



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:25 AM UTC

PDB ID : 8T1E / pdb_00008t1e
EMDB ID : EMD-40961
Title : Closed-state cryo-EM structure of full-length human TRPV4 in the presence of 4a-PDD
Authors : Talyzina, I.A.; Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on : 2023-06-02
Resolution : 2.77 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:

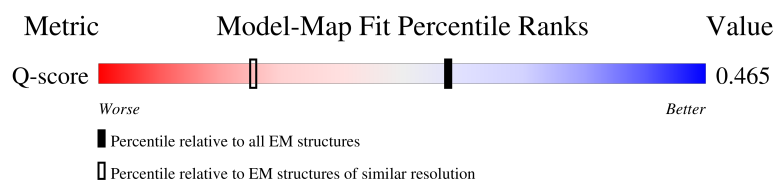
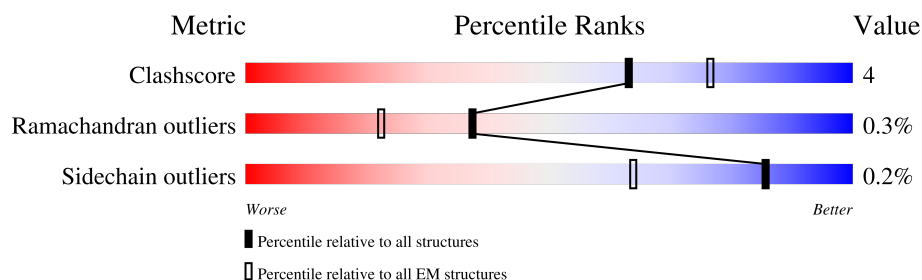
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.77 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	10695 (2.27 - 3.27)

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	1132	
1	B	1132	
1	C	1132	
1	D	1132	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22115 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 4, Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	629	Total	C	N	O	S	0	0
			5061	3296	838	900	27		
1	B	629	Total	C	N	O	S	0	0
			5061	3296	838	900	27		
1	C	629	Total	C	N	O	S	0	0
			5061	3296	838	900	27		
1	D	629	Total	C	N	O	S	0	0
			5061	3296	838	900	27		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	872	LEU	-	linker	UNP Q9HBA0
A	873	VAL	-	linker	UNP Q9HBA0
A	874	PRO	-	linker	UNP Q9HBA0
A	875	ARG	-	linker	UNP Q9HBA0
A	876	GLY	-	linker	UNP Q9HBA0
A	877	SER	-	linker	UNP Q9HBA0
A	878	ALA	-	linker	UNP Q9HBA0
A	879	ALA	-	linker	UNP Q9HBA0
A	880	ALA	-	linker	UNP Q9HBA0
A	881	ALA	-	linker	UNP Q9HBA0
A	1087	LYS	ALA	engineered mutation	UNP C5MKY7
A	1120	SER	-	expression tag	UNP C5MKY7
A	1121	GLY	-	expression tag	UNP C5MKY7
A	1122	LEU	-	expression tag	UNP C5MKY7
A	1123	ARG	-	expression tag	UNP C5MKY7
A	1124	SER	-	expression tag	UNP C5MKY7
A	1125	TRP	-	expression tag	UNP C5MKY7
A	1126	SER	-	expression tag	UNP C5MKY7
A	1127	HIS	-	expression tag	UNP C5MKY7
A	1128	PRO	-	expression tag	UNP C5MKY7
A	1129	GLN	-	expression tag	UNP C5MKY7

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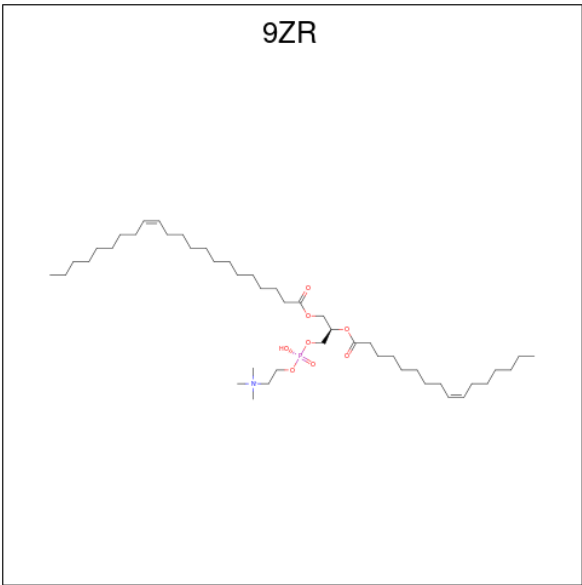
Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	PHE	-	expression tag	UNP C5MKY7
A	1131	GLU	-	expression tag	UNP C5MKY7
A	1132	LYS	-	expression tag	UNP C5MKY7
B	872	LEU	-	linker	UNP Q9HBA0
B	873	VAL	-	linker	UNP Q9HBA0
B	874	PRO	-	linker	UNP Q9HBA0
B	875	ARG	-	linker	UNP Q9HBA0
B	876	GLY	-	linker	UNP Q9HBA0
B	877	SER	-	linker	UNP Q9HBA0
B	878	ALA	-	linker	UNP Q9HBA0
B	879	ALA	-	linker	UNP Q9HBA0
B	880	ALA	-	linker	UNP Q9HBA0
B	881	ALA	-	linker	UNP Q9HBA0
B	1087	LYS	ALA	engineered mutation	UNP C5MKY7
B	1120	SER	-	expression tag	UNP C5MKY7
B	1121	GLY	-	expression tag	UNP C5MKY7
B	1122	LEU	-	expression tag	UNP C5MKY7
B	1123	ARG	-	expression tag	UNP C5MKY7
B	1124	SER	-	expression tag	UNP C5MKY7
B	1125	TRP	-	expression tag	UNP C5MKY7
B	1126	SER	-	expression tag	UNP C5MKY7
B	1127	HIS	-	expression tag	UNP C5MKY7
B	1128	PRO	-	expression tag	UNP C5MKY7
B	1129	GLN	-	expression tag	UNP C5MKY7
B	1130	PHE	-	expression tag	UNP C5MKY7
B	1131	GLU	-	expression tag	UNP C5MKY7
B	1132	LYS	-	expression tag	UNP C5MKY7
C	872	LEU	-	linker	UNP Q9HBA0
C	873	VAL	-	linker	UNP Q9HBA0
C	874	PRO	-	linker	UNP Q9HBA0
C	875	ARG	-	linker	UNP Q9HBA0
C	876	GLY	-	linker	UNP Q9HBA0
C	877	SER	-	linker	UNP Q9HBA0
C	878	ALA	-	linker	UNP Q9HBA0
C	879	ALA	-	linker	UNP Q9HBA0
C	880	ALA	-	linker	UNP Q9HBA0
C	881	ALA	-	linker	UNP Q9HBA0
C	1087	LYS	ALA	engineered mutation	UNP C5MKY7
C	1120	SER	-	expression tag	UNP C5MKY7
C	1121	GLY	-	expression tag	UNP C5MKY7
C	1122	LEU	-	expression tag	UNP C5MKY7
C	1123	ARG	-	expression tag	UNP C5MKY7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1124	SER	-	expression tag	UNP C5MKY7
C	1125	TRP	-	expression tag	UNP C5MKY7
C	1126	SER	-	expression tag	UNP C5MKY7
C	1127	HIS	-	expression tag	UNP C5MKY7
C	1128	PRO	-	expression tag	UNP C5MKY7
C	1129	GLN	-	expression tag	UNP C5MKY7
C	1130	PHE	-	expression tag	UNP C5MKY7
C	1131	GLU	-	expression tag	UNP C5MKY7
C	1132	LYS	-	expression tag	UNP C5MKY7
D	872	LEU	-	linker	UNP Q9HBA0
D	873	VAL	-	linker	UNP Q9HBA0
D	874	PRO	-	linker	UNP Q9HBA0
D	875	ARG	-	linker	UNP Q9HBA0
D	876	GLY	-	linker	UNP Q9HBA0
D	877	SER	-	linker	UNP Q9HBA0
D	878	ALA	-	linker	UNP Q9HBA0
D	879	ALA	-	linker	UNP Q9HBA0
D	880	ALA	-	linker	UNP Q9HBA0
D	881	ALA	-	linker	UNP Q9HBA0
D	1087	LYS	ALA	engineered mutation	UNP C5MKY7
D	1120	SER	-	expression tag	UNP C5MKY7
D	1121	GLY	-	expression tag	UNP C5MKY7
D	1122	LEU	-	expression tag	UNP C5MKY7
D	1123	ARG	-	expression tag	UNP C5MKY7
D	1124	SER	-	expression tag	UNP C5MKY7
D	1125	TRP	-	expression tag	UNP C5MKY7
D	1126	SER	-	expression tag	UNP C5MKY7
D	1127	HIS	-	expression tag	UNP C5MKY7
D	1128	PRO	-	expression tag	UNP C5MKY7
D	1129	GLN	-	expression tag	UNP C5MKY7
D	1130	PHE	-	expression tag	UNP C5MKY7
D	1131	GLU	-	expression tag	UNP C5MKY7
D	1132	LYS	-	expression tag	UNP C5MKY7

- Molecule 2 is [(2 {R})-2-[({Z})-hexadec-9-enoyl]oxy-3-[oxidanyl-[2-(trimethyl- $\text{l}^{\{4\}}$ -azanyl)ethoxy]phosphoryl]oxy-propyl] ({Z})-docos-13-enoate (CCD ID: 9ZR) (formula: $\text{C}_{46}\text{H}_{89}\text{NO}_8\text{P}$).



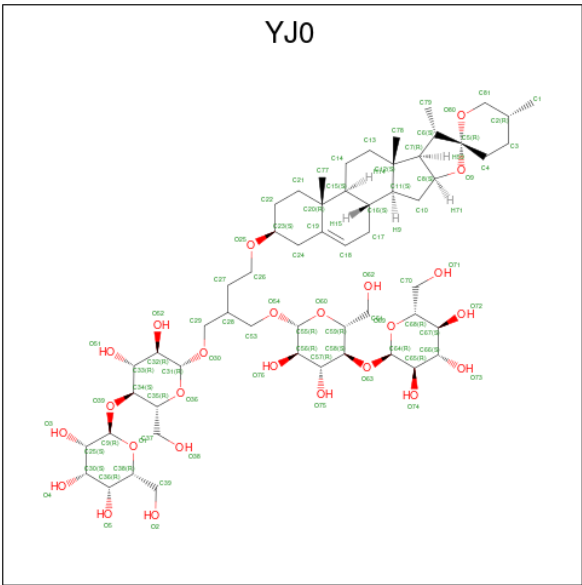
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	A	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	A	1	Total	C				0
			13	13				
2	A	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	A	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	A	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	A	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	B	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	B	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	B	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	B	1	Total	C				0
			13	13				
2	B	1	Total	C	N	O	P	0
			56	46	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	B	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	C	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	C	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	C	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	C	1	Total	C				0
			13	13				
2	C	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	C	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	C	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	D	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	D	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	D	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	D	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	D	1	Total	C				0
			13	13				
2	D	1	Total	C	N	O	P	0
			56	46	1	8	1	
2	D	1	Total	C	N	O	P	0
			56	46	1	8	1	

- Molecule 3 is (2R)-2-[[[(4-O-hexopyranosyl-beta-D-glucopyranosyl)oxy]methyl]-4-[[[(25R)-5 beta,14beta,17beta-spirostan-3beta-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: YJ0) (formula: C₅₆H₉₂O₂₅).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	32	3	
3	A	1	Total	C	O	0
			30	27	3	
3	B	1	Total	C	O	0
			30	27	3	
3	B	1	Total	C	O	0
			35	32	3	
3	C	1	Total	C	O	0
			30	27	3	
3	C	1	Total	C	O	0
			35	32	3	
3	D	1	Total	C	O	0
			30	27	3	
3	D	1	Total	C	O	0
			35	32	3	

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

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

- Molecule 5 is water.

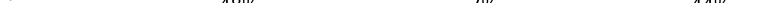
Mol	Chain	Residues	Atoms		AltConf
5	A	9	Total 9	O 9	0
5	B	9	Total 9	O 9	0
5	C	9	Total 9	O 9	0
5	D	9	Total 9	O 9	0

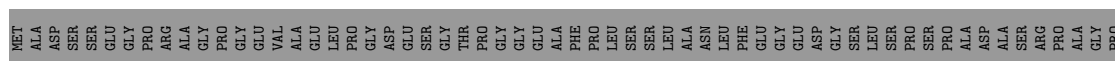
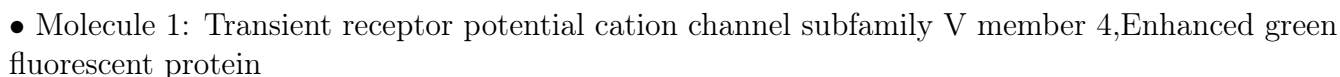
SER	THR	GLN	SER	LYS	SER	LYS	ASP	PRO	ASN	GLU	LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	LEU	LEU	GLY	MET	ASP	GLU	LEU	TYR	LYS	SER	GLY	LEU	ARG	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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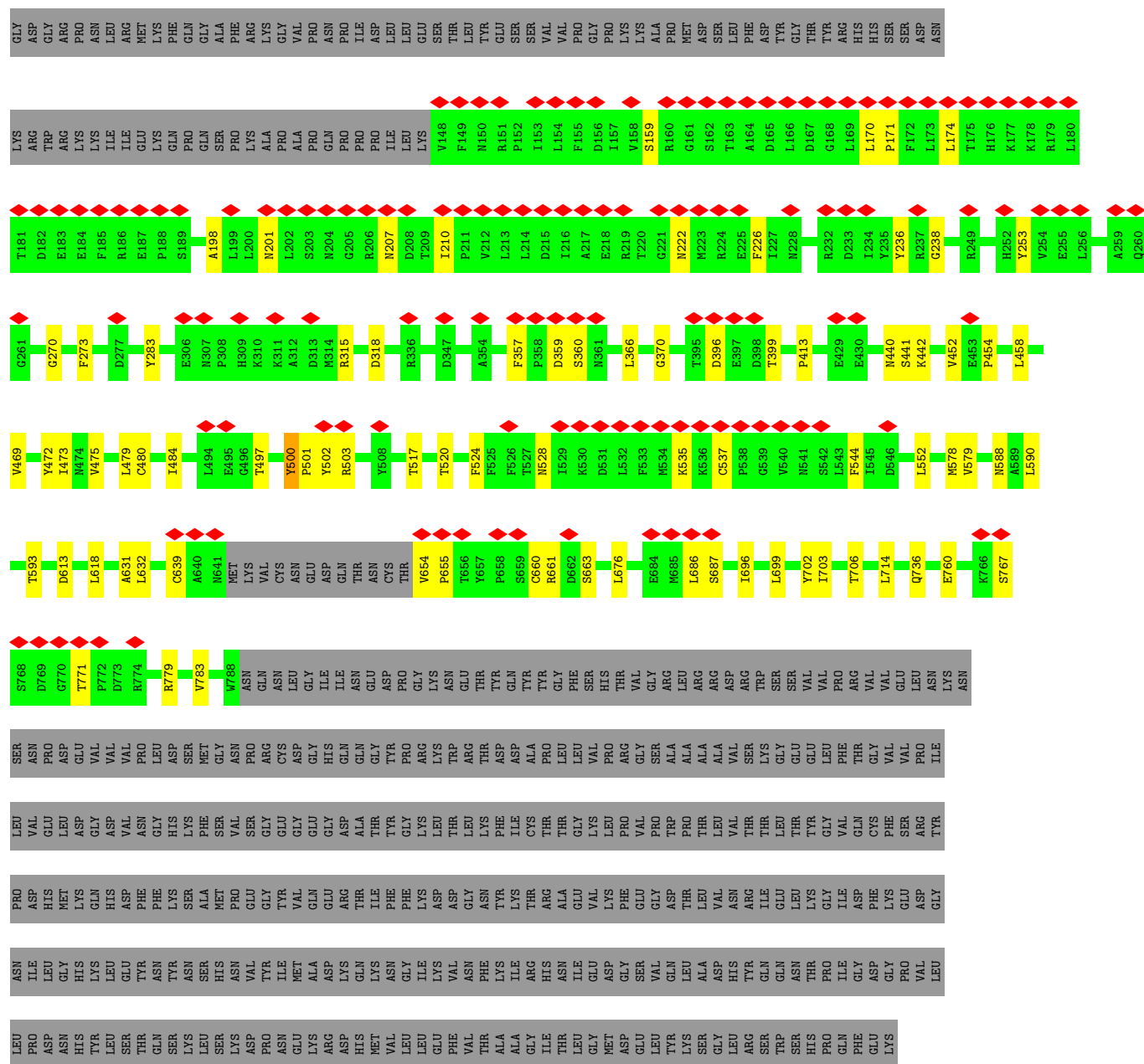
- Molecule 1: Transient receptor potential cation channel subfamily V member 4,Enhanced green fluorescent protein

[illegible]

ASP	ASN	HIS	TYR	LEU	THR	GLN	SER	GLY	PRO	G770	D613	V452	Q260	T181	LYS
ASN	HIS	GLY	LEU	ASN	THR	ASN	LEU	GLY	ASP	T771	L618	E453	G261	D182	ARG
HIS	TYR	GLY	LEU	GLY	VAL	GLY	ASP	GLY	VAL	P772	A631	V469	G270	E183	ARG
LEU	SER	ASP	GLY	ASN	VAL	ASN	VAL	VAL	VAL	R773	L632		F273	E184	LYS
THR	THR	PHE	TYR	ASN	PRO	LEU	LEU	PRO	PRO	R774		Y472		F185	ILE
GLN	ASN	PHE	ASN	GLY	LEU	GLY	GLY	GLY	GLY	R779	C639	I473	D277	R186	GLY
SER	SER	LYS	TYR	HIS	ASP	LYS	LYS	SER	ASP	V783	A640	N474		E187	LYS
LEU	LEU	ALA	LEU	PHE	MET	ASN	ASN	MET	MET	V788	A640	N475	Y283	P188	GLN
SER	SER	MET	HIS	SER	GLY	SER	GLY	GLY	GLY	V788	N641			S189	PRO
ASN	ASN	PRO	ASN	VAL	ASN	VAL	ASN	ASN	ASN		MET	L479	E506	A198	GLN
ASP	ASP	GLY	PRO	SER	PRO	PRO	PRO	PRO	PRO		LYS	C480	N307	L199	SER
PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		VAL	I484	P308	L199	PRO
ASN	ASN	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY		CYS		L200	L200	LYS
ILE	ILE	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY		ASN		H309	N201	ALA
LYS	LYS	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY		ASN	L494	K310	L202	PRO
ALA	ALA	GLN	ALA	GLY	GLY	GLY	GLY	GLY	GLY		ASP	E495	K311	L202	ALA
ARG	ARG	HIS	ASP	GLY	GLY	GLY	GLY	GLY	GLY		ASP	G496	A312	S203	PRO
ASP	ASP	ARG	ASP	ASP	ASP	ASP	ASP	ASP	ASP		THR	T497	D313	N204	GLN
HIS	HIS	THR	GLN	ALA	GLY	GLY	GLY	GLY	GLY		ASN		M314	G205	PRO
MET	MET	ILE	LYS	THR	THR	THR	THR	THR	THR		ASN	Y500	R315	R206	PRO
VAL	VAL	PHE	ASN	GLY	GLY	GLY	GLY	GLY	GLY		CYS			R206	PRO
LEU	LEU	PHE	LEU	GLY	GLY	GLY	GLY	GLY	GLY		THR	Y501	D318	N207	ILE
LEU	LEU	ILE	LYS	LYS	LYS	LYS	LYS	LYS	LYS		THR	Y502		N207	ILE
GLY	GLY	ASP	LYS	LYS	LYS	LYS	LYS	LYS	LYS		THR	R503	R336	D208	LEU
PHE	PHE	ASP	VAL	VAL	VAL	VAL	VAL	VAL	VAL		THR	Y508		T209	LYS
VAL	VAL	GLY	THR	THR	THR	THR	THR	THR	THR		THR		D347	V211	LYS
VAL	VAL	GLY	THR	THR	THR	THR	THR	THR	THR		THR	T517		V212	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	T520	A354	L213	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR		F357	L214	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	F524	D215	L214	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	F525	P359	I153	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	F526	I216	L154	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	F527	A217	F155	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	T527	S360	D156	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	N528	N361	I157	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	I529		R219	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	K530	L366	T220	LYS
THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR		THR	D531		G221	LY

- Chain C: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75146	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.497	Depositor
Minimum map value	-0.329	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.065	Depositor
Map size ($\text{\AA}$)	252.416, 252.416, 252.416	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.7888, 0.7888, 0.7888	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: NA, 9ZR, YJ0

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	0.41	0/5181	0.65	1/7027 (0.0%)
1	B	0.41	0/5181	0.65	1/7027 (0.0%)
1	C	0.41	0/5181	0.65	1/7027 (0.0%)
1	D	0.41	0/5181	0.65	1/7027 (0.0%)
All	All	0.41	0/20724	0.65	4/28108 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	663	SER	N-CA-CB	-5.50	107.90	114.17
1	B	663	SER	N-CA-CB	-5.49	107.91	114.17
1	A	663	SER	N-CA-CB	-5.47	107.94	114.17
1	C	663	SER	N-CA-CB	-5.47	107.94	114.17

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	452	VAL	Peptide
1	A	497	THR	Peptide
1	A	500	TYR	Peptide
1	A	537	CYS	Peptide
1	B	452	VAL	Peptide
1	B	497	THR	Peptide
1	B	500	TYR	Peptide
1	B	537	CYS	Peptide
1	C	452	VAL	Peptide
1	C	497	THR	Peptide
1	C	500	TYR	Peptide
1	C	537	CYS	Peptide
1	D	452	VAL	Peptide
1	D	497	THR	Peptide
1	D	500	TYR	Peptide
1	D	537	CYS	Peptide

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	5061	0	5128	45	0
1	B	5061	0	5128	46	0
1	C	5061	0	5128	46	0
1	D	5061	0	5128	44	0
2	A	393	0	0	0	0
2	B	393	0	0	0	0
2	C	393	0	0	0	0
2	D	393	0	0	0	0
3	A	65	0	0	4	0
3	B	65	0	0	3	0
3	C	65	0	0	3	0
3	D	65	0	0	3	0
4	A	3	0	0	0	0
5	A	9	0	0	4	0
5	B	9	0	0	4	0
5	C	9	0	0	4	0
5	D	9	0	0	4	0
All	All	22115	0	20512	179	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 (179) 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:660:CYS:SG	1:A:661:ARG:N	2.56	0.79
1:C:660:CYS:SG	1:C:661:ARG:N	2.56	0.78
1:B:660:CYS:SG	1:B:661:ARG:N	2.56	0.78
1:D:660:CYS:SG	1:D:661:ARG:N	2.56	0.77
1:B:315:ARG:NH2	5:B:1302:HOH:O	2.19	0.75
1:A:315:ARG:NH2	5:A:1302:HOH:O	2.19	0.75
1:D:315:ARG:NH2	5:D:1302:HOH:O	2.19	0.75
1:C:315:ARG:NH2	5:C:1302:HOH:O	2.19	0.74
1:C:222:ASN:O	1:C:226:PHE:N	2.21	0.73
1:A:222:ASN:O	1:A:226:PHE:N	2.21	0.73
1:B:222:ASN:O	1:B:226:PHE:N	2.21	0.73
1:B:360:SER:O	5:B:1302:HOH:O	2.07	0.73
1:A:360:SER:O	5:A:1302:HOH:O	2.07	0.73
1:D:613:ASP:O	5:D:1301:HOH:O	2.06	0.73
1:D:222:ASN:O	1:D:226:PHE:N	2.21	0.72
1:A:613:ASP:O	5:A:1301:HOH:O	2.07	0.72
1:C:613:ASP:O	5:C:1301:HOH:O	2.06	0.71
1:B:613:ASP:O	5:B:1301:HOH:O	2.06	0.71
1:D:360:SER:O	5:D:1302:HOH:O	2.07	0.71
1:A:578:MET:SD	5:A:1307:HOH:O	2.49	0.70
1:B:578:MET:SD	5:B:1307:HOH:O	2.50	0.70
1:B:760:GLU:OE2	1:B:779:ARG:NH1	2.25	0.70
1:C:360:SER:O	5:C:1302:HOH:O	2.07	0.70
1:D:760:GLU:OE2	1:D:779:ARG:NH1	2.25	0.70
1:A:760:GLU:OE2	1:A:779:ARG:NH1	2.25	0.69
1:C:760:GLU:OE2	1:C:779:ARG:NH1	2.25	0.69
1:D:578:MET:SD	5:D:1307:HOH:O	2.50	0.69
1:D:702:TYR:O	1:D:706:THR:OG1	2.07	0.69
1:C:578:MET:SD	5:C:1307:HOH:O	2.50	0.69
1:B:702:TYR:O	1:B:706:THR:OG1	2.07	0.67
1:B:579:VAL:HG13	1:C:631:ALA:HB1	1.78	0.65
1:A:702:TYR:O	1:A:706:THR:OG1	2.07	0.65
1:C:579:VAL:HG13	1:D:631:ALA:HB1	1.78	0.64
1:A:631:ALA:HB1	1:D:579:VAL:HG13	1.79	0.63
1:C:702:TYR:O	1:C:706:THR:OG1	2.07	0.62
1:A:170:LEU:HB3	1:A:171:PRO:HD3	1.83	0.61
1:D:170:LEU:HB3	1:D:171:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HB3	1:C:171:PRO:HD3	1.83	0.60
1:B:170:LEU:HB3	1:B:171:PRO:HD3	1.82	0.60
1:A:579:VAL:HG13	1:B:631:ALA:HB1	1.84	0.59
1:C:440:ASN:OD1	1:C:535:LYS:NZ	2.36	0.59
1:B:440:ASN:OD1	1:B:535:LYS:NZ	2.36	0.58
1:A:207:ASN:O	1:A:253:TYR:OH	2.21	0.58
1:A:440:ASN:OD1	1:A:535:LYS:NZ	2.36	0.58
1:C:207:ASN:O	1:C:253:TYR:OH	2.21	0.58
1:D:440:ASN:OD1	1:D:535:LYS:NZ	2.36	0.58
1:D:357:PHE:O	1:D:359:ASP:N	2.38	0.57
1:B:357:PHE:O	1:B:359:ASP:N	2.38	0.57
1:D:207:ASN:O	1:D:253:TYR:OH	2.21	0.56
1:C:357:PHE:O	1:C:359:ASP:N	2.38	0.56
1:A:357:PHE:O	1:A:359:ASP:N	2.38	0.56
1:A:396:ASP:OD1	1:A:399:THR:OG1	2.23	0.56
1:B:396:ASP:OD1	1:B:399:THR:OG1	2.23	0.56
1:B:207:ASN:O	1:B:253:TYR:OH	2.21	0.56
1:D:270:GLY:O	1:D:273:PHE:N	2.39	0.55
1:B:159:SER:O	1:B:201:ASN:ND2	2.40	0.55
1:D:396:ASP:OD1	1:D:399:THR:OG1	2.23	0.55
1:B:270:GLY:O	1:B:273:PHE:N	2.39	0.55
1:C:270:GLY:O	1:C:273:PHE:N	2.39	0.55
1:A:270:GLY:O	1:A:273:PHE:N	2.39	0.54
1:D:159:SER:O	1:D:201:ASN:ND2	2.40	0.54
1:C:159:SER:O	1:C:201:ASN:ND2	2.40	0.54
1:D:413:PRO:O	1:D:783:VAL:HG13	2.08	0.54
1:A:159:SER:O	1:A:201:ASN:ND2	2.40	0.54
1:A:413:PRO:O	1:A:783:VAL:HG13	2.08	0.54
1:B:413:PRO:O	1:B:783:VAL:HG13	2.08	0.53
1:C:396:ASP:OD1	1:C:399:THR:OG1	2.23	0.53
1:C:413:PRO:O	1:C:783:VAL:HG13	2.08	0.53
1:D:159:SER:OG	1:D:201:ASN:ND2	2.43	0.51
1:D:283:TYR:OH	1:D:318:ASP:OD2	2.25	0.51
1:A:441:SER:OG	1:A:442:LYS:N	2.44	0.50
1:B:441:SER:OG	1:B:442:LYS:N	2.45	0.50
1:C:472:TYR:HA	1:C:475:VAL:HG12	1.93	0.50
1:D:441:SER:OG	1:D:442:LYS:N	2.45	0.50
1:C:159:SER:OG	1:C:201:ASN:ND2	2.43	0.50
1:D:472:TYR:HA	1:D:475:VAL:HG12	1.93	0.50
1:B:472:TYR:HA	1:B:475:VAL:HG12	1.93	0.50
1:A:472:TYR:HA	1:A:475:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:LEU:O	1:B:690:LYS:NZ	2.33	0.49
1:B:159:SER:OG	1:B:201:ASN:ND2	2.43	0.49
1:A:159:SER:OG	1:A:201:ASN:ND2	2.43	0.49
1:C:441:SER:OG	1:C:442:LYS:N	2.44	0.49
1:B:517:THR:O	1:B:520:THR:OG1	2.30	0.48
1:C:500:TYR:O	1:C:502:TYR:N	2.47	0.48
1:A:500:TYR:O	1:A:502:TYR:N	2.47	0.48
1:C:283:TYR:OH	1:C:318:ASP:OD2	2.25	0.48
1:B:500:TYR:O	1:B:502:TYR:N	2.47	0.48
1:D:500:TYR:O	1:D:502:TYR:N	2.46	0.48
1:D:639:CYS:N	1:D:660:CYS:SG	2.87	0.48
1:C:475:VAL:HG22	1:C:479:LEU:HD23	1.96	0.48
1:A:639:CYS:N	1:A:660:CYS:SG	2.87	0.48
1:B:639:CYS:N	1:B:660:CYS:SG	2.87	0.48
1:A:696:ILE:HG21	3:A:1210:YJ0:C18	2.44	0.48
1:B:475:VAL:HG22	1:B:479:LEU:HD23	1.96	0.47
1:B:198:ALA:HB1	1:B:210:ILE:HD11	1.96	0.47
1:C:198:ALA:HB1	1:C:210:ILE:HD11	1.96	0.47
1:C:639:CYS:N	1:C:660:CYS:SG	2.87	0.47
3:B:1209:YJ0:C81	3:B:1209:YJ0:C79	2.93	0.47
1:C:170:LEU:O	1:C:174:LEU:HD23	2.14	0.47
1:D:475:VAL:HG22	1:D:479:LEU:HD23	1.96	0.47
1:A:475:VAL:HG22	1:A:479:LEU:HD23	1.96	0.47
1:A:693:VAL:HG22	3:A:1210:YJ0:C23	2.44	0.47
1:C:439:TYR:OH	1:C:743:ASP:OD1	2.28	0.47
1:D:170:LEU:O	1:D:174:LEU:HD23	2.14	0.47
1:A:198:ALA:HB1	1:A:210:ILE:HD11	1.96	0.47
3:C:1209:YJ0:C79	3:C:1209:YJ0:C81	2.93	0.47
3:D:1210:YJ0:C81	3:D:1210:YJ0:C79	2.93	0.47
1:A:170:LEU:O	1:A:174:LEU:HD23	2.14	0.46
1:B:170:LEU:O	1:B:174:LEU:HD23	2.15	0.46
1:D:198:ALA:HB1	1:D:210:ILE:HD11	1.96	0.46
3:A:1207:YJ0:C79	3:A:1207:YJ0:C81	2.93	0.46
1:C:517:THR:O	1:C:520:THR:OG1	2.31	0.46
1:A:480:CYS:O	1:A:484:ILE:HD12	2.17	0.45
3:A:1210:YJ0:C1	1:D:618:LEU:HD23	2.47	0.45
1:D:480:CYS:O	1:D:484:ILE:HD12	2.17	0.45
1:A:283:TYR:OH	1:A:318:ASP:OD2	2.25	0.45
1:A:618:LEU:HD23	3:B:1202:YJ0:C1	2.47	0.45
1:C:480:CYS:O	1:C:484:ILE:HD12	2.16	0.45
1:D:517:THR:O	1:D:520:THR:OG1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:CYS:O	1:B:484:ILE:HD12	2.17	0.44
1:B:618:LEU:HD23	3:C:1202:YJ0:C1	2.47	0.44
1:A:228:ASN:O	1:A:229:SER:OG	2.32	0.44
1:B:366:LEU:HD22	1:B:370:GLY:O	2.18	0.44
1:A:517:THR:O	1:A:520:THR:OG1	2.30	0.44
1:C:696:ILE:HG21	3:C:1202:YJ0:C18	2.48	0.44
1:C:618:LEU:HD23	3:D:1203:YJ0:C1	2.47	0.44
1:A:366:LEU:HD22	1:A:370:GLY:O	2.18	0.44
1:B:767:SER:N	1:B:771:THR:O	2.50	0.44
1:A:767:SER:N	1:A:771:THR:O	2.50	0.44
1:C:366:LEU:HD22	1:C:370:GLY:O	2.18	0.44
1:D:696:ILE:HG21	3:D:1203:YJ0:C18	2.48	0.44
1:C:392:ARG:NH2	1:C:402:LEU:O	2.50	0.43
1:D:366:LEU:HD22	1:D:370:GLY:O	2.18	0.43
1:A:469:VAL:O	1:A:473:ILE:HD12	2.19	0.43
1:C:469:VAL:O	1:C:473:ILE:HD12	2.19	0.43
1:C:632:LEU:HD21	1:C:699:LEU:CD1	2.49	0.43
1:D:469:VAL:O	1:D:473:ILE:HD12	2.19	0.43
1:D:632:LEU:HD21	1:D:699:LEU:CD1	2.49	0.43
1:B:469:VAL:O	1:B:473:ILE:HD12	2.19	0.43
1:D:767:SER:N	1:D:771:THR:O	2.50	0.43
1:A:632:LEU:HD21	1:A:699:LEU:CD1	2.49	0.42
1:B:632:LEU:HD21	1:B:699:LEU:CD1	2.49	0.42
1:A:524:PHE:O	1:A:528:ASN:ND2	2.53	0.42
1:B:524:PHE:O	1:B:528:ASN:ND2	2.53	0.42
1:B:236:TYR:O	1:B:238:GLY:N	2.52	0.42
1:D:524:PHE:O	1:D:528:ASN:ND2	2.53	0.42
1:A:686:LEU:O	1:A:687:SER:OG	2.31	0.42
1:B:494:LEU:O	1:C:690:LYS:NZ	2.37	0.42
1:C:524:PHE:O	1:C:528:ASN:ND2	2.53	0.42
1:C:552:LEU:HB3	1:C:588:ASN:HD21	1.85	0.42
1:D:654:VAL:HG23	1:D:655:PRO:HD3	2.02	0.42
1:A:654:VAL:HG23	1:A:655:PRO:HD3	2.02	0.42
1:B:228:ASN:O	1:B:229:SER:OG	2.32	0.42
1:C:436:ILE:O	1:C:440:ASN:N	2.51	0.42
1:D:236:TYR:O	1:D:238:GLY:N	2.52	0.42
1:B:654:VAL:HG23	1:B:655:PRO:HD3	2.02	0.42
1:C:767:SER:N	1:C:771:THR:O	2.50	0.42
1:D:686:LEU:O	1:D:687:SER:OG	2.31	0.42
1:B:552:LEU:HB3	1:B:588:ASN:HD21	1.85	0.42
1:D:552:LEU:HB3	1:D:588:ASN:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:TYR:OH	1:B:318:ASP:OD2	2.25	0.41
1:A:676:LEU:HD21	1:A:703:ILE:HG12	2.03	0.41
1:B:436:ILE:O	1:B:440:ASN:N	2.51	0.41
1:B:696:ILE:HG21	3:B:1202:YJ0:C18	2.51	0.41
1:D:590:LEU:O	1:D:593:THR:OG1	2.35	0.41
1:B:676:LEU:HD21	1:B:703:ILE:HG12	2.03	0.41
1:C:676:LEU:HD21	1:C:703:ILE:HG12	2.03	0.41
1:A:151:ARG:HB3	1:A:152:PRO:HD3	2.03	0.41
1:A:454:PRO:O	1:A:458:LEU:N	2.52	0.41
1:C:654:VAL:HG23	1:C:655:PRO:HD3	2.02	0.41
1:D:676:LEU:HD21	1:D:703:ILE:HG12	2.03	0.41
1:C:151:ARG:HB3	1:C:152:PRO:HD3	2.02	0.41
1:D:544:PHE:O	1:D:736:GLN:NE2	2.45	0.41
1:B:151:ARG:HB3	1:B:152:PRO:HD3	2.03	0.40
1:C:236:TYR:O	1:C:238:GLY:N	2.52	0.40
1:D:454:PRO:O	1:D:458:LEU:N	2.52	0.40
1:B:392:ARG:NH2	1:B:402:LEU:O	2.50	0.40
1:A:552:LEU:HB3	1:A:588:ASN:HD21	1.85	0.40
1:C:228:ASN:O	1:C:229:SER:OG	2.32	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	625/1132 (55%)	545 (87%)	78 (12%)	2 (0%)	36	63
1	B	625/1132 (55%)	545 (87%)	78 (12%)	2 (0%)	36	63
1	C	625/1132 (55%)	545 (87%)	78 (12%)	2 (0%)	36	63
1	D	625/1132 (55%)	545 (87%)	78 (12%)	2 (0%)	36	63
All	All	2500/4528 (55%)	2180 (87%)	312 (12%)	8 (0%)	37	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	PRO
1	B	501	PRO
1	C	501	PRO
1	D	501	PRO
1	A	503	ARG
1	B	503	ARG
1	C	503	ARG
1	D	503	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/987 (56%)	554 (100%)	1 (0%)	87	96
1	B	555/987 (56%)	554 (100%)	1 (0%)	87	96
1	C	555/987 (56%)	554 (100%)	1 (0%)	87	96
1	D	555/987 (56%)	554 (100%)	1 (0%)	87	96
All	All	2220/3948 (56%)	2216 (100%)	4 (0%)	85	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	714	LEU
1	B	714	LEU
1	C	714	LEU
1	D	714	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	299	HIS
1	A	528	ASN

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Mol	Chain	Res	Type
1	B	201	ASN
1	B	274	GLN
1	B	528	ASN
1	C	201	ASN
1	C	204	ASN
1	C	528	ASN
1	D	201	ASN
1	D	204	ASN
1	D	299	HIS
1	D	528	ASN

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](#)

Of 43 ligands modelled in this entry, 3 are monoatomic - leaving 40 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	9ZR	D	1207	-	12,12,55	0.18	0	11,11,63	0.11	0
2	9ZR	A	1205	-	55,55,55	0.31	0	61,63,63	0.43	0
2	9ZR	C	1207	-	55,55,55	0.31	0	61,63,63	0.43	0
2	9ZR	D	1204	-	55,55,55	0.29	0	61,63,63	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9ZR	C	1201	-	55,55,55	0.31	0	61,63,63	0.92	5 (8%)
2	9ZR	A	1203	-	43,43,55	0.31	0	49,51,63	0.35	0
3	YJ0	B	1209	-	40,40,90	0.34	0	63,64,138	0.64	1 (1%)
2	9ZR	A	1209	-	55,55,55	0.31	0	61,63,63	0.92	5 (8%)
2	9ZR	C	1205	-	43,43,55	0.31	0	49,51,63	0.35	0
2	9ZR	D	1206	-	43,43,55	0.32	0	49,51,63	0.35	0
2	9ZR	B	1208	-	55,55,55	0.30	0	61,63,63	0.30	0
2	9ZR	D	1202	-	55,55,55	0.31	0	61,63,63	0.92	5 (8%)
2	9ZR	B	1207	-	55,55,55	0.31	0	61,63,63	0.43	0
2	9ZR	D	1205	-	55,55,55	0.30	0	61,63,63	0.37	0
3	YJ0	D	1210	-	40,40,90	0.33	0	63,64,138	0.64	1 (1%)
2	9ZR	B	1205	-	43,43,55	0.32	0	49,51,63	0.35	0
3	YJ0	D	1203	-	35,35,90	0.41	0	58,58,138	0.63	0
2	9ZR	C	1203	-	55,55,55	0.29	0	61,63,63	0.34	0
3	YJ0	A	1207	-	40,40,90	0.33	0	63,64,138	0.64	1 (1%)
3	YJ0	B	1202	-	35,35,90	0.42	0	58,58,138	0.63	0
3	YJ0	C	1202	-	35,35,90	0.41	0	58,58,138	0.63	0
3	YJ0	C	1209	-	40,40,90	0.34	0	63,64,138	0.64	1 (1%)
2	9ZR	A	1204	-	12,12,55	0.18	0	11,11,63	0.12	0
2	9ZR	C	1208	-	55,55,55	0.30	0	61,63,63	0.30	0
2	9ZR	C	1210	-	55,55,55	0.32	0	61,63,63	0.48	1 (1%)
2	9ZR	C	1204	-	55,55,55	0.29	0	61,63,63	0.37	0
2	9ZR	A	1208	-	55,55,55	0.32	0	61,63,63	0.48	1 (1%)
2	9ZR	D	1209	-	55,55,55	0.30	0	61,63,63	0.30	0
2	9ZR	B	1203	-	55,55,55	0.29	0	61,63,63	0.34	0
2	9ZR	D	1208	-	55,55,55	0.31	0	61,63,63	0.43	0
2	9ZR	C	1206	-	12,12,55	0.18	0	11,11,63	0.12	0
2	9ZR	D	1201	-	55,55,55	0.32	0	61,63,63	0.48	1 (1%)
2	9ZR	B	1201	-	55,55,55	0.31	0	61,63,63	0.91	5 (8%)
2	9ZR	A	1206	-	55,55,55	0.30	0	61,63,63	0.30	0
2	9ZR	B	1204	-	55,55,55	0.30	0	61,63,63	0.37	0
2	9ZR	B	1210	-	55,55,55	0.32	0	61,63,63	0.48	1 (1%)
2	9ZR	A	1201	-	55,55,55	0.29	0	61,63,63	0.34	0
2	9ZR	B	1206	-	12,12,55	0.18	0	11,11,63	0.12	0
2	9ZR	A	1202	-	55,55,55	0.29	0	61,63,63	0.37	0
3	YJ0	A	1210	-	35,35,90	0.41	0	58,58,138	0.63	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	9ZR	D	1207	-	-	2/10/10/59	-
2	9ZR	A	1205	-	-	18/59/59/59	-
2	9ZR	C	1207	-	-	17/59/59/59	-
2	9ZR	D	1204	-	-	21/59/59/59	-
2	9ZR	C	1201	-	-	20/59/59/59	-
2	9ZR	A	1203	-	-	11/47/47/59	-
3	YJ0	B	1209	-	-	4/6/94/200	0/6/6/10
2	9ZR	A	1209	-	-	19/59/59/59	-
2	9ZR	C	1205	-	-	11/47/47/59	-
2	9ZR	D	1206	-	-	11/47/47/59	-
2	9ZR	B	1208	-	-	22/59/59/59	-
2	9ZR	D	1202	-	-	19/59/59/59	-
2	9ZR	B	1207	-	-	17/59/59/59	-
2	9ZR	D	1205	-	-	10/59/59/59	-
3	YJ0	D	1210	-	-	4/6/94/200	0/6/6/10
2	9ZR	B	1205	-	-	11/47/47/59	-
3	YJ0	D	1203	-	-	-	0/6/6/10
2	9ZR	C	1203	-	-	21/59/59/59	-
3	YJ0	A	1207	-	-	4/6/94/200	0/6/6/10
3	YJ0	B	1202	-	-	-	0/6/6/10
3	YJ0	C	1202	-	-	-	0/6/6/10
3	YJ0	C	1209	-	-	4/6/94/200	0/6/6/10
2	9ZR	A	1204	-	-	2/10/10/59	-
2	9ZR	C	1208	-	-	22/59/59/59	-
2	9ZR	C	1210	-	-	18/59/59/59	-
2	9ZR	C	1204	-	-	10/59/59/59	-
2	9ZR	A	1208	-	-	18/59/59/59	-
2	9ZR	D	1209	-	-	23/59/59/59	-
2	9ZR	B	1203	-	-	21/59/59/59	-
2	9ZR	D	1208	-	-	18/59/59/59	-
2	9ZR	C	1206	-	-	2/10/10/59	-
2	9ZR	D	1201	-	-	18/59/59/59	-
2	9ZR	B	1201	-	-	19/59/59/59	-
2	9ZR	A	1206	-	-	23/59/59/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9ZR	B	1204	-	-	10/59/59/59	-
2	9ZR	B	1210	-	-	18/59/59/59	-
2	9ZR	A	1201	-	-	20/59/59/59	-
2	9ZR	B	1206	-	-	3/10/10/59	-
2	9ZR	A	1202	-	-	11/59/59/59	-
3	YJ0	A	1210	-	-	-	0/6/6/10

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	9ZR	O39-C26-C27	3.32	120.24	108.34
2	D	1202	9ZR	O39-C26-C27	3.31	120.23	108.34
2	C	1201	9ZR	O39-C26-C27	3.28	120.12	108.34
2	A	1209	9ZR	C27-C26-C25	3.24	119.35	111.78
2	A	1209	9ZR	O39-C26-C27	3.24	119.95	108.34
2	C	1201	9ZR	C27-C26-C25	3.22	119.30	111.78
2	D	1202	9ZR	C27-C26-C25	3.18	119.19	111.78
2	B	1201	9ZR	C27-C26-C25	3.15	119.12	111.78
2	C	1201	9ZR	C8-C9-C10	3.04	147.62	124.83
2	B	1201	9ZR	C8-C9-C10	3.04	147.62	124.83
2	A	1209	9ZR	C8-C9-C10	3.04	147.61	124.83
2	D	1202	9ZR	C8-C9-C10	3.04	147.59	124.83
2	D	1202	9ZR	C51-C50-C49	2.94	146.84	124.83
2	B	1201	9ZR	C51-C50-C49	2.93	146.80	124.83
2	C	1201	9ZR	C51-C50-C49	2.93	146.78	124.83
2	A	1209	9ZR	C51-C50-C49	2.92	146.73	124.83
2	A	1209	9ZR	O39-C26-C25	2.66	117.89	108.34
2	B	1201	9ZR	O39-C26-C25	2.62	117.73	108.34
2	C	1201	9ZR	O39-C26-C25	2.61	117.71	108.34
3	D	1210	YJ0	C81-O80-C5	2.61	118.19	113.69
2	D	1202	9ZR	O39-C26-C25	2.61	117.70	108.34
3	A	1207	YJ0	C81-O80-C5	2.59	118.16	113.69
3	B	1209	YJ0	C81-O80-C5	2.59	118.15	113.69
3	C	1209	YJ0	C81-O80-C5	2.56	118.11	113.69
2	B	1210	9ZR	C26-O39-C40	2.26	123.19	117.80
2	A	1208	9ZR	C26-O39-C40	2.25	123.17	117.80
2	D	1201	9ZR	C26-O39-C40	2.23	123.14	117.80
2	C	1210	9ZR	C26-O39-C40	2.23	123.14	117.80

There are no chirality outliers.

All (502) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	9ZR	C33-O32-P29-O30
2	A	1201	9ZR	O32-C33-C34-N35
2	A	1203	9ZR	O32-C33-C34-N35
2	A	1203	9ZR	C27-O28-P29-O31
2	A	1205	9ZR	C21-C22-O24-C25
2	A	1205	9ZR	O23-C22-O24-C25
2	A	1205	9ZR	C27-O28-P29-O32
2	A	1206	9ZR	C34-C33-O32-P29
2	A	1206	9ZR	C33-O32-P29-O31
2	A	1206	9ZR	C33-O32-P29-O28
2	A	1206	9ZR	C27-O28-P29-O32
2	A	1208	9ZR	C33-O32-P29-O30
2	A	1208	9ZR	O32-C33-C34-N35
2	A	1208	9ZR	C42-C40-O39-C26
2	A	1208	9ZR	O41-C40-O39-C26
2	A	1209	9ZR	C33-O32-P29-O30
2	A	1209	9ZR	O32-C33-C34-N35
2	A	1209	9ZR	C27-O28-P29-O31
2	A	1209	9ZR	C27-O28-P29-O32
2	A	1209	9ZR	C27-O28-P29-O30
2	B	1201	9ZR	C33-O32-P29-O28
2	B	1201	9ZR	C33-O32-P29-O30
2	B	1201	9ZR	O32-C33-C34-N35
2	B	1201	9ZR	C27-O28-P29-O31
2	B	1201	9ZR	C27-O28-P29-O32
2	B	1201	9ZR	C27-O28-P29-O30
2	B	1203	9ZR	C33-O32-P29-O30
2	B	1203	9ZR	O32-C33-C34-N35
2	B	1205	9ZR	O32-C33-C34-N35
2	B	1205	9ZR	C27-O28-P29-O31
2	B	1207	9ZR	C21-C22-O24-C25
2	B	1207	9ZR	O23-C22-O24-C25
2	B	1207	9ZR	C27-O28-P29-O32
2	B	1208	9ZR	C34-C33-O32-P29
2	B	1208	9ZR	C33-O32-P29-O31
2	B	1208	9ZR	C33-O32-P29-O28
2	B	1208	9ZR	C27-O28-P29-O32
2	B	1210	9ZR	C33-O32-P29-O30
2	B	1210	9ZR	O32-C33-C34-N35
2	B	1210	9ZR	C42-C40-O39-C26
2	B	1210	9ZR	O41-C40-O39-C26
2	C	1201	9ZR	C33-O32-P29-O28

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Mol	Chain	Res	Type	Atoms
2	C	1201	9ZR	C33-O32-P29-O30
2	C	1201	9ZR	O32-C33-C34-N35
2	C	1201	9ZR	C27-O28-P29-O31
2	C	1201	9ZR	C27-O28-P29-O32
2	C	1201	9ZR	C27-O28-P29-O30
2	C	1203	9ZR	C33-O32-P29-O30
2	C	1203	9ZR	O32-C33-C34-N35
2	C	1205	9ZR	O32-C33-C34-N35
2	C	1205	9ZR	C27-O28-P29-O31
2	C	1207	9ZR	C21-C22-O24-C25
2	C	1207	9ZR	O23-C22-O24-C25
2	C	1207	9ZR	C27-O28-P29-O32
2	C	1208	9ZR	C34-C33-O32-P29
2	C	1208	9ZR	C33-O32-P29-O31
2	C	1208	9ZR	C33-O32-P29-O28
2	C	1208	9ZR	C27-O28-P29-O32
2	C	1210	9ZR	C33-O32-P29-O30
2	C	1210	9ZR	O32-C33-C34-N35
2	C	1210	9ZR	C42-C40-O39-C26
2	C	1210	9ZR	O41-C40-O39-C26
2	D	1201	9ZR	C33-O32-P29-O30
2	D	1201	9ZR	O32-C33-C34-N35
2	D	1201	9ZR	C42-C40-O39-C26
2	D	1201	9ZR	O41-C40-O39-C26
2	D	1202	9ZR	C33-O32-P29-O28
2	D	1202	9ZR	C33-O32-P29-O30
2	D	1202	9ZR	O32-C33-C34-N35
2	D	1202	9ZR	C27-O28-P29-O31
2	D	1202	9ZR	C27-O28-P29-O32
2	D	1202	9ZR	C27-O28-P29-O30
2	D	1204	9ZR	C33-O32-P29-O30
2	D	1204	9ZR	O32-C33-C34-N35
2	D	1206	9ZR	O32-C33-C34-N35
2	D	1206	9ZR	C27-O28-P29-O31
2	D	1208	9ZR	C21-C22-O24-C25
2	D	1208	9ZR	O23-C22-O24-C25
2	D	1208	9ZR	C27-O28-P29-O32
2	D	1209	9ZR	C34-C33-O32-P29
2	D	1209	9ZR	C33-O32-P29-O31
2	D	1209	9ZR	C33-O32-P29-O28
2	D	1209	9ZR	C27-O28-P29-O32
2	A	1206	9ZR	O24-C25-C26-O39

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Mol	Chain	Res	Type	Atoms
2	B	1208	9ZR	O24-C25-C26-O39
2	C	1208	9ZR	O24-C25-C26-O39
2	D	1209	9ZR	O24-C25-C26-O39
3	A	1207	YJ0	C26-C27-C28-C53
3	B	1209	YJ0	C26-C27-C28-C53
3	C	1209	YJ0	C26-C27-C28-C53
3	D	1210	YJ0	C26-C27-C28-C53
2	B	1205	9ZR	C19-C20-C21-C22
2	C	1205	9ZR	C19-C20-C21-C22
2	A	1203	9ZR	C19-C20-C21-C22
2	A	1205	9ZR	C40-C42-C43-C44
2	D	1206	9ZR	C19-C20-C21-C22
2	A	1206	9ZR	C19-C20-C21-C22
2	B	1207	9ZR	C40-C42-C43-C44
2	B	1208	9ZR	C19-C20-C21-C22
2	C	1208	9ZR	C19-C20-C21-C22
2	D	1209	9ZR	C19-C20-C21-C22
2	C	1207	9ZR	C40-C42-C43-C44
2	D	1208	9ZR	C40-C42-C43-C44
2	A	1202	9ZR	C19-C20-C21-C22
2	C	1204	9ZR	C19-C20-C21-C22
2	D	1205	9ZR	C19-C20-C21-C22
2	B	1204	9ZR	C19-C20-C21-C22
2	A	1201	9ZR	C19-C20-C21-C22
2	A	1208	9ZR	C43-C44-C45-C46
2	B	1210	9ZR	C43-C44-C45-C46
2	C	1210	9ZR	C43-C44-C45-C46
2	D	1201	9ZR	C43-C44-C45-C46
2	C	1201	9ZR	C2-C3-C4-C5
2	A	1209	9ZR	C2-C3-C4-C5
2	B	1201	9ZR	C2-C3-C4-C5
2	D	1202	9ZR	C2-C3-C4-C5
2	B	1203	9ZR	C19-C20-C21-C22
2	C	1203	9ZR	C19-C20-C21-C22
2	D	1204	9ZR	C19-C20-C21-C22
2	A	1208	9ZR	C12-C13-C14-C15
2	B	1210	9ZR	C12-C13-C14-C15
2	C	1210	9ZR	C12-C13-C14-C15
2	D	1201	9ZR	C12-C13-C14-C15
2	B	1208	9ZR	C12-C13-C14-C15
2	C	1208	9ZR	C12-C13-C14-C15
2	D	1209	9ZR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	A	1206	9ZR	C12-C13-C14-C15
2	A	1203	9ZR	C44-C45-C46-C47
2	C	1205	9ZR	C44-C45-C46-C47
2	D	1206	9ZR	C44-C45-C46-C47
2	B	1205	9ZR	C44-C45-C46-C47
2	B	1203	9ZR	C46-C47-C48-C49
2	C	1203	9ZR	C46-C47-C48-C49
2	D	1204	9ZR	C46-C47-C48-C49
2	D	1202	9ZR	C18-C19-C20-C21
2	B	1201	9ZR	C18-C19-C20-C21
2	C	1201	9ZR	C18-C19-C20-C21
2	A	1209	9ZR	C18-C19-C20-C21
2	A	1209	9ZR	O24-C25-C26-O39
2	B	1201	9ZR	O24-C25-C26-O39
2	C	1201	9ZR	O24-C25-C26-O39
2	D	1202	9ZR	O24-C25-C26-O39
2	C	1207	9ZR	C43-C44-C45-C46
2	A	1203	9ZR	C26-C27-O28-P29
2	B	1205	9ZR	C26-C27-O28-P29
2	C	1205	9ZR	C26-C27-O28-P29
2	D	1206	9ZR	C26-C27-O28-P29
2	D	1208	9ZR	C43-C44-C45-C46
2	A	1202	9ZR	C14-C15-C16-C17
2	B	1207	9ZR	C43-C44-C45-C46
2	C	1204	9ZR	C14-C15-C16-C17
2	B	1204	9ZR	C14-C15-C16-C17
2	D	1205	9ZR	C14-C15-C16-C17
3	A	1207	YJ0	C26-C27-C28-C29
3	B	1209	YJ0	C26-C27-C28-C29
3	C	1209	YJ0	C26-C27-C28-C29
3	D	1210	YJ0	C26-C27-C28-C29
2	A	1201	9ZR	C6-C7-C8-C9
2	A	1206	9ZR	C10-C11-C12-C13
2	A	1206	9ZR	C6-C7-C8-C9
2	B	1203	9ZR	C6-C7-C8-C9
2	B	1208	9ZR	C6-C7-C8-C9
2	C	1203	9ZR	C6-C7-C8-C9
2	C	1208	9ZR	C6-C7-C8-C9
2	D	1204	9ZR	C6-C7-C8-C9
2	D	1209	9ZR	C6-C7-C8-C9
2	A	1201	9ZR	C44-C45-C46-C47
2	C	1203	9ZR	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
2	B	1203	9ZR	C44-C45-C46-C47
2	A	1205	9ZR	C3-C4-C5-C6
2	A	1203	9ZR	C49-C50-C51-C52
2	B	1205	9ZR	C49-C50-C51-C52
2	C	1205	9ZR	C49-C50-C51-C52
2	D	1206	9ZR	C49-C50-C51-C52
2	B	1207	9ZR	C3-C4-C5-C6
2	C	1207	9ZR	C3-C4-C5-C6
2	A	1206	9ZR	C5-C6-C7-C8
2	B	1203	9ZR	C52-C53-C54-C55
2	D	1204	9ZR	C52-C53-C54-C55
2	A	1205	9ZR	O24-C25-C26-C27
2	A	1206	9ZR	O24-C25-C26-C27
2	B	1207	9ZR	O24-C25-C26-C27
2	B	1208	9ZR	O24-C25-C26-C27
2	C	1207	9ZR	O24-C25-C26-C27
2	C	1208	9ZR	O24-C25-C26-C27
2	D	1208	9ZR	O24-C25-C26-C27
2	D	1209	9ZR	O24-C25-C26-C27
2	A	1201	9ZR	C52-C53-C54-C55
2	B	1208	9ZR	C5-C6-C7-C8
2	C	1203	9ZR	C52-C53-C54-C55
2	C	1208	9ZR	C5-C6-C7-C8
2	D	1208	9ZR	C3-C4-C5-C6
2	D	1209	9ZR	C5-C6-C7-C8
2	A	1201	9ZR	C46-C47-C48-C49
2	B	1208	9ZR	C10-C11-C12-C13
2	C	1208	9ZR	C10-C11-C12-C13
2	D	1209	9ZR	C10-C11-C12-C13
2	A	1205	9ZR	C43-C44-C45-C46
2	D	1204	9ZR	C44-C45-C46-C47
2	C	1207	9ZR	C17-C18-C19-C20
2	A	1209	9ZR	O39-C26-C27-O28
2	C	1201	9ZR	O39-C26-C27-O28
2	A	1201	9ZR	O24-C25-C26-O39
2	B	1203	9ZR	O24-C25-C26-O39
2	C	1203	9ZR	O24-C25-C26-O39
2	D	1204	9ZR	O24-C25-C26-O39
2	A	1206	9ZR	C45-C46-C47-C48
2	B	1207	9ZR	C17-C18-C19-C20
2	D	1208	9ZR	C17-C18-C19-C20
2	D	1209	9ZR	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
2	A	1205	9ZR	C17-C18-C19-C20
2	C	1208	9ZR	C44-C45-C46-C47
2	A	1204	9ZR	C53-C54-C55-C56
2	A	1203	9ZR	C16-C17-C18-C19
2	B	1208	9ZR	C44-C45-C46-C47
2	D	1209	9ZR	C52-C53-C54-C55
2	B	1206	9ZR	C53-C54-C55-C56
2	C	1206	9ZR	C53-C54-C55-C56
2	D	1207	9ZR	C53-C54-C55-C56
2	A	1201	9ZR	C50-C51-C52-C53
2	A	1208	9ZR	C6-C7-C8-C9
2	D	1201	9ZR	C6-C7-C8-C9
2	A	1201	9ZR	C4-C5-C6-C7
2	B	1208	9ZR	C52-C53-C54-C55
2	C	1208	9ZR	C52-C53-C54-C55
2	A	1206	9ZR	C44-C45-C46-C47
2	B	1203	9ZR	C4-C5-C6-C7
2	B	1208	9ZR	C45-C46-C47-C48
2	C	1203	9ZR	C4-C5-C6-C7
2	D	1204	9ZR	C4-C5-C6-C7
2	C	1208	9ZR	C45-C46-C47-C48
2	B	1210	9ZR	C6-C7-C8-C9
2	C	1210	9ZR	C6-C7-C8-C9
2	A	1201	9ZR	O24-C25-C26-C27
2	B	1203	9ZR	O24-C25-C26-C27
2	C	1203	9ZR	O24-C25-C26-C27
2	D	1204	9ZR	O24-C25-C26-C27
2	A	1202	9ZR	C11-C12-C13-C14
2	C	1210	9ZR	C14-C15-C16-C17
2	D	1209	9ZR	C45-C46-C47-C48
2	B	1205	9ZR	C16-C17-C18-C19
2	A	1208	9ZR	C14-C15-C16-C17
2	B	1210	9ZR	C14-C15-C16-C17
2	D	1201	9ZR	C14-C15-C16-C17
2	D	1202	9ZR	O39-C26-C27-O28
2	B	1204	9ZR	C11-C12-C13-C14
2	C	1205	9ZR	C16-C17-C18-C19
2	C	1204	9ZR	C11-C12-C13-C14
2	D	1205	9ZR	C11-C12-C13-C14
2	D	1206	9ZR	C16-C17-C18-C19
2	A	1206	9ZR	C52-C53-C54-C55
2	A	1205	9ZR	O24-C25-C26-O39

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Mol	Chain	Res	Type	Atoms
2	A	1208	9ZR	O24-C25-C26-O39
2	B	1207	9ZR	O24-C25-C26-O39
2	B	1210	9ZR	O24-C25-C26-O39
2	C	1207	9ZR	O24-C25-C26-O39
2	C	1210	9ZR	O24-C25-C26-O39
2	D	1201	9ZR	O24-C25-C26-O39
2	D	1208	9ZR	O24-C25-C26-O39
3	A	1207	YJ0	C27-C26-O25-C23
3	B	1209	YJ0	C27-C26-O25-C23
3	C	1209	YJ0	C27-C26-O25-C23
3	D	1210	YJ0	C27-C26-O25-C23
2	B	1210	9ZR	C46-C47-C48-C49
2	C	1210	9ZR	C46-C47-C48-C49
2	D	1201	9ZR	C46-C47-C48-C49
2	A	1209	9ZR	C45-C46-C47-C48
2	B	1201	9ZR	O39-C26-C27-O28
2	A	1202	9ZR	O24-C25-C26-C27
2	B	1204	9ZR	O24-C25-C26-C27
2	C	1204	9ZR	O24-C25-C26-C27
2	D	1205	9ZR	O24-C25-C26-C27
2	A	1202	9ZR	O24-C25-C26-O39
2	A	1208	9ZR	C46-C47-C48-C49
2	B	1204	9ZR	O24-C25-C26-O39
2	C	1204	9ZR	O24-C25-C26-O39
2	D	1205	9ZR	O24-C25-C26-O39
2	B	1201	9ZR	C45-C46-C47-C48
2	C	1201	9ZR	C45-C46-C47-C48
2	D	1202	9ZR	C45-C46-C47-C48
2	A	1206	9ZR	O32-C33-C34-N35
2	B	1208	9ZR	O32-C33-C34-N35
2	C	1208	9ZR	O32-C33-C34-N35
2	D	1209	9ZR	O32-C33-C34-N35
2	B	1203	9ZR	C50-C51-C52-C53
2	C	1203	9ZR	C50-C51-C52-C53
2	D	1204	9ZR	C50-C51-C52-C53
2	B	1201	9ZR	C1-C2-C3-C4
2	A	1209	9ZR	C25-C26-C27-O28
2	B	1201	9ZR	C25-C26-C27-O28
2	C	1201	9ZR	C25-C26-C27-O28
2	D	1202	9ZR	C25-C26-C27-O28
2	A	1201	9ZR	C53-C54-C55-C56
2	C	1201	9ZR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	D	1202	9ZR	C1-C2-C3-C4
2	A	1209	9ZR	C49-C50-C51-C52
2	C	1201	9ZR	C49-C50-C51-C52
2	D	1202	9ZR	C49-C50-C51-C52
2	B	1203	9ZR	C53-C54-C55-C56
2	A	1203	9ZR	O39-C26-C27-O28
2	B	1205	9ZR	O39-C26-C27-O28
2	C	1205	9ZR	O39-C26-C27-O28
2	D	1206	9ZR	O39-C26-C27-O28
2	A	1205	9ZR	C46-C47-C48-C49
2	C	1207	9ZR	C46-C47-C48-C49
2	A	1209	9ZR	C1-C2-C3-C4
2	C	1203	9ZR	C53-C54-C55-C56
2	B	1201	9ZR	C49-C50-C51-C52
2	D	1204	9ZR	C53-C54-C55-C56
2	A	1208	9ZR	O24-C25-C26-C27
2	B	1210	9ZR	O24-C25-C26-C27
2	C	1210	9ZR	O24-C25-C26-C27
2	D	1201	9ZR	O24-C25-C26-C27
2	B	1207	9ZR	C46-C47-C48-C49
2	D	1208	9ZR	C46-C47-C48-C49
2	A	1205	9ZR	C27-O28-P29-O30
2	A	1206	9ZR	C27-O28-P29-O30
2	A	1209	9ZR	C33-O32-P29-O28
2	B	1207	9ZR	C27-O28-P29-O30
2	B	1208	9ZR	C27-O28-P29-O30
2	C	1207	9ZR	C27-O28-P29-O30
2	C	1208	9ZR	C27-O28-P29-O30
2	D	1208	9ZR	C27-O28-P29-O30
2	D	1209	9ZR	C27-O28-P29-O30
2	A	1206	9ZR	C26-C27-O28-P29
2	B	1204	9ZR	C17-C18-C19-C20
2	C	1210	9ZR	C49-C50-C51-C52
2	A	1201	9ZR	C13-C14-C15-C16
2	C	1203	9ZR	C13-C14-C15-C16
2	C	1204	9ZR	C17-C18-C19-C20
2	D	1204	9ZR	C13-C14-C15-C16
2	B	1203	9ZR	C13-C14-C15-C16
2	D	1205	9ZR	C17-C18-C19-C20
2	A	1202	9ZR	C17-C18-C19-C20
2	B	1210	9ZR	C49-C50-C51-C52
2	D	1201	9ZR	C49-C50-C51-C52

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Mol	Chain	Res	Type	Atoms
2	B	1208	9ZR	C26-C27-O28-P29
2	C	1208	9ZR	C26-C27-O28-P29
2	D	1209	9ZR	C26-C27-O28-P29
2	D	1205	9ZR	C18-C19-C20-C21
2	C	1204	9ZR	C18-C19-C20-C21
2	B	1201	9ZR	C16-C17-C18-C19
2	C	1201	9ZR	C16-C17-C18-C19
2	A	1208	9ZR	C16-C17-C18-C19
2	D	1209	9ZR	C15-C16-C17-C18
2	B	1208	9ZR	C15-C16-C17-C18
2	C	1208	9ZR	C15-C16-C17-C18
2	B	1210	9ZR	C16-C17-C18-C19
2	C	1210	9ZR	C16-C17-C18-C19
2	D	1201	9ZR	C16-C17-C18-C19
2	A	1202	9ZR	C18-C19-C20-C21
2	B	1204	9ZR	C18-C19-C20-C21
2	D	1202	9ZR	C16-C17-C18-C19
2	A	1209	9ZR	C16-C17-C18-C19
2	A	1208	9ZR	O39-C26-C27-O28
2	B	1210	9ZR	O39-C26-C27-O28
2	C	1210	9ZR	O39-C26-C27-O28
2	D	1201	9ZR	O39-C26-C27-O28
2	A	1201	9ZR	C11-C12-C13-C14
2	D	1204	9ZR	C11-C12-C13-C14
2	C	1203	9ZR	C11-C12-C13-C14
2	A	1208	9ZR	C49-C50-C51-C52
2	A	1201	9ZR	C26-C27-O28-P29
2	B	1203	9ZR	C11-C12-C13-C14
2	A	1206	9ZR	C15-C16-C17-C18
2	A	1202	9ZR	C7-C8-C9-C10
2	A	1206	9ZR	C9-C10-C11-C12
2	B	1201	9ZR	C47-C48-C49-C50
2	B	1208	9ZR	C9-C10-C11-C12
2	C	1208	9ZR	C9-C10-C11-C12
2	D	1209	9ZR	C9-C10-C11-C12
2	C	1204	9ZR	C7-C8-C9-C10
2	D	1205	9ZR	C7-C8-C9-C10
2	B	1203	9ZR	C26-C27-O28-P29
2	C	1203	9ZR	C26-C27-O28-P29
2	D	1204	9ZR	C26-C27-O28-P29
2	B	1204	9ZR	C7-C8-C9-C10
2	C	1203	9ZR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	D	1201	9ZR	C20-C21-C22-O24
2	B	1203	9ZR	C12-C13-C14-C15
2	D	1204	9ZR	C12-C13-C14-C15
2	A	1202	9ZR	C9-C10-C11-C12
2	A	1209	9ZR	C47-C48-C49-C50
2	B	1204	9ZR	C9-C10-C11-C12
2	C	1201	9ZR	C47-C48-C49-C50
2	C	1204	9ZR	C9-C10-C11-C12
2	D	1202	9ZR	C47-C48-C49-C50
2	D	1205	9ZR	C9-C10-C11-C12
2	B	1203	9ZR	C5-C6-C7-C8
2	A	1208	9ZR	C20-C21-C22-O24
2	B	1210	9ZR	C20-C21-C22-O24
2	A	1201	9ZR	C5-C6-C7-C8
2	C	1203	9ZR	C5-C6-C7-C8
2	A	1203	9ZR	C25-C26-C27-O28
2	B	1205	9ZR	C25-C26-C27-O28
2	C	1205	9ZR	C25-C26-C27-O28
2	D	1206	9ZR	C25-C26-C27-O28
2	C	1210	9ZR	C20-C21-C22-O24
2	A	1206	9ZR	C47-C48-C49-C50
2	B	1207	9ZR	C9-C10-C11-C12
2	B	1207	9ZR	C47-C48-C49-C50
2	C	1207	9ZR	C9-C10-C11-C12
2	C	1207	9ZR	C47-C48-C49-C50
2	D	1208	9ZR	C9-C10-C11-C12
2	D	1208	9ZR	C47-C48-C49-C50
2	D	1204	9ZR	C5-C6-C7-C8
2	A	1201	9ZR	C12-C13-C14-C15
2	B	1210	9ZR	C15-C16-C17-C18
2	C	1210	9ZR	C15-C16-C17-C18
2	A	1202	9ZR	C49-C50-C51-C52
2	B	1204	9ZR	C49-C50-C51-C52
2	B	1207	9ZR	C7-C8-C9-C10
2	C	1204	9ZR	C49-C50-C51-C52
2	C	1207	9ZR	C7-C8-C9-C10
2	D	1205	9ZR	C49-C50-C51-C52
2	D	1209	9ZR	C47-C48-C49-C50
2	A	1208	9ZR	C15-C16-C17-C18
2	D	1201	9ZR	C15-C16-C17-C18
2	A	1203	9ZR	C27-C26-O39-C40
2	B	1205	9ZR	C27-C26-O39-C40

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Mol	Chain	Res	Type	Atoms
2	C	1205	9ZR	C27-C26-O39-C40
2	D	1206	9ZR	C27-C26-O39-C40
2	A	1205	9ZR	C9-C10-C11-C12
2	A	1205	9ZR	C47-C48-C49-C50
2	C	1201	9ZR	C7-C8-C9-C10
2	D	1202	9ZR	C7-C8-C9-C10
2	D	1208	9ZR	C7-C8-C9-C10
2	A	1208	9ZR	C51-C52-C53-C54
2	A	1205	9ZR	C7-C8-C9-C10
2	B	1208	9ZR	C47-C48-C49-C50
2	A	1206	9ZR	C49-C50-C51-C52
2	A	1209	9ZR	C7-C8-C9-C10
2	B	1201	9ZR	C7-C8-C9-C10
2	B	1208	9ZR	C49-C50-C51-C52
2	C	1208	9ZR	C47-C48-C49-C50
2	A	1205	9ZR	C34-C33-O32-P29
2	C	1201	9ZR	C34-C33-O32-P29
2	D	1208	9ZR	C34-C33-O32-P29
2	A	1201	9ZR	C51-C52-C53-C54
2	C	1208	9ZR	C49-C50-C51-C52
2	D	1209	9ZR	C49-C50-C51-C52
2	C	1207	9ZR	C49-C50-C51-C52
2	D	1208	9ZR	C49-C50-C51-C52
2	B	1207	9ZR	C49-C50-C51-C52
2	C	1203	9ZR	C51-C52-C53-C54
2	B	1203	9ZR	C51-C52-C53-C54
2	B	1201	9ZR	C20-C21-C22-O24
2	B	1206	9ZR	C44-C45-C46-C47
2	C	1201	9ZR	C20-C21-C22-O24
2	D	1202	9ZR	C20-C21-C22-O24
2	A	1209	9ZR	C20-C21-C22-O24
2	D	1204	9ZR	C51-C52-C53-C54
2	C	1206	9ZR	C44-C45-C46-C47
2	D	1204	9ZR	O39-C40-C42-C43
2	A	1206	9ZR	C20-C21-C22-O24
2	D	1207	9ZR	C44-C45-C46-C47
2	B	1203	9ZR	O39-C40-C42-C43
2	C	1203	9ZR	O39-C40-C42-C43
2	C	1208	9ZR	C20-C21-C22-O24
2	D	1209	9ZR	C20-C21-C22-O24
2	B	1208	9ZR	C20-C21-C22-O24
3	A	1207	YJ0	C22-C23-O25-C26

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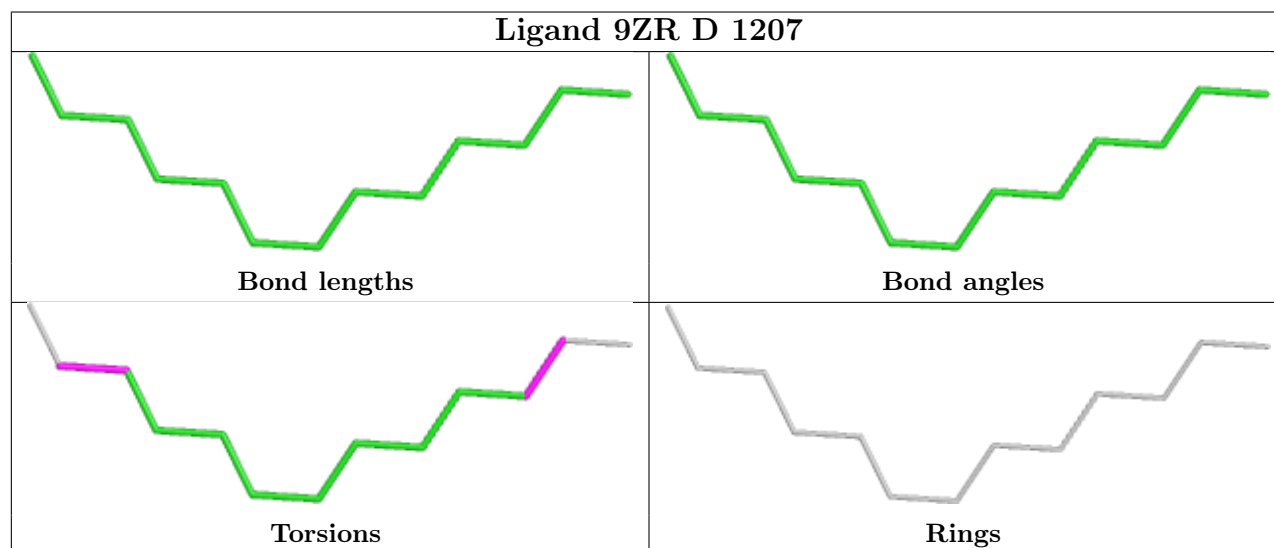
Mol	Chain	Res	Type	Atoms
3	B	1209	YJ0	C22-C23-O25-C26
3	C	1209	YJ0	C22-C23-O25-C26
3	D	1210	YJ0	C22-C23-O25-C26
2	A	1205	9ZR	C14-C15-C16-C17
2	D	1201	9ZR	C13-C14-C15-C16
2	A	1203	9ZR	C25-C26-O39-C40
2	B	1205	9ZR	C25-C26-O39-C40
2	C	1205	9ZR	C25-C26-O39-C40
2	D	1206	9ZR	C25-C26-O39-C40
2	B	1203	9ZR	C10-C11-C12-C13
2	C	1203	9ZR	C10-C11-C12-C13
2	D	1204	9ZR	C10-C11-C12-C13
2	B	1210	9ZR	C51-C52-C53-C54
2	B	1210	9ZR	C13-C14-C15-C16
2	A	1204	9ZR	C44-C45-C46-C47
2	B	1207	9ZR	C14-C15-C16-C17
2	C	1210	9ZR	C13-C14-C15-C16
2	C	1210	9ZR	C51-C52-C53-C54
2	A	1208	9ZR	C13-C14-C15-C16
2	D	1208	9ZR	C14-C15-C16-C17
2	A	1205	9ZR	C20-C21-C22-O24
2	B	1207	9ZR	C20-C21-C22-O24
2	D	1201	9ZR	C51-C52-C53-C54
2	C	1207	9ZR	C14-C15-C16-C17
2	C	1207	9ZR	C20-C21-C22-O24
2	D	1208	9ZR	C20-C21-C22-O24
2	B	1201	9ZR	C20-C21-C22-O23
2	C	1201	9ZR	C20-C21-C22-O23
2	D	1202	9ZR	C20-C21-C22-O23
2	D	1204	9ZR	O41-C40-C42-C43
2	B	1206	9ZR	C45-C46-C47-C48
2	A	1205	9ZR	C49-C50-C51-C52
2	A	1209	9ZR	C20-C21-C22-O23
2	C	1203	9ZR	O41-C40-C42-C43
2	A	1201	9ZR	C10-C11-C12-C13
2	A	1201	9ZR	O39-C40-C42-C43
2	B	1203	9ZR	O41-C40-C42-C43
2	A	1202	9ZR	C26-C25-O24-C22
2	A	1206	9ZR	C20-C21-C22-O23
2	D	1209	9ZR	C20-C21-C22-O23

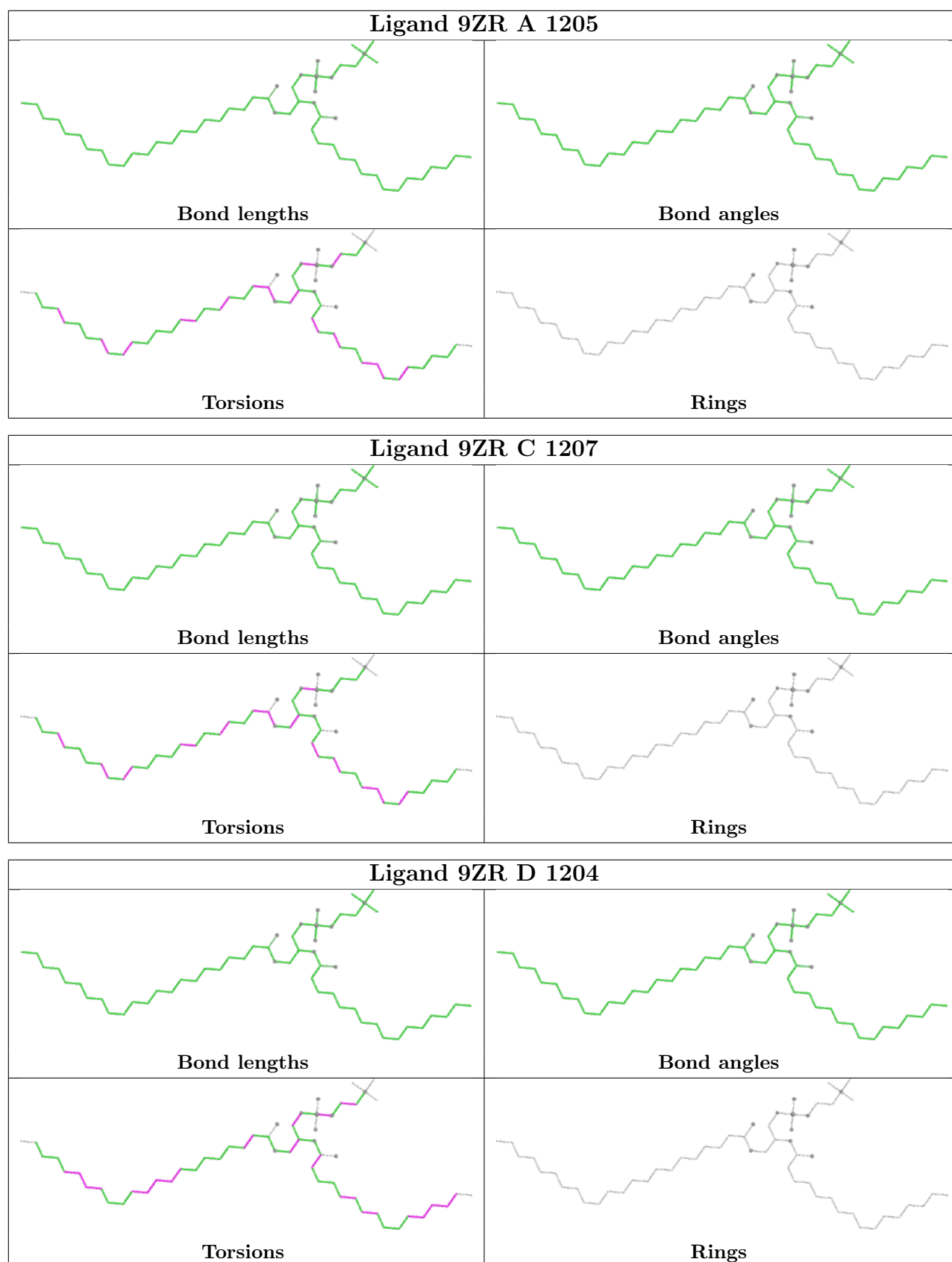
There are no ring outliers.

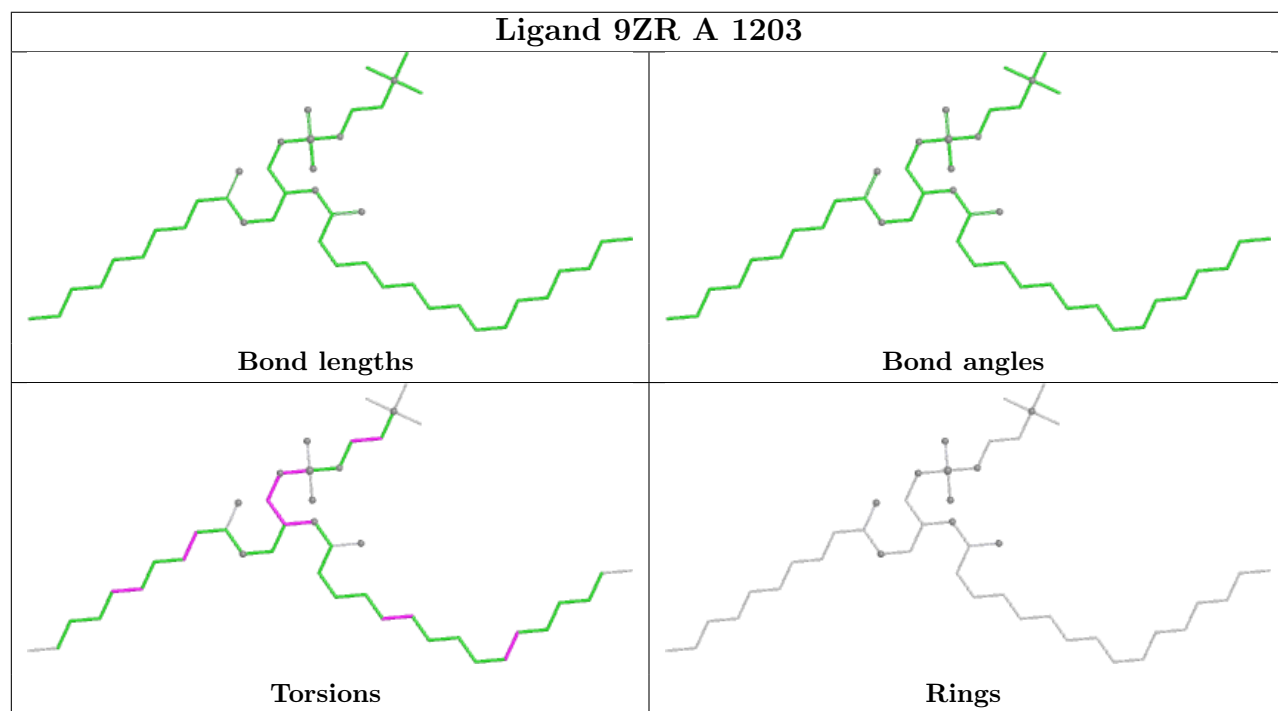
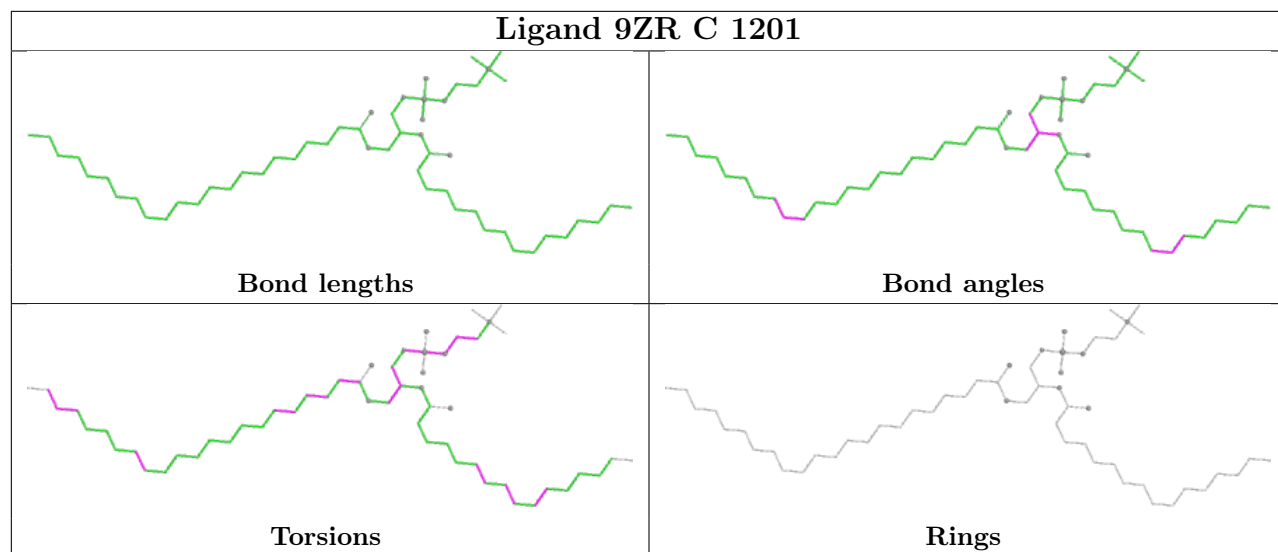
8 monomers are involved in 13 short contacts:

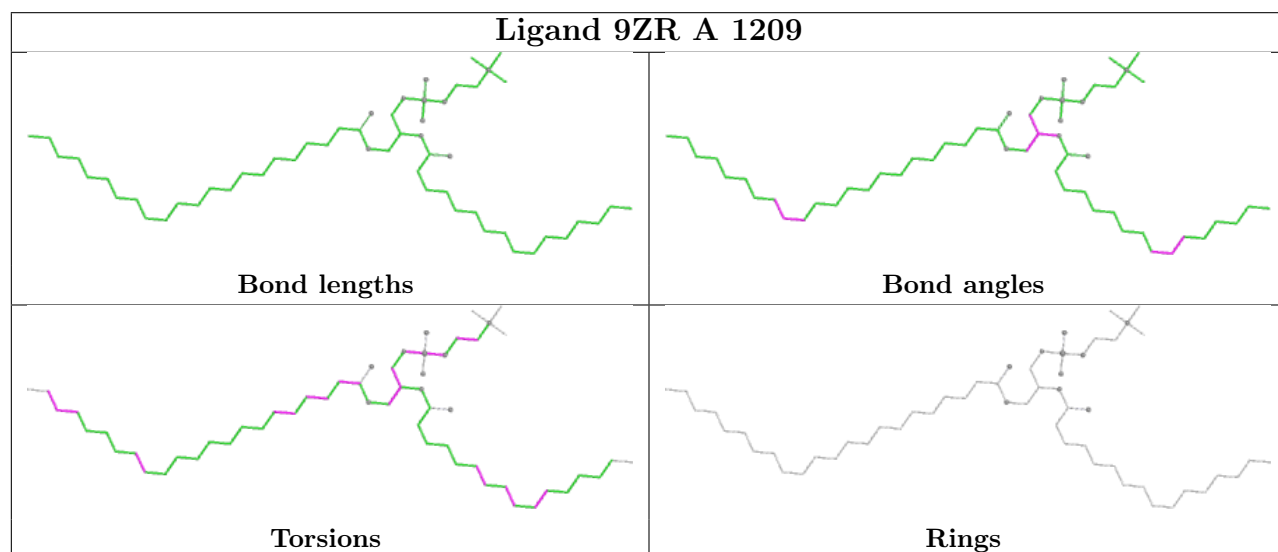
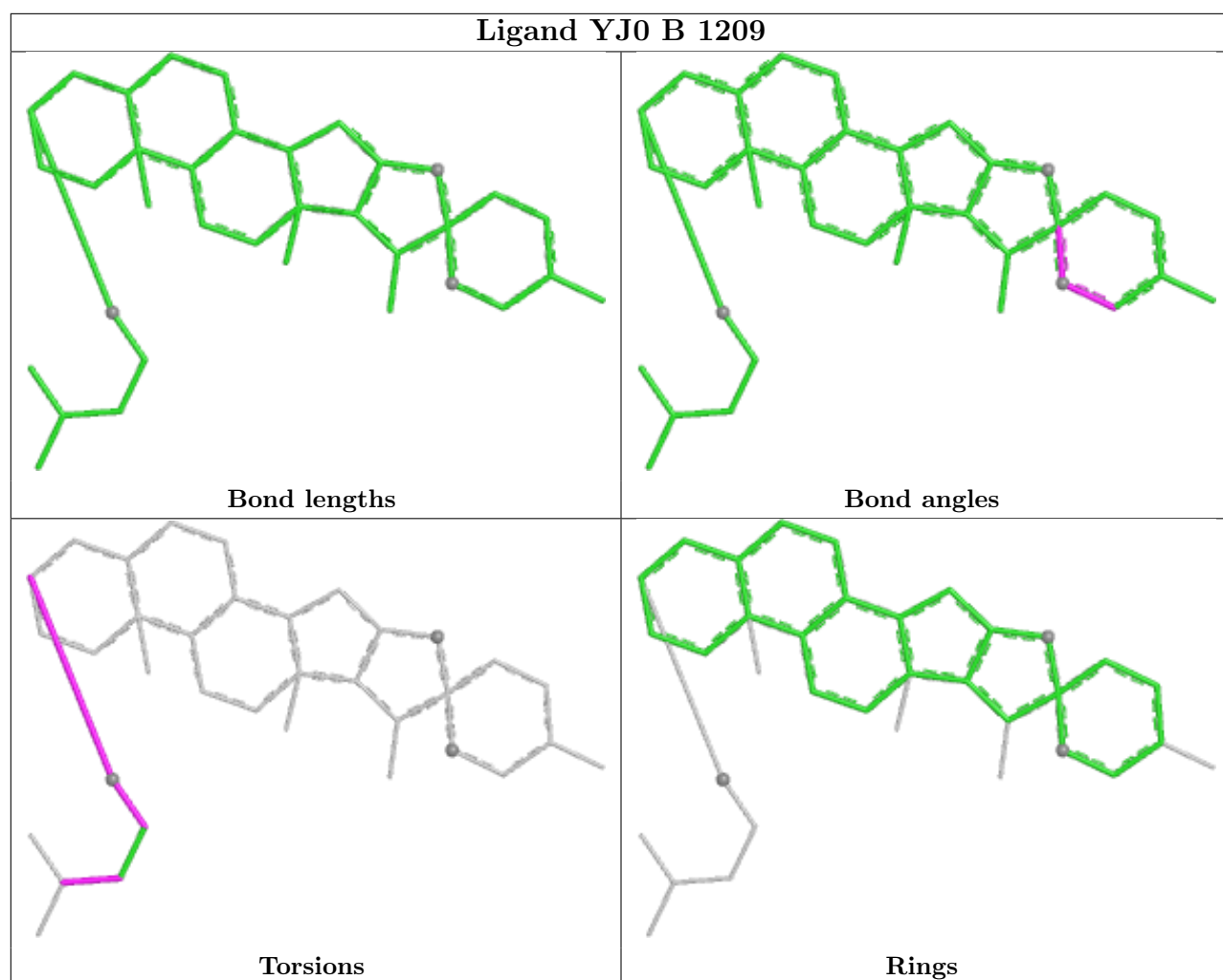
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1209	YJ0	1	0
3	D	1210	YJ0	1	0
3	D	1203	YJ0	2	0
3	A	1207	YJ0	1	0
3	B	1202	YJ0	2	0
3	C	1202	YJ0	2	0
3	C	1209	YJ0	1	0
3	A	1210	YJ0	3	0

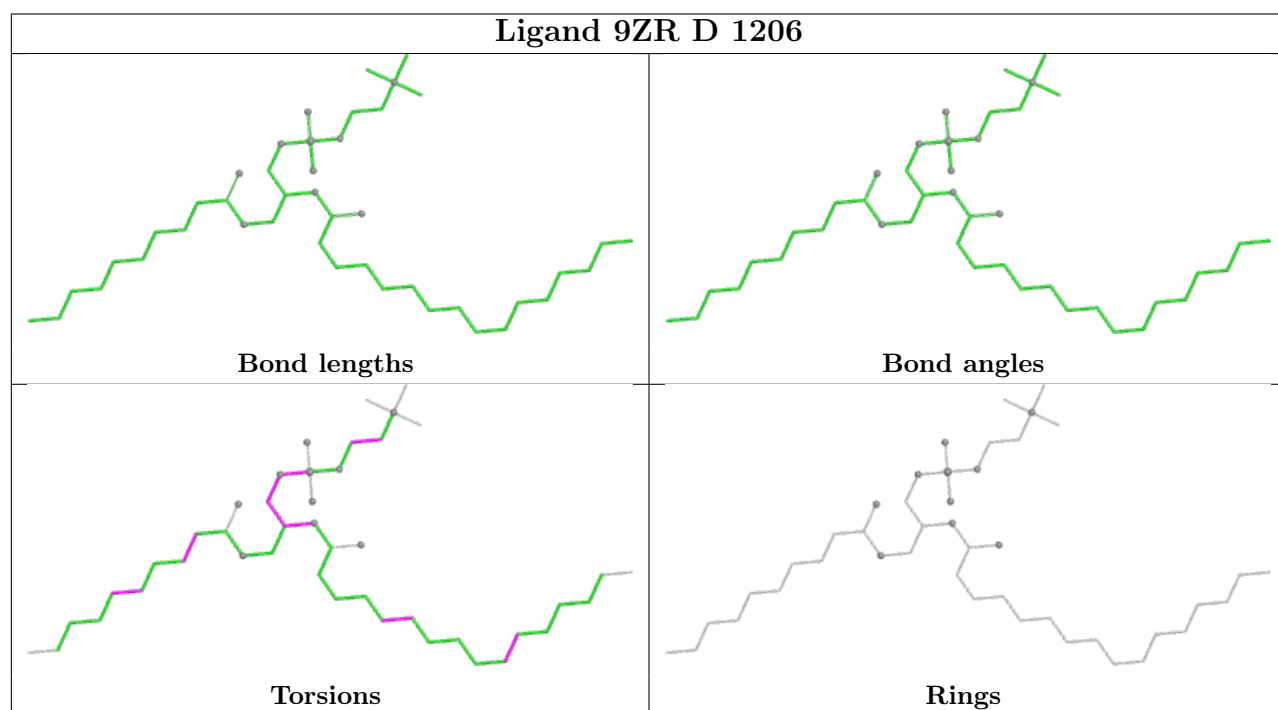
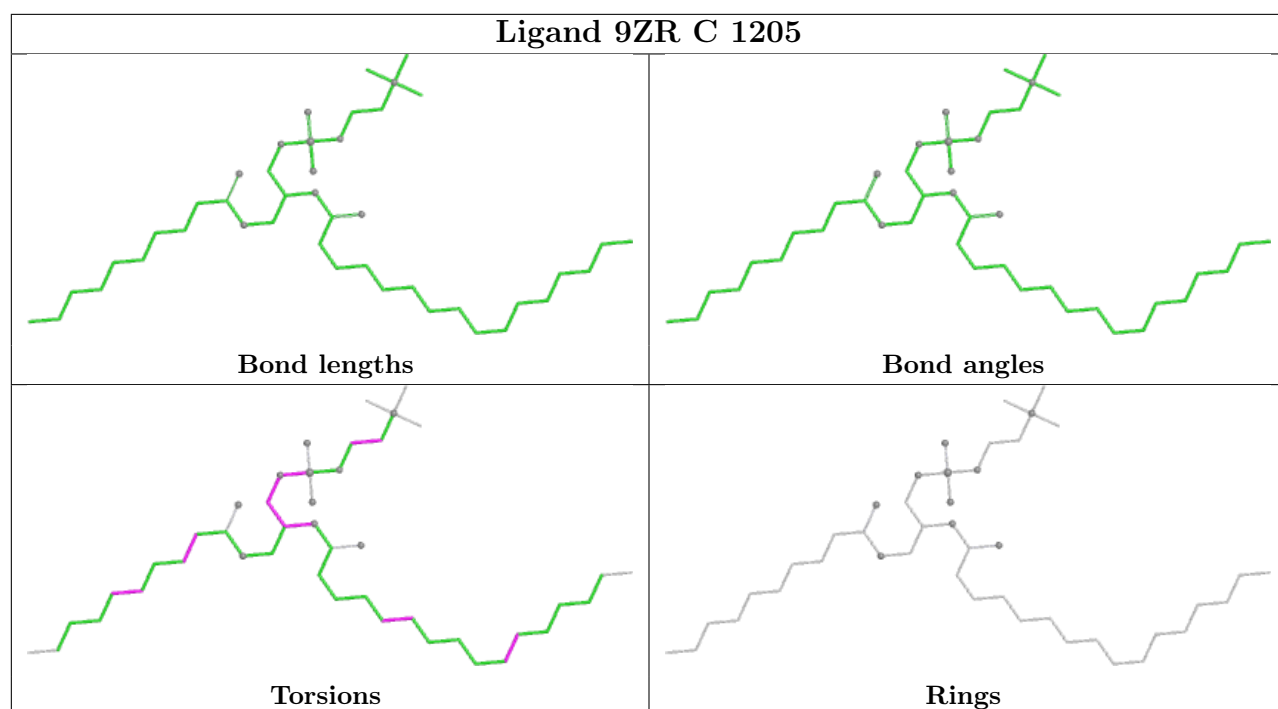
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

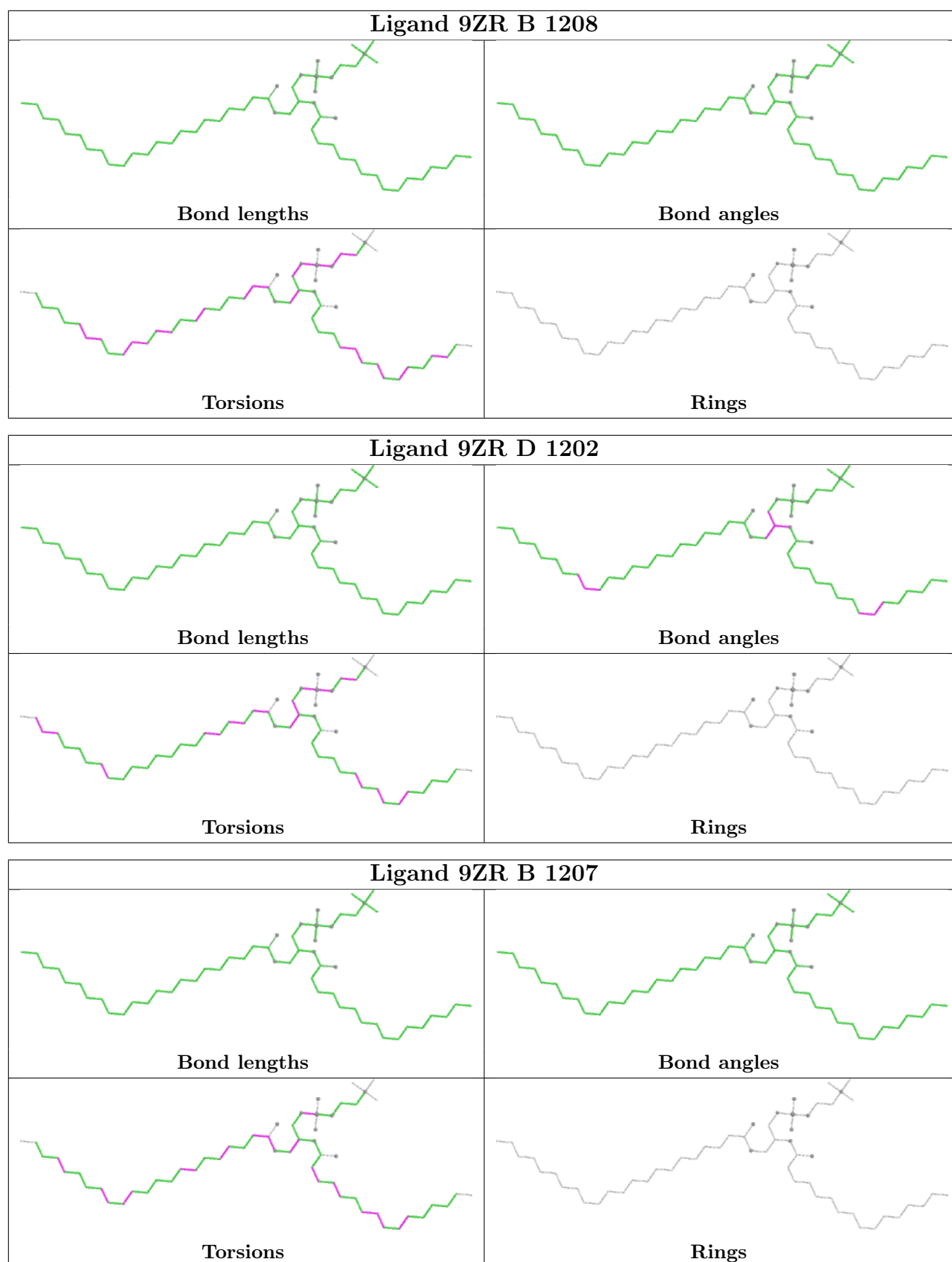


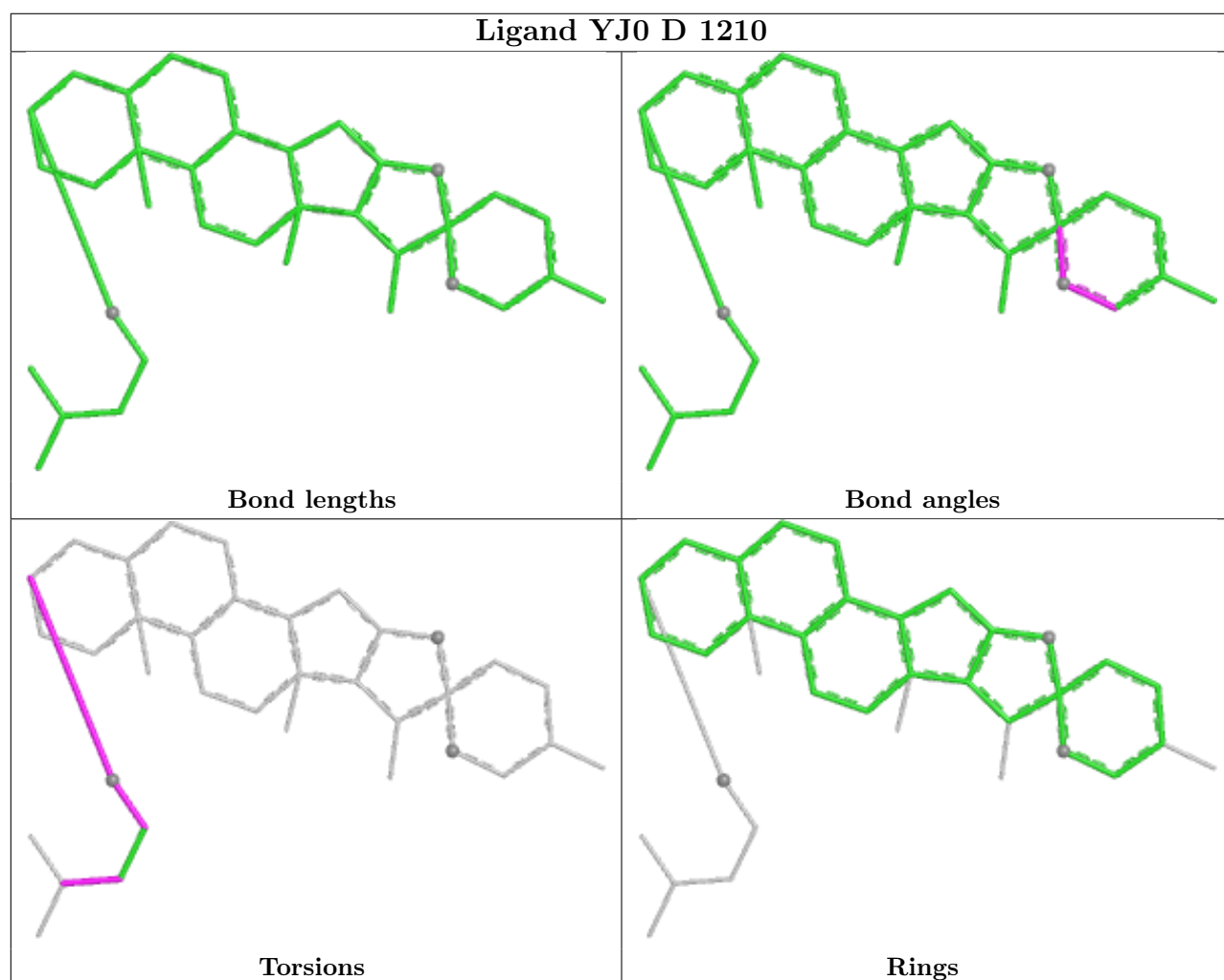
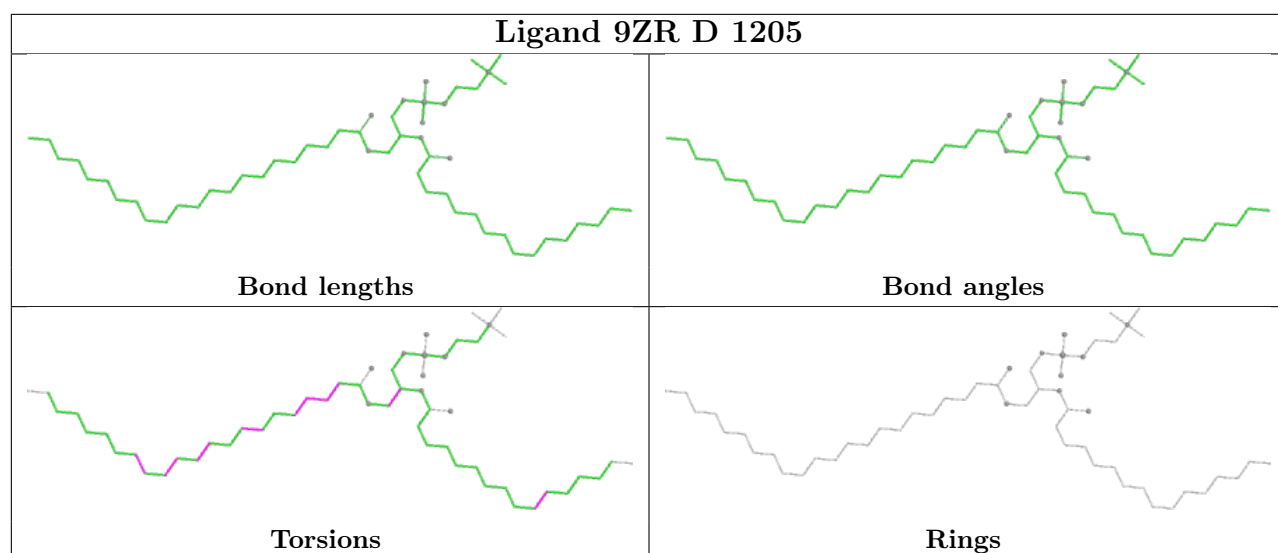


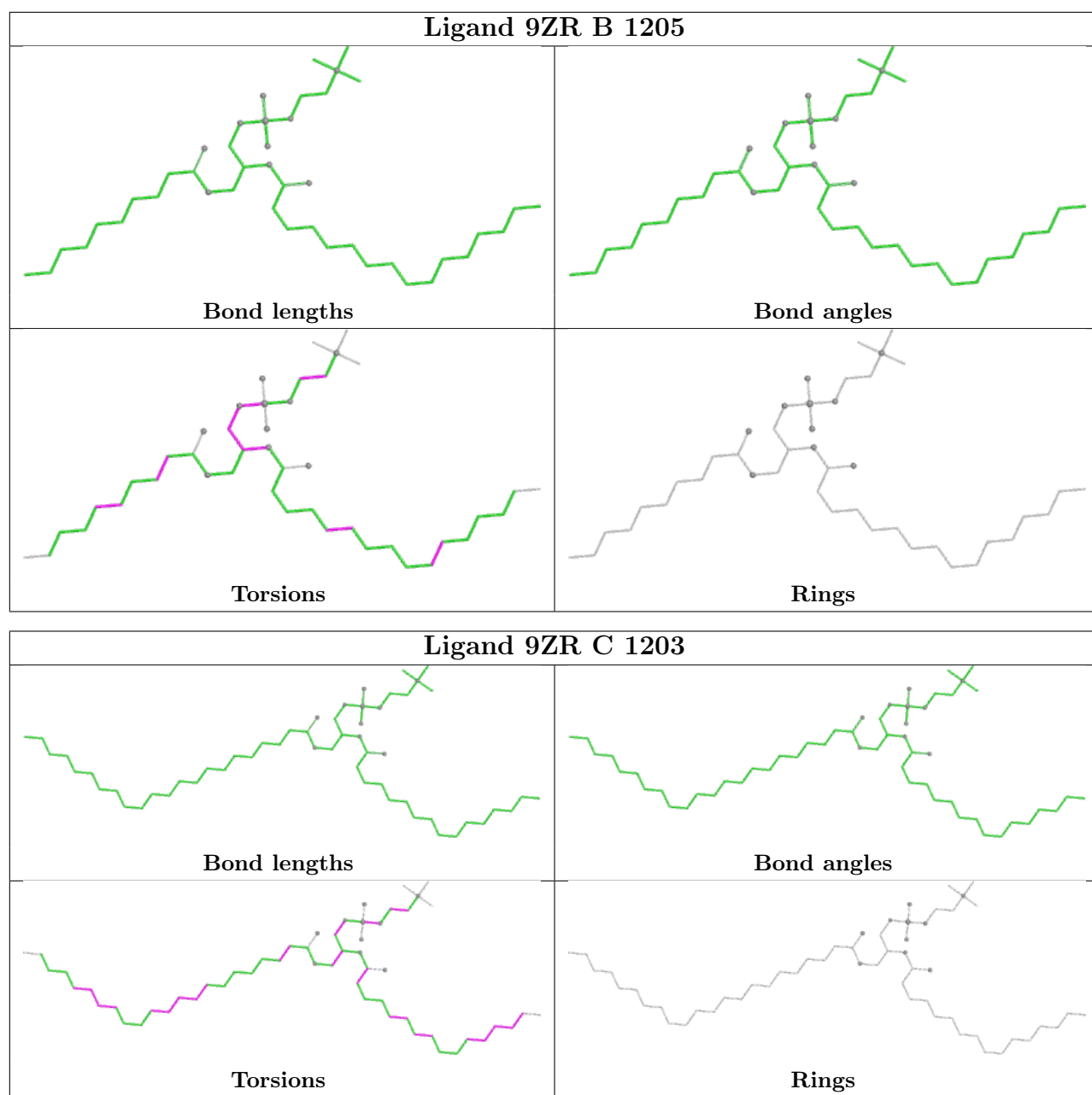


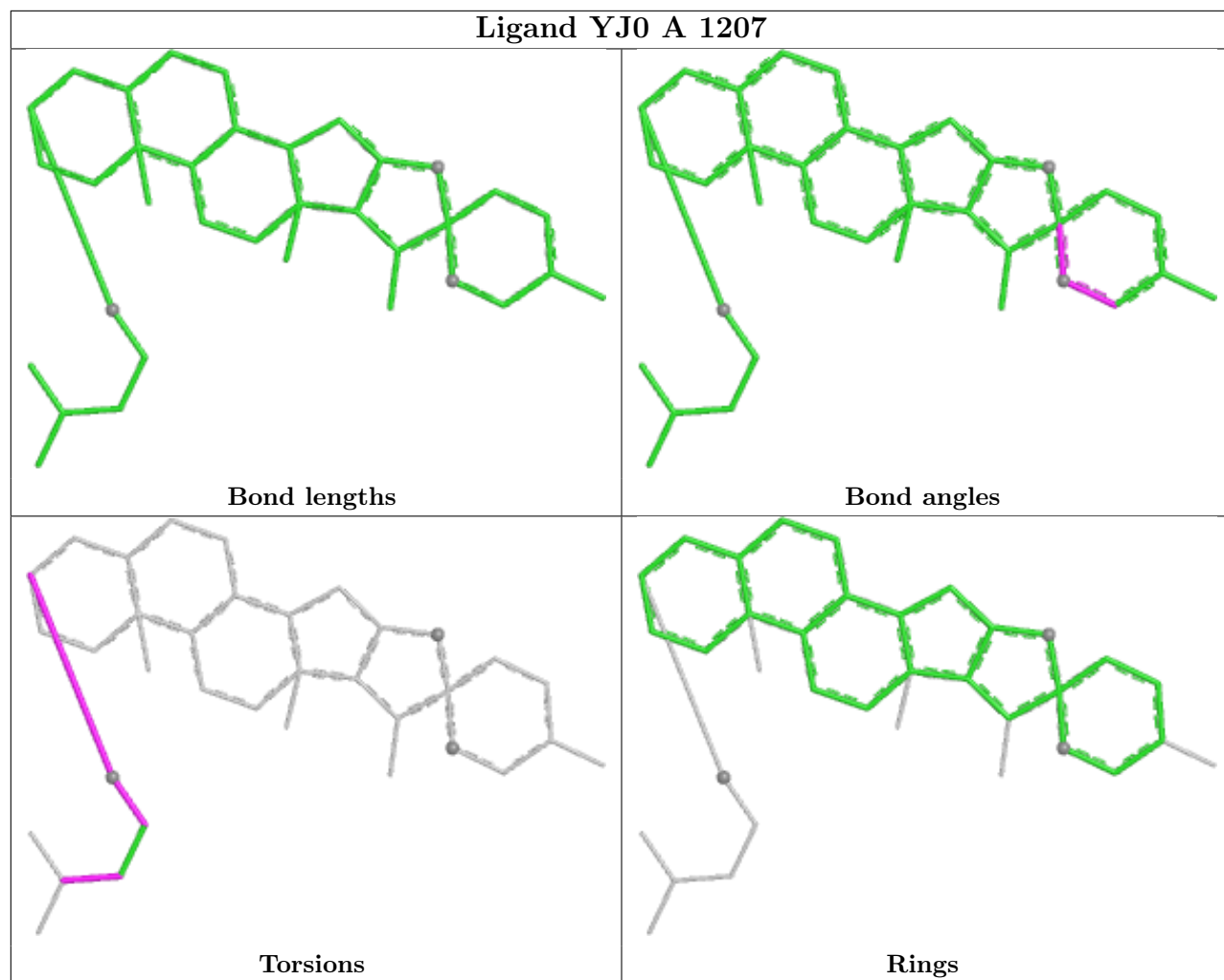


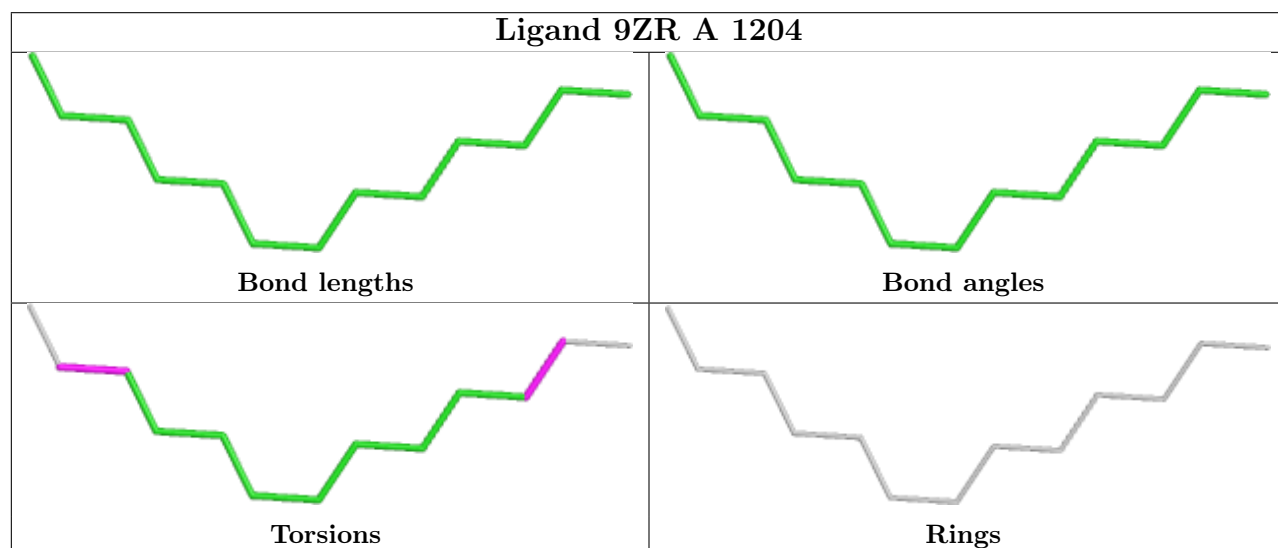
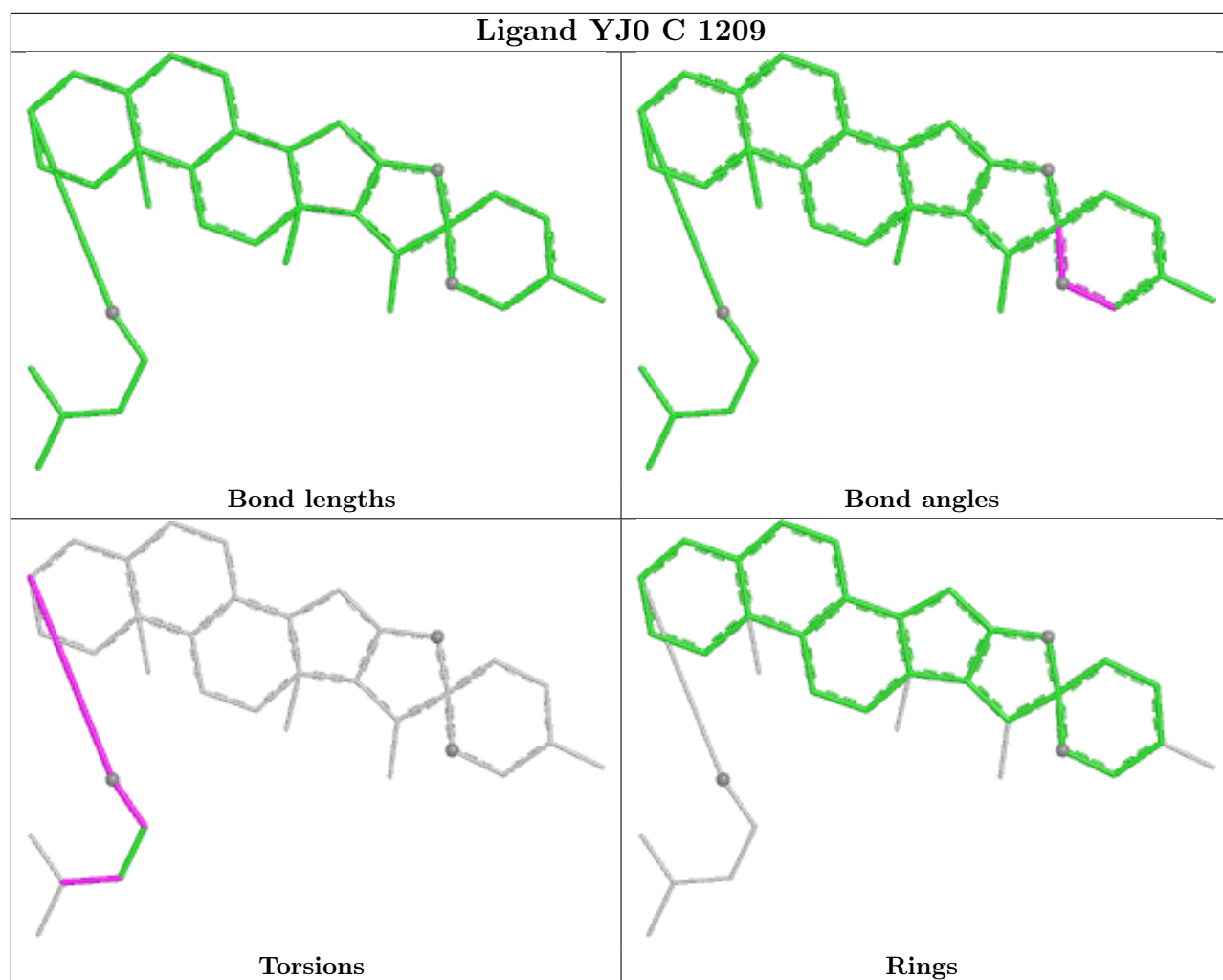


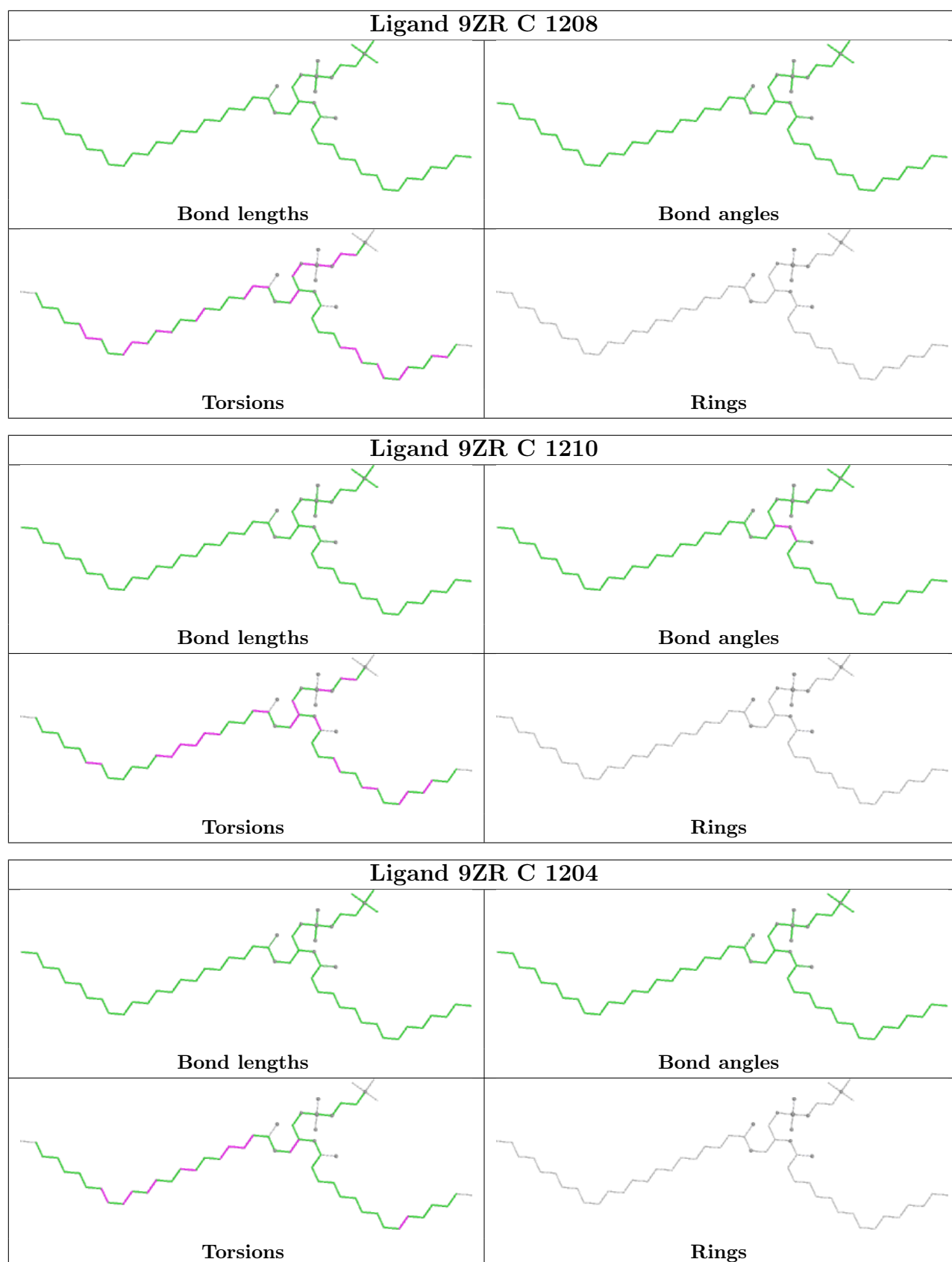


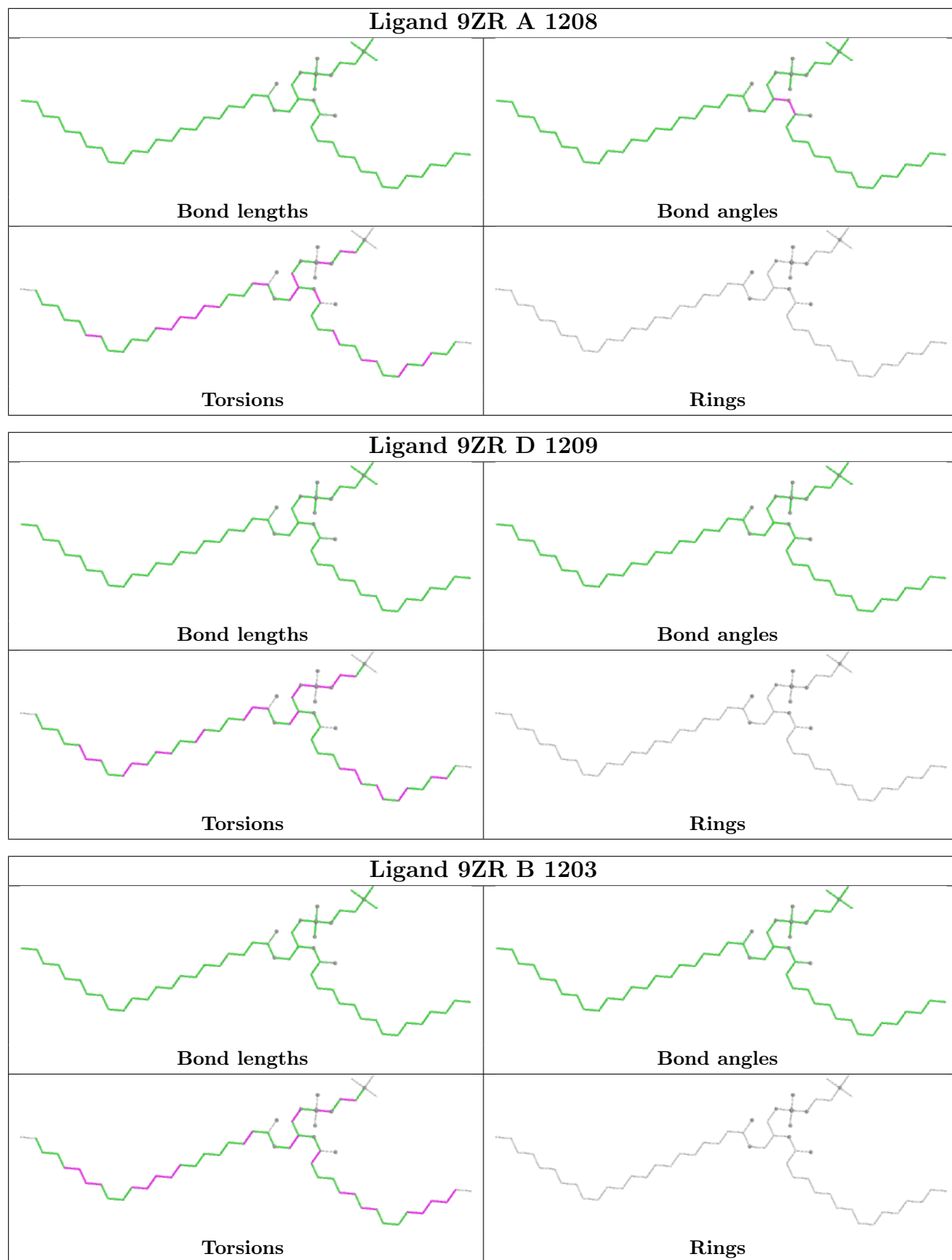


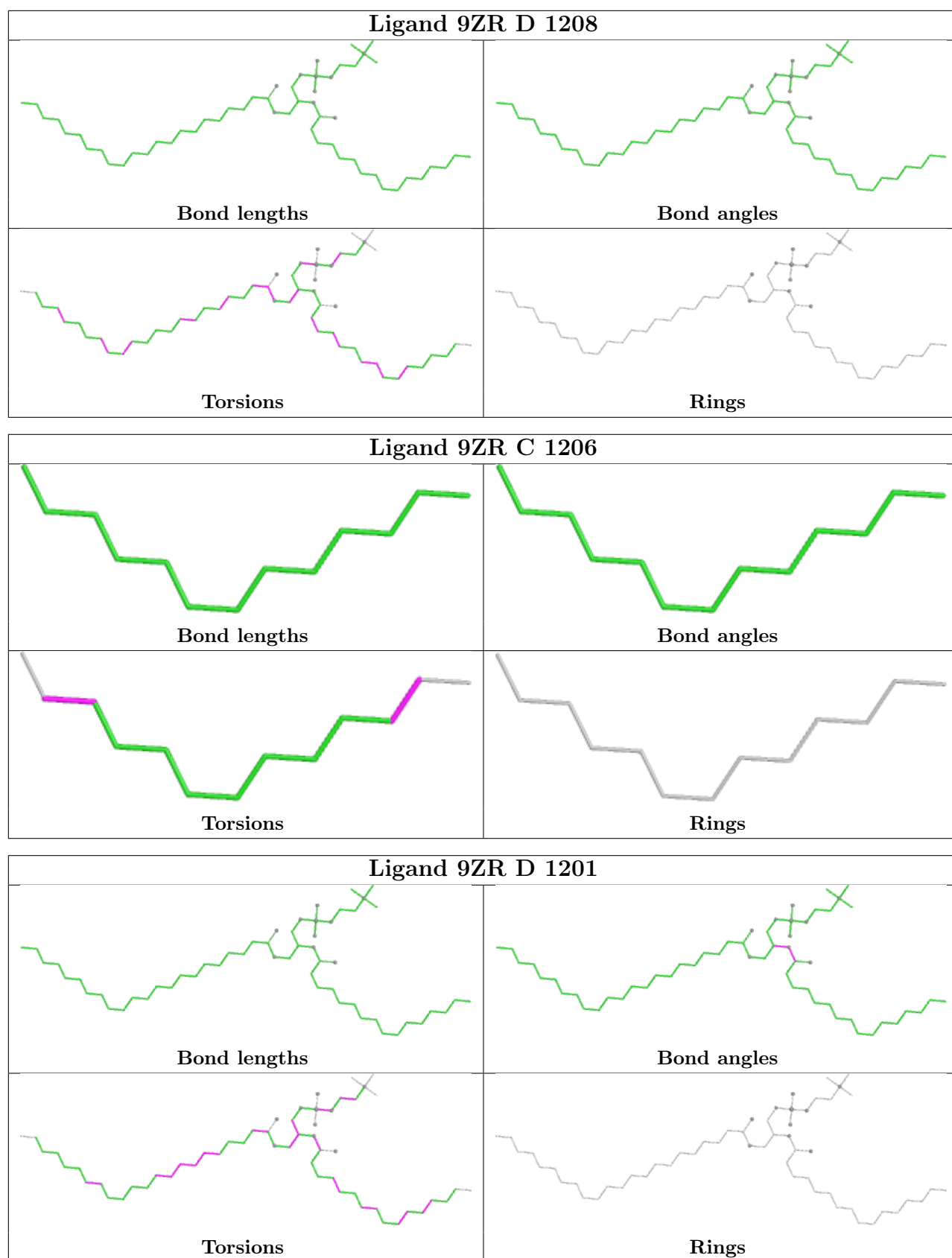


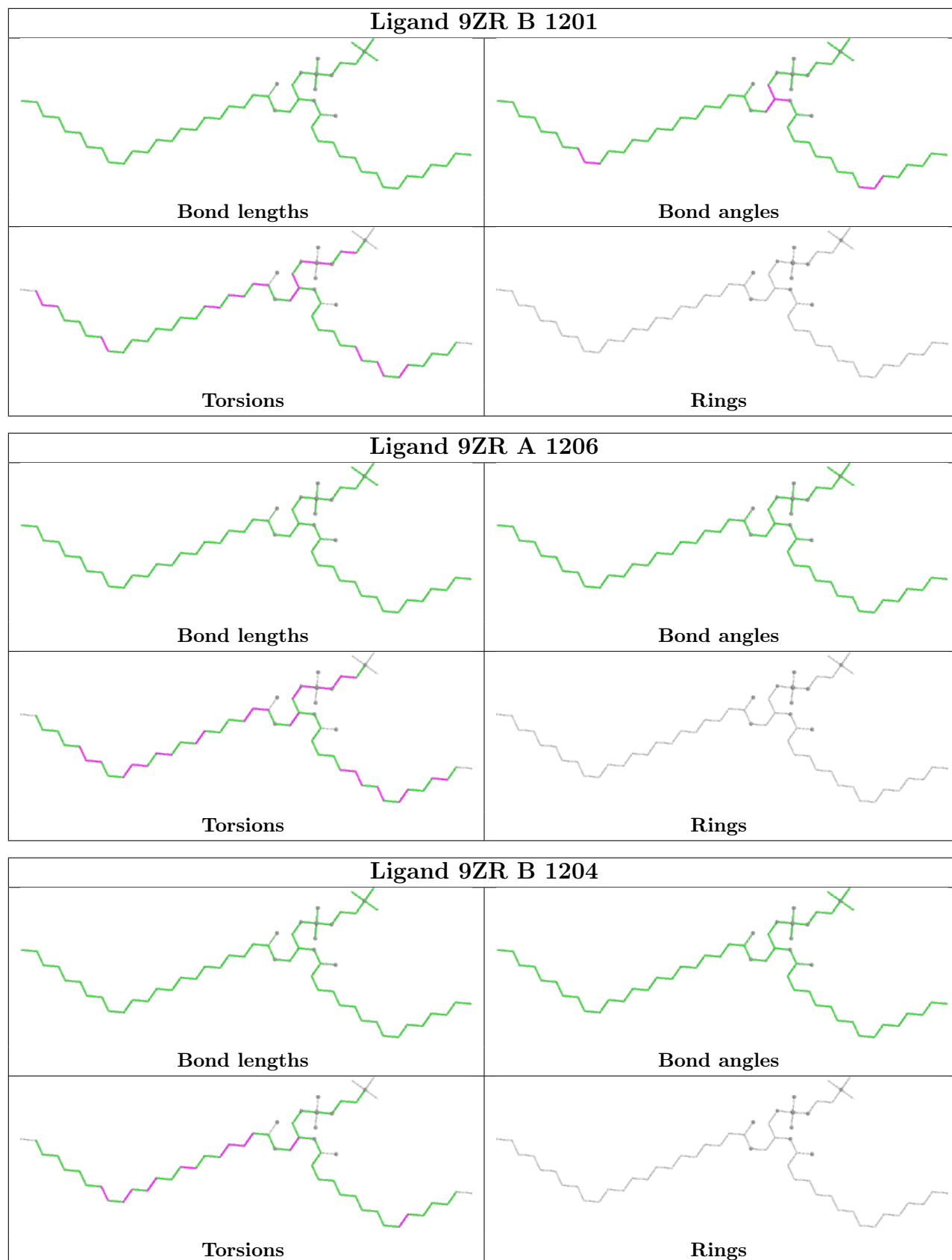


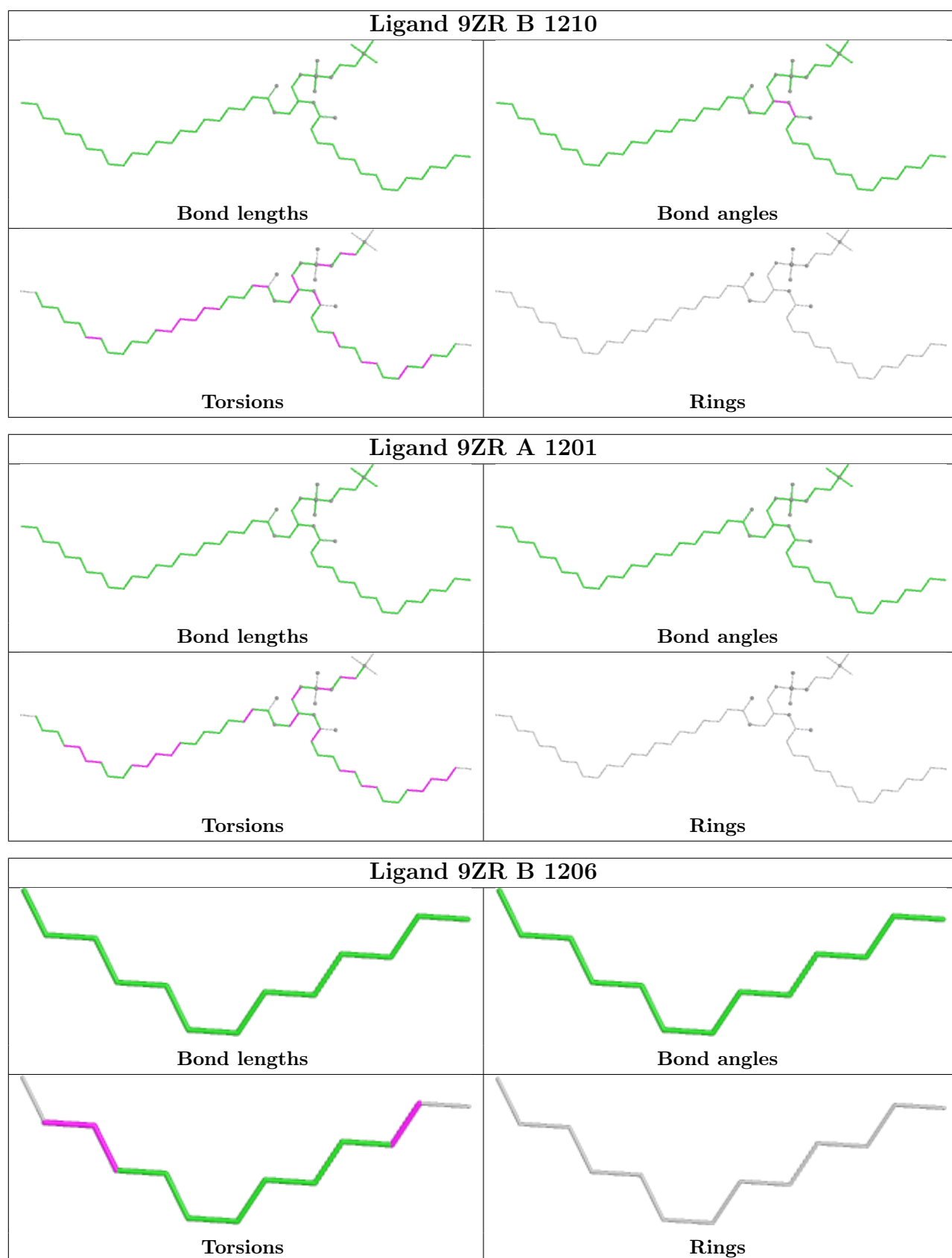


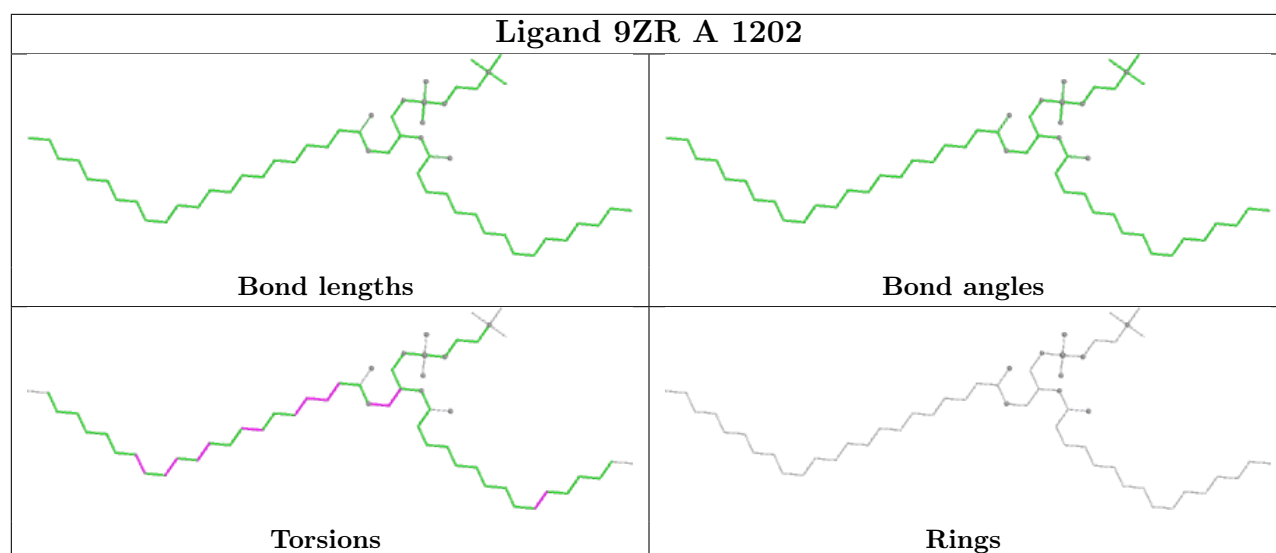












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

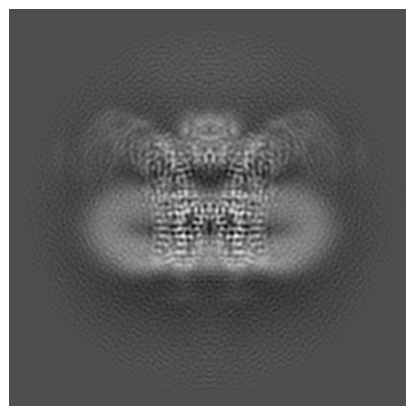
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40961. These allow visual inspection of the internal detail of the map and identification of artifacts.

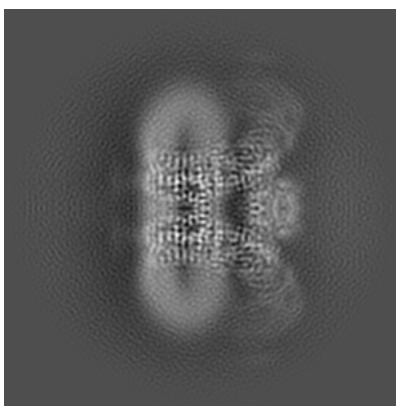
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

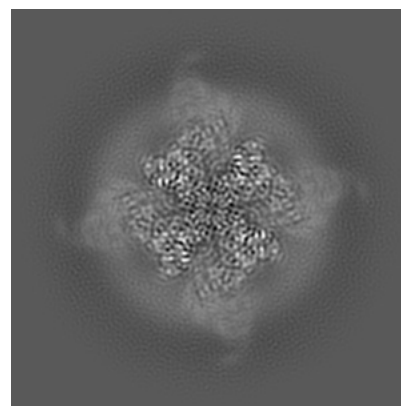
6.1.1 Primary map



X

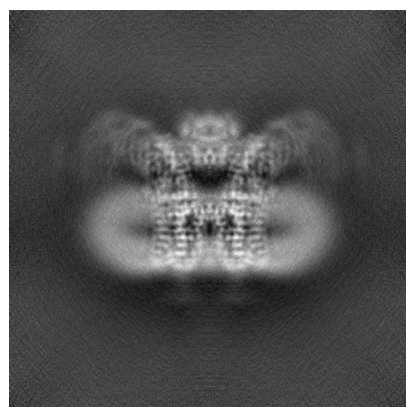


Y

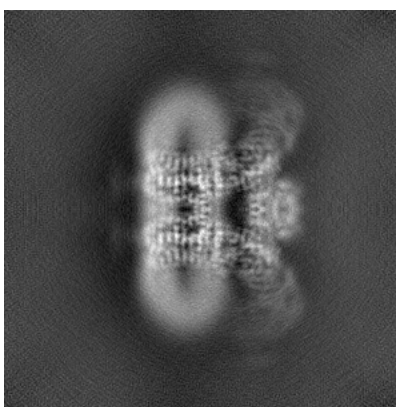


Z

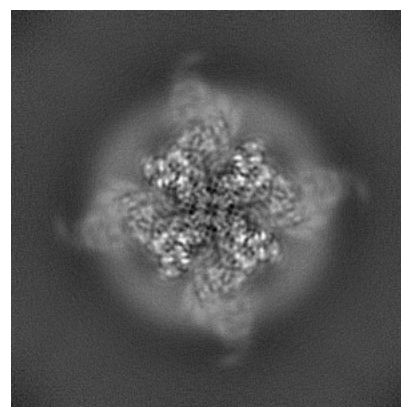
6.1.2 Raw map



X



Y

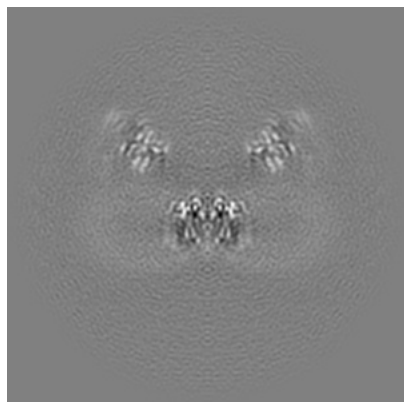


Z

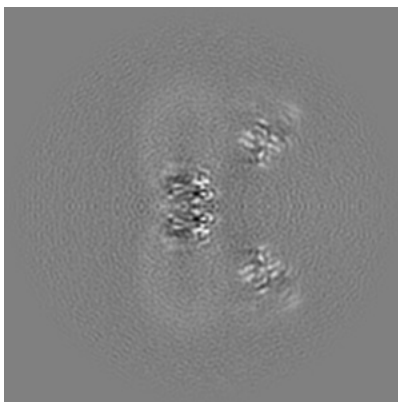
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

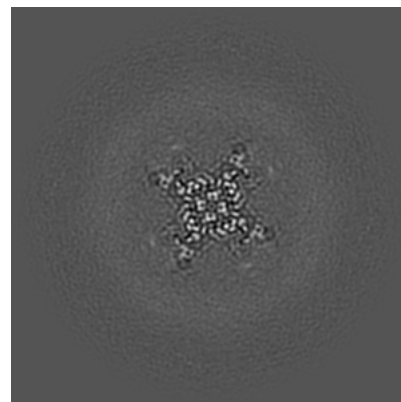
6.2.1 Primary map



X Index: 160

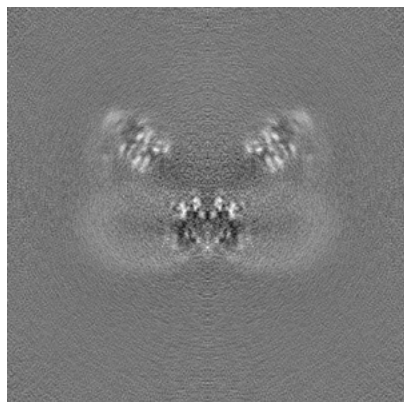


Y Index: 160

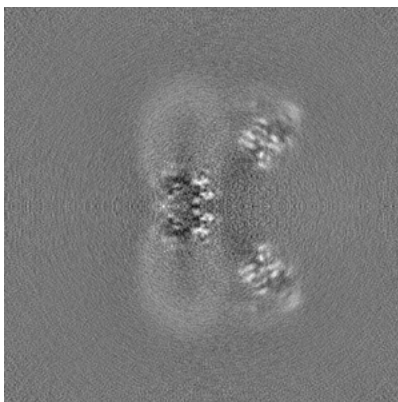


Z Index: 160

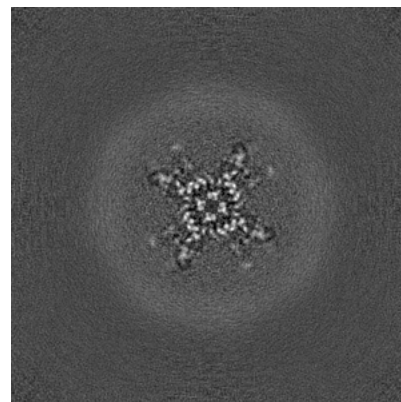
6.2.2 Raw map



X Index: 160



Y Index: 160

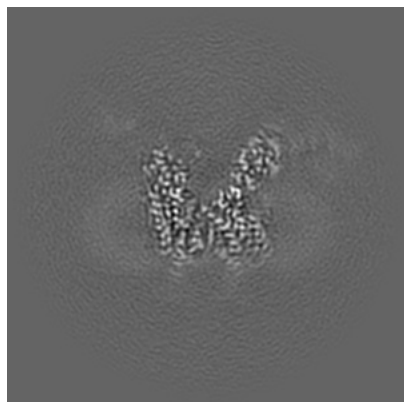


Z Index: 160

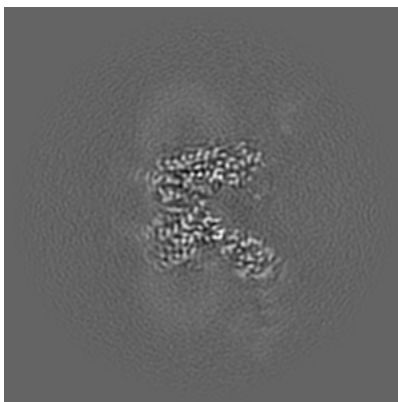
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

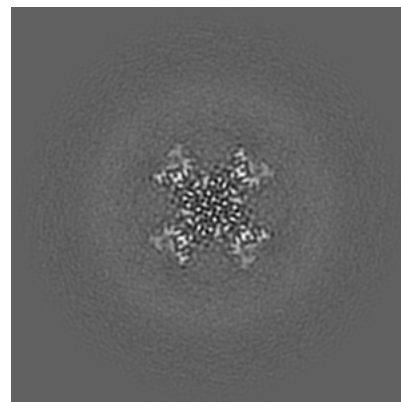
6.3.1 Primary map



X Index: 136

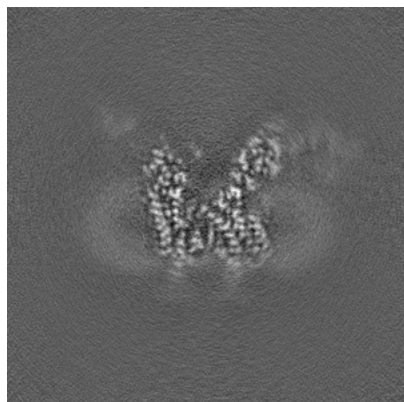


Y Index: 136

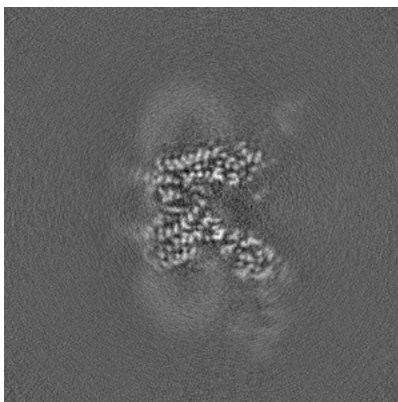


Z Index: 156

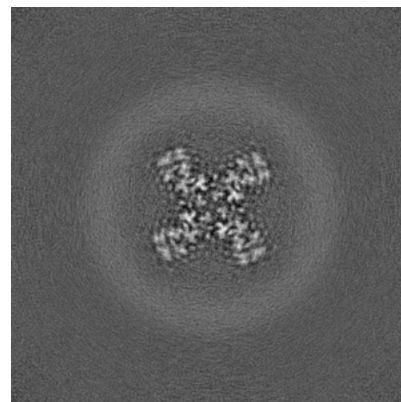
6.3.2 Raw map



X Index: 136



Y Index: 136

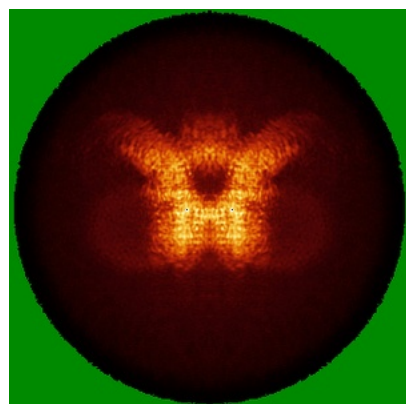


Z Index: 138

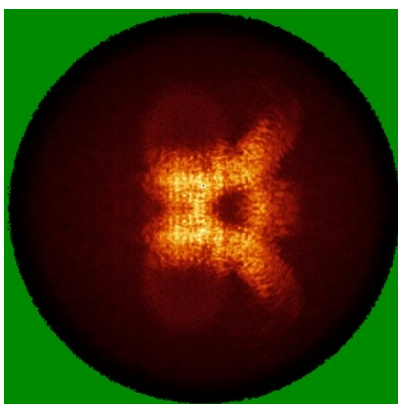
The images above show the largest variance slices of the map in three orthogonal directions.

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

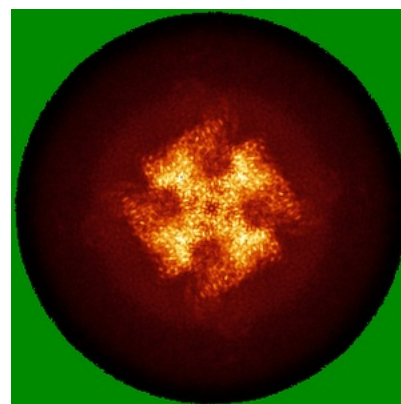
6.4.1 Primary map



X

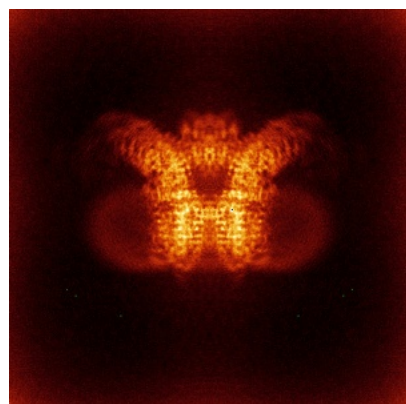


Y

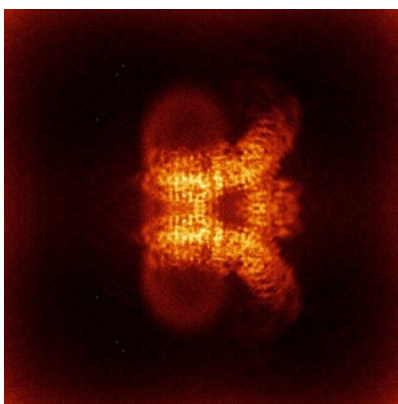


Z

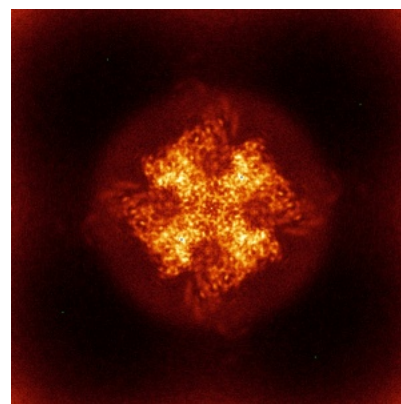
6.4.2 Raw map



X



Y

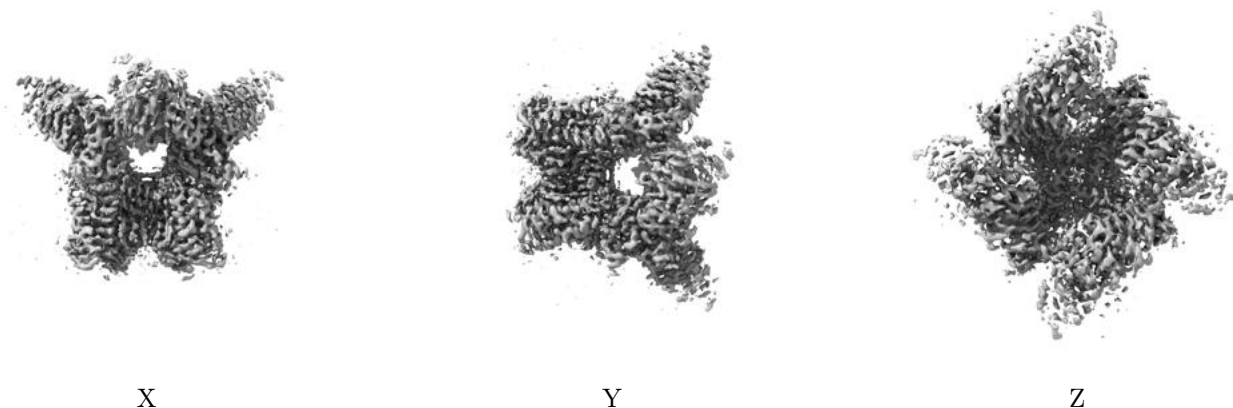


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

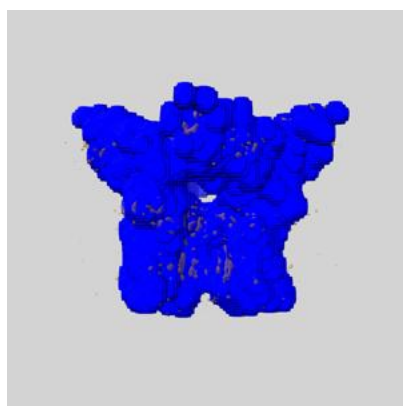
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

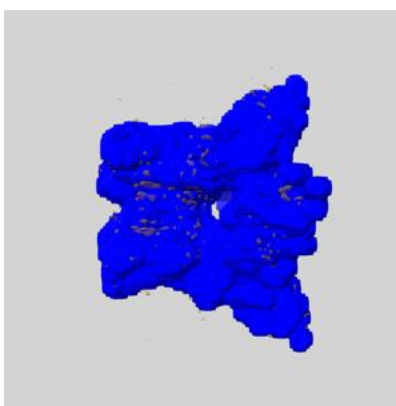
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

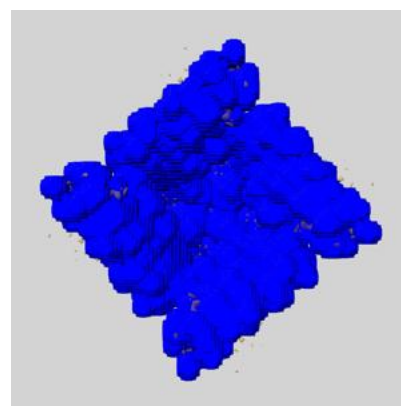
6.6.1 emd_40961_msk_1.map [i](#)



X



Y

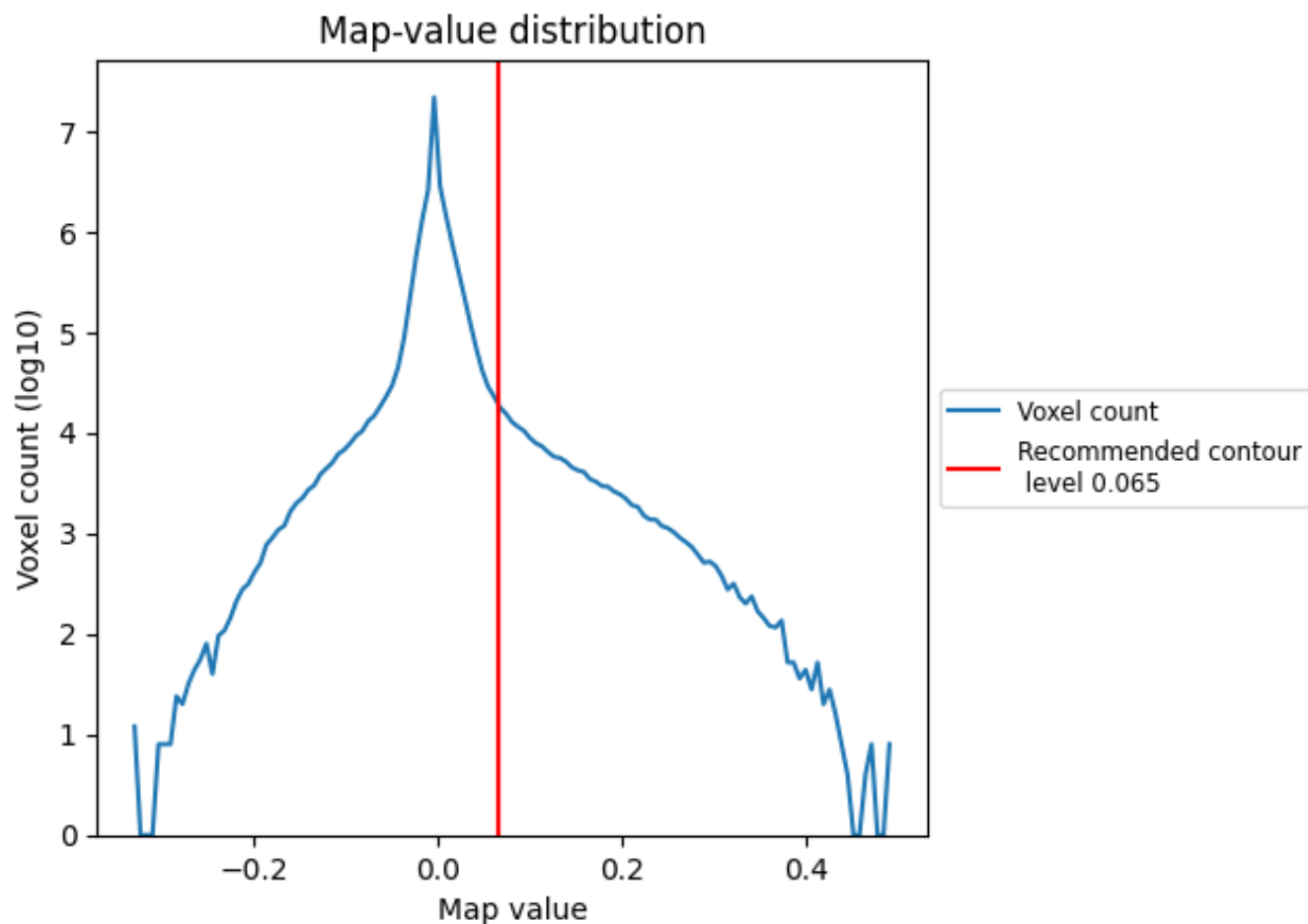


Z

7 Map analysis [i](#)

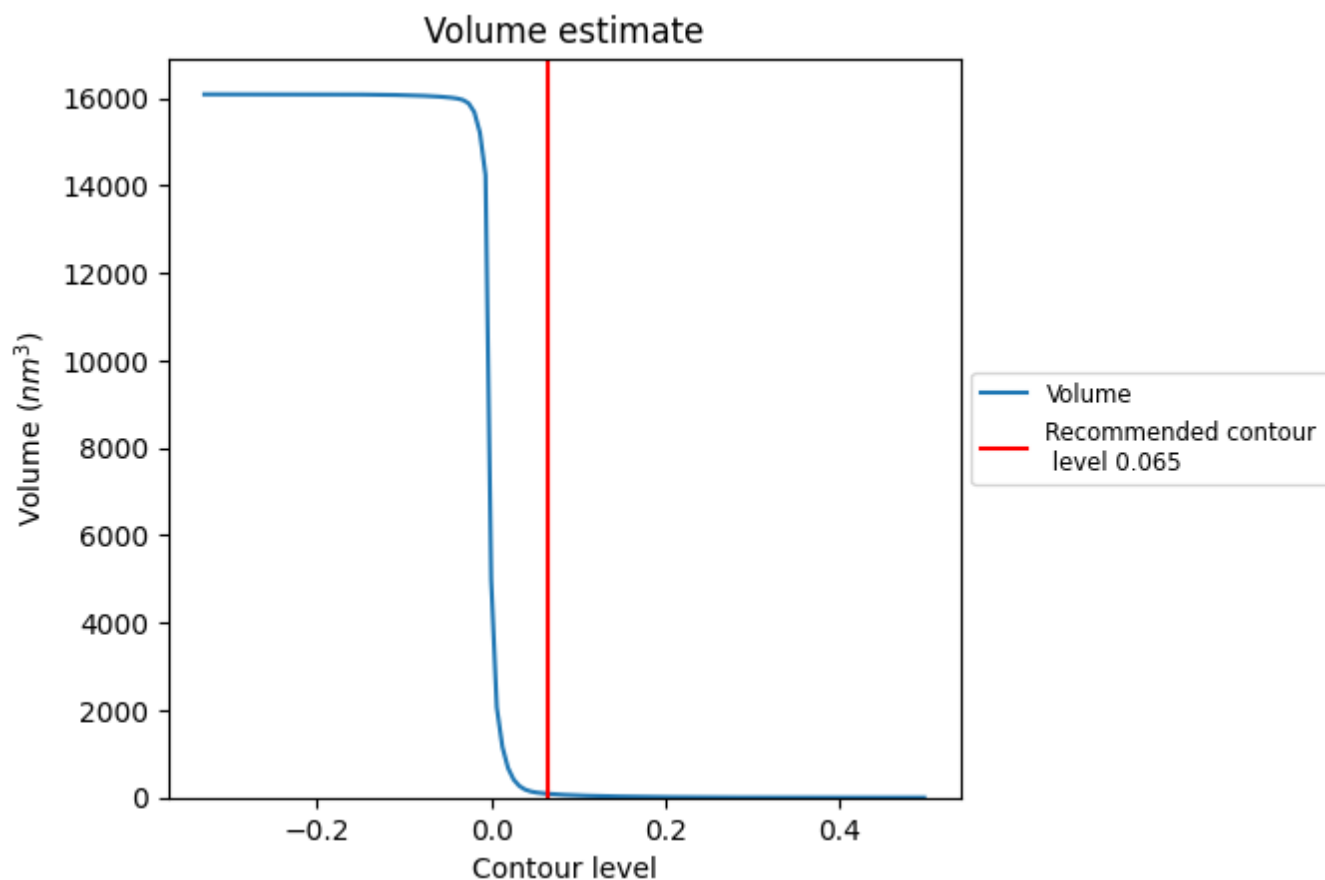
This section contains the results of statistical analysis of the map.

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.

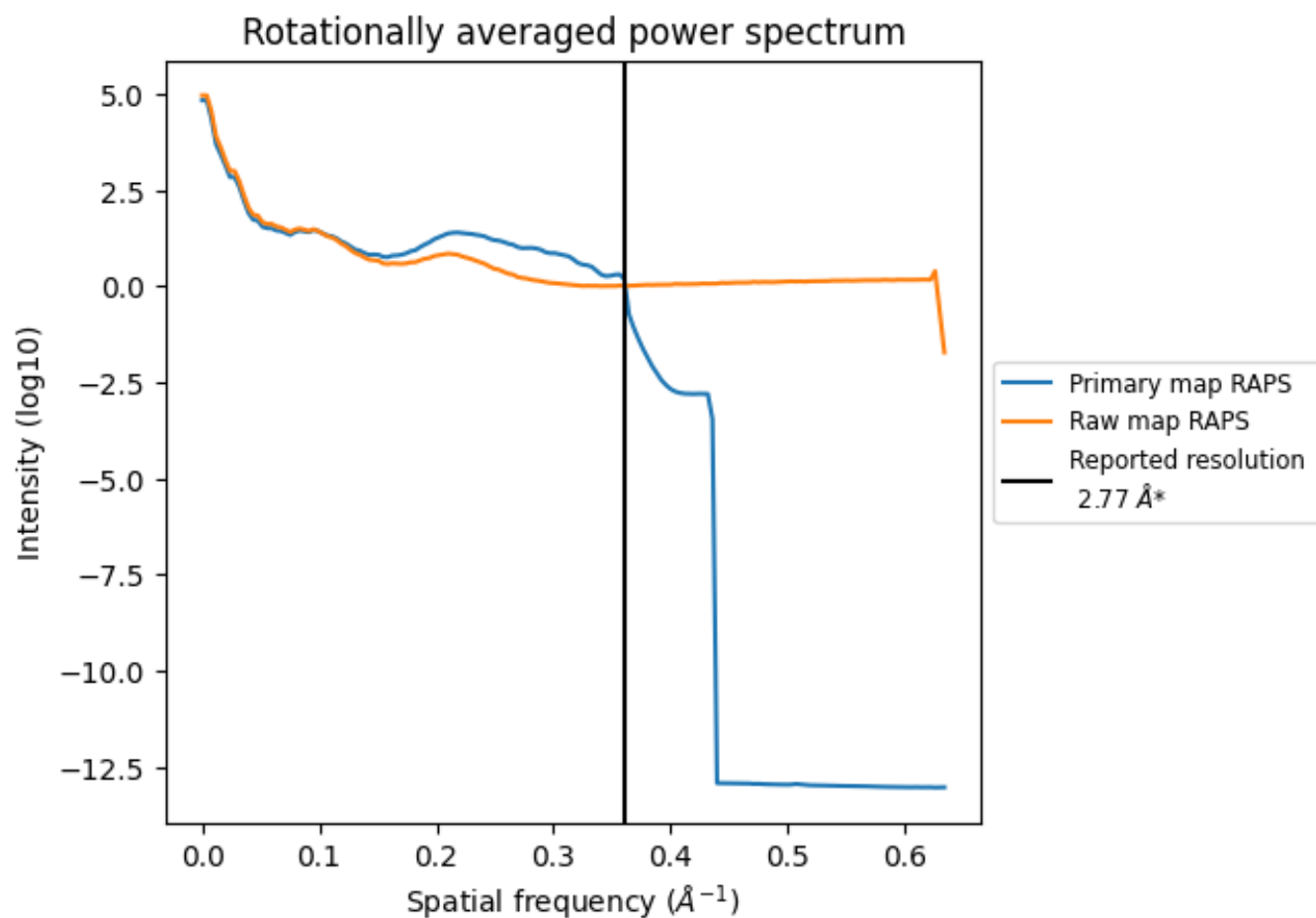
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 78 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 ⓘ

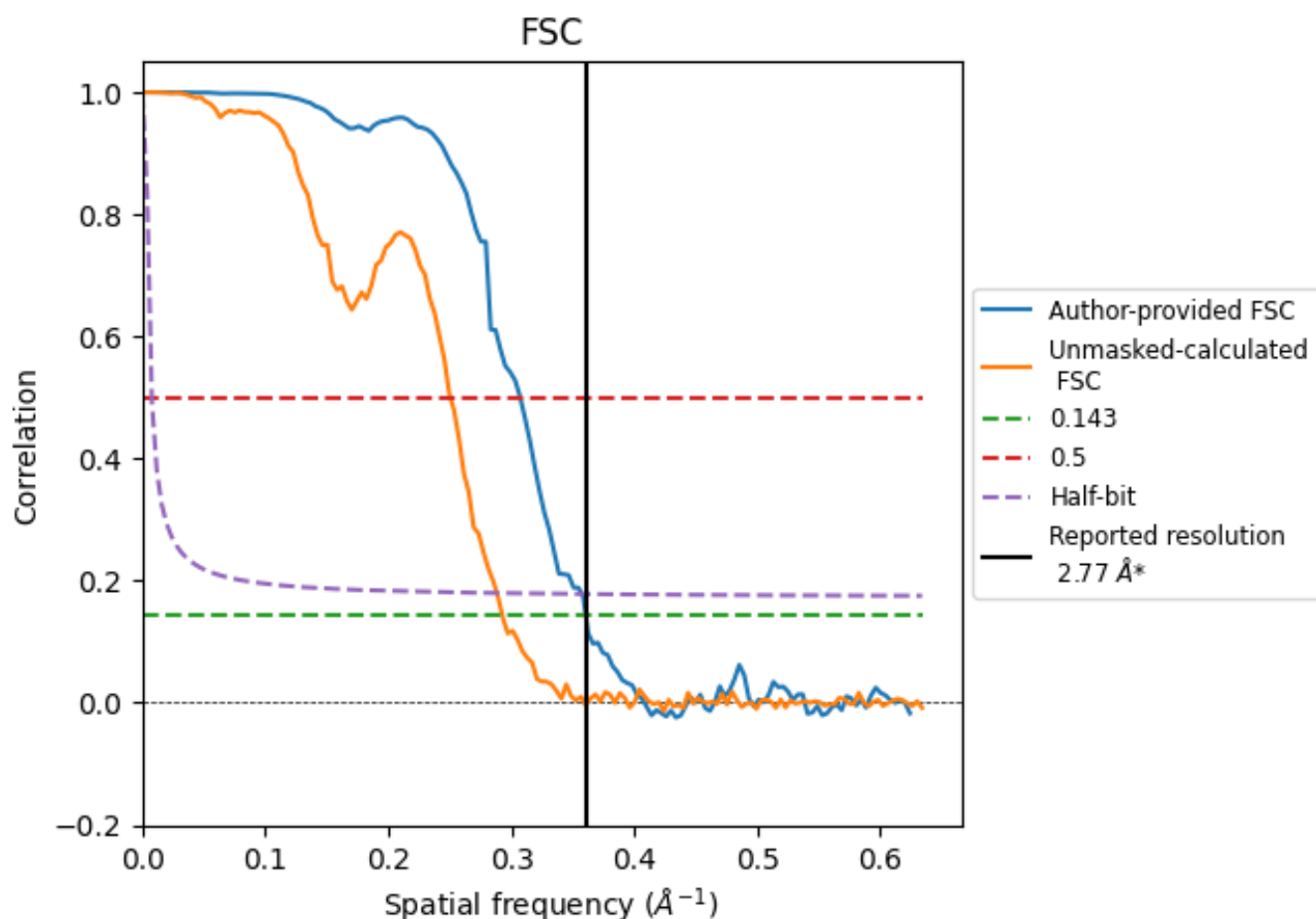


*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

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 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

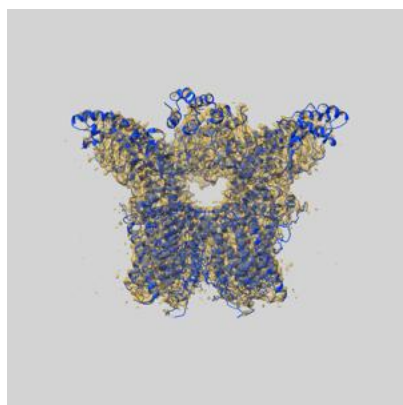
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.25	2.80
Unmasked-calculated*	3.42	3.99	3.47

*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 3.42 differs from the reported value 2.77 by more than 10 %

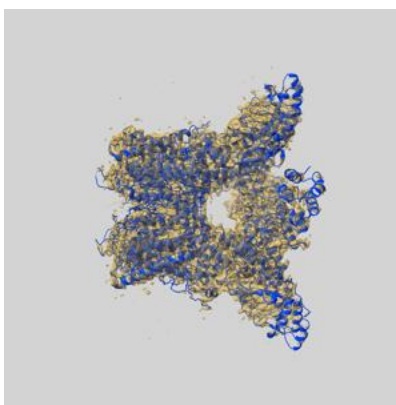
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40961 and PDB model 8T1E. Per-residue inclusion information can be found in section [3](#) on page [10](#).

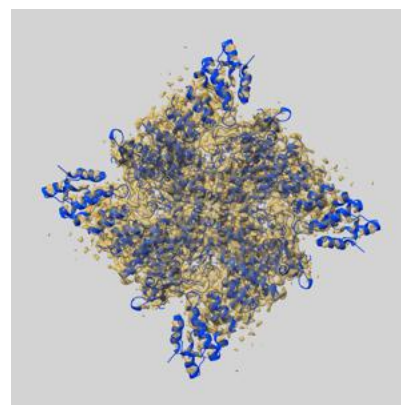
9.1 Map-model overlay [i](#)



X



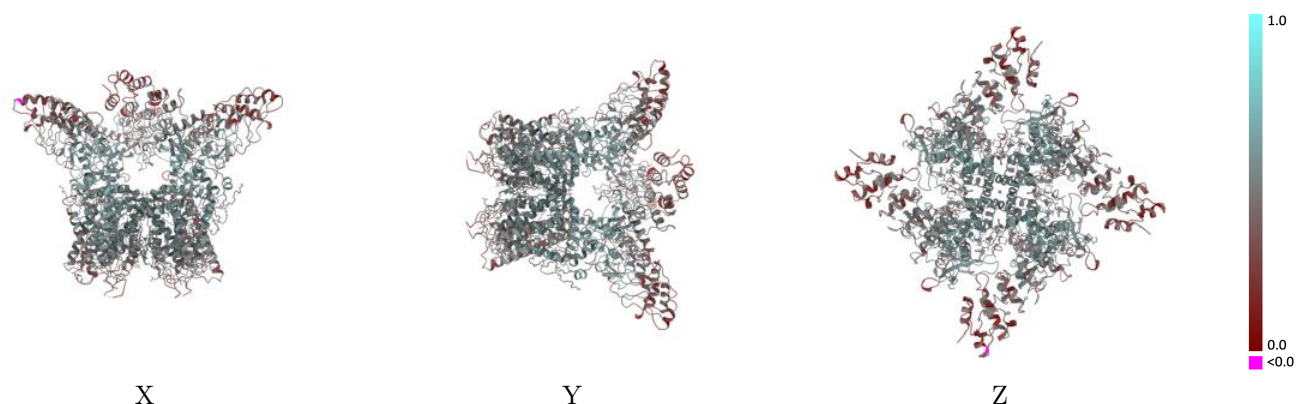
Y



Z

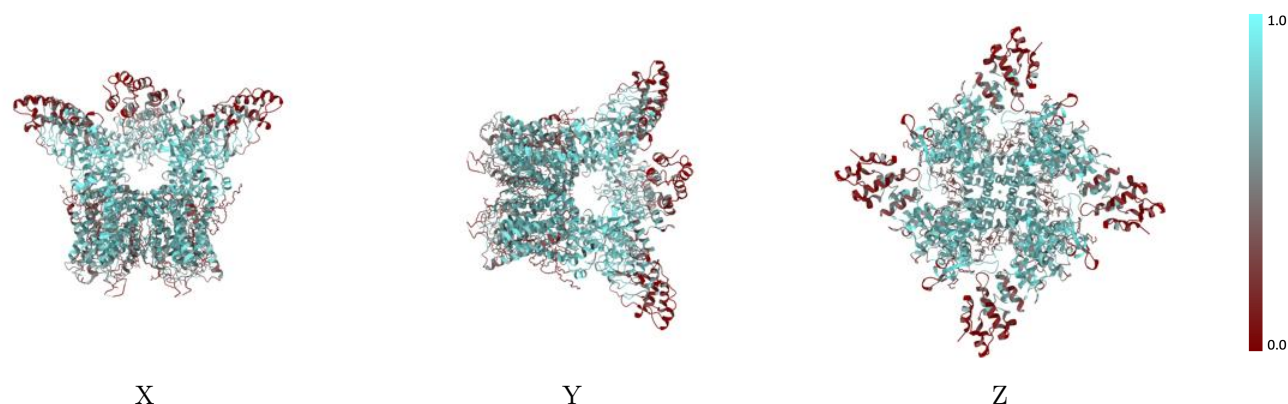
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



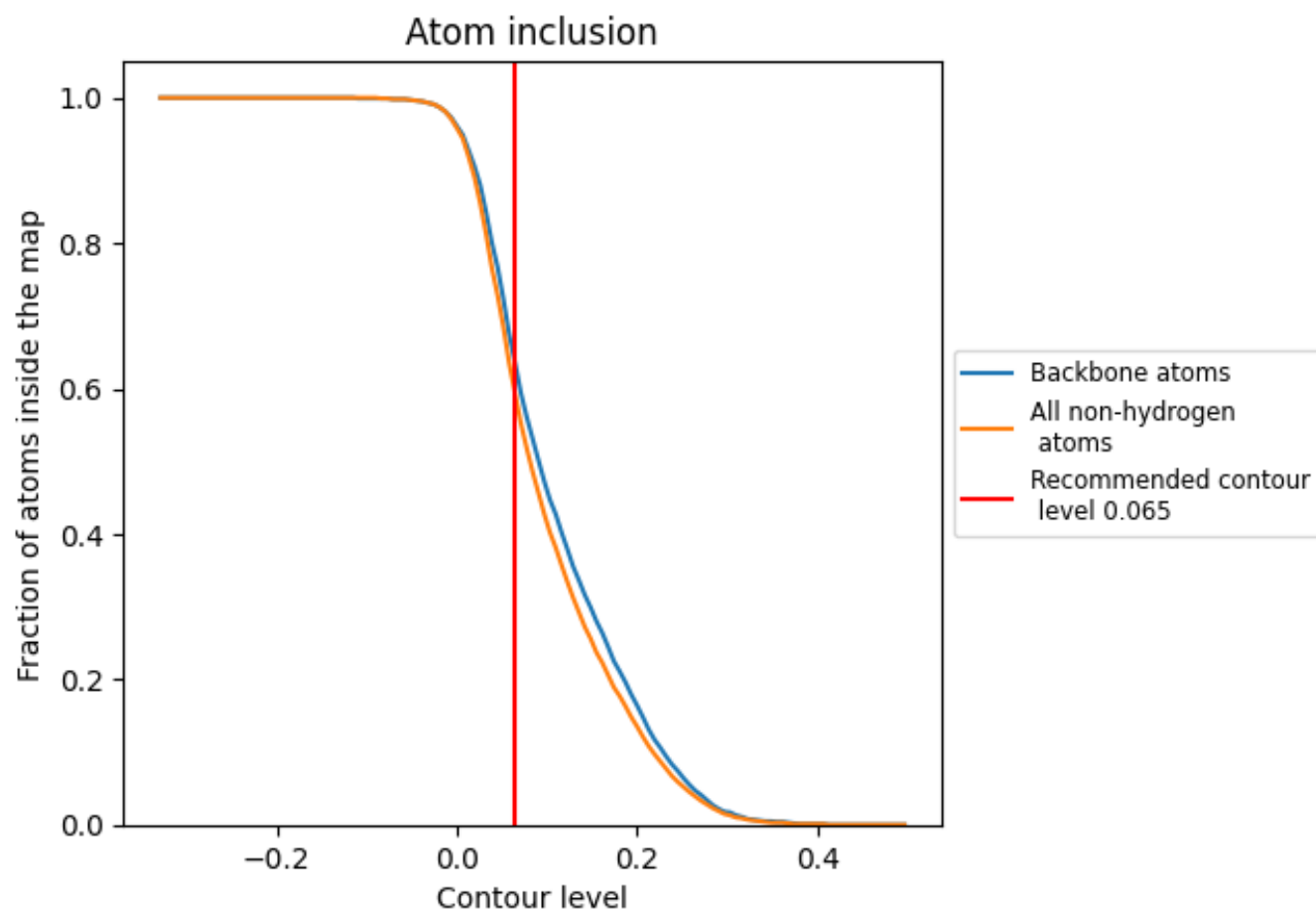
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 59% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.4650
A	0.5950	0.4640
B	0.5960	0.4640
C	0.5950	0.4650
D	0.5960	0.4650

