wwPDB EM Validation Summary Report (i)

Jun 24, 2023 – 12:26 PM EDT

PDB ID	:	8F7B
EMDB ID	:	EMD-28901
Title	:	LRRC8A(T48D):C conformation 2 top focus
Authors	:	Kern, D.M.; Brohawn, S.G.
Deposited on	:	2022-11-18
Resolution	:	3.15 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 (1)) were used in the production of this report:

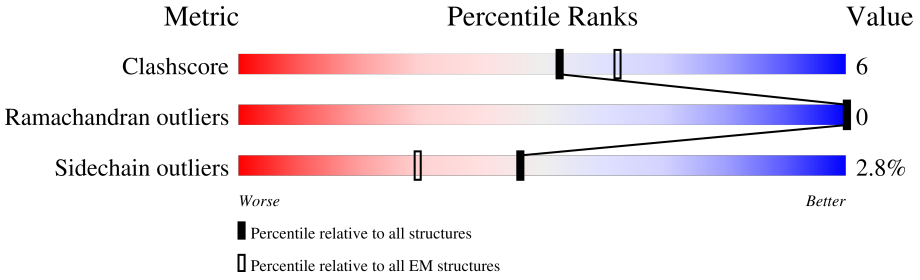
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.15 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	911	7% 30% 5% 65%
1	B	911	7% 30% 5% 65%
1	C	911	9% 27% 7% 65%
1	D	911	12% 28% 6% 65%
1	E	911	13% 29% 5% 65%
2	F	813	17% 31% 7% 62%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16166 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 Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	319	2672	1760	429	466	17	0	0
1	B	318	2668	1758	428	465	17	0	0
1	C	316	2654	1749	426	462	17	0	0
1	D	316	2648	1747	425	459	17	0	0
1	E	316	2652	1749	426	460	17	0	0

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ASP	THR	engineered mutation	UNP Q80WG5
A	68O	TRP	MET	conflict	UNP P0ABE7
A	72F	ILE	HIS	conflict	UNP P0ABE7
A	72J	LEU	PRO	conflict	UNP Q80WG5
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
B	48	ASP	THR	engineered mutation	UNP Q80WG5
B	68O	TRP	MET	conflict	UNP P0ABE7
B	72F	ILE	HIS	conflict	UNP P0ABE7
B	72J	LEU	PRO	conflict	UNP Q80WG5
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	813	SER	-	expression tag	UNP Q80WG5
B	814	LEU	-	expression tag	UNP Q80WG5
B	815	GLU	-	expression tag	UNP Q80WG5
B	816	VAL	-	expression tag	UNP Q80WG5
B	817	LEU	-	expression tag	UNP Q80WG5
B	818	PHE	-	expression tag	UNP Q80WG5
B	819	GLN	-	expression tag	UNP Q80WG5
C	48	ASP	THR	engineered mutation	UNP Q80WG5
C	68O	TRP	MET	conflict	UNP P0ABE7
C	72F	ILE	HIS	conflict	UNP P0ABE7
C	72J	LEU	PRO	conflict	UNP Q80WG5
C	811	SER	-	expression tag	UNP Q80WG5
C	812	ASN	-	expression tag	UNP Q80WG5
C	813	SER	-	expression tag	UNP Q80WG5
C	814	LEU	-	expression tag	UNP Q80WG5
C	815	GLU	-	expression tag	UNP Q80WG5
C	816	VAL	-	expression tag	UNP Q80WG5
C	817	LEU	-	expression tag	UNP Q80WG5
C	818	PHE	-	expression tag	UNP Q80WG5
C	819	GLN	-	expression tag	UNP Q80WG5
D	48	ASP	THR	engineered mutation	UNP Q80WG5
D	68O	TRP	MET	conflict	UNP P0ABE7
D	72F	ILE	HIS	conflict	UNP P0ABE7
D	72J	LEU	PRO	conflict	UNP Q80WG5
D	811	SER	-	expression tag	UNP Q80WG5
D	812	ASN	-	expression tag	UNP Q80WG5
D	813	SER	-	expression tag	UNP Q80WG5
D	814	LEU	-	expression tag	UNP Q80WG5
D	815	GLU	-	expression tag	UNP Q80WG5
D	816	VAL	-	expression tag	UNP Q80WG5
D	817	LEU	-	expression tag	UNP Q80WG5
D	818	PHE	-	expression tag	UNP Q80WG5
D	819	GLN	-	expression tag	UNP Q80WG5
E	48	ASP	THR	engineered mutation	UNP Q80WG5
E	68O	TRP	MET	conflict	UNP P0ABE7
E	72F	ILE	HIS	conflict	UNP P0ABE7
E	72J	LEU	PRO	conflict	UNP Q80WG5
E	811	SER	-	expression tag	UNP Q80WG5
E	812	ASN	-	expression tag	UNP Q80WG5
E	813	SER	-	expression tag	UNP Q80WG5
E	814	LEU	-	expression tag	UNP Q80WG5
E	815	GLU	-	expression tag	UNP Q80WG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	816	VAL	-	expression tag	UNP Q80WG5
E	817	LEU	-	expression tag	UNP Q80WG5
E	818	PHE	-	expression tag	UNP Q80WG5
E	819	GLN	-	expression tag	UNP Q80WG5

- Molecule 2 is a protein called Volume-regulated anion channel subunit LRRC8C.

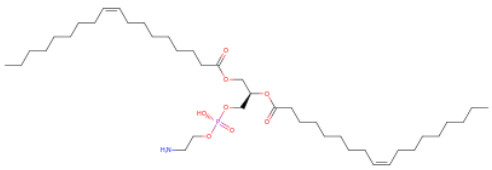
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	309	2569	1692	407	449	21	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	804	SER	-	expression tag	UNP Q8R502
F	805	ASN	-	expression tag	UNP Q8R502
F	806	SER	-	expression tag	UNP Q8R502
F	807	GLU	-	expression tag	UNP Q8R502
F	808	ASN	-	expression tag	UNP Q8R502
F	809	LEU	-	expression tag	UNP Q8R502
F	810	TYR	-	expression tag	UNP Q8R502
F	811	PHE	-	expression tag	UNP Q8R502
F	812	GLN	-	expression tag	UNP Q8R502
F	813	GLY	-	expression tag	UNP Q8R502

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).

PEE



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	23	15	1	6	1	0
			Total	C	O			
3	A	1	13	11	2			0
			Total	C	O			
3	A	1	13	11	2			0
			Total	C	N	O	P	
3	B	1	26	18	1	6	1	0
			Total	C	O			
3	B	1	11	9	2			0
			Total	C	O			
3	B	1	10	8	2			0
			Total	C	N	O	P	
3	C	1	26	18	1	6	1	0
			Total	C	O			
3	C	1	11	9	2			0
			Total	C	N	O	P	
3	D	1	38	28	1	8	1	0
			Total	C	O			
3	D	1	9	7	2			0
			Total	C	O			
3	D	1	11	9	2			0
			Total	C	N	O	P	
3	E	1	27	19	1	6	1	0
			Total	C	O			
3	E	1	10	8	2			0
			Total	C	O			
3	E	1	10	8	2			0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	F	1	40	30	1	8	1	0
			Total	C	O			
3	F	1	11	9	2			0
			Total	C	O			
3	F	1	8	6	2			0

- Molecule 4 is water.

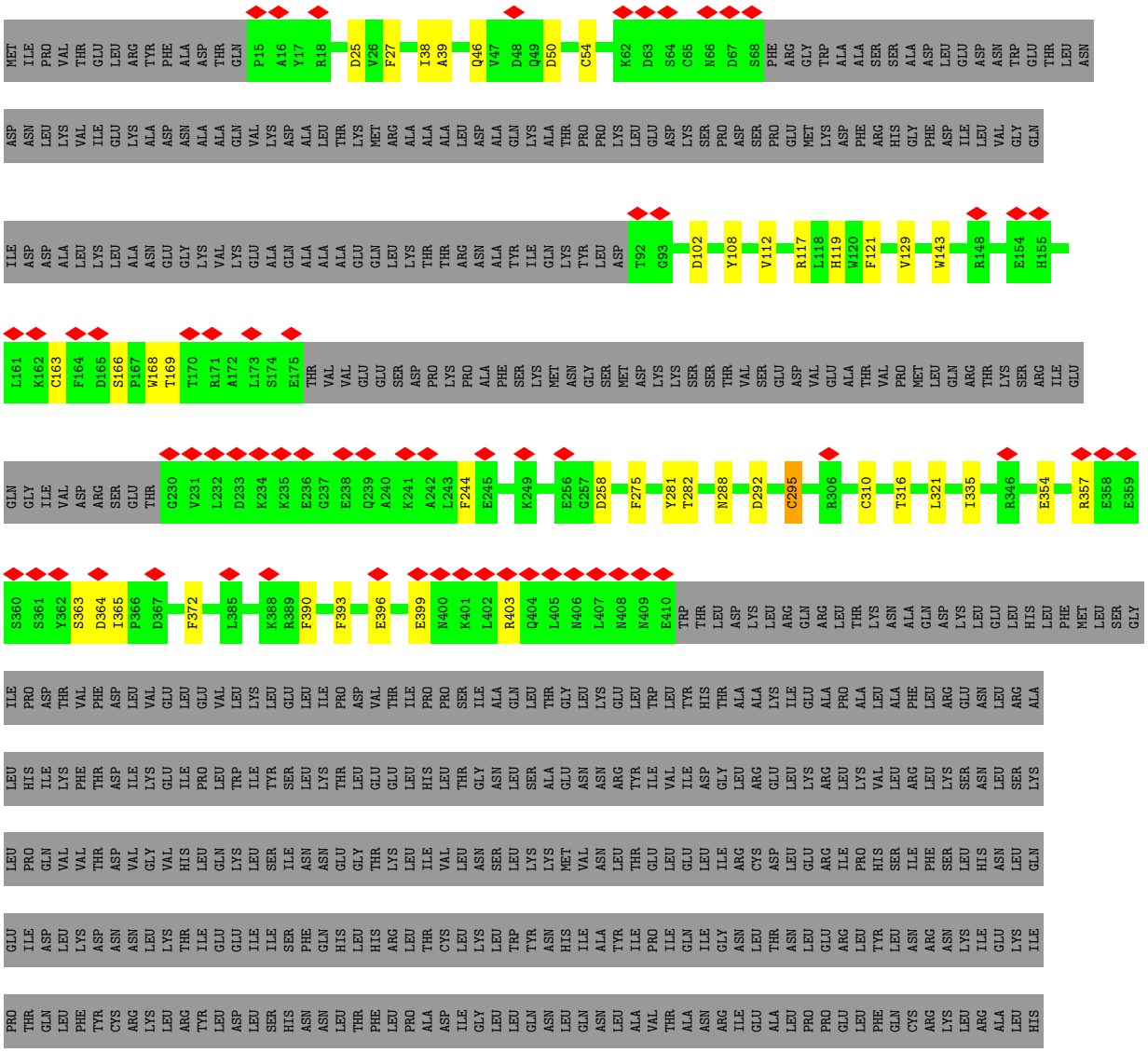
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
4	A	1	1	1	0
			Total	O	
4	B	1	1	1	0
			Total	O	
4	C	1	1	1	0
			Total	O	
4	D	1	1	1	0
			Total	O	
4	E	1	1	1	0
			Total	O	
4	F	1	1	1	0

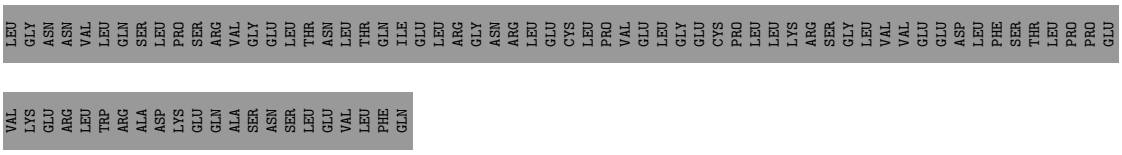
3 Residue-property plots (i)

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: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

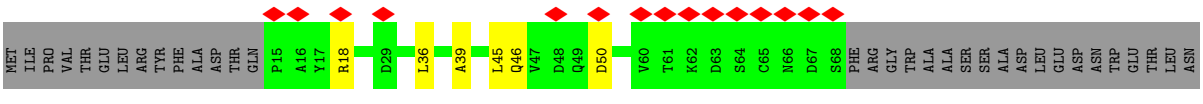
Chain A: 7% 30% 5% 65%

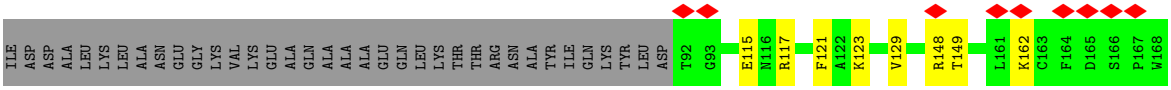


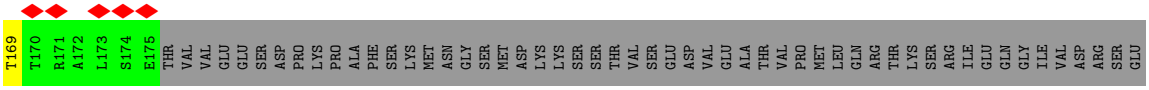


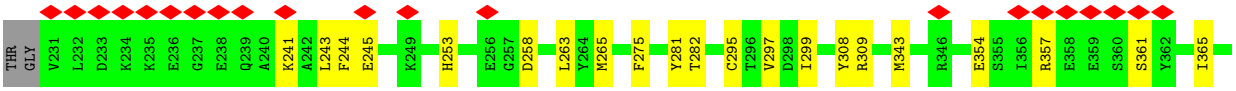
• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

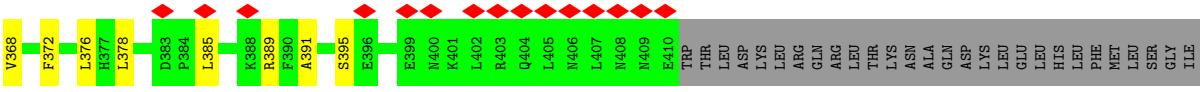
Chain B:

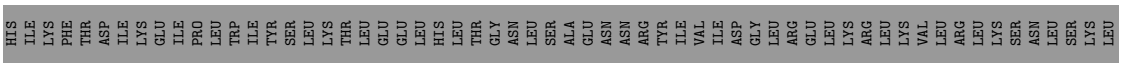


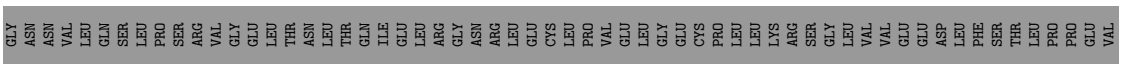


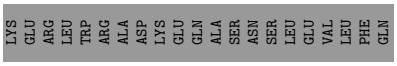






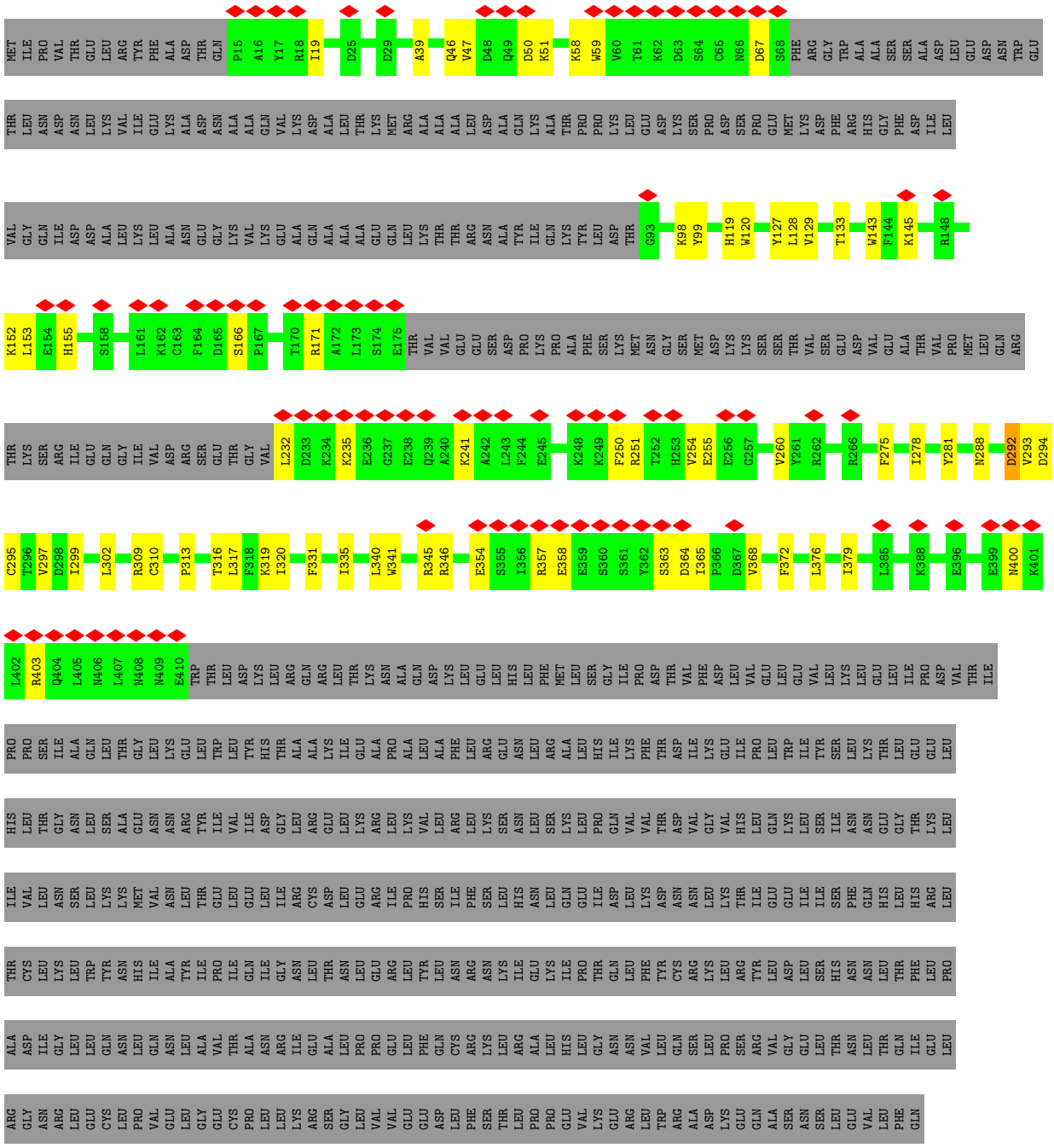






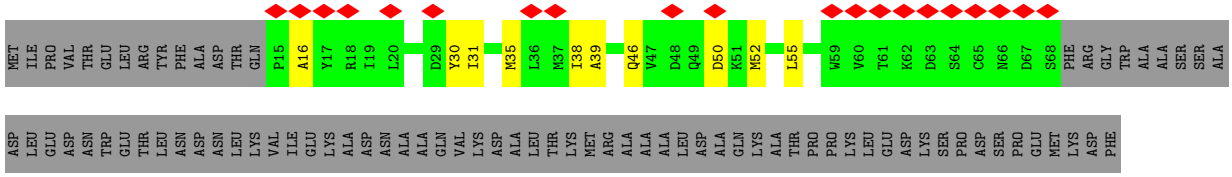
• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

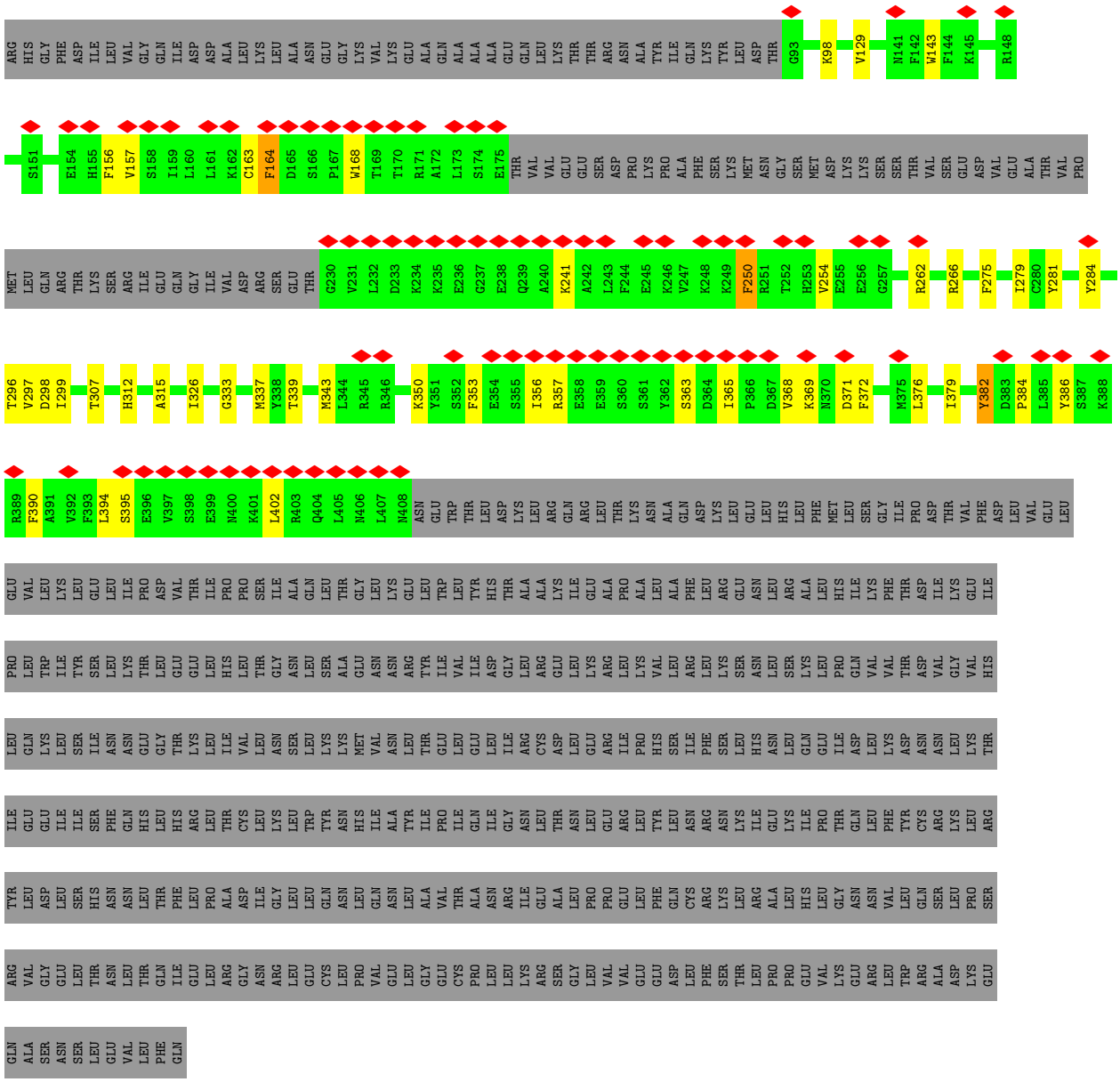
Chain C:



• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

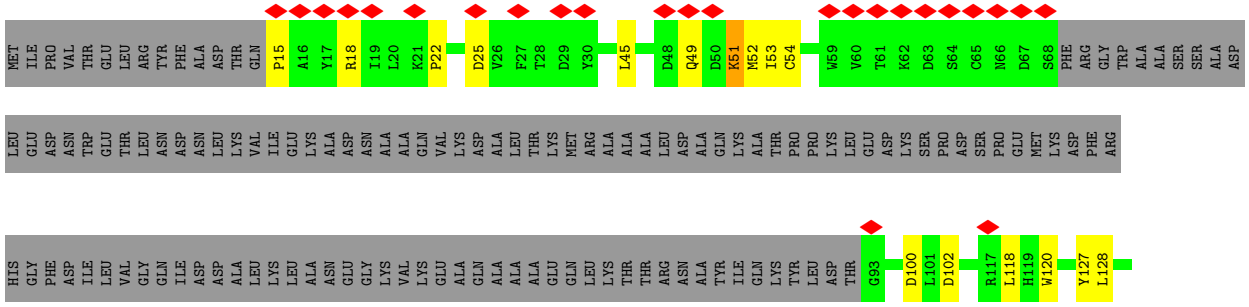
Chain D:

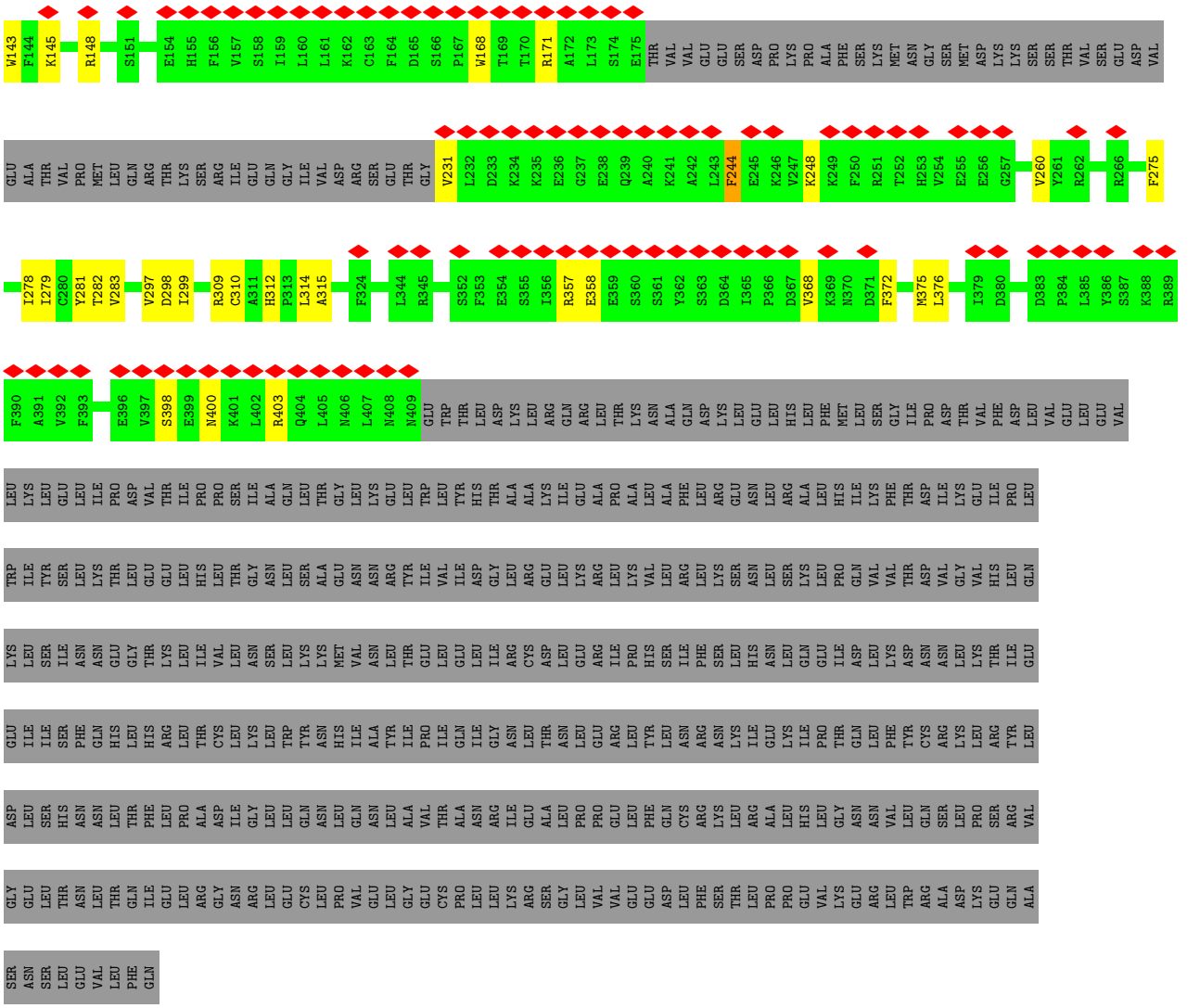




• Molecule 1: Volume-regulated anion channel subunit LRRC8A,Soluble cytochrome b562

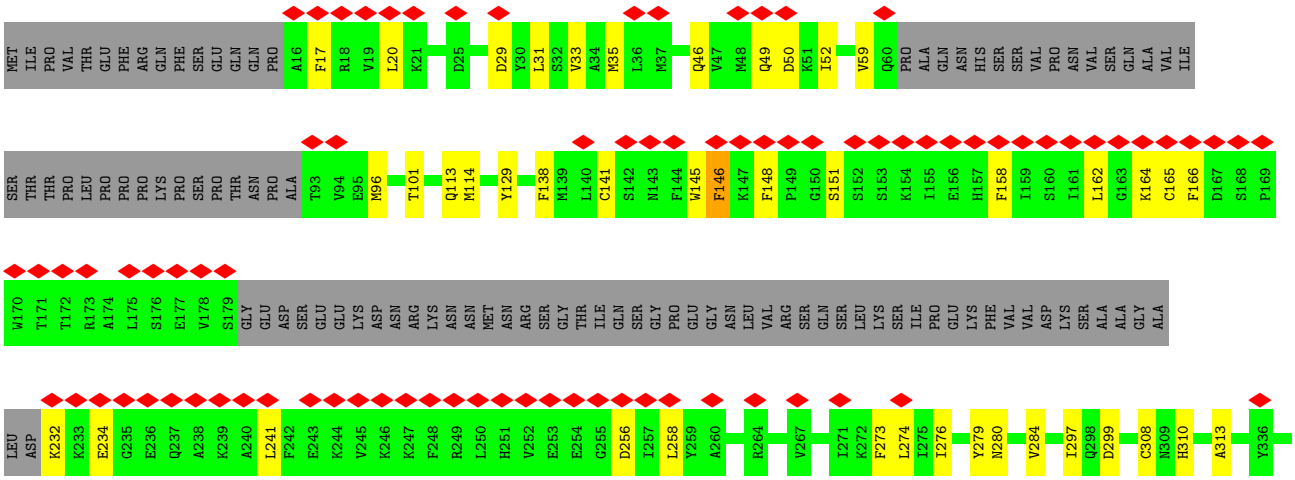
Chain E:

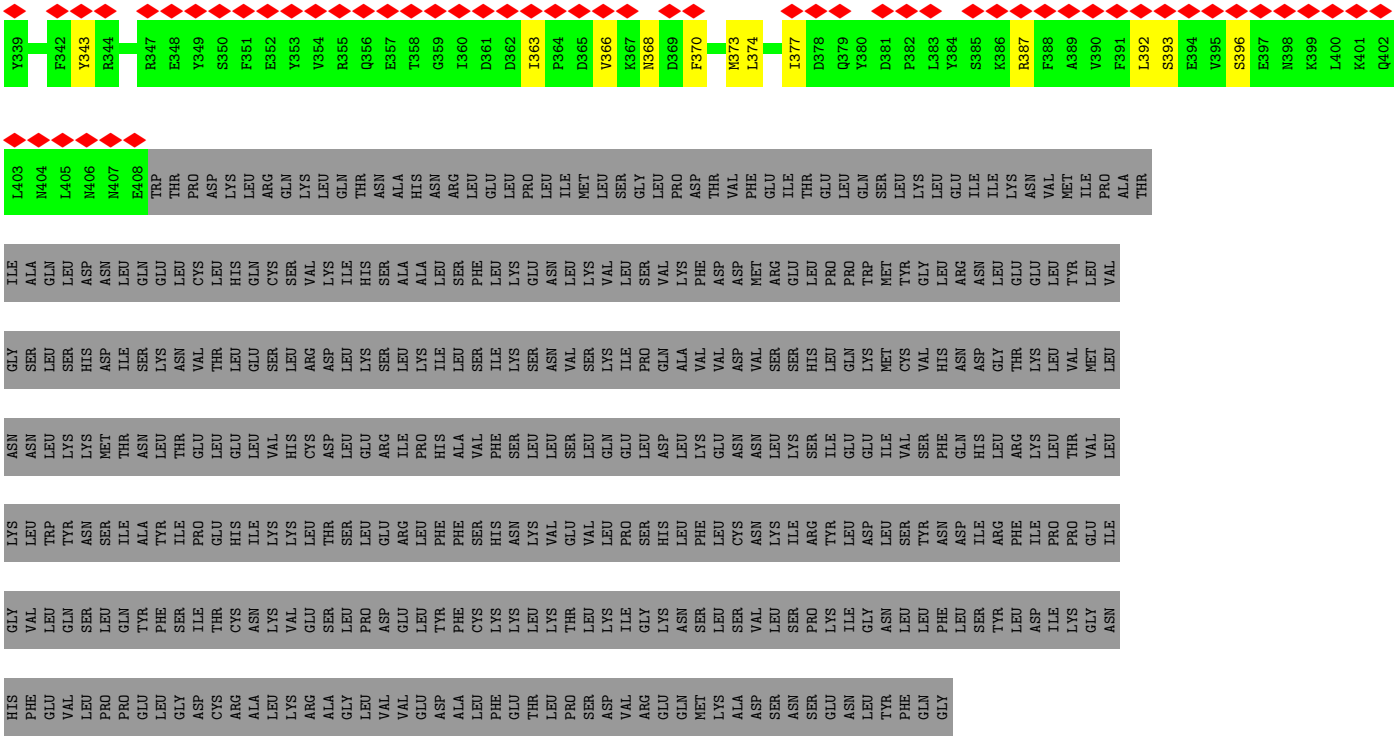




- Molecule 2: Volume-regulated anion channel subunit LRRC8C

Chain F:




Y339 F342 Y343 R344 R347 E348 Y349 S350 F351 E352 Y353 V354 R355 Q356 E357 T358 G359 I360 D361 D362 I363 P364 D365 V366 K367 N368 D369 F370 M373 L374 I377 D378 Q379 Y380 D381 P382 L383 Y384 S385 K386 R387 F388 A389 V390 F391 L392 S393 E394 V395 S396 E397 N398 K399 L400 K401 Q402
L403 N404 L405 N406 N407 E408 TRP THR PRO ASP LYS LEU ARG GLN LYS LEU GLN THR ASN ALA HIS ASN ARG LEU GLU LEU PRO LEU ILE MET LEU SER GLY LEU PRO ASP THR VAL PHE GLU ILE THR GLU LEU GLN SER LEU LYS LEU GLU ILE ILE LYS ASN VAL MET ILE PRO ALA THR
ILE ALA GLN LEU ASP ASN LEU GLN GLU LEU CYS LEU HIS GLN CYS SER VAL LYS ILE HIS SER ALA ALA LEU SER PHE LEU LYS GLU ASN LEU LYS VAL LEU SER VAL LYS PHE ASP ASP MET ARG GLU LEU PRO PRO TRP MET TYR GLY LEU ARG ASN LEU GLU GLU LEU TYR TRP VAL
GLY SER LEU SER HIS ASP ILE SER LYS ASN VAL THR LEU GLU SER LEU ARG ASP LEU LYS SER LEU ILE LEU SER ILE LYS SER ASN VAL SER LYS ILE PRO GLN ALA VAL VAL ASP VAL SER SER HIS LEU GLN GLN LYS MET CYS VAL HIS ASN ASP GLY THR LYS LEU VAL MET LEU
ASN ASN LEU LYS LYS MET THR ASN LEU THR GLU LEU GLU LEU VAL HIS CYS ASP LEU GLU ARG ILE PRO HIS ALA VAL PHE SER LEU LEU LEU SER LEU GLN GLU LEU ASP LEU LYS GLU ASN ASN LEU LYS SER ILE GLU GLU ILE VAL SER PHE GLN HIS LEU ARG LYS LEU THR VAL LEU
LYS LEU TRP TYR ASN SER ILE ALA TYR ILE PRO GLU HIS ILE LYS LYS LEU THR SER LEU GLU ARG LEU PHE PHE SER HIS ASN LYS VAL GLU VAL LEU PRO SER HIS LEU PHE LEU CYS ASN LYS ILE ARG TYR LEU ASP LEU SER TYR ASN ASP ILE ARG PHE ILE PRO PRO GLU ILE
GLY VAL LEU GLN SER LEU GLN TYR PHE SER ILE THR CYS ASN LYS VAL GLU SER LEU PRO ASP GLU LEU TYR PHE CYS LYS LYS LEU LYS THR LEU LYS ILE GLY LYS ASN SER LEU SER VAL LEU SER PRO LYS ILE GLY ASN LEU LEU PHE LEU SER TYR LEU ASP ILE LYS GLY ASN
HIS PHE GLU VAL LEU PRO PRO GLU LEU GLY ASP CYS ARG ALA LEU LYS ARG ALA GLY LEU VAL VAL GLU ASP ALA LEU PHE GLU THR LEU PRO SER ASP VAL ARG GLU GLN MET LYS ALA ASP SER ASN SER GLU ASN LEU TYR PHE GLN GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71566	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.279	Depositor
Minimum map value	-2.201	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	435.968, 435.968, 435.968	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: PEE

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	0.28	0/2747	0.50	0/3719
1	B	0.28	0/2743	0.47	0/3714
1	C	0.28	0/2729	0.50	0/3694
1	D	0.27	0/2723	0.48	0/3686
1	E	0.27	0/2727	0.49	0/3692
2	F	0.28	0/2636	0.48	0/3559
All	All	0.28	0/16305	0.49	0/22064

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	2672	0	2657	24	0
1	B	2668	0	2654	25	0
1	C	2654	0	2638	44	0
1	D	2648	0	2638	40	0
1	E	2652	0	2641	31	0
2	F	2569	0	2559	28	0
3	A	49	0	63	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	47	0	59	1	0
3	C	37	0	47	1	0
3	D	58	0	74	2	0
3	E	47	0	59	2	0
3	F	59	0	76	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	16166	0	16165	182	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 6.

The worst 5 of 182 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:D:350:LYS:HE2	1:D:369:LYS:CE	1.48	1.42
1:D:350:LYS:CE	1:D:369:LYS:HE2	1.66	1.23
1:D:350:LYS:CD	1:D:369:LYS:HG2	1.97	0.95
1:D:350:LYS:HD2	1:D:369:LYS:HG2	1.50	0.93
1:D:350:LYS:HE2	1:D:369:LYS:HE2	0.87	0.86

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	313/911 (34%)	307 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/911 (34%)	307 (98%)	5 (2%)	0	100	100
1	C	310/911 (34%)	303 (98%)	7 (2%)	0	100	100
1	D	310/911 (34%)	303 (98%)	7 (2%)	0	100	100
1	E	310/911 (34%)	298 (96%)	12 (4%)	0	100	100
2	F	303/813 (37%)	295 (97%)	8 (3%)	0	100	100
All	All	1858/5368 (35%)	1813 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/830 (36%)	289 (98%)	7 (2%)	49	76
1	B	296/830 (36%)	290 (98%)	6 (2%)	55	79
1	C	294/830 (35%)	287 (98%)	7 (2%)	49	76
1	D	293/830 (35%)	283 (97%)	10 (3%)	37	68
1	E	294/830 (35%)	288 (98%)	6 (2%)	55	79
2	F	286/756 (38%)	273 (96%)	13 (4%)	27	61
All	All	1759/4906 (36%)	1710 (97%)	49 (3%)	46	73

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	298	ASP
1	E	298	ASP
1	D	382	TYR
1	E	244	PHE
2	F	96	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	288	ASN
2	F	112	ASN
2	F	113	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
3	PEE	B	903	-	9,9,50	0.62	0	9,9,55	0.79	0
3	PEE	F	902	-	10,10,50	0.59	0	10,10,55	0.80	0
3	PEE	E	901	-	26,26,50	1.45	2 (7%)	28,29,55	1.11	1 (3%)
3	PEE	E	903	-	9,9,50	0.62	0	9,9,55	0.80	0
3	PEE	D	902	-	8,8,50	0.64	0	8,8,55	0.85	0
3	PEE	A	903	-	12,12,50	1.08	1 (8%)	12,12,55	1.11	1 (8%)
3	PEE	A	901	-	22,22,50	1.51	3 (13%)	24,25,55	1.26	2 (8%)
3	PEE	B	902	-	10,10,50	1.61	2 (20%)	10,10,55	1.55	2 (20%)
3	PEE	C	902	-	10,10,50	0.60	0	10,10,55	0.79	0
3	PEE	D	901	-	37,37,50	1.31	2 (5%)	40,42,55	0.99	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEE	F	901	-	39,39,50	1.39	3 (7%)	42,44,55	1.06	2 (4%)
3	PEE	F	903	-	7,7,50	0.68	0	7,7,55	0.87	0
3	PEE	D	903	-	10,10,50	0.59	0	10,10,55	0.80	0
3	PEE	C	901	-	25,25,50	1.47	3 (12%)	27,28,55	1.13	1 (3%)
3	PEE	E	902	-	9,9,50	0.62	0	9,9,55	0.81	0
3	PEE	B	901	-	25,25,50	1.49	2 (8%)	27,28,55	1.14	1 (3%)
3	PEE	A	902	-	12,12,50	1.09	1 (8%)	12,12,55	1.10	1 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	B	903	-	-	4/7/7/54	-
3	PEE	F	902	-	-	5/8/8/54	-
3	PEE	E	901	-	-	8/27/27/54	-
3	PEE	E	903	-	-	4/7/7/54	-
3	PEE	D	902	-	-	3/6/6/54	-
3	PEE	A	903	-	-	7/10/10/54	-
3	PEE	A	901	-	-	7/23/23/54	-
3	PEE	B	902	-	-	5/8/8/54	-
3	PEE	C	902	-	-	4/8/8/54	-
3	PEE	D	901	-	-	17/41/41/54	-
3	PEE	F	901	-	-	21/43/43/54	-
3	PEE	F	903	-	-	3/5/5/54	-
3	PEE	D	903	-	-	4/8/8/54	-
3	PEE	C	901	-	-	8/26/26/54	-
3	PEE	E	902	-	-	5/7/7/54	-
3	PEE	B	901	-	-	15/26/26/54	-
3	PEE	A	902	-	-	7/10/10/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	PEE	P-O4P	4.81	1.78	1.59
3	E	901	PEE	P-O4P	4.67	1.78	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	PEE	P-O4P	4.66	1.78	1.59
3	A	901	PEE	P-O4P	4.62	1.78	1.59
3	D	901	PEE	P-O4P	4.62	1.78	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	901	PEE	O2P-P-O1P	4.26	133.31	112.24
3	A	901	PEE	O2P-P-O1P	4.26	133.28	112.24
3	C	901	PEE	O2P-P-O1P	4.25	133.23	112.24
3	B	901	PEE	O2P-P-O1P	4.24	133.21	112.24
3	E	901	PEE	O2P-P-O1P	4.24	133.19	112.24

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	PEE	C17-C18-C19-C20
3	A	901	PEE	C4-O4P-P-O2P
3	A	901	PEE	O4P-C4-C5-N
3	B	901	PEE	C1-O3P-P-O1P
3	B	901	PEE	C4-O4P-P-O3P

There are no ring outliers.

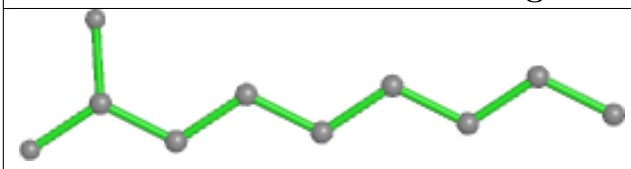
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	901	PEE	1	0
3	D	901	PEE	2	0
3	F	901	PEE	1	0
3	C	901	PEE	1	0
3	E	902	PEE	1	0
3	B	901	PEE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 PEE B 903



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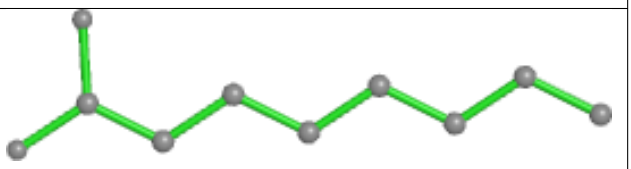

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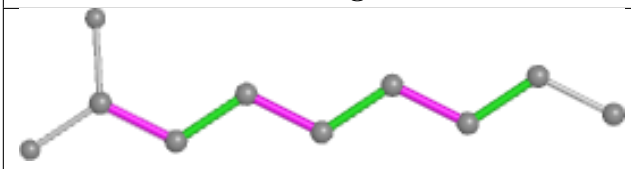

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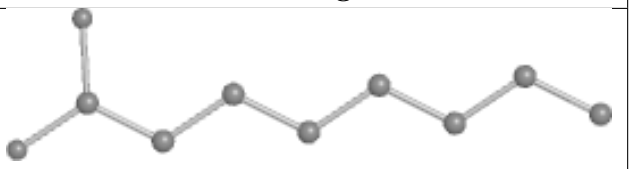
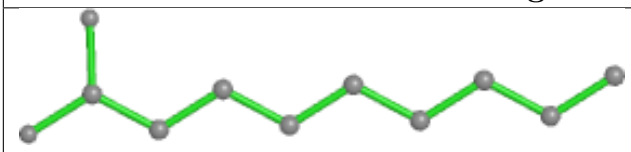


Rings

Ligand PEE F 902



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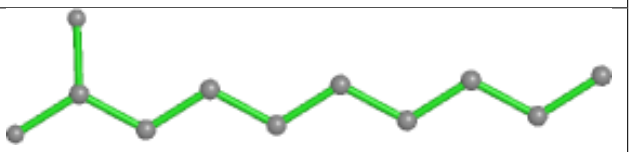

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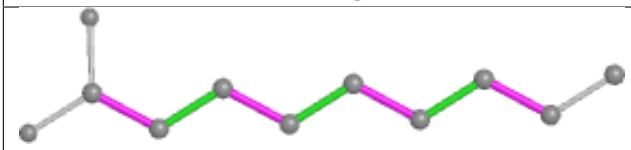

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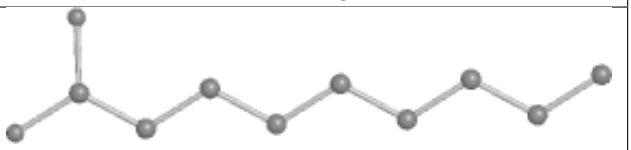
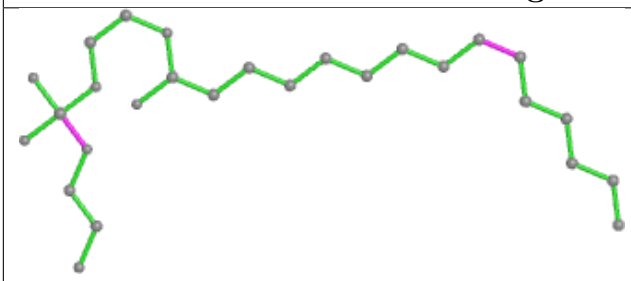


Rings

Ligand PEE E 901



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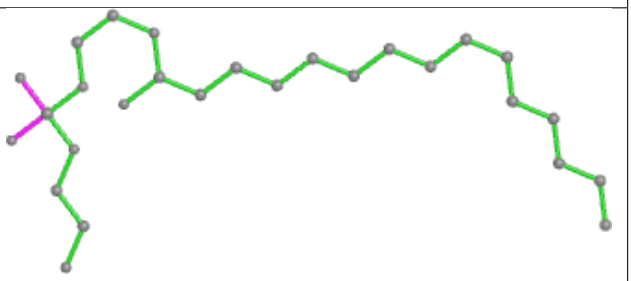

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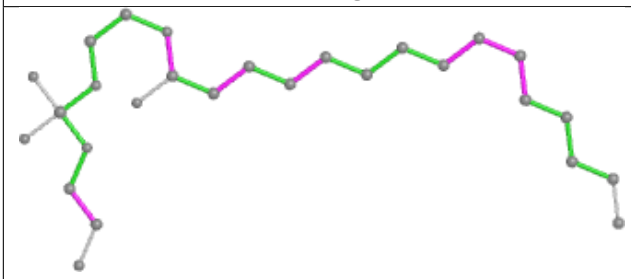
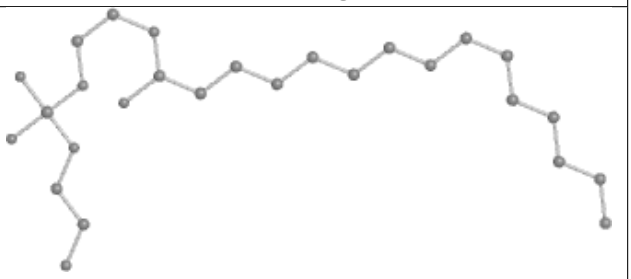


Torsions



Rings

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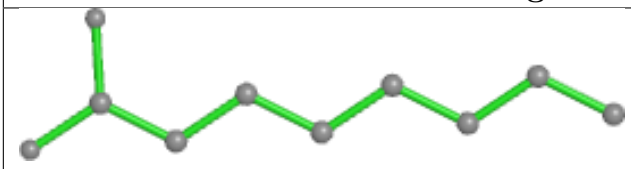
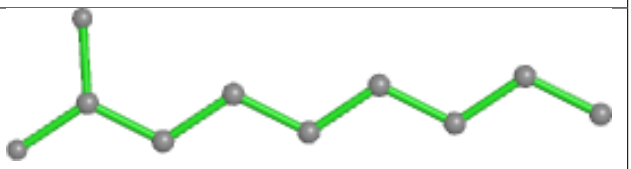
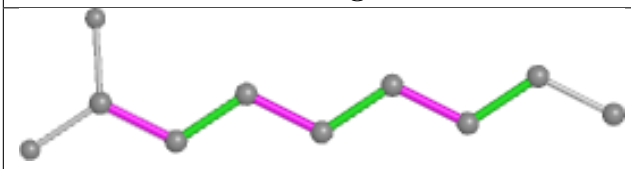
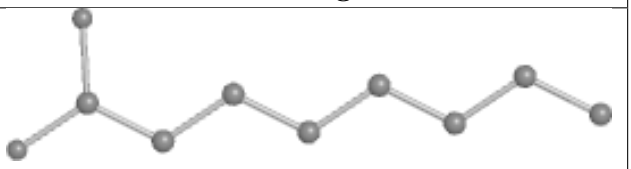
 Bond lengths	 Bond angles
 Torsions	 Rings

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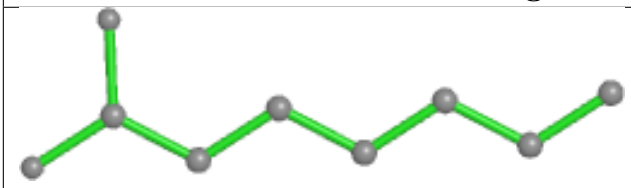
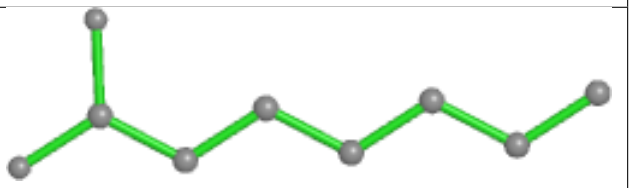
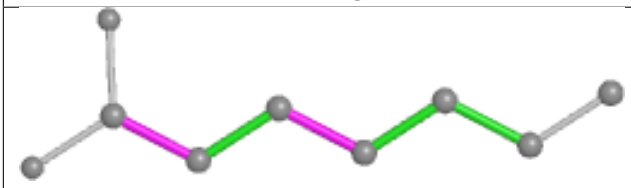
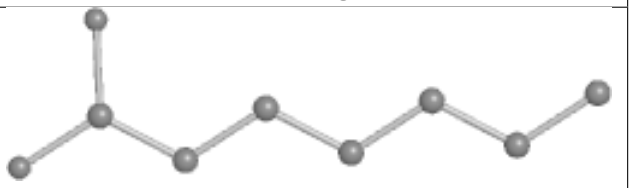
 Bond lengths	 Bond angles
 Torsions	 Rings

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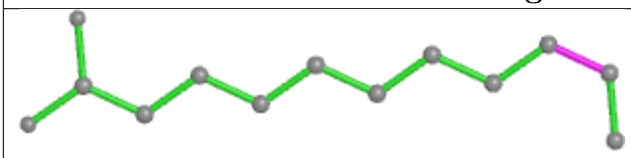
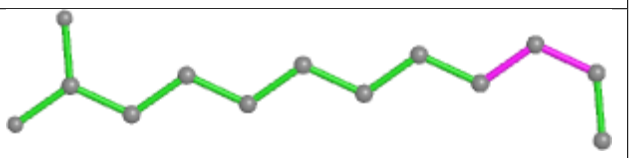
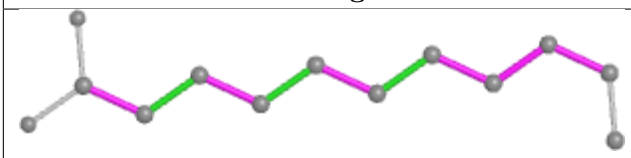
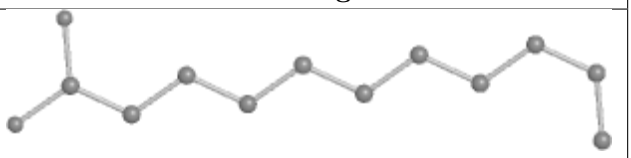
 Bond lengths	 Bond angles
 Torsions	 Rings

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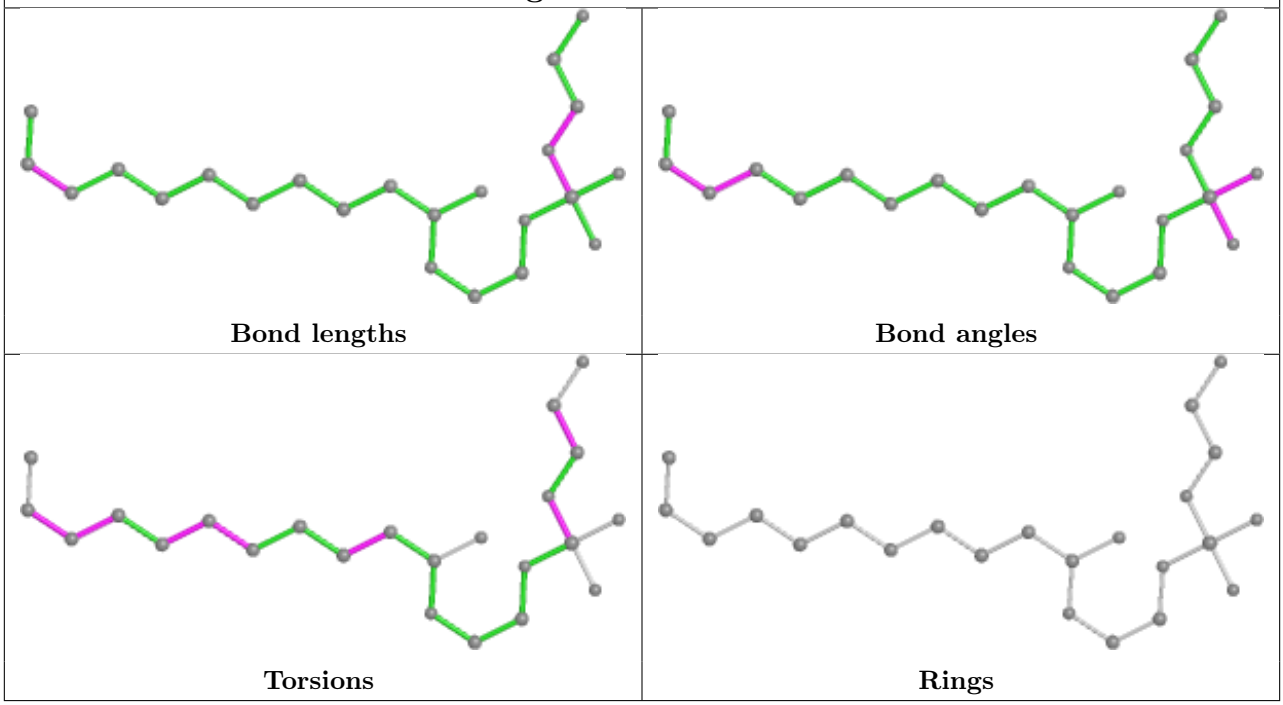

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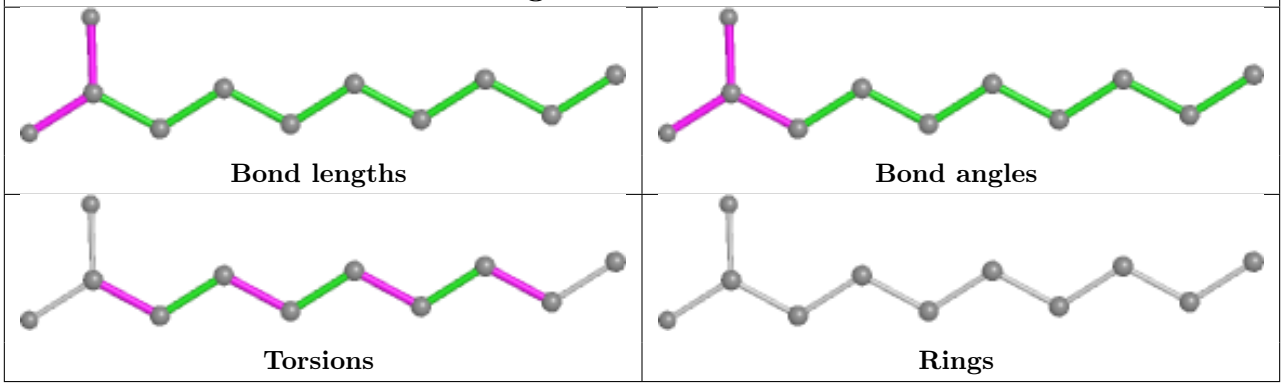

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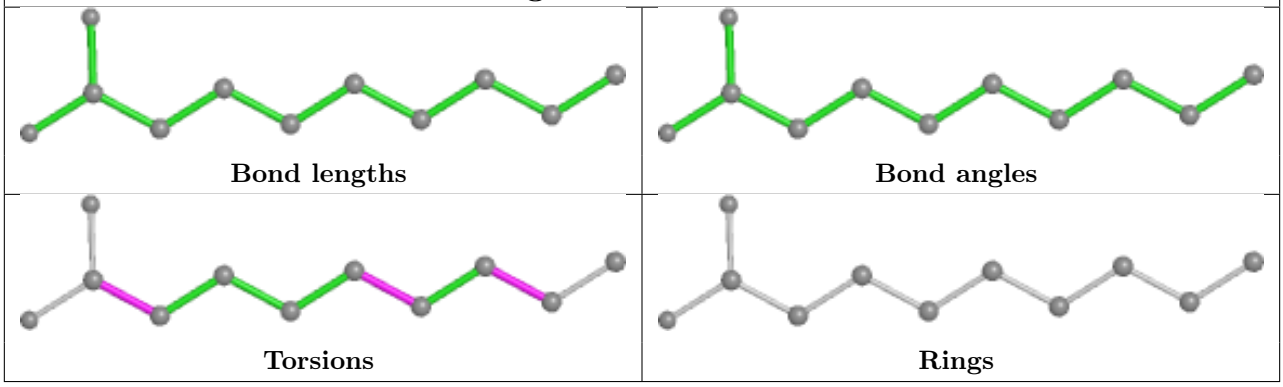
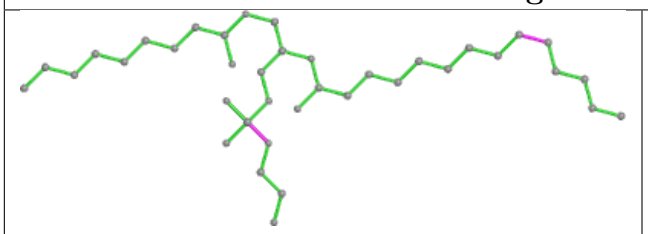
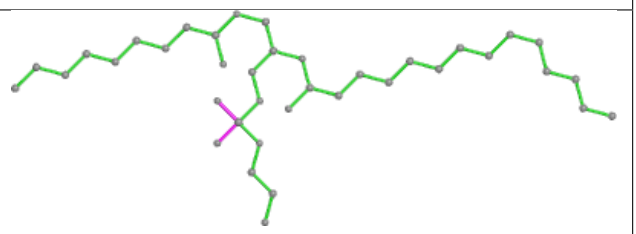


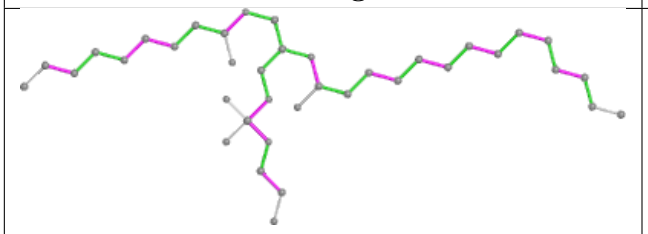
Ligand PEE D 901



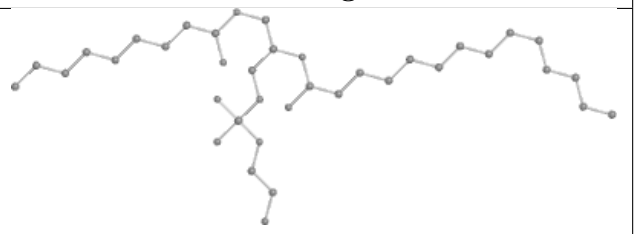
Bond lengths



Bond angles

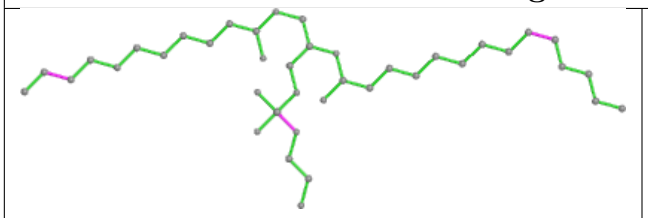


Torsions

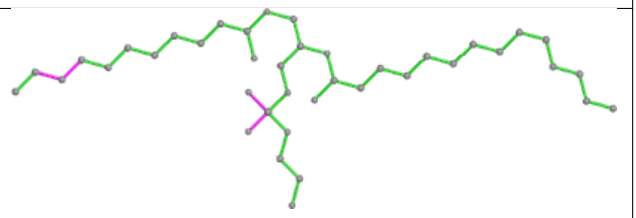


Rings

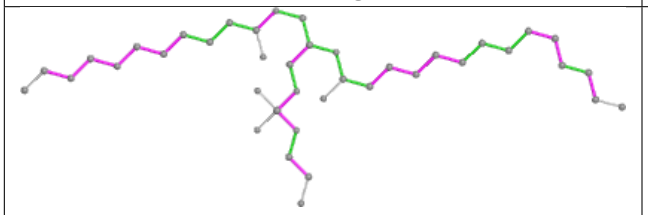
Ligand PEE F 901



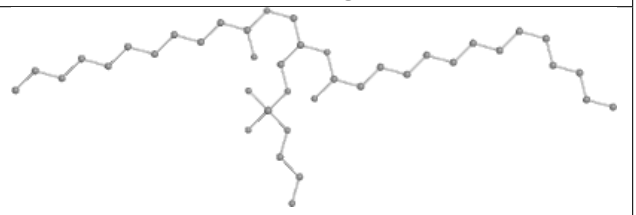
Bond lengths



Bond angles

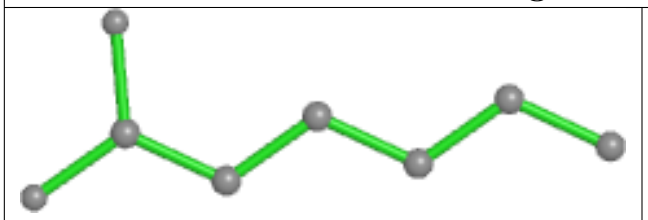


Torsions

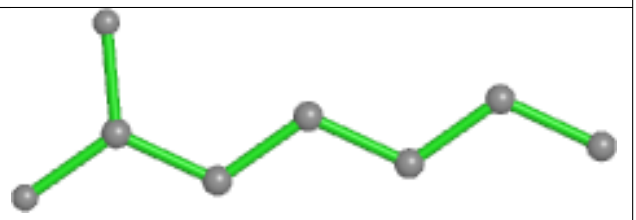


Rings

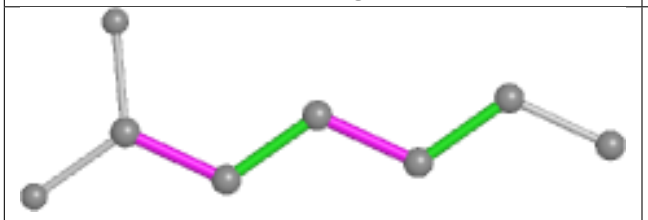
Ligand PEE F 903



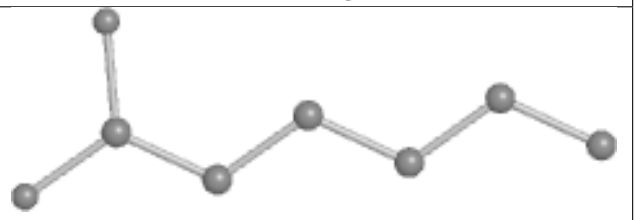
Bond lengths



Bond angles

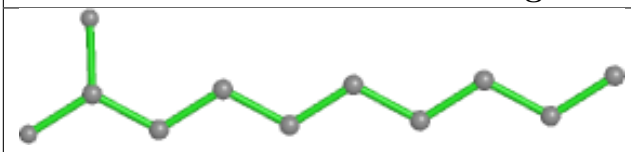


Torsions

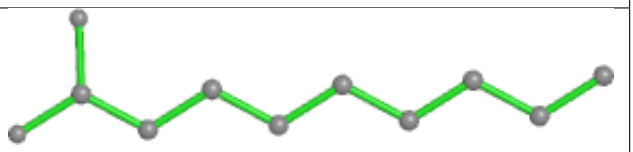


Rings

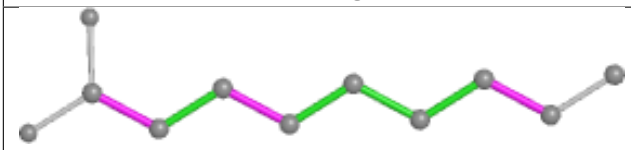
Ligand PEE D 903



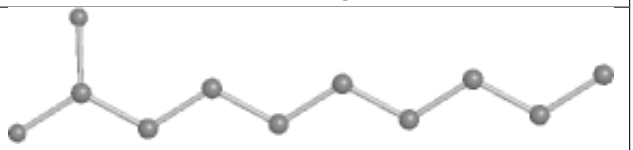
Bond lengths



Bond angles

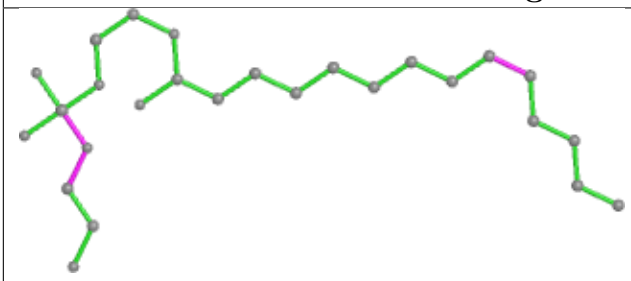


Torsions

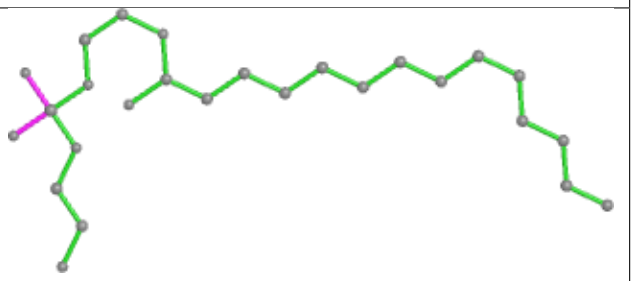


Rings

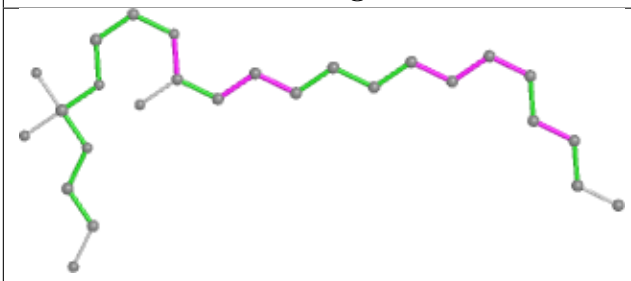
Ligand PEE C 901



Bond lengths



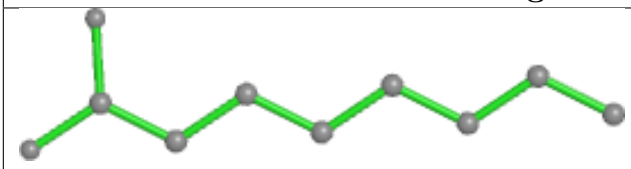
Bond angles



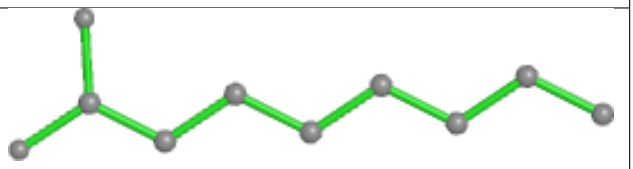
Torsions

Rings

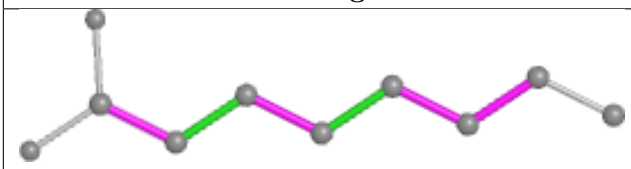
Ligand PEE E 902



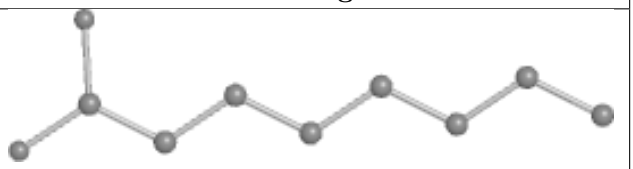
Bond lengths



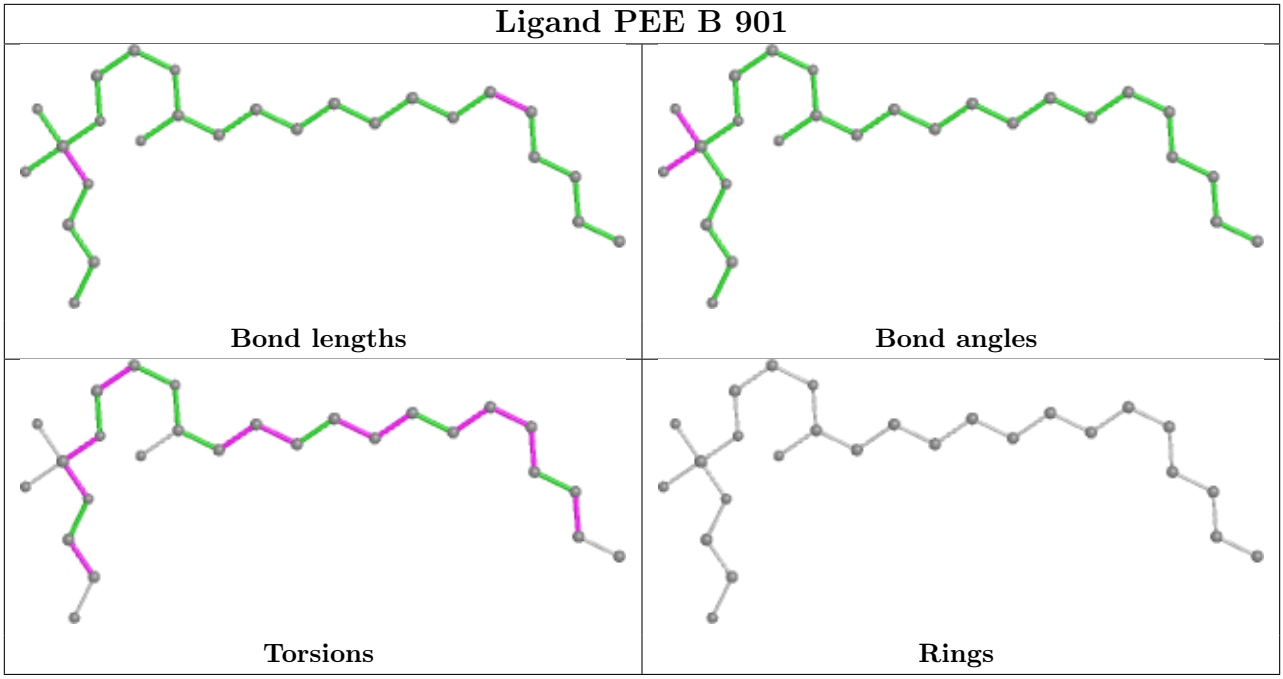
Bond angles

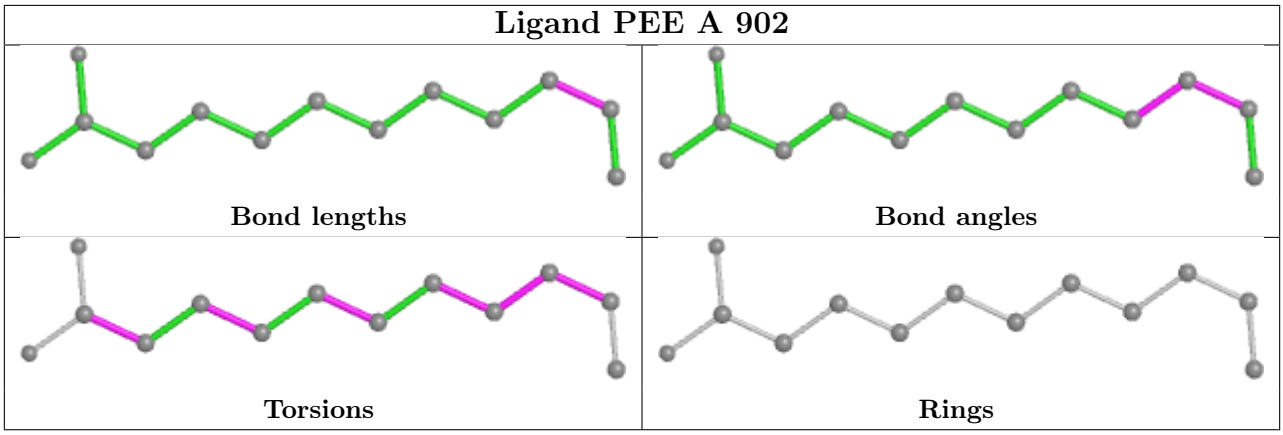


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

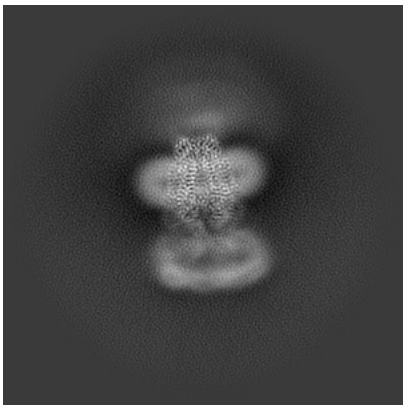
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-28901. These allow visual inspection of the internal detail of the map and identification of artifacts.

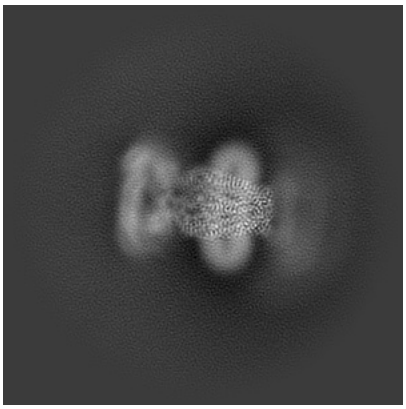
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

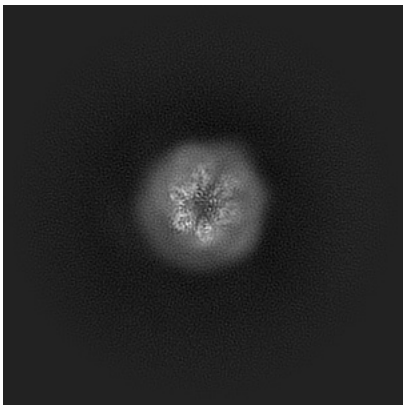
6.1.1 Primary map



X

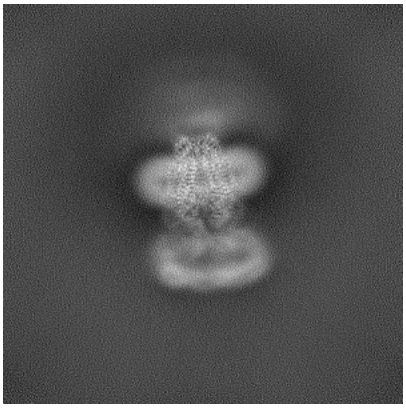


Y

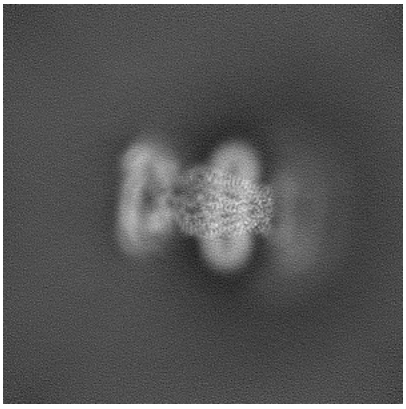


Z

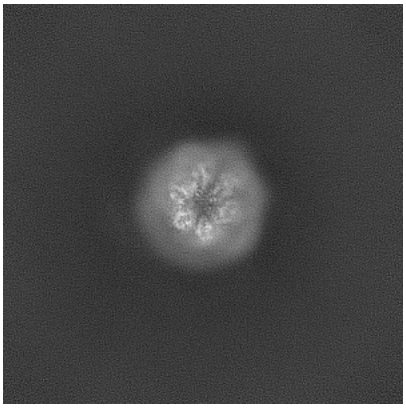
6.1.2 Raw map



X



Y

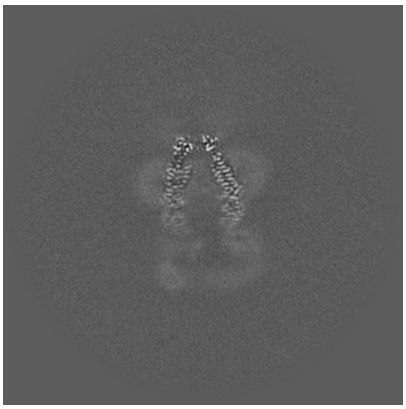


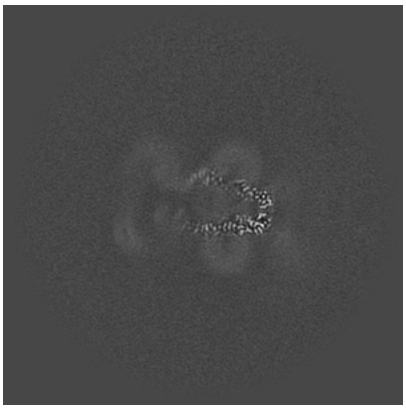
Z

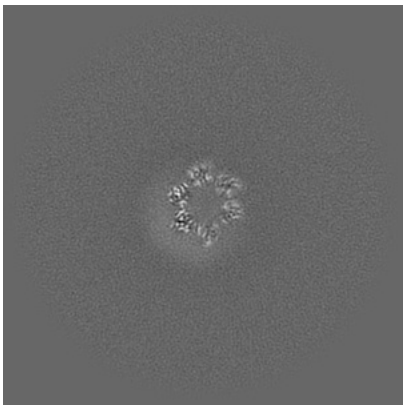
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

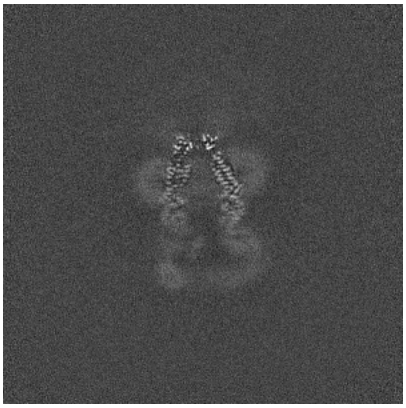
6.2.1 Primary map

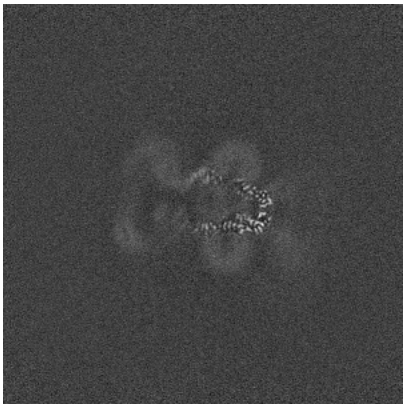

X Index: 208

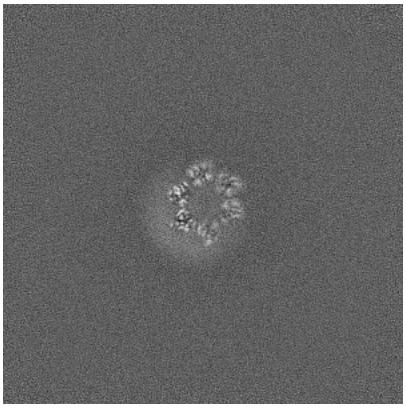

Y Index: 208


Z Index: 208

6.2.2 Raw map


X Index: 208

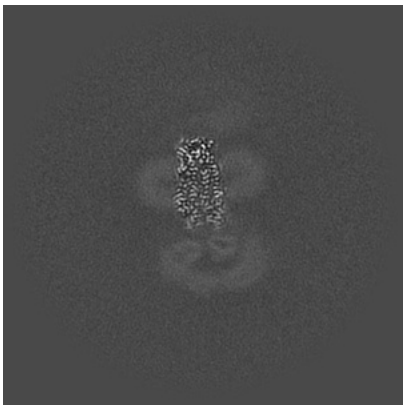

Y Index: 208


Z Index: 208

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

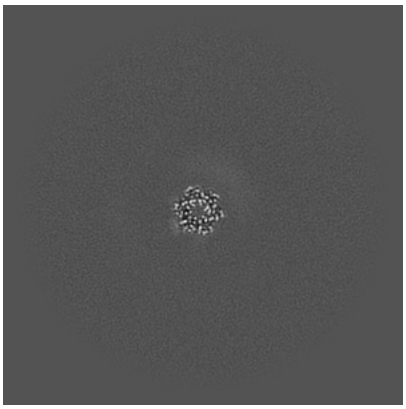
6.3 Largest variance slices (i)

6.3.1 Primary map



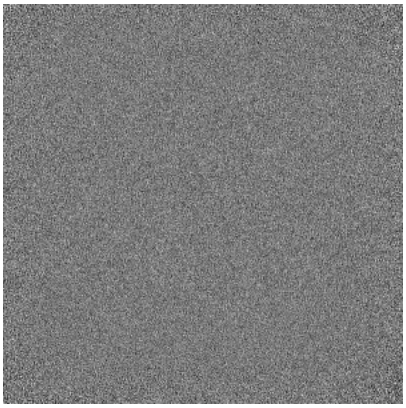
X Index: 187

Y Index: 188

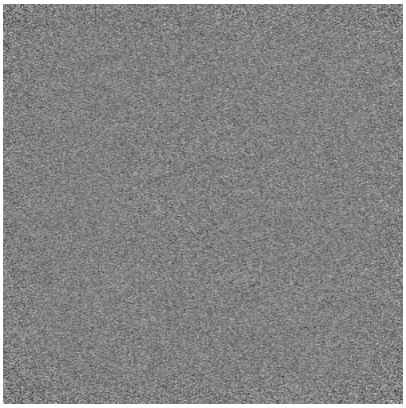


Z Index: 268

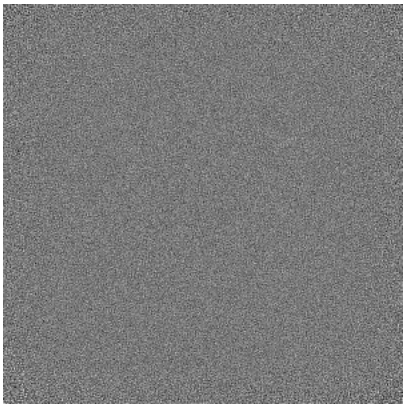
6.3.2 Raw map



X Index: 0



Y Index: 0

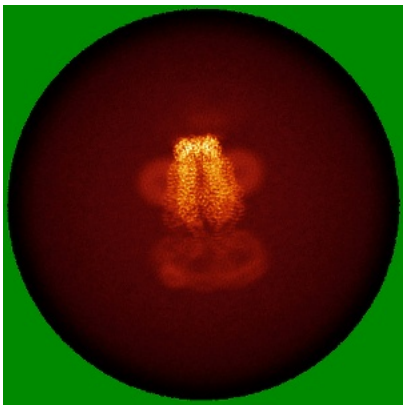


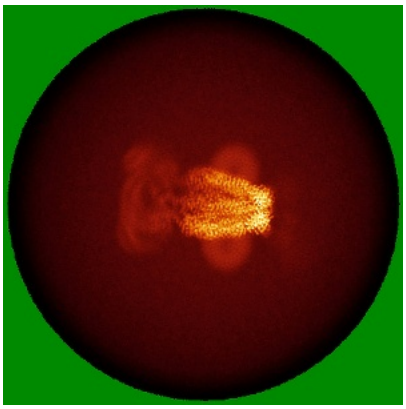
Z Index: 0

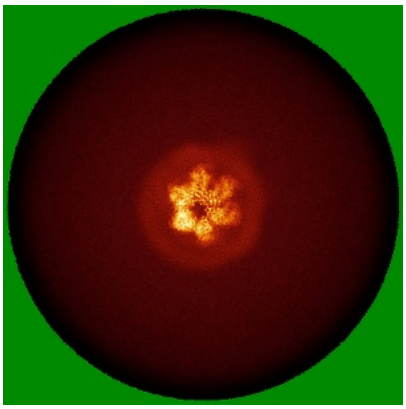
The images above show the largest variance slices of the map in three orthogonal directions.

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

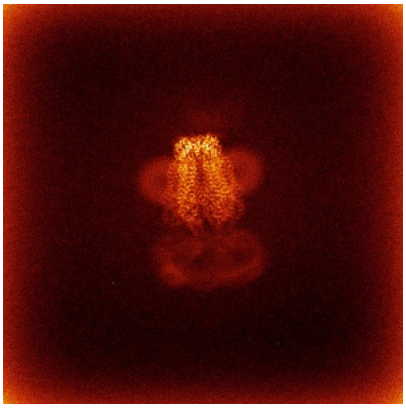
6.4.1 Primary map

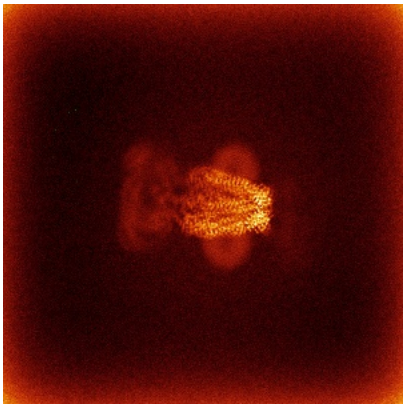

X

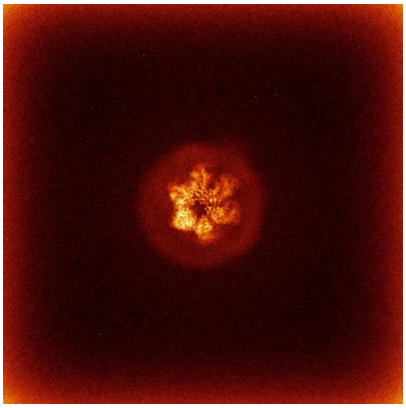

Y


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 0.7. 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.

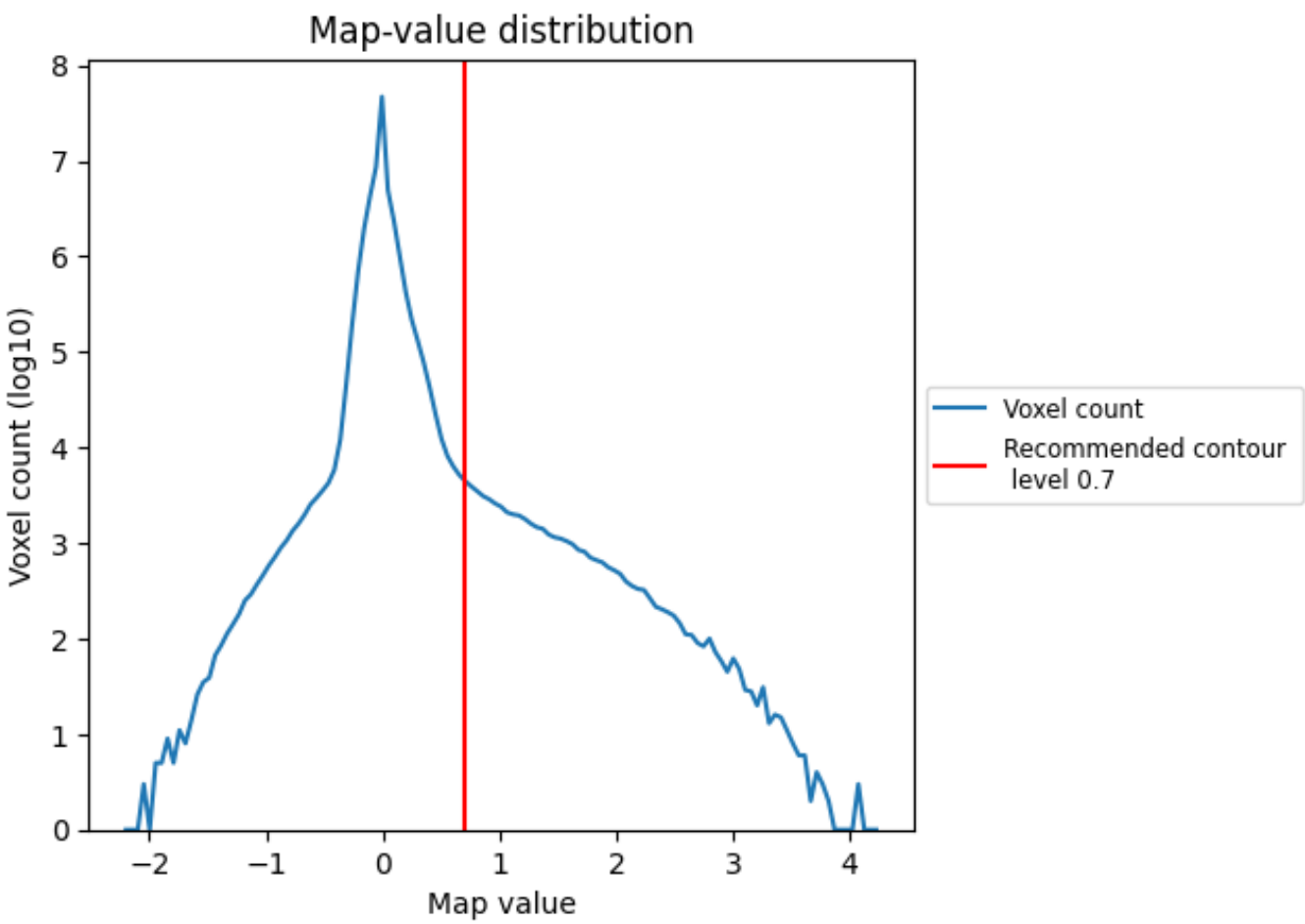
6.6 Mask visualisation (i)

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

7 Map analysis (i)

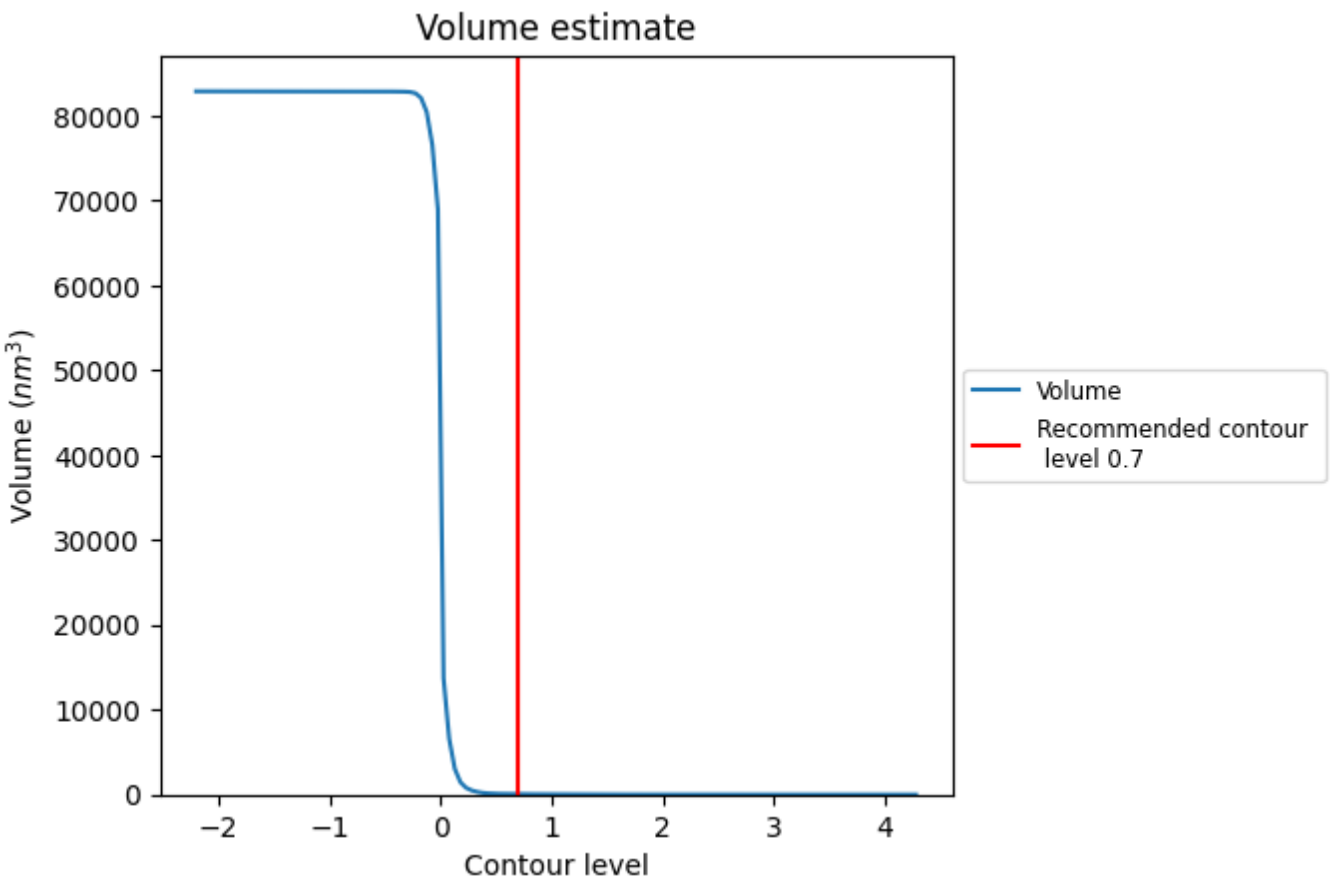
This section contains the results of statistical analysis of the map.

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.

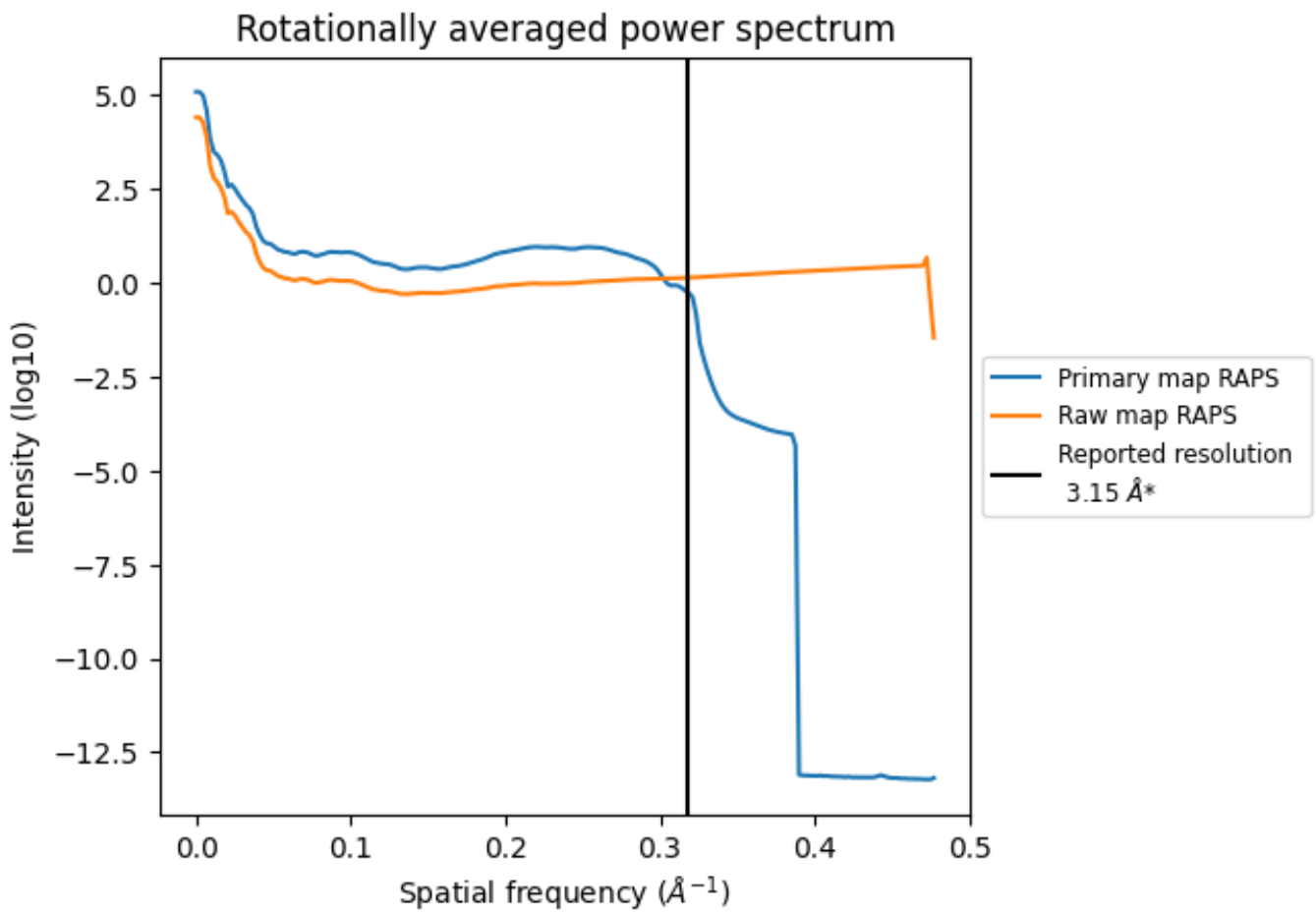
7.2 Volume estimate (i)



The volume at the recommended contour level is 58 nm^3; this corresponds to an approximate mass of 52 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)

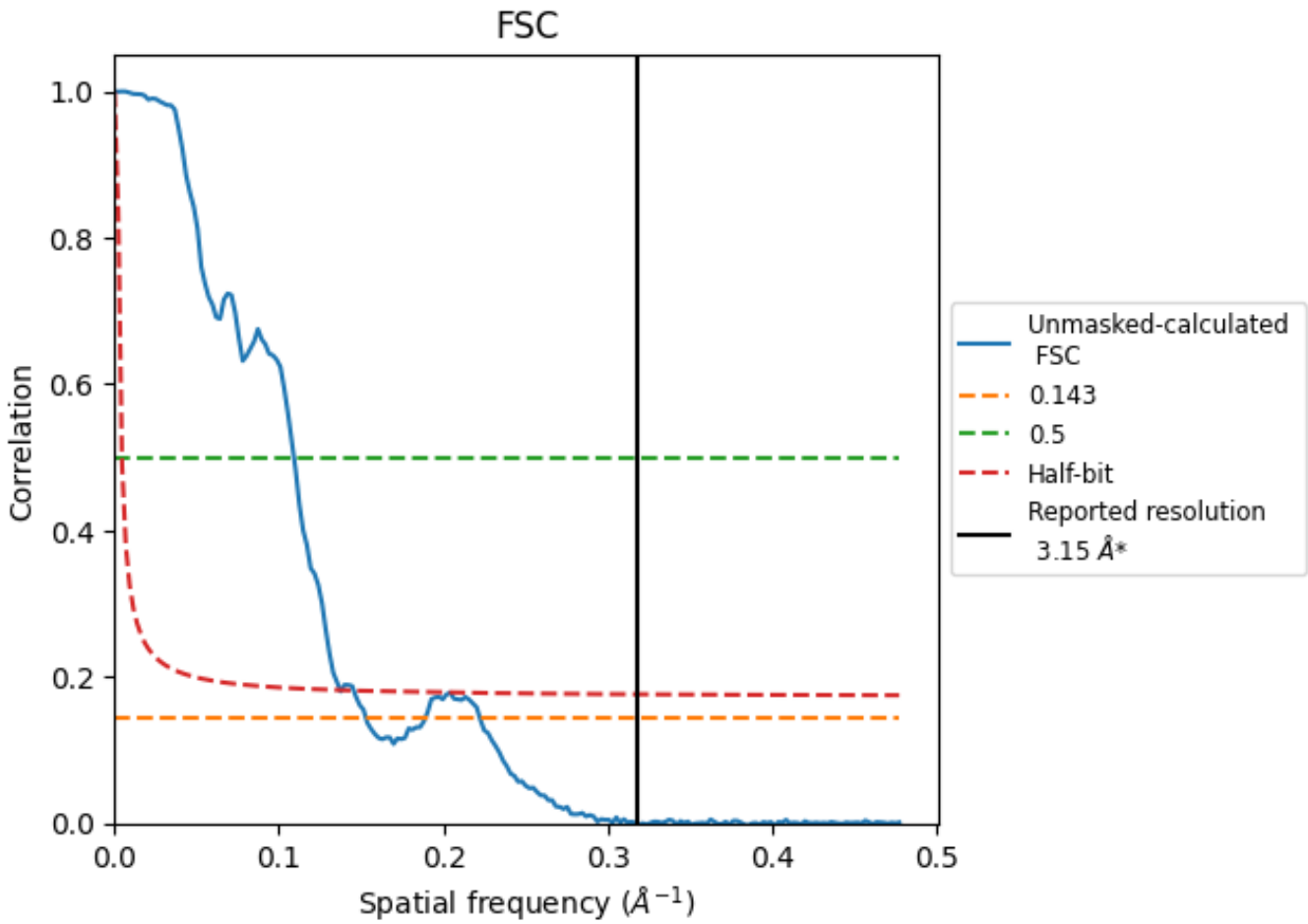


*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

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 0.317 Å^{-1}

8.2 Resolution estimates (i)

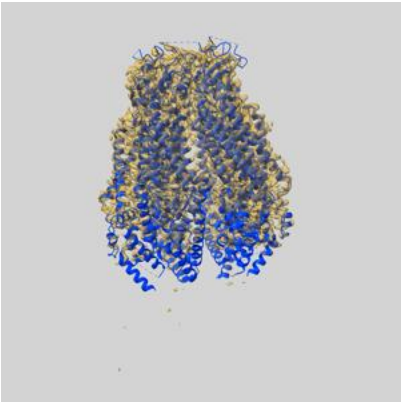
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.54	9.17	7.28

*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 6.54 differs from the reported value 3.15 by more than 10 %

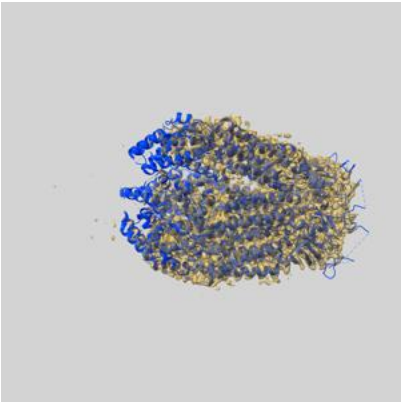
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-28901 and PDB model 8F7B. Per-residue inclusion information can be found in section 3 on page 8.

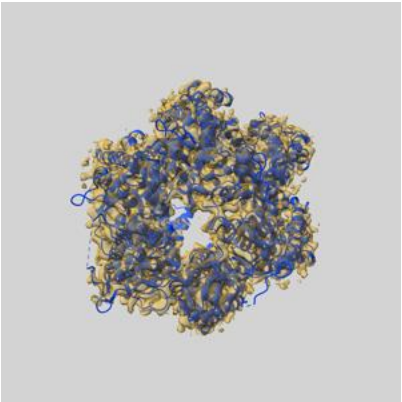
9.1 Map-model overlay (i)



X



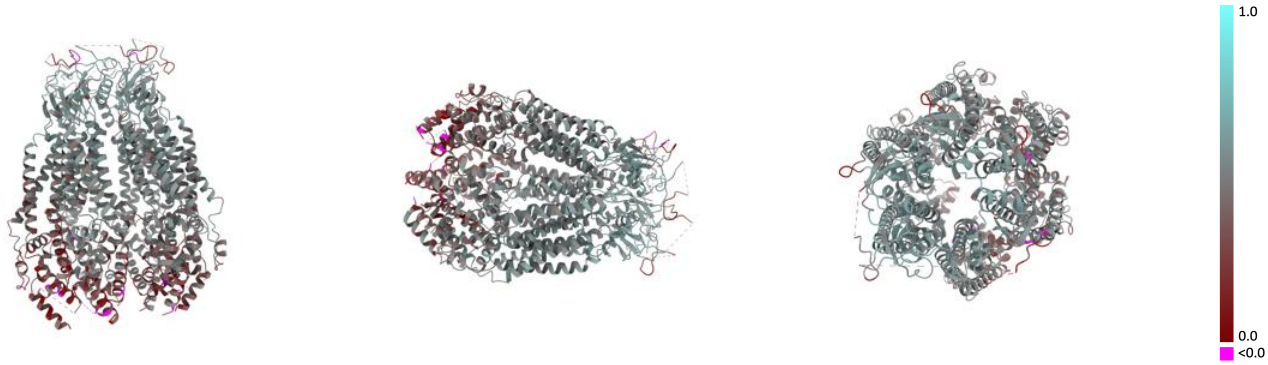
Y



Z

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

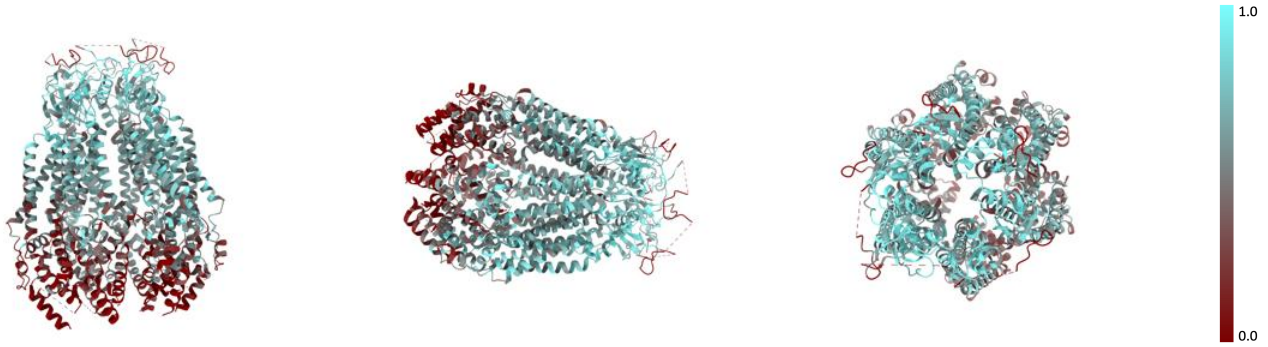
9.2 Q-score mapped to coordinate model (i)



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.

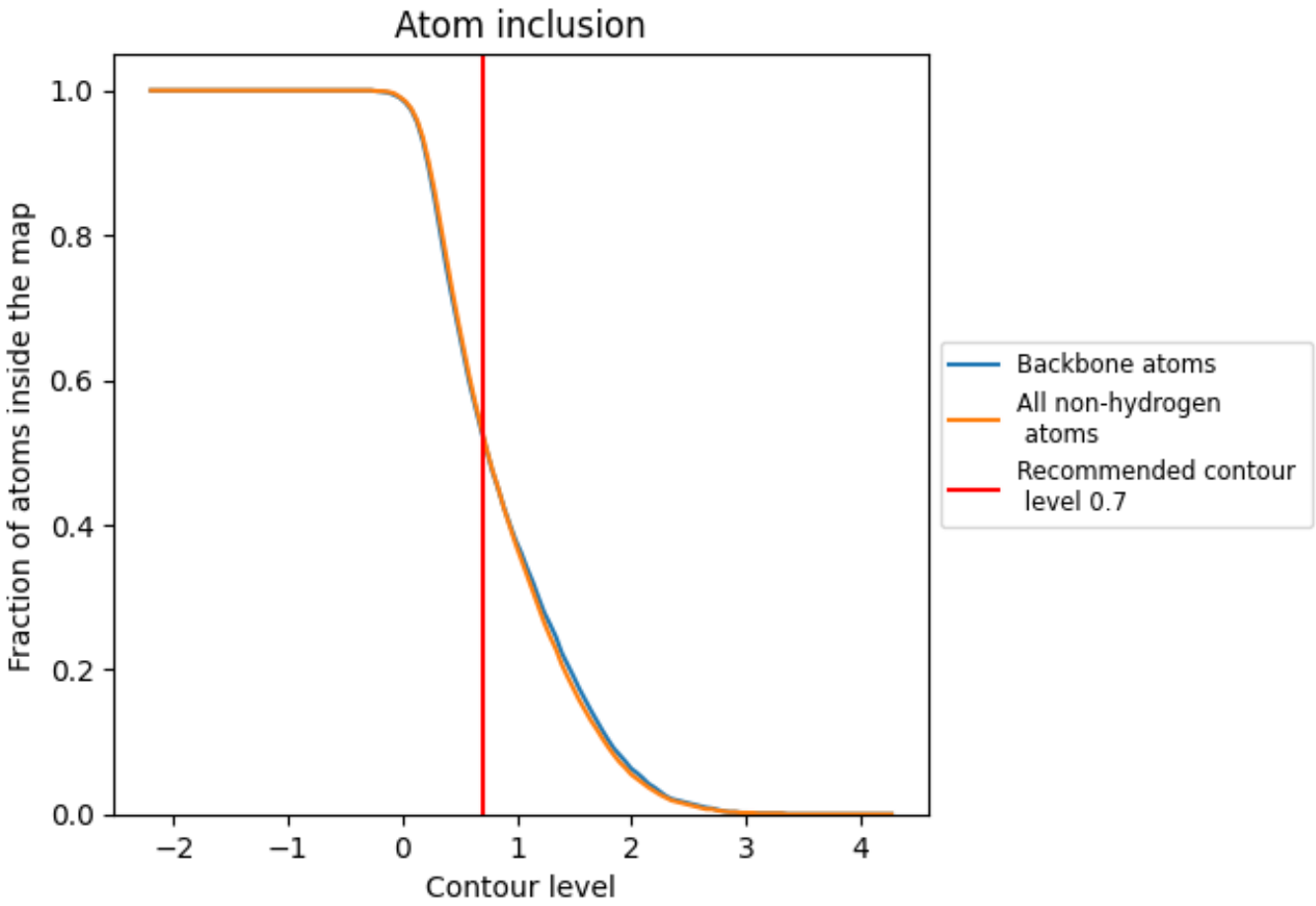
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5270	0.4630
A	0.6240	0.4970
B	0.6040	0.5010
C	0.5630	0.4730
D	0.5060	0.4560
E	0.4820	0.4380
F	0.4390	0.4140