



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 09:29 PM EST

PDB ID : 6VUM
EMDB ID : EMD-21390
Title : Structure of nevanimibe-bound human tetrameric ACAT1
Authors : Li, X.; Long, T.
Deposited on : 2020-02-16
Resolution : 3.67 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

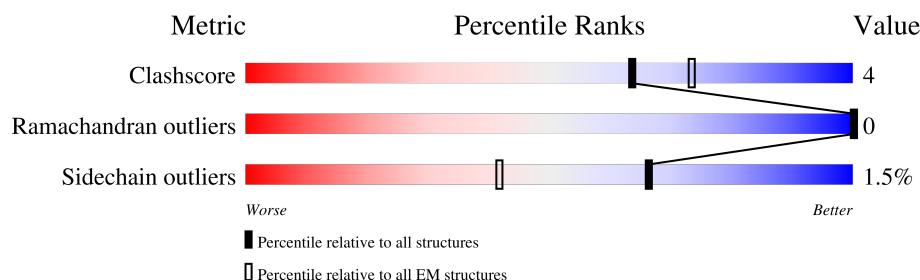
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	558	
1	B	558	
1	C	558	
1	D	558	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14388 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 Sterol O-acyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	409	Total	C	N	O	S	0	0
			3423	2329	537	540	17		
1	B	409	Total	C	N	O	S	0	0
			3423	2329	537	540	17		
1	C	409	Total	C	N	O	S	0	0
			3423	2329	537	540	17		
1	D	409	Total	C	N	O	S	0	0
			3423	2329	537	540	17		

There are 32 discrepancies between the modelled and reference sequences:

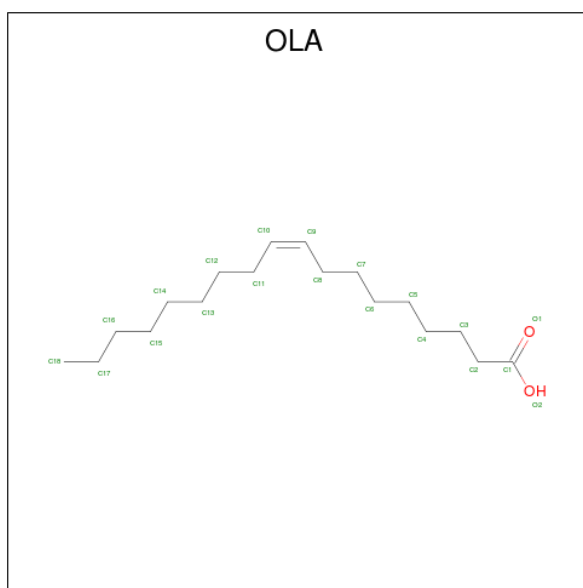
Chain	Residue	Modelled	Actual	Comment	Reference
A	551	ASP	-	expression tag	UNP P35610
A	552	TYR	-	expression tag	UNP P35610
A	553	LYS	-	expression tag	UNP P35610
A	554	ASP	-	expression tag	UNP P35610
A	555	ASP	-	expression tag	UNP P35610
A	556	ASP	-	expression tag	UNP P35610
A	557	ASP	-	expression tag	UNP P35610
A	558	LYS	-	expression tag	UNP P35610
B	551	ASP	-	expression tag	UNP P35610
B	552	TYR	-	expression tag	UNP P35610
B	553	LYS	-	expression tag	UNP P35610
B	554	ASP	-	expression tag	UNP P35610
B	555	ASP	-	expression tag	UNP P35610
B	556	ASP	-	expression tag	UNP P35610
B	557	ASP	-	expression tag	UNP P35610
B	558	LYS	-	expression tag	UNP P35610
C	551	ASP	-	expression tag	UNP P35610
C	552	TYR	-	expression tag	UNP P35610
C	553	LYS	-	expression tag	UNP P35610
C	554	ASP	-	expression tag	UNP P35610
C	555	ASP	-	expression tag	UNP P35610
C	556	ASP	-	expression tag	UNP P35610

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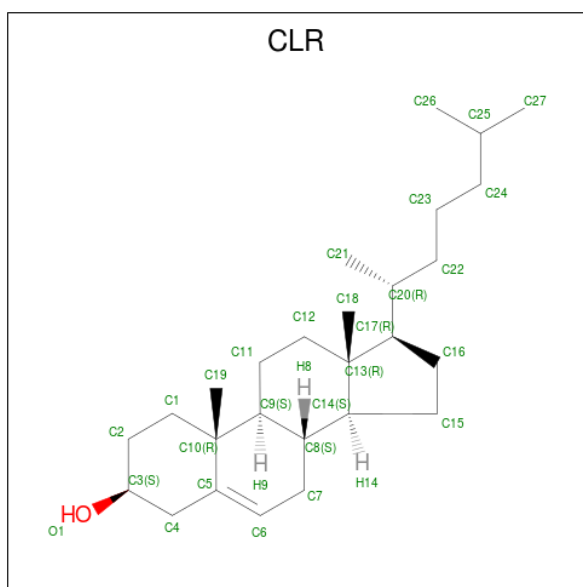
Chain	Residue	Modelled	Actual	Comment	Reference
C	557	ASP	-	expression tag	UNP P35610
C	558	LYS	-	expression tag	UNP P35610
D	551	ASP	-	expression tag	UNP P35610
D	552	TYR	-	expression tag	UNP P35610
D	553	LYS	-	expression tag	UNP P35610
D	554	ASP	-	expression tag	UNP P35610
D	555	ASP	-	expression tag	UNP P35610
D	556	ASP	-	expression tag	UNP P35610
D	557	ASP	-	expression tag	UNP P35610
D	558	LYS	-	expression tag	UNP P35610

- Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



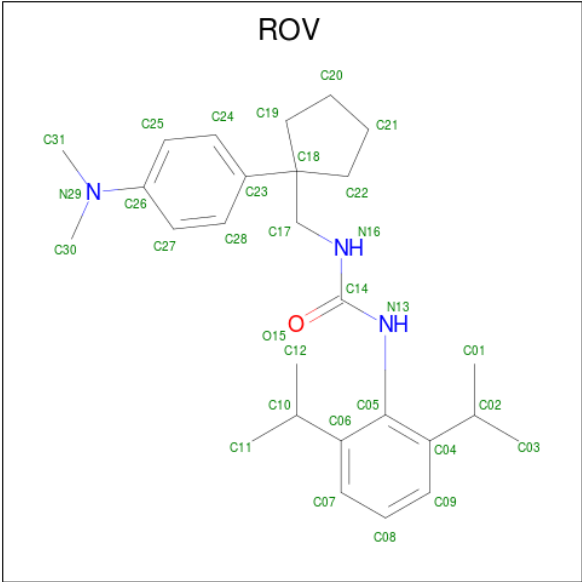
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			20	18	2	
2	B	1	Total	C	O	0
			20	18	2	
2	C	1	Total	C	O	0
			20	18	2	
2	D	1	Total	C	O	0
			20	18	2	

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



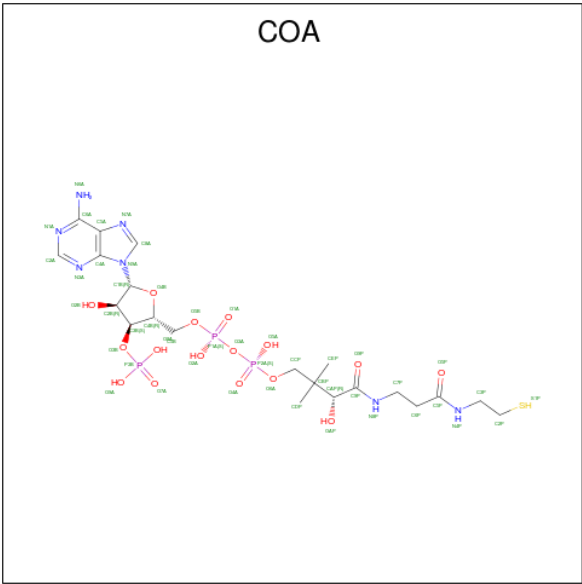
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			84	81	3	
3	A	1	Total	C	O	0
			84	81	3	
3	A	1	Total	C	O	0
			84	81	3	
3	B	1	Total	C	O	0
			56	54	2	
3	B	1	Total	C	O	0
			56	54	2	
3	C	1	Total	C	O	0
			84	81	3	
3	C	1	Total	C	O	0
			84	81	3	
3	C	1	Total	C	O	0
			84	81	3	
3	D	1	Total	C	O	0
			56	54	2	
3	D	1	Total	C	O	0
			56	54	2	

- Molecule 4 is nevanimibe (three-letter code: ROV) (formula: $C_{27}H_{39}N_3O$) (labeled as "Ligand of Interest" by depositor).



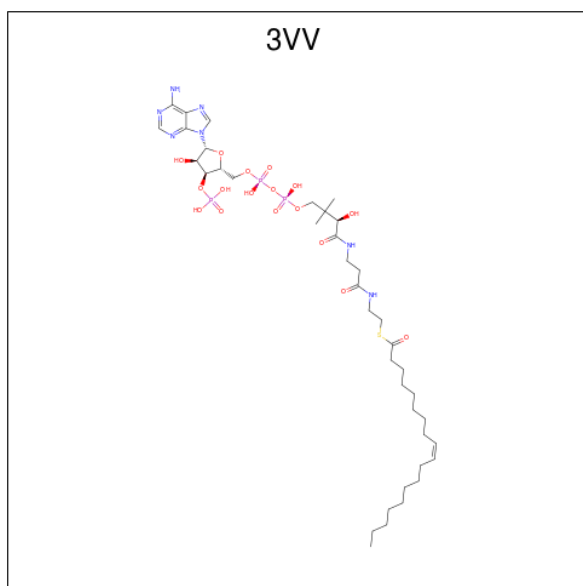
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			31	27	3	1	
4	B	1	Total	C	N	O	0
			31	27	3	1	
4	C	1	Total	C	N	O	0
			31	27	3	1	
4	D	1	Total	C	N	O	0
			31	27	3	1	

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	
5	C	1	Total	C	N	O	P	S	0
			48	21	7	16	3	1	

- Molecule 6 is S-{(3R,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4,6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} (9Z)-octadec-9-ene thioate (non-preferred name) (three-letter code: 3VV) (formula: C₃₉H₆₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).

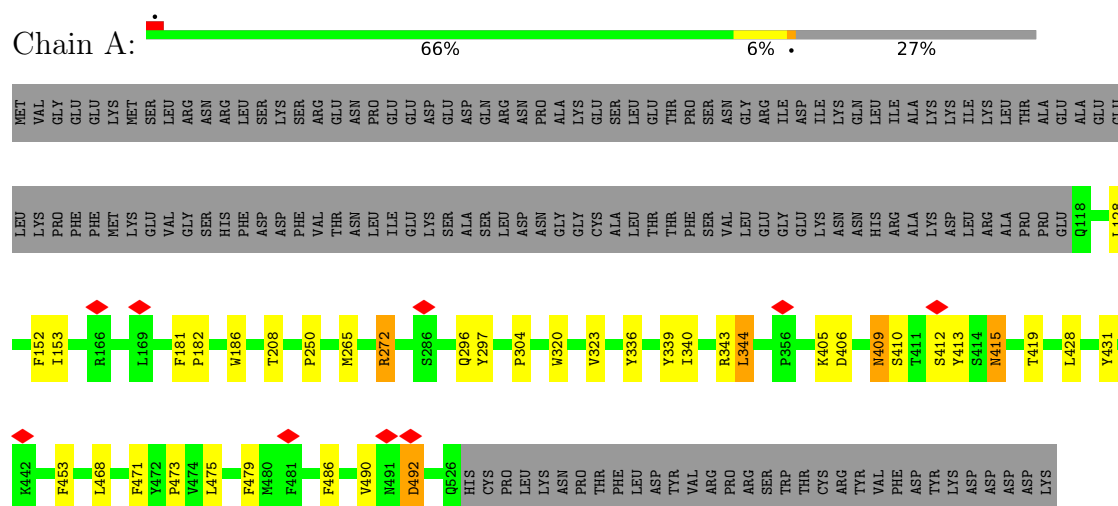


Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	N	O	P	S	0
			58	30	7	17	3	1	
6	D	1	Total	C	N	O	P	S	0
			58	30	7	17	3	1	

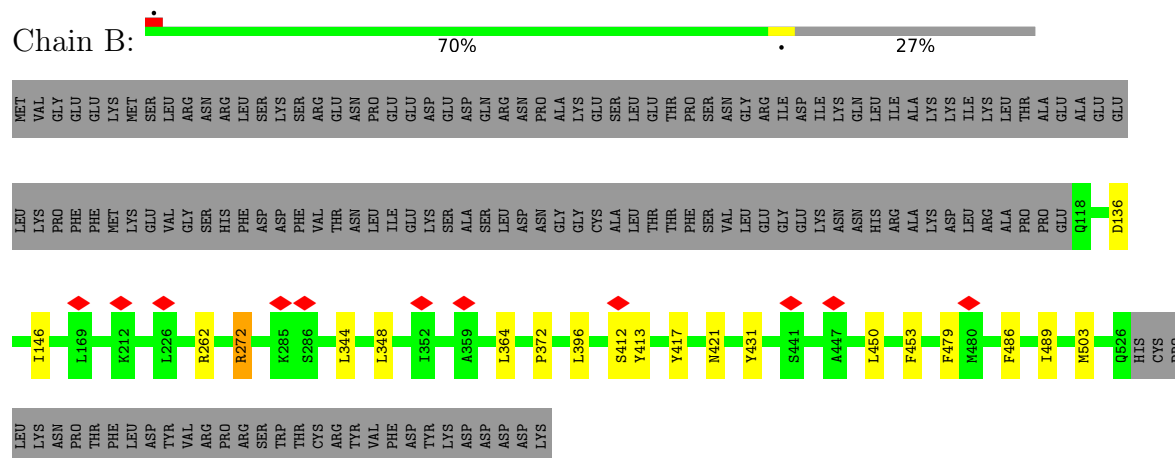
3 Residue-property plots

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: Sterol O-acyltransferase 1

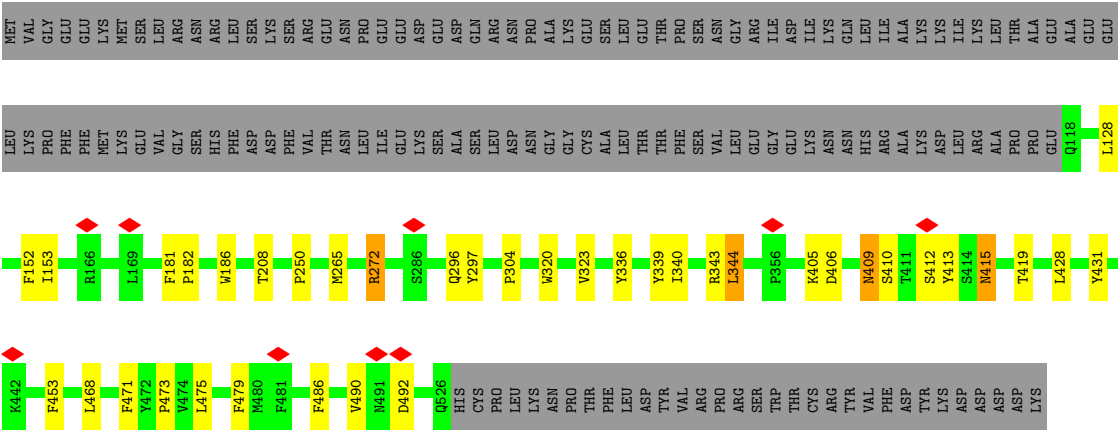


• Molecule 1: Sterol O-acyltransferase 1

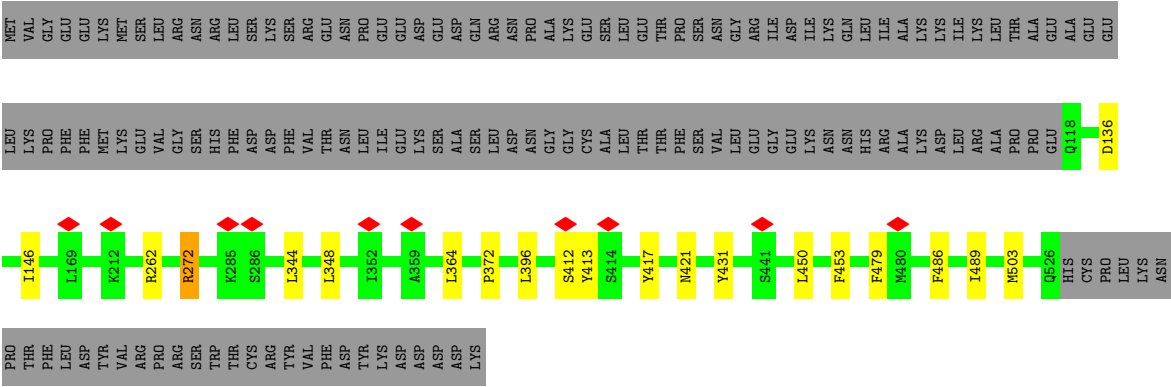


• Molecule 1: Sterol O-acyltransferase 1





● Molecule 1: Sterol O-acyltransferase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0094	Depositor
Map size (\AA)	274.89, 274.89, 274.89	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83300006, 0.83300006, 0.83300006	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: COA, CLR, 3VV, OLA, ROV

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	0/3552	0.55	0/4840
1	B	0.41	0/3552	0.55	0/4840
1	C	0.41	0/3552	0.55	0/4840
1	D	0.41	0/3552	0.55	0/4840
All	All	0.41	0/14208	0.55	0/19360

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3358	44	0
1	B	3423	0	3358	14	0
1	C	3423	0	3358	42	0
1	D	3423	0	3358	14	0
2	A	20	0	33	4	0
2	B	20	0	33	1	0
2	C	20	0	33	4	0
2	D	20	0	33	1	0
3	A	84	0	138	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	92	1	0
3	C	84	0	138	7	0
3	D	56	0	92	1	0
4	A	31	0	0	0	0
4	B	31	0	0	1	0
4	C	31	0	0	0	0
4	D	31	0	0	1	0
5	A	48	0	32	2	0
5	C	48	0	32	2	0
6	B	58	0	45	4	0
6	D	58	0	45	4	0
All	All	14388	0	14178	122	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 (122) 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)
6:B:702:3VV:C49	6:B:702:3VV:O48	1.69	1.25
6:D:702:3VV:O48	6:D:702:3VV:C49	1.69	1.18
1:C:340:ILE:HD12	1:C:344:LEU:HD21	1.70	0.73
1:A:340:ILE:HD12	1:A:344:LEU:HD21	1.70	0.73
1:C:340:ILE:HA	1:C:344:LEU:HD13	1.72	0.71
3:A:703:CLR:H212	3:A:703:CLR:H183	1.73	0.70
1:A:340:ILE:HG23	1:A:344:LEU:HD22	1.74	0.70
3:C:703:CLR:H212	3:C:703:CLR:H183	1.73	0.70
1:A:340:ILE:HA	1:A:344:LEU:HD13	1.72	0.69
1:C:340:ILE:HG23	1:C:344:LEU:HD22	1.74	0.68
1:C:340:ILE:HD12	1:C:344:LEU:CD2	2.24	0.68
1:A:340:ILE:HD12	1:A:344:LEU:CD2	2.24	0.67
1:C:152:PHE:CE2	1:C:344:LEU:HD11	2.33	0.64
1:A:152:PHE:CE2	1:A:344:LEU:HD11	2.33	0.64
1:C:428:LEU:HD21	2:C:701:OLA:H181	1.80	0.63
1:A:428:LEU:HD21	2:A:701:OLA:H181	1.80	0.63
1:C:412:SER:O	1:C:490:VAL:HG11	2.00	0.62
1:D:262:ARG:HE	2:D:701:OLA:H31	1.66	0.61
1:B:262:ARG:HE	2:B:701:OLA:H31	1.66	0.60
1:A:412:SER:O	1:A:490:VAL:HG11	2.00	0.60
1:D:344:LEU:HB3	1:D:372:PRO:HG3	1.85	0.59
1:C:410:SER:HB2	1:C:415:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HB3	1:B:372:PRO:HG3	1.85	0.58
1:A:410:SER:HB2	1:A:415:ASN:HD21	1.67	0.58
1:C:343:ARG:NH2	1:D:364:LEU:HD22	2.20	0.57
1:C:344:LEU:HD12	1:C:344:LEU:N	2.21	0.56
1:C:340:ILE:O	1:C:344:LEU:HB2	2.06	0.56
1:A:409:ASN:OD1	1:A:409:ASN:N	2.38	0.56
1:A:344:LEU:HD12	1:A:344:LEU:N	2.21	0.56
1:A:340:ILE:O	1:A:344:LEU:HB2	2.06	0.56
1:A:343:ARG:NH2	1:B:364:LEU:HD22	2.21	0.55
1:C:413:TYR:CG	1:C:486:PHE:HB3	2.44	0.52
1:B:413:TYR:CD2	1:B:486:PHE:HB3	2.45	0.52
1:A:413:TYR:CG	1:A:486:PHE:HB3	2.44	0.52
3:A:703:CLR:H273	3:A:703:CLR:H221	1.91	0.52
1:D:413:TYR:CD2	1:D:486:PHE:HB3	2.45	0.52
1:A:336:TYR:CE1	1:A:340:ILE:HD11	2.45	0.52
3:C:703:CLR:H221	3:C:703:CLR:H273	1.91	0.52
1:D:421:ASN:ND2	4:D:705:ROV:O15	2.43	0.52
1:B:413:TYR:HB3	1:B:417:TYR:CE2	2.45	0.51
1:B:421:ASN:ND2	4:B:705:ROV:O15	2.43	0.51
1:C:340:ILE:HA	1:C:344:LEU:HD22	1.92	0.51
1:C:409:ASN:OD1	1:C:409:ASN:N	2.38	0.51
1:A:340:ILE:HA	1:A:344:LEU:HD22	1.92	0.51
1:C:128:LEU:HD21	1:C:406:ASP:HB3	1.92	0.50
1:C:304:PRO:HA	2:C:701:OLA:H31	1.93	0.50
1:C:336:TYR:CE1	1:C:340:ILE:HD11	2.45	0.50
1:A:428:LEU:HD21	2:A:701:OLA:C18	2.41	0.50
1:A:304:PRO:HA	2:A:701:OLA:H31	1.92	0.50
1:D:413:TYR:HB3	1:D:417:TYR:CE2	2.46	0.50
1:A:128:LEU:HD21	1:A:406:ASP:HB3	1.92	0.50
1:C:428:LEU:HD21	2:C:701:OLA:C18	2.41	0.49
1:C:272:ARG:HG2	3:C:703:CLR:H181	1.94	0.49
1:C:475:LEU:HD11	1:C:479:PHE:CZ	2.48	0.49
1:A:475:LEU:HD11	1:A:479:PHE:CZ	2.48	0.48
1:A:272:ARG:HG2	3:A:703:CLR:H181	1.94	0.48
1:B:453:PHE:HE1	6:B:702:3VV:H41	1.79	0.48
1:B:412:SER:HA	1:B:503:MET:HG3	1.96	0.48
1:C:265:MET:CE	2:C:701:OLA:H162	2.44	0.48
1:A:153:ILE:HG12	1:A:339:TYR:CZ	2.49	0.48
1:A:265:MET:CE	2:A:701:OLA:H162	2.44	0.48
1:A:479:PHE:CE1	5:A:706:COA:H21	2.50	0.47
1:D:412:SER:HA	1:D:503:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:N	1:A:182:PRO:HD2	2.30	0.47
1:C:153:ILE:HG12	1:C:339:TYR:CZ	2.49	0.47
1:C:181:PHE:N	1:C:182:PRO:HD2	2.30	0.47
1:D:453:PHE:HE1	6:D:702:3VV:H41	1.79	0.47
1:C:479:PHE:CE1	5:C:706:COA:H21	2.49	0.46
3:C:702:CLR:H222	3:C:702:CLR:H121	1.97	0.46
1:C:410:SER:HB2	1:C:415:ASN:ND2	2.31	0.46
3:A:702:CLR:H121	3:A:702:CLR:H222	1.97	0.46
1:B:272:ARG:HD2	1:B:431:TYR:CD1	2.51	0.46
1:C:340:ILE:HA	1:C:344:LEU:CD1	2.43	0.45
1:B:453:PHE:CE1	6:B:702:3VV:H41	2.51	0.45
1:C:471:PHE:CZ	1:C:473:PRO:HG3	2.51	0.45
1:A:471:PHE:CZ	1:A:473:PRO:HG3	2.52	0.45
1:D:146:ILE:CD1	3:D:703:CLR:H271	2.46	0.45
1:C:409:ASN:ND2	1:D:136:ASP:O	2.49	0.45
1:B:146:ILE:CD1	3:B:703:CLR:H271	2.46	0.45
1:A:296:GLN:O	1:A:297:TYR:HB3	2.17	0.45
1:A:409:ASN:ND2	1:B:136:ASP:O	2.50	0.45
1:D:453:PHE:CE1	6:D:702:3VV:H41	2.51	0.45
1:C:344:LEU:N	1:C:344:LEU:CD1	2.80	0.45
1:C:272:ARG:HD2	1:C:431:TYR:CD1	2.52	0.44
1:D:413:TYR:HB2	1:D:486:PHE:O	2.17	0.44
1:C:296:GLN:O	1:C:297:TYR:HB3	2.17	0.44
1:D:272:ARG:HD2	1:D:431:TYR:CD1	2.51	0.44
1:A:410:SER:HB2	1:A:415:ASN:ND2	2.30	0.44
1:C:128:LEU:CD2	1:C:406:ASP:HB3	2.47	0.44
1:A:128:LEU:CD2	1:A:406:ASP:HB3	2.47	0.44
1:C:340:ILE:CA	1:C:344:LEU:HD13	2.45	0.44
1:B:413:TYR:HB2	1:B:486:PHE:O	2.17	0.44
1:A:272:ARG:HD2	1:A:431:TYR:CD1	2.52	0.44
1:A:320:TRP:HA	1:A:323:VAL:HG22	1.99	0.44
1:C:453:PHE:HE1	5:C:706:COA:OAP	2.01	0.44
1:A:344:LEU:N	1:A:344:LEU:CD1	2.80	0.43
1:A:340:ILE:HA	1:A:344:LEU:CD1	2.44	0.43
1:C:320:TRP:HA	1:C:323:VAL:HG22	1.99	0.43
1:A:453:PHE:HE1	5:A:706:COA:OAP	2.02	0.43
1:C:405:LYS:HD2	1:C:419:THR:HG22	2.01	0.43
1:C:475:LEU:HD11	1:C:479:PHE:CE2	2.54	0.43
1:A:405:LYS:HD2	1:A:419:THR:HG22	2.00	0.42
1:A:343:ARG:HB2	1:A:344:LEU:HD12	2.01	0.42
3:A:704:CLR:H212	3:A:704:CLR:H121	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:704:CLR:H121	3:C:704:CLR:H212	2.01	0.42
1:A:340:ILE:CG2	1:A:344:LEU:HD22	2.48	0.42
1:C:186:TRP:NE1	3:C:702:CLR:H192	2.35	0.42
1:B:479:PHE:CD1	6:B:702:3VV:H9	2.55	0.42
1:A:343:ARG:C	1:A:344:LEU:HD12	2.40	0.42
1:A:475:LEU:HD11	1:A:479:PHE:CE2	2.54	0.42
1:C:250:PRO:HB3	1:C:468:LEU:HD23	2.02	0.42
1:C:343:ARG:HB2	1:C:344:LEU:HD12	2.01	0.41
1:D:479:PHE:CD1	6:D:702:3VV:H9	2.55	0.41
3:A:702:CLR:H222	3:A:702:CLR:H183	2.02	0.41
1:A:413:TYR:CD2	1:A:486:PHE:CD1	3.08	0.41
1:A:250:PRO:HB3	1:A:468:LEU:HD23	2.02	0.41
1:A:492:ASP:OD1	1:A:492:ASP:N	2.54	0.41
3:C:702:CLR:H222	3:C:702:CLR:H183	2.02	0.41
1:C:343:ARG:C	1:C:344:LEU:HD12	2.40	0.41
1:A:186:TRP:NE1	3:A:702:CLR:H192	2.35	0.41
1:C:413:TYR:CD2	1:C:486:PHE:CD1	3.08	0.40
1:A:340:ILE:CA	1:A:344:LEU:HD13	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	407/558 (73%)	362 (89%)	45 (11%)	0	100	100
1	B	407/558 (73%)	365 (90%)	42 (10%)	0	100	100
1	C	407/558 (73%)	362 (89%)	45 (11%)	0	100	100
1	D	407/558 (73%)	365 (90%)	42 (10%)	0	100	100
All	All	1628/2232 (73%)	1454 (89%)	174 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/503 (71%)	351 (98%)	6 (2%)	60	79
1	B	357/503 (71%)	352 (99%)	5 (1%)	67	82
1	C	357/503 (71%)	351 (98%)	6 (2%)	60	79
1	D	357/503 (71%)	352 (99%)	5 (1%)	67	82
All	All	1428/2012 (71%)	1406 (98%)	22 (2%)	66	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	272	ARG
1	A	344	LEU
1	A	409	ASN
1	A	415	ASN
1	A	492	ASP
1	B	272	ARG
1	B	348	LEU
1	B	396	LEU
1	B	450	LEU
1	B	489	ILE
1	C	208	THR
1	C	272	ARG
1	C	344	LEU
1	C	409	ASN
1	C	415	ASN
1	C	492	ASP
1	D	272	ARG
1	D	348	LEU
1	D	396	LEU
1	D	450	LEU
1	D	489	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	415	ASN
1	A	500	ASN
1	B	386	HIS
1	B	500	ASN
1	C	329	GLN
1	C	415	ASN
1	C	500	ASN
1	D	386	HIS
1	D	500	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CLR	C	704	-	31,31,31	0.58	0	48,48,48	1.18	4 (8%)
3	CLR	C	703	-	31,31,31	0.62	0	48,48,48	1.35	6 (12%)
3	CLR	A	702	-	31,31,31	0.72	0	48,48,48	1.61	10 (20%)
2	OLA	D	701	-	19,19,19	0.50	0	19,19,19	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLR	B	704	-	31,31,31	0.59	0	48,48,48	1.35	5 (10%)
3	CLR	A	704	-	31,31,31	0.58	0	48,48,48	1.18	4 (8%)
4	ROV	C	705	-	31,33,33	2.63	10 (32%)	44,47,47	0.98	2 (4%)
3	CLR	A	703	-	31,31,31	0.62	0	48,48,48	1.35	6 (12%)
4	ROV	B	705	-	31,33,33	2.67	10 (32%)	44,47,47	1.29	3 (6%)
3	CLR	D	704	-	31,31,31	0.59	0	48,48,48	1.35	5 (10%)
2	OLA	A	701	-	19,19,19	0.48	0	19,19,19	0.60	0
6	3VV	D	702	-	52,60,69	4.12	18 (34%)	63,86,95	1.57	12 (19%)
4	ROV	A	705	-	31,33,33	2.63	10 (32%)	44,47,47	0.98	2 (4%)
3	CLR	C	702	-	31,31,31	0.73	0	48,48,48	1.61	12 (25%)
5	COA	A	706	-	41,50,50	3.77	13 (31%)	52,75,75	1.60	11 (21%)
4	ROV	D	705	-	31,33,33	2.67	10 (32%)	44,47,47	1.29	3 (6%)
2	OLA	C	701	-	19,19,19	0.48	0	19,19,19	0.60	0
3	CLR	B	703	-	31,31,31	0.56	0	48,48,48	1.24	5 (10%)
5	COA	C	706	-	41,50,50	3.76	13 (31%)	52,75,75	1.60	11 (21%)
6	3VV	B	702	-	52,60,69	4.12	18 (34%)	63,86,95	1.57	12 (19%)
3	CLR	D	703	-	31,31,31	0.56	0	48,48,48	1.24	5 (10%)
2	OLA	B	701	-	19,19,19	0.50	0	19,19,19	0.71	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
3	CLR	C	704	-	-	0/10/68/68	0/4/4/4
3	CLR	C	703	-	-	3/10/68/68	0/4/4/4
3	CLR	A	702	-	-	10/10/68/68	0/4/4/4
2	OLA	D	701	-	-	12/17/17/17	-
3	CLR	B	704	-	-	2/10/68/68	0/4/4/4
3	CLR	A	704	-	-	0/10/68/68	0/4/4/4
4	ROV	C	705	-	-	16/28/37/37	0/3/3/3
3	CLR	A	703	-	-	3/10/68/68	0/4/4/4
4	ROV	B	705	-	-	11/28/37/37	0/3/3/3
3	CLR	D	704	-	-	2/10/68/68	0/4/4/4
2	OLA	A	701	-	-	10/17/17/17	-
6	3VV	D	702	-	-	23/55/75/84	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ROV	A	705	-	-	16/28/37/37	0/3/3/3
3	CLR	C	702	-	-	10/10/68/68	0/4/4/4
5	COA	A	706	-	-	17/44/64/64	0/3/3/3
4	ROV	D	705	-	-	11/28/37/37	0/3/3/3
2	OLA	C	701	-	-	10/17/17/17	-
3	CLR	B	703	-	-	0/10/68/68	0/4/4/4
5	COA	C	706	-	-	17/44/64/64	0/3/3/3
6	3VV	B	702	-	-	23/55/75/84	0/3/3/3
3	CLR	D	703	-	-	0/10/68/68	0/4/4/4
2	OLA	B	701	-	-	12/17/17/17	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	702	3VV	O48-C49	20.03	1.69	1.41
6	B	702	3VV	O48-C49	20.02	1.69	1.41
5	A	706	COA	O4B-C1B	15.36	1.62	1.41
5	C	706	COA	O4B-C1B	15.35	1.62	1.41
6	D	702	3VV	C50-C49	-14.88	1.31	1.53
6	B	702	3VV	C50-C49	-14.83	1.31	1.53
5	A	706	COA	C2B-C1B	-12.39	1.35	1.53
5	C	706	COA	C2B-C1B	-12.37	1.35	1.53
4	C	705	ROV	C14-N16	7.79	1.51	1.35
4	A	705	ROV	C14-N16	7.77	1.51	1.35
4	B	705	ROV	C14-N16	7.75	1.51	1.35
4	D	705	ROV	C14-N16	7.70	1.51	1.35
5	A	706	COA	O4B-C4B	-7.17	1.29	1.45
5	C	706	COA	O4B-C4B	-7.13	1.29	1.45
6	D	702	3VV	O48-C47	-6.94	1.29	1.45
6	B	702	3VV	O48-C47	-6.92	1.29	1.45
5	A	706	COA	C9P-N8P	6.83	1.48	1.33
5	C	706	COA	C9P-N8P	6.81	1.48	1.33
4	D	705	ROV	C14-N13	6.61	1.51	1.37
4	B	705	ROV	C14-N13	6.57	1.51	1.37
4	A	705	ROV	C14-N13	6.37	1.50	1.37
4	C	705	ROV	C14-N13	6.36	1.50	1.37
6	D	702	3VV	C29-N28	6.20	1.47	1.33
6	B	702	3VV	C29-N28	6.16	1.47	1.33
6	B	702	3VV	C24-N23	5.93	1.46	1.33
6	D	702	3VV	C24-N23	5.90	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	702	3VV	P54-O53	5.27	1.69	1.59
6	D	702	3VV	P54-O53	5.21	1.69	1.59
5	A	706	COA	C5P-N4P	5.13	1.45	1.33
5	C	706	COA	C5P-N4P	5.10	1.45	1.33
4	A	705	ROV	C06-C10	4.71	1.59	1.52
4	C	705	ROV	C06-C10	4.69	1.59	1.52
4	B	705	ROV	C06-C10	4.63	1.59	1.52
4	D	705	ROV	C06-C10	4.60	1.59	1.52
4	D	705	ROV	C19-C20	-4.39	1.37	1.52
4	B	705	ROV	C19-C20	-4.39	1.37	1.52
4	A	705	ROV	C19-C20	-4.38	1.37	1.52
4	C	705	ROV	C19-C20	-4.37	1.37	1.52
4	B	705	ROV	C26-N29	4.04	1.47	1.37
4	D	705	ROV	C26-N29	4.01	1.46	1.37
4	A	705	ROV	C26-N29	3.65	1.46	1.37
4	C	705	ROV	C26-N29	3.64	1.46	1.37
5	C	706	COA	P3B-O3B	3.30	1.65	1.59
5	A	706	COA	P3B-O3B	3.27	1.65	1.59
4	A	705	ROV	C05-N13	3.13	1.49	1.43
4	D	705	ROV	C05-C06	3.11	1.46	1.41
4	C	705	ROV	C05-N13	3.10	1.49	1.43
6	D	702	3VV	O51-C50	3.09	1.50	1.43
6	B	702	3VV	O51-C50	3.09	1.50	1.43
4	D	705	ROV	C05-N13	3.08	1.49	1.43
4	B	705	ROV	C05-N13	3.06	1.49	1.43
4	B	705	ROV	C05-C06	3.01	1.45	1.41
5	C	706	COA	C6A-N6A	2.86	1.44	1.34
5	A	706	COA	C6A-N6A	2.85	1.44	1.34
4	C	705	ROV	C05-C06	2.77	1.45	1.41
6	D	702	3VV	C62-N63	2.74	1.44	1.34
6	B	702	3VV	C62-N63	2.74	1.44	1.34
4	A	705	ROV	C05-C06	2.73	1.45	1.41
6	D	702	3VV	C18-S20	2.72	1.82	1.76
5	C	706	COA	O2B-C2B	2.71	1.49	1.43
6	B	702	3VV	C18-S20	2.71	1.82	1.76
5	A	706	COA	O2B-C2B	2.70	1.49	1.43
6	B	702	3VV	O30-C29	-2.64	1.18	1.23
6	D	702	3VV	O30-C29	-2.61	1.18	1.23
6	B	702	3VV	O25-C24	-2.60	1.18	1.23
6	B	702	3VV	O53-C52	-2.56	1.34	1.44
4	D	705	ROV	C22-C21	2.56	1.60	1.52
6	D	702	3VV	O53-C52	-2.55	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	702	3VV	O25-C24	-2.55	1.18	1.23
4	B	705	ROV	C22-C21	2.52	1.60	1.52
4	C	705	ROV	C22-C21	2.51	1.60	1.52
6	B	702	3VV	C17-C18	2.49	1.53	1.50
4	A	705	ROV	C22-C21	2.49	1.60	1.52
6	D	702	3VV	C17-C18	2.48	1.53	1.50
6	B	702	3VV	C65-N66	2.46	1.36	1.32
6	D	702	3VV	C65-N66	2.45	1.36	1.32
6	D	702	3VV	C50-C52	2.41	1.58	1.52
6	B	702	3VV	C50-C52	2.37	1.58	1.52
5	C	706	COA	O5P-C5P	-2.26	1.18	1.23
5	A	706	COA	O5P-C5P	-2.26	1.18	1.23
5	A	706	COA	P1A-O5B	2.24	1.68	1.59
5	C	706	COA	P1A-O5B	2.24	1.68	1.59
6	D	702	3VV	C26-C24	2.23	1.55	1.51
4	C	705	ROV	C18-C23	2.19	1.57	1.53
6	B	702	3VV	C26-C24	2.19	1.55	1.51
4	C	705	ROV	C08-C09	2.18	1.43	1.38
4	A	705	ROV	C08-C09	2.18	1.43	1.38
5	A	706	COA	O9P-C9P	-2.17	1.19	1.23
4	A	705	ROV	C18-C23	2.17	1.57	1.53
5	C	706	COA	O9P-C9P	-2.17	1.19	1.23
4	B	705	ROV	C08-C09	2.15	1.43	1.38
4	D	705	ROV	C08-C09	2.13	1.43	1.38
5	C	706	COA	O3B-C3B	-2.11	1.36	1.44
6	D	702	3VV	C46-C47	2.10	1.58	1.51
6	B	702	3VV	C46-C47	2.09	1.58	1.51
5	A	706	COA	O3B-C3B	-2.08	1.36	1.44
6	D	702	3VV	P38-O37	2.08	1.67	1.59
6	B	702	3VV	P38-O37	2.08	1.67	1.59
4	D	705	ROV	C18-C23	2.06	1.57	1.53
5	A	706	COA	C3B-C4B	2.06	1.58	1.52
4	B	705	ROV	C18-C23	2.06	1.57	1.53
5	C	706	COA	C3B-C4B	2.04	1.58	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	702	3VV	C17-C18-S20	6.13	120.59	113.46
6	D	702	3VV	C17-C18-S20	6.11	120.56	113.46
5	A	706	COA	N3A-C2A-N1A	-4.89	121.04	128.68
5	C	706	COA	N3A-C2A-N1A	-4.87	121.06	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	705	ROV	N13-C14-N16	4.84	122.20	113.87
4	B	705	ROV	N13-C14-N16	4.83	122.17	113.87
3	A	704	CLR	C8-C7-C6	-4.64	106.06	112.73
3	C	704	CLR	C8-C7-C6	-4.63	106.08	112.73
3	D	703	CLR	C8-C7-C6	-4.50	106.26	112.73
3	B	703	CLR	C8-C7-C6	-4.49	106.27	112.73
5	C	706	COA	O9P-C9P-N8P	-4.33	113.70	122.99
5	A	706	COA	O9P-C9P-N8P	-4.32	113.72	122.99
5	C	706	COA	P2A-O3A-P1A	-4.13	118.65	132.83
5	A	706	COA	P2A-O3A-P1A	-4.12	118.70	132.83
3	C	703	CLR	C8-C7-C6	-3.83	107.23	112.73
3	A	703	CLR	C8-C7-C6	-3.82	107.25	112.73
6	D	702	3VV	O30-C29-N28	-3.77	114.90	122.99
6	B	702	3VV	O30-C29-N28	-3.73	114.98	122.99
3	A	702	CLR	C11-C9-C8	3.73	117.12	111.75
3	C	702	CLR	C11-C9-C8	3.72	117.11	111.75
3	B	704	CLR	C8-C7-C6	-3.66	107.47	112.73
3	D	704	CLR	C8-C7-C6	-3.66	107.47	112.73
6	B	702	3VV	N66-C65-N64	-3.63	123.00	128.68
6	D	702	3VV	N66-C65-N64	-3.61	123.03	128.68
3	A	703	CLR	C17-C13-C14	3.61	104.35	100.07
3	C	703	CLR	C17-C13-C14	3.59	104.33	100.07
5	A	706	COA	C7P-C6P-C5P	-3.53	106.47	112.36
5	C	706	COA	C7P-C6P-C5P	-3.48	106.56	112.36
3	A	702	CLR	C19-C10-C5	3.35	113.76	108.34
3	C	702	CLR	C19-C10-C5	3.32	113.72	108.34
3	A	703	CLR	C11-C9-C8	3.26	116.45	111.75
3	C	703	CLR	C11-C9-C8	3.24	116.43	111.75
3	C	702	CLR	C4-C5-C10	3.19	120.66	116.42
3	A	702	CLR	C4-C5-C10	3.19	120.65	116.42
6	D	702	3VV	P42-O41-P38	-3.16	121.98	132.83
6	B	702	3VV	P42-O41-P38	-3.15	122.02	132.83
4	A	705	ROV	N13-C14-N16	3.15	119.28	113.87
3	D	704	CLR	C12-C11-C9	3.14	118.55	113.11
4	C	705	ROV	N13-C14-N16	3.14	119.27	113.87
3	B	704	CLR	C12-C11-C9	3.11	118.51	113.11
6	D	702	3VV	C31-C29-N28	3.09	122.72	116.58
6	B	702	3VV	C31-C29-N28	3.07	122.69	116.58
4	D	705	ROV	O15-C14-N13	-3.04	118.48	123.62
4	B	705	ROV	O15-C14-N13	-3.01	118.53	123.62
5	C	706	COA	CAP-C9P-N8P	2.98	122.52	116.58
5	A	706	COA	CAP-C9P-N8P	2.96	122.46	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	CLR	C22-C20-C17	2.94	116.36	110.28
3	C	702	CLR	C22-C20-C17	2.94	116.36	110.28
6	B	702	3VV	O19-C18-C17	-2.93	120.53	123.99
6	D	702	3VV	O19-C18-C17	-2.90	120.56	123.99
6	D	702	3VV	O19-C18-S20	-2.89	118.86	122.61
6	B	702	3VV	O19-C18-S20	-2.88	118.87	122.61
6	B	702	3VV	C52-C50-C49	2.80	106.09	99.89
3	A	702	CLR	C13-C14-C8	-2.78	110.27	114.38
6	D	702	3VV	C52-C50-C49	2.77	106.03	99.89
3	C	702	CLR	C13-C14-C8	-2.76	110.30	114.38
3	A	703	CLR	C7-C8-C14	2.72	114.85	110.91
3	C	703	CLR	C7-C8-C14	2.71	114.84	110.91
5	C	706	COA	C4A-C5A-N7A	-2.68	106.61	109.40
3	A	702	CLR	C9-C10-C5	-2.64	105.51	109.65
5	A	706	COA	C4A-C5A-N7A	-2.64	106.65	109.40
3	C	702	CLR	C9-C10-C5	-2.61	105.57	109.65
3	C	702	CLR	C2-C3-C4	2.58	113.84	110.31
5	C	706	COA	CDP-CBP-CAP	-2.54	104.41	108.82
3	A	702	CLR	C12-C13-C17	-2.54	112.77	116.57
3	C	702	CLR	C12-C13-C17	-2.54	112.77	116.57
5	A	706	COA	CDP-CBP-CAP	-2.53	104.43	108.82
3	A	702	CLR	C2-C3-C4	2.52	113.76	110.31
3	A	702	CLR	C4-C5-C6	-2.49	117.01	120.61
3	A	702	CLR	C16-C17-C20	2.49	115.99	112.15
3	C	702	CLR	C16-C17-C20	2.48	115.99	112.15
3	B	704	CLR	C11-C9-C8	2.48	115.32	111.75
3	B	703	CLR	C12-C11-C9	2.46	117.38	113.11
3	C	702	CLR	C4-C5-C6	-2.46	117.06	120.61
3	D	703	CLR	C12-C11-C9	2.45	117.36	113.11
6	D	702	3VV	C22-N23-C24	-2.44	118.30	122.84
3	D	704	CLR	C11-C9-C8	2.43	115.26	111.75
6	B	702	3VV	C22-N23-C24	-2.42	118.34	122.84
3	C	704	CLR	C15-C14-C8	-2.39	115.15	119.08
3	A	704	CLR	C15-C14-C8	-2.35	115.20	119.08
3	A	703	CLR	C12-C11-C9	2.31	117.12	113.11
3	C	703	CLR	C12-C11-C9	2.29	117.08	113.11
3	D	703	CLR	C4-C5-C10	2.26	119.43	116.42
3	B	703	CLR	C4-C5-C10	2.26	119.42	116.42
6	B	702	3VV	C67-C61-N60	-2.23	107.07	109.40
3	D	703	CLR	C15-C14-C8	-2.21	115.44	119.08
6	D	702	3VV	C67-C61-N60	-2.21	107.09	109.40
3	B	703	CLR	C15-C14-C8	-2.19	115.47	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	702	3VV	O25-C24-N23	-2.18	118.91	123.01
4	A	705	ROV	O15-C14-N13	-2.17	119.95	123.62
6	D	702	3VV	O25-C24-N23	-2.17	118.93	123.01
4	C	705	ROV	O15-C14-N13	-2.16	119.97	123.62
3	D	704	CLR	C15-C14-C8	-2.15	115.55	119.08
5	A	706	COA	C6P-C7P-N8P	-2.14	107.57	111.90
3	B	704	CLR	C15-C14-C8	-2.13	115.57	119.08
5	C	706	COA	C6P-C7P-N8P	-2.12	107.62	111.90
4	B	705	ROV	C20-C19-C18	2.09	107.51	105.00
3	A	704	CLR	C12-C11-C9	2.08	116.72	113.11
5	C	706	COA	C3P-N4P-C5P	-2.08	118.98	122.84
4	D	705	ROV	C20-C19-C18	2.08	107.50	105.00
5	C	706	COA	CDP-CBP-CCP	2.07	111.60	108.23
3	C	703	CLR	C21-C20-C17	2.06	116.08	112.92
3	C	704	CLR	C12-C11-C9	2.06	116.68	113.11
6	D	702	3VV	C26-C24-N23	2.06	119.88	116.42
3	C	704	CLR	C11-C9-C8	2.05	114.71	111.75
5	A	706	COA	C3P-N4P-C5P	-2.05	119.03	122.84
3	A	704	CLR	C11-C9-C8	2.05	114.71	111.75
3	D	703	CLR	C22-C20-C17	2.05	114.52	110.28
3	A	703	CLR	C21-C20-C17	2.05	116.06	112.92
5	A	706	COA	CDP-CBP-CCP	2.04	111.57	108.23
6	B	702	3VV	C26-C24-N23	2.04	119.86	116.42
3	B	704	CLR	C4-C5-C10	2.04	119.13	116.42
3	C	702	CLR	C10-C9-C8	-2.02	109.70	112.73
3	B	703	CLR	C22-C20-C17	2.02	114.46	110.28
5	C	706	COA	C3B-C2B-C1B	2.02	104.36	99.89
5	A	706	COA	C3B-C2B-C1B	2.01	104.35	99.89
3	C	702	CLR	C17-C13-C14	2.01	102.46	100.07
3	D	704	CLR	C4-C5-C10	2.01	119.09	116.42

There are no chirality outliers.

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	CLR	C13-C17-C20-C22
3	C	702	CLR	C13-C17-C20-C22
4	A	705	ROV	N16-C17-C18-C19
4	A	705	ROV	C17-C18-C23-C24
4	A	705	ROV	C22-C18-C23-C24
4	B	705	ROV	N16-C17-C18-C19
4	C	705	ROV	N16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	C	705	ROV	C17-C18-C23-C24
4	C	705	ROV	C22-C18-C23-C24
4	D	705	ROV	N16-C17-C18-C19
5	A	706	COA	C5B-O5B-P1A-O1A
5	A	706	COA	C5B-O5B-P1A-O2A
5	A	706	COA	C5B-O5B-P1A-O3A
5	A	706	COA	CCP-O6A-P2A-O4A
5	A	706	COA	CBP-CCP-O6A-P2A
5	A	706	COA	CDP-CBP-CCP-O6A
5	A	706	COA	CEP-CBP-CCP-O6A
5	A	706	COA	CAP-CBP-CCP-O6A
5	A	706	COA	O9P-C9P-CAP-CBP
5	A	706	COA	N8P-C9P-CAP-CBP
5	A	706	COA	N8P-C9P-CAP-OAP
5	A	706	COA	CAP-C9P-N8P-C7P
5	A	706	COA	C5P-C6P-C7P-N8P
5	C	706	COA	C5B-O5B-P1A-O1A
5	C	706	COA	C5B-O5B-P1A-O2A
5	C	706	COA	C5B-O5B-P1A-O3A
5	C	706	COA	CCP-O6A-P2A-O4A
5	C	706	COA	CBP-CCP-O6A-P2A
5	C	706	COA	CDP-CBP-CCP-O6A
5	C	706	COA	CEP-CBP-CCP-O6A
5	C	706	COA	CAP-CBP-CCP-O6A
5	C	706	COA	O9P-C9P-CAP-CBP
5	C	706	COA	N8P-C9P-CAP-CBP
5	C	706	COA	N8P-C9P-CAP-OAP
5	C	706	COA	CAP-C9P-N8P-C7P
5	C	706	COA	C5P-C6P-C7P-N8P
6	B	702	3VV	C15-C16-C17-C18
6	B	702	3VV	C24-C26-C27-N28
6	B	702	3VV	C31-C29-N28-C27
6	B	702	3VV	N28-C29-C31-O32
6	B	702	3VV	N28-C29-C31-C33
6	B	702	3VV	O30-C29-C31-C33
6	B	702	3VV	C31-C33-C36-O37
6	B	702	3VV	C34-C33-C36-O37
6	D	702	3VV	C15-C16-C17-C18
6	D	702	3VV	C24-C26-C27-N28
6	D	702	3VV	C31-C29-N28-C27
6	D	702	3VV	N28-C29-C31-O32
6	D	702	3VV	N28-C29-C31-C33

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Mol	Chain	Res	Type	Atoms
6	D	702	3VV	O30-C29-C31-C33
6	D	702	3VV	C31-C33-C36-O37
6	D	702	3VV	C34-C33-C36-O37
4	A	705	ROV	C25-C26-N29-C30
4	A	705	ROV	C25-C26-N29-C31
4	A	705	ROV	C27-C26-N29-C30
4	A	705	ROV	C27-C26-N29-C31
4	B	705	ROV	C05-C06-C10-C11
4	C	705	ROV	C25-C26-N29-C30
4	C	705	ROV	C25-C26-N29-C31
4	C	705	ROV	C27-C26-N29-C30
4	C	705	ROV	C27-C26-N29-C31
4	D	705	ROV	C05-C06-C10-C11
4	B	705	ROV	C07-C06-C10-C11
4	D	705	ROV	C07-C06-C10-C11
3	A	702	CLR	C20-C22-C23-C24
3	C	702	CLR	C20-C22-C23-C24
6	B	702	3VV	C26-C24-N23-C22
6	D	702	3VV	C26-C24-N23-C22
5	A	706	COA	O9P-C9P-N8P-C7P
5	C	706	COA	O9P-C9P-N8P-C7P
6	B	702	3VV	O30-C29-N28-C27
6	D	702	3VV	O30-C29-N28-C27
6	B	702	3VV	O25-C24-N23-C22
6	D	702	3VV	O25-C24-N23-C22
2	A	701	OLA	C13-C14-C15-C16
2	C	701	OLA	C13-C14-C15-C16
4	B	705	ROV	C25-C26-N29-C30
4	D	705	ROV	C25-C26-N29-C30
3	A	702	CLR	C17-C20-C22-C23
3	C	702	CLR	C17-C20-C22-C23
4	B	705	ROV	C27-C26-N29-C31
4	D	705	ROV	C27-C26-N29-C31
3	A	702	CLR	C16-C17-C20-C21
3	C	702	CLR	C16-C17-C20-C21
3	A	702	CLR	C21-C20-C22-C23
3	C	702	CLR	C21-C20-C22-C23
3	A	702	CLR	C16-C17-C20-C22
3	C	702	CLR	C16-C17-C20-C22
4	D	705	ROV	C27-C26-N29-C30
4	B	705	ROV	C27-C26-N29-C30
4	B	705	ROV	C25-C26-N29-C31

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Mol	Chain	Res	Type	Atoms
4	D	705	ROV	C25-C26-N29-C31
6	B	702	3VV	O45-C46-C47-C52
6	D	702	3VV	O45-C46-C47-C52
6	B	702	3VV	C35-C33-C36-O37
6	D	702	3VV	C35-C33-C36-O37
6	B	702	3VV	C13-C14-C15-C16
6	D	702	3VV	C13-C14-C15-C16
2	A	701	OLA	C2-C3-C4-C5
2	C	701	OLA	C2-C3-C4-C5
6	B	702	3VV	C14-C15-C16-C17
6	D	702	3VV	C14-C15-C16-C17
2	B	701	OLA	C3-C4-C5-C6
2	D	701	OLA	C3-C4-C5-C6
2	A	701	OLA	C4-C5-C6-C7
2	C	701	OLA	C4-C5-C6-C7
2	D	701	OLA	C11-C12-C13-C14
2	A	701	OLA	C15-C16-C17-C18
2	B	701	OLA	C11-C12-C13-C14
2	C	701	OLA	C15-C16-C17-C18
2	A	701	OLA	C10-C11-C12-C13
2	C	701	OLA	C10-C11-C12-C13
6	B	702	3VV	C12-C13-C14-C15
6	D	702	3VV	C12-C13-C14-C15
2	B	701	OLA	C4-C5-C6-C7
2	D	701	OLA	C4-C5-C6-C7
3	A	702	CLR	C22-C23-C24-C25
3	C	702	CLR	C22-C23-C24-C25
5	A	706	COA	O9P-C9P-CAP-OAP
5	C	706	COA	O9P-C9P-CAP-OAP
6	B	702	3VV	O30-C29-C31-O32
6	D	702	3VV	O30-C29-C31-O32
2	A	701	OLA	C6-C7-C8-C9
2	C	701	OLA	C6-C7-C8-C9
3	B	704	CLR	C20-C22-C23-C24
3	D	704	CLR	C20-C22-C23-C24
3	A	702	CLR	C13-C17-C20-C21
3	C	702	CLR	C13-C17-C20-C21
6	B	702	3VV	C10-C11-C12-C13
6	D	702	3VV	C10-C11-C12-C13
6	B	702	3VV	C11-C12-C13-C14
6	D	702	3VV	C11-C12-C13-C14
2	A	701	OLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	C	701	OLA	C11-C12-C13-C14
2	B	701	OLA	C10-C11-C12-C13
2	D	701	OLA	C10-C11-C12-C13
6	D	702	3VV	O45-C46-C47-O48
2	B	701	OLA	C14-C15-C16-C17
2	D	701	OLA	C14-C15-C16-C17
3	A	702	CLR	C23-C24-C25-C26
3	C	702	CLR	C23-C24-C25-C26
6	B	702	3VV	P38-O41-P42-O45
6	D	702	3VV	P38-O41-P42-O45
6	B	702	3VV	O45-C46-C47-O48
4	A	705	ROV	C07-C06-C10-C11
4	C	705	ROV	C07-C06-C10-C11
5	A	706	COA	CCP-O6A-P2A-O3A
5	C	706	COA	CCP-O6A-P2A-O3A
2	B	701	OLA	C6-C7-C8-C9
2	D	701	OLA	C6-C7-C8-C9
2	D	701	OLA	C15-C16-C17-C18
3	A	702	CLR	C23-C24-C25-C27
3	C	702	CLR	C23-C24-C25-C27
2	B	701	OLA	C15-C16-C17-C18
5	A	706	COA	CCP-O6A-P2A-O5A
5	C	706	COA	CCP-O6A-P2A-O5A
4	A	705	ROV	C05-C06-C10-C11
4	C	705	ROV	C05-C06-C10-C11
4	A	705	ROV	C17-C18-C23-C28
4	A	705	ROV	C19-C18-C23-C24
4	A	705	ROV	C19-C18-C23-C28
4	A	705	ROV	C22-C18-C23-C28
4	B	705	ROV	C19-C18-C23-C24
4	B	705	ROV	C19-C18-C23-C28
4	C	705	ROV	C17-C18-C23-C28
4	C	705	ROV	C19-C18-C23-C24
4	C	705	ROV	C19-C18-C23-C28
4	C	705	ROV	C22-C18-C23-C28
4	D	705	ROV	C19-C18-C23-C24
4	D	705	ROV	C19-C18-C23-C28
2	D	701	OLA	C13-C14-C15-C16
2	B	701	OLA	C13-C14-C15-C16
2	B	701	OLA	C2-C3-C4-C5
2	D	701	OLA	C2-C3-C4-C5
3	A	703	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	C	703	CLR	C20-C22-C23-C24
4	C	705	ROV	C07-C06-C10-C12
4	A	705	ROV	C07-C06-C10-C12
2	B	701	OLA	O2-C1-C2-C3
2	D	701	OLA	O2-C1-C2-C3
2	A	701	OLA	C3-C4-C5-C6
2	C	701	OLA	C3-C4-C5-C6
6	B	702	3VV	C22-C21-S20-C18
6	D	702	3VV	C22-C21-S20-C18
2	B	701	OLA	O1-C1-C2-C3
2	D	701	OLA	O1-C1-C2-C3
4	A	705	ROV	C05-C06-C10-C12
4	C	705	ROV	C05-C06-C10-C12
2	A	701	OLA	C9-C10-C11-C12
2	C	701	OLA	C9-C10-C11-C12
2	B	701	OLA	C9-C10-C11-C12
2	D	701	OLA	C9-C10-C11-C12
4	A	705	ROV	N16-C17-C18-C23
4	B	705	ROV	N16-C17-C18-C23
4	C	705	ROV	N16-C17-C18-C23
4	D	705	ROV	N16-C17-C18-C23
3	B	704	CLR	C22-C23-C24-C25
3	D	704	CLR	C22-C23-C24-C25
6	B	702	3VV	C46-O45-P42-O41
6	D	702	3VV	C46-O45-P42-O41
3	C	703	CLR	C22-C23-C24-C25
3	A	703	CLR	C22-C23-C24-C25
3	A	703	CLR	C23-C24-C25-C27
3	C	703	CLR	C23-C24-C25-C27
4	B	705	ROV	N16-C17-C18-C22
4	D	705	ROV	N16-C17-C18-C22
2	A	701	OLA	C7-C8-C9-C10
2	C	701	OLA	C7-C8-C9-C10

There are no ring outliers.

18 monomers are involved in 40 short contacts:

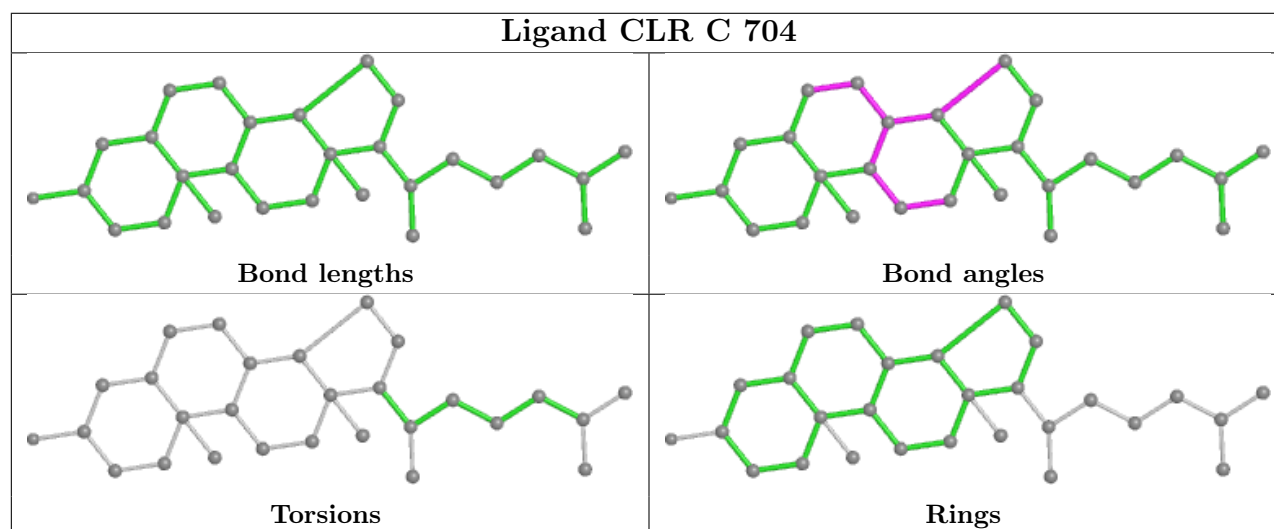
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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3	C	703	CLR	3	0
3	A	702	CLR	3	0
2	D	701	OLA	1	0

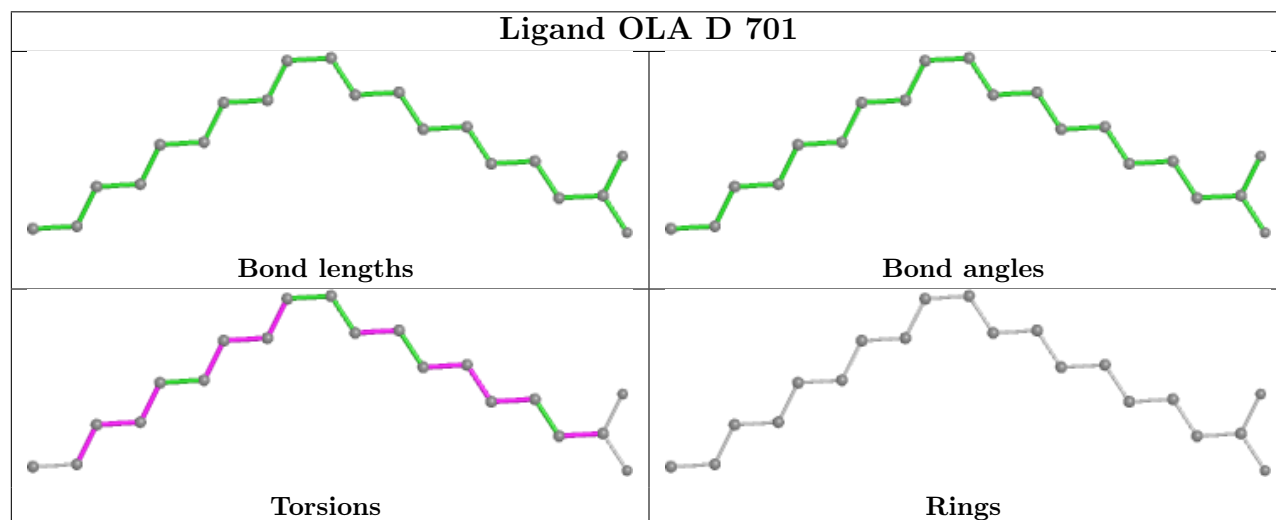
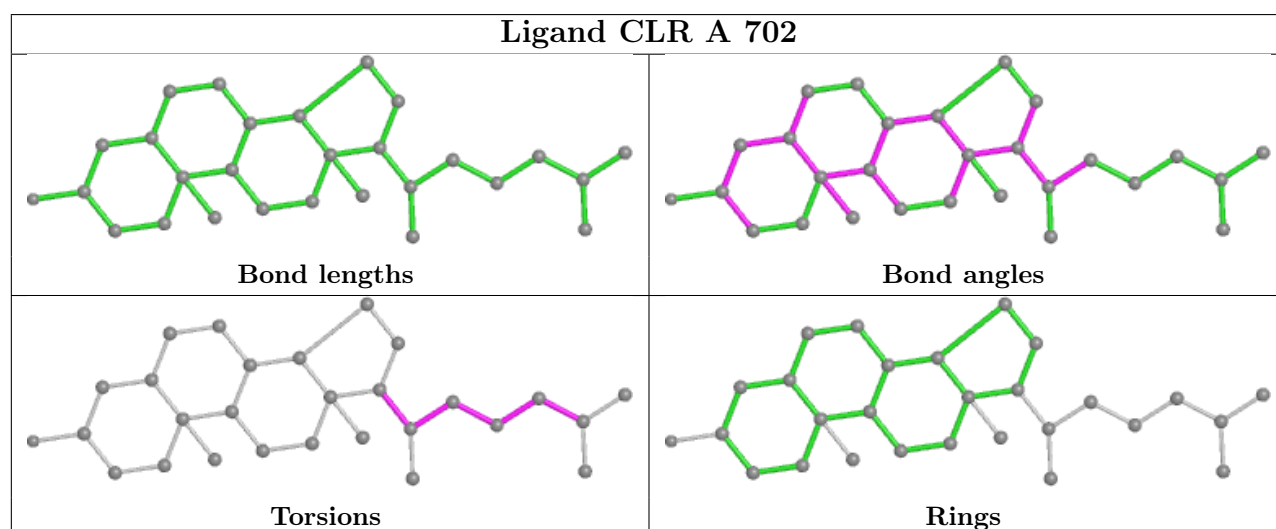
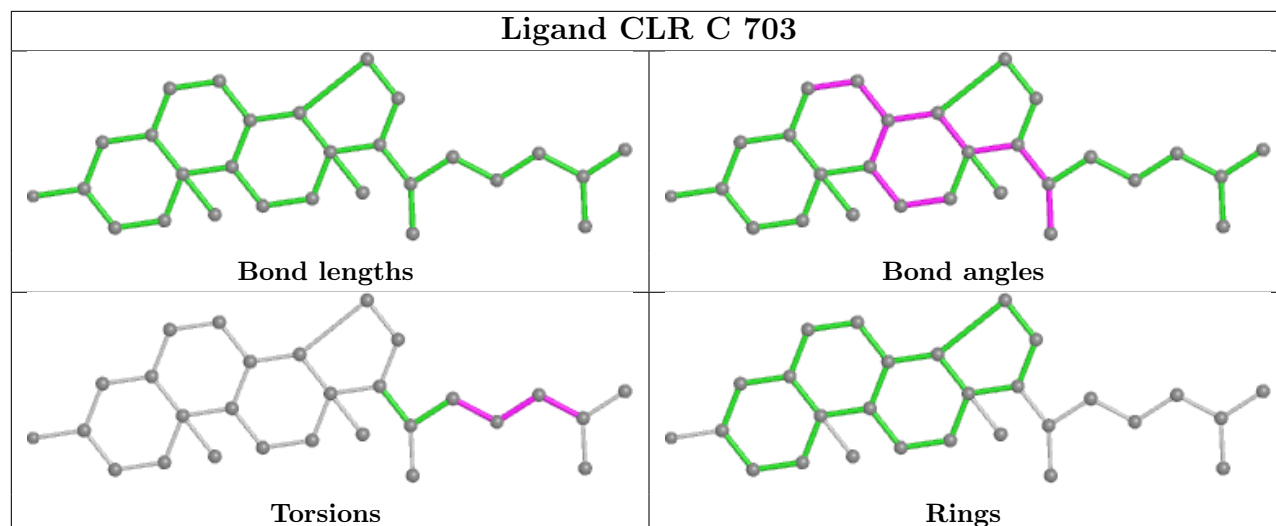
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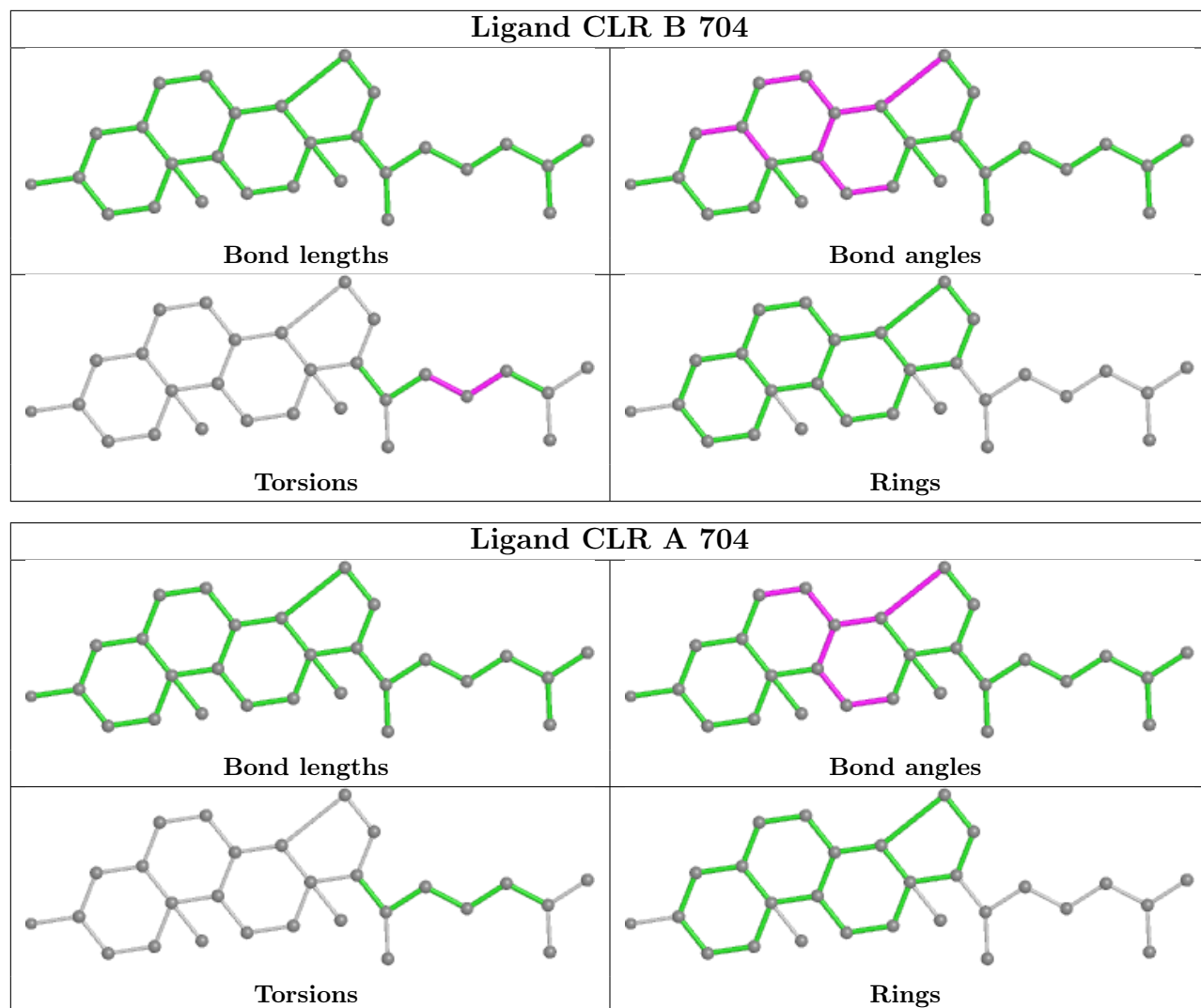
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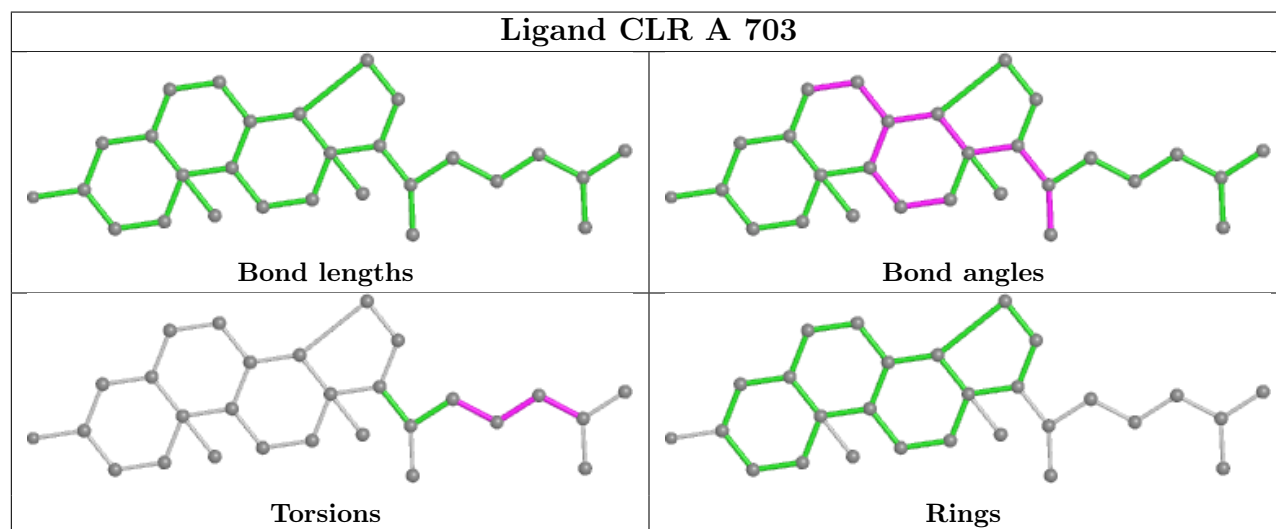
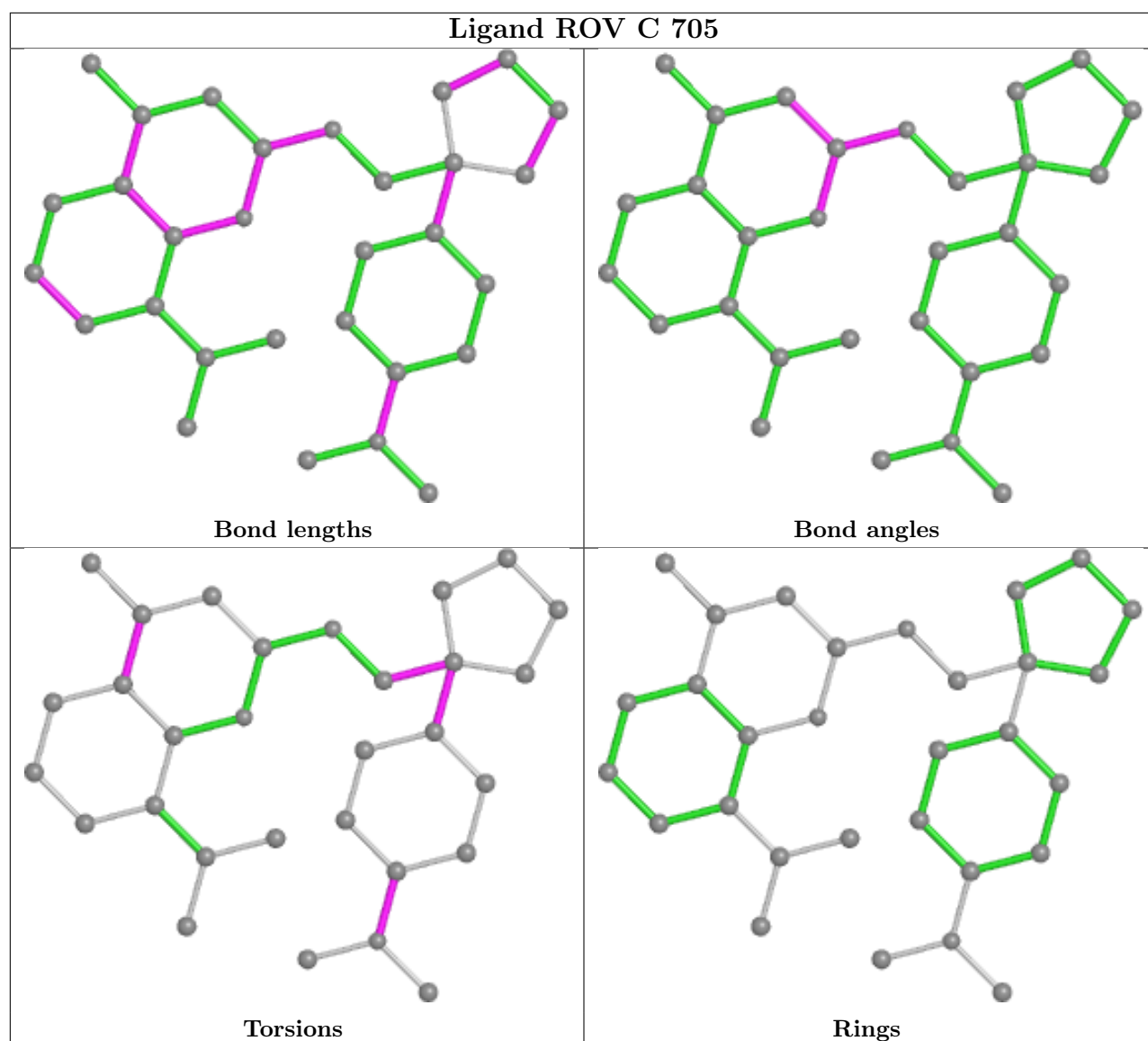
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	CLR	1	0
3	A	703	CLR	3	0
4	B	705	ROV	1	0
2	A	701	OLA	4	0
6	D	702	3VV	4	0
3	C	702	CLR	3	0
5	A	706	COA	2	0
4	D	705	ROV	1	0
2	C	701	OLA	4	0
3	B	703	CLR	1	0
5	C	706	COA	2	0
6	B	702	3VV	4	0
3	D	703	CLR	1	0
2	B	701	OLA	1	0

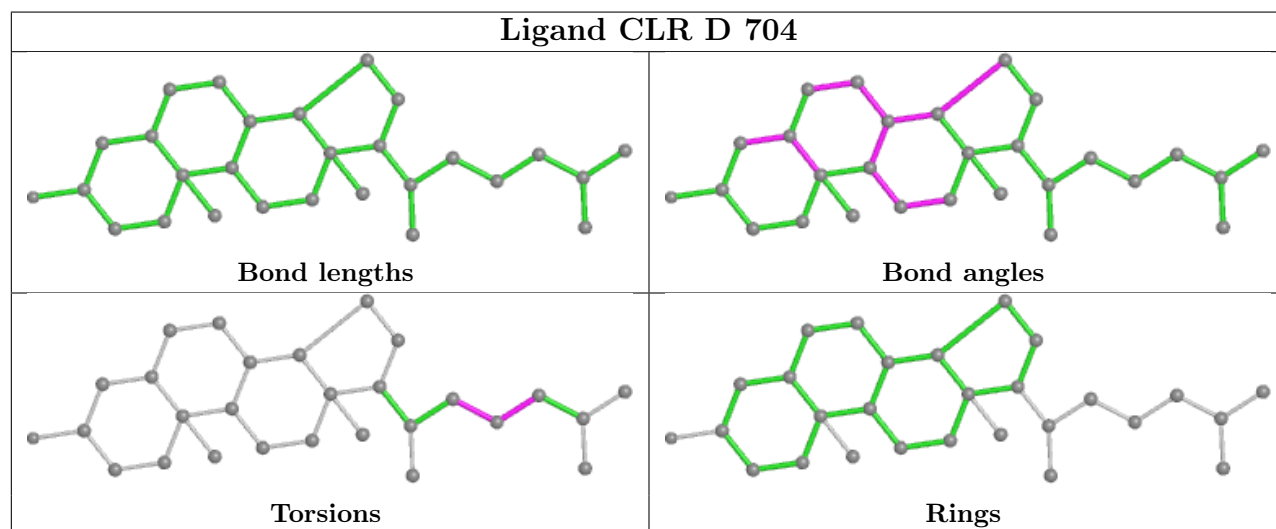
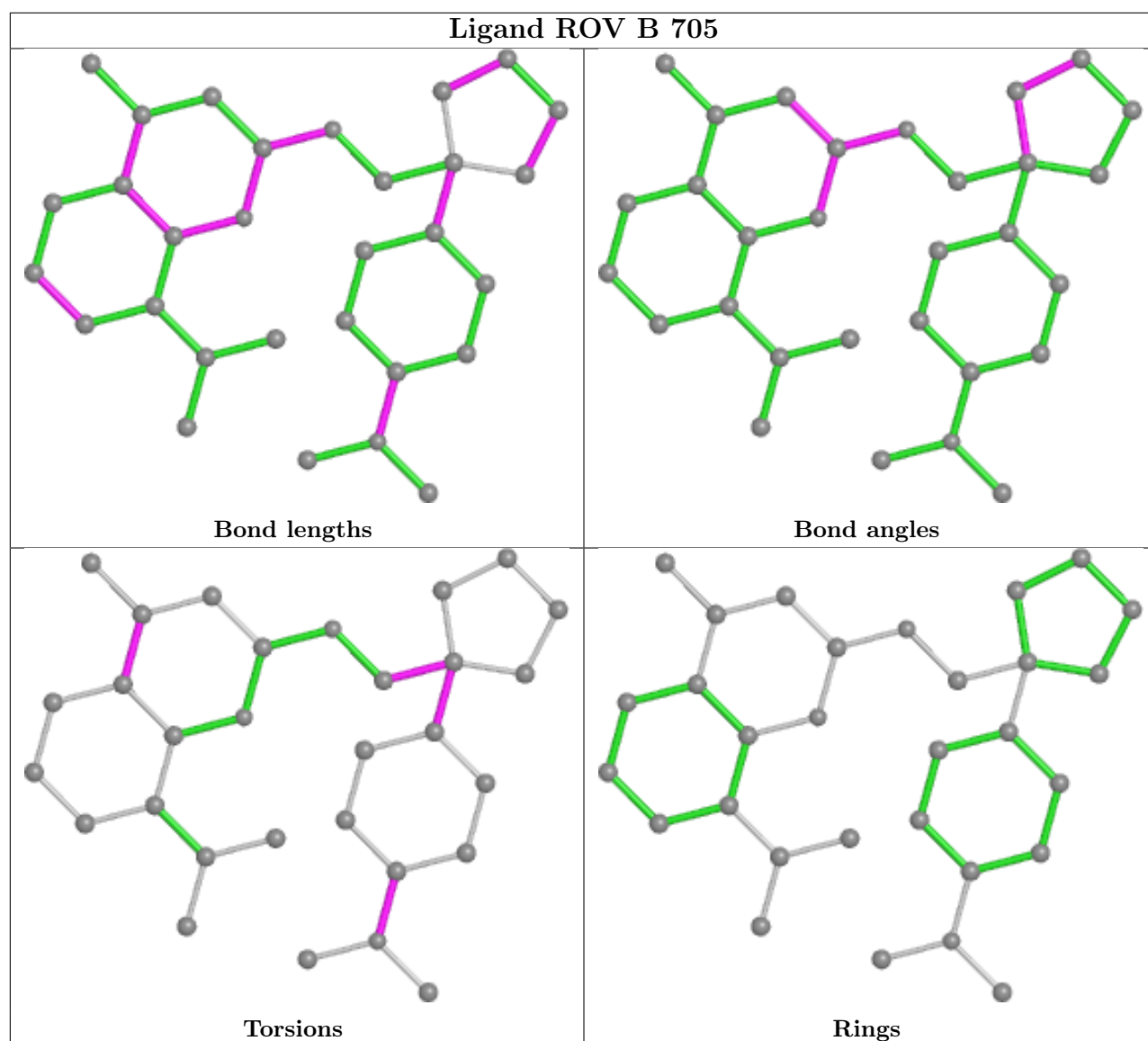
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

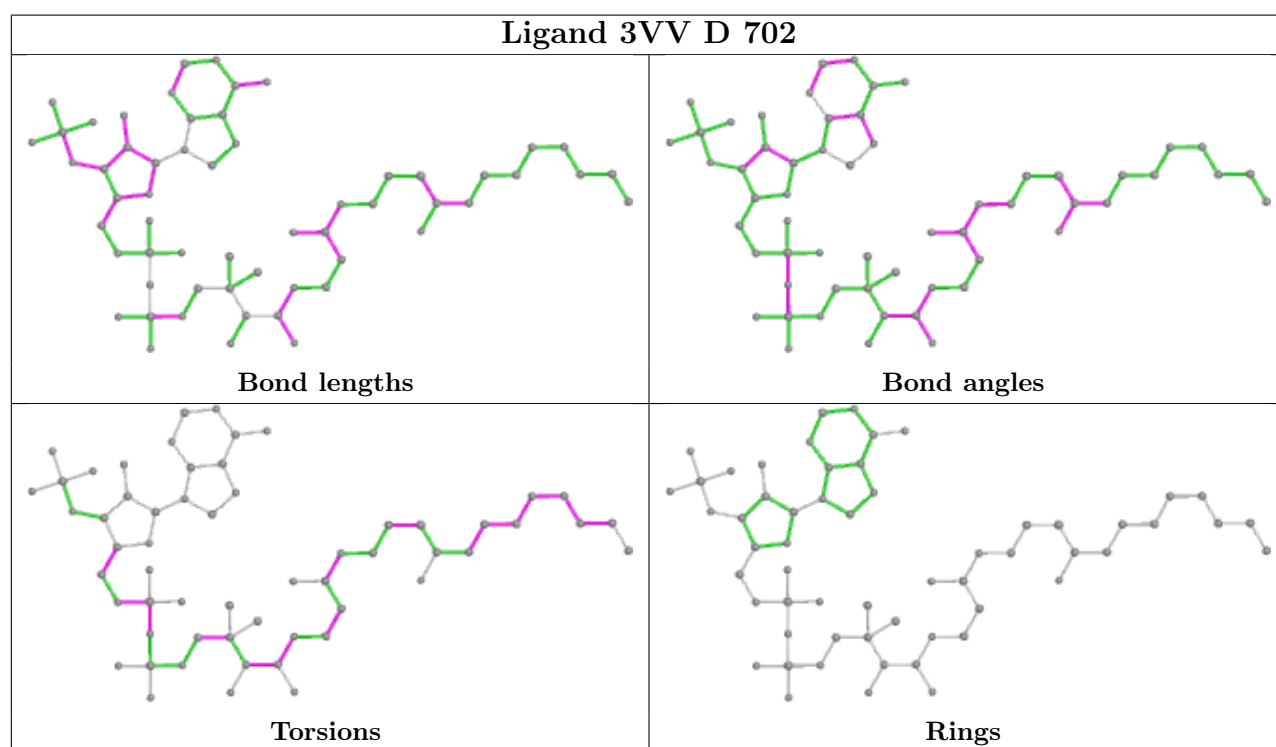
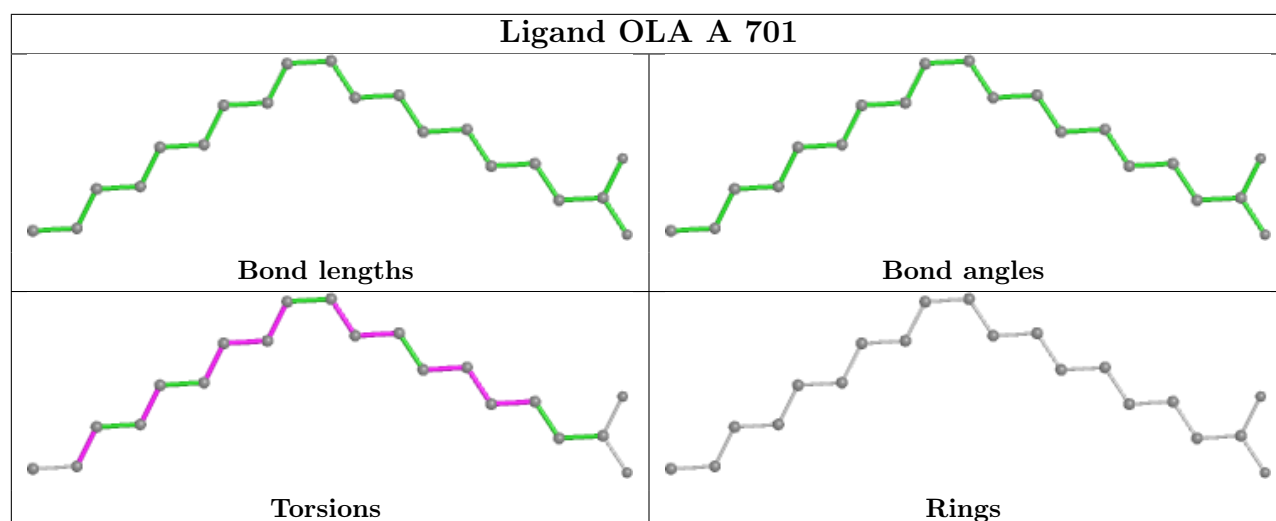


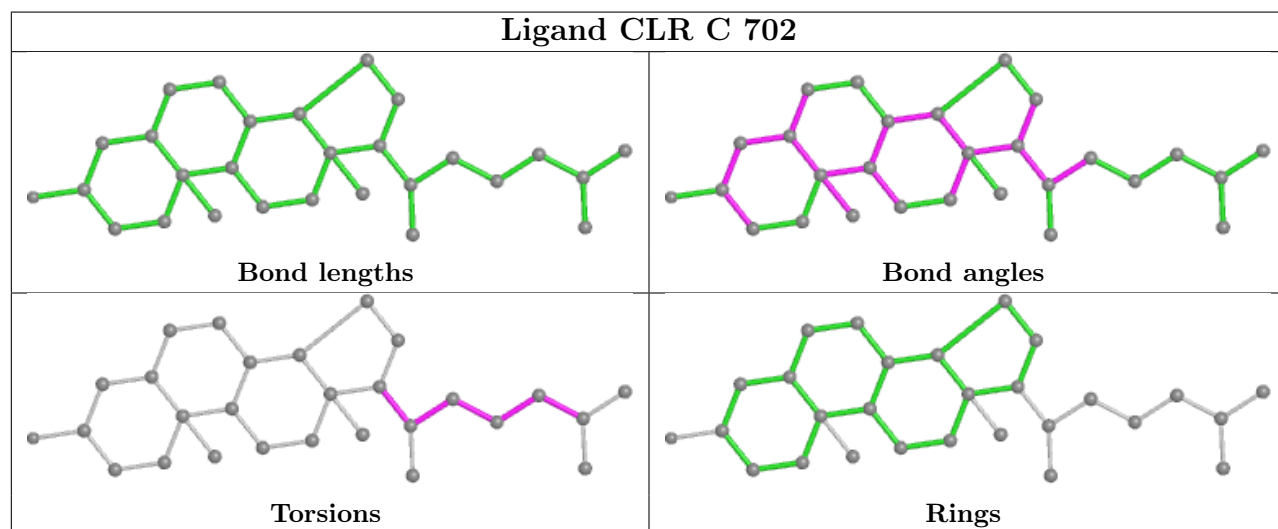
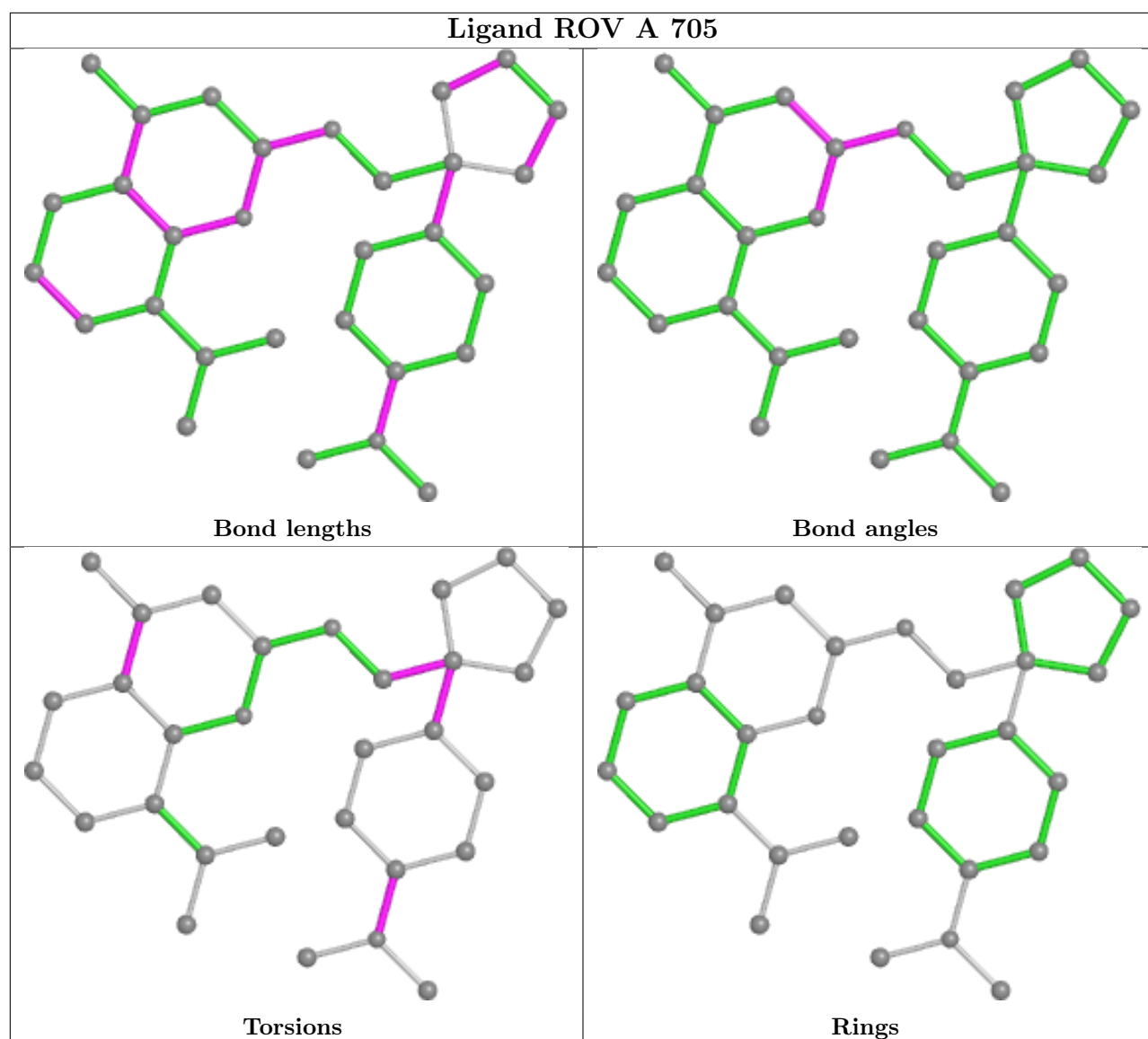


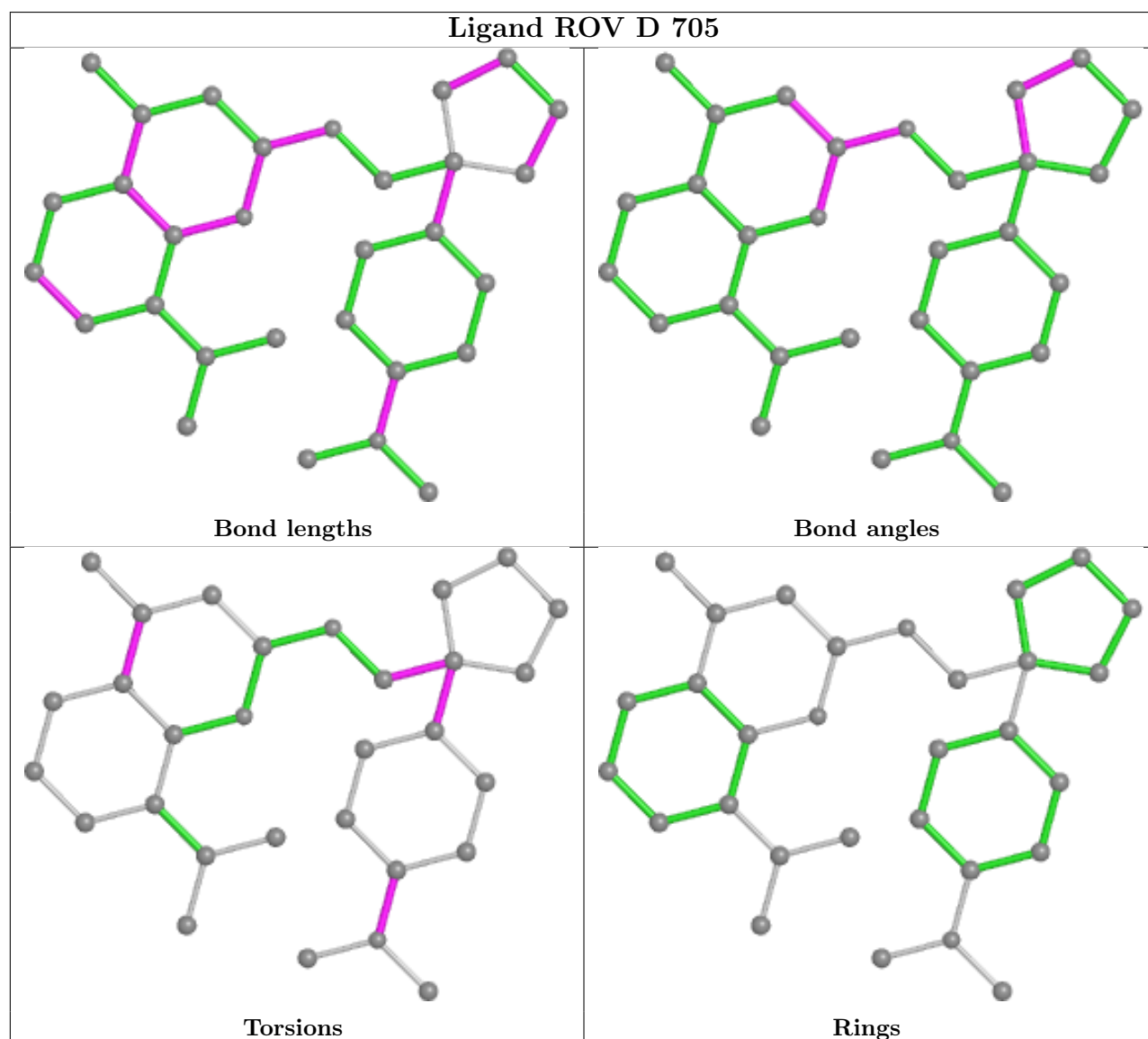
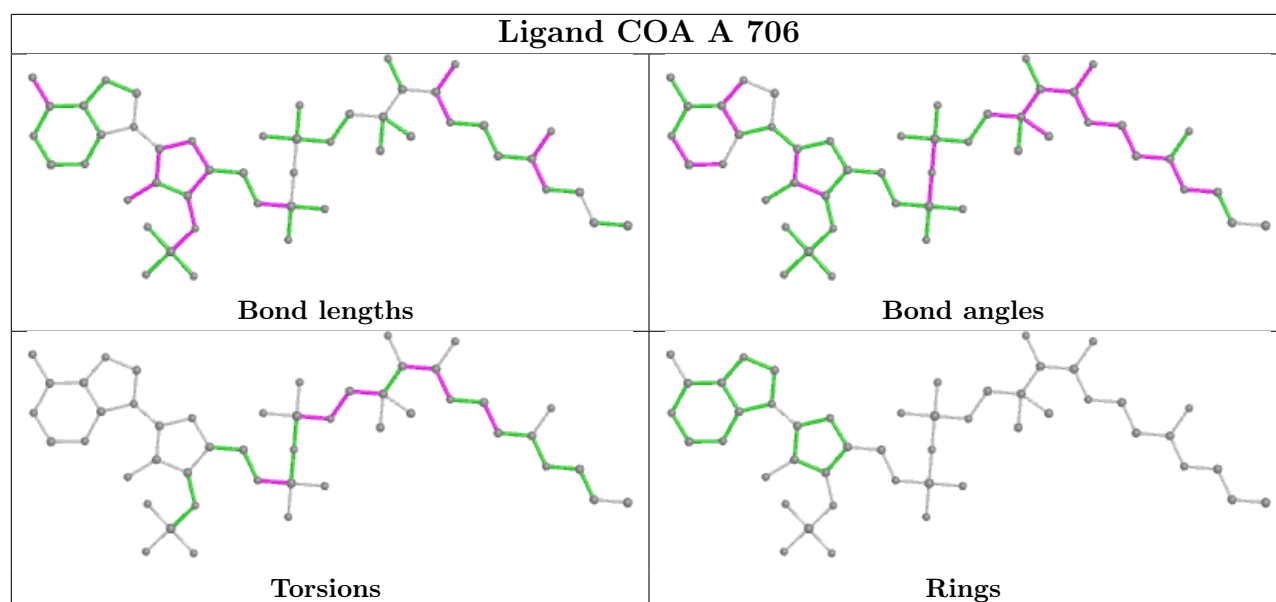


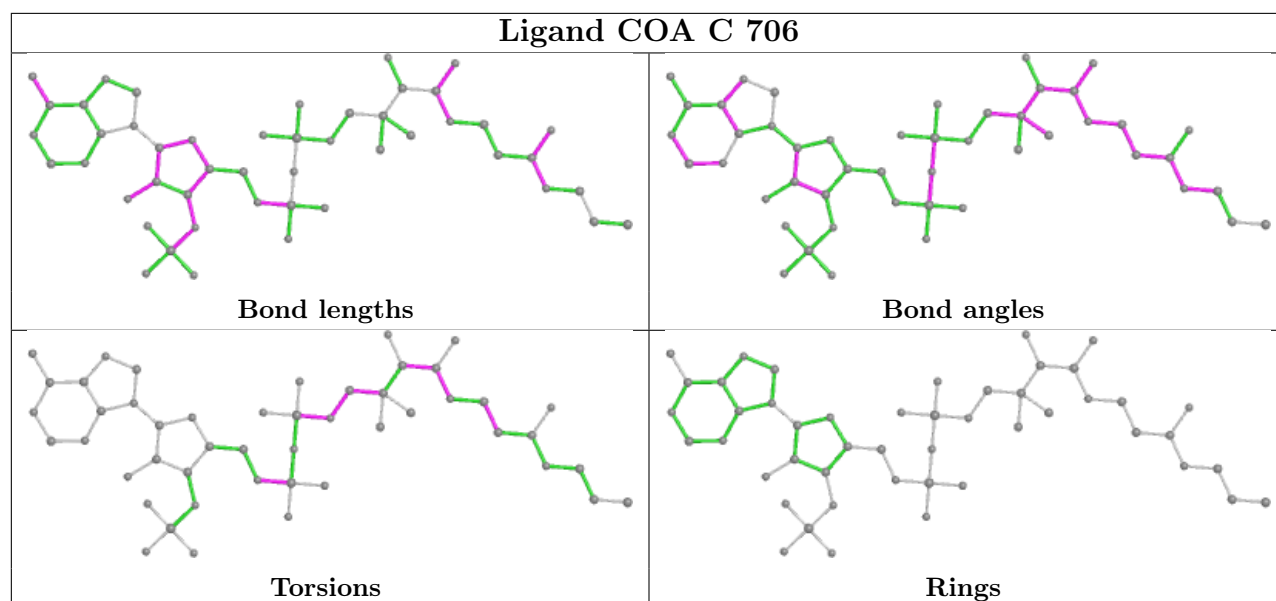
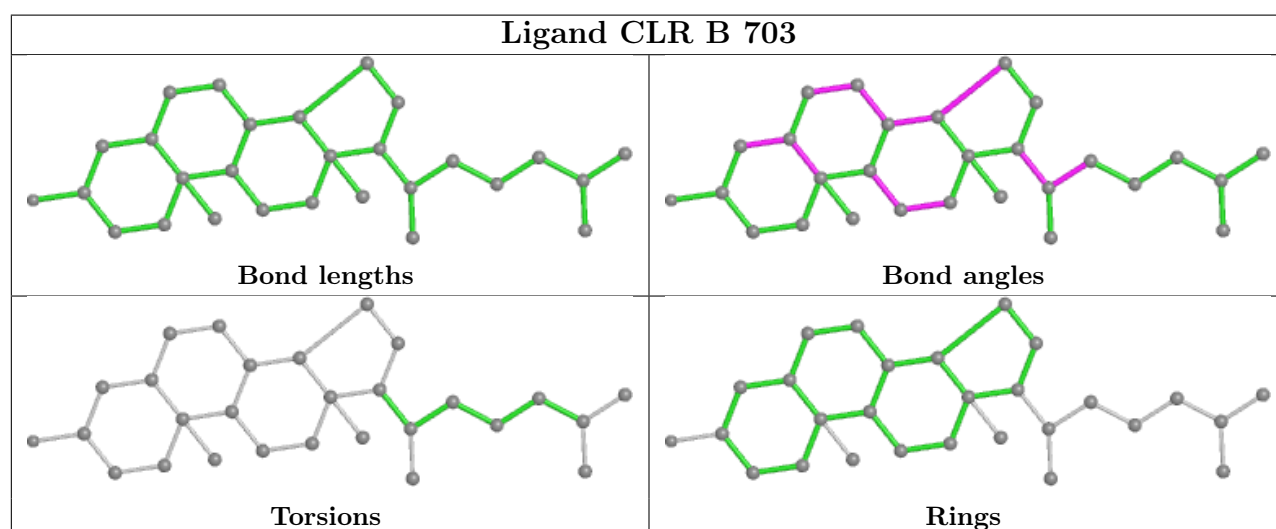
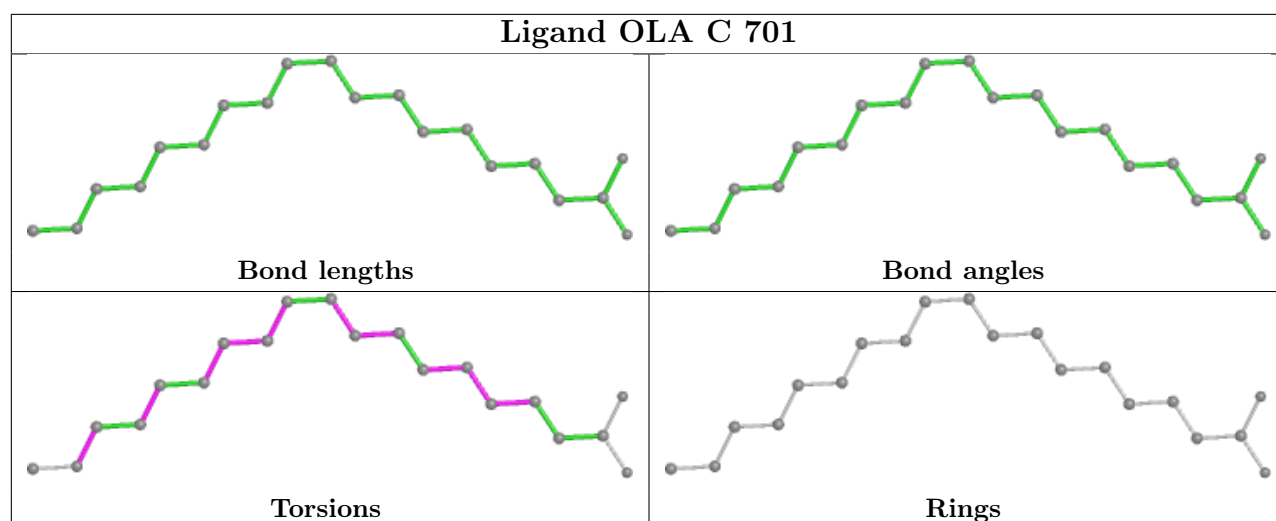


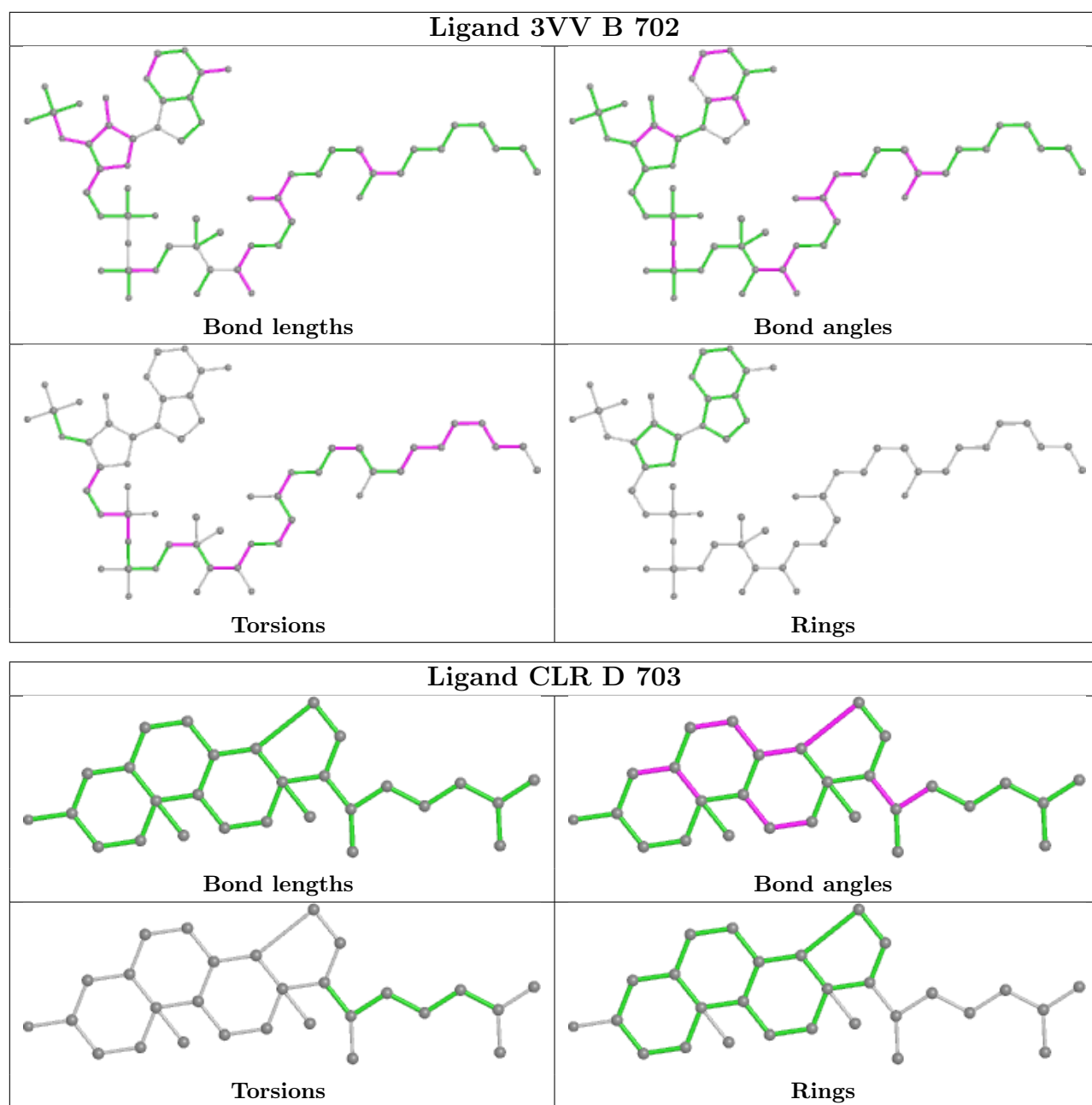


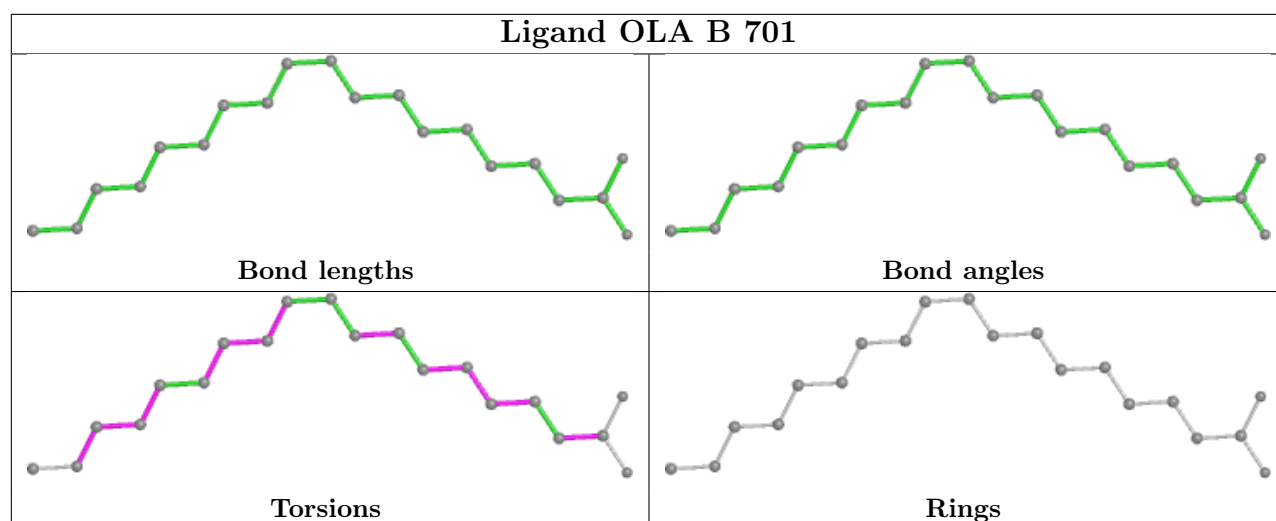












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

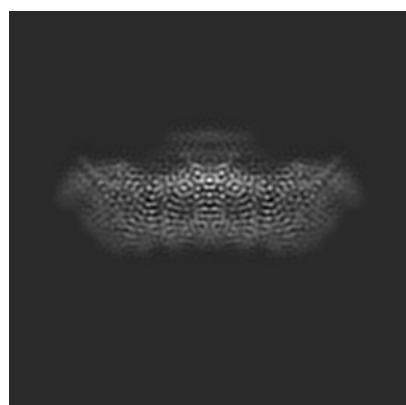
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21390. These allow visual inspection of the internal detail of the map and identification of artifacts.

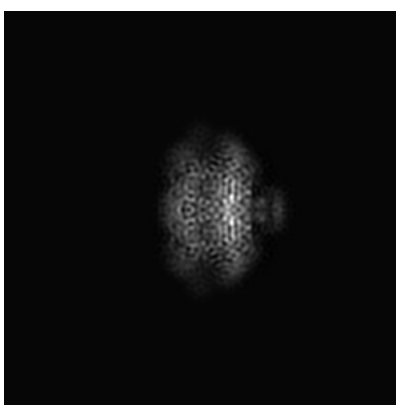
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

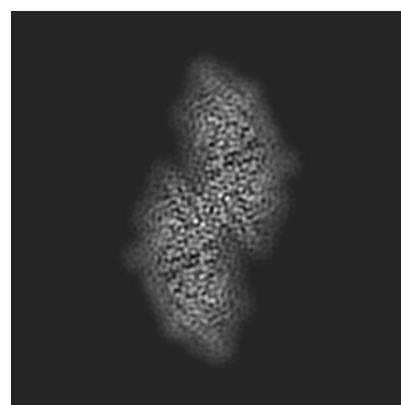
6.1.1 Primary map



X



Y



Z

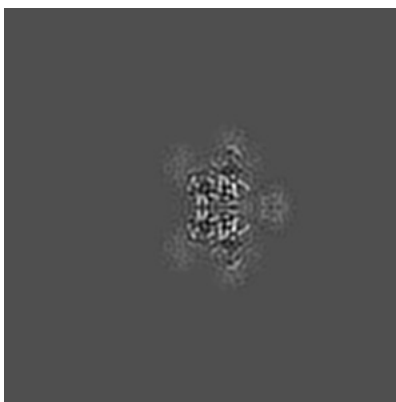
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

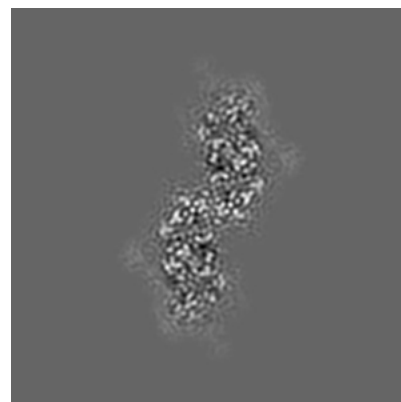
6.2.1 Primary map



X Index: 165



Y Index: 165

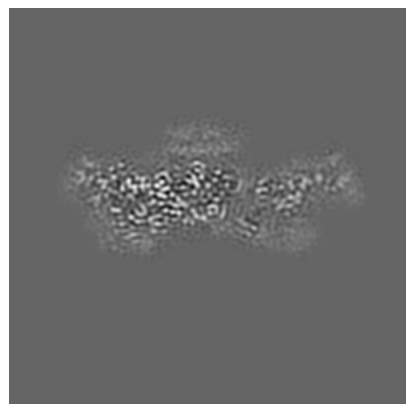


Z Index: 165

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

6.3 Largest variance slices [i](#)

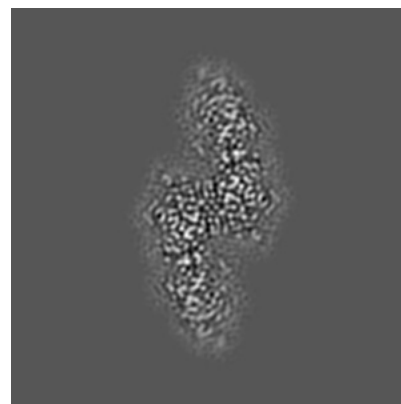
6.3.1 Primary map



X Index: 158



Y Index: 155



Z Index: 188

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0094. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

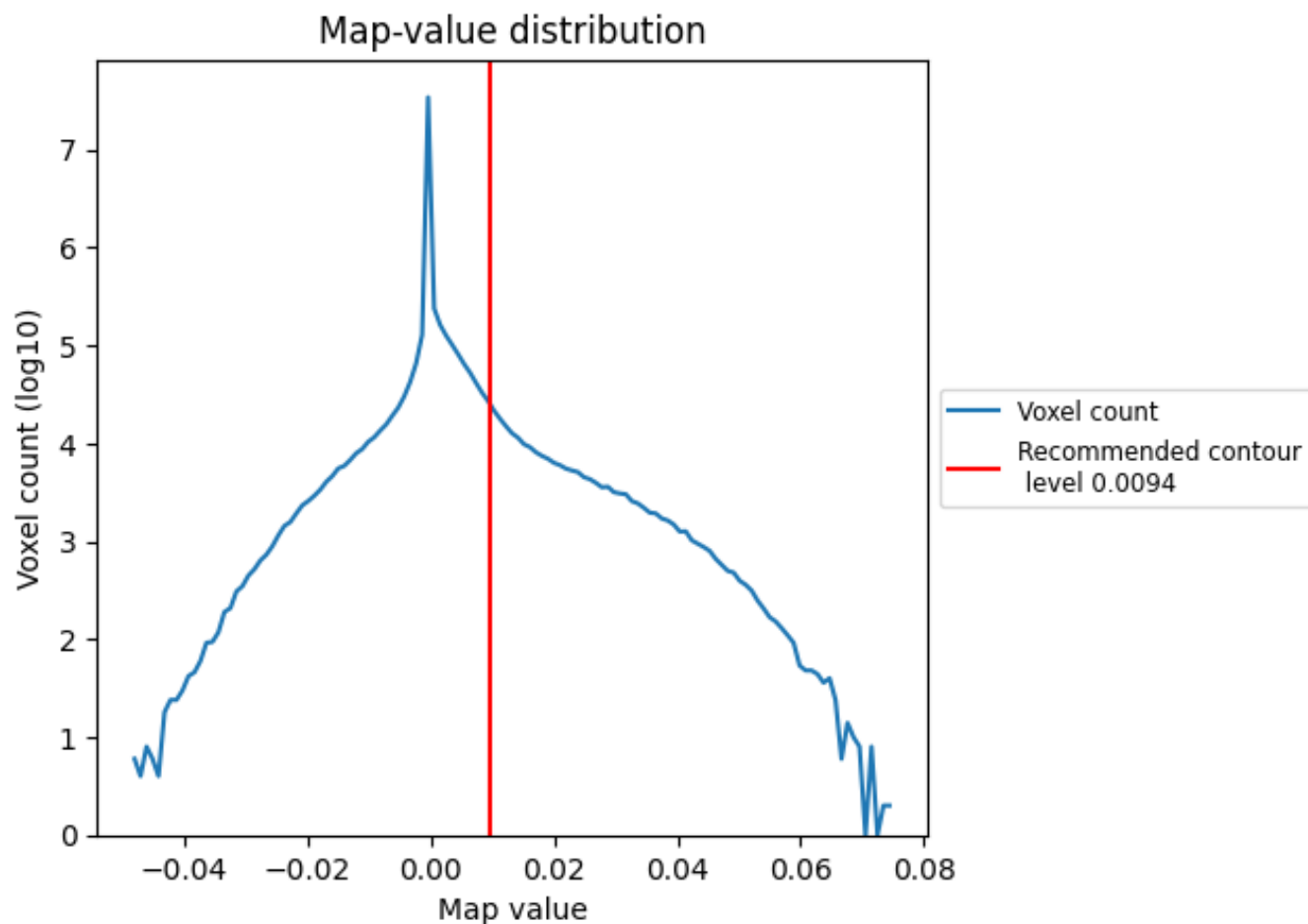
6.5 Mask visualisation

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

7 Map analysis [i](#)

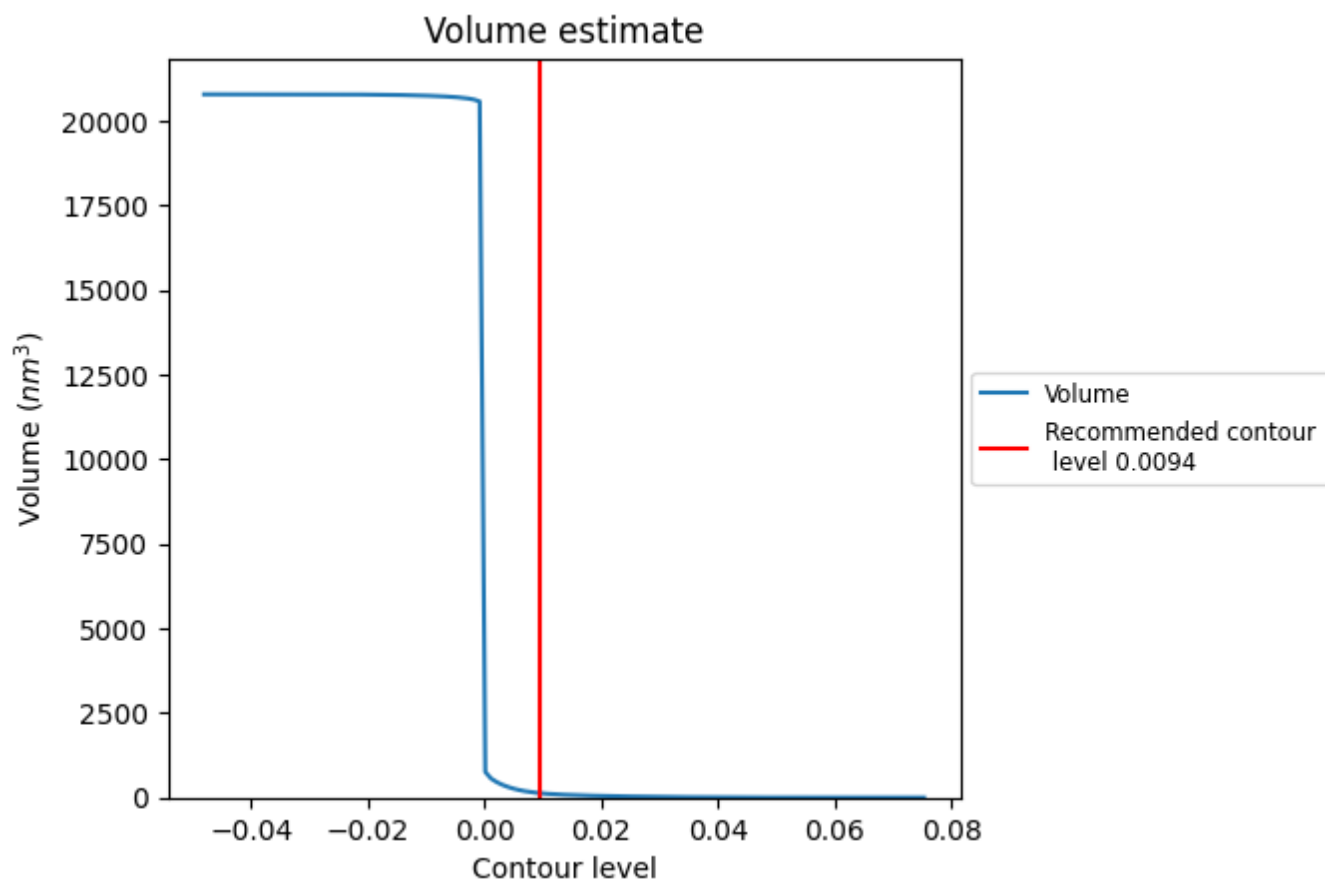
This section contains the results of statistical analysis of the map.

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.

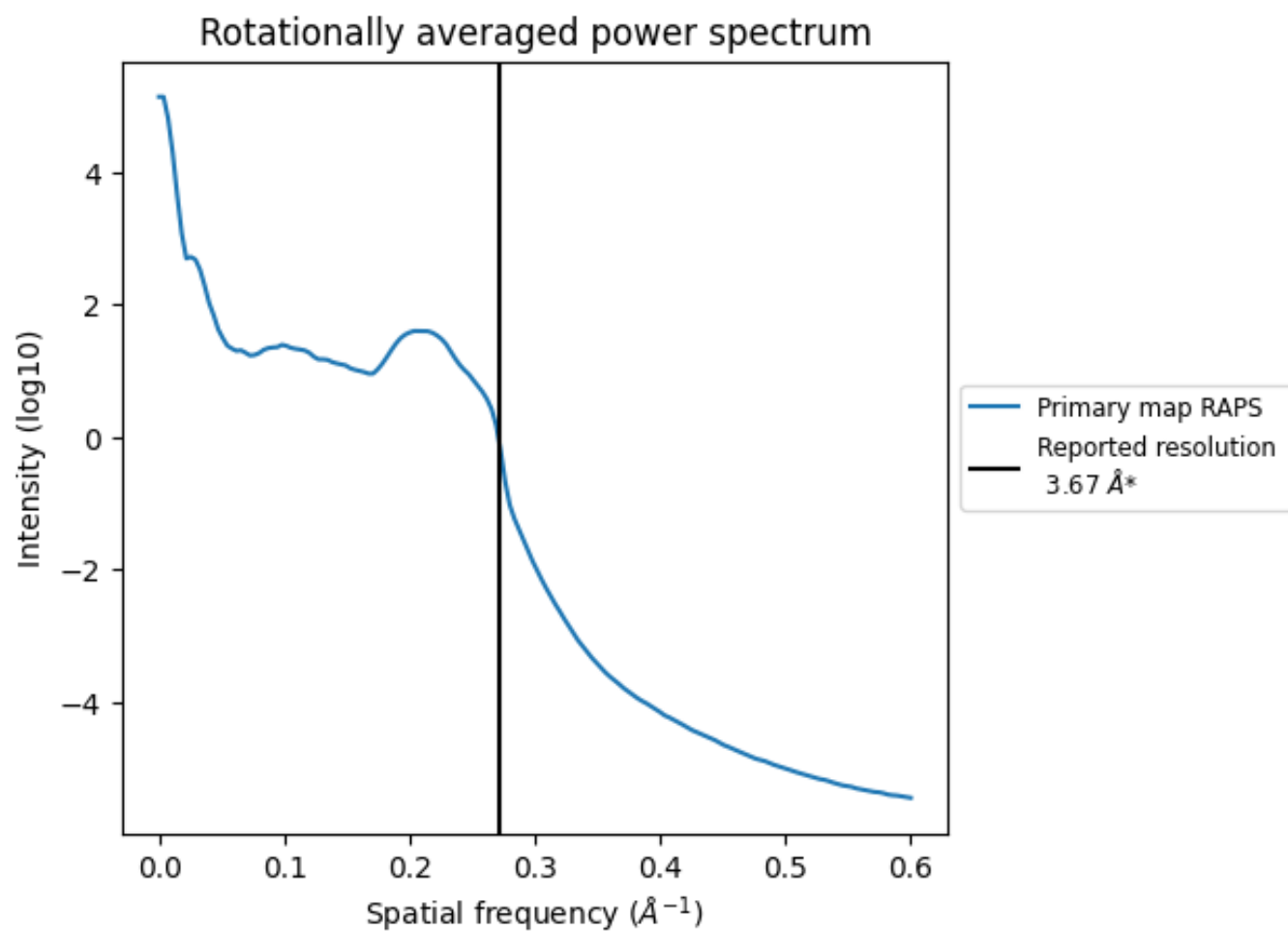
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 0.272 Å⁻¹

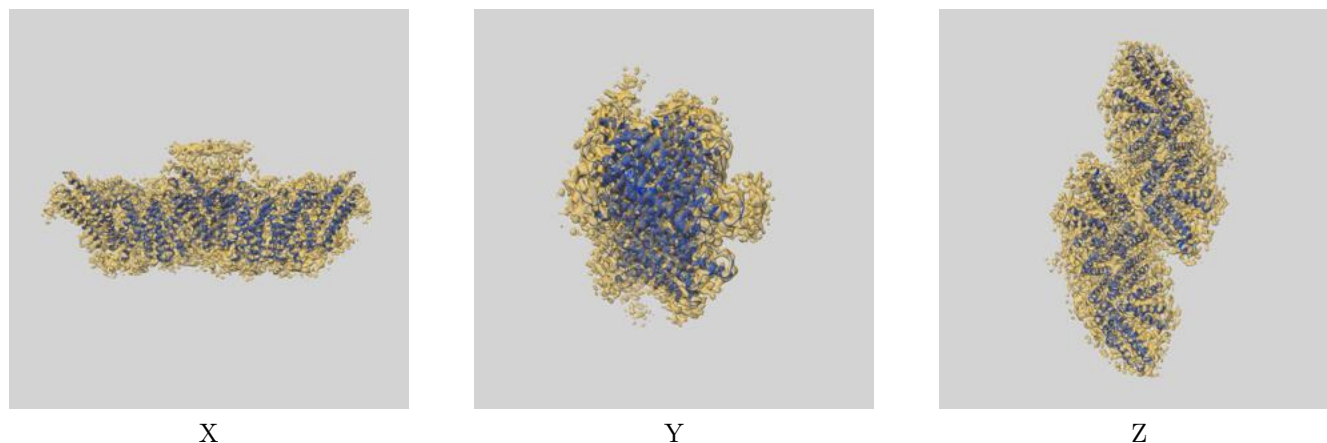
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

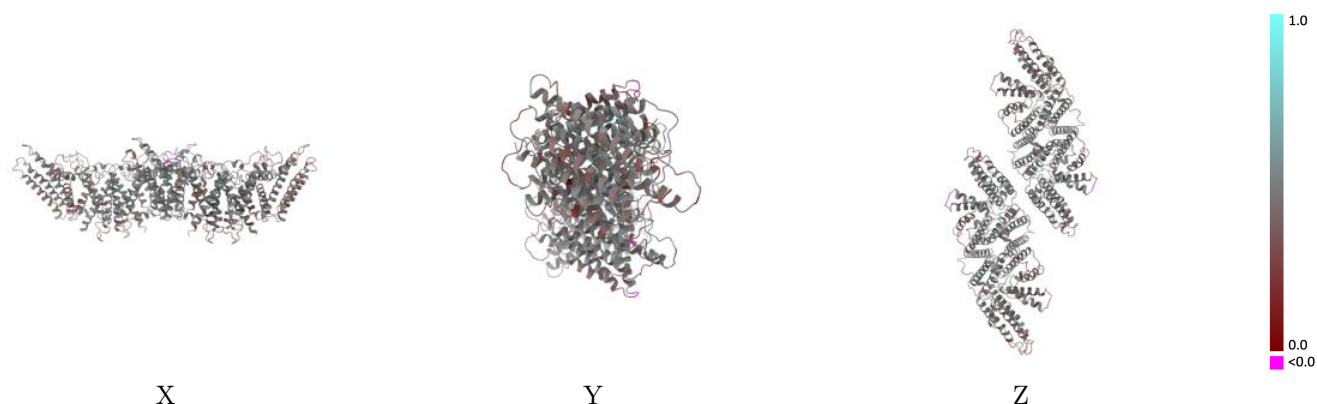
This section contains information regarding the fit between EMDB map EMD-21390 and PDB model 6VUM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



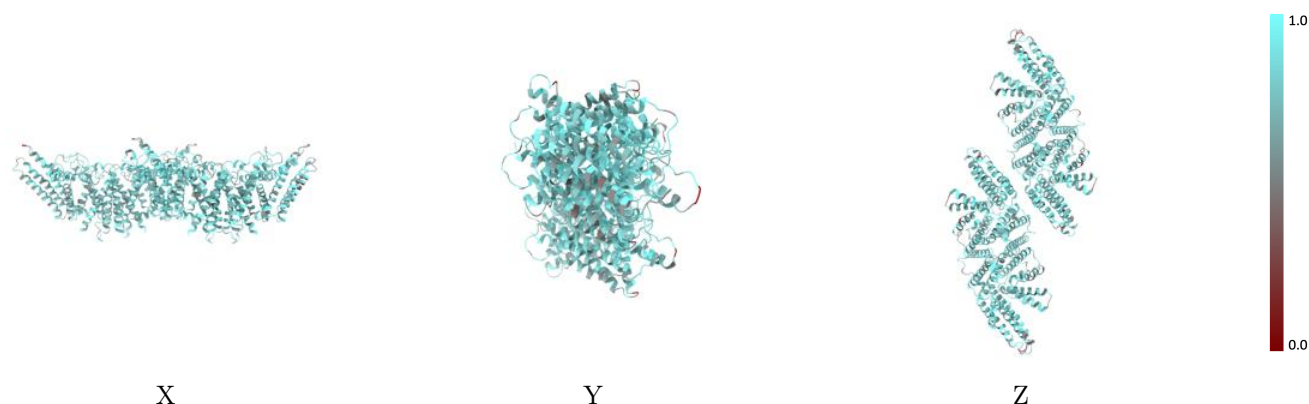
The images above show the 3D surface view of the map at the recommended contour level 0.0094 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



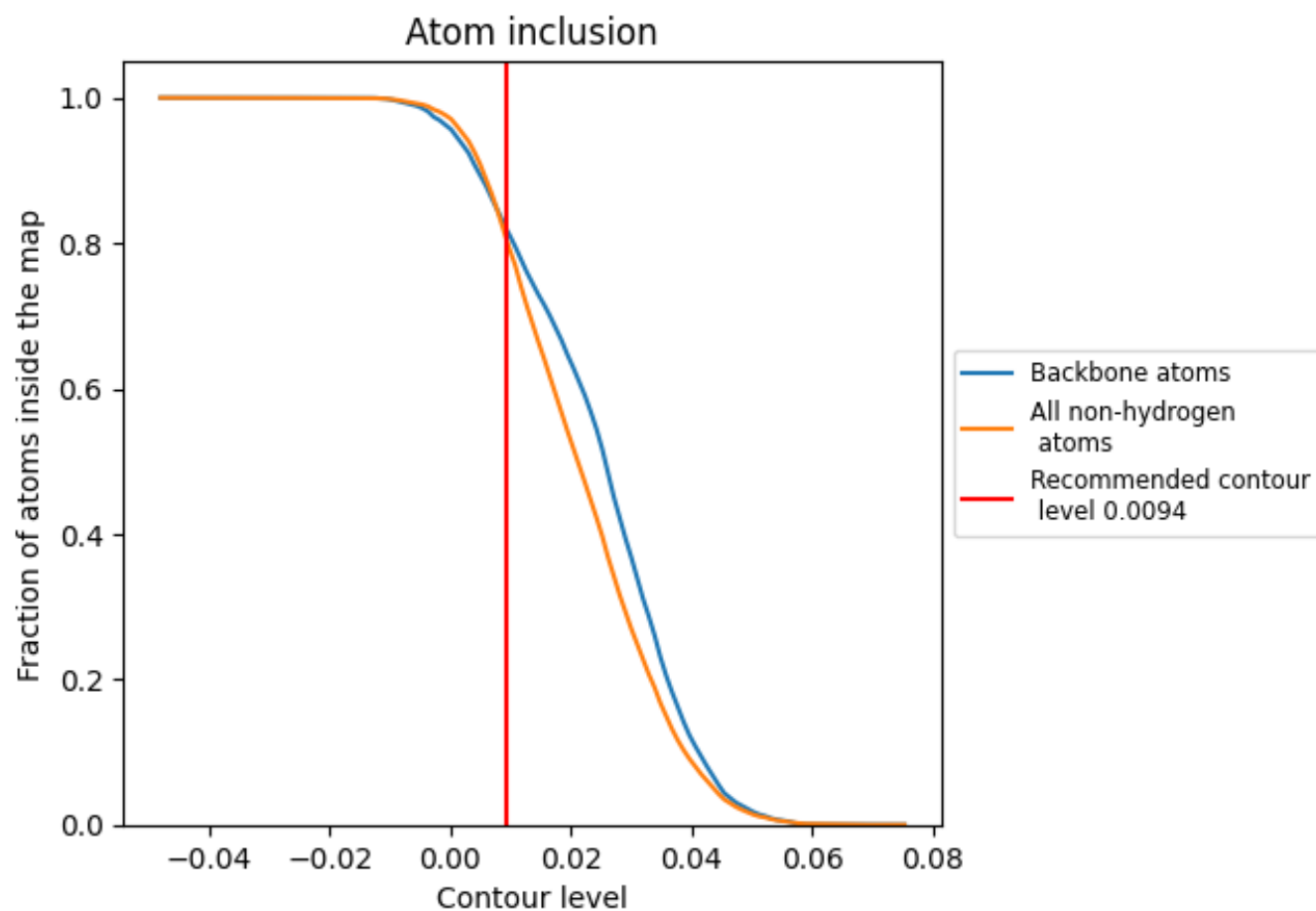
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0094).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.0094) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8026	<div></div> 0.4500
A	<div></div> 0.8129	<div></div> 0.4590
B	<div></div> 0.7912	<div></div> 0.4410
C	<div></div> 0.8129	<div></div> 0.4600
D	<div></div> 0.7932	<div></div> 0.4420

