



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:03 AM UTC

PDB ID : 9Z9H / pdb_00009z9h
EMDB ID : EMD-73942
Title : Stable open state sheep connexin-50 in DMPC nanodiscs at low pH
Authors : Jarodsky, J.M.; Myers, J.B.; Reichow, S.L.
Deposited on : 2025-11-18
Resolution : 2.50 Å(reported)
Based on initial model : 7jjp

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

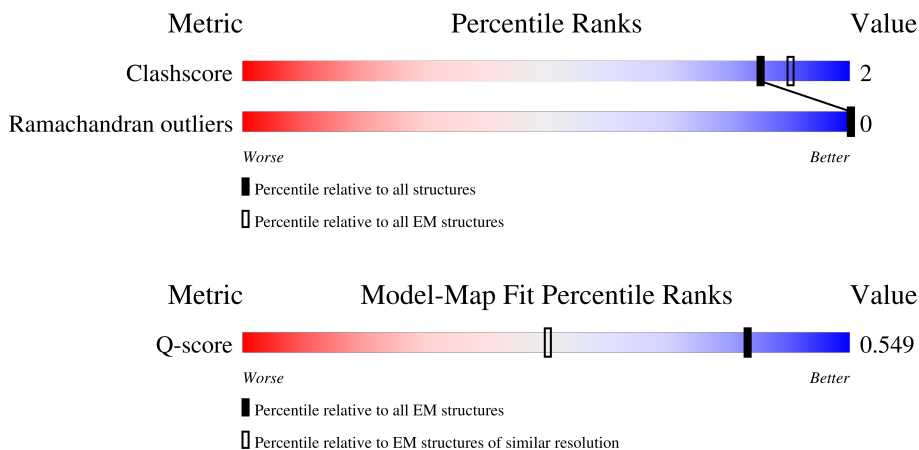
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	440	
1	B	440	
1	C	440	
1	D	440	
1	E	440	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	440	 40% • 58%
1	G	440	 40% • 58%
1	H	440	 40% • 58%
1	I	440	 40% • 58%
1	J	440	 41% • 58%
1	K	440	 41% • 58%
1	L	440	 40% • 58%

2 Entry composition

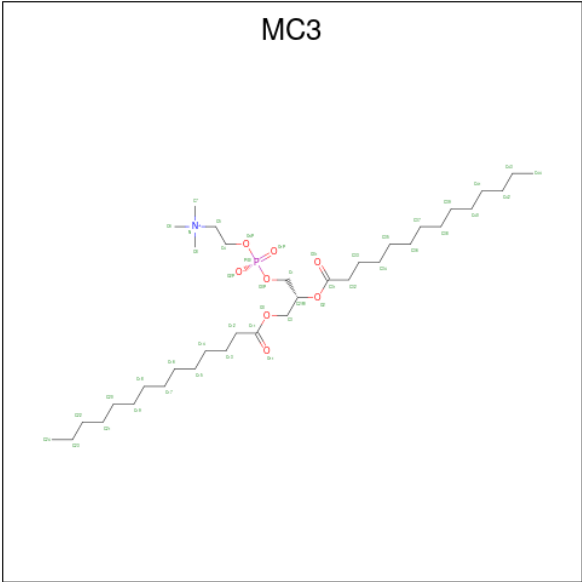
There are 3 unique types of molecules in this entry. The entry contains 42612 atoms, of which 21780 are hydrogens and 0 are deuteriums.

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 Gap junction alpha-8 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	B	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	C	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	D	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	E	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	F	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	G	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	H	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	I	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	J	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	K	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0
1	L	185	Total 2997	C 994	H 1495	N 245	O 253	S 10	0	0

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H			0
			33	11	22			
2	A	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	A	1	Total	C	H			0
			30	10	20			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			30	10	20			
2	A	1	Total	C	H			0
			33	11	22			
2	A	1	Total	C	H			0
			24	8	16			
2	A	1	Total	C	H			0
			24	8	16			
2	A	1	Total	C	H			0
			27	9	18			
2	A	1	Total	C	H			0
			39	13	26			
2	A	1	Total	C	H			0
			30	10	20			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			33	11	22			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H			0
			21	7	14			
2	B	1	Total	C	H			0
			39	13	26			
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			33	11	22			
2	B	1	Total	C	H			0
			21	7	14			
2	B	1	Total	C	H			0
			33	11	22			
2	B	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H			0
			33	11	22			
2	B	1	Total	C	H			0
			24	8	16			
2	B	1	Total	C	H			0
			24	8	16			
2	B	1	Total	C	H			0
			27	9	18			
2	C	1	Total	C	H			0
			39	13	26			
2	C	1	Total	C	H			0
			30	10	20			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			33	11	22			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	H			0
			21	7	14			
2	C	1	Total	C	H			0
			33	11	22			
2	C	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	C	1	Total	C	H			0
			30	10	20			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			30	10	20			
2	C	1	Total	C	H			0
			33	11	22			
2	C	1	Total	C	H			0
			24	8	16			
2	C	1	Total	C	H			0
			24	8	16			
2	C	1	Total	C	H			0
			27	9	18			
2	D	1	Total	C	H			0
			39	13	26			
2	D	1	Total	C	H			0
			30	10	20			
2	D	1	Total	C	H			0
			36	12	24			
2	D	1	Total	C	H			0
			36	12	24			
2	D	1	Total	C	H			0
			33	11	22			
2	D	1	Total	C	H			0
			21	7	14			
2	D	1	Total	C	H			0
			33	11	22			
2	D	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	D	1	Total	C	H			0
			30	10	20			
2	D	1	Total	C	H			0
			36	12	24			
2	D	1	Total	C	H			0
			30	10	20			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	H			0
			33	11	22			
2	D	1	Total	C	H			0
			24	8	16			
2	D	1	Total	C	H			0
			24	8	16			
2	D	1	Total	C	H			0
			27	9	18			
2	E	1	Total	C	H			0
			39	13	26			
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			33	11	22			
2	E	1	Total	C	H			0
			21	7	14			
2	E	1	Total	C	H			0
			33	11	22			
2	E	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H			0
			33	11	22			
2	E	1	Total	C	H			0
			24	8	16			
2	E	1	Total	C	H			0
			24	8	16			
2	E	1	Total	C	H			0
			27	9	18			
2	F	1	Total	C	H			0
			39	13	26			
2	F	1	Total	C	H			0
			30	10	20			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			33	11	22			
2	F	1	Total	C	H			0
			21	7	14			
2	F	1	Total	C	H			0
			33	11	22			
2	F	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	F	1	Total	C	H			0
			30	10	20			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			30	10	20			
2	F	1	Total	C	H			0
			33	11	22			
2	F	1	Total	C	H			0
			24	8	16			
2	F	1	Total	C	H			0
			24	8	16			
2	F	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H			0
			33	11	22			
2	G	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			33	11	22			
2	G	1	Total	C	H			0
			24	8	16			
2	G	1	Total	C	H			0
			24	8	16			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			33	11	22			
2	G	1	Total	C	H			0
			21	7	14			
2	H	1	Total	C	H			0
			39	13	26			
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			33	11	22			
2	H	1	Total	C	H			0
			21	7	14			
2	H	1	Total	C	H			0
			33	11	22			
2	H	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			33	11	22			
2	H	1	Total	C	H			0
			24	8	16			
2	H	1	Total	C	H			0
			24	8	16			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	H	1	Total	C	H			0
			27	9	18			
2	I	1	Total	C	H			0
			39	13	26			
2	I	1	Total	C	H			0
			30	10	20			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			33	11	22			
2	I	1	Total	C	H			0
			21	7	14			
2	I	1	Total	C	H			0
			33	11	22			
2	I	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	I	1	Total	C	H			0
			30	10	20			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			30	10	20			
2	I	1	Total	C	H			0
			33	11	22			
2	I	1	Total	C	H			0
			24	8	16			
2	I	1	Total	C	H			0
			24	8	16			
2	I	1	Total	C	H			0
			27	9	18			
2	J	1	Total	C	H			0
			39	13	26			
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			33	11	22			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	J	1	Total	C	H			0
			21	7	14			
2	J	1	Total	C	H			0
			33	11	22			
2	J	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H			0
			33	11	22			
2	J	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			27	9	18			
2	K	1	Total	C	H			0
			39	13	26			
2	K	1	Total	C	H			0
			30	10	20			
2	K	1	Total	C	H			0
			36	12	24			
2	K	1	Total	C	H			0
			36	12	24			
2	K	1	Total	C	H			0
			33	11	22			
2	K	1	Total	C	H			0
			21	7	14			
2	K	1	Total	C	H			0
			33	11	22			
2	K	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	K	1	Total	C	H			0
			30	10	20			
2	K	1	Total	C	H			0
			36	12	24			
2	K	1	Total	C	H			0
			30	10	20			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total	C	H			0
			33	11	22			
2	K	1	Total	C	H			0
			24	8	16			
2	K	1	Total	C	H			0
			24	8	16			
2	K	1	Total	C	H			0
			27	9	18			
2	L	1	Total	C	H			0
			39	13	26			
2	L	1	Total	C	H			0
			30	10	20			
2	L	1	Total	C	H			0
			36	12	24			
2	L	1	Total	C	H			0
			36	12	24			
2	L	1	Total	C	H			0
			33	11	22			
2	L	1	Total	C	H			0
			21	7	14			
2	L	1	Total	C	H			0
			33	11	22			
2	L	1	Total	C	H	O	P	0
			56	17	32	6	1	
2	L	1	Total	C	H			0
			30	10	20			
2	L	1	Total	C	H			0
			36	12	24			
2	L	1	Total	C	H			0
			30	10	20			
2	L	1	Total	C	H			0
			33	11	22			
2	L	1	Total	C	H			0
			24	8	16			
2	L	1	Total	C	H			0
			24	8	16			
2	L	1	Total	C	H			0
			27	9	18			

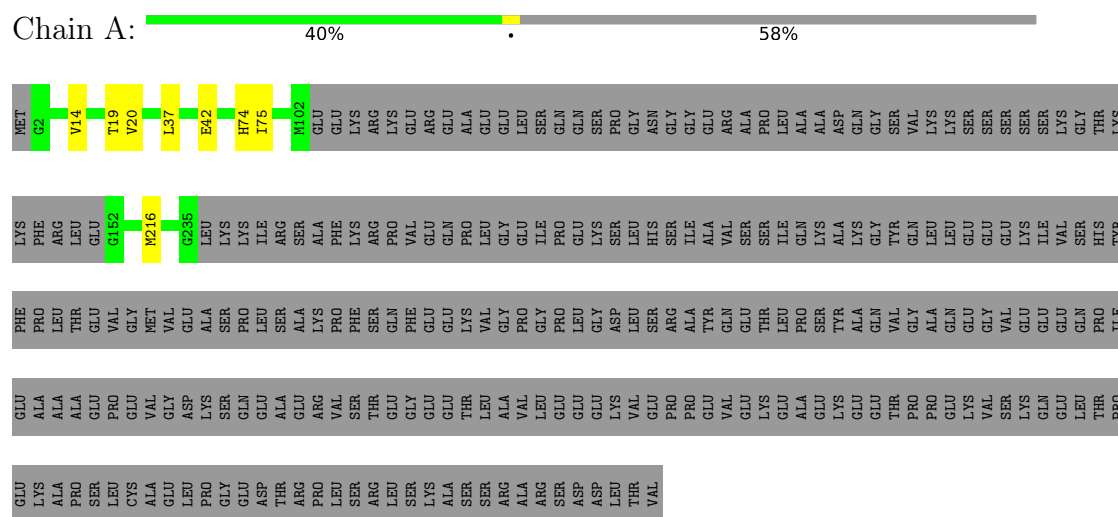
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	66	Total 66	O 66	0
3	B	66	Total 66	O 66	0
3	C	66	Total 66	O 66	0
3	D	66	Total 66	O 66	0
3	E	66	Total 66	O 66	0
3	F	66	Total 66	O 66	0
3	G	66	Total 66	O 66	0
3	H	66	Total 66	O 66	0
3	I	66	Total 66	O 66	0
3	J	66	Total 66	O 66	0
3	K	66	Total 66	O 66	0
3	L	66	Total 66	O 66	0

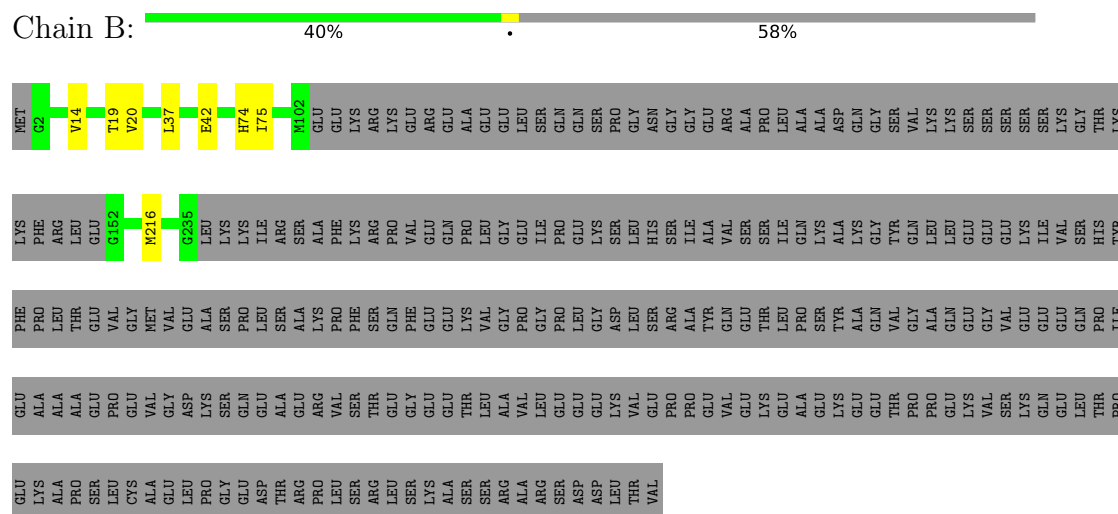
3 Residue-property plots [i](#)

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

- Molecule 1: Gap junction alpha-8 protein



- Molecule 1: Gap junction alpha-8 protein



- Molecule 1: Gap junction alpha-8 protein

[illegible]

Chain D: 41% 58%

[illegible]

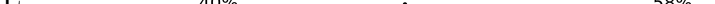
Chain E: 41% . 58%

SER	GLU	GLU	GLU
LEU	PRO	VAL	VAL
CYS	GLU	GLY	GLY
ALA	VAL	MET	MET
GLU	GLY	VAL	G2
LEU	ASP	GLU	V14
PRO	LYS	ALA	T19
GLY	SER	SER	V20
GLU	GLN	PRO	H74
ASP	GLU	ILE	I75
THR	ALA	SER	M102
ARG	GLU	ALA	GLU
PRO	ARG	LYS	GLU
LEU	VAL	PHE	LYS
LEU	SER	PRO	LYS
ARG	THR	ARG	ARG
GLU	GLY	PRO	LYS
SER	GLY	PHE	GLU
LYS	GLU	GLU	ARG
ALA	GLU	GLN	GLU
SER	THR	LYS	ALA
SER	LEU	VAL	GLU
ARG	ALA	GLY	GLU
ALA	VAL	PRO	LEU
ARG	LEU	GLY	SER
SER	GLU	ILE	SER
ASP	GLU	PRO	GLN
ASP	GLU	LEU	GLN
LEU	GLY	LYS	SER
THR	VAL	ASP	PRO
VAL	VAL	LEU	GLY
	GLU	SER	ASN
	PRO	ARG	SER
	GLU	ILE	GLY
	GLU	TYR	GLU
	VAL	GLN	ARG
	GLU	GLU	PRO
	LYS	THR	ALA
	GLU	VAL	ALA
	GLU	TYR	ALA
	LYS	SER	ASP
	GLU	ALA	GLN
	GLU	GLN	GLY
	PRO	ALA	VAL
	PRO	ALA	LYS
	GLU	LEU	LYS
	LYS	GLU	SER
	VAL	GLY	SER
	SER	VAL	SER
	GLN	ILE	SER
	GLU	GLU	LYS
	LEU	GLU	LYS
	THR	GLN	GLY
	PRO	PRO	THR
	GLU	ILE	LYS
	LYS	GLU	LYS
	ALA	ALA	PHE
	PRO	ALA	ARG
		ALA	LEU



SER
LEU
CYS
ALA
GLU
LEU
PRO
GLY
GLU
ASP
THR
ARG
PRO
LEU
SER
ARG
LEU
SER
LYS
ALA
SER
SER
ARG
ALA
ARG
SER
ASP
ASP
LEU
THR
VAL

- Molecule 1: Gap junction alpha-8 protein

Chain L:  40% . 58%

LYS PHE ARG ARG LEU GLU G152 M216 G235 LEU LYS LYS LYS ARG ARG ALA PHE LYS ARG VAL VAL GLU GLN PRO LEU LEU GLU ILE ILE PRO GLU LYS SER SER LEU LEU HIS SER ILE ILE VAL VAL SER SER ILE GLN ALA ALA SER SER ILE LYS LYS LYS LYS VAL VAL SER SER LYS LYS

PHE PRO LEU LEU THR GLU VAL GLY MET VAL GLU ALA SER PRO LEU SER SER LYS PHE SER GLN PHE GLU GLU LYS VAL VAL GLY PRO PRO LEU LEU ASP SER SER ARG ALA ALA TYR GLN GLU GLU THR LEU LEU PRO SER TYR ALA ALA GLN VAL GLY GLN GLN GLU GLY VAL GLU GLU GLU GLU PHE

GLU	ALA	ALA	ALA	ALA	GLU	PRO	GLU	VAL	GLY	ASP	LYS	SER	GLN	GLU	ALA	ALA	GLU	ARG	VAL	SER	THR	GLY	GLU	GLU	GLU	THR	LEU	VAL	LYS	VAL	GLU	PRO	PRO	GLU	VAL	GLU	LYS	GLU	GLU	ALA	GLU	LYS	THR	PRO	PRO	GLU	VAL	GLU	LYS	SER	GLN	GLU	LEU	THR	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLU	LYS	ALA	PRO	SER	LEU	CYS	ALA	GLU	LEU	PRO	GLY	GLU	ASP	THR	ARG	PRO	LEU	SER	ARG	LEU	SER	LYS	ALA	SER	SER	ARG	ALA	ARG	SER	ASP	ASP	LEU	THR	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	42656	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 ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.484	Depositor
Minimum map value	-1.691	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	307.8144, 307.8144, 307.8144	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8016, 0.8016, 0.8016	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MC3

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	0.09	0/1547	0.26	0/2108
1	B	0.09	0/1547	0.26	0/2108
1	C	0.10	0/1547	0.26	0/2108
1	D	0.09	0/1547	0.26	0/2108
1	E	0.09	0/1547	0.26	0/2108
1	F	0.09	0/1547	0.26	0/2108
1	G	0.09	0/1547	0.26	0/2108
1	H	0.09	0/1547	0.26	0/2108
1	I	0.09	0/1547	0.26	0/2108
1	J	0.09	0/1547	0.26	0/2108
1	K	0.09	0/1547	0.26	0/2108
1	L	0.09	0/1547	0.26	0/2108
All	All	0.09	0/18564	0.26	0/25296

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1502	1495	1485	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1502	1495	1485	8	0
1	C	1502	1495	1485	8	0
1	D	1502	1495	1485	7	0
1	E	1502	1495	1485	6	0
1	F	1502	1495	1485	8	0
1	G	1502	1495	1485	8	0
1	H	1502	1495	1485	8	0
1	I	1502	1495	1485	8	0
1	J	1502	1495	1485	7	0
1	K	1502	1495	1485	6	0
1	L	1502	1495	1485	8	0
2	A	168	320	278	0	0
2	B	168	320	278	0	0
2	C	168	320	278	0	0
2	D	168	320	278	0	0
2	E	168	320	278	0	0
2	F	168	320	278	0	0
2	G	168	320	278	0	0
2	H	168	320	278	0	0
2	I	168	320	278	0	0
2	J	168	320	278	0	0
2	K	168	320	278	0	0
2	L	168	320	278	0	0
3	A	66	0	0	4	0
3	B	66	0	0	4	0
3	C	66	0	0	4	0
3	D	66	0	0	4	0
3	E	66	0	0	4	0
3	F	66	0	0	4	0
3	G	66	0	0	4	0
3	H	66	0	0	4	0
3	I	66	0	0	4	0
3	J	66	0	0	4	0
3	K	66	0	0	4	0
3	L	66	0	0	4	0
All	All	20832	21780	21156	90	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 (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:HIS:HD2	3:A:640:HOH:O	1.67	0.77
1:G:74:HIS:HD2	3:G:640:HOH:O	1.67	0.77
1:F:74:HIS:HD2	3:F:640:HOH:O	1.67	0.77
1:L:74:HIS:HD2	3:L:640:HOH:O	1.67	0.77
1:H:74:HIS:HD2	3:H:640:HOH:O	1.67	0.77
1:B:74:HIS:HD2	3:B:640:HOH:O	1.67	0.77
1:C:74:HIS:HD2	3:C:640:HOH:O	1.67	0.76
1:I:74:HIS:HD2	3:I:640:HOH:O	1.67	0.76
1:K:74:HIS:HD2	3:K:640:HOH:O	1.67	0.76
1:E:74:HIS:HD2	3:E:640:HOH:O	1.67	0.76
1:D:74:HIS:HD2	3:D:640:HOH:O	1.67	0.76
1:J:74:HIS:HD2	3:J:640:HOH:O	1.67	0.75
1:D:74:HIS:CD2	3:D:640:HOH:O	2.48	0.61
1:B:74:HIS:CD2	3:B:640:HOH:O	2.48	0.60
1:J:74:HIS:CD2	3:J:640:HOH:O	2.49	0.60
1:H:74:HIS:CD2	3:H:640:HOH:O	2.49	0.60
1:A:74:HIS:CD2	3:A:640:HOH:O	2.48	0.60
1:G:74:HIS:CD2	3:G:640:HOH:O	2.49	0.59
1:F:74:HIS:CD2	3:F:640:HOH:O	2.49	0.59
1:L:74:HIS:CD2	3:L:640:HOH:O	2.48	0.59
1:E:74:HIS:CD2	3:E:640:HOH:O	2.49	0.57
1:K:74:HIS:CD2	3:K:640:HOH:O	2.49	0.57
1:I:74:HIS:CD2	3:I:640:HOH:O	2.48	0.53
1:C:74:HIS:CD2	3:C:640:HOH:O	2.49	0.53
1:H:216:MET:HE3	3:H:653:HOH:O	2.09	0.52
1:B:216:MET:HE3	3:B:653:HOH:O	2.09	0.52
1:E:216:MET:HE3	3:E:653:HOH:O	2.09	0.52
1:F:216:MET:HE3	3:F:653:HOH:O	2.09	0.52
1:A:216:MET:HE3	3:A:653:HOH:O	2.09	0.52
1:K:216:MET:HE3	3:K:653:HOH:O	2.09	0.52
1:L:216:MET:HE3	3:L:653:HOH:O	2.09	0.52
1:G:216:MET:HE3	3:G:653:HOH:O	2.09	0.52
1:I:216:MET:HE3	3:I:653:HOH:O	2.09	0.51
1:C:216:MET:HE3	3:C:653:HOH:O	2.09	0.51
1:D:75:ILE:HD12	3:E:633:HOH:O	2.11	0.51
1:J:75:ILE:HD12	3:K:633:HOH:O	2.11	0.51
1:C:75:ILE:HD12	3:D:633:HOH:O	2.11	0.50
1:D:216:MET:HE3	3:D:653:HOH:O	2.09	0.50
1:I:75:ILE:HD12	3:J:633:HOH:O	2.11	0.50
1:A:75:ILE:HD12	3:B:633:HOH:O	2.11	0.50
1:G:75:ILE:HD12	3:H:633:HOH:O	2.11	0.50
1:J:216:MET:HE3	3:J:653:HOH:O	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:75:ILE:HD12	3:L:633:HOH:O	2.11	0.50
3:A:633:HOH:O	1:F:75:ILE:HD12	2.11	0.50
1:E:75:ILE:HD12	3:F:633:HOH:O	2.11	0.50
3:G:633:HOH:O	1:L:75:ILE:HD12	2.11	0.49
1:B:75:ILE:HD12	3:C:633:HOH:O	2.11	0.49
1:H:75:ILE:HD12	3:I:633:HOH:O	2.11	0.49
1:A:19:THR:HG22	1:A:20:VAL:N	2.28	0.48
1:F:19:THR:HG22	1:F:20:VAL:N	2.28	0.48
1:G:19:THR:HG22	1:G:20:VAL:N	2.28	0.48
1:L:19:THR:HG22	1:L:20:VAL:N	2.28	0.48
1:E:14:VAL:HG22	1:E:14:VAL:O	2.14	0.48
1:E:19:THR:HG22	1:E:20:VAL:N	2.28	0.48
1:K:14:VAL:O	1:K:14:VAL:HG22	2.14	0.48
1:F:14:VAL:HG22	1:F:14:VAL:O	2.14	0.47
1:K:19:THR:HG22	1:K:20:VAL:N	2.28	0.47
1:L:14:VAL:HG22	1:L:14:VAL:O	2.14	0.47
1:B:19:THR:HG22	1:B:20:VAL:N	2.28	0.47
1:C:19:THR:HG22	1:C:20:VAL:N	2.28	0.47
1:H:19:THR:HG22	1:H:20:VAL:N	2.28	0.47
1:I:19:THR:HG22	1:I:20:VAL:N	2.28	0.47
1:I:14:VAL:HG22	1:I:14:VAL:O	2.14	0.47
1:C:14:VAL:O	1:C:14:VAL:HG22	2.14	0.47
1:B:14:VAL:HG22	1:B:14:VAL:O	2.14	0.47
1:H:14:VAL:HG22	1:H:14:VAL:O	2.14	0.46
1:D:19:THR:HG22	1:D:20:VAL:N	2.28	0.46
1:J:19:THR:HG22	1:J:20:VAL:N	2.28	0.46
1:D:14:VAL:HG22	1:D:14:VAL:O	2.14	0.46
1:J:14:VAL:O	1:J:14:VAL:HG22	2.14	0.46
1:G:14:VAL:O	1:G:14:VAL:HG22	2.14	0.46
1:A:14:VAL:HG22	1:A:14:VAL:O	2.14	0.46
1:I:37:LEU:O	1:I:42:GLU:HG3	2.21	0.41
1:C:19:THR:HG22	1:C:20:VAL:H	1.86	0.41
1:C:37:LEU:O	1:C:42:GLU:HG3	2.21	0.41
1:F:37:LEU:O	1:F:42:GLU:HG3	2.21	0.41
1:G:37:LEU:O	1:G:42:GLU:HG3	2.21	0.41
1:I:19:THR:HG22	1:I:20:VAL:H	1.86	0.41
1:A:37:LEU:O	1:A:42:GLU:HG3	2.21	0.41
1:F:19:THR:HG22	1:F:20:VAL:H	1.86	0.41
1:J:19:THR:HG22	1:J:20:VAL:H	1.86	0.41
1:L:37:LEU:O	1:L:42:GLU:HG3	2.21	0.41
1:B:37:LEU:O	1:B:42:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:THR:HG22	1:D:20:VAL:H	1.86	0.41
1:H:37:LEU:O	1:H:42:GLU:HG3	2.21	0.41
1:L:19:THR:HG22	1:L:20:VAL:H	1.86	0.41
1:G:19:THR:HG22	1:G:20:VAL:H	1.86	0.40
1:A:19:THR:HG22	1:A:20:VAL:H	1.86	0.40
1:B:19:THR:HG22	1:B:20:VAL:H	1.86	0.40
1:H:19:THR:HG22	1:H:20:VAL:H	1.86	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	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	B	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	C	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	D	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	E	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	F	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	G	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	H	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	I	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	J	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	K	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
1	L	181/440 (41%)	180 (99%)	1 (1%)	0	100	100
All	All	2172/5280 (41%)	2160 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

180 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	MC3	I	511	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	H	508	-	23,23,45	0.48	0	26,26,53	0.60	1 (3%)
2	MC3	I	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	B	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	A	509	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	B	510	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	B	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	E	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	G	513	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	B	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	C	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	J	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	F	503	-	11,11,45	0.35	0	10,10,53	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	G	512	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	K	509	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	C	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	K	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	A	515	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	F	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	G	511	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	C	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	J	511	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	D	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	D	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	D	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	F	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	J	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	J	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	L	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	G	509	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	G	508	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	L	515	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	F	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	B	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	A	502	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	H	513	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	C	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	C	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	D	511	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	J	510	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	H	505	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	B	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	C	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	D	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	F	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	E	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	E	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	K	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	J	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	D	505	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	A	504	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	B	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	E	511	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	F	510	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	E	505	-	10,10,45	0.35	0	9,9,53	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	K	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	A	503	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	L	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	H	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	H	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	F	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	C	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	A	501	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	L	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	G	503	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	C	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	A	514	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	G	502	-	23,23,45	0.48	0	26,26,53	0.60	1 (3%)
2	MC3	H	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	K	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	G	514	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	G	501	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	I	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	I	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	D	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	G	506	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	E	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	H	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	L	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	B	505	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	I	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	L	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	B	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	H	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	D	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	E	507	-	10,10,45	0.34	0	9,9,53	0.84	0
2	MC3	E	510	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	K	505	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	H	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	D	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	L	506	-	6,6,45	0.36	0	5,5,53	0.71	0
2	MC3	J	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	J	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	J	508	-	23,23,45	0.48	0	26,26,53	0.60	1 (3%)
2	MC3	F	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	D	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	D	512	-	10,10,45	0.35	0	9,9,53	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	E	506	-	6,6,45	0.37	0	5,5,53	0.70	0
2	MC3	J	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	H	511	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	E	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	H	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	A	512	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	B	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	B	511	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	F	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	L	505	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	G	505	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	F	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	I	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	K	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	B	512	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	D	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	I	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	K	510	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	I	505	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	A	510	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	K	511	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	L	514	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	J	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	K	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	A	511	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	L	503	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	F	507	-	10,10,45	0.34	0	9,9,53	0.84	0
2	MC3	B	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	L	511	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	L	510	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	F	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	L	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	K	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	C	510	-	11,11,45	0.35	0	10,10,53	0.83	0
2	MC3	A	506	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	C	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	A	505	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	F	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	K	507	-	10,10,45	0.34	0	9,9,53	0.84	0
2	MC3	D	515	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	K	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	A	508	-	7,7,45	0.36	0	6,6,53	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	J	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	L	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	B	514	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	C	511	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	I	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	C	501	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	K	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	H	509	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	I	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	J	506	-	6,6,45	0.37	0	5,5,53	0.71	0
2	MC3	G	507	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	E	515	-	8,8,45	0.36	0	7,7,53	0.78	0
2	MC3	D	510	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	G	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	C	505	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	B	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	H	510	-	11,11,45	0.36	0	10,10,53	0.84	0
2	MC3	J	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	A	507	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	E	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	I	509	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	I	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	F	511	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	D	513	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	E	501	-	12,12,45	0.34	0	11,11,53	0.86	0
2	MC3	E	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	G	510	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	K	502	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	G	515	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	H	506	-	6,6,45	0.36	0	5,5,53	0.70	0
2	MC3	J	505	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	I	510	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	I	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	H	507	-	10,10,45	0.34	0	9,9,53	0.83	0
2	MC3	L	512	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	C	514	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	C	515	-	8,8,45	0.36	0	7,7,53	0.78	0
2	MC3	F	505	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	E	508	-	23,23,45	0.48	0	26,26,53	0.61	1 (3%)
2	MC3	I	504	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	A	513	-	11,11,45	0.35	0	10,10,53	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	511	-	-	0/7/7/49	-
2	MC3	H	508	-	-	12/22/22/49	-
2	MC3	I	501	-	-	0/10/10/49	-
2	MC3	B	508	-	-	12/22/22/49	-
2	MC3	A	509	-	-	0/6/6/49	-
2	MC3	B	510	-	-	0/9/9/49	-
2	MC3	B	515	-	-	0/6/6/49	-
2	MC3	E	509	-	-	0/7/7/49	-
2	MC3	G	513	-	-	0/9/9/49	-
2	MC3	B	506	-	-	0/4/4/49	-
2	MC3	C	502	-	-	0/7/7/49	-
2	MC3	J	514	-	-	0/5/5/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	G	512	-	-	0/9/9/49	-
2	MC3	K	509	-	-	0/7/7/49	-
2	MC3	C	509	-	-	0/7/7/49	-
2	MC3	K	515	-	-	0/6/6/49	-
2	MC3	A	515	-	-	0/4/4/49	-
2	MC3	F	501	-	-	0/10/10/49	-
2	MC3	G	511	-	-	0/7/7/49	-
2	MC3	C	504	-	-	0/9/9/49	-
2	MC3	J	511	-	-	0/7/7/49	-
2	MC3	D	514	-	-	0/5/5/49	-
2	MC3	D	508	-	-	12/22/22/49	-
2	MC3	D	506	-	-	0/4/4/49	-
2	MC3	F	512	-	-	0/8/8/49	-
2	MC3	J	501	-	-	0/10/10/49	-
2	MC3	J	513	-	-	0/5/5/49	-
2	MC3	L	508	-	-	12/22/22/49	-
2	MC3	G	509	-	-	0/6/6/49	-
2	MC3	G	508	-	-	0/5/5/49	-
2	MC3	L	515	-	-	0/6/6/49	-
2	MC3	F	502	-	-	0/7/7/49	-
2	MC3	B	507	-	-	0/8/8/49	-
2	MC3	A	502	-	-	12/22/22/49	-
2	MC3	H	513	-	-	0/5/5/49	-
2	MC3	C	508	-	-	12/22/22/49	-
2	MC3	C	506	-	-	0/4/4/49	-
2	MC3	D	511	-	-	0/7/7/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	J	510	-	-	0/9/9/49	-
2	MC3	H	505	-	-	0/8/8/49	-
2	MC3	B	502	-	-	0/7/7/49	-
2	MC3	C	513	-	-	0/5/5/49	-
2	MC3	D	502	-	-	0/7/7/49	-
2	MC3	F	504	-	-	0/9/9/49	-
2	MC3	E	502	-	-	0/7/7/49	-
2	MC3	E	512	-	-	0/8/8/49	-
2	MC3	K	513	-	-	0/5/5/49	-
2	MC3	J	504	-	-	0/9/9/49	-
2	MC3	D	505	-	-	0/8/8/49	-
2	MC3	A	504	-	-	0/9/9/49	-
2	MC3	B	509	-	-	0/7/7/49	-
2	MC3	E	511	-	-	0/7/7/49	-
2	MC3	F	510	-	-	0/9/9/49	-
2	MC3	E	505	-	-	0/8/8/49	-
2	MC3	K	512	-	-	0/8/8/49	-
2	MC3	A	503	-	-	0/7/7/49	-
2	MC3	L	507	-	-	0/8/8/49	-
2	MC3	H	514	-	-	0/5/5/49	-
2	MC3	H	515	-	-	0/6/6/49	-
2	MC3	F	514	-	-	0/5/5/49	-
2	MC3	C	512	-	-	0/8/8/49	-
2	MC3	A	501	-	-	0/8/8/49	-
2	MC3	L	502	-	-	0/7/7/49	-
2	MC3	G	503	-	-	0/7/7/49	-
2	MC3	C	507	-	-	0/8/8/49	-
2	MC3	A	514	-	-	0/8/8/49	-
2	MC3	G	502	-	-	12/22/22/49	-
2	MC3	H	512	-	-	0/8/8/49	-
2	MC3	K	503	-	-	0/9/9/49	-
2	MC3	G	514	-	-	0/8/8/49	-
2	MC3	G	501	-	-	0/8/8/49	-
2	MC3	I	508	-	-	12/22/22/49	-
2	MC3	I	515	-	-	0/6/6/49	-
2	MC3	D	501	-	-	0/10/10/49	-
2	MC3	G	506	-	-	0/8/8/49	-
2	MC3	E	514	-	-	0/5/5/49	-
2	MC3	H	502	-	-	0/7/7/49	-
2	MC3	L	509	-	-	0/7/7/49	-
2	MC3	B	505	-	-	0/8/8/49	-
2	MC3	I	506	-	-	0/4/4/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	L	504	-	-	0/9/9/49	-
2	MC3	B	503	-	-	0/9/9/49	-
2	MC3	H	504	-	-	0/9/9/49	-
2	MC3	D	507	-	-	0/8/8/49	-
2	MC3	E	507	-	-	0/8/8/49	-
2	MC3	E	510	-	-	0/9/9/49	-
2	MC3	K	505	-	-	0/8/8/49	-
2	MC3	H	503	-	-	0/9/9/49	-
2	MC3	D	504	-	-	0/9/9/49	-
2	MC3	L	506	-	-	0/4/4/49	-
2	MC3	J	509	-	-	0/7/7/49	-
2	MC3	J	507	-	-	0/8/8/49	-
2	MC3	J	508	-	-	12/22/22/49	-
2	MC3	F	509	-	-	0/7/7/49	-
2	MC3	D	503	-	-	0/9/9/49	-
2	MC3	D	512	-	-	0/8/8/49	-
2	MC3	E	506	-	-	0/4/4/49	-
2	MC3	J	515	-	-	0/6/6/49	-
2	MC3	H	511	-	-	0/7/7/49	-
2	MC3	E	513	-	-	0/5/5/49	-
2	MC3	H	501	-	-	0/10/10/49	-
2	MC3	A	512	-	-	0/9/9/49	-
2	MC3	B	501	-	-	0/10/10/49	-
2	MC3	B	511	-	-	0/7/7/49	-
2	MC3	F	506	-	-	0/4/4/49	-
2	MC3	L	505	-	-	0/8/8/49	-
2	MC3	G	505	-	-	0/7/7/49	-
2	MC3	F	513	-	-	0/5/5/49	-
2	MC3	I	512	-	-	0/8/8/49	-
2	MC3	K	514	-	-	0/5/5/49	-
2	MC3	B	512	-	-	0/8/8/49	-
2	MC3	D	509	-	-	0/7/7/49	-
2	MC3	I	502	-	-	0/7/7/49	-
2	MC3	K	510	-	-	0/9/9/49	-
2	MC3	I	505	-	-	0/8/8/49	-
2	MC3	A	510	-	-	0/10/10/49	-
2	MC3	K	511	-	-	0/7/7/49	-
2	MC3	L	514	-	-	0/5/5/49	-
2	MC3	J	503	-	-	0/9/9/49	-
2	MC3	K	501	-	-	0/10/10/49	-
2	MC3	A	511	-	-	0/7/7/49	-
2	MC3	L	503	-	-	0/9/9/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	F	507	-	-	0/8/8/49	-
2	MC3	B	504	-	-	0/9/9/49	-
2	MC3	L	511	-	-	0/7/7/49	-
2	MC3	L	510	-	-	0/9/9/49	-
2	MC3	F	508	-	-	12/22/22/49	-
2	MC3	L	501	-	-	0/10/10/49	-
2	MC3	K	506	-	-	0/4/4/49	-
2	MC3	C	510	-	-	0/9/9/49	-
2	MC3	A	506	-	-	0/8/8/49	-
2	MC3	C	503	-	-	0/9/9/49	-
2	MC3	A	505	-	-	0/7/7/49	-
2	MC3	F	515	-	-	0/6/6/49	-
2	MC3	K	507	-	-	0/8/8/49	-
2	MC3	D	515	-	-	0/6/6/49	-
2	MC3	K	508	-	-	12/22/22/49	-
2	MC3	A	508	-	-	0/5/5/49	-
2	MC3	J	502	-	-	0/7/7/49	-
2	MC3	L	513	-	-	0/5/5/49	-
2	MC3	B	514	-	-	0/5/5/49	-
2	MC3	C	511	-	-	0/7/7/49	-
2	MC3	I	513	-	-	0/5/5/49	-
2	MC3	C	501	-	-	0/10/10/49	-
2	MC3	K	504	-	-	0/9/9/49	-
2	MC3	H	509	-	-	0/7/7/49	-
2	MC3	I	514	-	-	0/5/5/49	-
2	MC3	J	506	-	-	0/4/4/49	-
2	MC3	G	507	-	-	0/5/5/49	-
2	MC3	E	515	-	-	0/6/6/49	-
2	MC3	D	510	-	-	0/9/9/49	-
2	MC3	G	504	-	-	0/9/9/49	-
2	MC3	C	505	-	-	0/8/8/49	-
2	MC3	B	513	-	-	0/5/5/49	-
2	MC3	H	510	-	-	0/9/9/49	-
2	MC3	J	512	-	-	0/8/8/49	-
2	MC3	A	507	-	-	0/5/5/49	-
2	MC3	E	504	-	-	0/9/9/49	-
2	MC3	I	509	-	-	0/7/7/49	-
2	MC3	I	507	-	-	0/8/8/49	-
2	MC3	F	511	-	-	0/7/7/49	-
2	MC3	D	513	-	-	0/5/5/49	-
2	MC3	E	501	-	-	0/10/10/49	-
2	MC3	E	503	-	-	0/9/9/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	510	-	-	0/10/10/49	-
2	MC3	K	502	-	-	0/7/7/49	-
2	MC3	G	515	-	-	0/4/4/49	-
2	MC3	H	506	-	-	0/4/4/49	-
2	MC3	J	505	-	-	0/8/8/49	-
2	MC3	I	510	-	-	0/9/9/49	-
2	MC3	I	503	-	-	0/9/9/49	-
2	MC3	H	507	-	-	0/8/8/49	-
2	MC3	L	512	-	-	0/8/8/49	-
2	MC3	C	514	-	-	0/5/5/49	-
2	MC3	C	515	-	-	0/6/6/49	-
2	MC3	F	505	-	-	0/8/8/49	-
2	MC3	E	508	-	-	12/22/22/49	-
2	MC3	I	504	-	-	0/9/9/49	-
2	MC3	A	513	-	-	0/9/9/49	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	508	MC3	O2P-P-O1P	2.25	119.60	110.83
2	E	508	MC3	O2P-P-O1P	2.24	119.58	110.83
2	I	508	MC3	O2P-P-O1P	2.24	119.57	110.83
2	B	508	MC3	O2P-P-O1P	2.24	119.57	110.83
2	A	502	MC3	O2P-P-O1P	2.24	119.56	110.83
2	K	508	MC3	O2P-P-O1P	2.24	119.56	110.83
2	F	508	MC3	O2P-P-O1P	2.24	119.55	110.83
2	C	508	MC3	O2P-P-O1P	2.24	119.55	110.83
2	L	508	MC3	O2P-P-O1P	2.24	119.55	110.83
2	J	508	MC3	O2P-P-O1P	2.24	119.54	110.83
2	G	502	MC3	O2P-P-O1P	2.23	119.54	110.83
2	H	508	MC3	O2P-P-O1P	2.23	119.53	110.83

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	MC3	O11-C11-O3-C3
2	B	508	MC3	O11-C11-O3-C3
2	C	508	MC3	O11-C11-O3-C3
2	D	508	MC3	O11-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	508	MC3	O11-C11-O3-C3
2	F	508	MC3	O11-C11-O3-C3
2	G	502	MC3	O11-C11-O3-C3
2	H	508	MC3	O11-C11-O3-C3
2	I	508	MC3	O11-C11-O3-C3
2	J	508	MC3	O11-C11-O3-C3
2	K	508	MC3	O11-C11-O3-C3
2	L	508	MC3	O11-C11-O3-C3
2	A	502	MC3	C12-C11-O3-C3
2	B	508	MC3	C12-C11-O3-C3
2	C	508	MC3	C12-C11-O3-C3
2	D	508	MC3	C12-C11-O3-C3
2	E	508	MC3	C12-C11-O3-C3
2	F	508	MC3	C12-C11-O3-C3
2	G	502	MC3	C12-C11-O3-C3
2	H	508	MC3	C12-C11-O3-C3
2	I	508	MC3	C12-C11-O3-C3
2	J	508	MC3	C12-C11-O3-C3
2	K	508	MC3	C12-C11-O3-C3
2	L	508	MC3	C12-C11-O3-C3
2	A	502	MC3	C18-C19-C20-C21
2	B	508	MC3	C18-C19-C20-C21
2	C	508	MC3	C18-C19-C20-C21
2	D	508	MC3	C18-C19-C20-C21
2	E	508	MC3	C18-C19-C20-C21
2	F	508	MC3	C18-C19-C20-C21
2	G	502	MC3	C18-C19-C20-C21
2	H	508	MC3	C18-C19-C20-C21
2	I	508	MC3	C18-C19-C20-C21
2	J	508	MC3	C18-C19-C20-C21
2	K	508	MC3	C18-C19-C20-C21
2	L	508	MC3	C18-C19-C20-C21
2	C	508	MC3	C17-C18-C19-C20
2	G	502	MC3	C17-C18-C19-C20
2	H	508	MC3	C17-C18-C19-C20
2	J	508	MC3	C17-C18-C19-C20
2	A	502	MC3	C17-C18-C19-C20
2	B	508	MC3	C17-C18-C19-C20
2	D	508	MC3	C17-C18-C19-C20
2	E	508	MC3	C17-C18-C19-C20
2	F	508	MC3	C17-C18-C19-C20
2	I	508	MC3	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	508	MC3	C17-C18-C19-C20
2	L	508	MC3	C17-C18-C19-C20
2	A	502	MC3	C14-C15-C16-C17
2	C	508	MC3	C14-C15-C16-C17
2	F	508	MC3	C14-C15-C16-C17
2	G	502	MC3	C14-C15-C16-C17
2	I	508	MC3	C14-C15-C16-C17
2	K	508	MC3	C14-C15-C16-C17
2	L	508	MC3	C14-C15-C16-C17
2	B	508	MC3	C14-C15-C16-C17
2	D	508	MC3	C14-C15-C16-C17
2	J	508	MC3	C14-C15-C16-C17
2	E	508	MC3	C14-C15-C16-C17
2	H	508	MC3	C14-C15-C16-C17
2	A	502	MC3	C11-C12-C13-C14
2	B	508	MC3	C11-C12-C13-C14
2	C	508	MC3	C11-C12-C13-C14
2	D	508	MC3	C11-C12-C13-C14
2	E	508	MC3	C11-C12-C13-C14
2	I	508	MC3	C11-C12-C13-C14
2	J	508	MC3	C11-C12-C13-C14
2	K	508	MC3	C11-C12-C13-C14
2	L	508	MC3	C11-C12-C13-C14
2	F	508	MC3	C11-C12-C13-C14
2	G	502	MC3	C11-C12-C13-C14
2	H	508	MC3	C11-C12-C13-C14
2	F	508	MC3	C21-C22-C23-C24
2	J	508	MC3	C21-C22-C23-C24
2	A	502	MC3	C21-C22-C23-C24
2	B	508	MC3	C21-C22-C23-C24
2	C	508	MC3	C21-C22-C23-C24
2	D	508	MC3	C21-C22-C23-C24
2	E	508	MC3	C21-C22-C23-C24
2	G	502	MC3	C21-C22-C23-C24
2	H	508	MC3	C21-C22-C23-C24
2	I	508	MC3	C21-C22-C23-C24
2	K	508	MC3	C21-C22-C23-C24
2	L	508	MC3	C21-C22-C23-C24
2	A	502	MC3	C19-C20-C21-C22
2	B	508	MC3	C19-C20-C21-C22
2	E	508	MC3	C19-C20-C21-C22
2	G	502	MC3	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	508	MC3	C19-C20-C21-C22
2	J	508	MC3	C19-C20-C21-C22
2	C	508	MC3	C19-C20-C21-C22
2	D	508	MC3	C19-C20-C21-C22
2	F	508	MC3	C19-C20-C21-C22
2	I	508	MC3	C19-C20-C21-C22
2	K	508	MC3	C19-C20-C21-C22
2	L	508	MC3	C19-C20-C21-C22
2	G	502	MC3	C13-C14-C15-C16
2	C	508	MC3	C13-C14-C15-C16
2	F	508	MC3	C13-C14-C15-C16
2	H	508	MC3	C13-C14-C15-C16
2	K	508	MC3	C13-C14-C15-C16
2	A	502	MC3	C13-C14-C15-C16
2	B	508	MC3	C13-C14-C15-C16
2	E	508	MC3	C13-C14-C15-C16
2	I	508	MC3	C13-C14-C15-C16
2	J	508	MC3	C13-C14-C15-C16
2	L	508	MC3	C13-C14-C15-C16
2	D	508	MC3	C13-C14-C15-C16
2	A	502	MC3	C1-C2-C3-O3
2	B	508	MC3	C1-C2-C3-O3
2	C	508	MC3	C1-C2-C3-O3
2	D	508	MC3	C1-C2-C3-O3
2	E	508	MC3	C1-C2-C3-O3
2	F	508	MC3	C1-C2-C3-O3
2	G	502	MC3	C1-C2-C3-O3
2	H	508	MC3	C1-C2-C3-O3
2	I	508	MC3	C1-C2-C3-O3
2	J	508	MC3	C1-C2-C3-O3
2	K	508	MC3	C1-C2-C3-O3
2	L	508	MC3	C1-C2-C3-O3
2	A	502	MC3	O3P-C1-C2-C3
2	B	508	MC3	O3P-C1-C2-C3
2	C	508	MC3	O3P-C1-C2-C3
2	D	508	MC3	O3P-C1-C2-C3
2	E	508	MC3	O3P-C1-C2-C3
2	F	508	MC3	O3P-C1-C2-C3
2	G	502	MC3	O3P-C1-C2-C3
2	H	508	MC3	O3P-C1-C2-C3
2	I	508	MC3	O3P-C1-C2-C3
2	J	508	MC3	O3P-C1-C2-C3

Continued on next page...

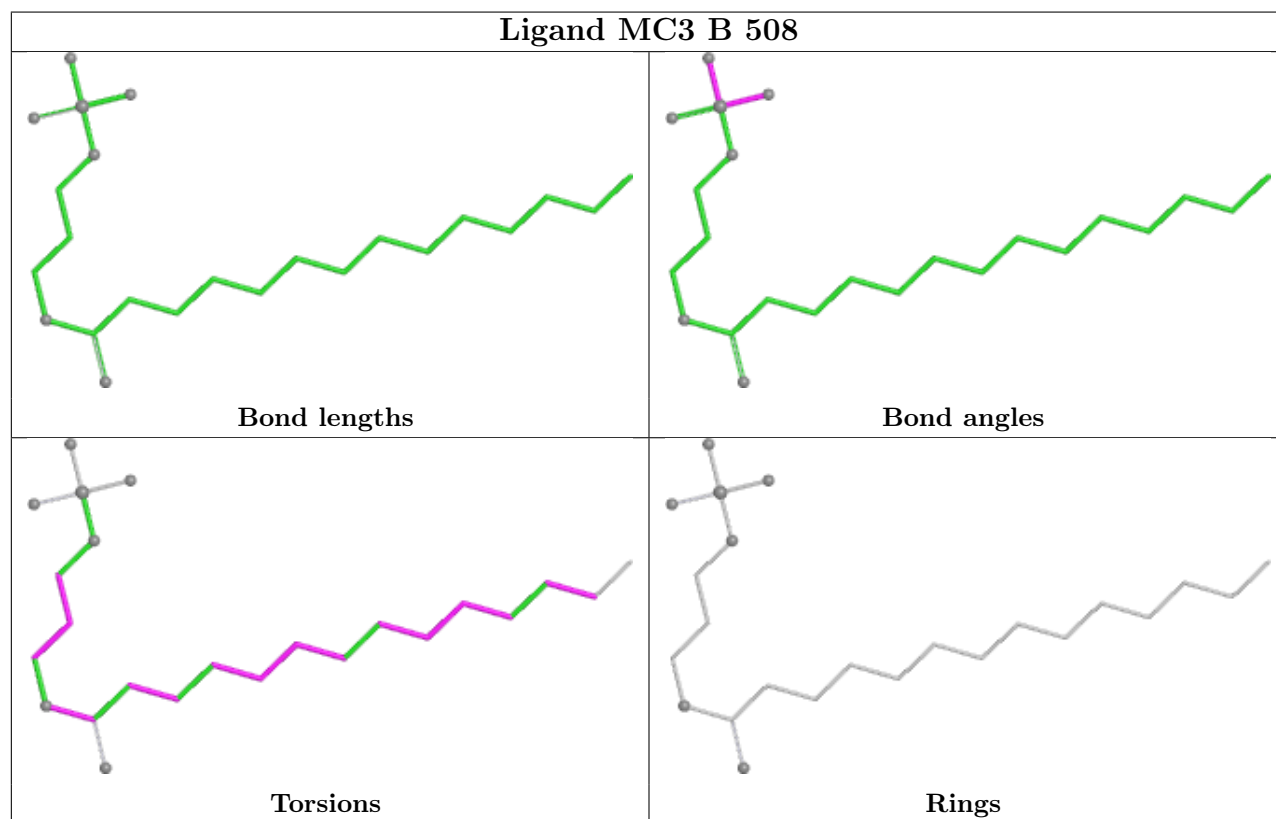
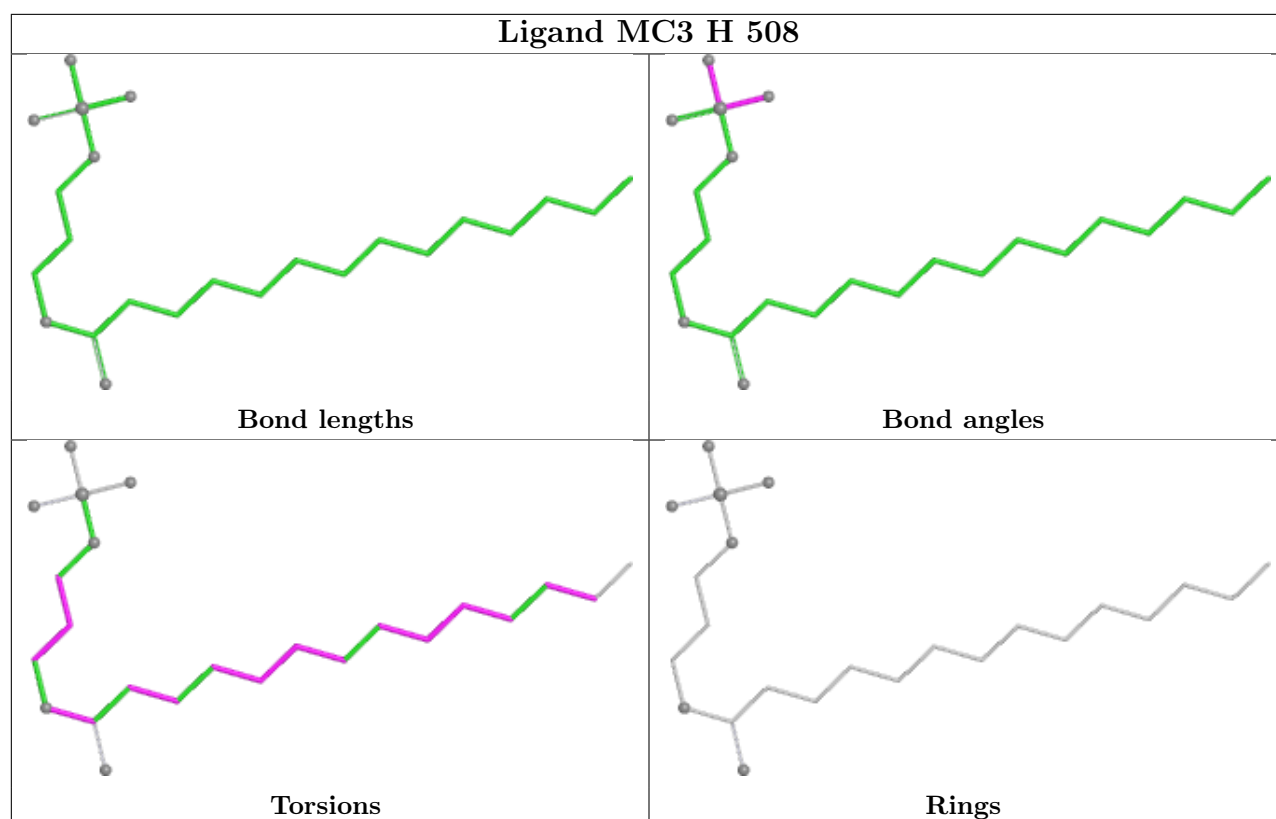
Continued from previous page...

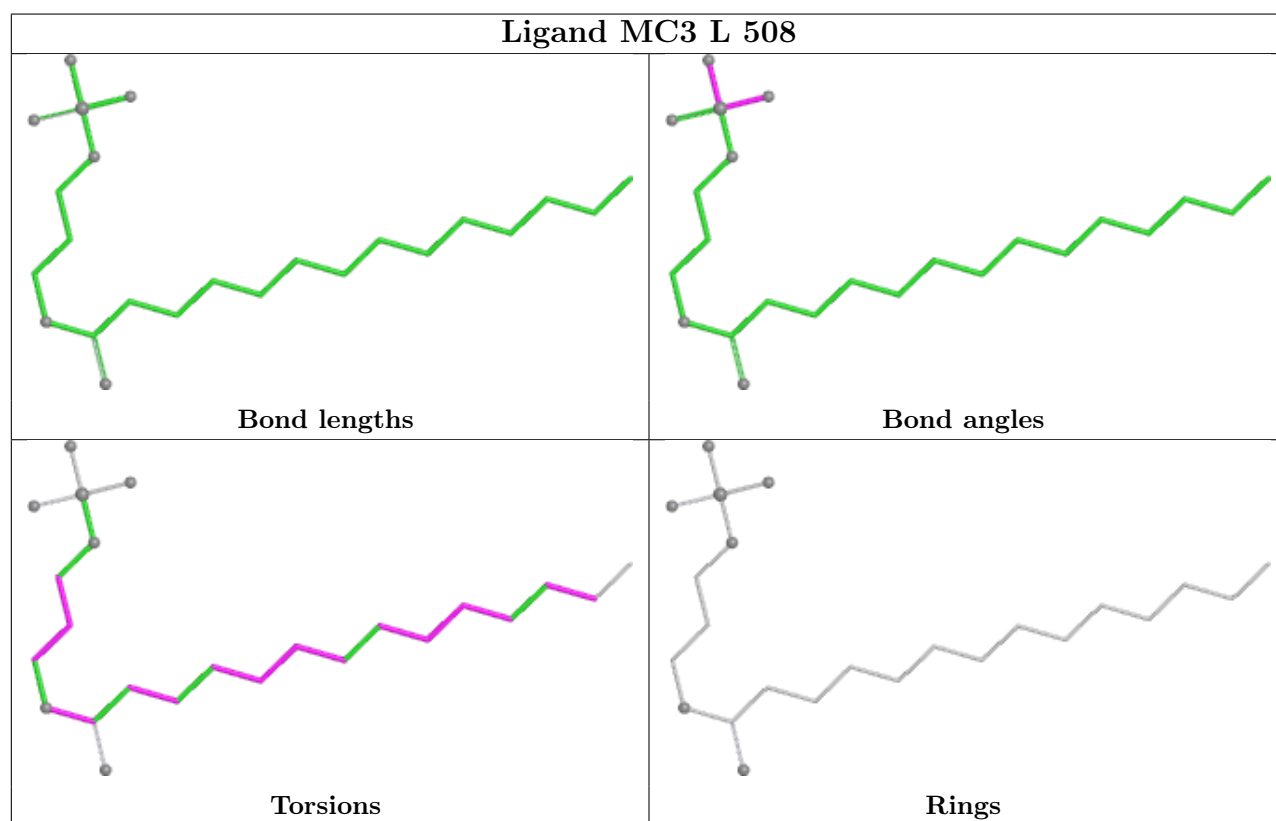
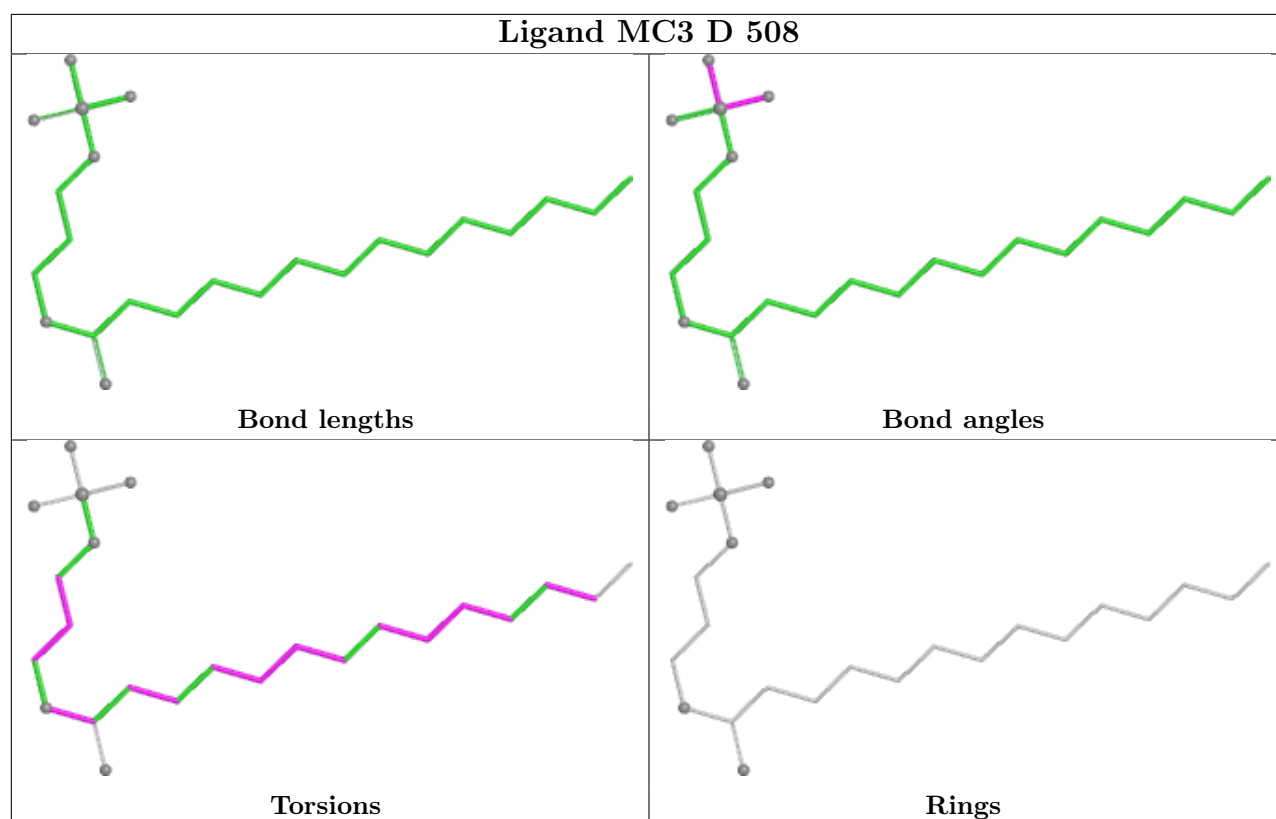
Mol	Chain	Res	Type	Atoms
2	K	508	MC3	O3P-C1-C2-C3
2	L	508	MC3	O3P-C1-C2-C3
2	C	508	MC3	C15-C16-C17-C18
2	F	508	MC3	C15-C16-C17-C18
2	G	502	MC3	C15-C16-C17-C18
2	H	508	MC3	C15-C16-C17-C18
2	I	508	MC3	C15-C16-C17-C18
2	A	502	MC3	C15-C16-C17-C18
2	E	508	MC3	C15-C16-C17-C18
2	J	508	MC3	C15-C16-C17-C18
2	B	508	MC3	C15-C16-C17-C18
2	K	508	MC3	C15-C16-C17-C18
2	D	508	MC3	C15-C16-C17-C18
2	L	508	MC3	C15-C16-C17-C18

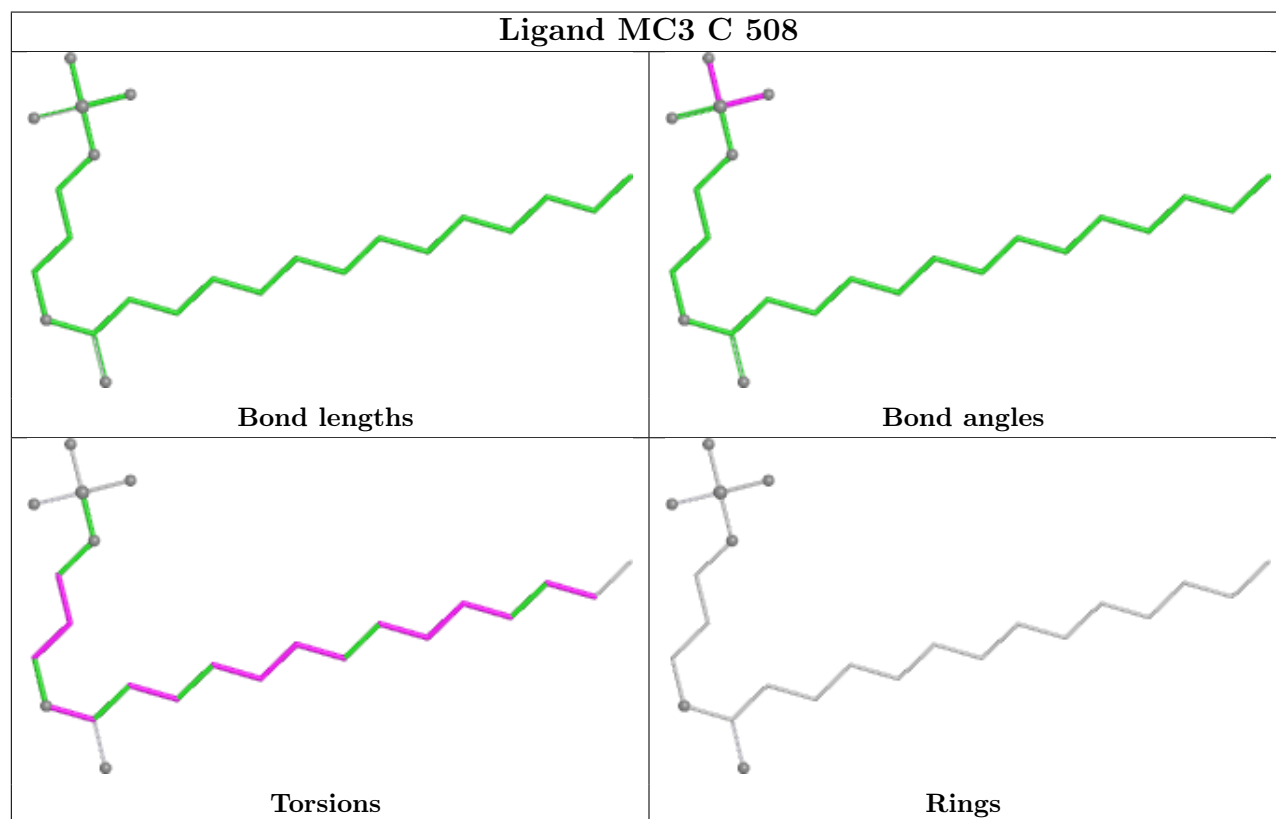
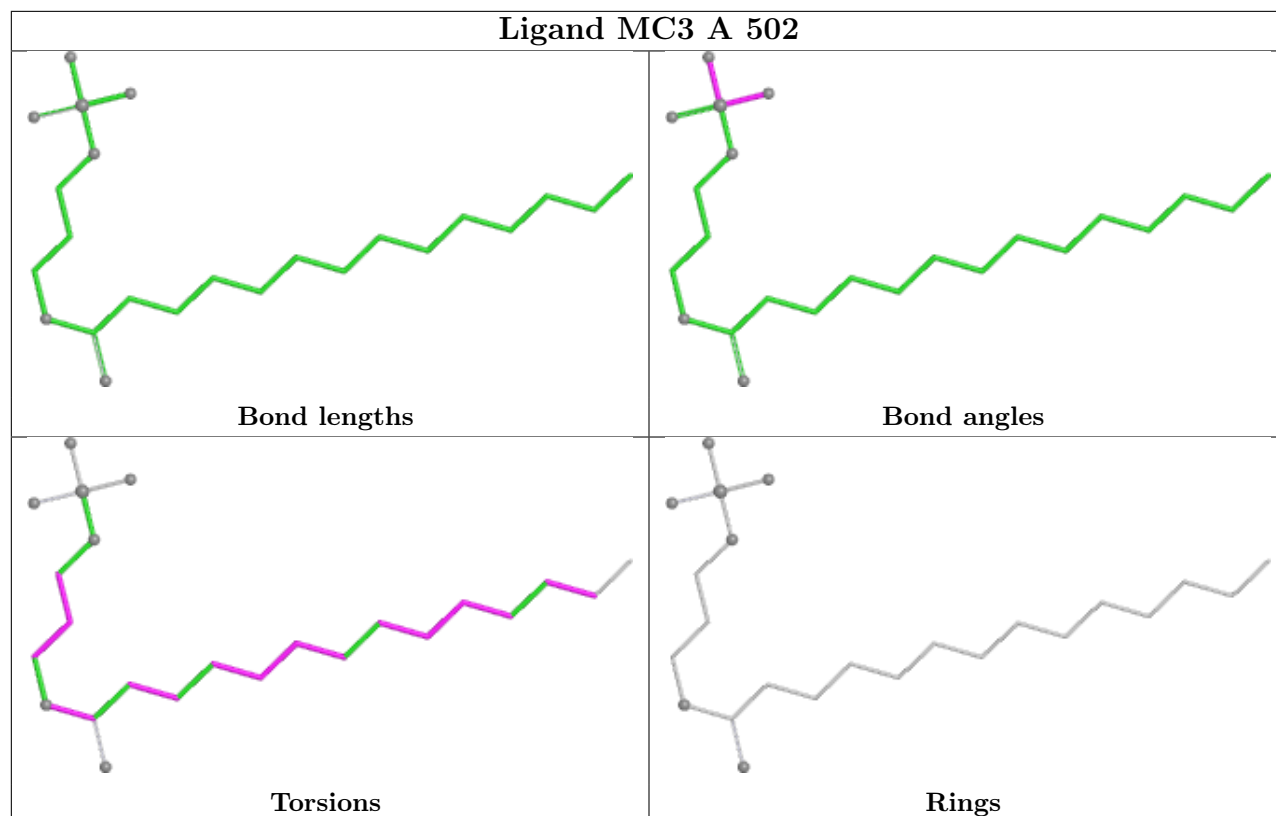
There are no ring outliers.

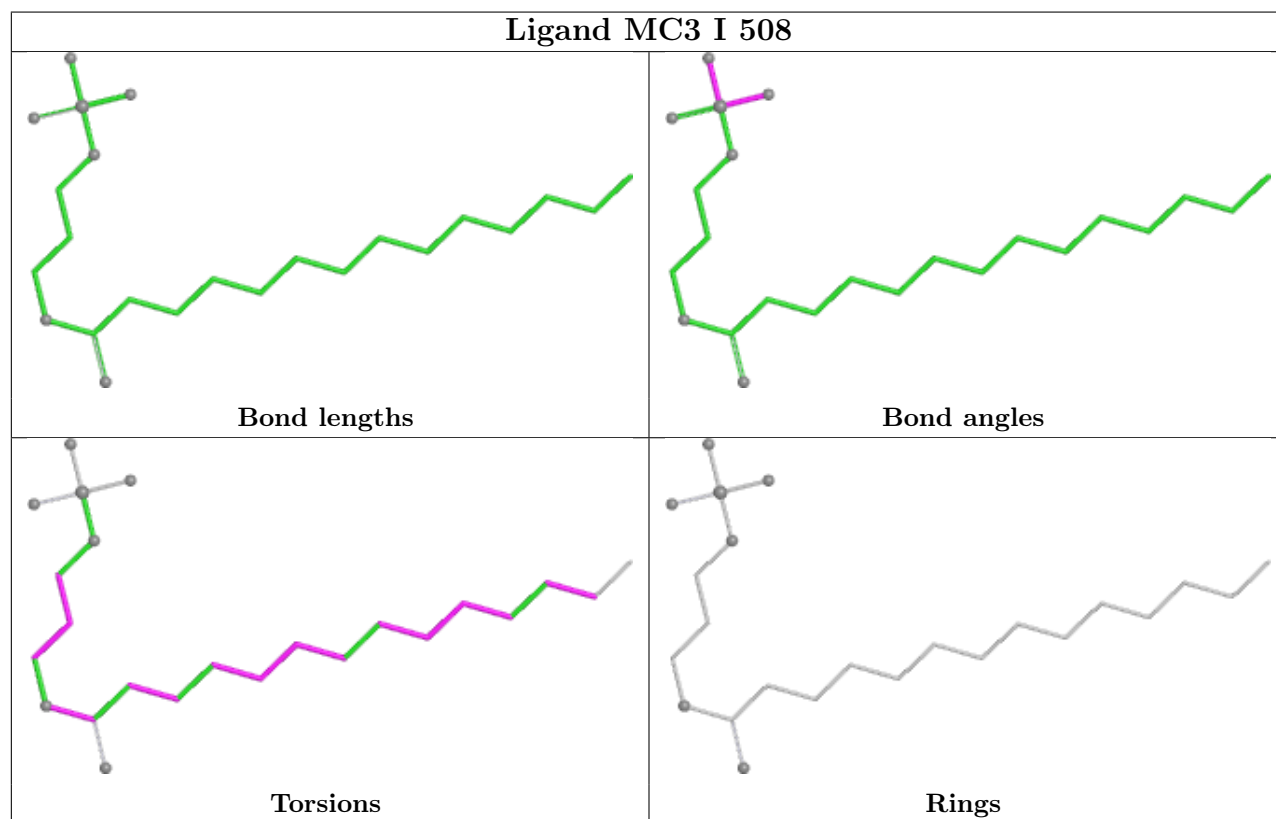
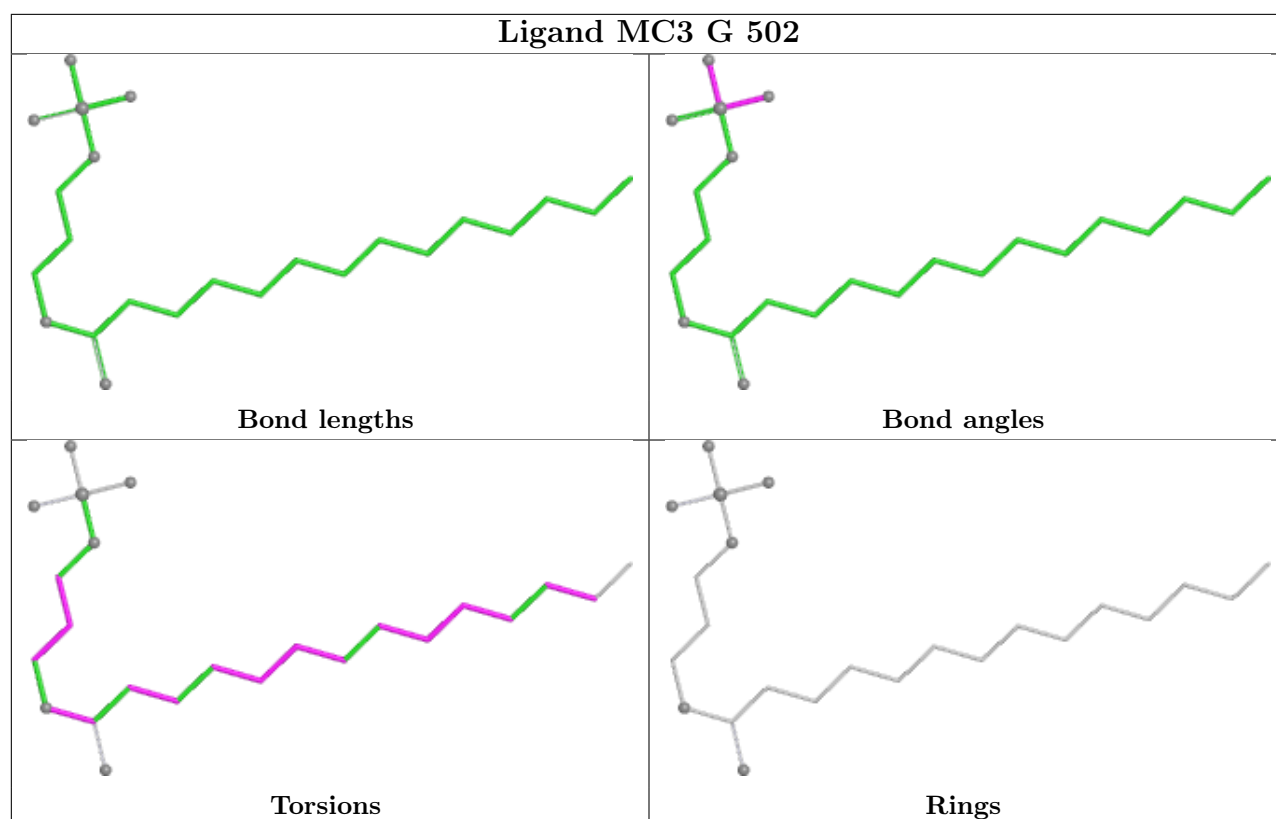
No monomer is involved in short contacts.

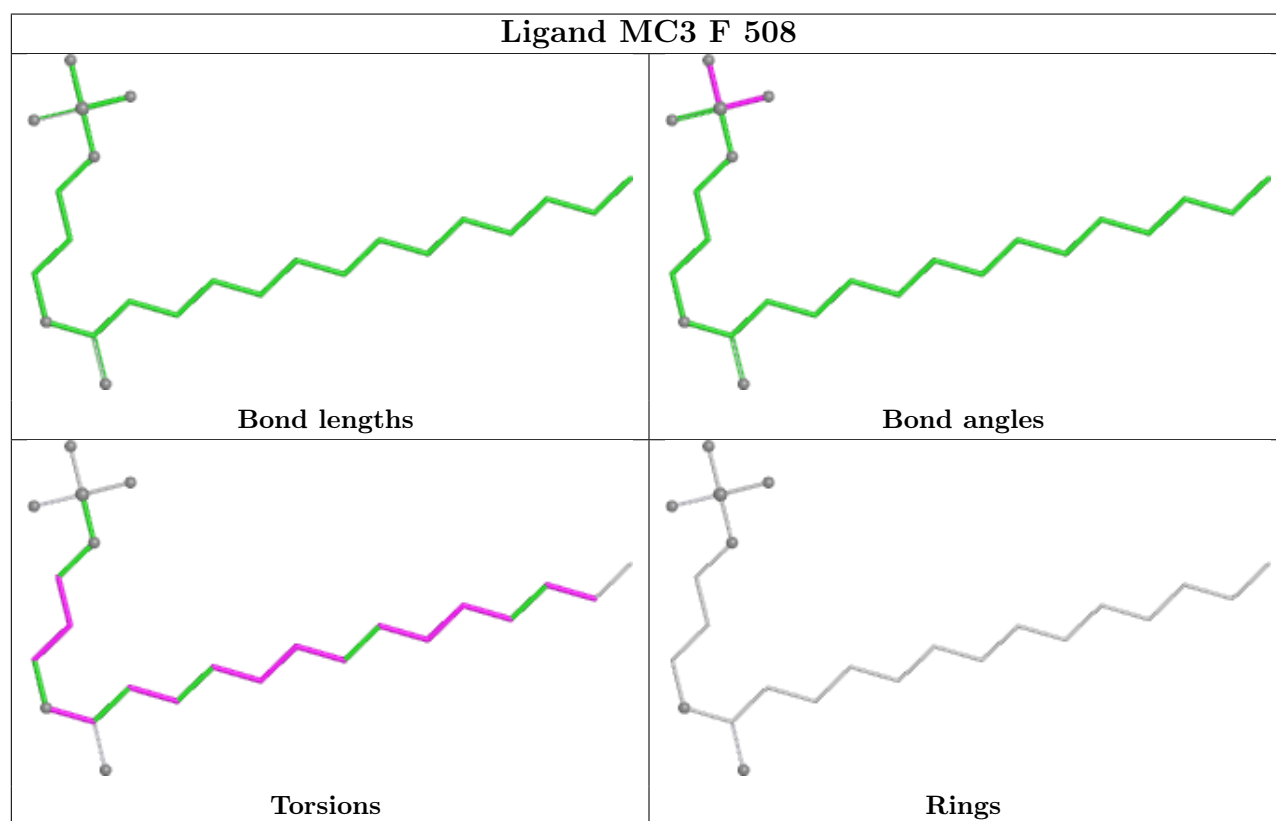
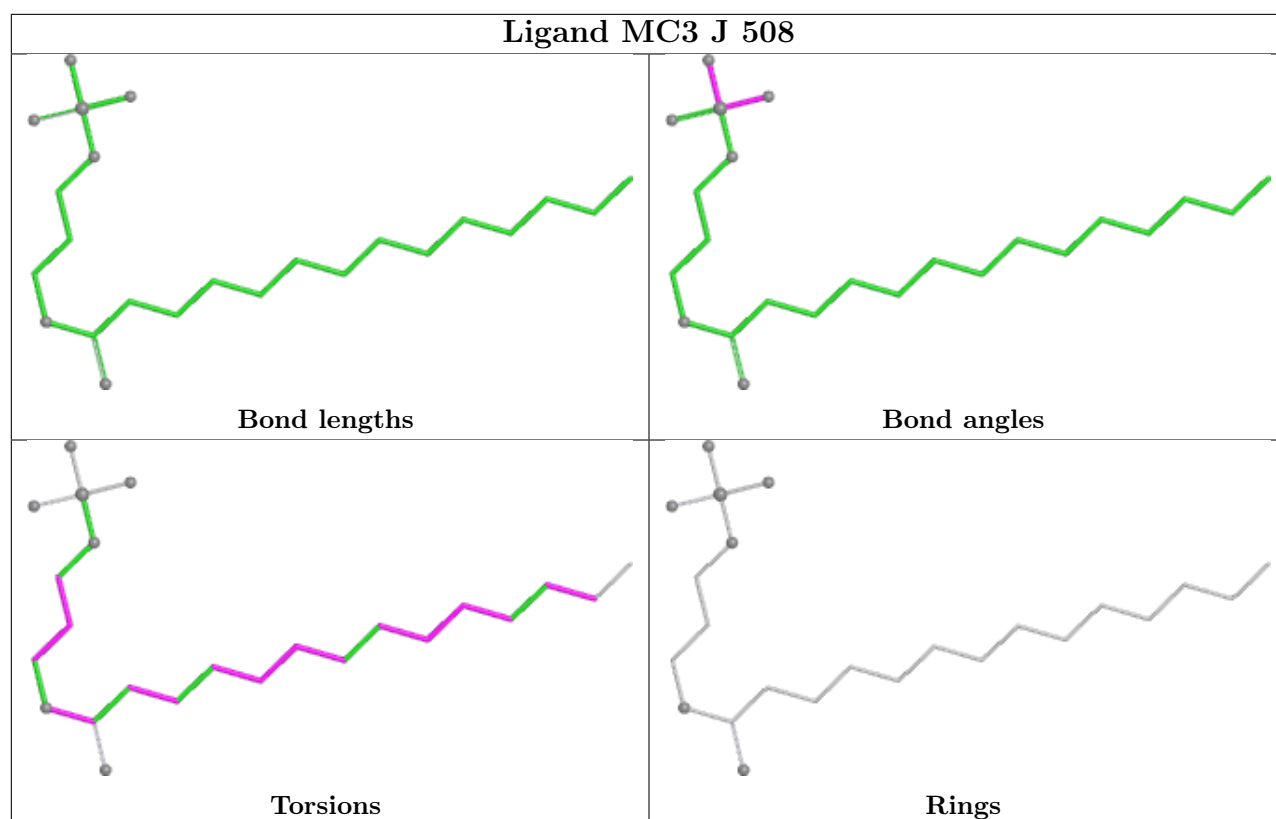
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

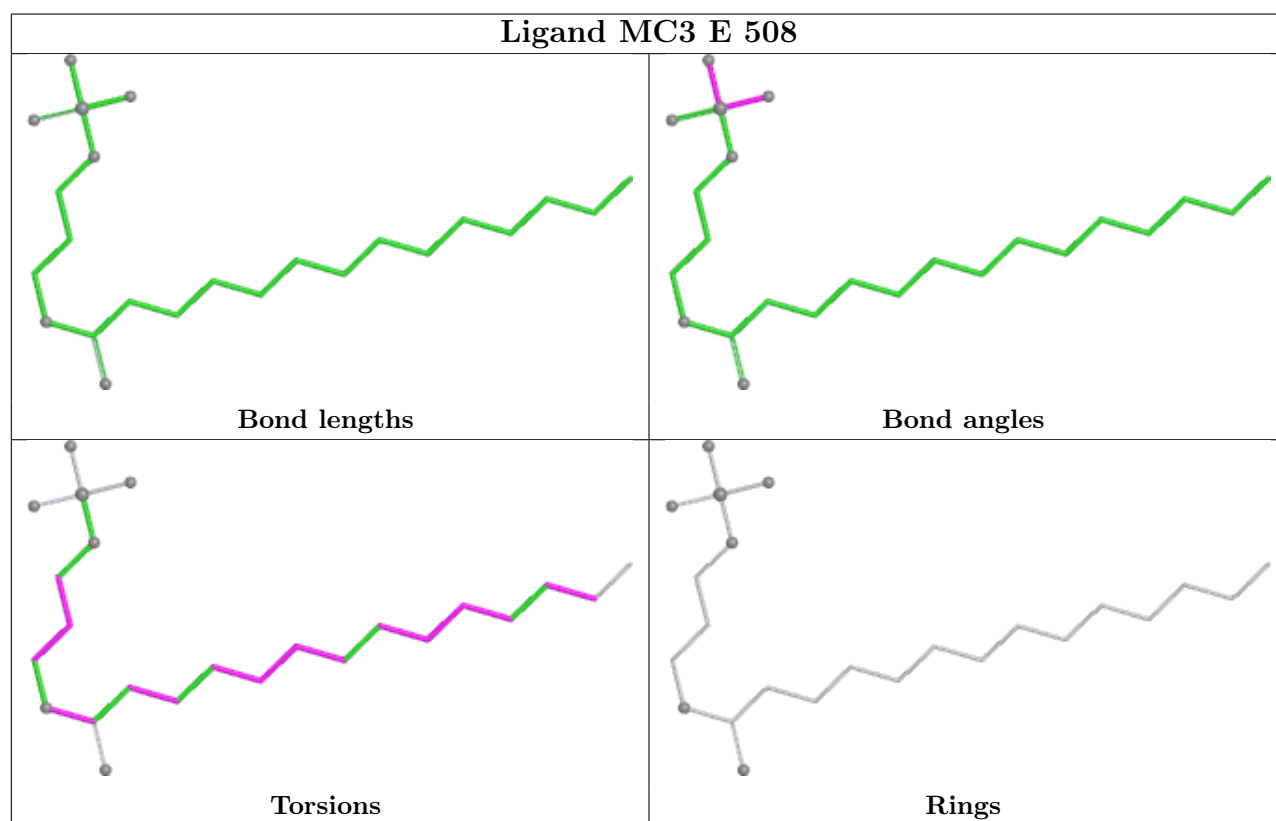
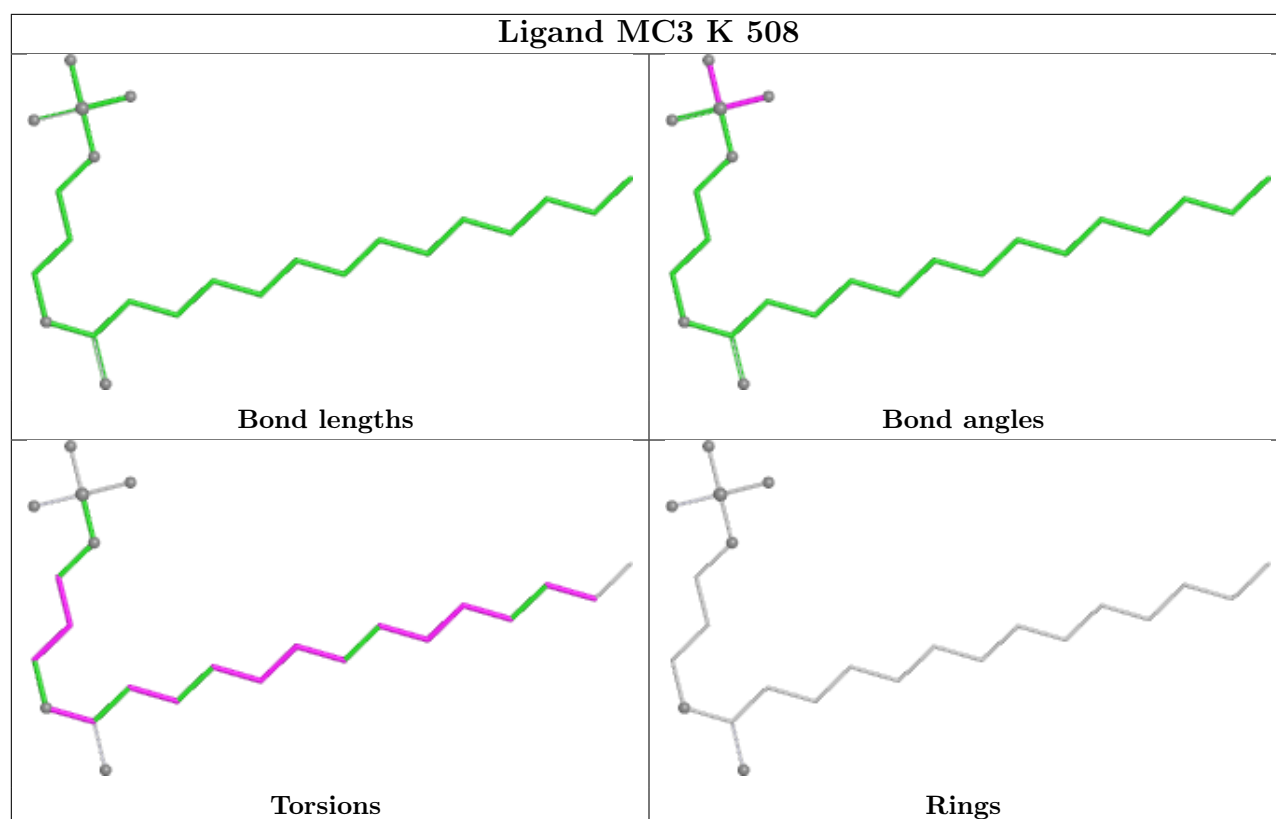












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

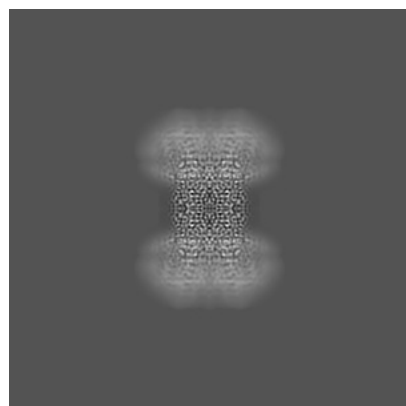
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73942. These allow visual inspection of the internal detail of the map and identification of artifacts.

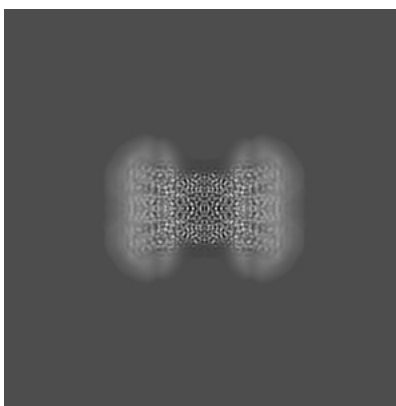
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

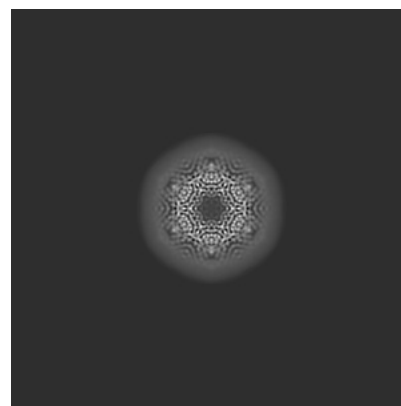
6.1.1 Primary map



X

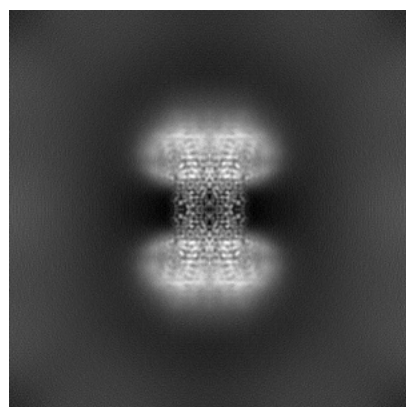


Y

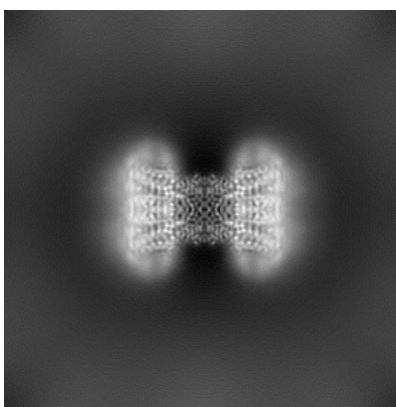


Z

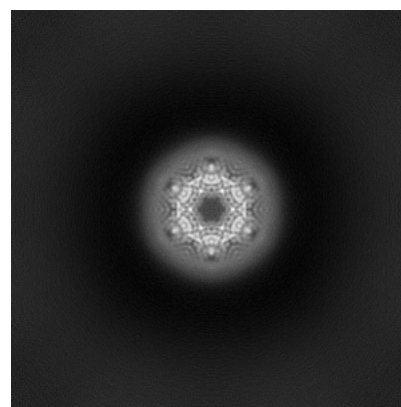
6.1.2 Raw map



X



Y

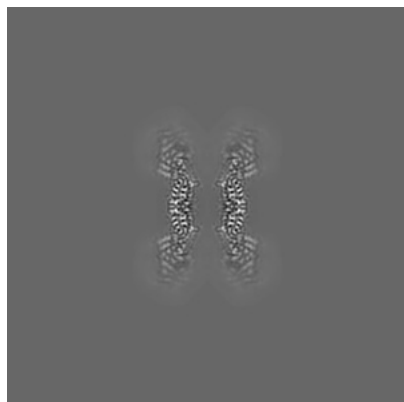


Z

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

6.2 Central slices [i](#)

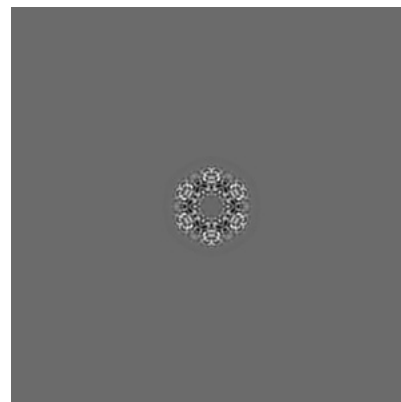
6.2.1 Primary map



X Index: 192

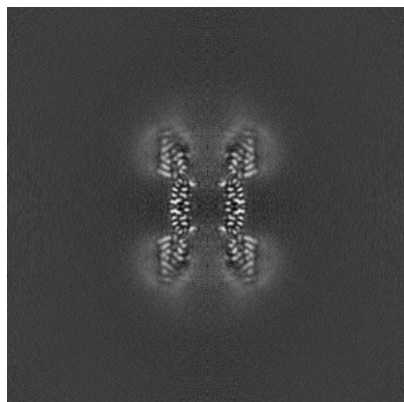


Y Index: 192

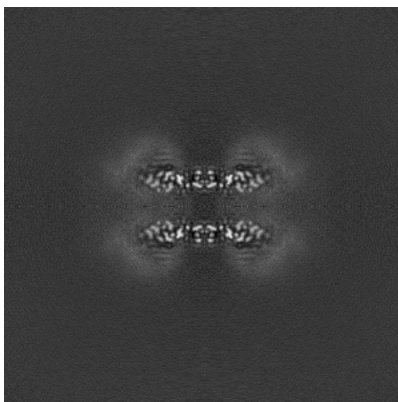


Z Index: 192

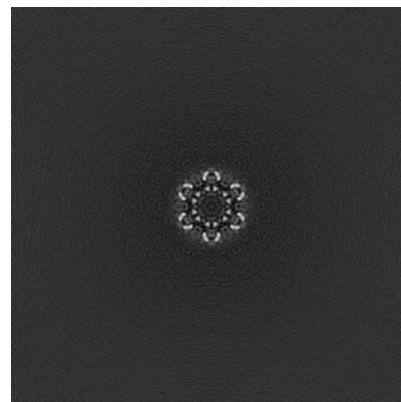
6.2.2 Raw map



X Index: 192



Y Index: 192

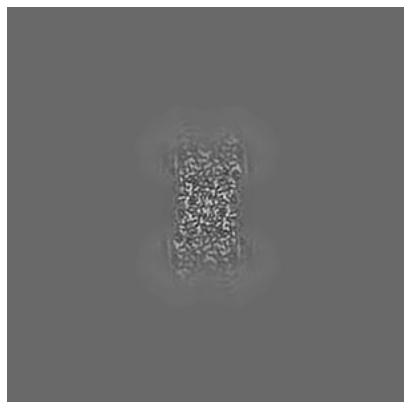


Z Index: 192

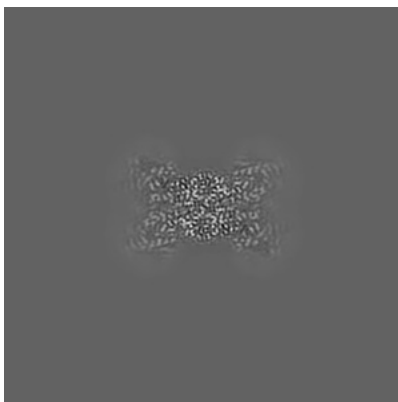
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

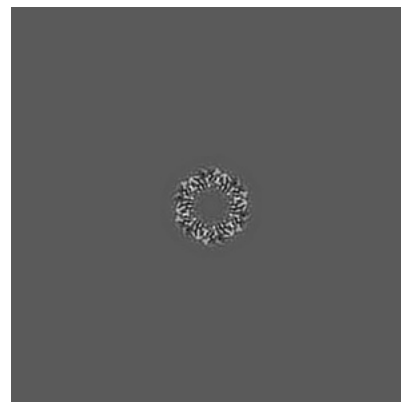
6.3.1 Primary map



X Index: 212

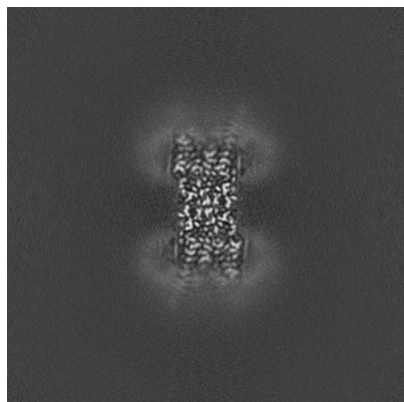


Y Index: 210

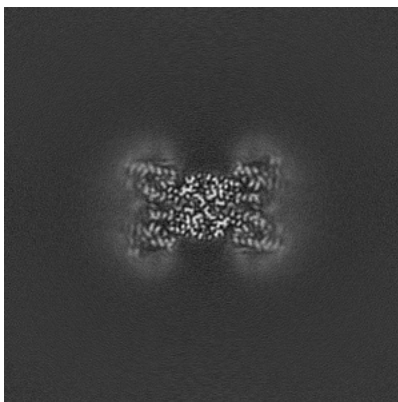


Z Index: 200

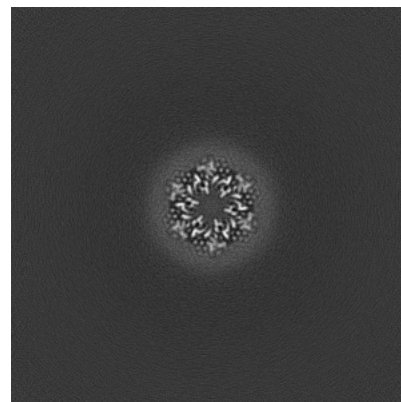
6.3.2 Raw map



X Index: 172



Y Index: 174

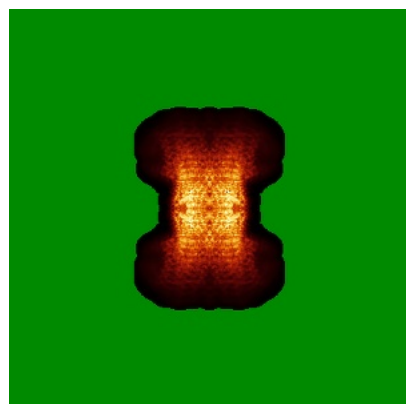


Z Index: 223

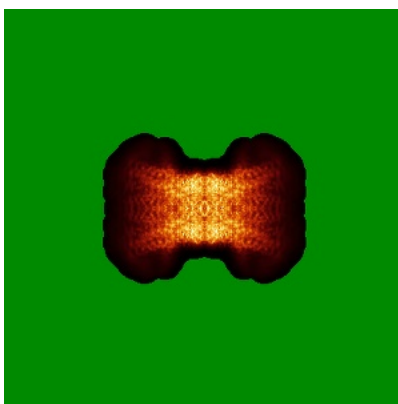
The images above show the largest variance slices of the map in three orthogonal directions.

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

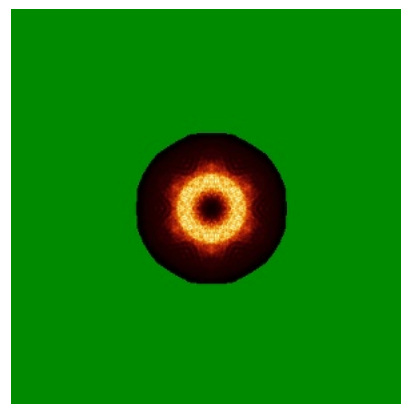
6.4.1 Primary map



X

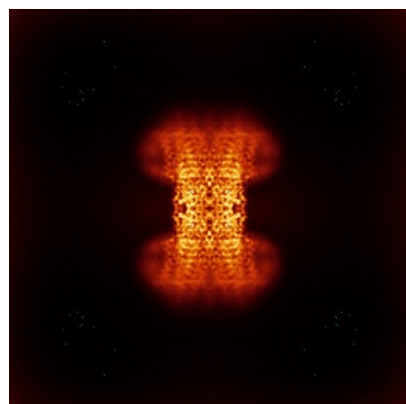


Y

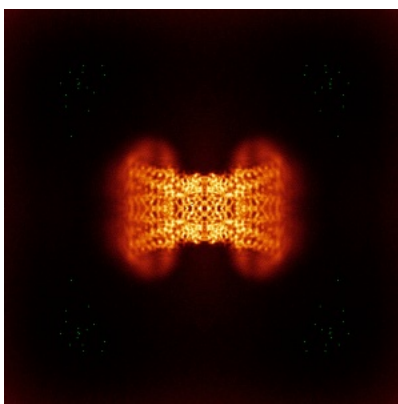


Z

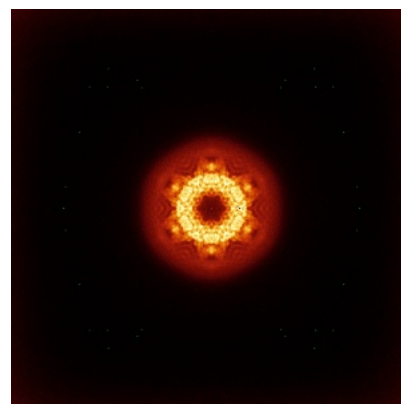
6.4.2 Raw map



X



Y

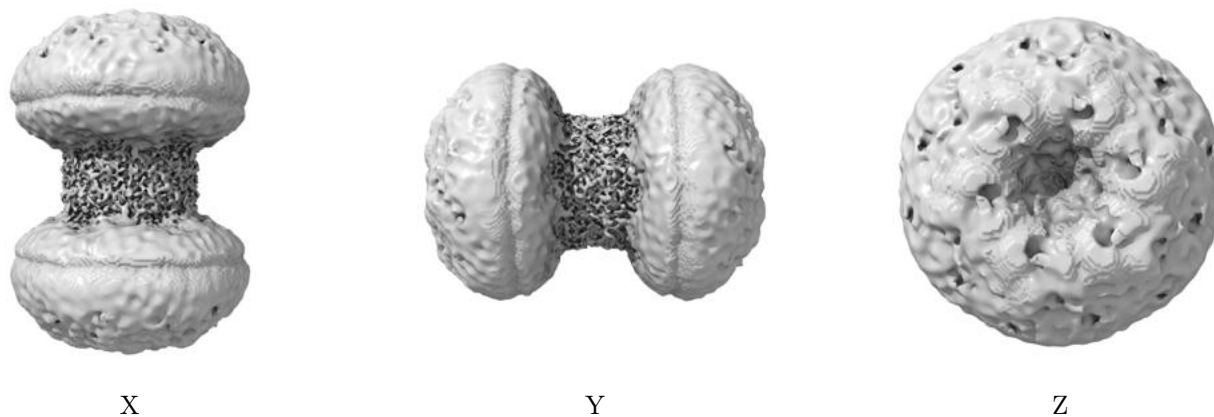


Z

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.

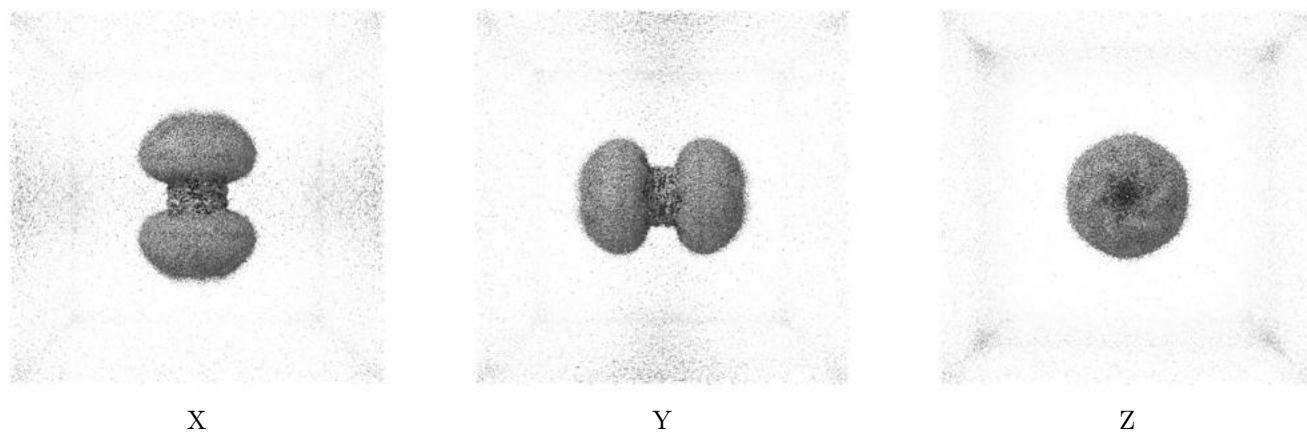
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

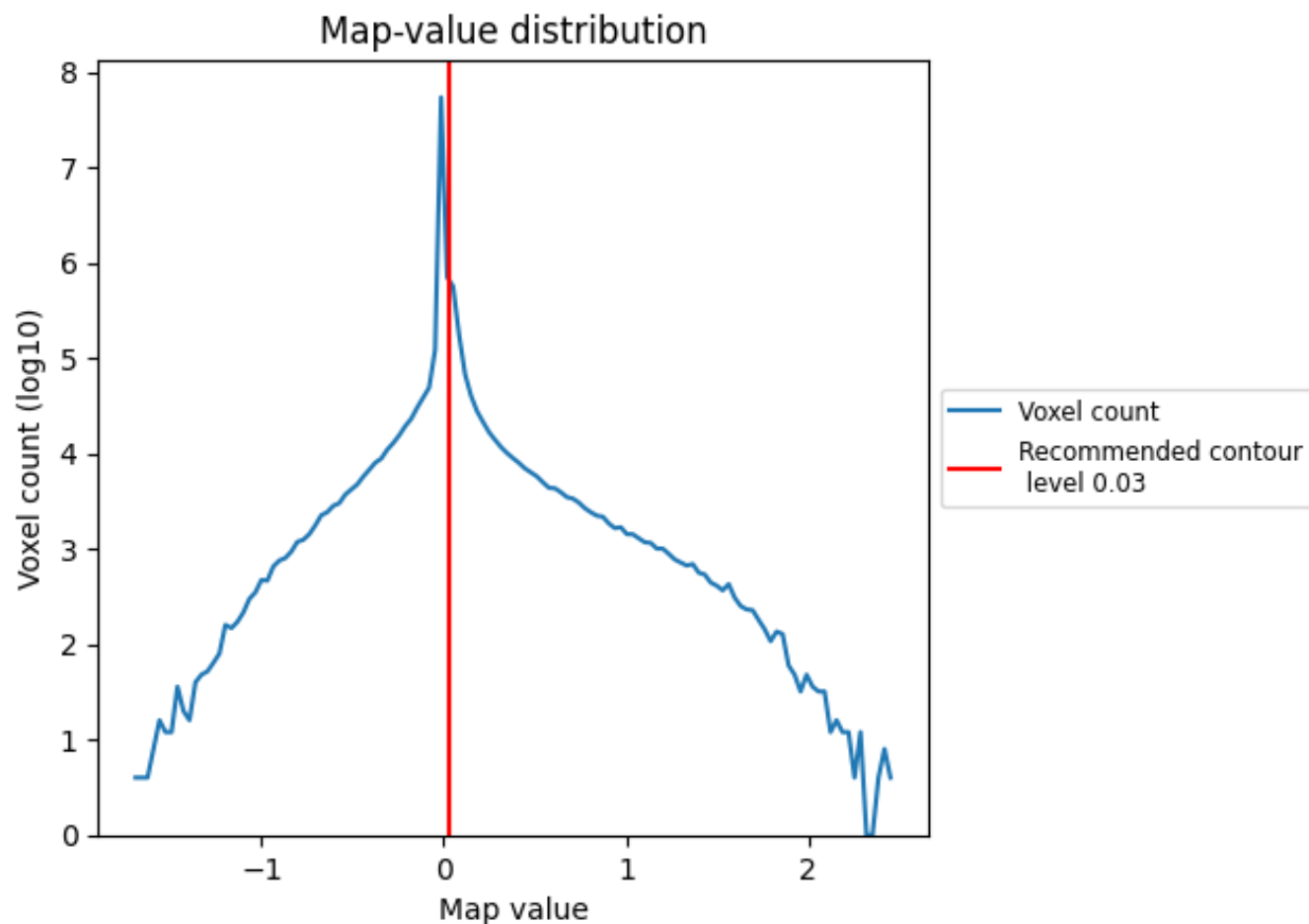
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

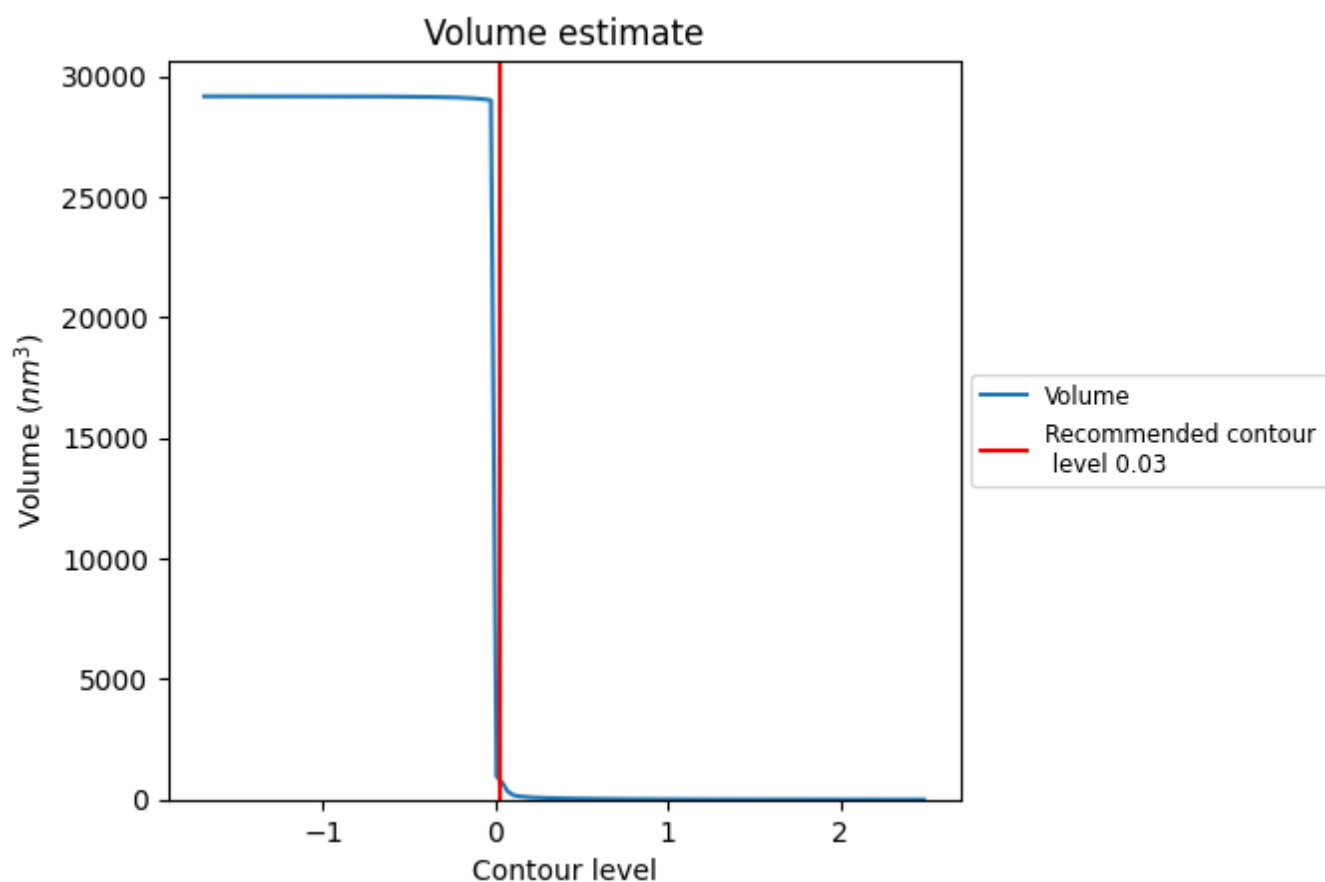
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

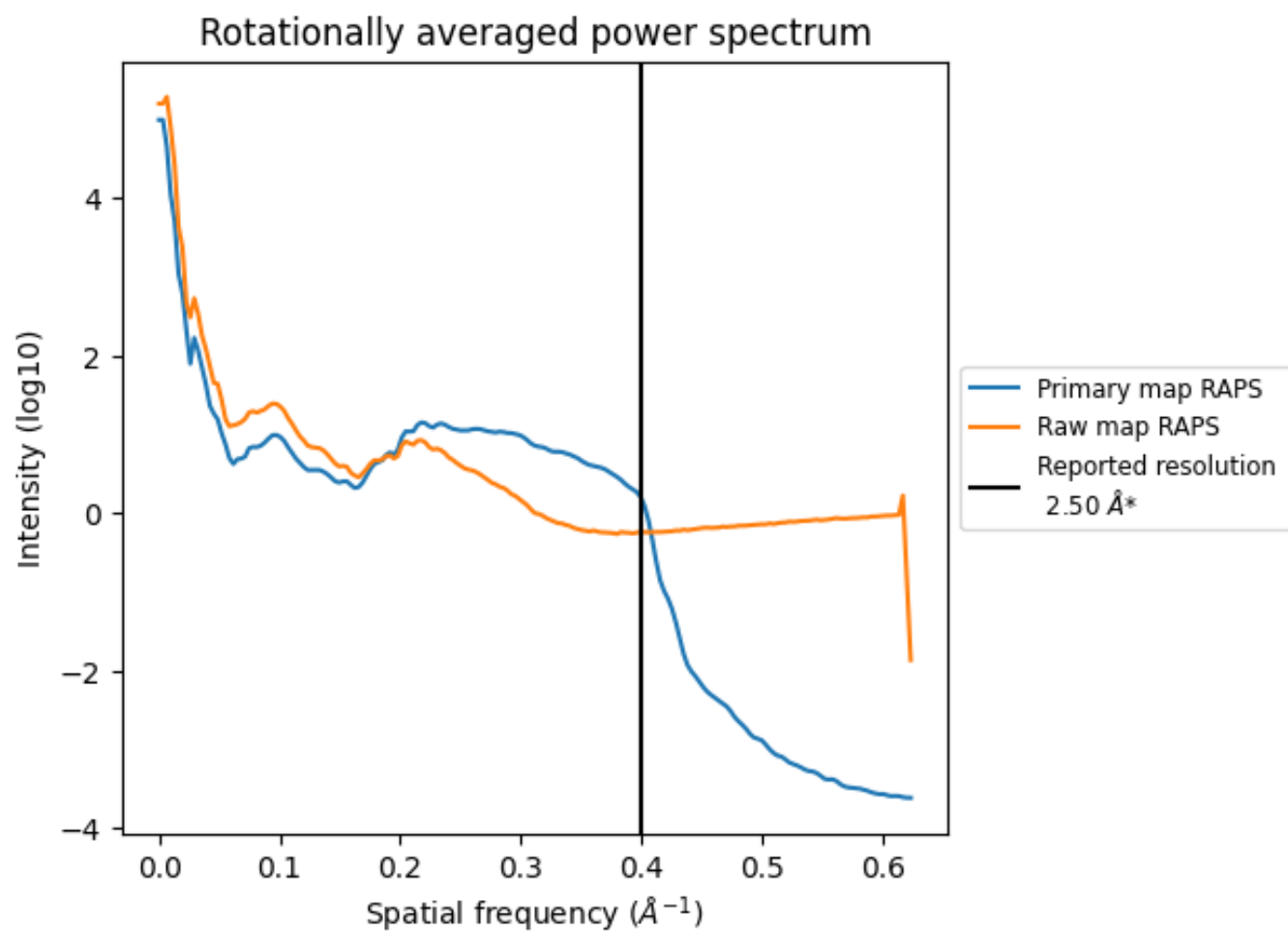
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 767 nm³; this corresponds to an approximate mass of 693 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 ⓘ

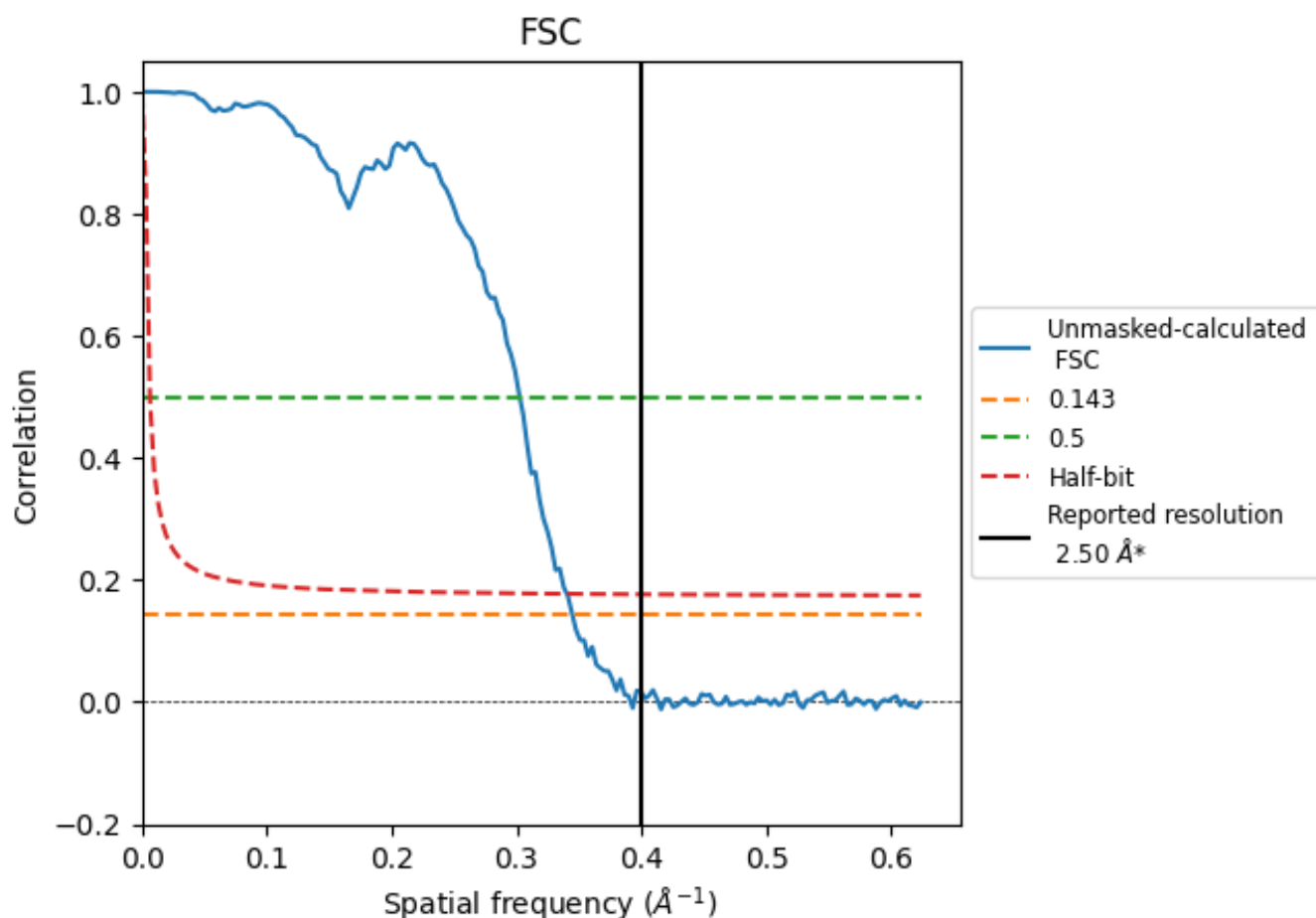


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.400 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

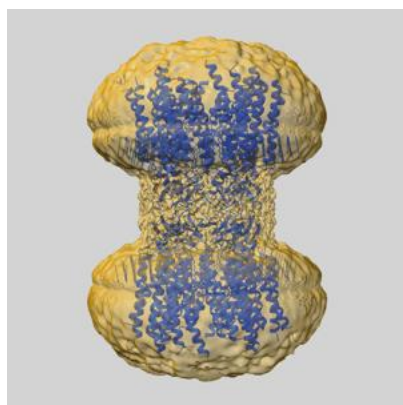
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.90	3.30	2.94

*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 2.90 differs from the reported value 2.5 by more than 10 %

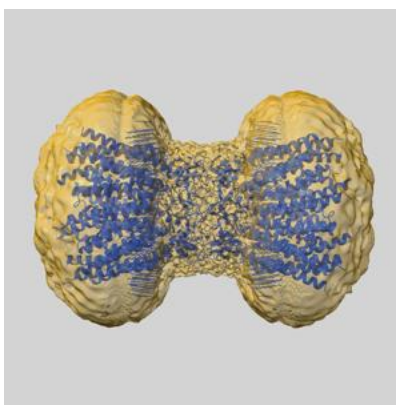
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73942 and PDB model 9Z9H. Per-residue inclusion information can be found in section [3](#) on page [15](#).

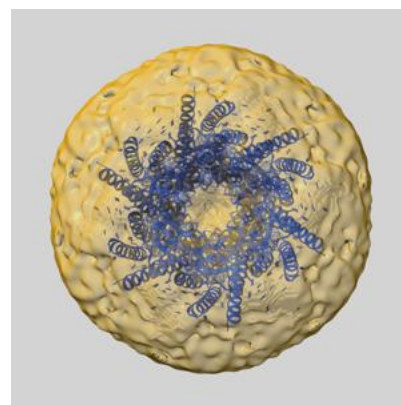
9.1 Map-model overlay [i](#)



X



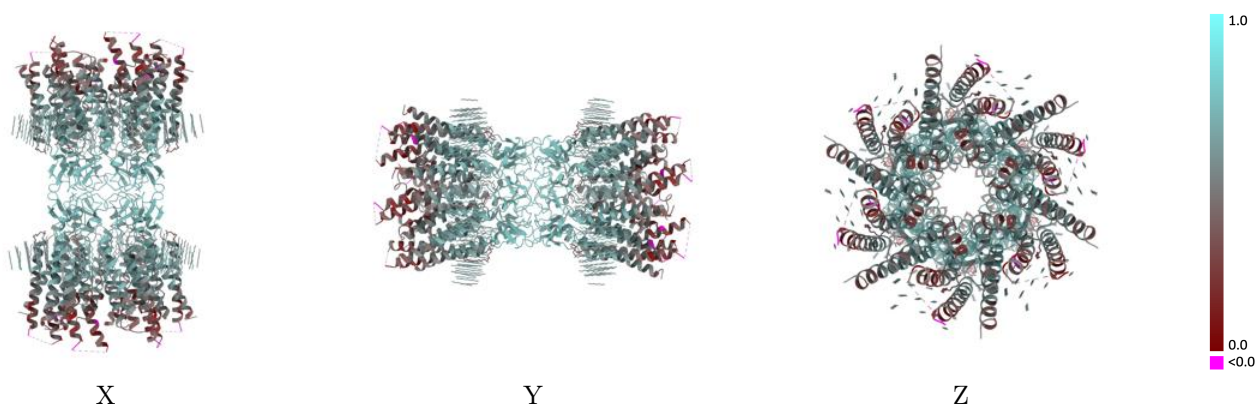
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

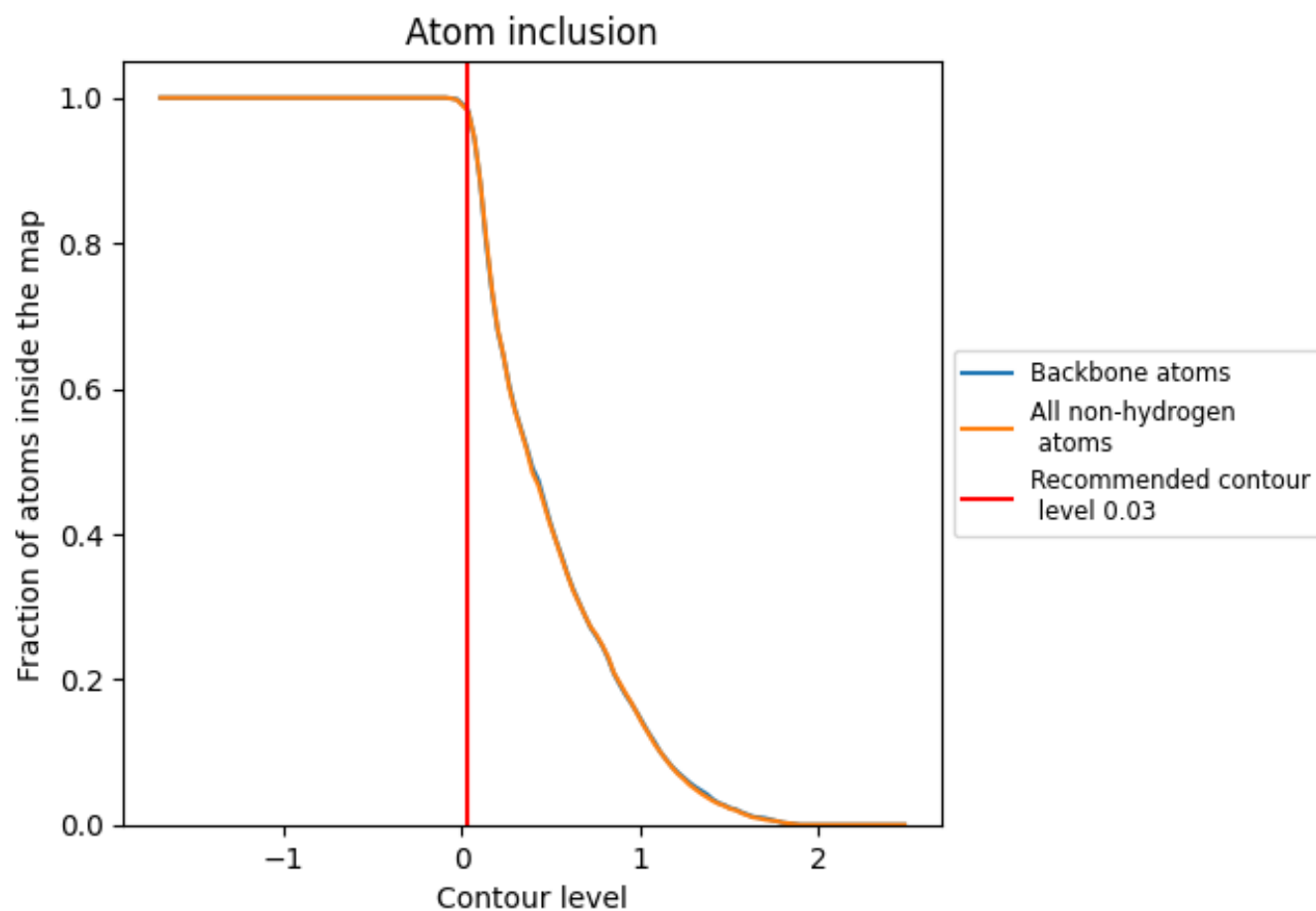


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9830	0.5490
A	0.9820	0.5500
B	0.9810	0.5510
C	0.9820	0.5490
D	0.9820	0.5490
E	0.9810	0.5500
F	0.9820	0.5500
G	0.9820	0.5490
H	0.9810	0.5500
I	0.9820	0.5490
J	0.9830	0.5500
K	0.9810	0.5490
L	0.9820	0.5470

1.0

0.0

<0.0