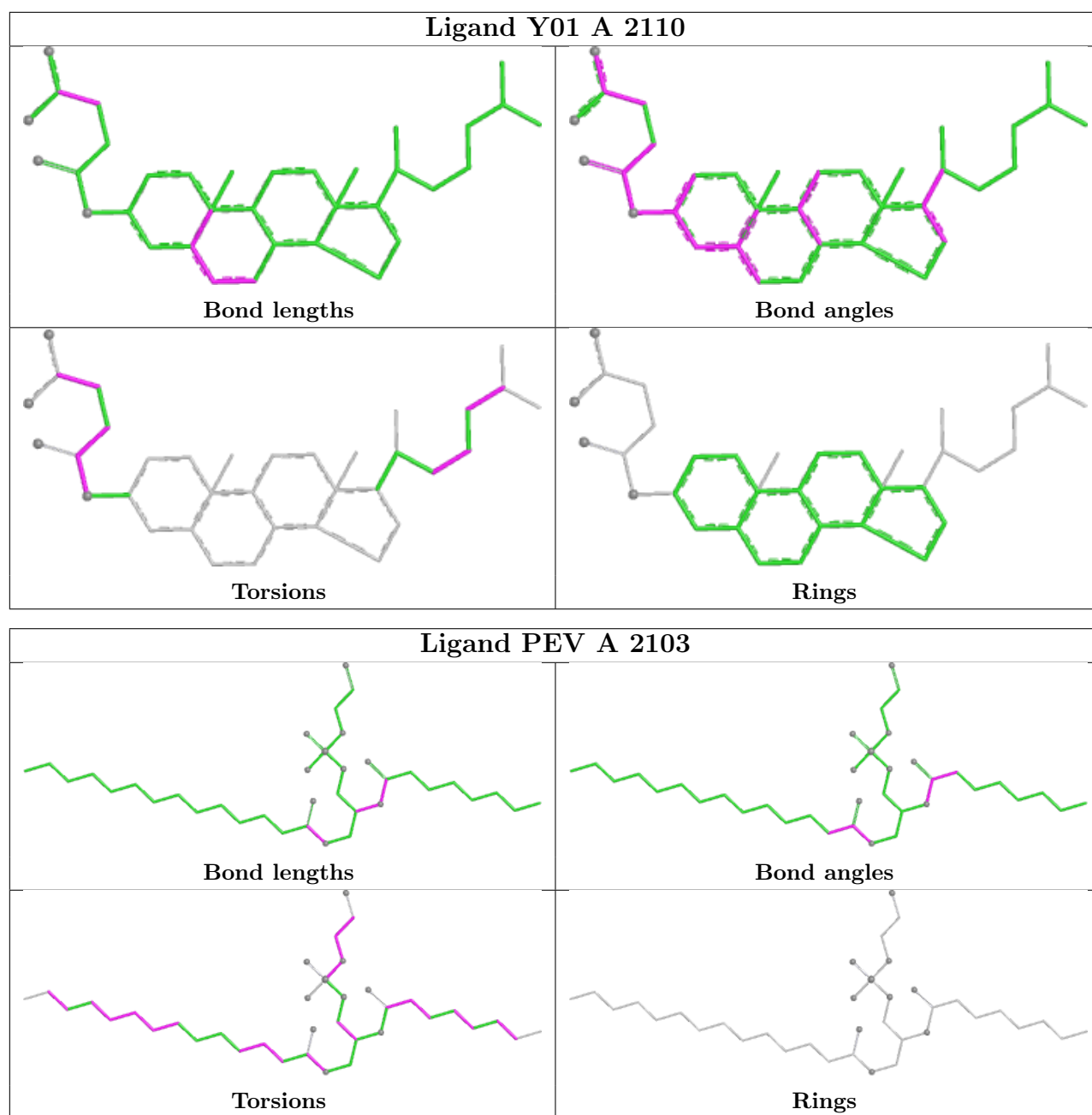
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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

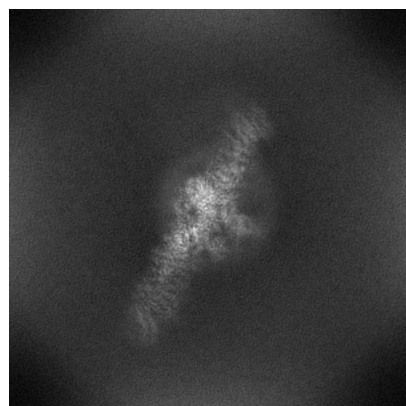
6 Map visualisation [i](#)

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.

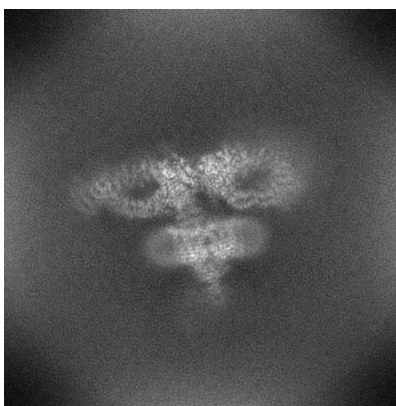
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

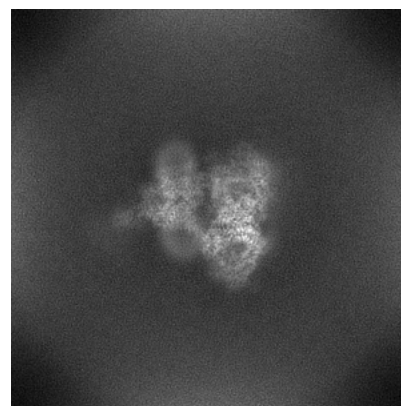
6.1.1 Primary map



X

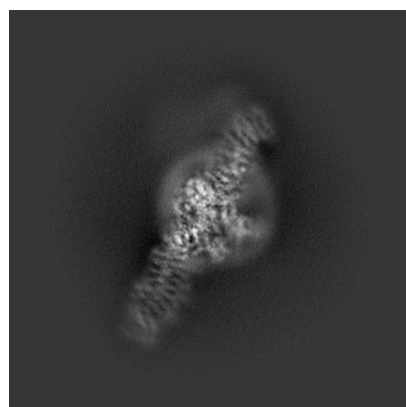


Y

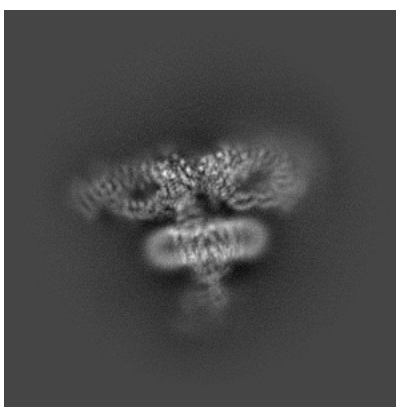


Z

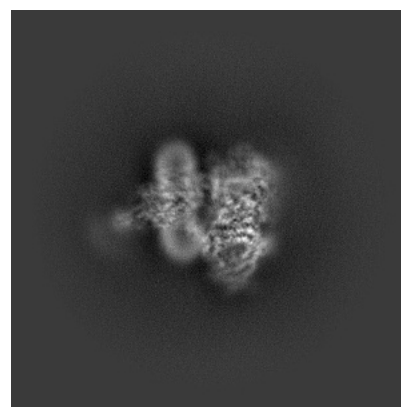
6.1.2 Raw map



X



Y



Z

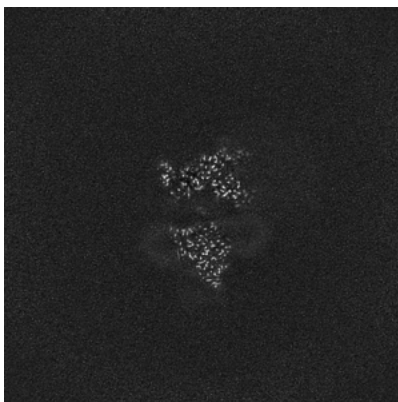
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

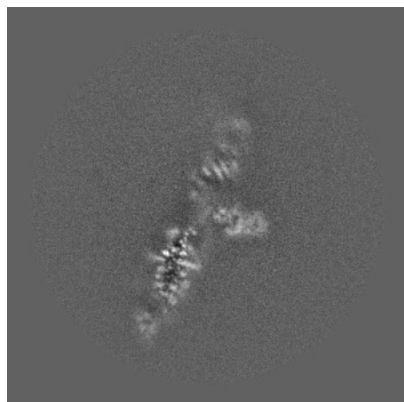


Y Index: 200

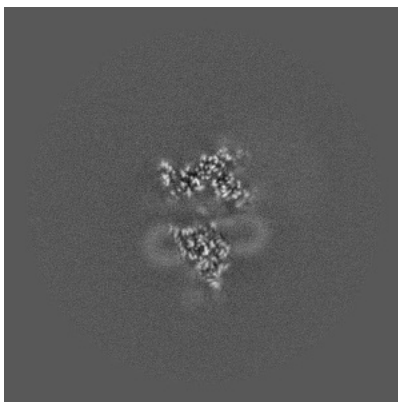


Z Index: 200

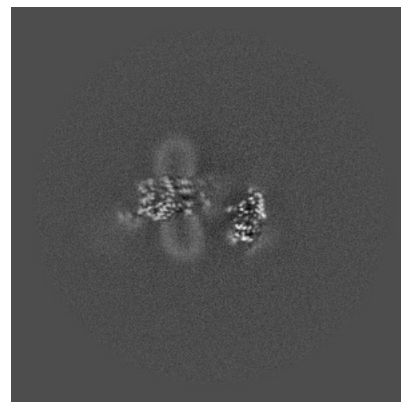
6.2.2 Raw map



X Index: 200



Y Index: 200

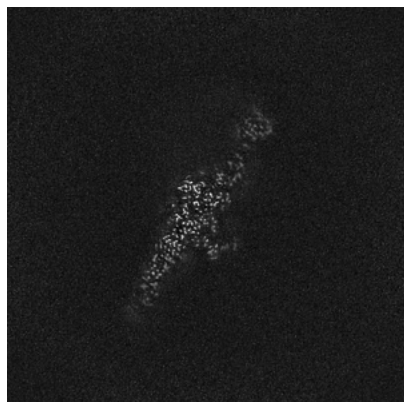


Z Index: 200

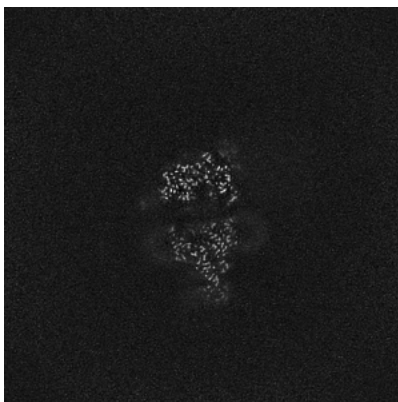
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 238

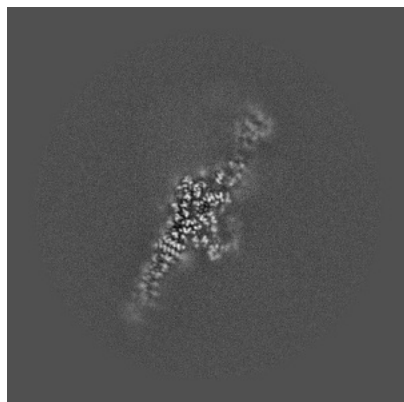


Y Index: 192

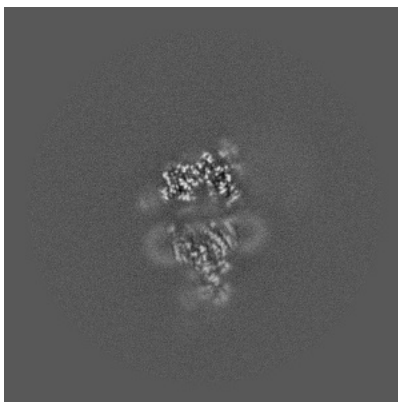


Z Index: 209

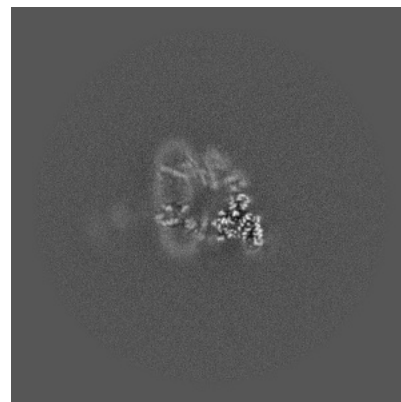
6.3.2 Raw map



X Index: 237



Y Index: 192

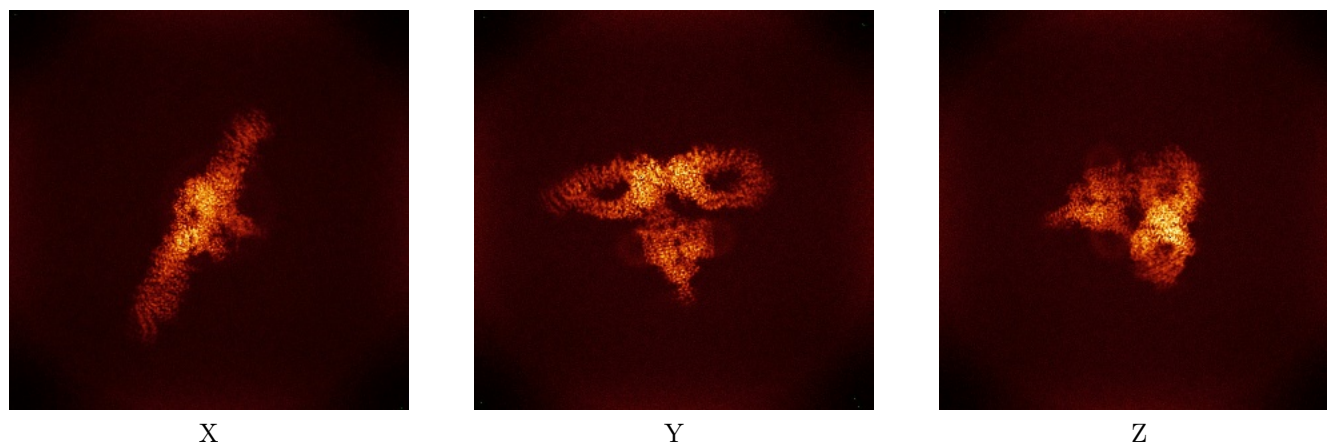


Z Index: 178

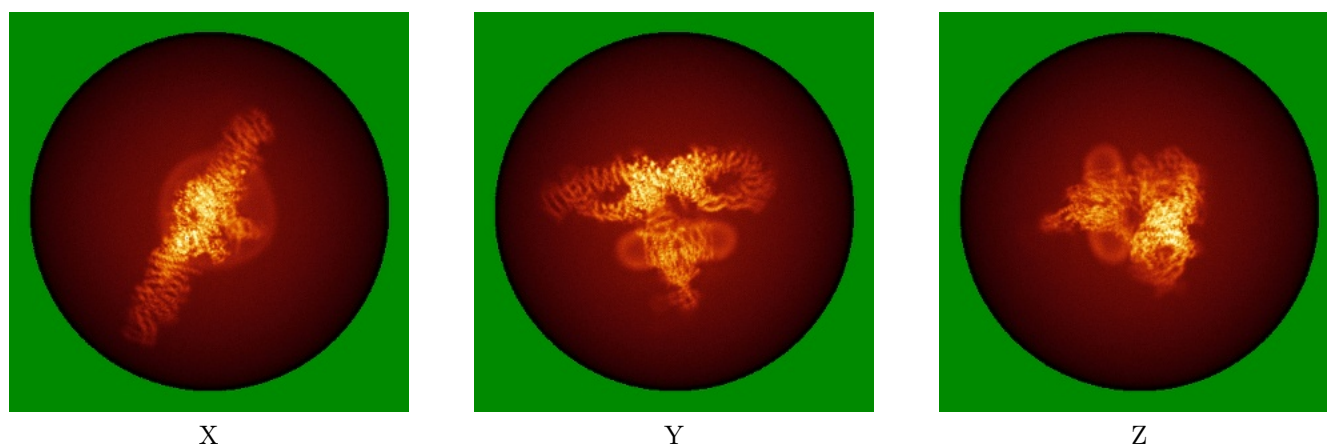
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

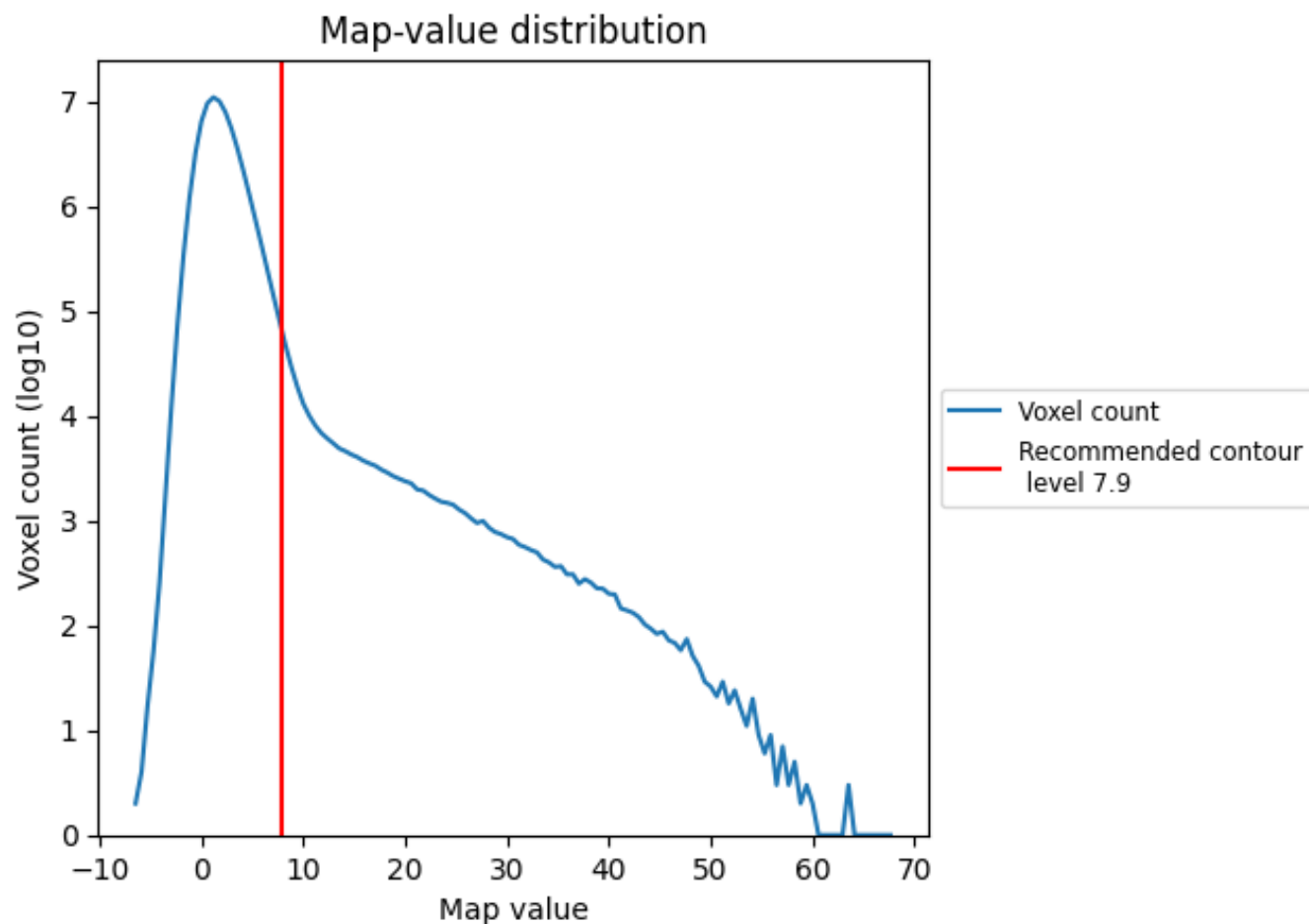
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

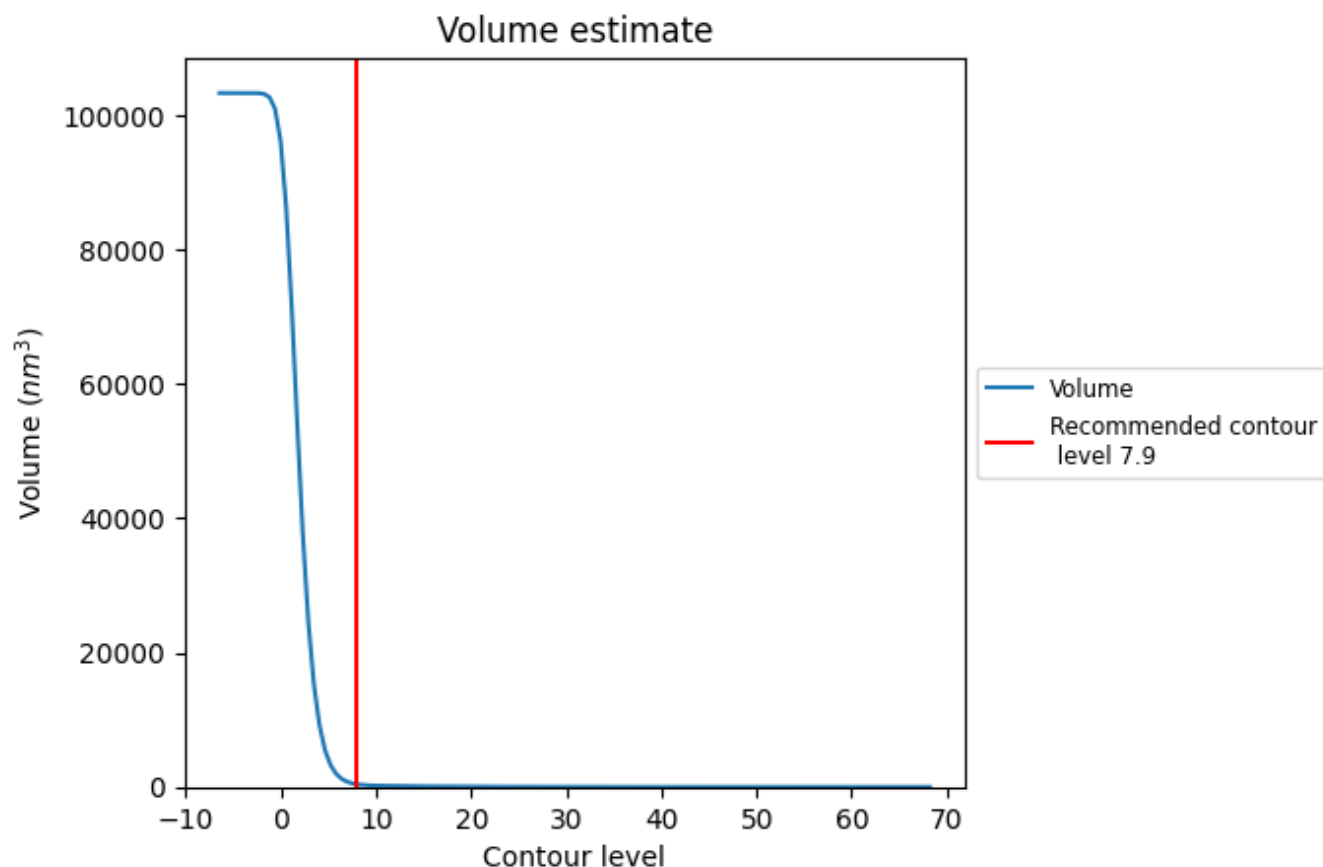
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

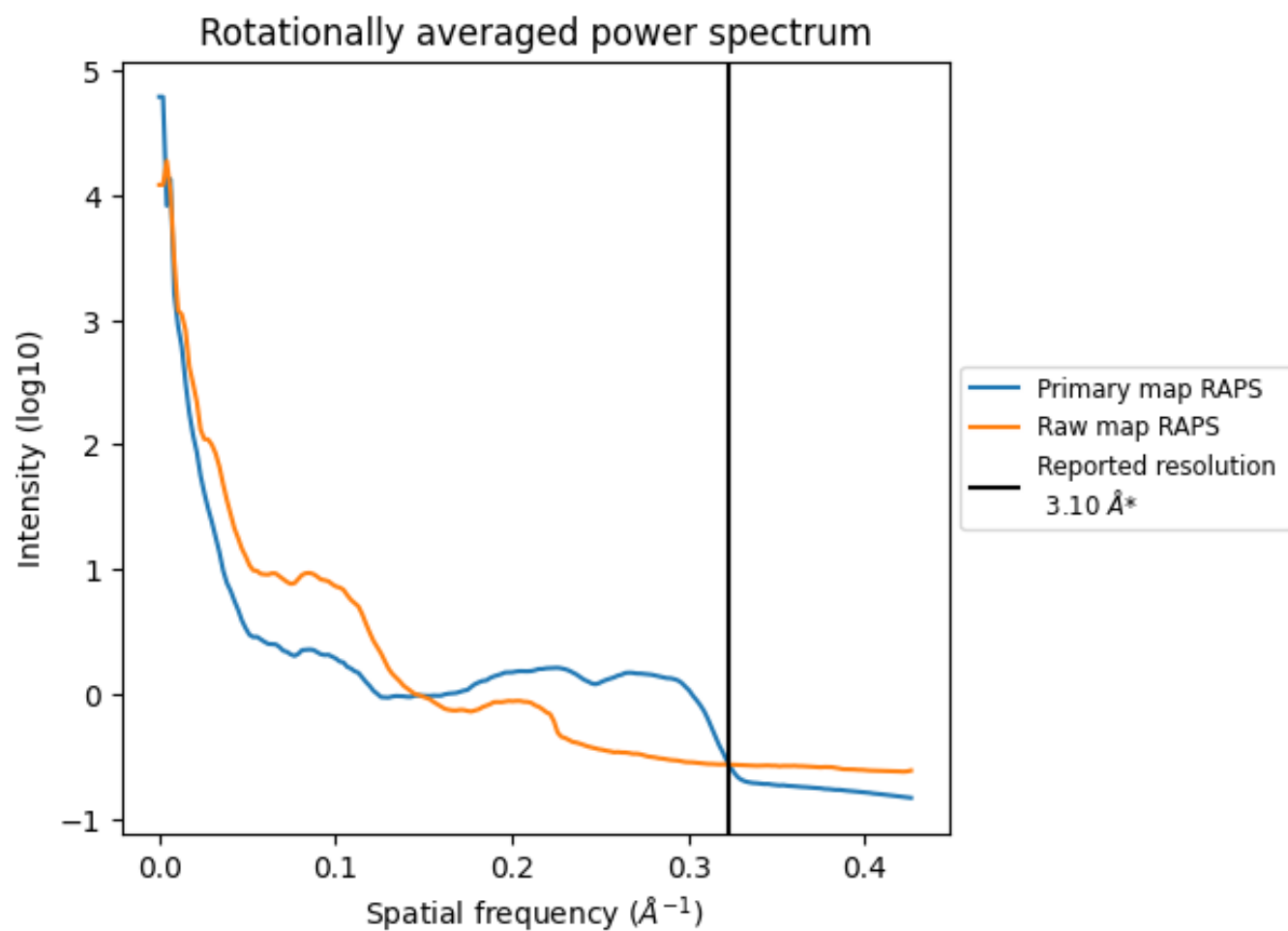
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

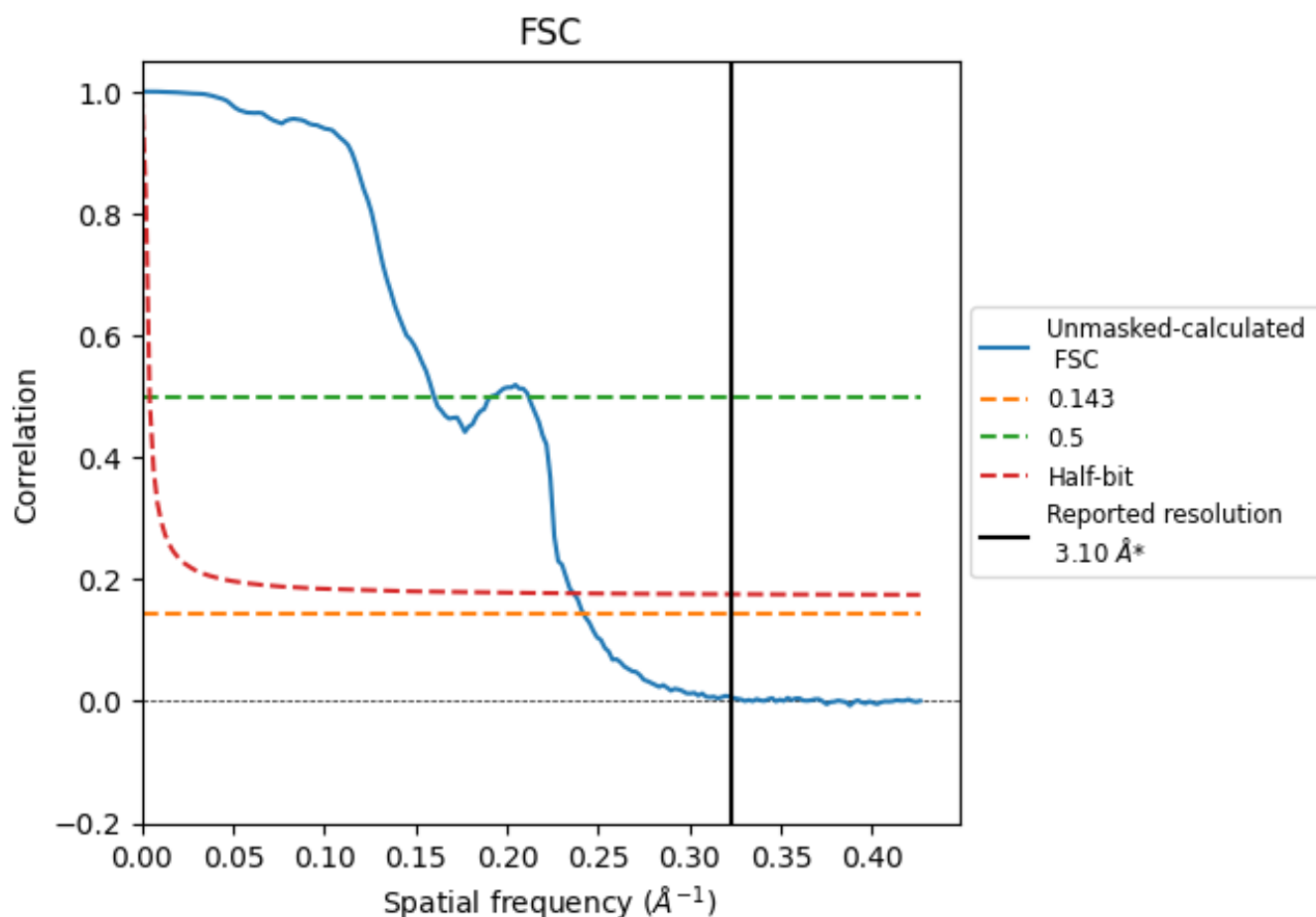


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

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 [i](#)

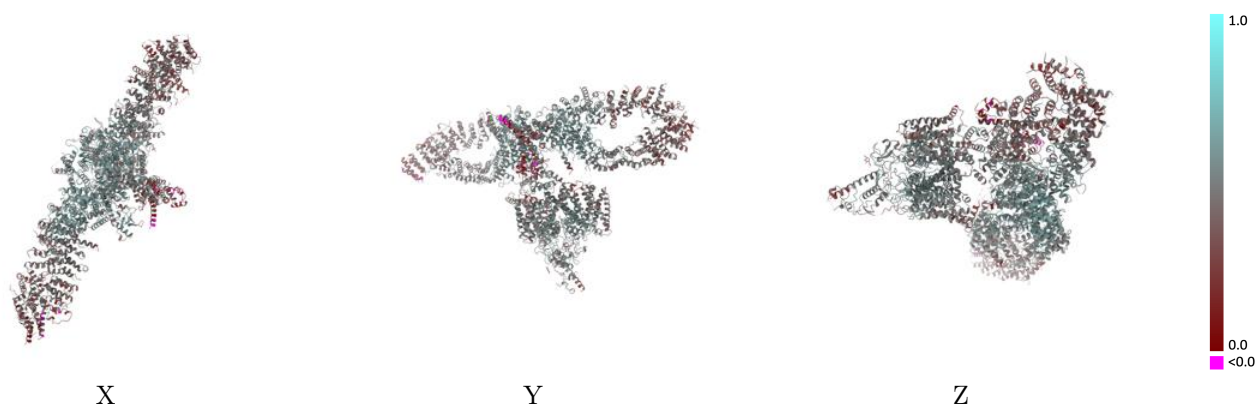
This section contains information regarding the fit between EMDB map EMD-25492 and PDB model 7SX3. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



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](#)

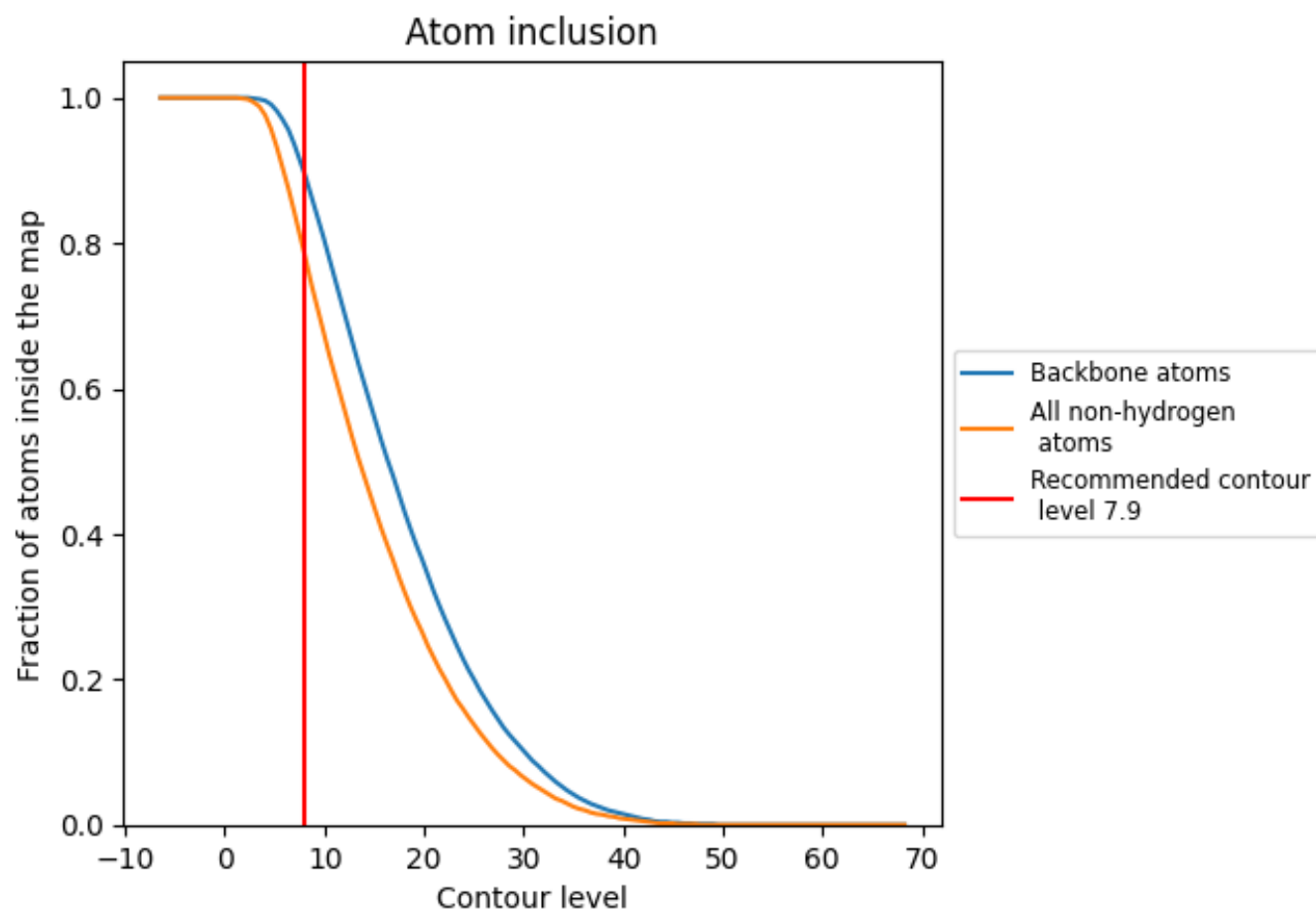


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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

