



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:43 PM UTC

PDB ID : 6NZZ / pdb_00006nzz
EMDB ID : EMD-0563
Title : LRRC8A-DCPIB in MSP1E3D1 nanodisc expanded state
Authors : Kern, D.M.; Hite, R.K.; Brohawn, S.G.
Deposited on : 2019-02-14
Resolution : 3.32 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:

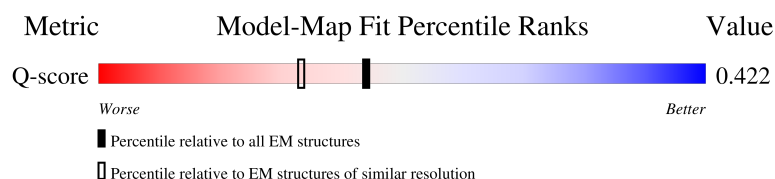
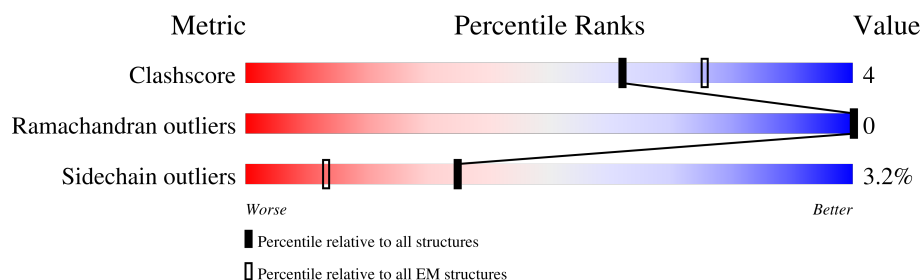
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.32 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	14518 (2.82 - 3.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	820	
1	B	820	
1	C	820	
1	D	820	

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Mol	Chain	Length	Quality of chain
1	E	820	16% 33% 5% 63%
1	F	820	16% 32% 5% 63%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31327 atoms, of which 15669 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.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	306	Total	C	H	N	O	S	0	0
			5123	1697	2555	411	443	17		
1	B	306	Total	C	H	N	O	S	0	0
			5123	1697	2555	411	443	17		
1	C	306	Total	C	H	N	O	S	0	0
			5123	1697	2555	411	443	17		
1	D	306	Total	C	H	N	O	S	0	0
			5123	1697	2555	411	443	17		
1	E	306	Total	C	H	N	O	S	0	0
			5123	1697	2555	411	443	17		
1	F	306	Total	C	H	N	O	S	0	0
			5123	1697	2555	411	443	17		

There are 60 discrepancies between the modelled and reference sequences:

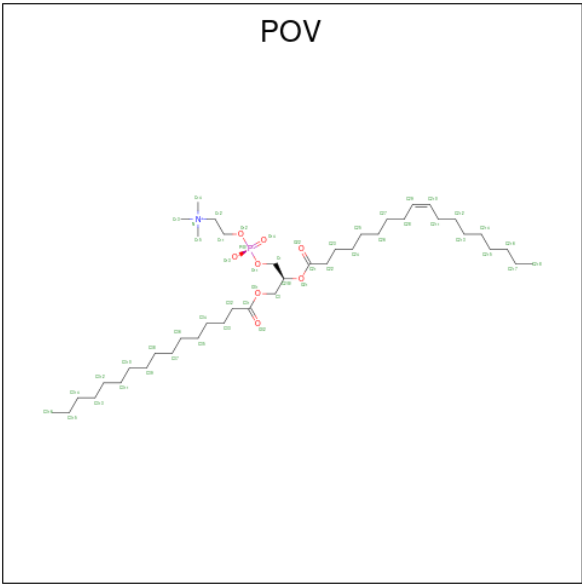
Chain	Residue	Modelled	Actual	Comment	Reference
A	811	SER	-	expression tag	UNP Q80WG5
A	812	ASN	-	expression tag	UNP Q80WG5
A	813	SER	-	expression tag	UNP Q80WG5
A	814	LEU	-	expression tag	UNP Q80WG5
A	815	GLU	-	expression tag	UNP Q80WG5
A	816	VAL	-	expression tag	UNP Q80WG5
A	817	LEU	-	expression tag	UNP Q80WG5
A	818	PHE	-	expression tag	UNP Q80WG5
A	819	GLN	-	expression tag	UNP Q80WG5
A	820	GLY	-	expression tag	UNP Q80WG5
B	811	SER	-	expression tag	UNP Q80WG5
B	812	ASN	-	expression tag	UNP Q80WG5
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	819	GLN	-	expression tag	UNP Q80WG5
B	820	GLY	-	expression tag	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
C	820	GLY	-	expression tag	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
D	820	GLY	-	expression tag	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
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
E	820	GLY	-	expression tag	UNP Q80WG5
F	811	SER	-	expression tag	UNP Q80WG5
F	812	ASN	-	expression tag	UNP Q80WG5
F	813	SER	-	expression tag	UNP Q80WG5
F	814	LEU	-	expression tag	UNP Q80WG5
F	815	GLU	-	expression tag	UNP Q80WG5
F	816	VAL	-	expression tag	UNP Q80WG5
F	817	LEU	-	expression tag	UNP Q80WG5
F	818	PHE	-	expression tag	UNP Q80WG5
F	819	GLN	-	expression tag	UNP Q80WG5
F	820	GLY	-	expression tag	UNP Q80WG5

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



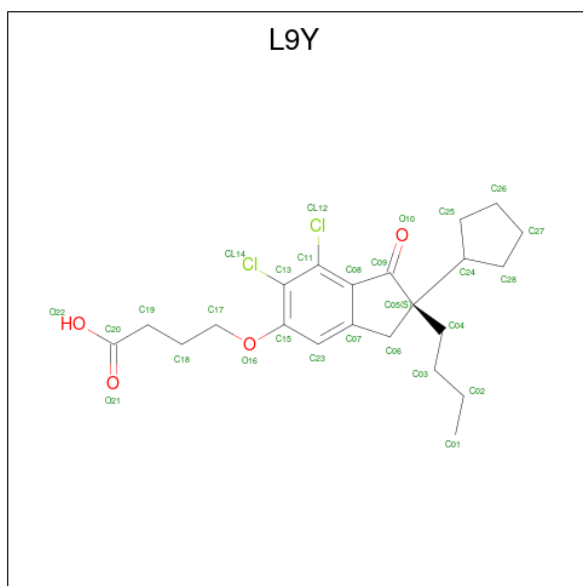
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			38	13	23	2	
2	A	1	Total	C	H	O	0
			28	10	16	2	
2	A	1	Total	C	H	O	0
			23	8	13	2	
2	B	1	Total	C	H	O	0
			38	13	23	2	
2	B	1	Total	C	H	O	0
			28	10	16	2	
2	B	1	Total	C	H	O	0
			23	8	13	2	
2	C	1	Total	C	H	O	0
			38	13	23	2	
2	C	1	Total	C	H	O	0
			28	10	16	2	
2	C	1	Total	C	H	O	0
			23	8	13	2	
2	D	1	Total	C	H	O	0
			38	13	23	2	
2	D	1	Total	C	H	O	0
			28	10	16	2	
2	D	1	Total	C	H	O	0
			23	8	13	2	

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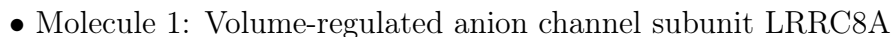
Mol	Chain	Residues	Atoms				AltConf
2	E	1	Total	C	H	O	0
			38	13	23	2	
2	E	1	Total	C	H	O	0
			28	10	16	2	
2	E	1	Total	C	H	O	0
			23	8	13	2	
2	F	1	Total	C	H	O	0
			38	13	23	2	
2	F	1	Total	C	H	O	0
			28	10	16	2	
2	F	1	Total	C	H	O	0
			23	8	13	2	

- Molecule 3 is 4-{{[(2S)-2-butyl-6,7-dichloro-2-cyclopentyl-1-oxo-2,3-dihydro-1H-inden-5-yl]oxy}butanoic acid (CCD ID: L9Y) (formula: C₂₂H₂₈Cl₂O₄).

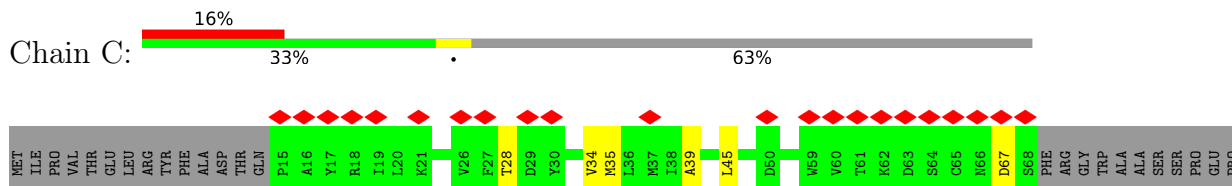


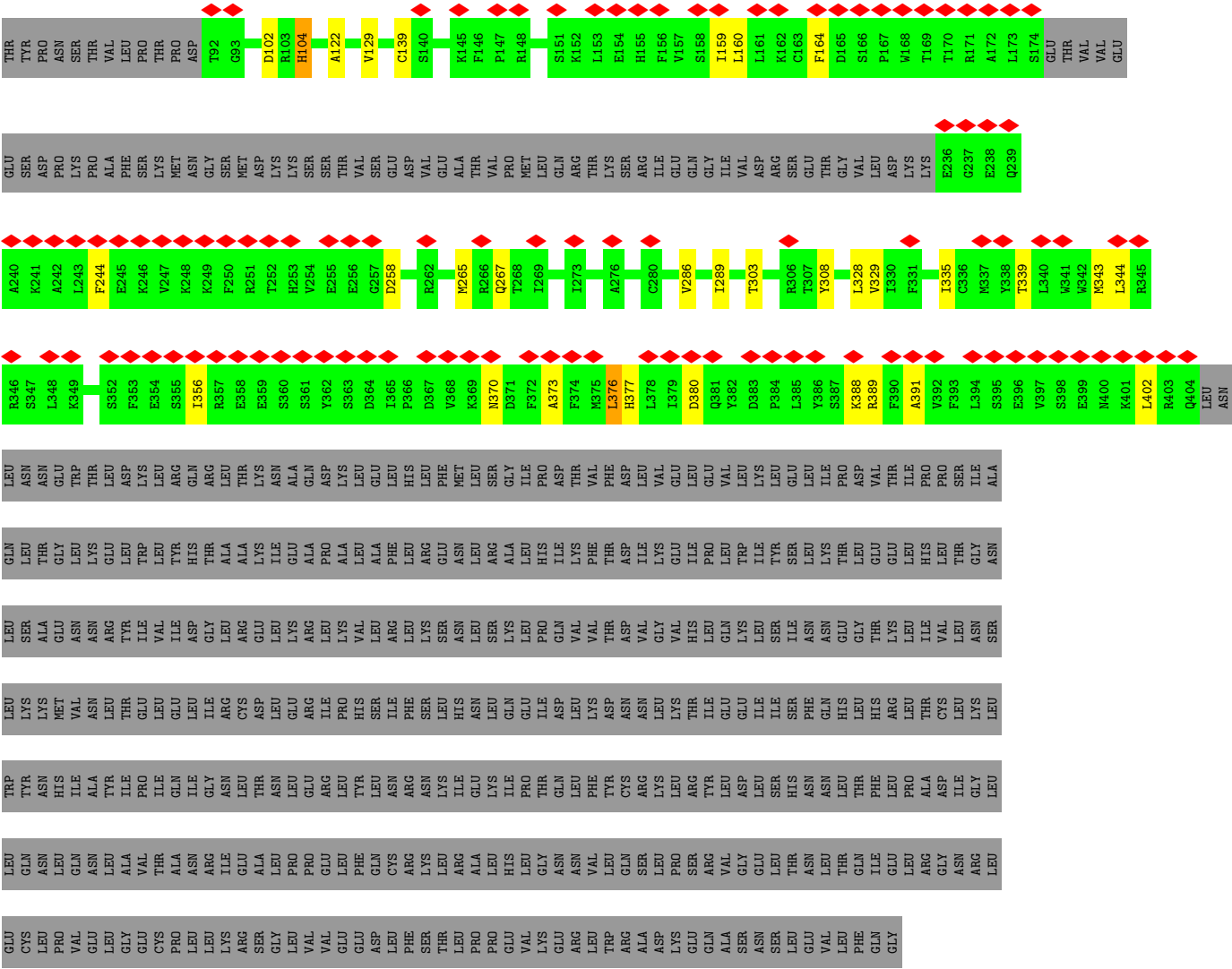
Mol	Chain	Residues	Atoms				AltConf
3	F	1	Total	C	Cl	H	O
			55	22	2	27	4
							0

Chain B:

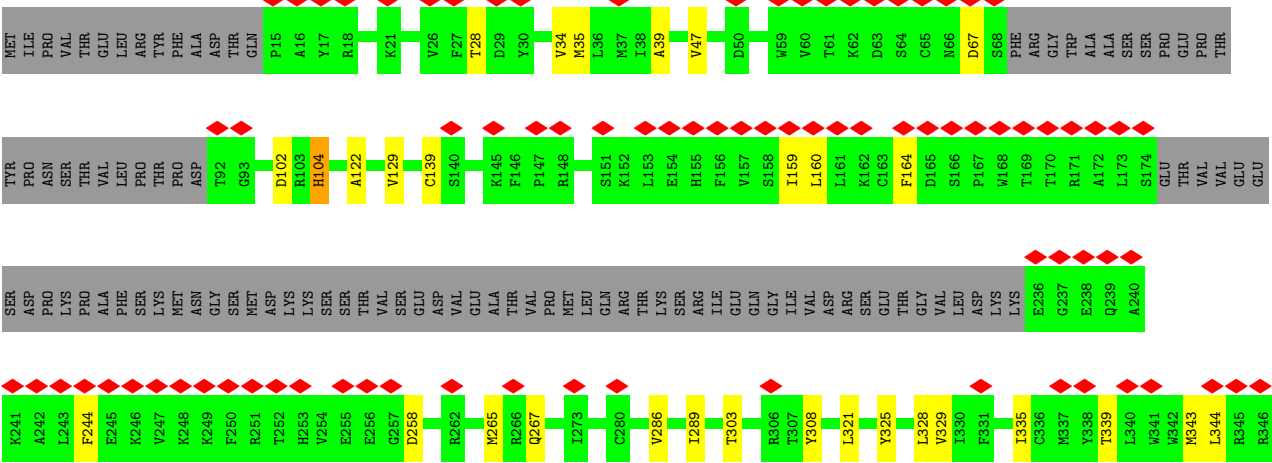


Chain C:

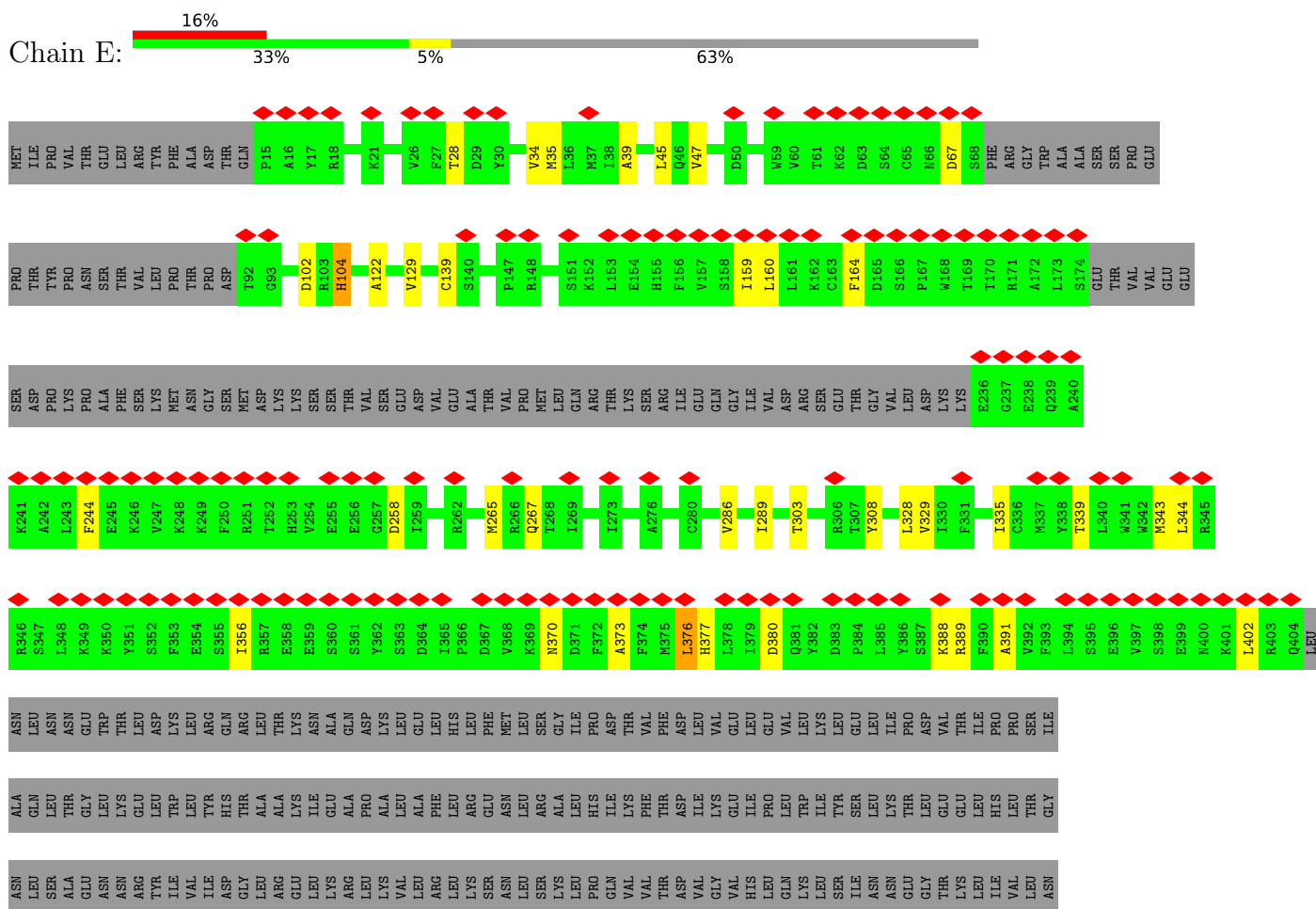




● Molecule 1: Volume-regulated anion channel subunit LRRC8A



- Molecule 1: Volume-regulated anion channel subunit LRRC8A



[illegible]

- Molecule 1: Volume-regulated anion channel subunit LRRC8A



GLY	ASN	ARG	LEU	LEU	GLY	ASP	CYS	VAL	LEU	PRO	R403	K343	Q239	GLU	TYR	MET
ASN	ARG	LEU	LEU	LEU	THR	ILE	LYS	LEU	THR	SER	Q404	L344	A240	GLU	PRO	ILE
LEU	LEU	LEU	LEU	LEU	ASN	ALA	LEU	ASN	ASN	ALA	LEU	R346	A241	SER	ASN	PRO
CYS	LEU	LEU	LEU	LEU	LEU	GLN	TRP	LEU	LEU	GLN	ASN	R346	A242	SER	THR	VAL
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	LEU	LEU	THR	ASN	S347	A243	VAL	LEU	GLY
PRO	LEU	LEU	LEU	LEU	GLY	GLY	GLY	ASN	ASN	GLY	ASN	L348	F244	PRO	LEU	ARG
VAL	VAL	VAL	VAL	VAL	ASN	LEU	THR	VAL	ASN	LEU	GLU	K349	E245	PHE	PRO	LEU
ASN	ASN	ASN	ASN	ASN	ASN	LEU	TRP	ASN	ASN	LEU	TRP	K350	E246	THR	THR	THR
ALA	ALA	ALA	ALA	ALA	LYS	GLU	THR	LYS	LYS	GLU	THR	Y351	V247	SER	PRO	ARG
LEU	LEU	LEU	LEU	LEU	ARG	LEU	LEU	LEU	LEU	LEU	ASP	S352	K248	THR	THR	THR
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	LEU	LEU	LEU	ASP	F353	E249	ASP	ALA	ASP
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	LEU	LEU	LEU	LEU	E354	K249	THR	THR	THR
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	LEU	LEU	LEU	LEU	S355	F250	THR	THR	THR
LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	THR	THR	HIS	ARG	R356	R251	ASP	ALA	ASP
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	ARG	ARG	GLN	ARG	T252	T252	LYS	LYS	LYS
LEU	LEU	LEU	LEU	LEU	ARG	ALA	ALA	ALA	ALA	LEU	LEU	R357	H253	SER	GLY	GLN
LEU	LEU	LEU	LEU	LEU	ASP	ALA	ALA	ALA	ALA	THR	LYS	E358	E255	SER	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	ILE	ILE	LYS	LYS	ILE	LYS	V254	E256	THR	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	GLU	GLU	LYS	LYS	GLU	ASN	E359	E257	THR	ASN	K21
LEU	LEU	LEU	LEU	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ASN	S360	E258	VAL	ASN	K21
LEU	LEU	LEU	LEU	LEU	ALA	ALA	ALA	ALA	ALA	ALA	GLN	S361	E259	VAL	ASN	K21
LEU	LEU	LEU	LEU	LEU	ASN	ASN	ASN	ASN	ASN	ASN	ASP	Y362	E260	SER	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	VAL	VAL	VAL	VAL	LEU	LYS	S363	E261	GLU	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	D364	E262	VAL	ASN	K21
LEU	LEU	LEU	LEU	LEU	ARG	ARG	ARG	ARG	ARG	PHE	GLU	T365	E263	GLU	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	HIS	R366	E264	ALA	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ARG	LEU	D367	E265	THR	ASN	K21
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	PHE	T368	E266	VAL	PRO	K35
LEU	LEU	LEU	LEU	LEU	ASN	ASN	ASN	ASN	ASN	ASN	MET	V368	Q267	VAL	P147	K35
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	K369	E268	MET	R148	A39
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ARG	SER	R370	E269	LEU	K145	Y30
LEU	LEU	LEU	LEU	LEU	LYS	LYS	ILE	GLN	GLN	ALA	GLY	D371	E270	GLN	S151	L45
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ILE	F372	E273	ARG	K152	Q46
LEU	LEU	LEU	LEU	LEU	PRO	PRO	PRO	ILE	ILE	HIS	PRO	Y372	E274	THR	L153	Q46
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	LYS	LYS	LYS	ASP	A373	E280	LYS	E154	Q47
LEU	LEU	LEU	LEU	LEU	VAL	VAL	VAL	VAL	VAL	PHE	THR	F374	E286	ARG	E155	D50
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	R376	E286	ILE	F156	M59
LEU	LEU	LEU	LEU	LEU	ASP	ASP	ASP	ASP	ASP	ASP	PHE	L376	E289	GLU	V157	V60
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	ILE	ILE	ILE	LEU	R377	E289	GLN	S158	T61
LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	VAL	L378	E303	ILE	I159	K62
LEU	LEU	LEU	LEU	LEU	VAL	VAL	VAL	VAL	VAL	ILE	GLU	L379	E303	ILE	L160	D63
LEU	LEU	LEU	LEU	LEU	GLU	GLU	GLU	GLU	GLU	GLU	LEU	D380	E306	ASP	L161	S64
LEU	LEU	LEU	LEU	LEU	PRO	PRO	PRO	PRO	PRO	PRO	GLU	Q381	E307	VAL	K162	C85
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	VAL	L382	E308	ARG	C163	N66
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	ILE	ILE	ILE	LYS	D383	E311	SER	F164	D67
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	LEU	P384	E325	THR	D165	S68
LEU	LEU	LEU	LEU	LEU	ASN	ASN	ASN	ASN	ASN	ASN	GLU	L385	E325	VAL	S166	PHE
LEU	LEU	LEU	LEU	LEU	ASN	ASN	ASN	ASN	ASN	ASN	LEU	R386	E325	VAL	S166	ARG
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ILE	S387	E328	LEU	S167	THR
LEU	LEU	LEU	LEU	LEU	GLU	GLU	GLU	GLU	GLU	GLU	THR	K388	E329	ASP	P167	GLY
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	PRO	L390	E330	LYS	W168	THR
LEU	LEU	LEU	LEU	LEU	ASP	ASP	ASP	ASP	ASP	ASP	VAL	R389	E331	GLU	T169	ALA
LEU	LEU	LEU	LEU	LEU	VAL	VAL	VAL	VAL	VAL	VAL	THR	F390	E331	THR	L170	ALA
LEU	LEU	LEU	LEU	LEU	ILE	ILE	ILE	ILE	ILE	ILE	ILE	R391	E335	ILE	R171	SER
LEU	LEU	LEU	LEU	LEU	PRO	PRO	PRO	PRO	PRO	PRO	PRO	V392	E336	THR	A172	PRO
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	F393	E337	THR	L173	PRO
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	L394	E338	GLU	T170	PRO
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	S395	E339	THR	S174	THR
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	R396	E340	THR	S174	THR
LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	V397	E341	THR	S174	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	35435	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	64.370	Depositor
Minimum map value	-35.093	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10	Depositor
Map size (Å)	396.032, 396.032, 396.032	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	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: L9Y, 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	0.22	0/2643	0.47	0/3580
1	B	0.22	0/2643	0.47	0/3580
1	C	0.22	0/2643	0.47	0/3580
1	D	0.22	0/2643	0.47	0/3580
1	E	0.22	0/2643	0.47	0/3580
1	F	0.22	0/2643	0.47	0/3580
All	All	0.22	0/15858	0.47	0/21480

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	2568	2555	2555	25	0
1	B	2568	2555	2555	23	0
1	C	2568	2555	2555	23	0
1	D	2568	2555	2555	23	0
1	E	2568	2555	2555	22	0
1	F	2568	2555	2555	26	0
2	A	37	52	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	52	50	0	0
2	C	37	52	50	0	0
2	D	37	52	50	0	0
2	E	37	52	50	0	0
2	F	37	52	50	0	0
3	F	28	27	0	0	0
All	All	15658	15669	15630	135	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 4.

All (135) 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:C:265:MET:HE1	1:C:344:LEU:HD21	1.54	0.90
1:F:265:MET:HE1	1:F:344:LEU:HD21	1.54	0.90
1:D:265:MET:HE1	1:D:344:LEU:HD21	1.54	0.90
1:E:265:MET:HE1	1:E:344:LEU:HD21	1.54	0.90
1:A:265:MET:HE1	1:A:344:LEU:HD21	1.54	0.89
1:B:265:MET:HE1	1:B:344:LEU:HD21	1.54	0.89
1:F:34:VAL:HG13	1:F:328:LEU:HD21	1.75	0.69
1:A:34:VAL:HG13	1:A:328:LEU:HD21	1.75	0.69
1:B:34:VAL:HG13	1:B:328:LEU:HD21	1.75	0.69
1:E:34:VAL:HG13	1:E:328:LEU:HD21	1.75	0.69
1:D:34:VAL:HG13	1:D:328:LEU:HD21	1.75	0.69
1:C:34:VAL:HG13	1:C:328:LEU:HD21	1.75	0.68
1:A:122:ALA:HB2	1:A:289:ILE:HG22	1.76	0.68
1:F:122:ALA:HB2	1:F:289:ILE:HG22	1.76	0.67
1:B:122:ALA:HB2	1:B:289:ILE:HG22	1.76	0.67
1:E:122:ALA:HB2	1:E:289:ILE:HG22	1.76	0.67
1:C:122:ALA:HB2	1:C:289:ILE:HG22	1.76	0.66
1:D:122:ALA:HB2	1:D:289:ILE:HG22	1.76	0.66
1:A:45:LEU:HD12	1:F:47:VAL:HG21	1.78	0.66
1:D:303:THR:HG1	1:D:308:TYR:HH	1.45	0.65
1:E:303:THR:HG1	1:E:308:TYR:HH	1.47	0.63
1:C:303:THR:HG1	1:C:308:TYR:HH	1.47	0.63
1:D:139:CYS:O	1:D:267:GLN:NE2	2.33	0.62
1:A:139:CYS:O	1:A:267:GLN:NE2	2.33	0.62
1:F:139:CYS:O	1:F:267:GLN:NE2	2.33	0.62
1:C:139:CYS:O	1:C:267:GLN:NE2	2.33	0.62
1:E:139:CYS:O	1:E:267:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:CYS:O	1:B:267:GLN:NE2	2.33	0.61
1:B:303:THR:OG1	1:B:308:TYR:OH	2.21	0.59
1:A:39:ALA:HB2	1:A:129:VAL:HG23	1.85	0.58
1:F:39:ALA:HB2	1:F:129:VAL:HG23	1.85	0.58
1:E:39:ALA:HB2	1:E:129:VAL:HG23	1.85	0.58
1:F:303:THR:OG1	1:F:308:TYR:OH	2.21	0.58
1:D:39:ALA:HB2	1:D:129:VAL:HG23	1.85	0.58
1:B:39:ALA:HB2	1:B:129:VAL:HG23	1.85	0.58
1:C:39:ALA:HB2	1:C:129:VAL:HG23	1.85	0.57
1:F:160:LEU:HD21	1:F:376:LEU:CD2	2.34	0.57
1:D:160:LEU:HD21	1:D:376:LEU:CD2	2.34	0.57
1:E:160:LEU:HD21	1:E:376:LEU:CD2	2.34	0.57
1:C:160:LEU:HD21	1:C:376:LEU:CD2	2.34	0.57
1:B:160:LEU:HD21	1:B:376:LEU:CD2	2.34	0.56
1:A:160:LEU:HD21	1:A:376:LEU:CD2	2.34	0.56
1:E:47:VAL:HG21	1:F:45:LEU:HD12	1.87	0.56
1:F:164:PHE:O	1:F:389:ARG:NH2	2.39	0.56
1:B:339:THR:O	1:B:343:MET:N	2.39	0.56
1:C:164:PHE:O	1:C:389:ARG:NH2	2.39	0.56
1:C:339:THR:O	1:C:343:MET:N	2.39	0.55
1:F:339:THR:O	1:F:343:MET:N	2.39	0.55
1:D:339:THR:O	1:D:343:MET:N	2.39	0.55
1:E:164:PHE:O	1:E:389:ARG:NH2	2.39	0.55
1:A:339:THR:O	1:A:343:MET:N	2.39	0.55
1:E:339:THR:O	1:E:343:MET:N	2.39	0.54
1:C:356:ILE:HD12	1:C:388:LYS:HG2	1.90	0.54
1:B:373:ALA:O	1:B:377:HIS:N	2.41	0.54
1:D:356:ILE:HD12	1:D:388:LYS:HG2	1.90	0.54
1:D:373:ALA:O	1:D:377:HIS:N	2.41	0.54
1:B:356:ILE:HD12	1:B:388:LYS:HG2	1.90	0.53
1:E:373:ALA:O	1:E:377:HIS:N	2.41	0.53
1:F:373:ALA:O	1:F:377:HIS:N	2.41	0.53
1:C:373:ALA:O	1:C:377:HIS:N	2.41	0.53
1:E:356:ILE:HD12	1:E:388:LYS:HG2	1.90	0.53
1:A:164:PHE:O	1:A:389:ARG:NH2	2.39	0.53
1:D:164:PHE:O	1:D:389:ARG:NH2	2.39	0.53
1:B:164:PHE:O	1:B:389:ARG:NH2	2.39	0.53
1:A:373:ALA:O	1:A:377:HIS:N	2.41	0.53
1:B:47:VAL:HG21	1:C:45:LEU:HD12	1.91	0.53
1:A:356:ILE:HD12	1:A:388:LYS:HG2	1.90	0.52
1:D:244:PHE:CE2	1:D:402:LEU:HD22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:PHE:CE2	1:E:402:LEU:HD22	2.44	0.52
1:F:356:ILE:HD12	1:F:388:LYS:HG2	1.90	0.52
1:B:244:PHE:CE2	1:B:402:LEU:HD22	2.44	0.52
1:C:244:PHE:CE2	1:C:402:LEU:HD22	2.44	0.52
1:A:47:VAL:HG21	1:B:45:LEU:HD12	1.91	0.52
1:F:244:PHE:CE2	1:F:402:LEU:HD22	2.44	0.52
1:A:244:PHE:CE2	1:A:402:LEU:HD22	2.44	0.51
1:E:370:ASN:N	1:E:370:ASN:OD1	2.45	0.50
1:D:47:VAL:HG21	1:E:45:LEU:HD12	1.94	0.50
1:F:370:ASN:OD1	1:F:370:ASN:N	2.44	0.50
1:B:370:ASN:N	1:B:370:ASN:OD1	2.44	0.49
1:C:370:ASN:N	1:C:370:ASN:OD1	2.44	0.49
1:D:370:ASN:N	1:D:370:ASN:OD1	2.45	0.49
1:A:370:ASN:N	1:A:370:ASN:OD1	2.44	0.49
1:D:356:ILE:HD13	1:D:391:ALA:CB	2.45	0.47
1:E:356:ILE:HD13	1:E:391:ALA:CB	2.44	0.47
1:A:45:LEU:HD12	1:F:47:VAL:CG2	2.43	0.47
1:A:316:THR:OG1	1:F:115:GLU:OE2	2.27	0.47
1:C:356:ILE:HD13	1:C:391:ALA:CB	2.45	0.47
1:F:356:ILE:HD13	1:F:391:ALA:CB	2.45	0.47
1:A:356:ILE:HD13	1:A:391:ALA:CB	2.45	0.46
1:A:303:THR:OG1	1:A:308:TYR:OH	2.21	0.46
1:B:356:ILE:HD13	1:B:391:ALA:CB	2.45	0.46
1:E:356:ILE:HD12	1:E:388:LYS:CG	2.46	0.45
1:F:356:ILE:HD12	1:F:388:LYS:CG	2.46	0.45
1:D:356:ILE:HD12	1:D:388:LYS:CG	2.46	0.45
1:C:356:ILE:HD12	1:C:388:LYS:CG	2.46	0.45
1:B:356:ILE:HD12	1:B:388:LYS:CG	2.46	0.45
1:F:258:ASP:OD1	1:F:258:ASP:N	2.50	0.45
1:A:356:ILE:HD12	1:A:388:LYS:CG	2.46	0.44
1:C:303:THR:OG1	1:C:308:TYR:OH	2.21	0.44
1:E:258:ASP:OD1	1:E:258:ASP:N	2.50	0.44
1:C:102:ASP:OD1	1:C:104:HIS:N	2.51	0.43
1:D:102:ASP:OD1	1:D:104:HIS:N	2.51	0.43
1:A:39:ALA:CB	1:A:129:VAL:HG23	2.50	0.42
1:B:244:PHE:CD2	1:B:402:LEU:HD22	2.54	0.42
1:E:102:ASP:OD1	1:E:104:HIS:N	2.51	0.42
1:A:321:LEU:O	1:A:325:TYR:N	2.51	0.42
1:B:102:ASP:OD1	1:B:104:HIS:N	2.51	0.42
1:A:343:MET:C	1:A:344:LEU:HD22	2.45	0.42
1:D:39:ALA:CB	1:D:129:VAL:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:MET:C	1:F:344:LEU:HD22	2.45	0.42
1:C:244:PHE:CD2	1:C:402:LEU:HD22	2.54	0.42
1:D:321:LEU:O	1:D:325:TYR:N	2.51	0.42
1:D:343:MET:C	1:D:344:LEU:HD22	2.45	0.42
1:F:244:PHE:CD2	1:F:402:LEU:HD22	2.54	0.42
1:A:244:PHE:CD2	1:A:402:LEU:HD22	2.54	0.42
1:E:244:PHE:CD2	1:E:402:LEU:HD22	2.55	0.42
1:E:343:MET:C	1:E:344:LEU:HD22	2.45	0.42
1:B:39:ALA:CB	1:B:129:VAL:HG23	2.50	0.41
1:C:343:MET:C	1:C:344:LEU:HD22	2.45	0.41
1:F:39:ALA:CB	1:F:129:VAL:HG23	2.50	0.41
1:C:258:ASP:OD1	1:C:258:ASP:N	2.50	0.41
1:F:321:LEU:O	1:F:325:TYR:N	2.51	0.41
1:B:343:MET:C	1:B:344:LEU:HD22	2.45	0.41
1:F:102:ASP:OD1	1:F:104:HIS:N	2.51	0.41
1:A:102:ASP:OD1	1:A:104:HIS:N	2.51	0.41
1:B:321:LEU:O	1:B:325:TYR:N	2.51	0.41
1:D:244:PHE:CD2	1:D:402:LEU:HD22	2.55	0.41
1:D:258:ASP:OD1	1:D:258:ASP:N	2.50	0.41
1:D:35:MET:HG3	1:D:328:LEU:HD23	2.03	0.41
1:E:35:MET:HG3	1:E:328:LEU:HD23	2.03	0.41
1:F:35:MET:HG3	1:F:328:LEU:HD23	2.03	0.41
1:C:39:ALA:CB	1:C:129:VAL:HG23	2.50	0.41
1:C:35:MET:HG3	1:C:328:LEU:HD23	2.03	0.40
1:A:35:MET:HG3	1:A:328:LEU:HD23	2.03	0.40
1:B:35:MET:HG3	1:B:328:LEU:HD23	2.03	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	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	B	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	C	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	D	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	E	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
1	F	300/820 (37%)	284 (95%)	16 (5%)	0	100	100
All	All	1800/4920 (37%)	1704 (95%)	96 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/758 (38%)	275 (97%)	9 (3%)	34	60
1	B	284/758 (38%)	275 (97%)	9 (3%)	34	60
1	C	284/758 (38%)	275 (97%)	9 (3%)	34	60
1	D	284/758 (38%)	275 (97%)	9 (3%)	34	60
1	E	284/758 (38%)	275 (97%)	9 (3%)	34	60
1	F	284/758 (38%)	275 (97%)	9 (3%)	34	60
All	All	1704/4548 (38%)	1650 (97%)	54 (3%)	35	60

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	67	ASP
1	A	104	HIS
1	A	159	ILE
1	A	286	VAL
1	A	329	VAL
1	A	335	ILE

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	380	ASP
1	B	28	THR
1	B	67	ASP
1	B	104	HIS
1	B	159	ILE
1	B	286	VAL
1	B	329	VAL
1	B	335	ILE
1	B	376	LEU
1	B	380	ASP
1	C	28	THR
1	C	67	ASP
1	C	104	HIS
1	C	159	ILE
1	C	286	VAL
1	C	329	VAL
1	C	335	ILE
1	C	376	LEU
1	C	380	ASP
1	D	28	THR
1	D	67	ASP
1	D	104	HIS
1	D	159	ILE
1	D	286	VAL
1	D	329	VAL
1	D	335	ILE
1	D	376	LEU
1	D	380	ASP
1	E	28	THR
1	E	67	ASP
1	E	104	HIS
1	E	159	ILE
1	E	286	VAL
1	E	329	VAL
1	E	335	ILE
1	E	376	LEU
1	E	380	ASP
1	F	28	THR
1	F	67	ASP
1	F	104	HIS
1	F	159	ILE

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Mol	Chain	Res	Type
1	F	286	VAL
1	F	329	VAL
1	F	335	ILE
1	F	376	LEU
1	F	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	155	HIS
1	A	267	GLN
1	A	381	GLN
1	B	105	GLN
1	B	155	HIS
1	B	267	GLN
1	C	105	GLN
1	C	155	HIS
1	C	267	GLN
1	C	381	GLN
1	D	267	GLN
1	D	381	GLN
1	E	105	GLN
1	E	155	HIS
1	E	267	GLN
1	E	381	GLN
1	F	155	HIS
1	F	267	GLN
1	F	381	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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
2	POV	D	902	-	11,11,51	0.51	0	11,11,59	1.04	1 (9%)
2	POV	D	901	-	14,14,51	1.33	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	D	903	-	9,9,51	0.54	0	9,9,59	1.05	1 (11%)
3	L9Y	F	904	-	28,30,30	2.03	9 (32%)	33,43,43	3.17	13 (39%)
2	POV	C	902	-	11,11,51	0.50	0	11,11,59	1.03	1 (9%)
2	POV	E	902	-	11,11,51	0.50	0	11,11,59	1.03	1 (9%)
2	POV	B	902	-	11,11,51	0.51	0	11,11,59	1.04	1 (9%)
2	POV	E	901	-	14,14,51	1.33	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	B	901	-	14,14,51	1.33	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	C	903	-	9,9,51	0.54	0	9,9,59	1.05	1 (11%)
2	POV	B	903	-	9,9,51	0.54	0	9,9,59	1.05	1 (11%)
2	POV	F	902	-	11,11,51	0.51	0	11,11,59	1.04	1 (9%)
2	POV	C	901	-	14,14,51	1.32	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	A	901	-	14,14,51	1.33	2 (14%)	14,14,59	1.49	3 (21%)
2	POV	A	903	-	9,9,51	0.54	0	9,9,59	1.05	1 (11%)
2	POV	E	903	-	9,9,51	0.53	0	9,9,59	1.05	1 (11%)
2	POV	F	903	-	9,9,51	0.53	0	9,9,59	1.05	1 (11%)
2	POV	A	902	-	11,11,51	0.51	0	11,11,59	1.03	1 (9%)
2	POV	F	901	-	14,14,51	1.33	2 (14%)	14,14,59	1.49	3 (21%)

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	902	-	-	5/9/9/55	-
2	POV	D	901	-	-	2/12/12/55	-
2	POV	D	903	-	-	3/7/7/55	-
3	L9Y	F	904	-	-	13/18/40/40	0/3/3/3
2	POV	C	902	-	-	5/9/9/55	-
2	POV	E	902	-	-	5/9/9/55	-
2	POV	B	902	-	-	5/9/9/55	-
2	POV	E	901	-	-	2/12/12/55	-
2	POV	B	901	-	-	2/12/12/55	-
2	POV	C	903	-	-	3/7/7/55	-
2	POV	B	903	-	-	3/7/7/55	-
2	POV	F	902	-	-	5/9/9/55	-
2	POV	C	901	-	-	2/12/12/55	-
2	POV	A	901	-	-	2/12/12/55	-
2	POV	A	903	-	-	3/7/7/55	-
2	POV	E	903	-	-	3/7/7/55	-
2	POV	F	903	-	-	3/7/7/55	-
2	POV	A	902	-	-	5/9/9/55	-
2	POV	F	901	-	-	2/12/12/55	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	904	L9Y	C06-C07	5.23	1.57	1.50
2	E	901	POV	O32-C31	4.29	1.36	1.22
2	B	901	POV	O32-C31	4.29	1.36	1.22
2	A	901	POV	O32-C31	4.28	1.36	1.22
2	D	901	POV	O32-C31	4.27	1.36	1.22
2	C	901	POV	O32-C31	4.27	1.36	1.22
2	F	901	POV	O32-C31	4.26	1.36	1.22
3	F	904	L9Y	C18-C17	3.52	1.65	1.51
3	F	904	L9Y	C23-C15	3.19	1.44	1.38
3	F	904	L9Y	O10-C09	3.11	1.26	1.21
3	F	904	L9Y	O16-C17	2.95	1.53	1.43
3	F	904	L9Y	O16-C15	2.90	1.43	1.37
3	F	904	L9Y	C04-C05	2.79	1.59	1.54
2	F	901	POV	O31-C31	-2.48	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	POV	O31-C31	-2.48	1.22	1.30
2	E	901	POV	O31-C31	-2.46	1.22	1.30
2	B	901	POV	O31-C31	-2.46	1.22	1.30
2	D	901	POV	O31-C31	-2.45	1.22	1.30
2	C	901	POV	O31-C31	-2.45	1.22	1.30
3	F	904	L9Y	C19-C20	2.42	1.56	1.50
3	F	904	L9Y	C13-CL14	-2.10	1.68	1.72

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	904	L9Y	C06-C05-C09	-13.41	91.60	103.66
3	F	904	L9Y	C23-C15-C13	-4.50	115.59	120.99
3	F	904	L9Y	C06-C07-C23	4.50	136.55	128.94
3	F	904	L9Y	O16-C15-C13	4.39	122.83	115.77
3	F	904	L9Y	C28-C24-C25	-3.74	100.11	104.35
3	F	904	L9Y	C06-C07-C08	-3.73	104.69	110.49
2	E	901	POV	O31-C31-C32	3.43	124.84	114.00
2	A	901	POV	O31-C31-C32	3.42	124.80	114.00
2	F	901	POV	O31-C31-C32	3.42	124.79	114.00
2	B	901	POV	O31-C31-C32	3.41	124.78	114.00
2	D	901	POV	O31-C31-C32	3.41	124.76	114.00
2	C	901	POV	O31-C31-C32	3.40	124.74	114.00
3	F	904	L9Y	O10-C09-C08	-3.22	123.84	130.69
3	F	904	L9Y	C26-C25-C24	2.66	109.10	105.03
3	F	904	L9Y	O16-C17-C18	2.61	117.91	108.30
2	B	901	POV	C33-C32-C31	-2.60	107.73	114.51
2	C	901	POV	C33-C32-C31	-2.59	107.74	114.51
2	E	901	POV	C33-C32-C31	-2.58	107.77	114.51
2	F	901	POV	C33-C32-C31	-2.58	107.78	114.51
2	A	901	POV	C33-C32-C31	-2.58	107.78	114.51
2	D	901	POV	C33-C32-C31	-2.58	107.79	114.51
2	F	902	POV	C33-C32-C31	-2.49	108.00	114.51
2	E	902	POV	C33-C32-C31	-2.49	108.00	114.51
2	D	902	POV	C33-C32-C31	-2.49	108.01	114.51
2	A	902	POV	C33-C32-C31	-2.48	108.03	114.51
2	C	902	POV	C33-C32-C31	-2.48	108.05	114.51
2	B	902	POV	C33-C32-C31	-2.48	108.05	114.51
3	F	904	L9Y	C19-C18-C17	2.46	117.26	112.33
2	E	901	POV	O32-C31-C32	-2.40	115.50	123.09
2	F	901	POV	O32-C31-C32	-2.39	115.50	123.09
2	A	901	POV	O32-C31-C32	-2.39	115.50	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	POV	O32-C31-C32	-2.38	115.53	123.09
2	B	901	POV	O32-C31-C32	-2.38	115.54	123.09
2	C	901	POV	O32-C31-C32	-2.37	115.59	123.09
2	A	903	POV	C23-C22-C21	-2.35	108.38	114.51
2	D	903	POV	C23-C22-C21	-2.35	108.38	114.51
2	F	903	POV	C23-C22-C21	-2.35	108.39	114.51
2	E	903	POV	C23-C22-C21	-2.35	108.39	114.51
2	C	903	POV	C23-C22-C21	-2.34	108.40	114.51
2	B	903	POV	C23-C22-C21	-2.33	108.43	114.51
3	F	904	L9Y	C27-C28-C24	2.06	108.19	105.03
3	F	904	L9Y	C23-C07-C08	-2.05	118.73	121.53
3	F	904	L9Y	C11-C08-C07	-2.02	120.17	121.52

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	904	L9Y	C04-C05-C24-C25
3	F	904	L9Y	C04-C05-C24-C28
3	F	904	L9Y	C06-C05-C24-C25
3	F	904	L9Y	C06-C05-C24-C28
3	F	904	L9Y	C09-C05-C24-C25
3	F	904	L9Y	C09-C05-C24-C28
3	F	904	L9Y	C13-C15-O16-C17
2	A	903	POV	C21-C22-C23-C24
2	B	903	POV	C21-C22-C23-C24
2	C	903	POV	C21-C22-C23-C24
2	D	903	POV	C21-C22-C23-C24
2	E	903	POV	C21-C22-C23-C24
2	F	903	POV	C21-C22-C23-C24
3	F	904	L9Y	C02-C03-C04-C05
2	F	901	POV	C33-C34-C35-C36
2	B	901	POV	C33-C34-C35-C36
2	C	901	POV	C33-C34-C35-C36
2	D	901	POV	C33-C34-C35-C36
2	E	901	POV	C33-C34-C35-C36
2	A	901	POV	C33-C34-C35-C36
3	F	904	L9Y	C17-C18-C19-C20
3	F	904	L9Y	C03-C04-C05-C24
2	D	902	POV	C36-C37-C38-C39
2	E	902	POV	C36-C37-C38-C39
2	F	902	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	F	904	L9Y	C03-C04-C05-C09
2	B	902	POV	C36-C37-C38-C39
2	C	902	POV	C36-C37-C38-C39
2	A	902	POV	C36-C37-C38-C39
3	F	904	L9Y	C23-C15-O16-C17
3	F	904	L9Y	C18-C17-O16-C15
2	A	902	POV	C34-C35-C36-C37
2	B	902	POV	C34-C35-C36-C37
2	C	902	POV	C34-C35-C36-C37
2	D	902	POV	C34-C35-C36-C37
2	F	902	POV	C34-C35-C36-C37
2	E	902	POV	C34-C35-C36-C37
2	A	903	POV	O21-C21-C22-C23
2	B	903	POV	O21-C21-C22-C23
2	C	903	POV	O21-C21-C22-C23
2	D	903	POV	O21-C21-C22-C23
2	E	903	POV	O21-C21-C22-C23
2	F	903	POV	O21-C21-C22-C23
2	B	903	POV	O22-C21-C22-C23
2	A	903	POV	O22-C21-C22-C23
2	C	903	POV	O22-C21-C22-C23
2	D	903	POV	O22-C21-C22-C23
2	E	903	POV	O22-C21-C22-C23
2	F	903	POV	O22-C21-C22-C23
2	A	902	POV	O32-C31-C32-C33
2	B	902	POV	O32-C31-C32-C33
2	E	902	POV	O32-C31-C32-C33
2	F	902	POV	O32-C31-C32-C33
2	C	902	POV	O32-C31-C32-C33
2	D	902	POV	O32-C31-C32-C33
2	E	901	POV	C32-C33-C34-C35
2	D	901	POV	C32-C33-C34-C35
2	F	901	POV	C32-C33-C34-C35
2	C	901	POV	C32-C33-C34-C35
2	B	901	POV	C32-C33-C34-C35
2	A	901	POV	C32-C33-C34-C35
2	A	902	POV	O31-C31-C32-C33
2	D	902	POV	O31-C31-C32-C33
2	E	902	POV	O31-C31-C32-C33
2	F	902	POV	O31-C31-C32-C33
2	C	902	POV	O31-C31-C32-C33
2	B	902	POV	O31-C31-C32-C33

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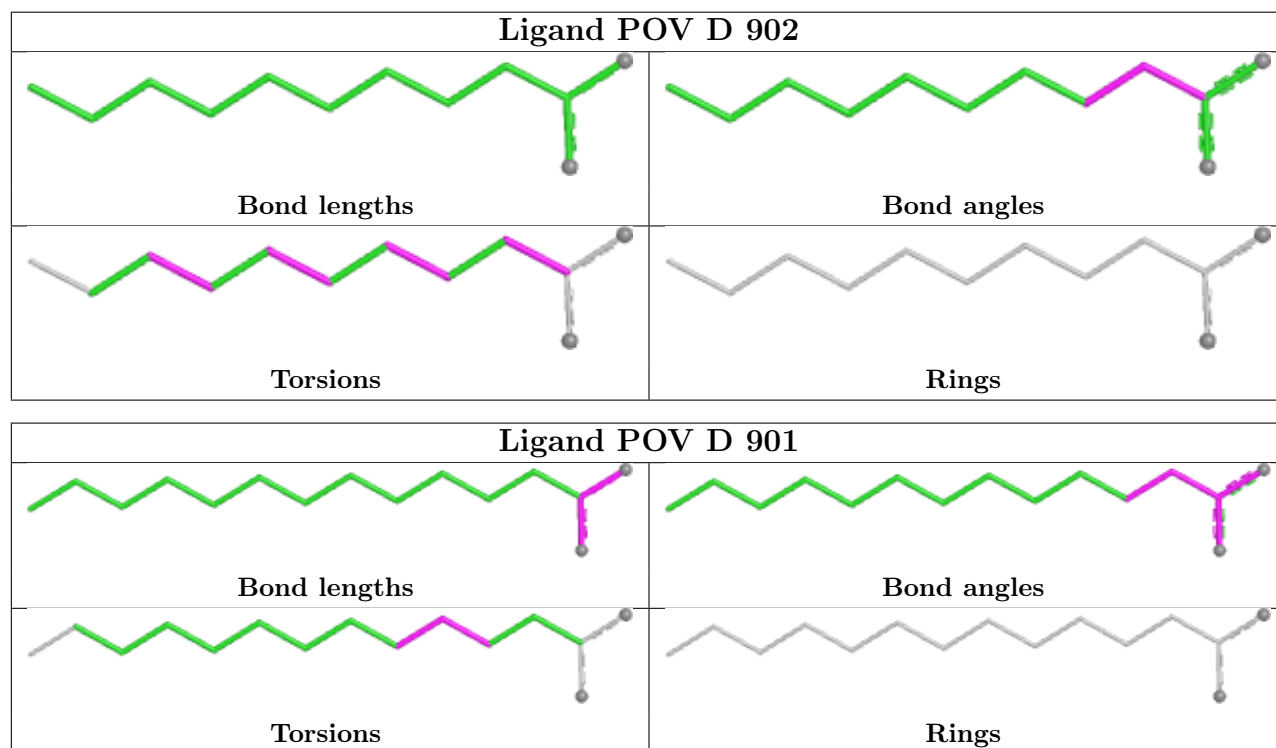
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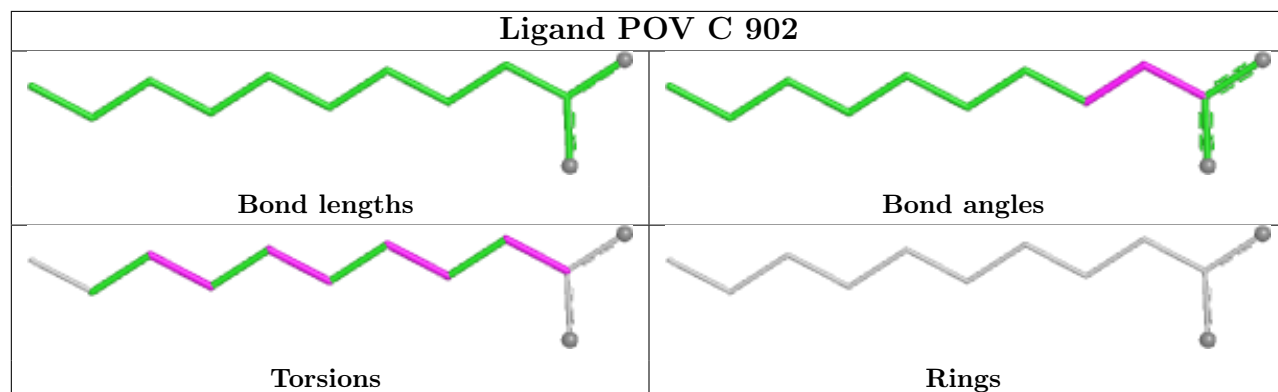
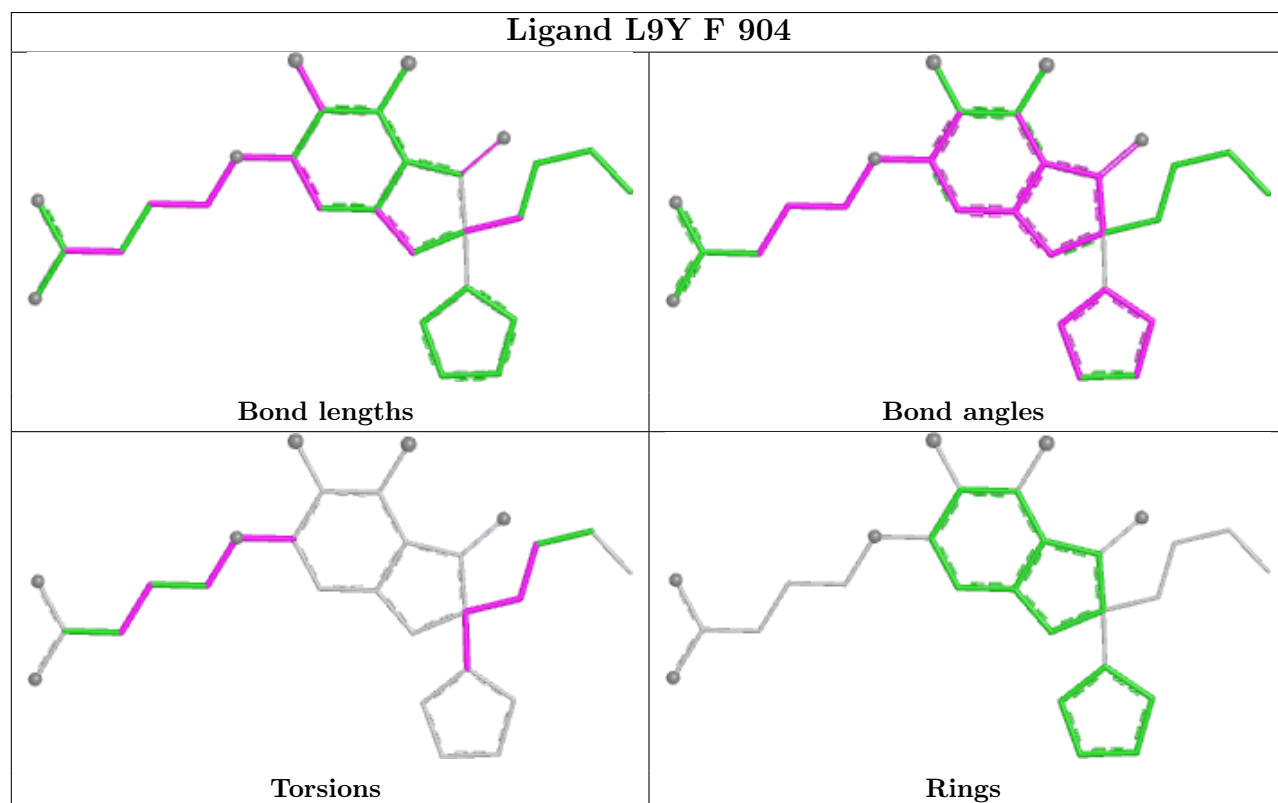
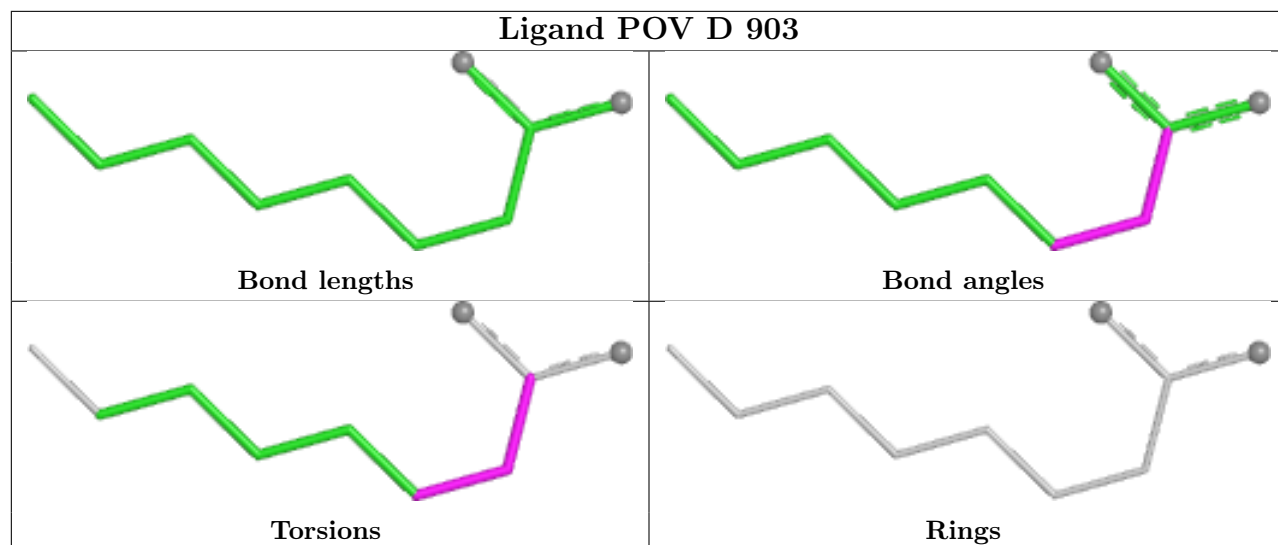
Mol	Chain	Res	Type	Atoms
2	D	902	POV	C32-C33-C34-C35
2	F	902	POV	C32-C33-C34-C35
2	B	902	POV	C32-C33-C34-C35
2	E	902	POV	C32-C33-C34-C35
2	A	902	POV	C32-C33-C34-C35
2	C	902	POV	C32-C33-C34-C35

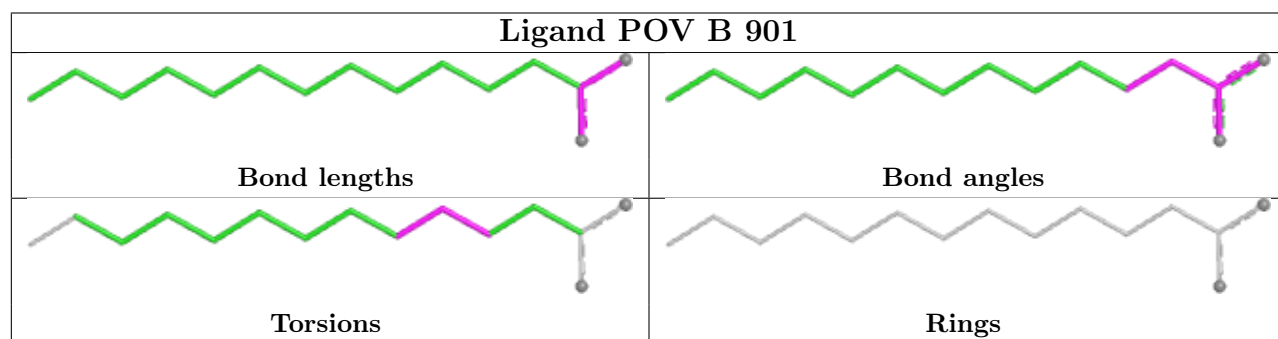
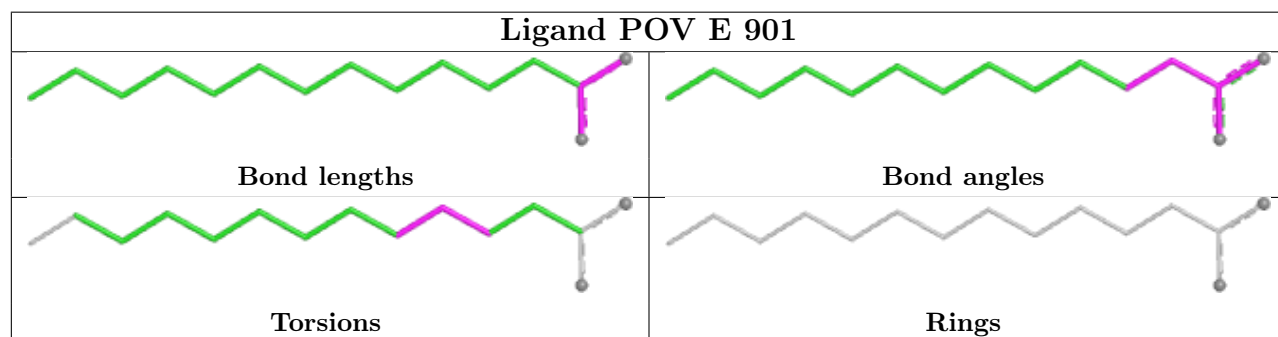
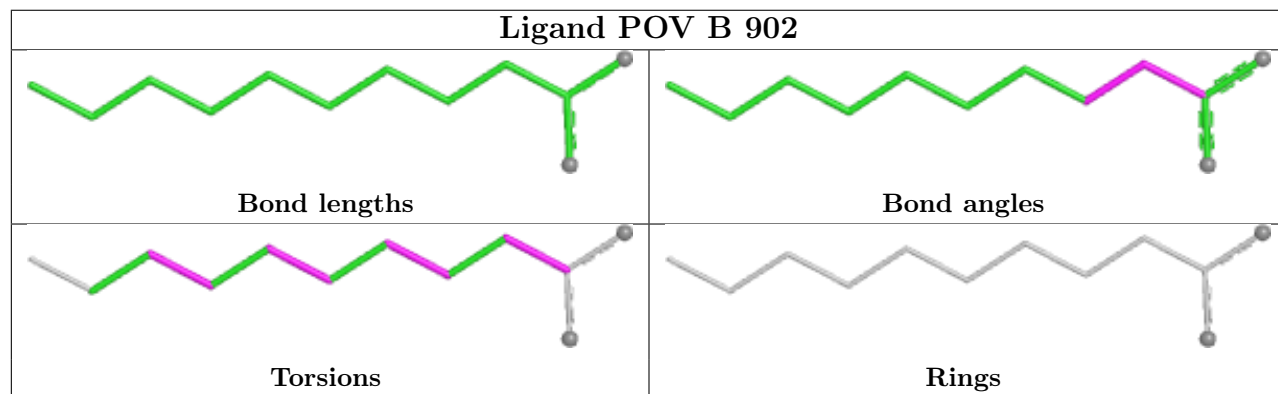
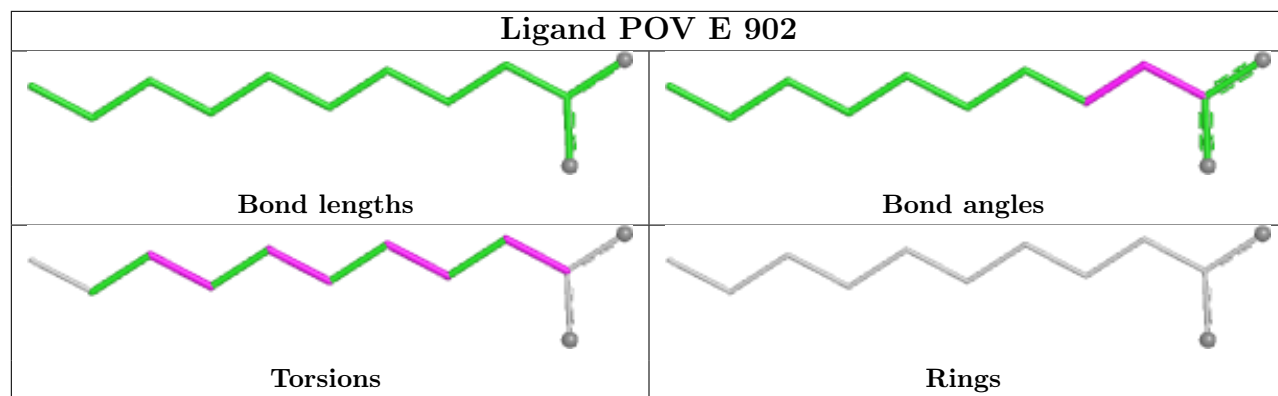
There are no ring outliers.

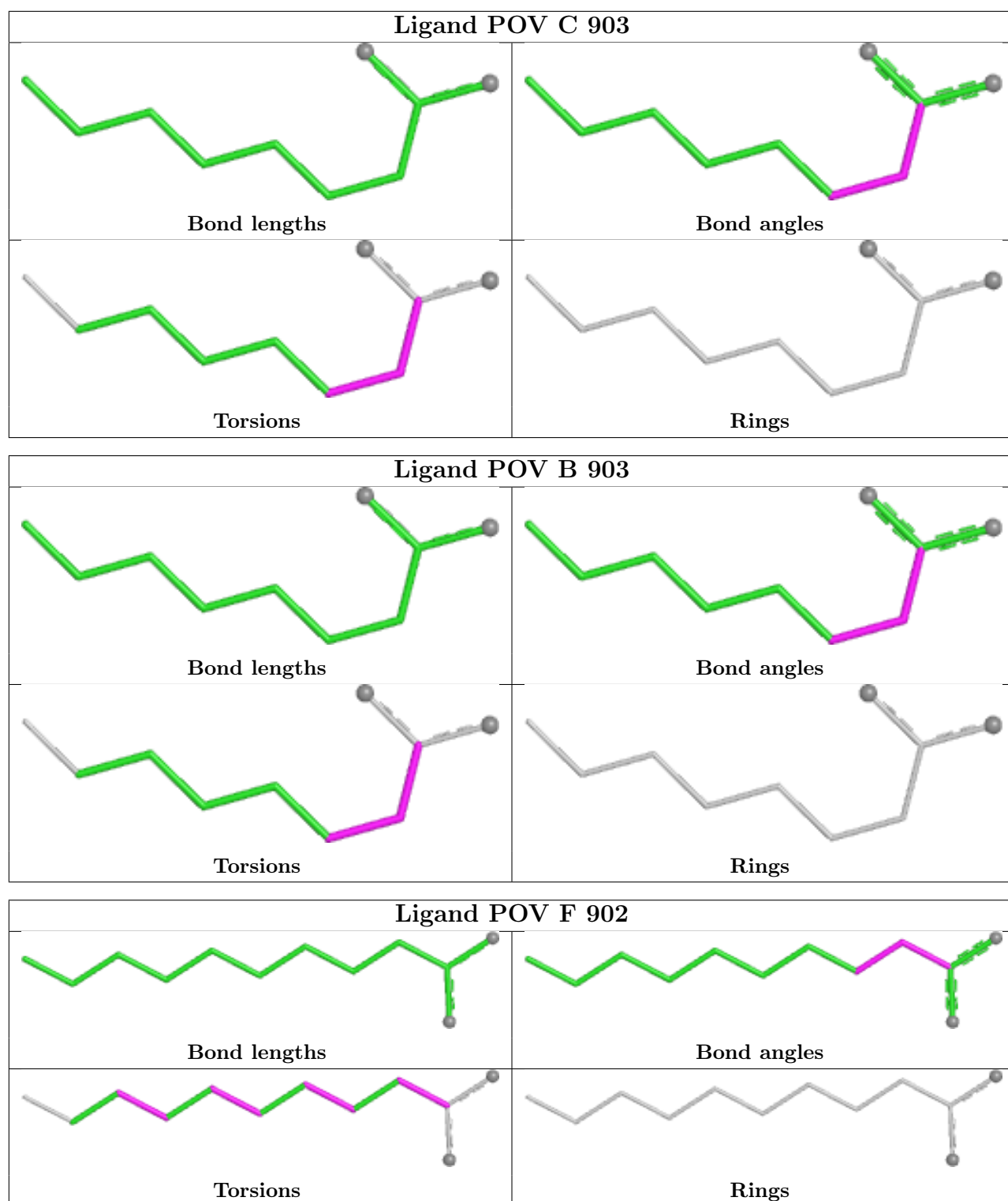
No monomer is involved in short contacts.

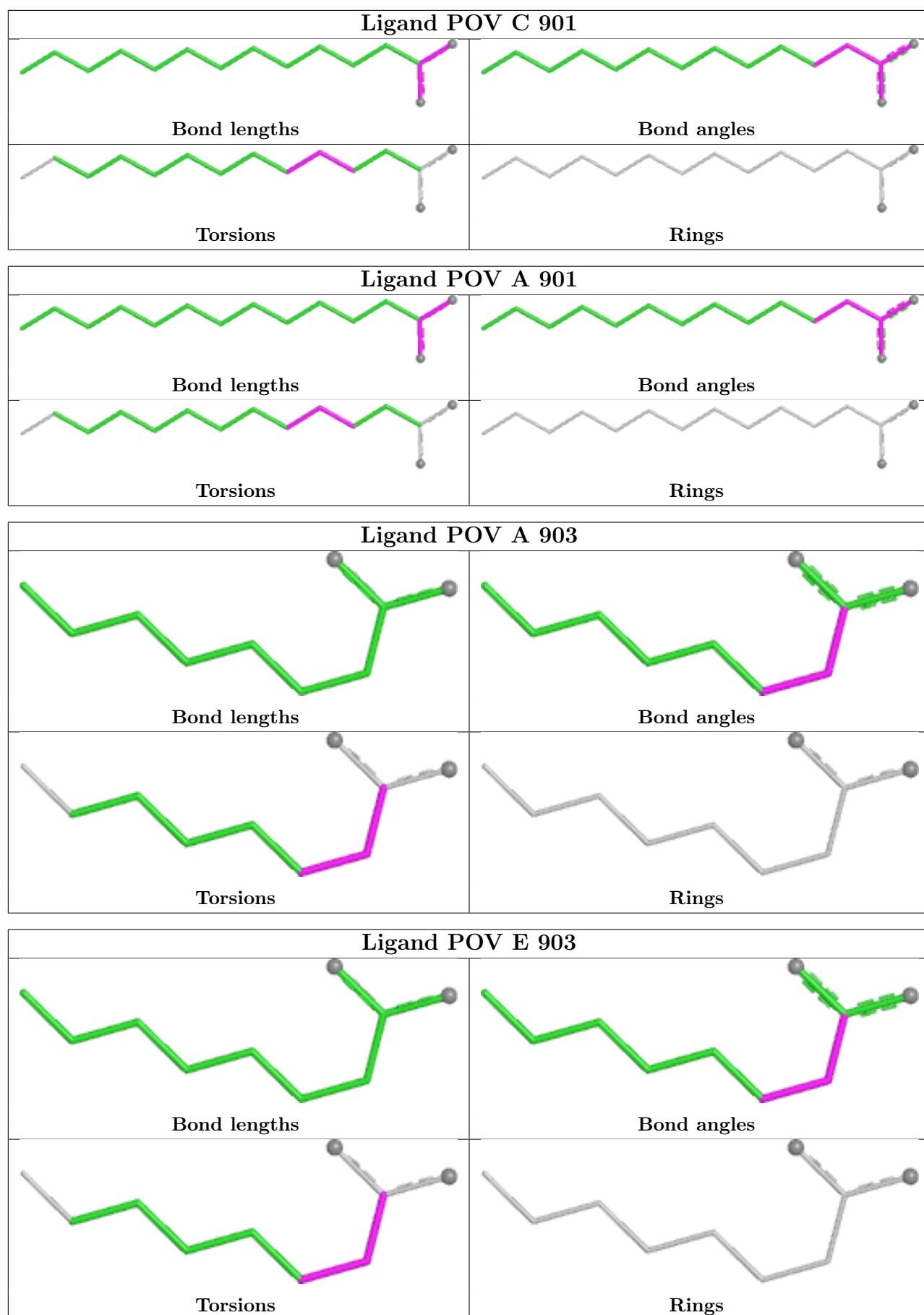
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

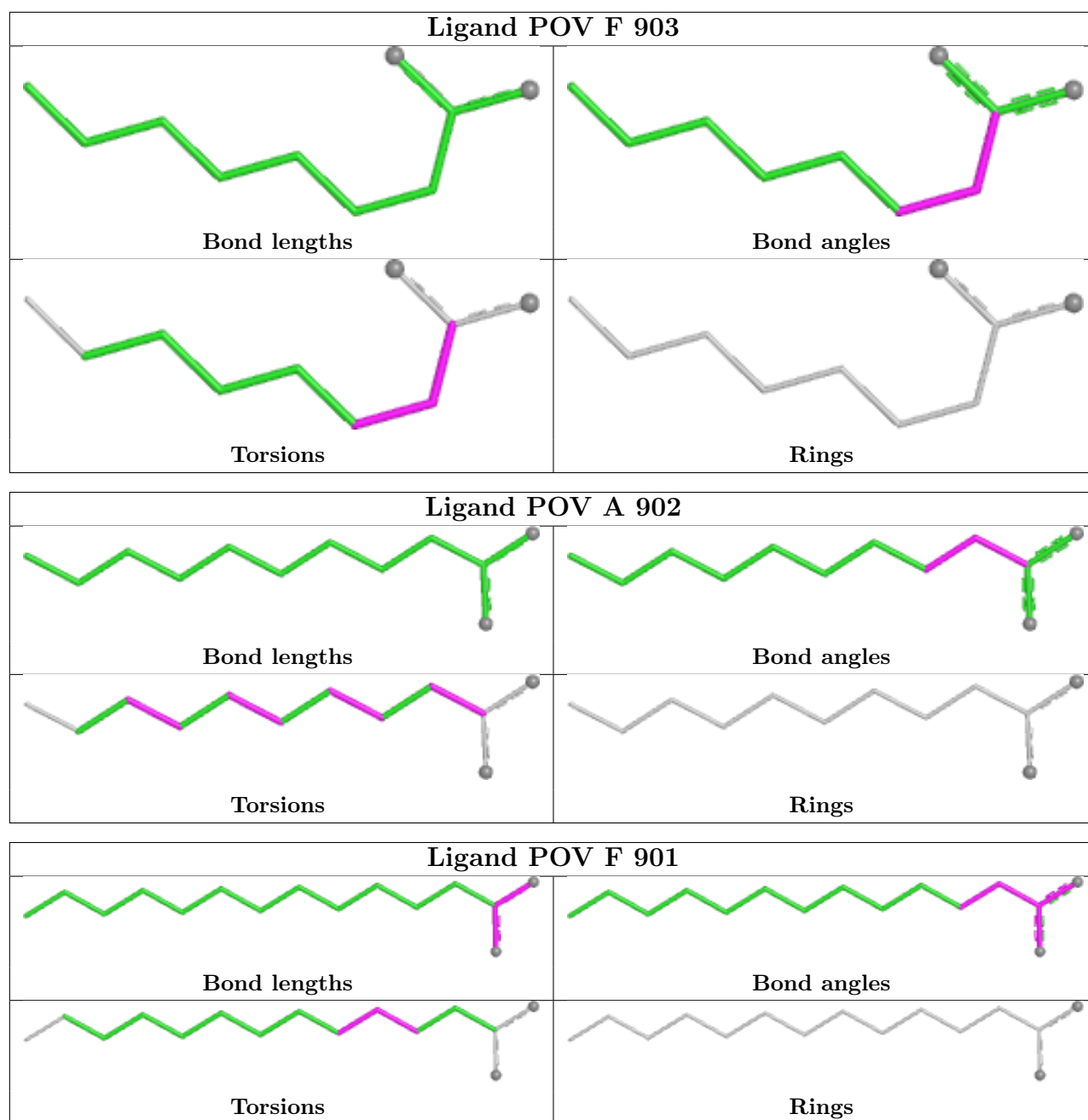












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

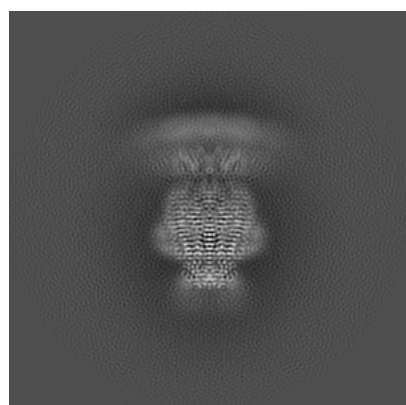
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0563. These allow visual inspection of the internal detail of the map and identification of artifacts.

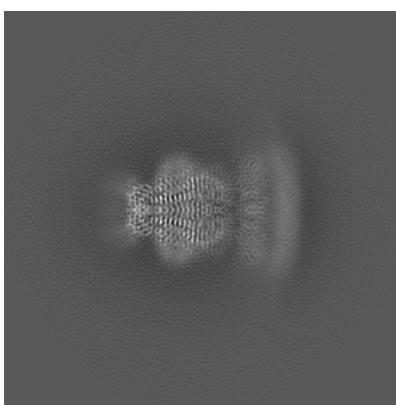
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

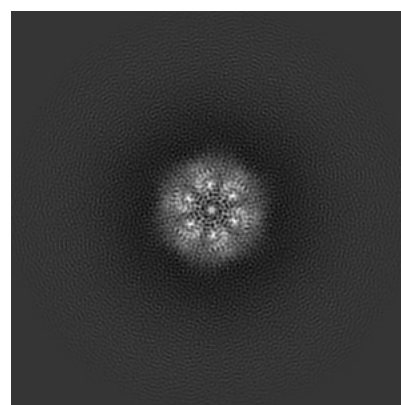
6.1.1 Primary map



X



Y

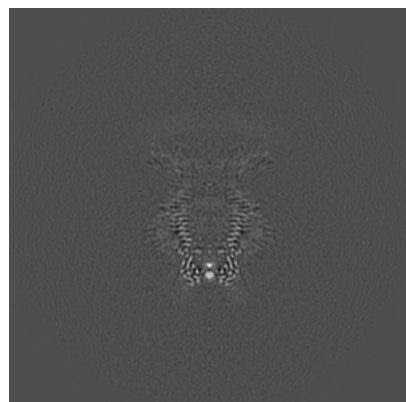


Z

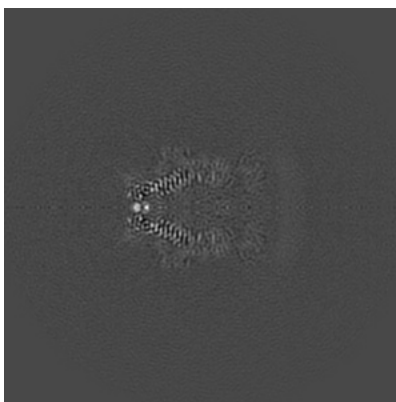
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

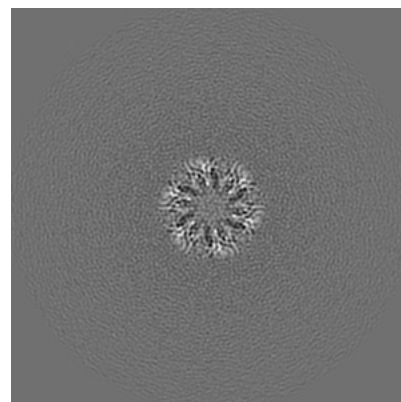
6.2.1 Primary map



X Index: 182



Y Index: 182

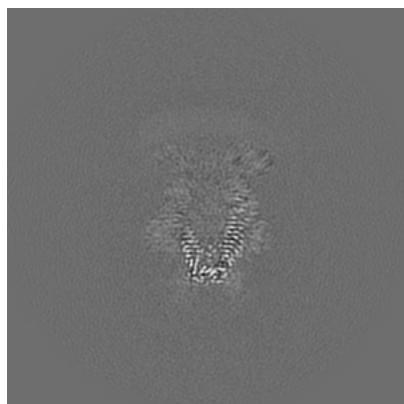


Z Index: 182

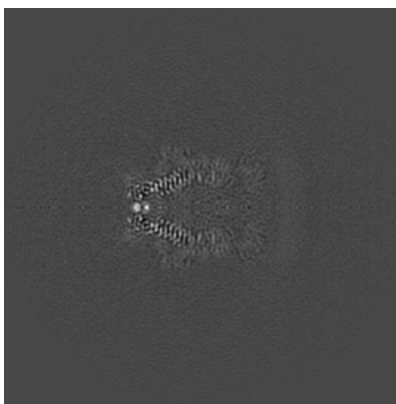
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

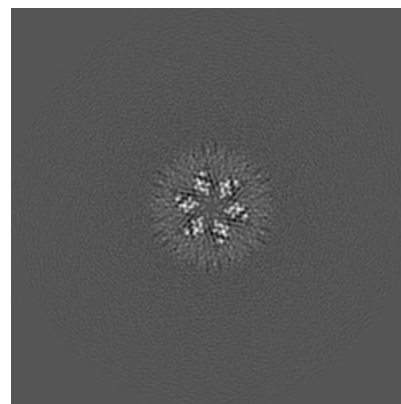
6.3.1 Primary map



X Index: 172



Y Index: 182

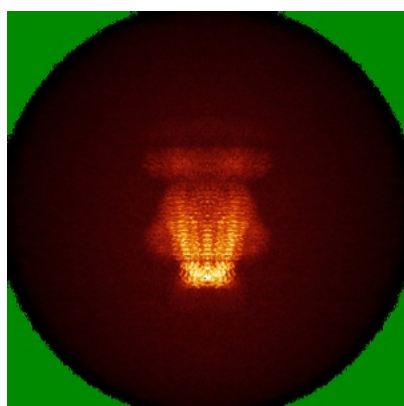


Z Index: 151

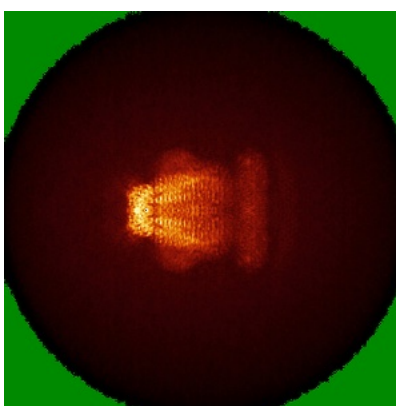
The images above show the largest variance slices of the map in three orthogonal directions.

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

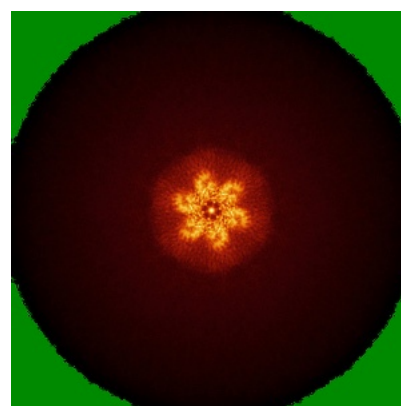
6.4.1 Primary map



X



Y

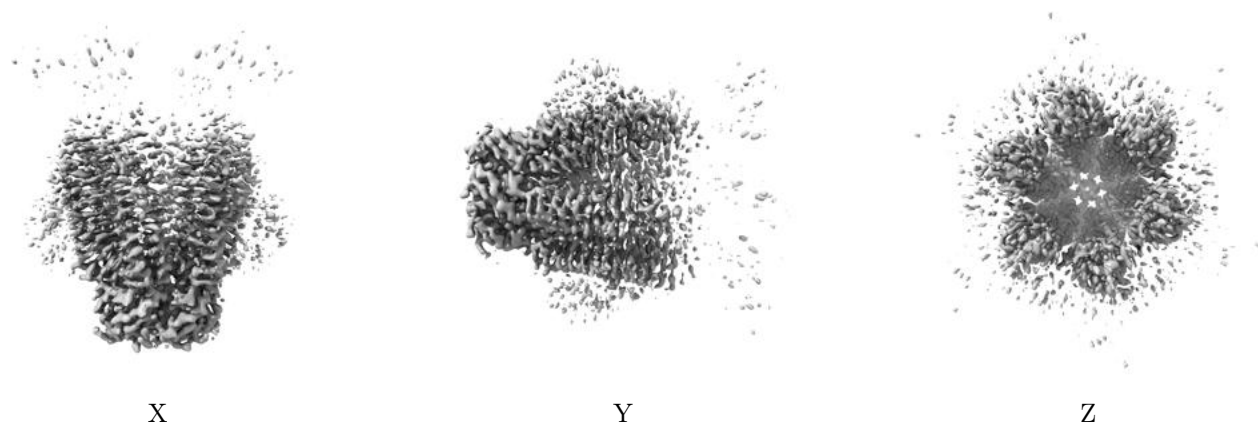


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

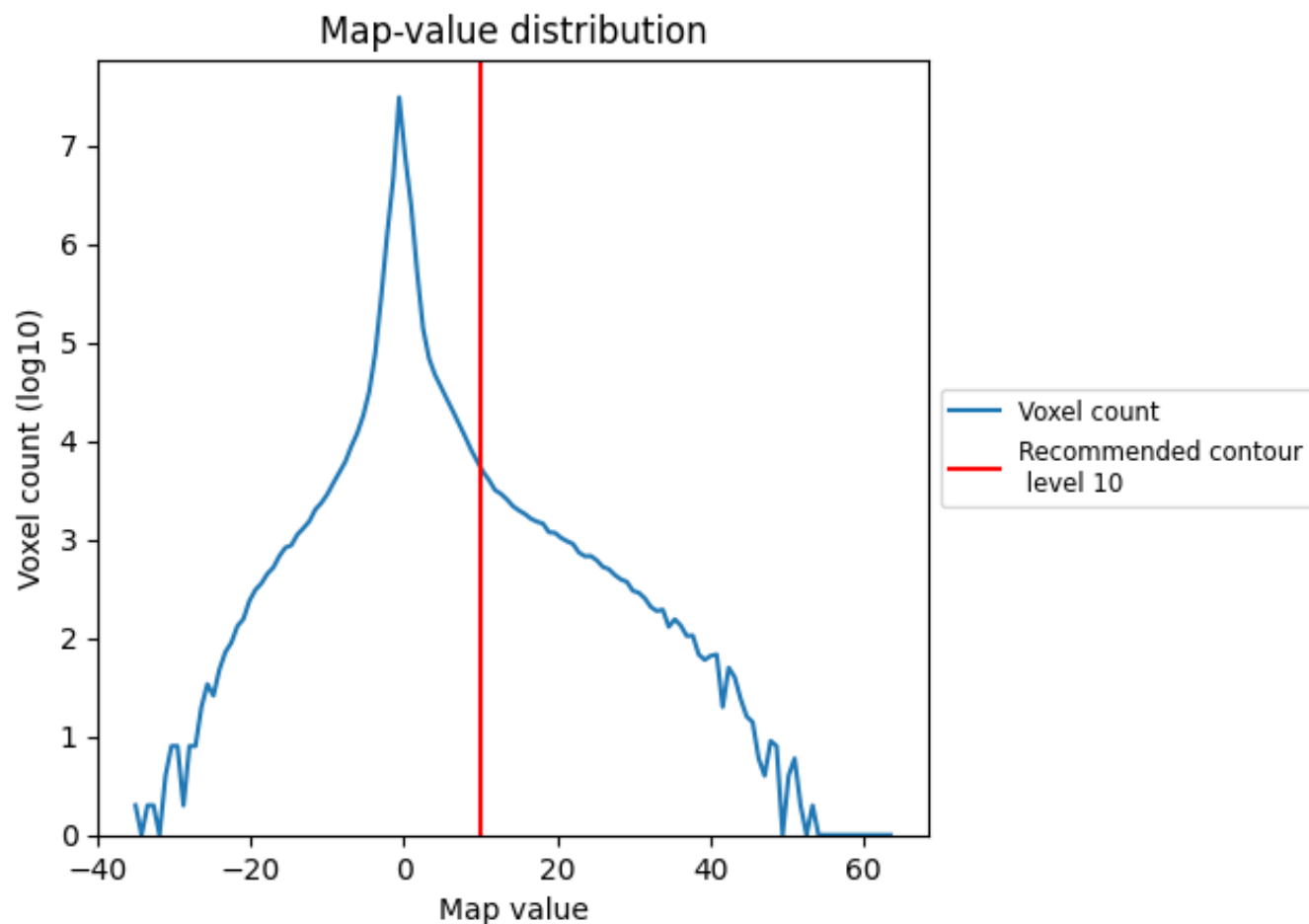
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

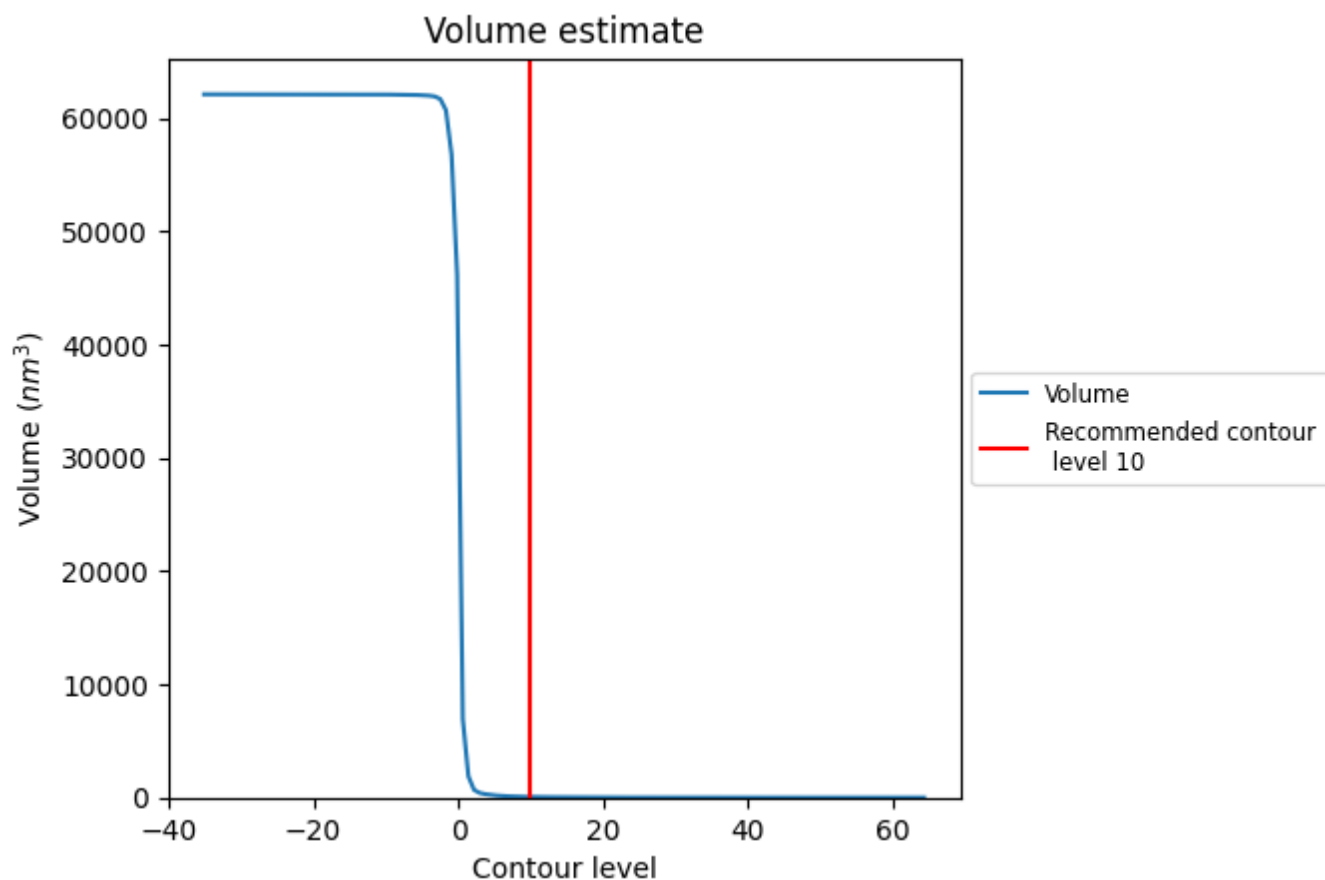
This section contains the results of statistical analysis of the map.

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.

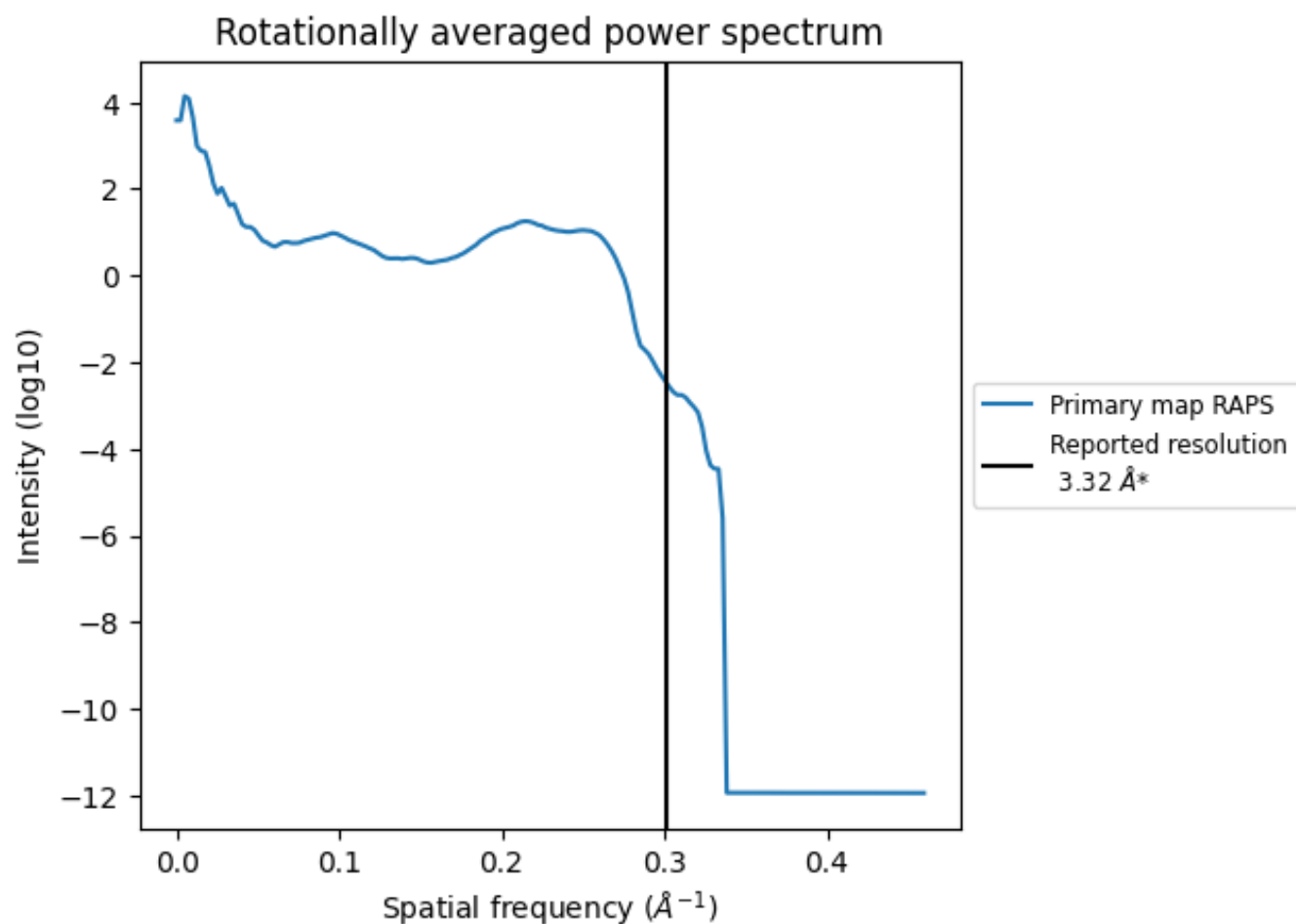
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm^3 ; this corresponds to an approximate mass of 50 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

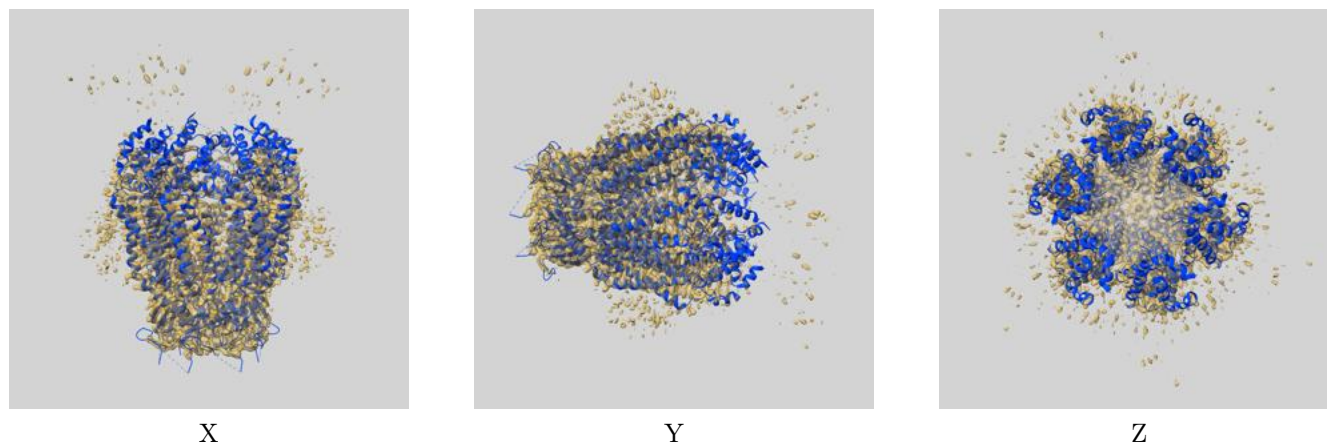
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

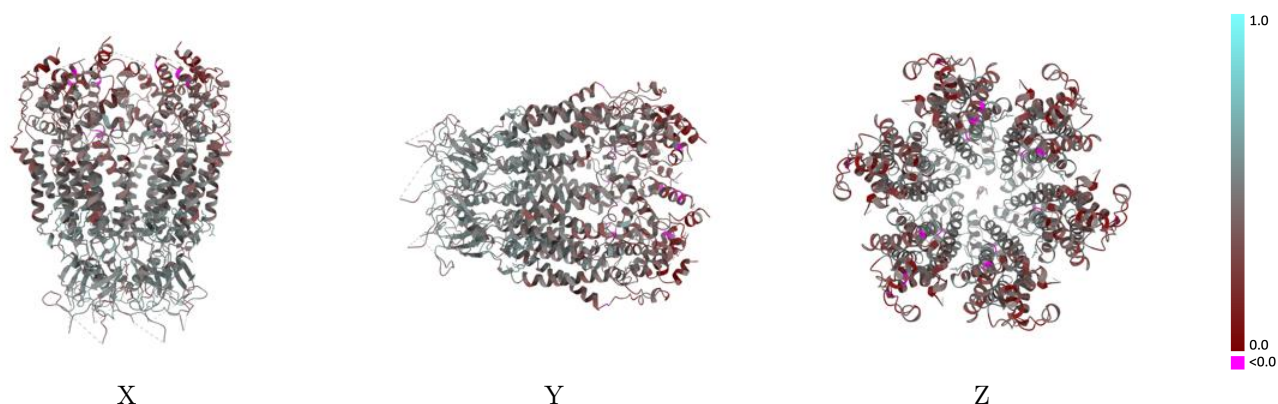
This section contains information regarding the fit between EMDB map EMD-0563 and PDB model 6NZZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



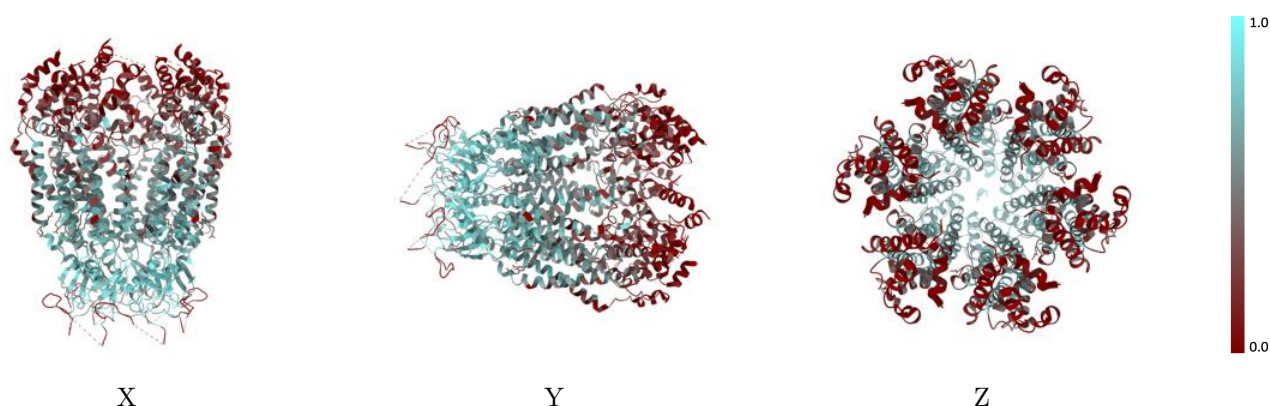
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



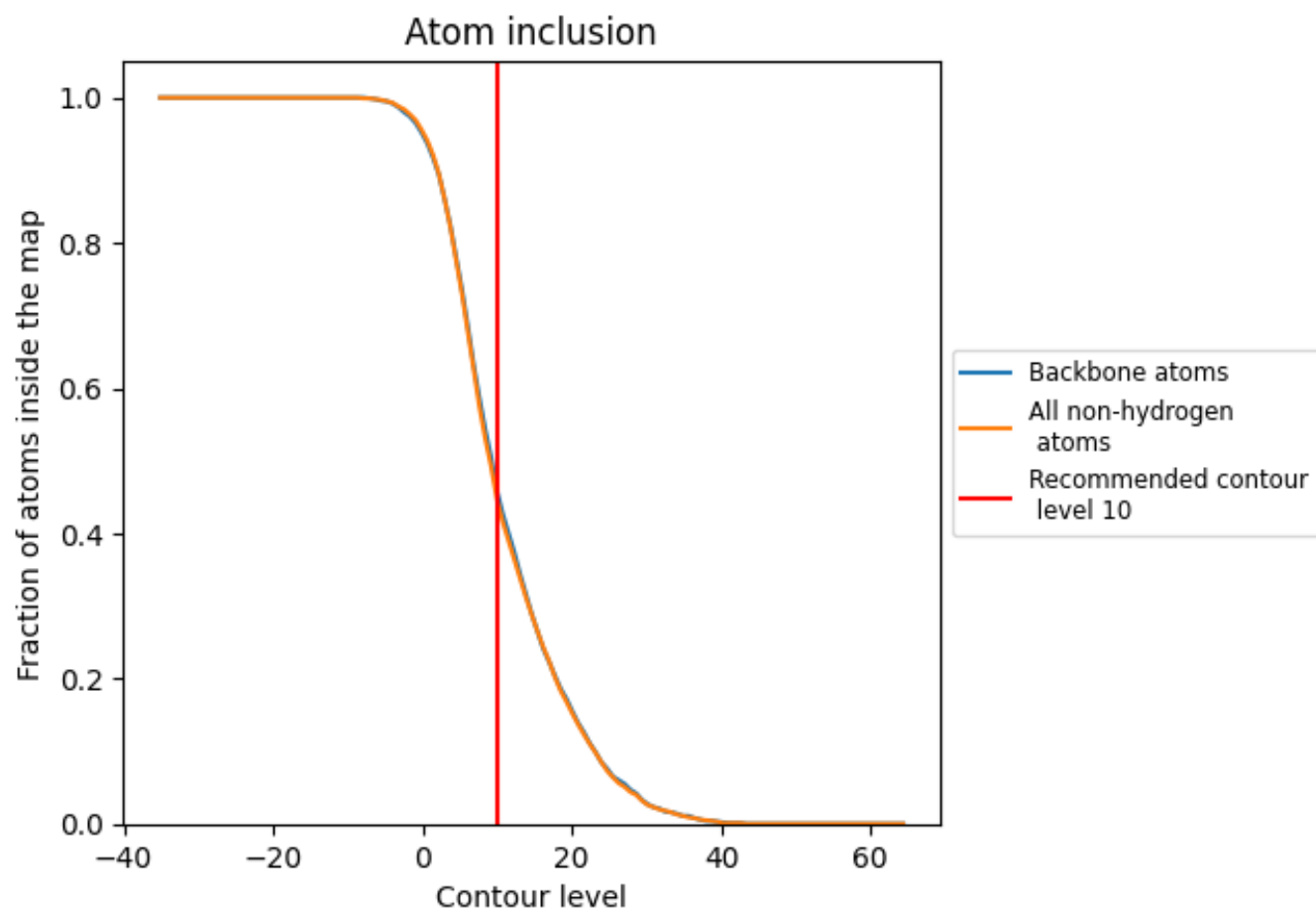
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4460	0.4220
A	0.4620	0.4250
B	0.4620	0.4240
C	0.4560	0.4210
D	0.4650	0.4240
E	0.4540	0.4190
F	0.4670	0.4230

1.0

0.0

<0.0