Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:59 AM UTC

PDB ID	:	8V6M / pdb_00008v6m
EMDB ID	:	EMD-42996
Title	:	Inactivated-state cryo-EM structure of human TRPV3 in presence of tetrahydrocannabivarin (THCV) in cNW30 nanodiscs
Authors	:	Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2023-12-01
Resolution	:	3.63 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:

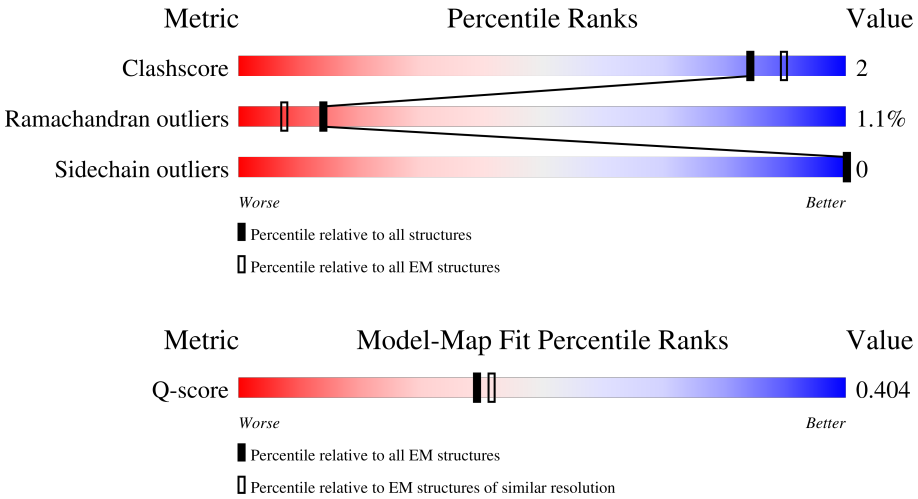
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.63 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	11696 (3.13 - 4.13)

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	808	7% 72% 7% 21%
1	B	808	7% 72% 7% 21%
1	C	808	7% 72% 7% 21%
1	D	808	7% 72% 7% 21%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 43727 atoms, of which 22180 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	640	Total	C	H	N	O	S	0	0
			10482	3386	5273	864	927	32		
1	B	640	Total	C	H	N	O	S	0	0
			10482	3386	5273	864	927	32		
1	C	640	Total	C	H	N	O	S	0	0
			10482	3386	5273	864	927	32		
1	D	640	Total	C	H	N	O	S	0	0
			10482	3386	5273	864	927	32		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	792	LEU	-	expression tag	UNP Q8NET8
A	793	VAL	-	expression tag	UNP Q8NET8
A	794	PRO	-	expression tag	UNP Q8NET8
A	795	ARG	-	expression tag	UNP Q8NET8
A	796	GLY	-	expression tag	UNP Q8NET8
A	797	SER	-	expression tag	UNP Q8NET8
A	798	ALA	-	expression tag	UNP Q8NET8
A	799	ALA	-	expression tag	UNP Q8NET8
A	800	ALA	-	expression tag	UNP Q8NET8
A	801	TRP	-	expression tag	UNP Q8NET8
A	802	SER	-	expression tag	UNP Q8NET8
A	803	HIS	-	expression tag	UNP Q8NET8
A	804	PRO	-	expression tag	UNP Q8NET8
A	805	GLN	-	expression tag	UNP Q8NET8
A	806	PHE	-	expression tag	UNP Q8NET8
A	807	GLU	-	expression tag	UNP Q8NET8
A	808	LYS	-	expression tag	UNP Q8NET8
B	792	LEU	-	expression tag	UNP Q8NET8
B	793	VAL	-	expression tag	UNP Q8NET8
B	794	PRO	-	expression tag	UNP Q8NET8
B	795	ARG	-	expression tag	UNP Q8NET8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	796	GLY	-	expression tag	UNP Q8NET8
B	797	SER	-	expression tag	UNP Q8NET8
B	798	ALA	-	expression tag	UNP Q8NET8
B	799	ALA	-	expression tag	UNP Q8NET8
B	800	ALA	-	expression tag	UNP Q8NET8
B	801	TRP	-	expression tag	UNP Q8NET8
B	802	SER	-	expression tag	UNP Q8NET8
B	803	HIS	-	expression tag	UNP Q8NET8
B	804	PRO	-	expression tag	UNP Q8NET8
B	805	GLN	-	expression tag	UNP Q8NET8
B	806	PHE	-	expression tag	UNP Q8NET8
B	807	GLU	-	expression tag	UNP Q8NET8
B	808	LYS	-	expression tag	UNP Q8NET8
C	792	LEU	-	expression tag	UNP Q8NET8
C	793	VAL	-	expression tag	UNP Q8NET8
C	794	PRO	-	expression tag	UNP Q8NET8
C	795	ARG	-	expression tag	UNP Q8NET8
C	796	GLY	-	expression tag	UNP Q8NET8
C	797	SER	-	expression tag	UNP Q8NET8
C	798	ALA	-	expression tag	UNP Q8NET8
C	799	ALA	-	expression tag	UNP Q8NET8
C	800	ALA	-	expression tag	UNP Q8NET8
C	801	TRP	-	expression tag	UNP Q8NET8
C	802	SER	-	expression tag	UNP Q8NET8
C	803	HIS	-	expression tag	UNP Q8NET8
C	804	PRO	-	expression tag	UNP Q8NET8
C	805	GLN	-	expression tag	UNP Q8NET8
C	806	PHE	-	expression tag	UNP Q8NET8
C	807	GLU	-	expression tag	UNP Q8NET8
C	808	LYS	-	expression tag	UNP Q8NET8
D	792	LEU	-	expression tag	UNP Q8NET8
D	793	VAL	-	expression tag	UNP Q8NET8
D	794	PRO	-	expression tag	UNP Q8NET8
D	795	ARG	-	expression tag	UNP Q8NET8
D	796	GLY	-	expression tag	UNP Q8NET8
D	797	SER	-	expression tag	UNP Q8NET8
D	798	ALA	-	expression tag	UNP Q8NET8
D	799	ALA	-	expression tag	UNP Q8NET8
D	800	ALA	-	expression tag	UNP Q8NET8
D	801	TRP	-	expression tag	UNP Q8NET8
D	802	SER	-	expression tag	UNP Q8NET8
D	803	HIS	-	expression tag	UNP Q8NET8

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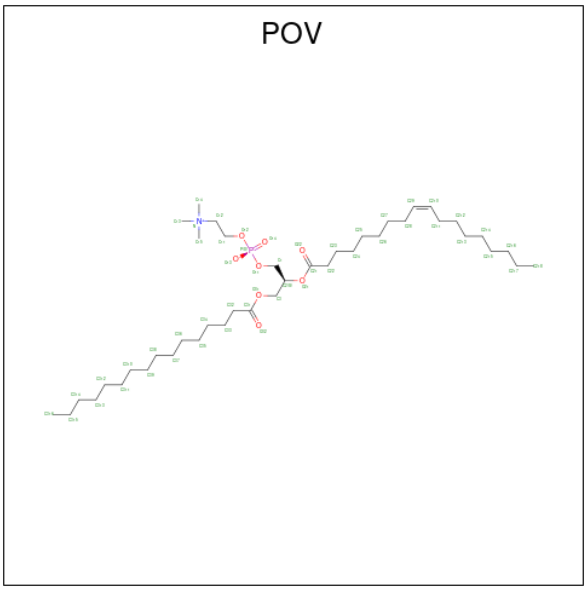
Chain	Residue	Modelled	Actual	Comment	Reference
D	804	PRO	-	expression tag	UNP Q8NET8
D	805	GLN	-	expression tag	UNP Q8NET8
D	806	PHE	-	expression tag	UNP Q8NET8
D	807	GLU	-	expression tag	UNP Q8NET8
D	808	LYS	-	expression tag	UNP Q8NET8

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

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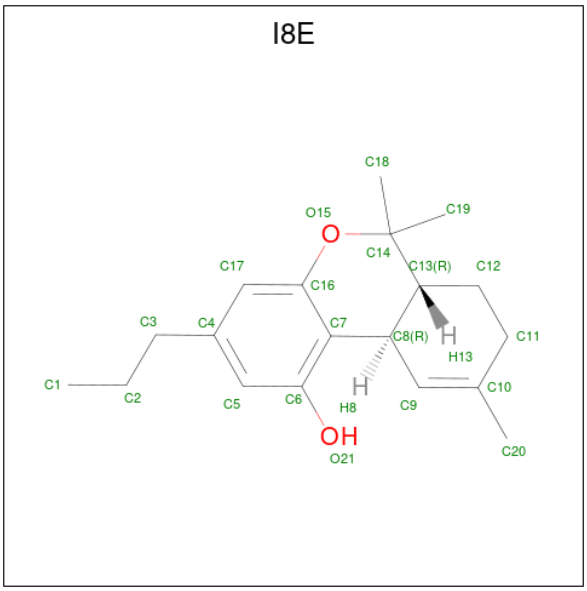
Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

- Molecule 3 is Tetrahydrocannabivarin (CCD ID: I8E) (formula: $C_{19}H_{26}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			47	19	26	2	
3	B	1	Total	C	H	O	0
			47	19	26	2	
3	C	1	Total	C	H	O	0
			47	19	26	2	
3	D	1	Total	C	H	O	0
			47	19	26	2	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

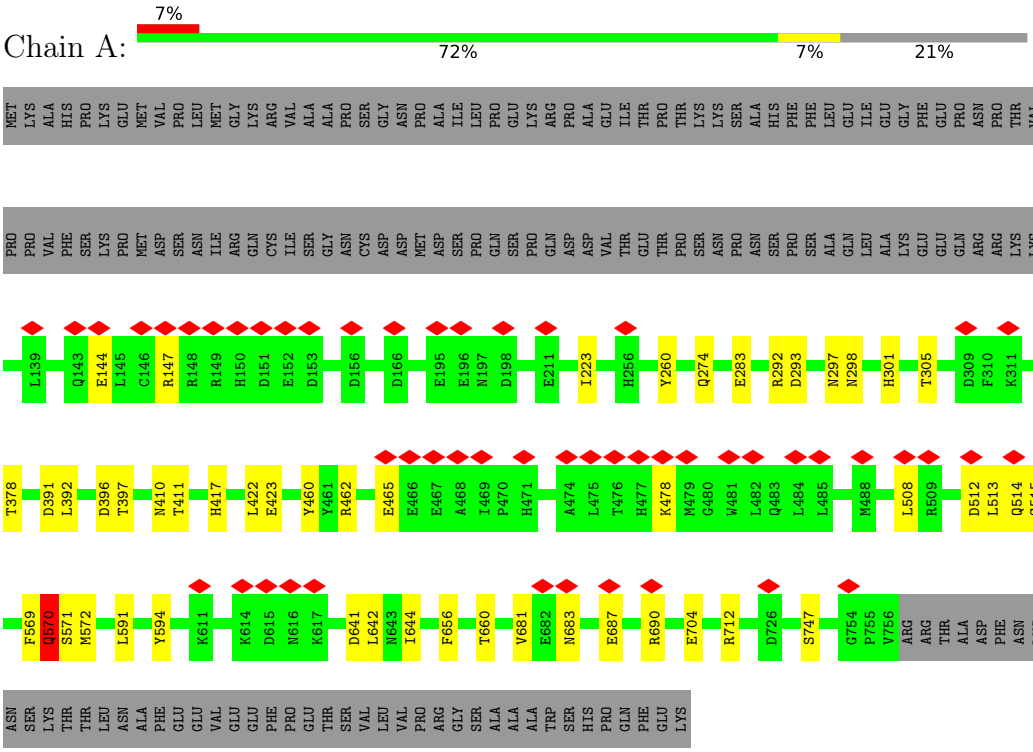
Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Na	0
			3	3	

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.

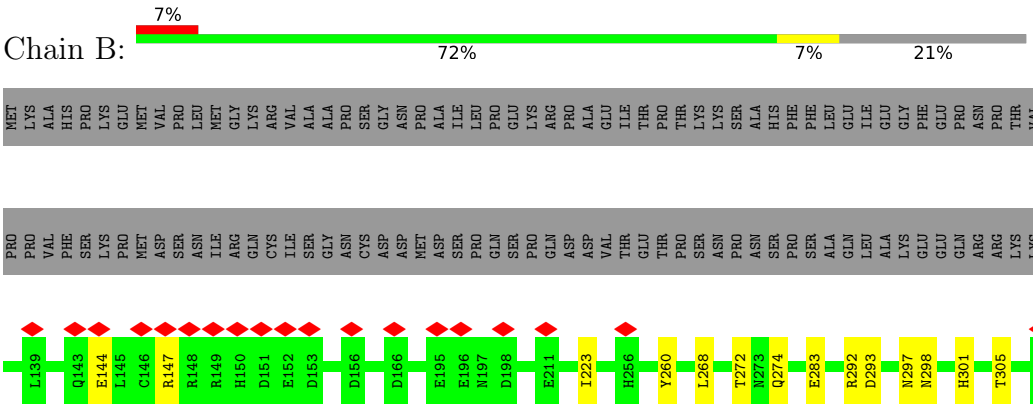
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

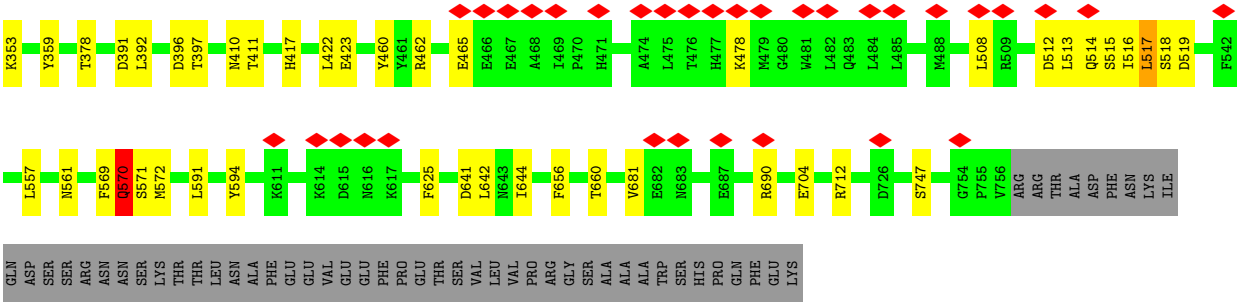
Chain A:



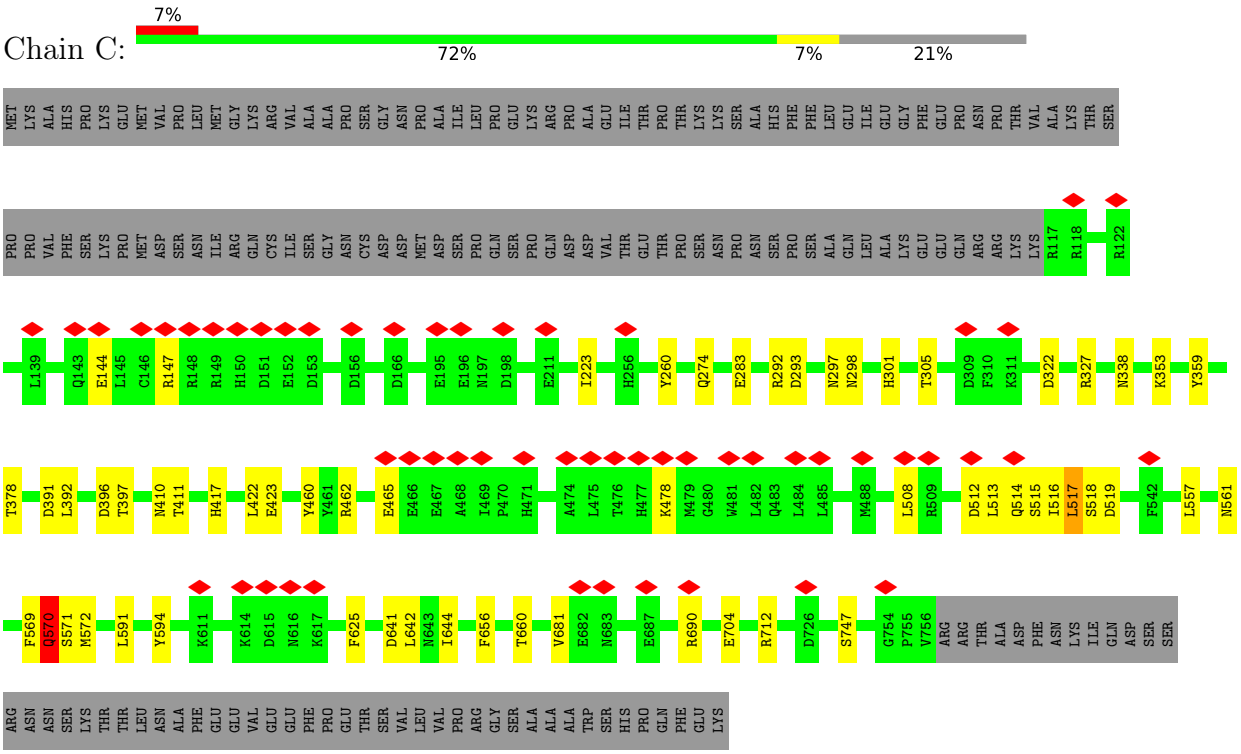
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain B:

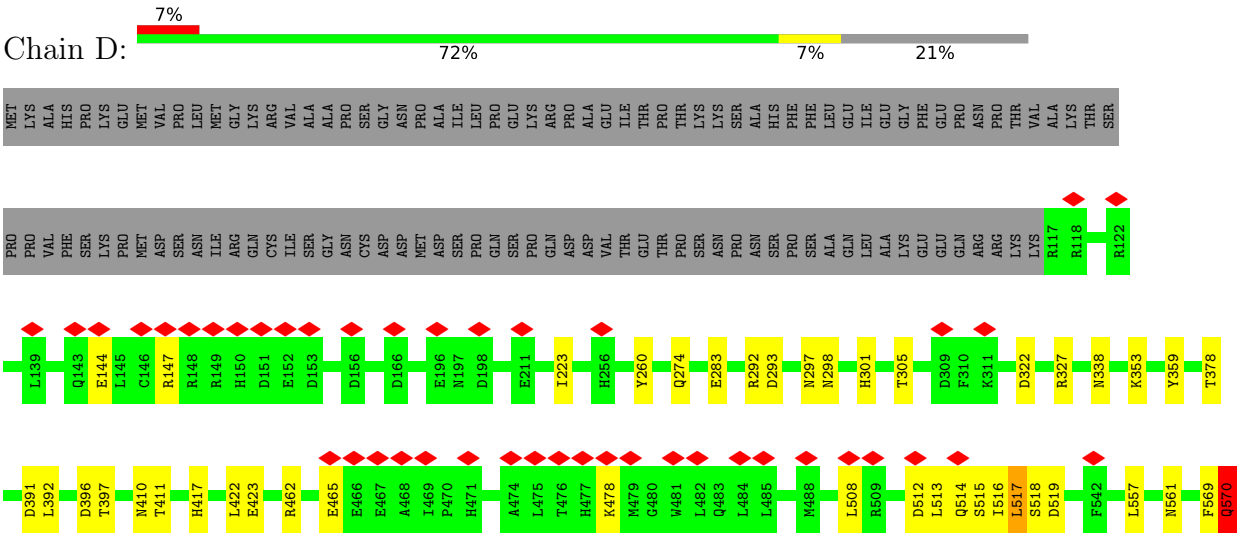


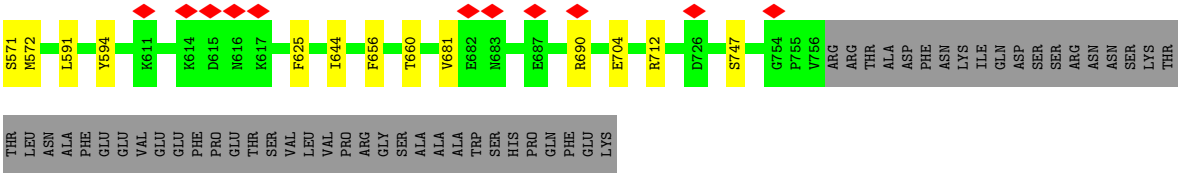


• Molecule 1: Transient receptor potential cation channel subfamily V member 3



• Molecule 1: Transient receptor potential cation channel subfamily V member 3




S571
M572
L591
Y594
K611
K614
D615
N616
K617
F625
I644
F656
T660
V681
E682
N683
E687
R690
E704
R712
D726
S747
G754
P755
V756
ARG
ARG
THR
ALA
ASP
PHE
ASN
LYS
ILE
GLN
ASP
SER
SER
ARG
ASN
ASN
SER
LYS
THR
THR
LEU
ASN
ALA
PHE
GLU
GLU
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GLU
GLU
PHE
PRO
GLU
THR
SER
VAL
LEU
VAL
PRO
ARG
GLY
SER
ALA
ALA
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	52193	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.701	Depositor
Minimum map value	-0.444	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0877	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: I8E, NA, POV

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	0.26	0/5325	0.63	3/7206 (0.0%)
1	B	0.26	0/5325	0.63	3/7206 (0.0%)
1	C	0.26	0/5325	0.63	3/7206 (0.0%)
1	D	0.26	0/5325	0.63	3/7206 (0.0%)
All	All	0.26	0/21300	0.63	12/28824 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	517	LEU	CA-C-N	5.30	131.66	121.54
1	B	517	LEU	C-N-CA	5.30	131.66	121.54
1	D	517	LEU	CA-C-N	5.30	131.66	121.54
1	D	517	LEU	C-N-CA	5.30	131.66	121.54
1	C	517	LEU	CA-C-N	5.28	131.63	121.54
1	C	517	LEU	C-N-CA	5.28	131.63	121.54
1	A	517	LEU	CA-C-N	5.28	131.62	121.54
1	A	517	LEU	C-N-CA	5.28	131.62	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	681	VAL	CG1-CB-CG2	5.14	122.12	110.80
1	D	681	VAL	CG1-CB-CG2	5.14	122.10	110.80
1	A	681	VAL	CG1-CB-CG2	5.13	122.08	110.80
1	B	681	VAL	CG1-CB-CG2	5.12	122.05	110.80

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	422	LEU	Peptide
1	A	423	GLU	Peptide
1	A	518	SER	Peptide
1	A	519	ASP	Peptide
1	A	569	PHE	Peptide
1	A	570	GLN	Peptide
1	B	422	LEU	Peptide
1	B	423	GLU	Peptide
1	B	518	SER	Peptide
1	B	519	ASP	Peptide
1	B	569	PHE	Peptide
1	B	570	GLN	Peptide
1	C	422	LEU	Peptide
1	C	423	GLU	Peptide
1	C	518	SER	Peptide
1	C	519	ASP	Peptide
1	C	569	PHE	Peptide
1	C	570	GLN	Peptide
1	D	422	LEU	Peptide
1	D	423	GLU	Peptide
1	D	518	SER	Peptide
1	D	519	ASP	Peptide
1	D	569	PHE	Peptide
1	D	570	GLN	Peptide

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	5209	5273	5272	26	0
1	B	5209	5273	5272	27	0
1	C	5209	5273	5272	26	0
1	D	5209	5273	5272	24	0
2	A	156	246	246	0	0
2	B	156	246	246	0	0
2	C	156	246	246	0	0
2	D	156	246	246	0	0
3	A	21	26	0	0	0
3	B	21	26	0	0	0
3	C	21	26	0	0	0
3	D	21	26	0	0	0
4	A	3	0	0	0	0
All	All	21547	22180	22072	100	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 2.

All (100) 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:B:656:PHE:O	1:B:660:THR:OG1	2.06	0.70
1:A:293:ASP:OD1	1:A:297:ASN:N	2.27	0.68
1:D:570:GLN:O	1:D:572:MET:N	2.27	0.68
1:C:570:GLN:O	1:C:572:MET:N	2.27	0.68
1:D:656:PHE:O	1:D:660:THR:OG1	2.06	0.68
1:A:570:GLN:O	1:A:572:MET:N	2.27	0.67
1:B:293:ASP:OD1	1:B:297:ASN:N	2.27	0.67
1:C:293:ASP:OD1	1:C:297:ASN:N	2.27	0.67
1:D:293:ASP:OD1	1:D:297:ASN:N	2.27	0.67
1:B:292:ARG:NH1	1:B:338:ASN:O	2.27	0.67
1:C:292:ARG:NH1	1:C:338:ASN:O	2.27	0.67
1:A:292:ARG:NH1	1:A:338:ASN:O	2.27	0.67
1:B:570:GLN:O	1:B:572:MET:N	2.27	0.67
1:A:656:PHE:O	1:A:660:THR:OG1	2.06	0.66
1:D:292:ARG:NH1	1:D:338:ASN:O	2.27	0.66
1:B:462:ARG:NH1	1:B:465:GLU:OE1	2.29	0.65
1:D:462:ARG:NH1	1:D:465:GLU:OE1	2.29	0.65
1:C:462:ARG:NH1	1:C:465:GLU:OE1	2.29	0.65
1:A:462:ARG:NH1	1:A:465:GLU:OE1	2.29	0.65
1:D:322:ASP:OD1	1:D:359:TYR:OH	2.15	0.65
1:C:322:ASP:OD1	1:C:359:TYR:OH	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASP:OD1	1:A:359:TYR:OH	2.15	0.64
1:B:322:ASP:OD1	1:B:359:TYR:OH	2.15	0.64
1:C:656:PHE:O	1:C:660:THR:OG1	2.06	0.63
1:B:144:GLU:OE1	1:B:147:ARG:NH2	2.35	0.60
1:C:144:GLU:OE1	1:C:147:ARG:NH2	2.35	0.60
1:D:144:GLU:OE1	1:D:147:ARG:NH2	2.35	0.60
1:A:144:GLU:OE1	1:A:147:ARG:NH2	2.35	0.59
1:D:557:LEU:O	1:D:561:ASN:ND2	2.38	0.57
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.37	0.57
1:A:298:ASN:OD1	1:A:301:HIS:ND1	2.37	0.57
1:C:557:LEU:O	1:C:561:ASN:ND2	2.38	0.57
1:B:704:GLU:O	1:B:712:ARG:NH2	2.38	0.57
1:A:557:LEU:O	1:A:561:ASN:ND2	2.38	0.56
1:B:557:LEU:O	1:B:561:ASN:ND2	2.37	0.56
1:D:704:GLU:O	1:D:712:ARG:NH2	2.38	0.56
1:B:298:ASN:OD1	1:B:301:HIS:ND1	2.37	0.56
1:A:704:GLU:O	1:A:712:ARG:NH2	2.38	0.56
1:C:704:GLU:O	1:C:712:ARG:NH2	2.38	0.55
1:B:378:THR:OG1	1:B:747:SER:O	2.26	0.54
1:B:417:HIS:O	1:B:690:ARG:NH2	2.42	0.53
1:D:417:HIS:O	1:D:690:ARG:NH2	2.42	0.53
1:C:378:THR:OG1	1:C:747:SER:O	2.26	0.53
1:A:378:THR:OG1	1:A:747:SER:O	2.26	0.52
1:C:417:HIS:O	1:C:690:ARG:NH2	2.42	0.52
1:A:417:HIS:O	1:A:690:ARG:NH2	2.42	0.52
1:A:460:TYR:OH	1:B:625:PHE:N	2.42	0.52
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.37	0.52
1:D:378:THR:OG1	1:D:747:SER:O	2.26	0.52
1:A:305:THR:O	1:A:353:LYS:NZ	2.46	0.49
1:B:305:THR:O	1:B:353:LYS:NZ	2.46	0.49
1:D:305:THR:O	1:D:353:LYS:NZ	2.46	0.49
1:C:305:THR:O	1:C:353:LYS:NZ	2.46	0.48
1:A:260:TYR:OH	1:A:293:ASP:OD2	2.30	0.48
1:C:260:TYR:OH	1:C:293:ASP:OD2	2.30	0.48
1:B:460:TYR:OH	1:C:625:PHE:N	2.46	0.47
1:D:260:TYR:OH	1:D:293:ASP:OD2	2.30	0.47
1:B:283:GLU:OE2	1:B:327:ARG:NH2	2.48	0.47
1:A:223:ILE:O	1:A:274:GLN:NE2	2.45	0.46
1:A:283:GLU:OE2	1:A:327:ARG:NH2	2.48	0.46
1:D:283:GLU:OE2	1:D:327:ARG:NH2	2.48	0.46
1:B:391:ASP:OD1	1:B:392:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLU:OE2	1:C:327:ARG:NH2	2.48	0.46
1:A:391:ASP:OD1	1:A:392:LEU:N	2.49	0.45
1:B:223:ILE:O	1:B:274:GLN:NE2	2.45	0.45
1:D:223:ILE:O	1:D:274:GLN:NE2	2.45	0.45
1:B:260:TYR:OH	1:B:293:ASP:OD2	2.30	0.45
1:D:391:ASP:OD1	1:D:392:LEU:N	2.49	0.45
1:C:391:ASP:OD1	1:C:392:LEU:N	2.49	0.45
1:A:396:ASP:OD1	1:A:397:THR:N	2.49	0.45
1:D:591:LEU:O	1:D:594:TYR:N	2.50	0.45
1:B:591:LEU:O	1:B:594:TYR:N	2.50	0.44
1:C:591:LEU:O	1:C:594:TYR:N	2.50	0.44
1:B:644:ILE:HG23	1:B:644:ILE:O	2.18	0.44
1:A:591:LEU:O	1:A:594:TYR:N	2.50	0.44
1:A:644:ILE:HG23	1:A:644:ILE:O	2.18	0.44
1:A:410:ASN:OD1	1:A:411:THR:N	2.51	0.44
1:B:410:ASN:OD1	1:B:411:THR:N	2.51	0.44
1:D:644:ILE:O	1:D:644:ILE:HG23	2.18	0.44
1:C:396:ASP:OD1	1:C:397:THR:N	2.49	0.43
1:C:644:ILE:O	1:C:644:ILE:HG23	2.18	0.43
1:D:396:ASP:OD1	1:D:397:THR:N	2.49	0.43
1:C:410:ASN:OD1	1:C:411:THR:N	2.51	0.43
1:B:508:LEU:O	1:B:508:LEU:HD23	2.19	0.43
1:C:460:TYR:OH	1:D:625:PHE:N	2.47	0.43
1:D:508:LEU:HD23	1:D:508:LEU:O	2.19	0.43
1:A:508:LEU:HD23	1:A:508:LEU:O	2.19	0.43
1:C:508:LEU:O	1:C:508:LEU:HD23	2.19	0.43
1:B:512:ASP:OD1	1:B:513:LEU:N	2.52	0.43
1:C:223:ILE:O	1:C:274:GLN:NE2	2.45	0.43
1:D:410:ASN:OD1	1:D:411:THR:N	2.51	0.42
1:A:512:ASP:OD1	1:A:513:LEU:N	2.52	0.42
1:D:512:ASP:OD1	1:D:513:LEU:N	2.52	0.42
1:C:512:ASP:OD1	1:C:513:LEU:N	2.52	0.42
1:B:641:ASP:OD1	1:B:642:LEU:N	2.53	0.42
1:A:641:ASP:OD1	1:A:642:LEU:N	2.53	0.42
1:B:396:ASP:OD1	1:B:397:THR:N	2.49	0.42
1:B:268:LEU:O	1:B:272:THR:OG1	2.27	0.41
1:C:641:ASP:OD1	1:C:642:LEU:N	2.53	0.41
1:A:683:ASN:O	1:A:687:GLU:N	2.44	0.40

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	638/808 (79%)	563 (88%)	68 (11%)	7 (1%)	11	40
1	B	638/808 (79%)	563 (88%)	68 (11%)	7 (1%)	11	40
1	C	638/808 (79%)	563 (88%)	68 (11%)	7 (1%)	11	40
1	D	638/808 (79%)	563 (88%)	68 (11%)	7 (1%)	11	40
All	All	2552/3232 (79%)	2252 (88%)	272 (11%)	28 (1%)	14	40

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	GLN
1	A	571	SER
1	B	570	GLN
1	B	571	SER
1	C	570	GLN
1	C	571	SER
1	D	570	GLN
1	D	571	SER
1	A	517	LEU
1	B	517	LEU
1	C	517	LEU
1	D	517	LEU
1	A	514	GLN
1	A	515	SER
1	B	514	GLN
1	B	515	SER
1	C	514	GLN
1	C	515	SER
1	D	514	GLN
1	D	515	SER
1	A	478	LYS
1	B	478	LYS

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Mol	Chain	Res	Type
1	C	478	LYS
1	D	478	LYS
1	A	516	ILE
1	B	516	ILE
1	C	516	ILE
1	D	516	ILE

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	567/716 (79%)	567 (100%)	0	100	100
1	B	567/716 (79%)	567 (100%)	0	100	100
1	C	567/716 (79%)	567 (100%)	0	100	100
1	D	567/716 (79%)	567 (100%)	0	100	100
All	All	2268/2864 (79%)	2268 (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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	647	ASN
1	B	220	ASN
1	B	647	ASN
1	B	683	ASN
1	C	220	ASN
1	C	647	ASN
1	C	683	ASN
1	D	220	ASN
1	D	647	ASN
1	D	683	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	POV	D	903	-	51,51,51	0.38	0	57,59,59	0.80	2 (3%)
2	POV	B	904	-	51,51,51	0.30	0	57,59,59	0.46	0
2	POV	C	904	-	51,51,51	0.30	0	57,59,59	0.46	0
3	I8E	A	903	-	23,23,23	0.17	0	33,35,35	0.71	1 (3%)
3	I8E	B	903	-	23,23,23	0.17	0	33,35,35	0.72	1 (3%)
3	I8E	C	903	-	23,23,23	0.16	0	33,35,35	0.72	1 (3%)
2	POV	D	901	-	51,51,51	0.30	0	57,59,59	0.46	0
2	POV	C	901	-	51,51,51	0.32	0	57,59,59	0.47	1 (1%)
2	POV	B	901	-	51,51,51	0.32	0	57,59,59	0.46	1 (1%)
2	POV	A	901	-	51,51,51	0.32	0	57,59,59	0.47	1 (1%)
2	POV	A	904	-	51,51,51	0.30	0	57,59,59	0.46	0
2	POV	B	902	-	51,51,51	0.37	0	57,59,59	0.81	2 (3%)
2	POV	C	902	-	51,51,51	0.38	0	57,59,59	0.81	2 (3%)
2	POV	D	902	-	51,51,51	0.32	0	57,59,59	0.47	1 (1%)
2	POV	A	902	-	51,51,51	0.38	0	57,59,59	0.81	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	I8E	D	904	-	23,23,23	0.16	0	33,35,35	0.72	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	903	-	-	23/55/55/55	-
2	POV	B	904	-	-	23/55/55/55	-
2	POV	C	904	-	-	23/55/55/55	-
3	I8E	A	903	-	-	1/3/31/31	0/3/3/3
3	I8E	B	903	-	-	1/3/31/31	0/3/3/3
3	I8E	C	903	-	-	1/3/31/31	0/3/3/3
2	POV	D	901	-	-	23/55/55/55	-
2	POV	C	901	-	-	17/55/55/55	-
2	POV	B	901	-	-	17/55/55/55	-
2	POV	A	901	-	-	17/55/55/55	-
2	POV	A	904	-	-	22/55/55/55	-
2	POV	B	902	-	-	23/55/55/55	-
2	POV	C	902	-	-	23/55/55/55	-
2	POV	D	902	-	-	17/55/55/55	-
2	POV	A	902	-	-	23/55/55/55	-
3	I8E	D	904	-	-	1/3/31/31	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	902	POV	O21-C2-C3	-3.45	95.98	108.34
2	C	902	POV	O21-C2-C3	-3.41	96.12	108.34
2	A	902	POV	O21-C2-C3	-3.40	96.15	108.34
2	D	903	POV	O21-C2-C3	-3.28	96.59	108.34
3	B	903	I8E	C13-C8-C9	-2.82	104.47	110.00
3	C	903	I8E	C13-C8-C9	-2.81	104.48	110.00
3	D	904	I8E	C13-C8-C9	-2.81	104.48	110.00
3	A	903	I8E	C13-C8-C9	-2.78	104.54	110.00
2	D	902	POV	C2-O21-C21	2.18	123.02	117.80
2	A	901	POV	C2-O21-C21	2.17	123.00	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	901	POV	C2-O21-C21	2.16	122.98	117.80
2	B	901	POV	C2-O21-C21	2.16	122.97	117.80
2	D	903	POV	C3-O31-C31	2.06	124.65	117.12
2	A	902	POV	C3-O31-C31	2.05	124.59	117.12
2	C	902	POV	C3-O31-C31	2.04	124.57	117.12
2	B	902	POV	C3-O31-C31	2.02	124.52	117.12

There are no chirality outliers.

All (255) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	POV	C11-O12-P-O11
2	A	901	POV	C11-O12-P-O14
2	A	901	POV	C22-C21-O21-C2
2	A	901	POV	O22-C21-O21-C2
2	A	902	POV	C11-O12-P-O11
2	A	902	POV	C11-O12-P-O13
2	A	902	POV	C11-O12-P-O14
2	A	902	POV	C32-C31-O31-C3
2	A	902	POV	O32-C31-O31-C3
2	A	904	POV	C1-O11-P-O12
2	A	904	POV	C1-O11-P-O13
2	A	904	POV	C11-O12-P-O11
2	A	904	POV	O21-C2-C3-O31
2	A	904	POV	O12-C11-C12-N
2	A	904	POV	O22-C21-O21-C2
2	B	901	POV	C11-O12-P-O11
2	B	901	POV	C11-O12-P-O14
2	B	901	POV	C22-C21-O21-C2
2	B	901	POV	O22-C21-O21-C2
2	B	902	POV	C11-O12-P-O11
2	B	902	POV	C11-O12-P-O13
2	B	902	POV	C11-O12-P-O14
2	B	902	POV	C32-C31-O31-C3
2	B	902	POV	O32-C31-O31-C3
2	B	904	POV	C1-O11-P-O12
2	B	904	POV	C1-O11-P-O13
2	B	904	POV	C11-O12-P-O11
2	B	904	POV	O21-C2-C3-O31
2	B	904	POV	O12-C11-C12-N
2	B	904	POV	O22-C21-O21-C2
2	C	901	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	C11-O12-P-O14
2	C	901	POV	C22-C21-O21-C2
2	C	901	POV	O22-C21-O21-C2
2	C	902	POV	C11-O12-P-O11
2	C	902	POV	C11-O12-P-O13
2	C	902	POV	C11-O12-P-O14
2	C	902	POV	C32-C31-O31-C3
2	C	902	POV	O32-C31-O31-C3
2	C	904	POV	C1-O11-P-O12
2	C	904	POV	C1-O11-P-O13
2	C	904	POV	C11-O12-P-O11
2	C	904	POV	O21-C2-C3-O31
2	C	904	POV	O12-C11-C12-N
2	C	904	POV	O22-C21-O21-C2
2	D	901	POV	C1-O11-P-O12
2	D	901	POV	C1-O11-P-O13
2	D	901	POV	C11-O12-P-O11
2	D	901	POV	O21-C2-C3-O31
2	D	901	POV	O12-C11-C12-N
2	D	901	POV	O22-C21-O21-C2
2	D	902	POV	C11-O12-P-O11
2	D	902	POV	C11-O12-P-O14
2	D	902	POV	C22-C21-O21-C2
2	D	902	POV	O22-C21-O21-C2
2	D	903	POV	C11-O12-P-O11
2	D	903	POV	C11-O12-P-O13
2	D	903	POV	C11-O12-P-O14
2	D	903	POV	C32-C31-O31-C3
2	D	903	POV	O32-C31-O31-C3
2	A	904	POV	C22-C21-O21-C2
2	B	904	POV	C22-C21-O21-C2
2	C	904	POV	C22-C21-O21-C2
2	D	901	POV	C22-C21-O21-C2
2	A	902	POV	C21-C22-C23-C24
2	B	902	POV	C21-C22-C23-C24
2	C	902	POV	C21-C22-C23-C24
2	D	901	POV	C31-C32-C33-C34
2	D	903	POV	C11-C12-N-C14
2	D	903	POV	C11-C12-N-C15
2	C	904	POV	C31-C32-C33-C34
2	D	903	POV	C21-C22-C23-C24
2	A	904	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	B	904	POV	C31-C32-C33-C34
2	A	902	POV	C11-C12-N-C14
2	A	902	POV	C11-C12-N-C15
2	B	902	POV	C11-C12-N-C14
2	B	902	POV	C11-C12-N-C15
2	C	902	POV	C11-C12-N-C14
2	C	902	POV	C11-C12-N-C15
2	A	902	POV	C32-C33-C34-C35
2	B	902	POV	C32-C33-C34-C35
2	C	902	POV	C32-C33-C34-C35
2	D	902	POV	C25-C26-C27-C28
2	D	903	POV	C32-C33-C34-C35
2	C	901	POV	C25-C26-C27-C28
2	B	904	POV	C21-C22-C23-C24
2	B	901	POV	C25-C26-C27-C28
2	A	901	POV	C25-C26-C27-C28
2	B	902	POV	C11-C12-N-C13
2	A	904	POV	C21-C22-C23-C24
2	C	904	POV	C21-C22-C23-C24
2	D	901	POV	C21-C22-C23-C24
2	A	901	POV	C312-C313-C314-C315
2	D	902	POV	C37-C38-C39-C310
2	D	902	POV	C312-C313-C314-C315
2	B	901	POV	C312-C313-C314-C315
2	C	901	POV	C312-C313-C314-C315
2	C	901	POV	C37-C38-C39-C310
2	A	901	POV	C37-C38-C39-C310
2	B	901	POV	C37-C38-C39-C310
2	A	902	POV	C210-C211-C212-C213
2	B	902	POV	C210-C211-C212-C213
2	C	902	POV	C210-C211-C212-C213
2	D	903	POV	C210-C211-C212-C213
2	A	902	POV	C11-C12-N-C13
2	C	902	POV	C11-C12-N-C13
2	D	903	POV	C11-C12-N-C13
2	D	903	POV	C312-C313-C314-C315
2	A	902	POV	C312-C313-C314-C315
2	C	902	POV	C312-C313-C314-C315
2	B	902	POV	C312-C313-C314-C315
2	A	901	POV	O21-C2-C3-O31
2	B	901	POV	O21-C2-C3-O31
2	C	901	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	D	902	POV	O21-C2-C3-O31
2	A	904	POV	C210-C211-C212-C213
2	B	904	POV	C210-C211-C212-C213
2	D	901	POV	C210-C211-C212-C213
2	D	903	POV	C23-C24-C25-C26
2	C	904	POV	C210-C211-C212-C213
2	A	902	POV	C23-C24-C25-C26
2	B	902	POV	C23-C24-C25-C26
2	C	902	POV	C23-C24-C25-C26
2	C	901	POV	C36-C37-C38-C39
2	B	901	POV	C36-C37-C38-C39
2	D	902	POV	C36-C37-C38-C39
2	A	901	POV	C36-C37-C38-C39
2	A	901	POV	C23-C24-C25-C26
2	B	901	POV	C33-C34-C35-C36
2	C	904	POV	C310-C311-C312-C313
2	A	904	POV	C1-C2-C3-O31
2	B	904	POV	C1-C2-C3-O31
2	C	904	POV	C1-C2-C3-O31
2	D	901	POV	C1-C2-C3-O31
2	A	904	POV	C310-C311-C312-C313
2	B	904	POV	C214-C215-C216-C217
2	A	904	POV	C214-C215-C216-C217
2	B	904	POV	C310-C311-C312-C313
2	C	904	POV	C214-C215-C216-C217
2	D	901	POV	C310-C311-C312-C313
2	A	901	POV	C34-C35-C36-C37
2	C	901	POV	C33-C34-C35-C36
2	D	902	POV	C33-C34-C35-C36
2	D	902	POV	C34-C35-C36-C37
2	D	901	POV	C214-C215-C216-C217
2	C	901	POV	C34-C35-C36-C37
2	A	901	POV	C33-C34-C35-C36
2	A	904	POV	C24-C25-C26-C27
2	B	901	POV	C23-C24-C25-C26
2	B	904	POV	C24-C25-C26-C27
2	C	904	POV	C24-C25-C26-C27
2	D	901	POV	C24-C25-C26-C27
2	B	901	POV	C34-C35-C36-C37
2	A	902	POV	O11-C1-C2-C3
2	B	902	POV	O11-C1-C2-C3
2	C	902	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	903	POV	O11-C1-C2-C3
2	C	901	POV	C23-C24-C25-C26
2	A	901	POV	C1-C2-C3-O31
2	B	901	POV	C1-C2-C3-O31
2	C	901	POV	C1-C2-C3-O31
2	D	902	POV	C1-C2-C3-O31
2	B	902	POV	C311-C312-C313-C314
2	A	902	POV	C311-C312-C313-C314
2	C	902	POV	C311-C312-C313-C314
2	D	903	POV	C311-C312-C313-C314
2	D	903	POV	C2-C1-O11-P
2	D	902	POV	C23-C24-C25-C26
2	A	901	POV	C1-O11-P-O14
2	A	901	POV	C11-O12-P-O13
2	A	904	POV	C11-O12-P-O14
2	B	901	POV	C1-O11-P-O14
2	B	901	POV	C11-O12-P-O13
2	B	904	POV	C11-O12-P-O14
2	C	901	POV	C1-O11-P-O14
2	C	901	POV	C11-O12-P-O13
2	C	904	POV	C11-O12-P-O14
2	D	901	POV	C11-O12-P-O14
2	D	902	POV	C1-O11-P-O14
2	D	902	POV	C11-O12-P-O13
2	A	902	POV	C2-C1-O11-P
2	B	902	POV	C2-C1-O11-P
2	C	902	POV	C2-C1-O11-P
2	A	902	POV	C1-C2-O21-C21
2	B	902	POV	C1-C2-O21-C21
2	C	902	POV	C1-C2-O21-C21
2	A	902	POV	O11-C1-C2-O21
2	B	902	POV	O11-C1-C2-O21
2	C	902	POV	O11-C1-C2-O21
2	D	903	POV	O11-C1-C2-O21
3	A	903	I8E	C1-C2-C3-C4
3	B	903	I8E	C1-C2-C3-C4
3	C	903	I8E	C1-C2-C3-C4
3	D	904	I8E	C1-C2-C3-C4
2	D	901	POV	C37-C38-C39-C310
2	D	903	POV	C1-C2-O21-C21
2	C	904	POV	C37-C38-C39-C310
2	A	904	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
2	C	904	POV	C25-C26-C27-C28
2	B	904	POV	C37-C38-C39-C310
2	B	904	POV	C25-C26-C27-C28
2	A	904	POV	C25-C26-C27-C28
2	D	901	POV	C25-C26-C27-C28
2	C	902	POV	C25-C26-C27-C28
2	B	902	POV	C25-C26-C27-C28
2	A	904	POV	C215-C216-C217-C218
2	D	901	POV	C215-C216-C217-C218
2	A	902	POV	C25-C26-C27-C28
2	B	904	POV	C215-C216-C217-C218
2	D	903	POV	C25-C26-C27-C28
2	A	901	POV	C29-C210-C211-C212
2	B	901	POV	C29-C210-C211-C212
2	B	904	POV	C27-C28-C29-C210
2	D	901	POV	C27-C28-C29-C210
2	D	902	POV	C29-C210-C211-C212
2	D	903	POV	C3-C2-O21-C21
2	A	904	POV	C27-C28-C29-C210
2	C	901	POV	C29-C210-C211-C212
2	C	904	POV	C215-C216-C217-C218
2	C	904	POV	C27-C28-C29-C210
2	C	902	POV	O31-C31-C32-C33
2	A	902	POV	O31-C31-C32-C33
2	B	902	POV	O31-C31-C32-C33
2	D	903	POV	O31-C31-C32-C33
2	D	901	POV	C33-C34-C35-C36
2	D	901	POV	O21-C21-C22-C23
2	A	904	POV	C33-C34-C35-C36
2	A	904	POV	O21-C21-C22-C23
2	B	904	POV	O21-C21-C22-C23
2	C	904	POV	O21-C21-C22-C23
2	C	904	POV	C33-C34-C35-C36
2	D	902	POV	C214-C215-C216-C217
2	A	904	POV	O22-C21-C22-C23
2	B	901	POV	C214-C215-C216-C217
2	C	901	POV	C214-C215-C216-C217
2	B	904	POV	C33-C34-C35-C36
2	A	901	POV	C214-C215-C216-C217
2	B	904	POV	O22-C21-C22-C23
2	D	901	POV	O22-C21-C22-C23
2	A	902	POV	C313-C314-C315-C316

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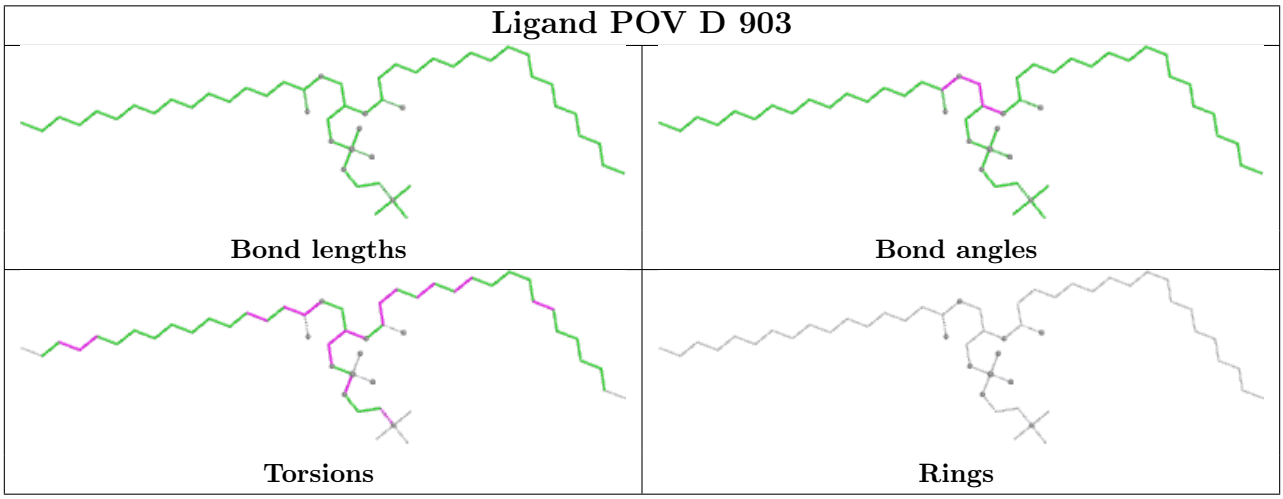
Mol	Chain	Res	Type	Atoms
2	C	902	POV	C313-C314-C315-C316
2	B	902	POV	O32-C31-C32-C33
2	C	904	POV	O22-C21-C22-C23
2	D	903	POV	O32-C31-C32-C33
2	B	902	POV	C313-C314-C315-C316
2	A	902	POV	O32-C31-C32-C33
2	C	902	POV	O32-C31-C32-C33
2	A	902	POV	O21-C21-C22-C23
2	D	901	POV	O31-C31-C32-C33
2	D	903	POV	O21-C21-C22-C23
2	B	902	POV	O21-C21-C22-C23
2	B	904	POV	O31-C31-C32-C33
2	C	902	POV	O21-C21-C22-C23
2	C	904	POV	O31-C31-C32-C33

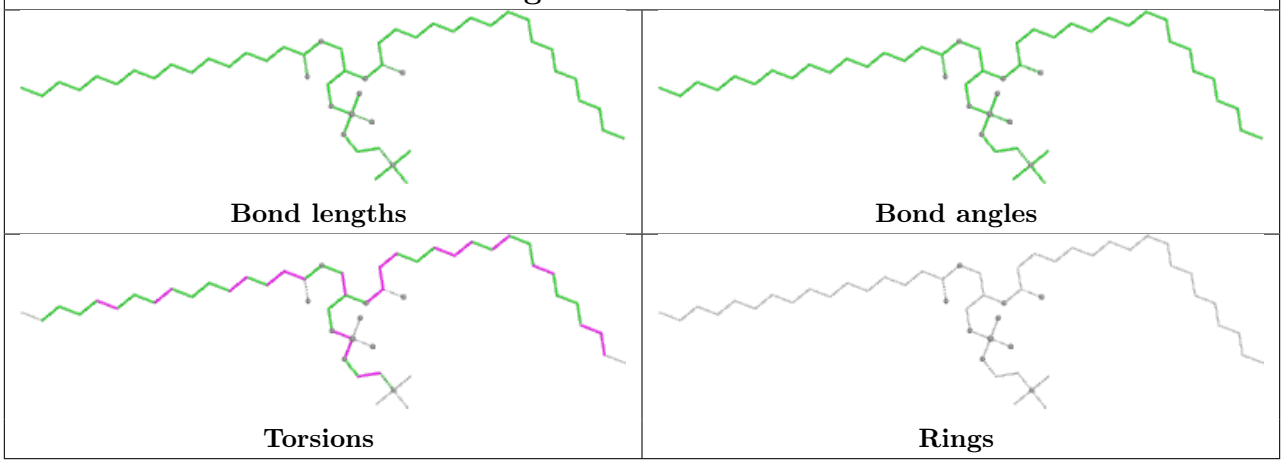
There are no ring outliers.

No monomer is involved in short contacts.

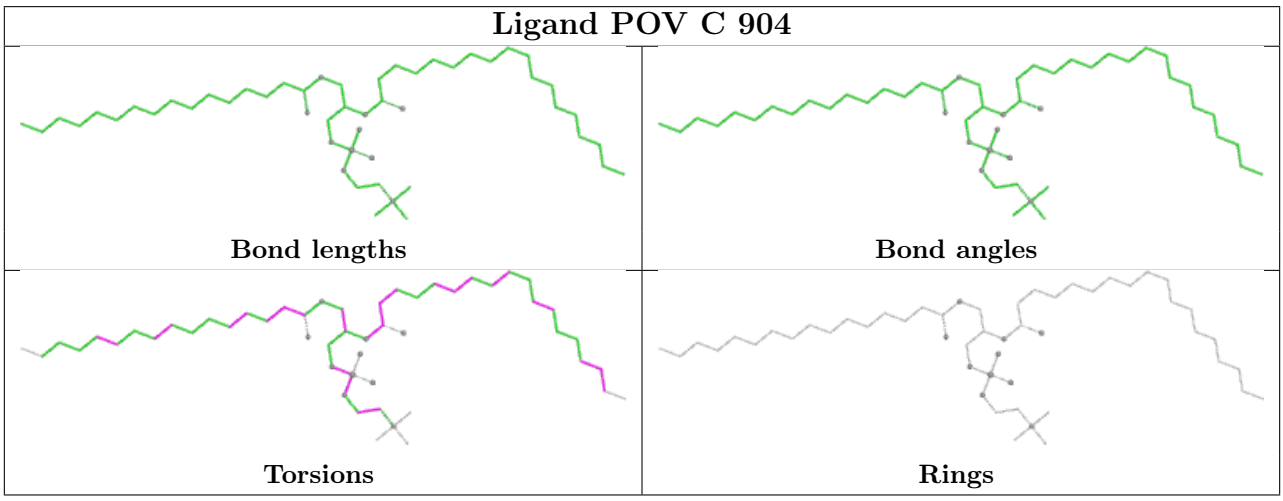
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



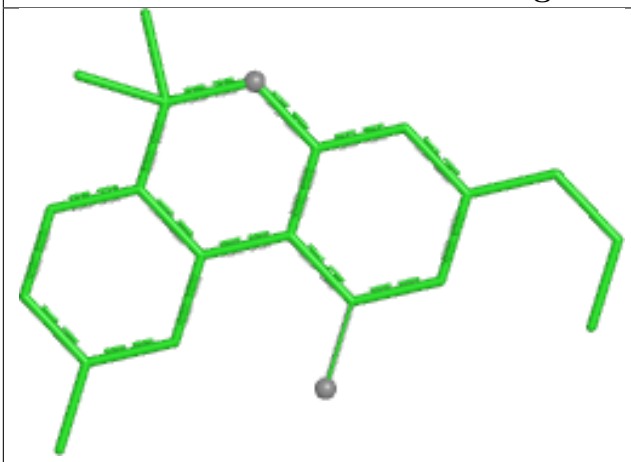
Ligand POV B 904



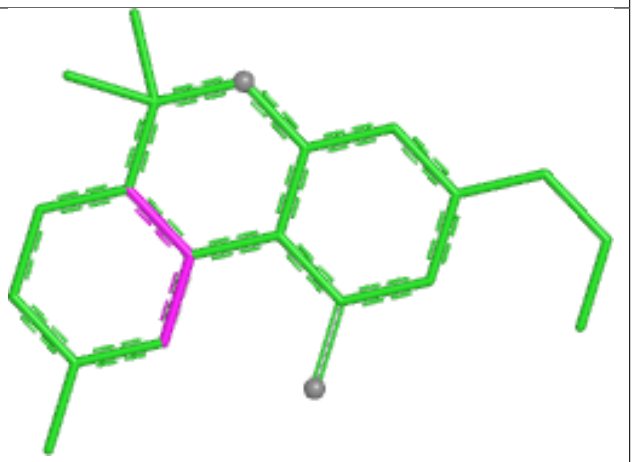
Ligand POV C 904



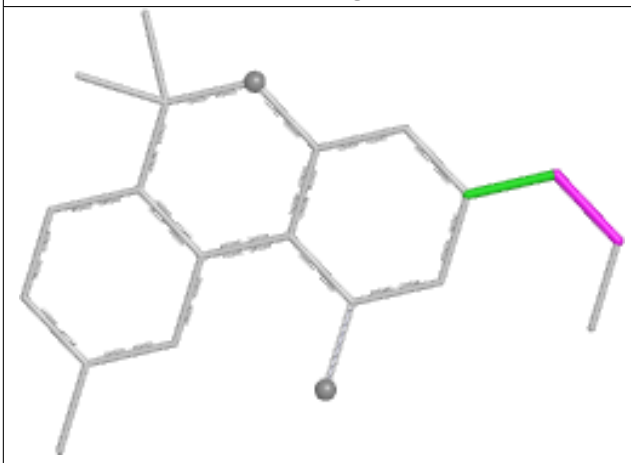
Ligand I8E A 903



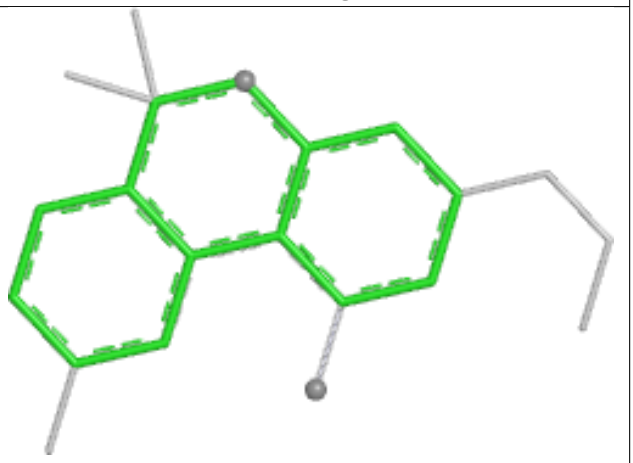
Bond lengths



Bond angles

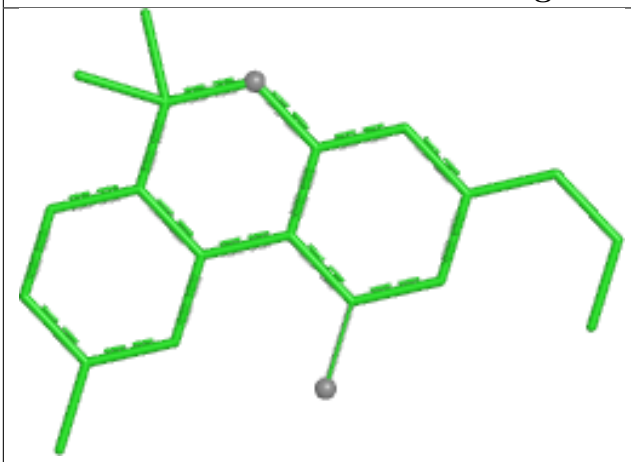


Torsions



Rings

Ligand I8E B 903



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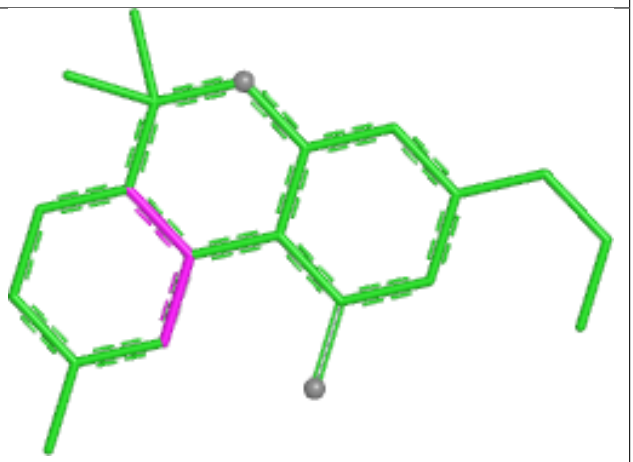
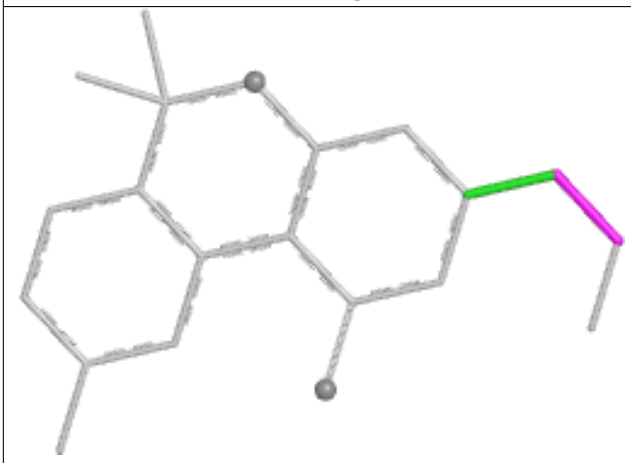
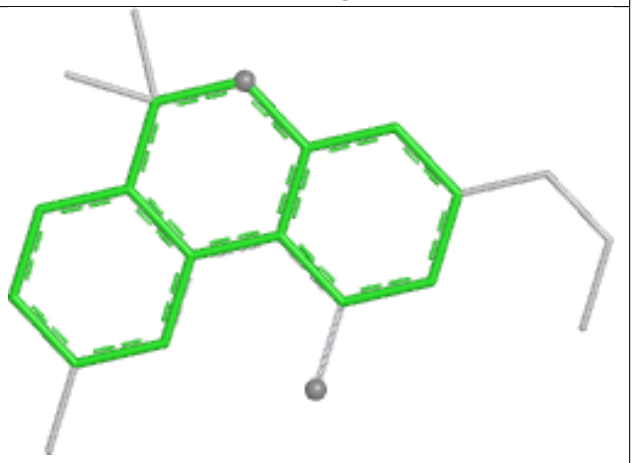


Bond angles

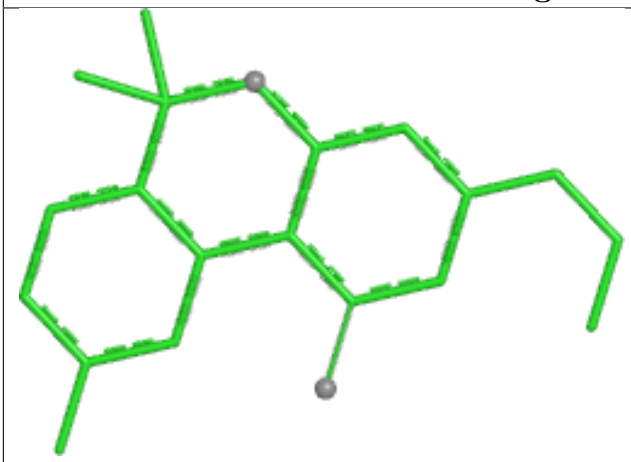


Torsions

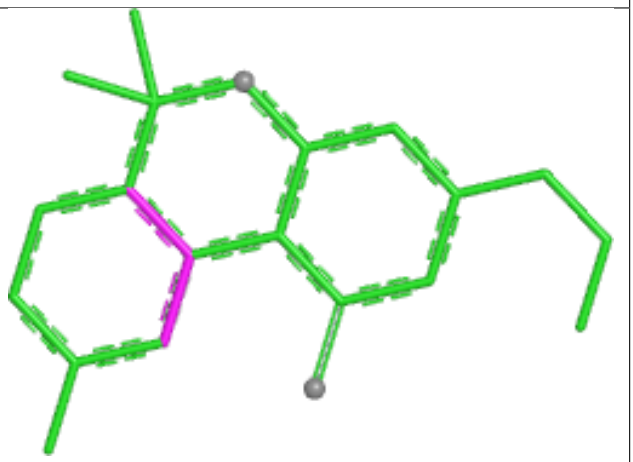


Rings

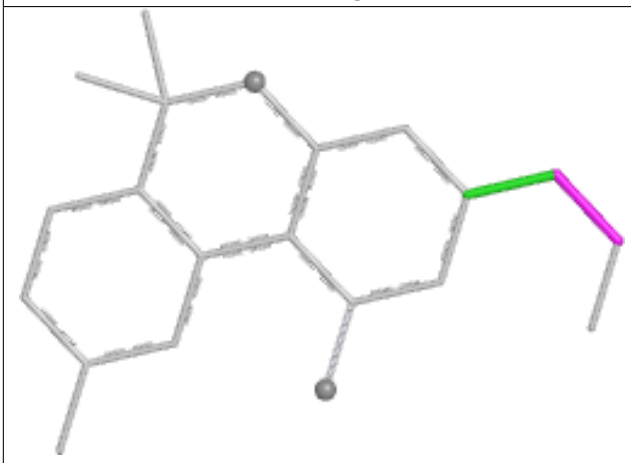
Ligand I8E C 903



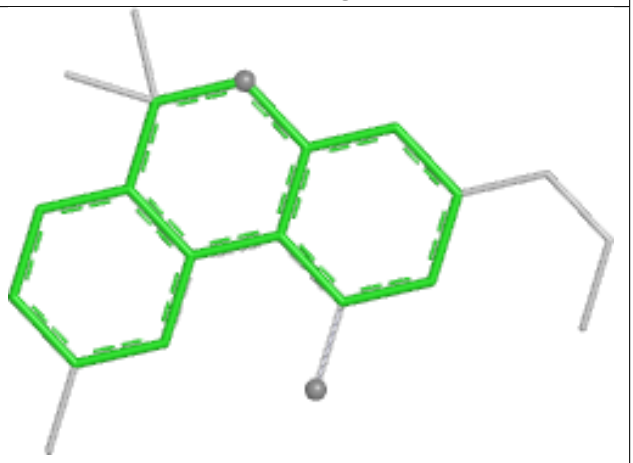
Bond lengths



Bond angles

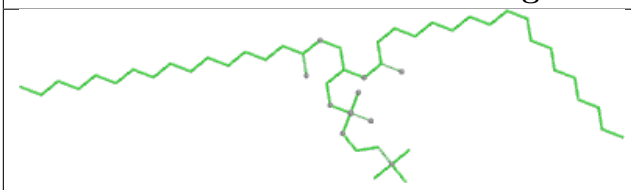


Torsions

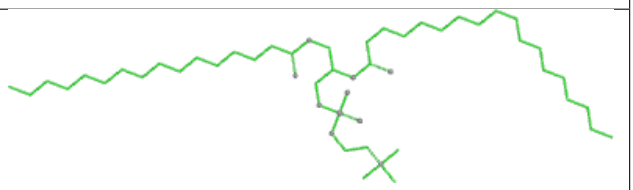


Rings

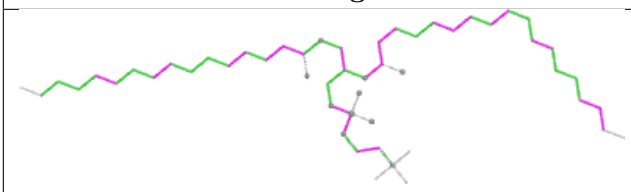
Ligand POV D 901



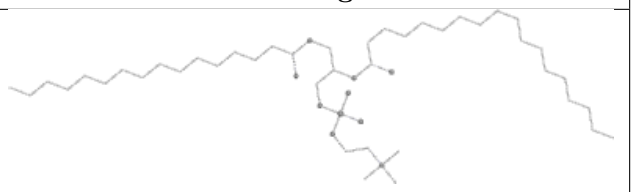
Bond lengths



Bond angles

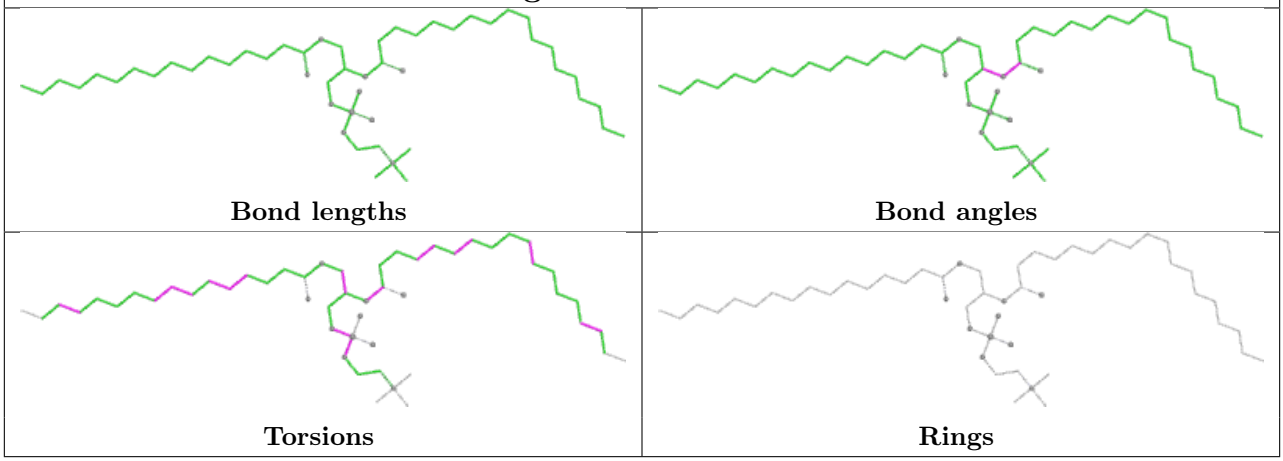


Torsions

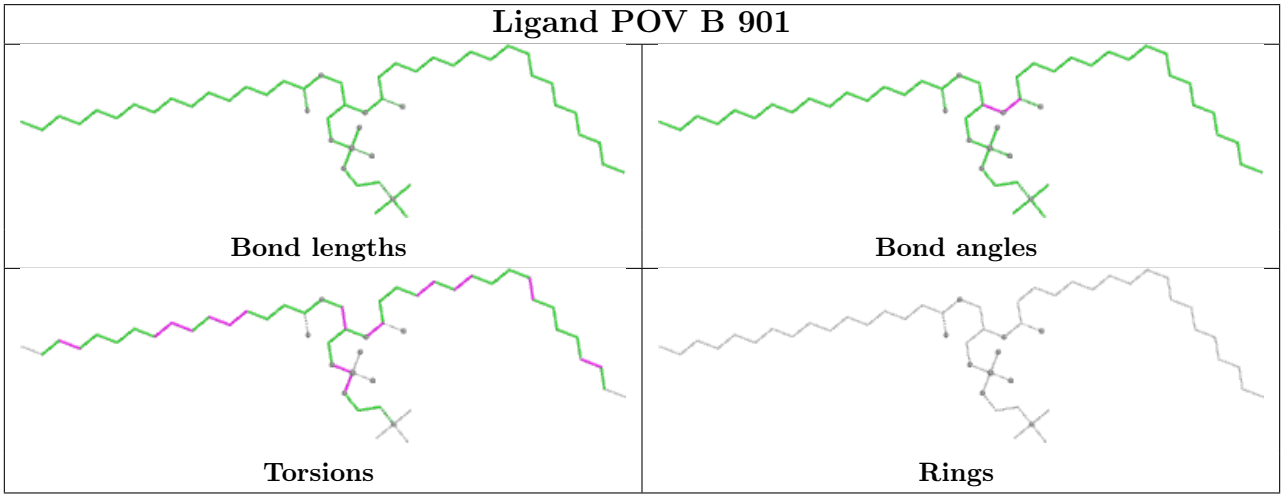


Rings

Ligand POV C 901



Ligand POV B 901



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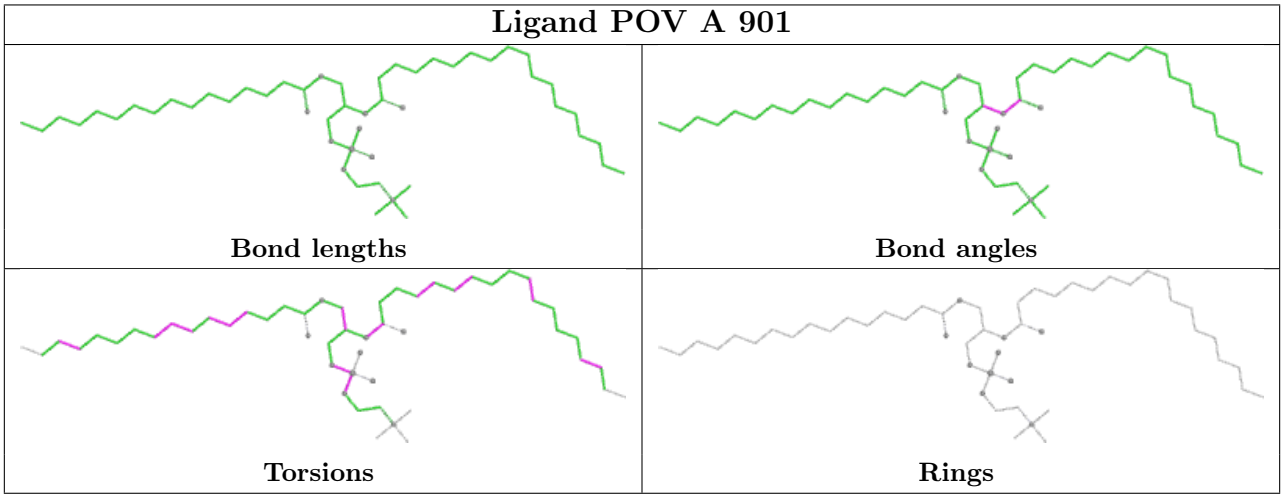

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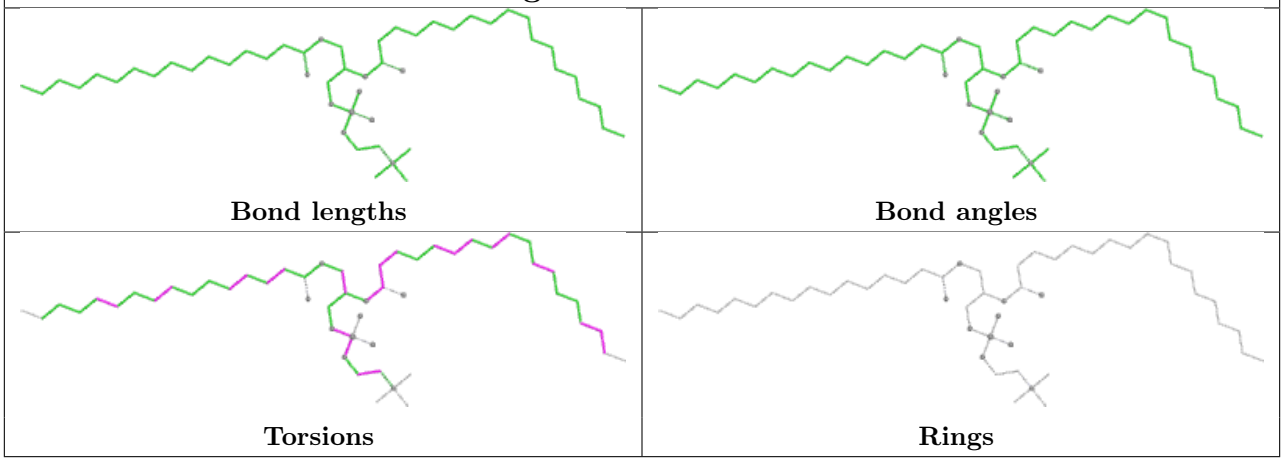

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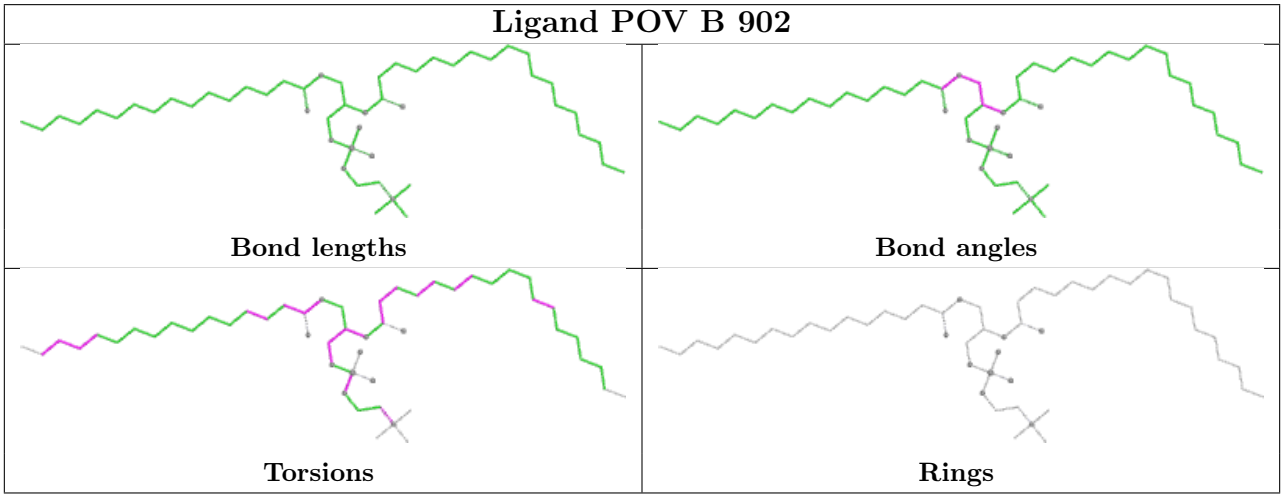

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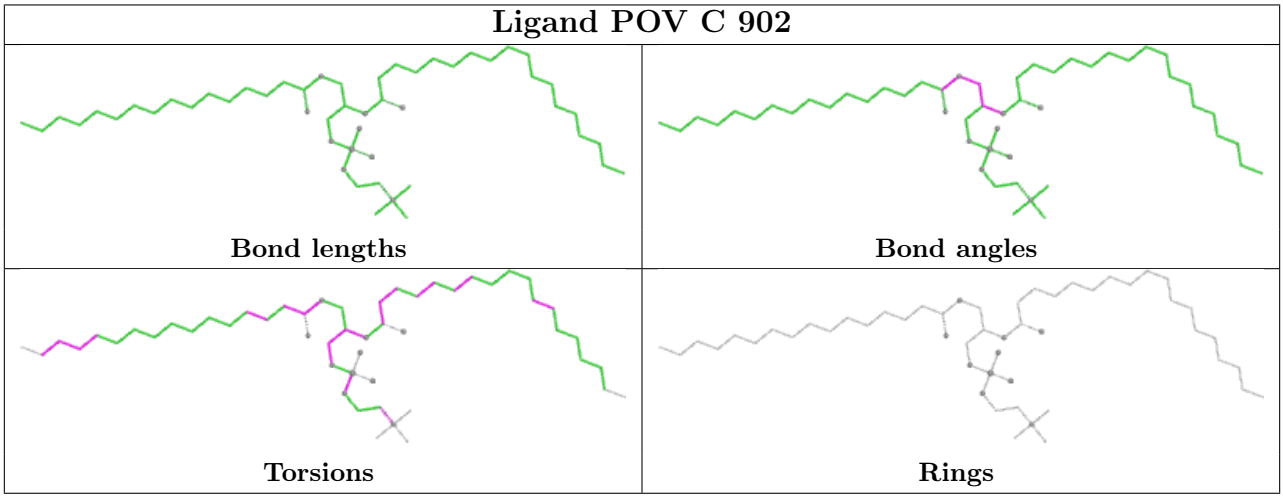

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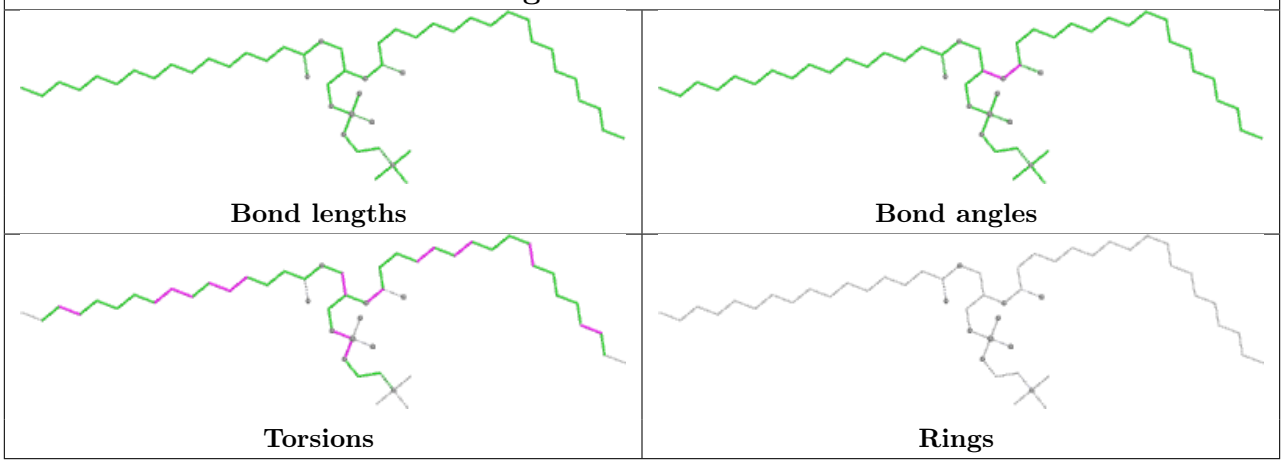

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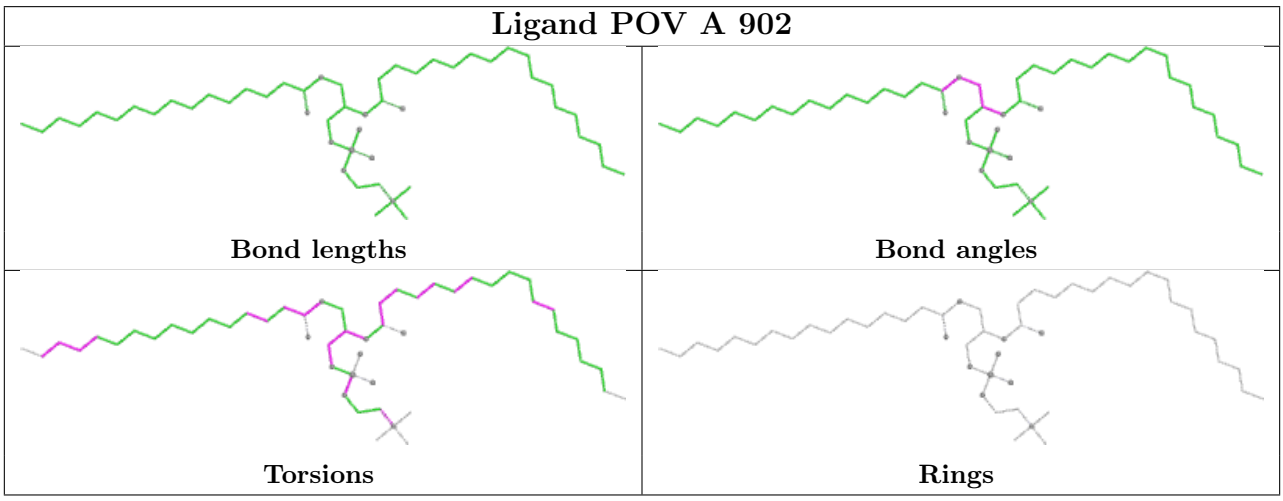
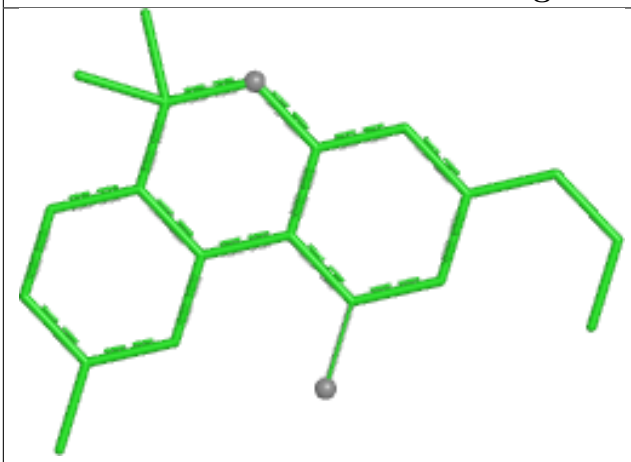
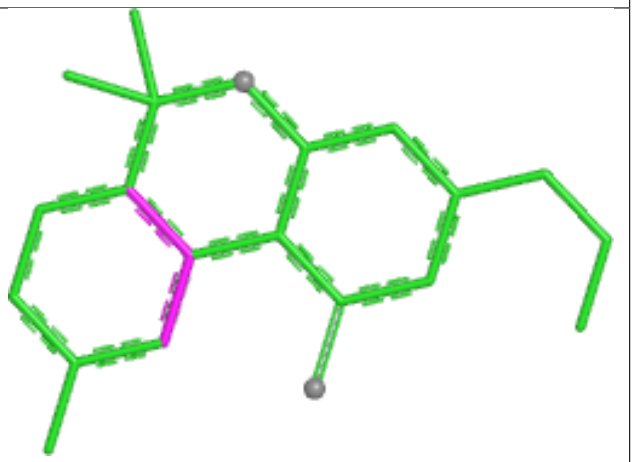


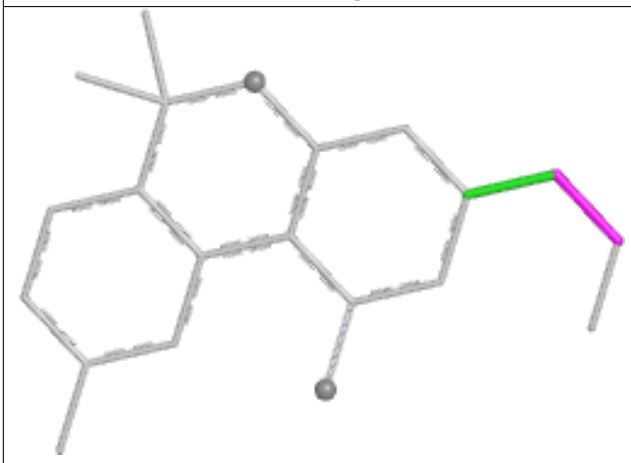
Ligand I8E D 904



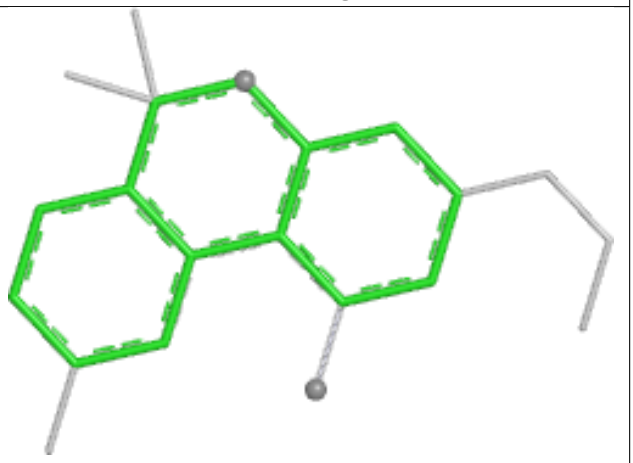
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

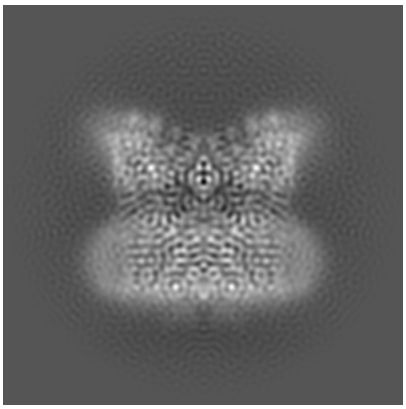
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42996. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map



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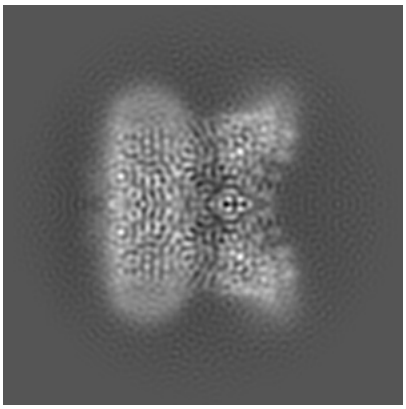

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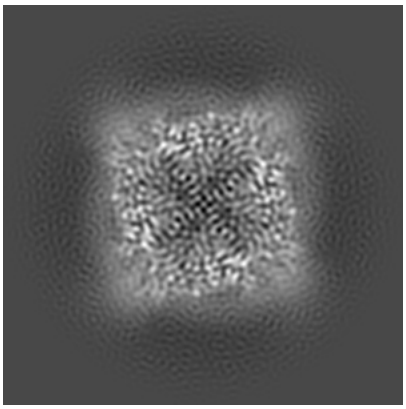
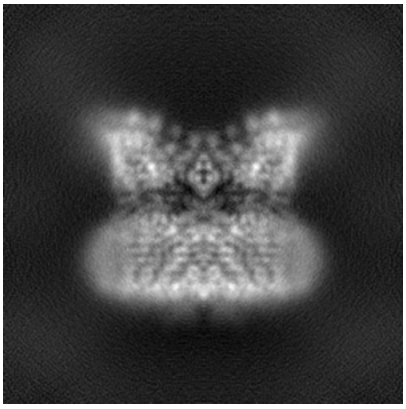
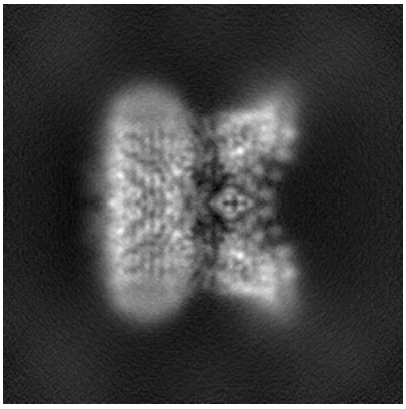


Z

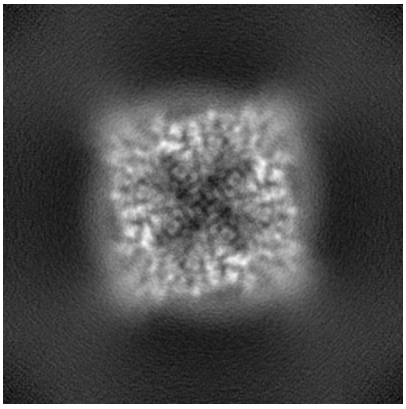
6.1.2 Raw map



X



Y

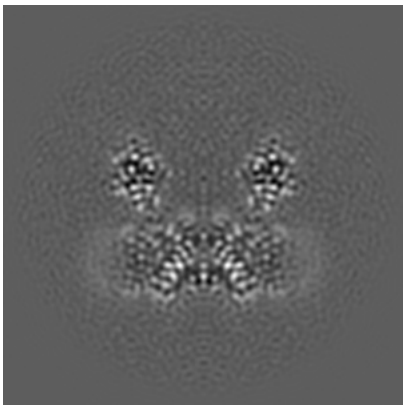


Z

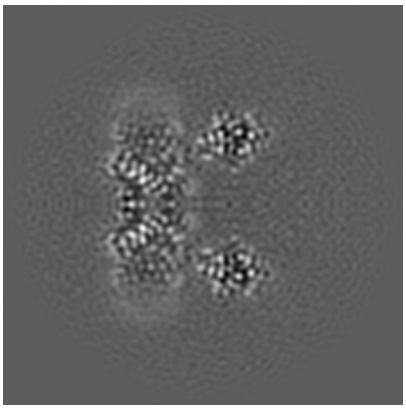
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

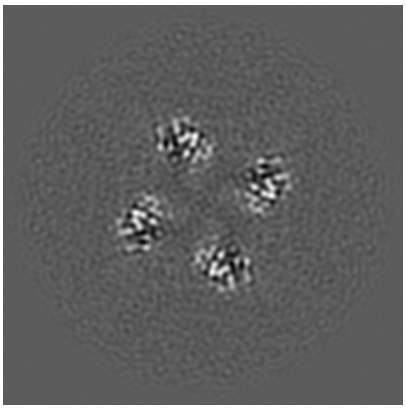
6.2.1 Primary map



X Index: 128

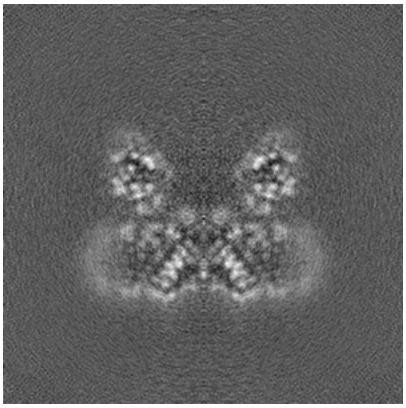


Y Index: 128

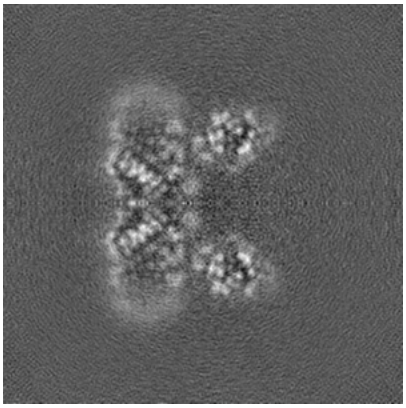


Z Index: 128

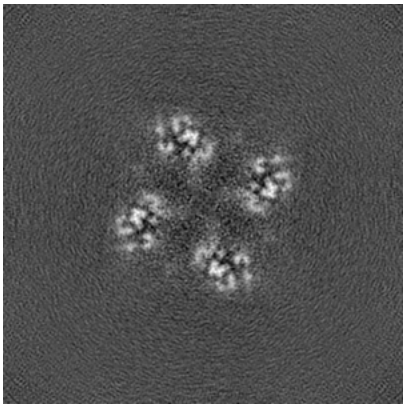
6.2.2 Raw map



X Index: 128



Y Index: 128

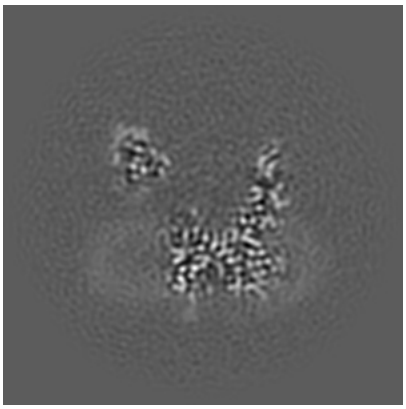


Z Index: 128

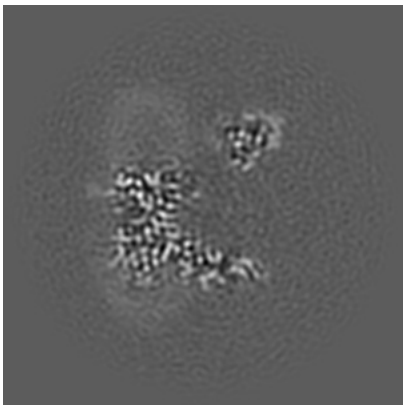
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

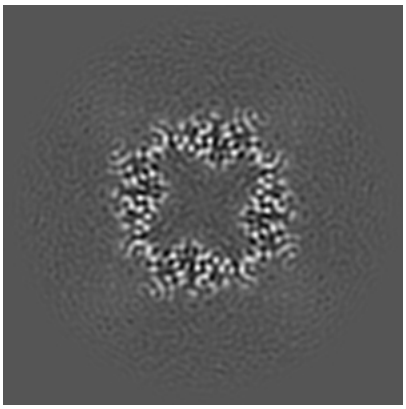
6.3.1 Primary map



X Index: 111

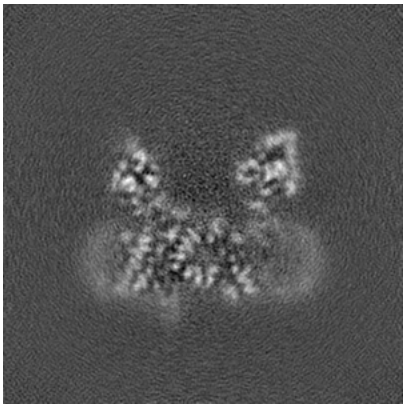


Y Index: 111

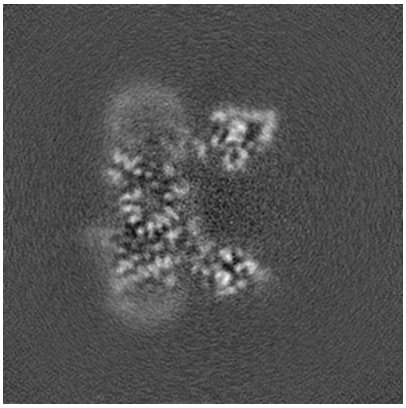


Z Index: 151

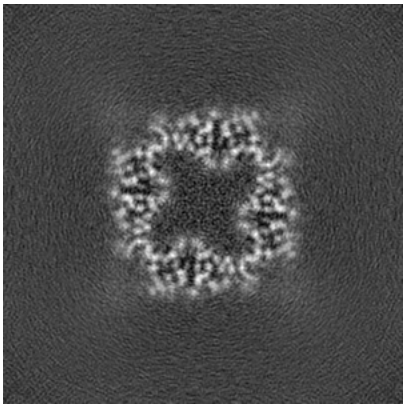
6.3.2 Raw map



X Index: 132



Y Index: 124

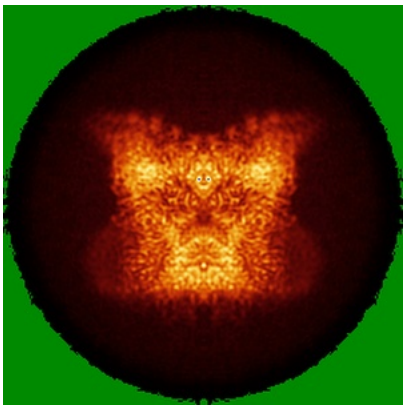


Z Index: 151

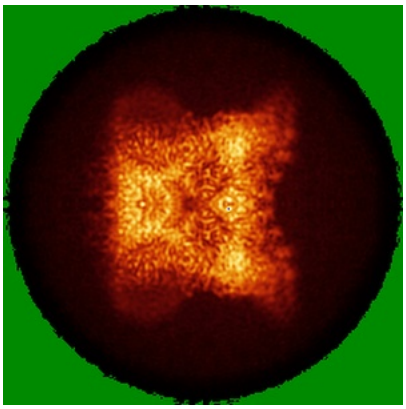
The images above show the largest variance slices of the map in three orthogonal directions.

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

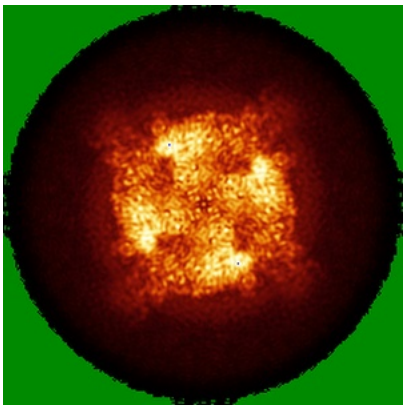
6.4.1 Primary map



X

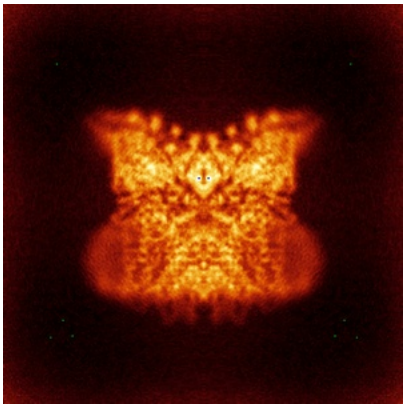


Y

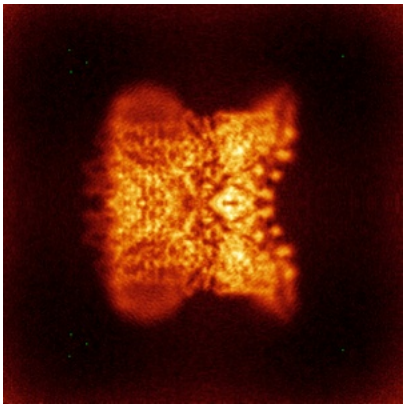


Z

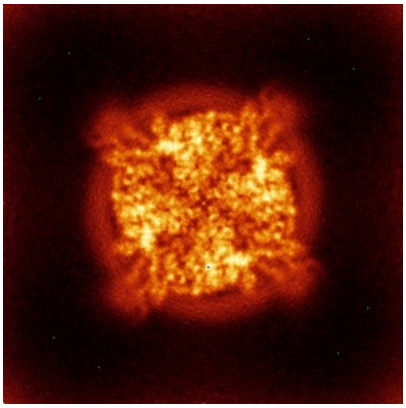
6.4.2 Raw map



X



Y

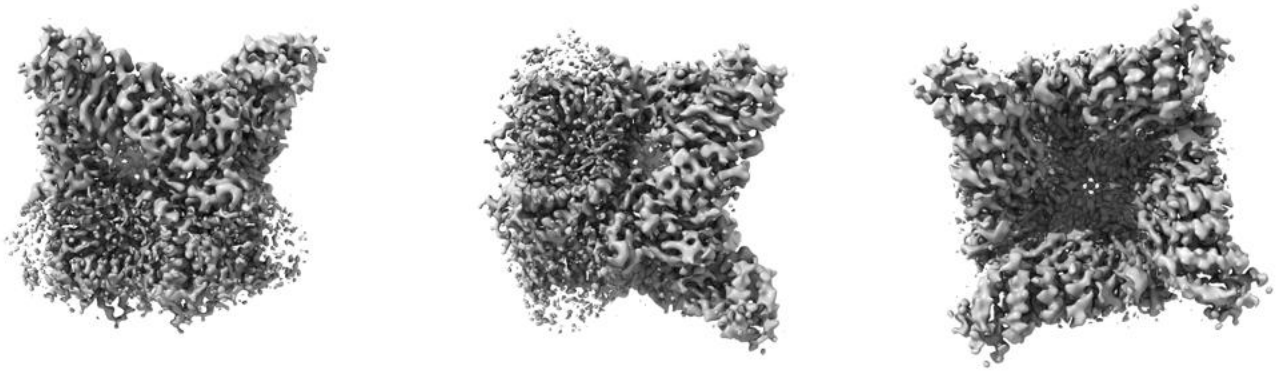


Z

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 0.0877. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

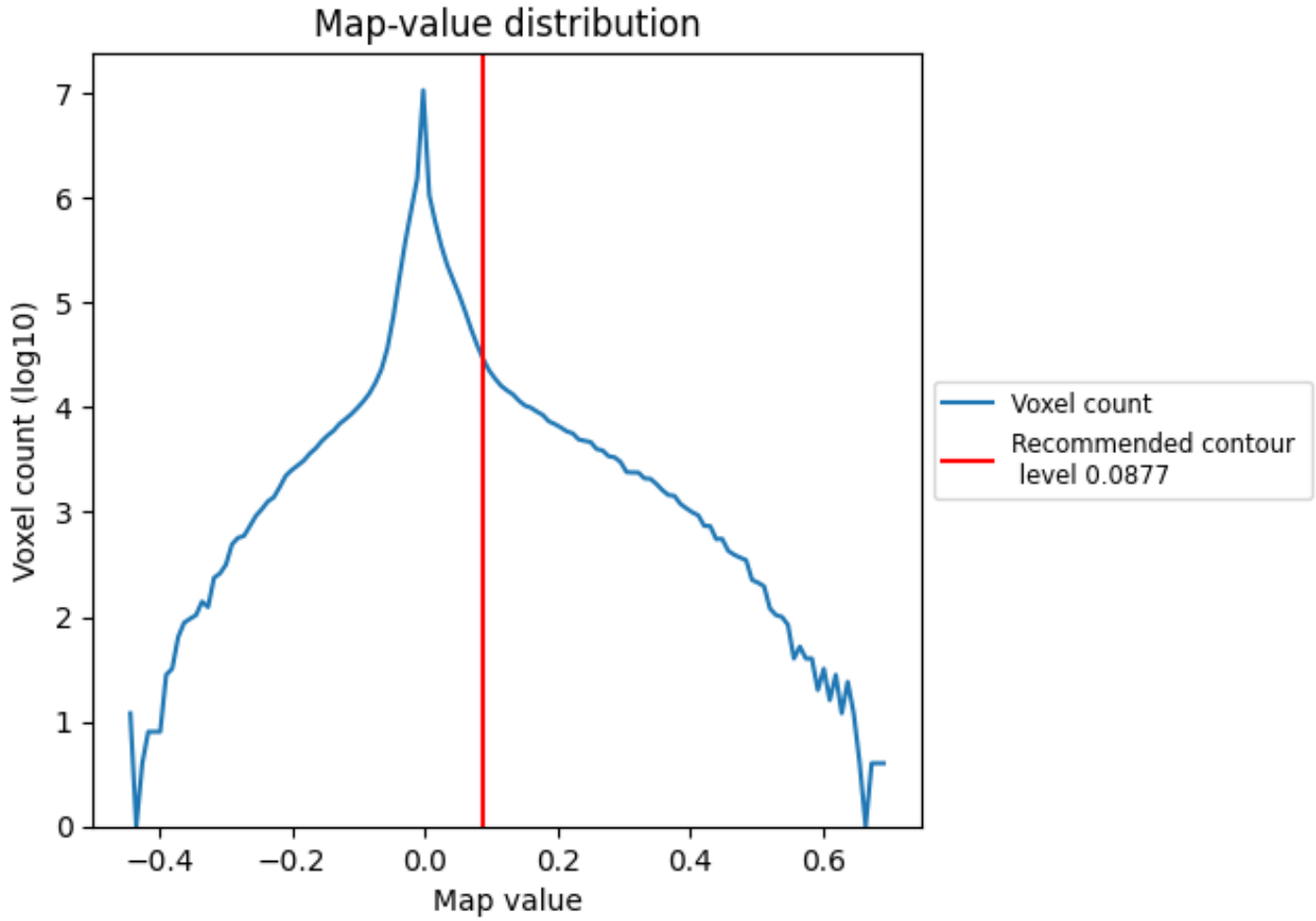
6.6 Mask visualisation (i)

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

7 Map analysis

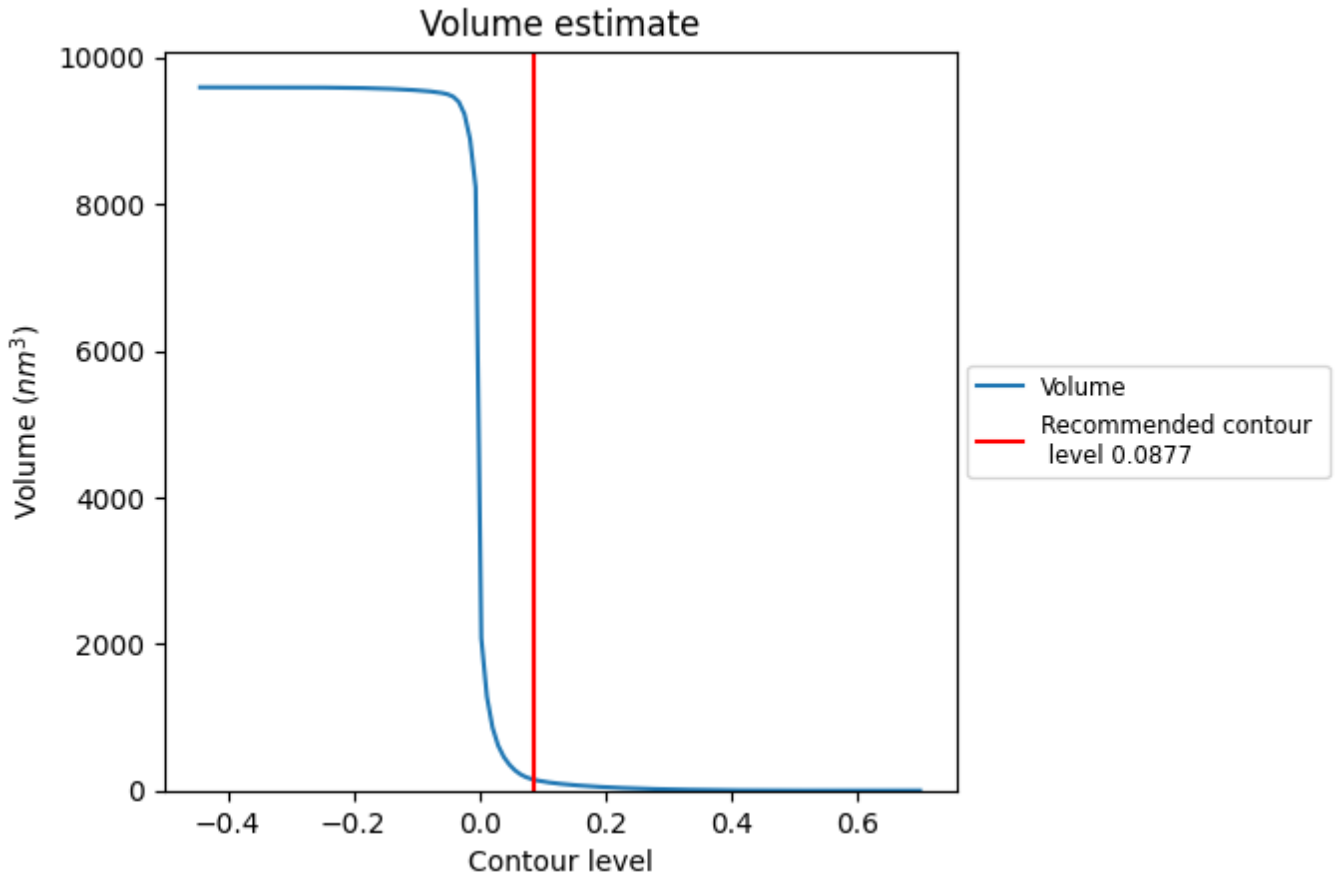
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

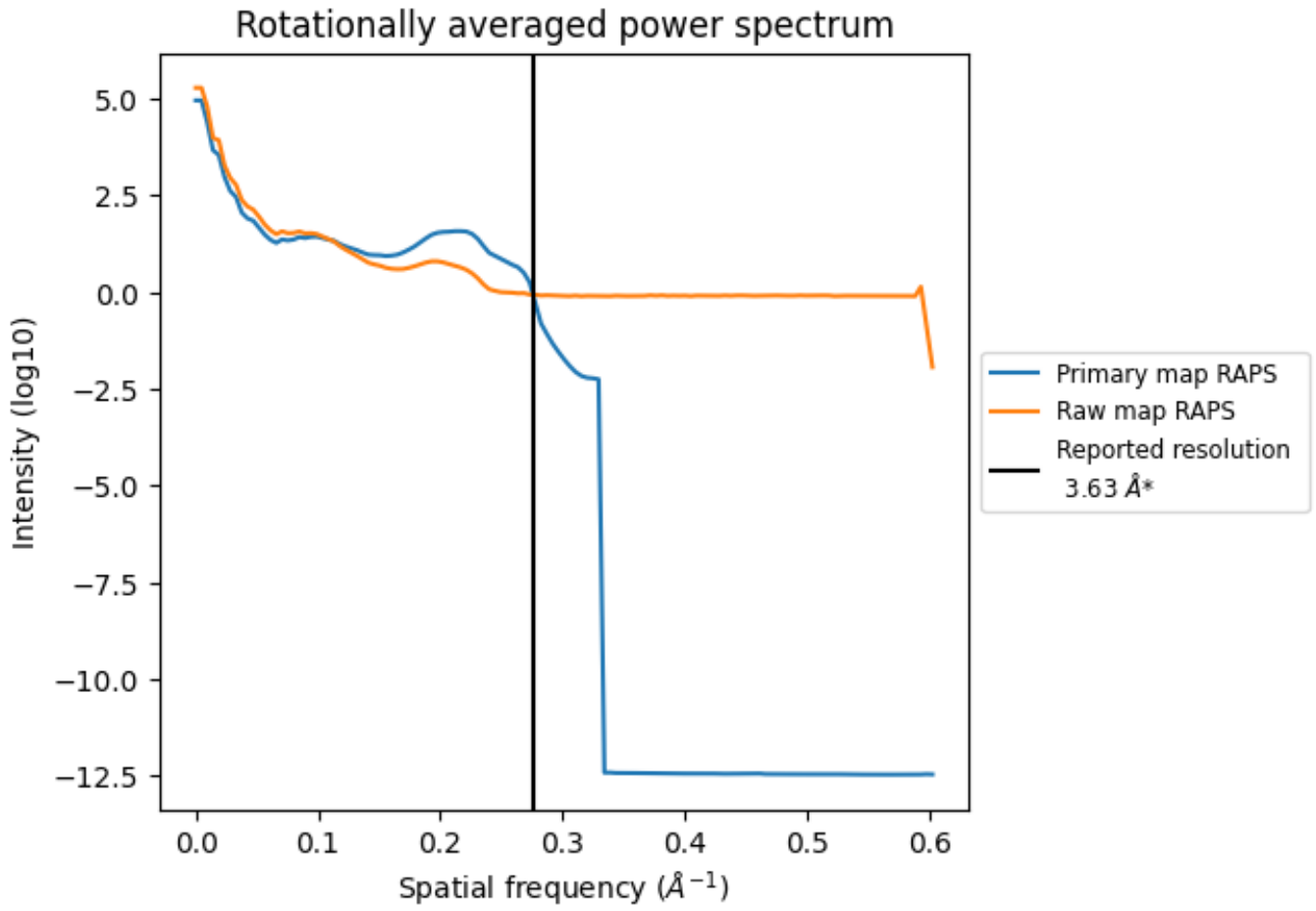
7.2 Volume estimate



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 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)

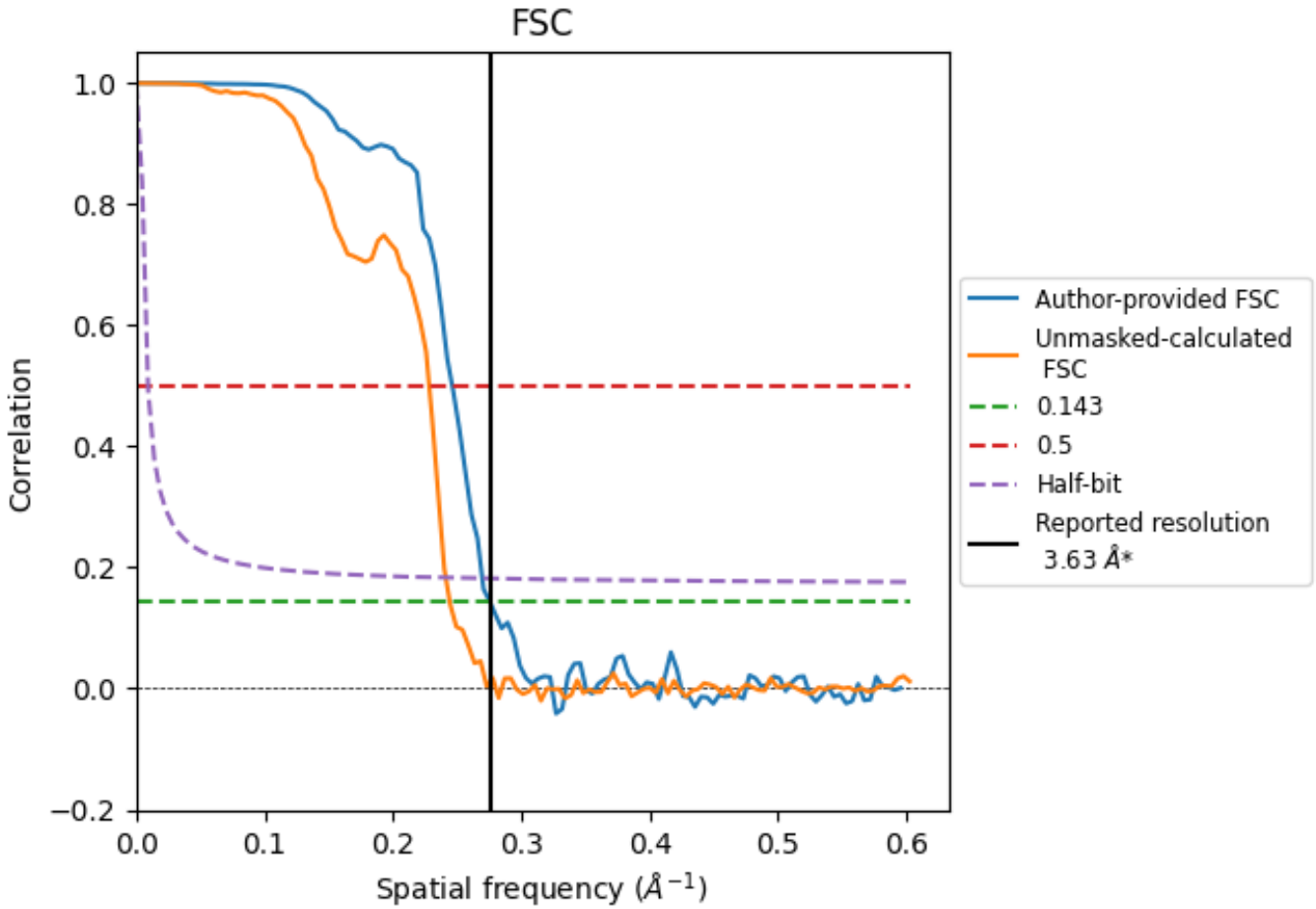


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8.2 Resolution estimates (i)

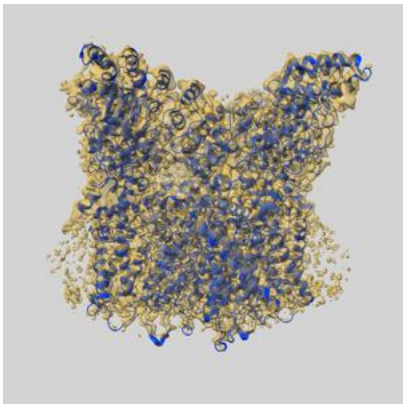
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	3.63	4.06	3.71
Unmasked-calculated*	4.09	4.38	4.15

*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 4.09 differs from the reported value 3.63 by more than 10 %

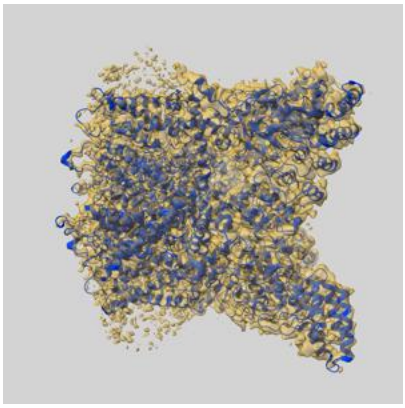
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42996 and PDB model 8V6M. Per-residue inclusion information can be found in section 3 on page 7.

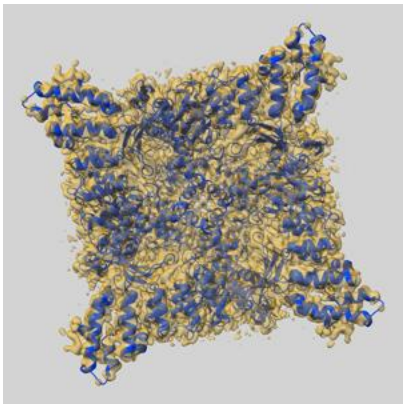
9.1 Map-model overlay



X



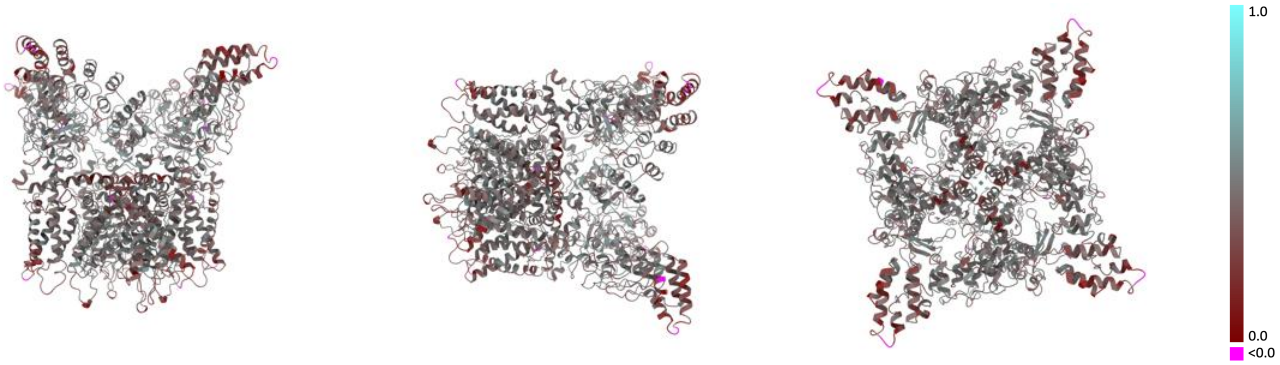
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0877 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.

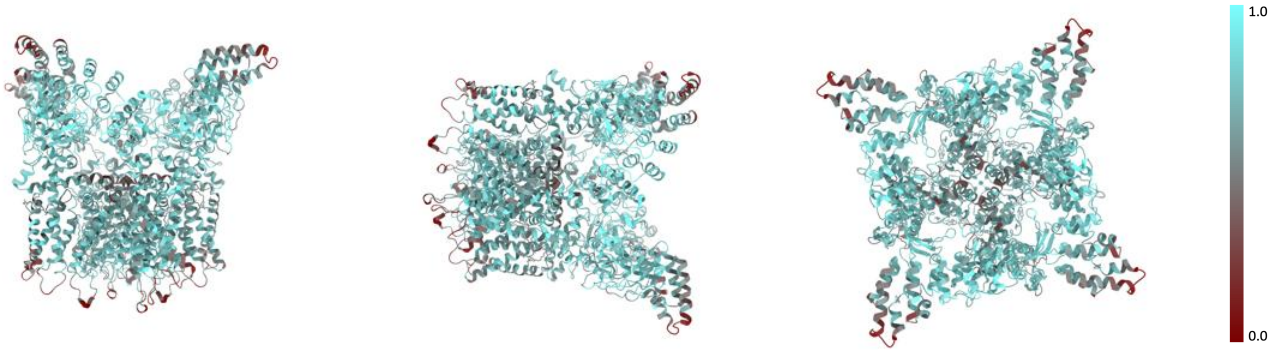
9.2 Q-score mapped to coordinate model (i)



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.

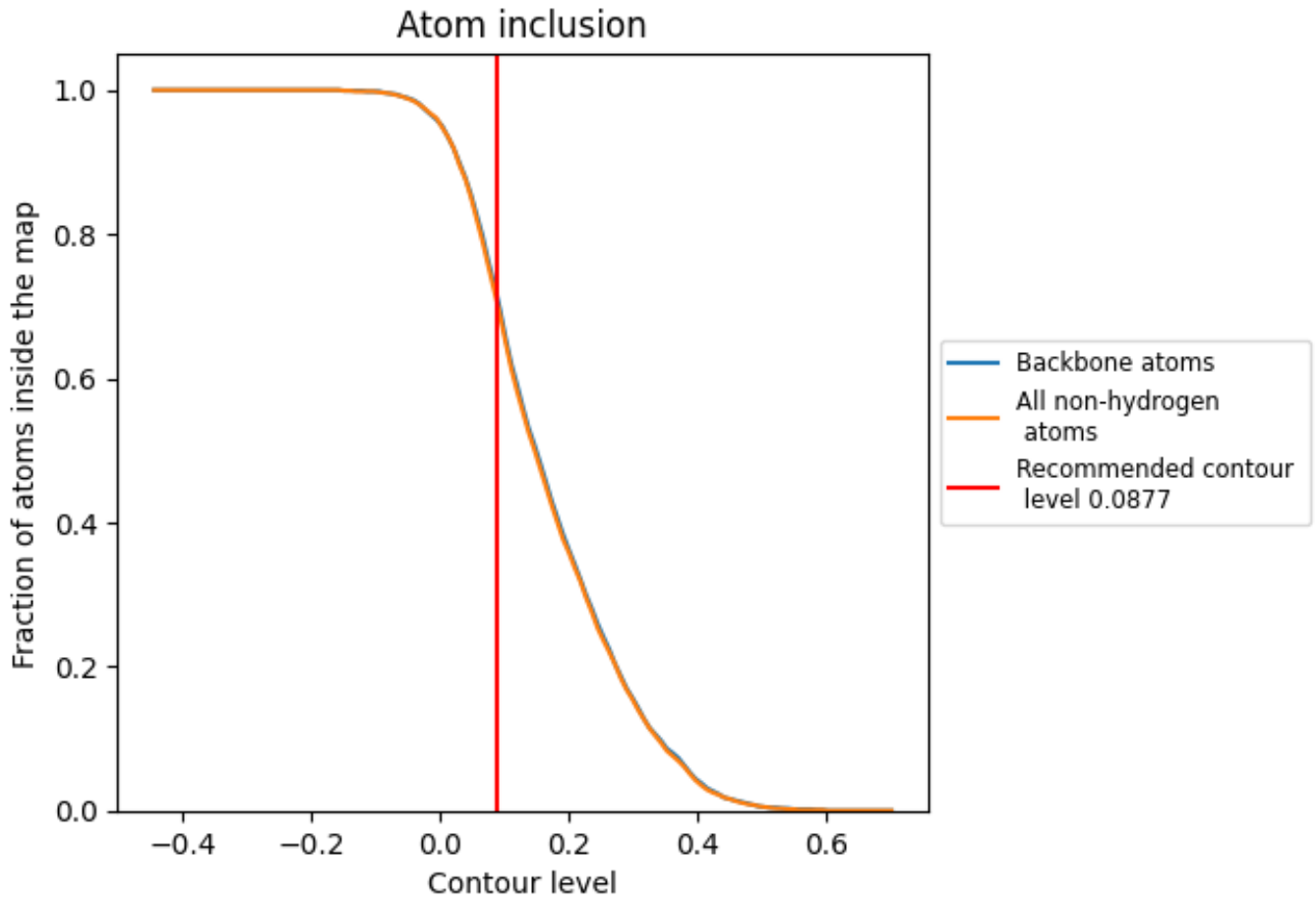
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0877).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.0877) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7080	0.4040
A	0.7080	0.4050
B	0.7070	0.4050
C	0.7080	0.4040
D	0.7070	0.4040