



## Full wwPDB EM Validation Report ⓘ

Oct 30, 2023 – 01:11 PM EDT

PDB ID : 8TK8  
EMDB ID : EMD-41323  
Title : Human Type 3 IP3 Receptor - Resting State (+IP3/ATP)  
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.  
Deposited on : 2023-07-25  
Resolution : 2.70 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70  
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) : 2.36

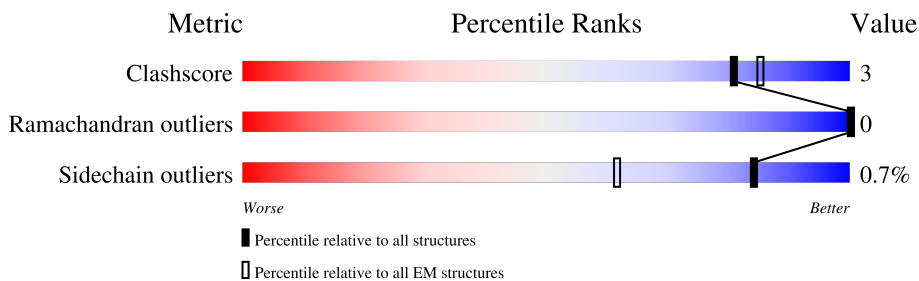
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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  $\geq 3$ , 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	2671	79% 6% 15%
1	B	2671	5% 79% 6% 15%
1	C	2671	79% 6% 15%
1	D	2671	79% 6% 15%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 148540 atoms, of which 74460 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.

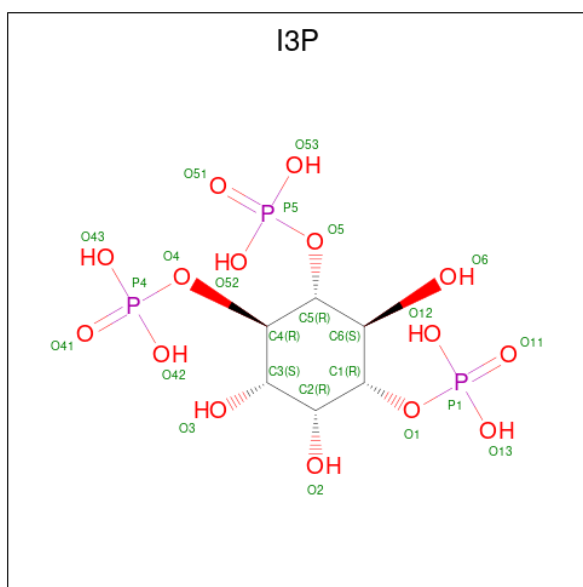
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2268	36394	11601	18207	3116	3355	115	0	0
1	B	2268	36395	11601	18208	3116	3355	115	0	0
1	C	2268	36394	11601	18207	3116	3355	115	0	0
1	D	2268	36395	11601	18208	3116	3355	115	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

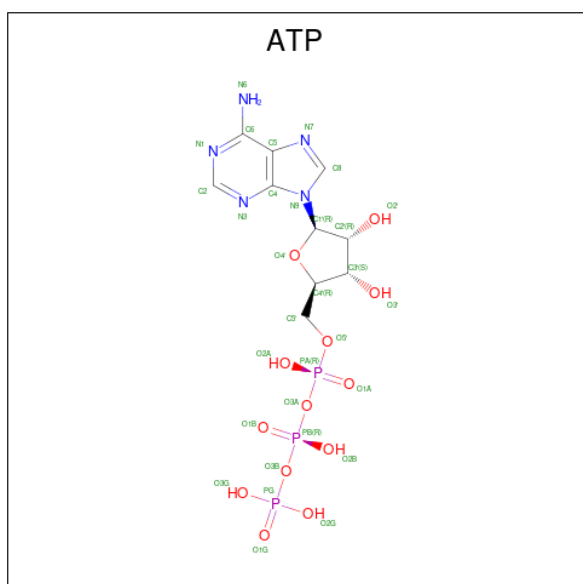
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>15</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



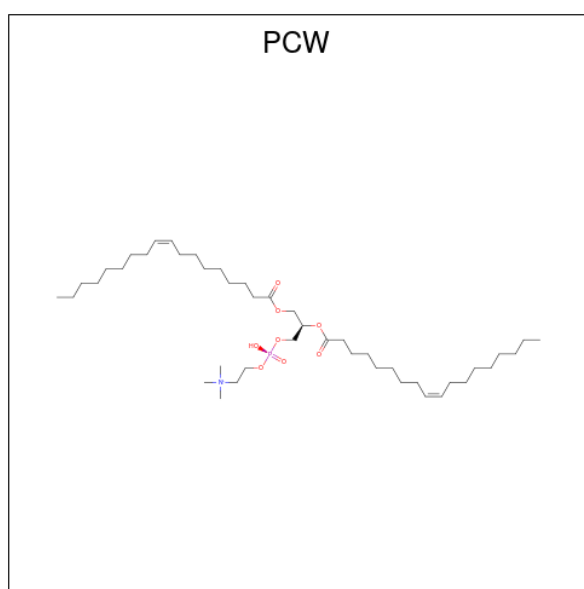
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
4	A	1	43	10	12	5	13	3	0
4	B	1	43	10	12	5	13	3	0
4	C	1	43	10	12	5	13	3	0
4	D	1	43	10	12	5	13	3	0

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
5	A	1	101	33	58	1	8	1	0
5	A	1	117	38	69	1	8	1	0
5	A	1	98	31	57	1	8	1	0
5	A	1	108	36	62	1	8	1	0
5	A	1	112	38	64	1	8	1	0
5	A	1	108	36	62	1	8	1	0
5	A	1	126	41	75	1	8	1	0

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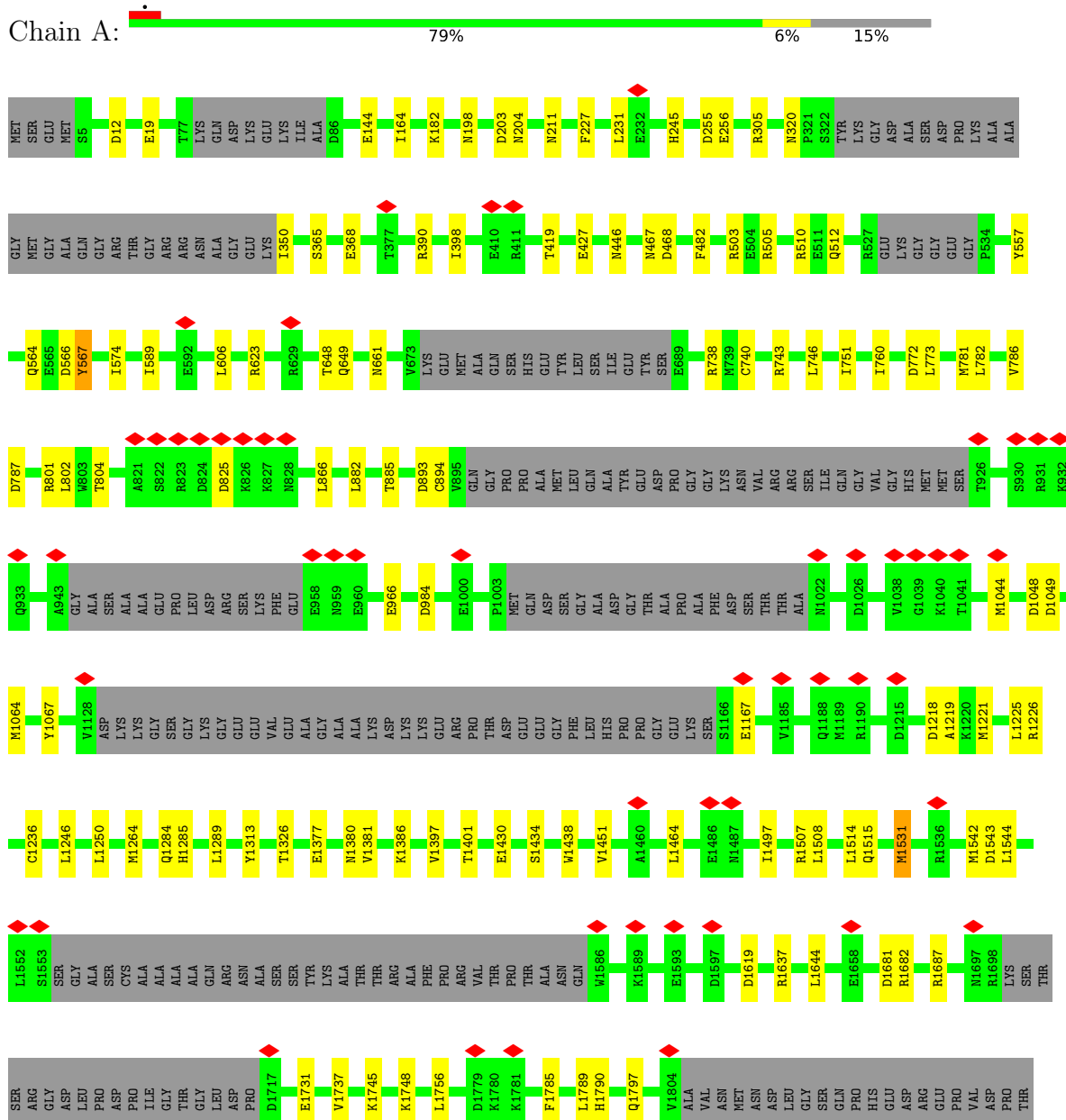
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
5	B	1	Total 126	C 41	H 75	N 1	O 8	P 1	0
5	B	1	Total 101	C 33	H 58	N 1	O 8	P 1	0
5	B	1	Total 117	C 38	H 69	N 1	O 8	P 1	0
5	B	1	Total 98	C 31	H 57	N 1	O 8	P 1	0
5	B	1	Total 112	C 38	H 64	N 1	O 8	P 1	0
5	C	1	Total 126	C 41	H 75	N 1	O 8	P 1	0
5	C	1	Total 101	C 33	H 58	N 1	O 8	P 1	0
5	C	1	Total 117	C 38	H 69	N 1	O 8	P 1	0
5	C	1	Total 98	C 31	H 57	N 1	O 8	P 1	0
5	C	1	Total 108	C 36	H 62	N 1	O 8	P 1	0
5	C	1	Total 113	C 38	H 65	N 1	O 8	P 1	0
5	C	1	Total 108	C 36	H 62	N 1	O 8	P 1	0
5	D	1	Total 117	C 38	H 69	N 1	O 8	P 1	0
5	D	1	Total 126	C 41	H 75	N 1	O 8	P 1	0
5	D	1	Total 101	C 33	H 58	N 1	O 8	P 1	0
5	D	1	Total 117	C 38	H 69	N 1	O 8	P 1	0
5	D	1	Total 98	C 31	H 57	N 1	O 8	P 1	0

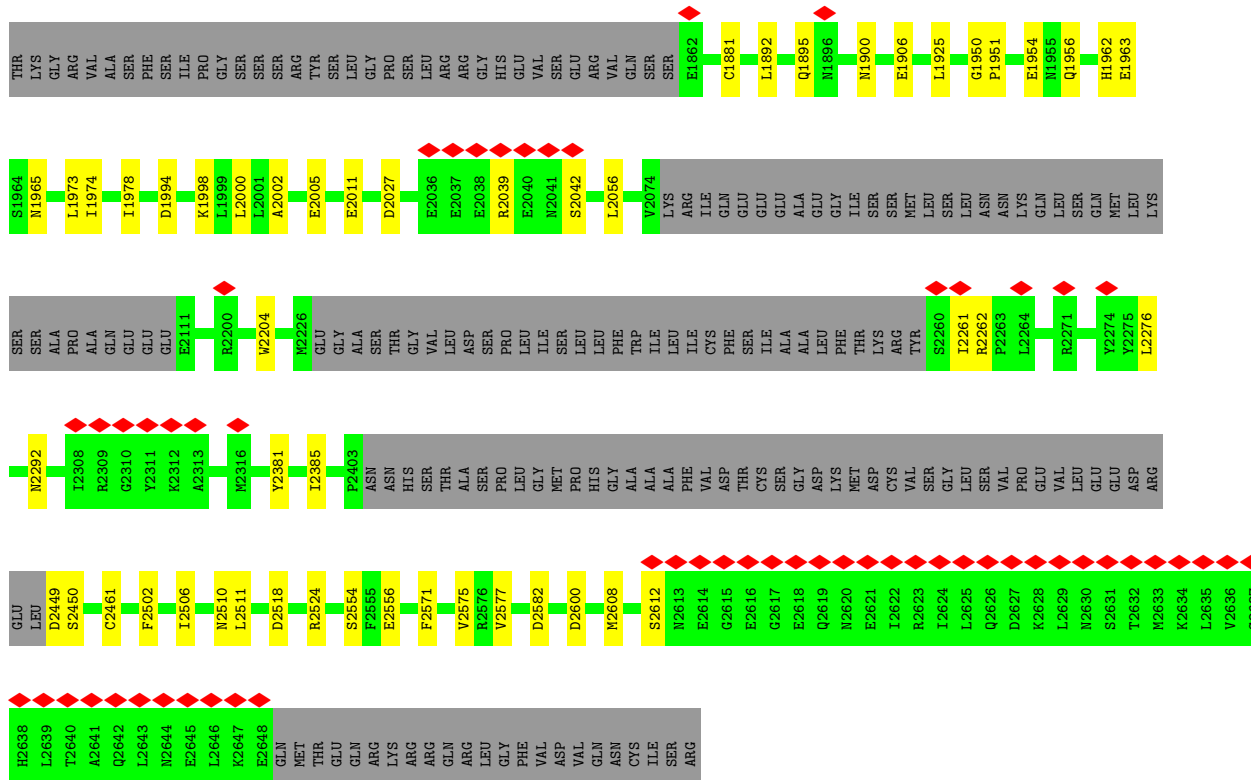
### 3 Residue-property plots

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.

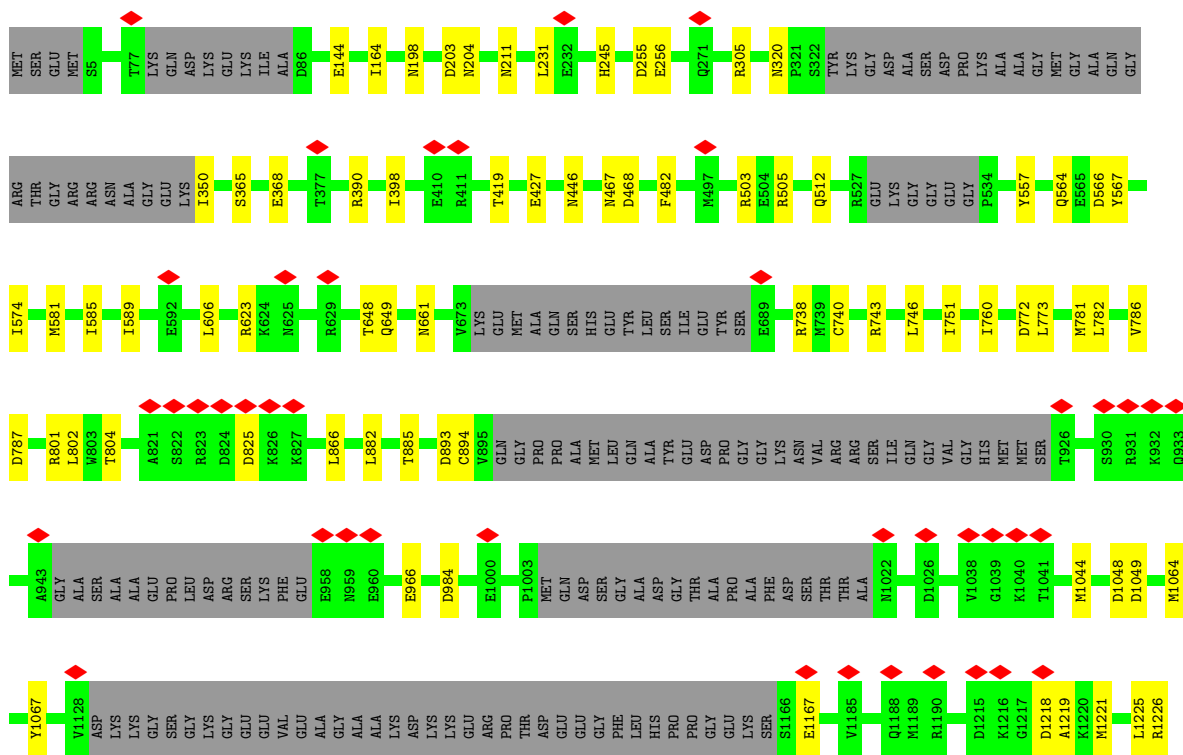
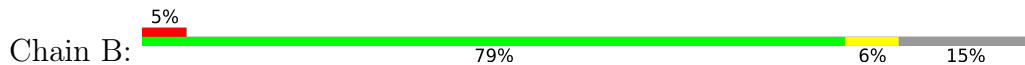
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain A:

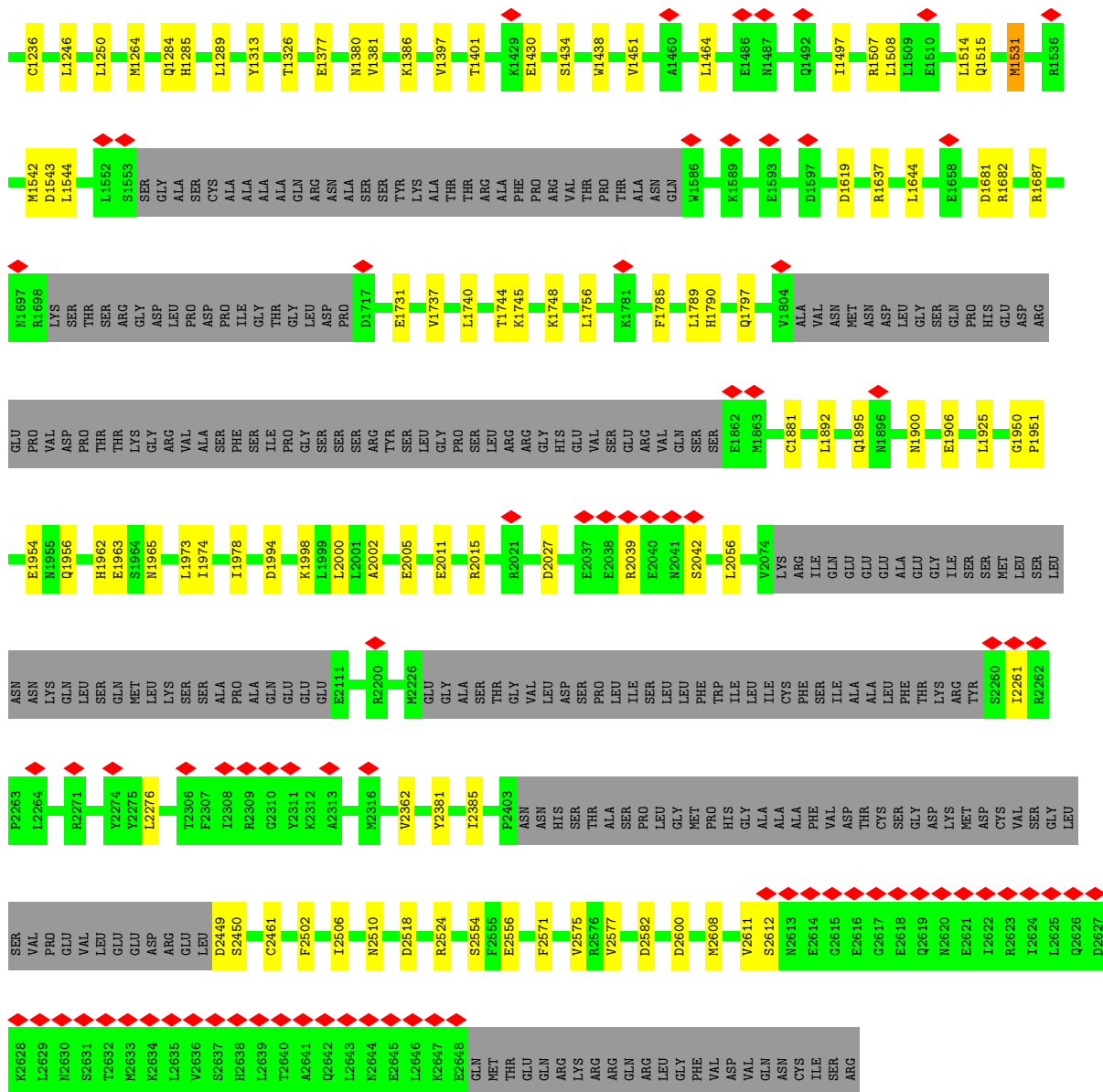




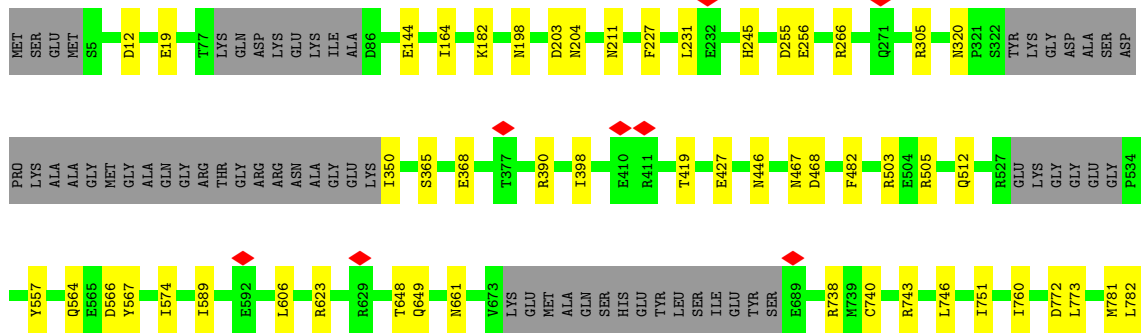
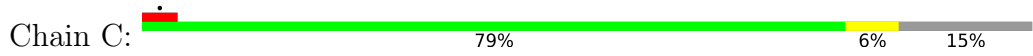
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

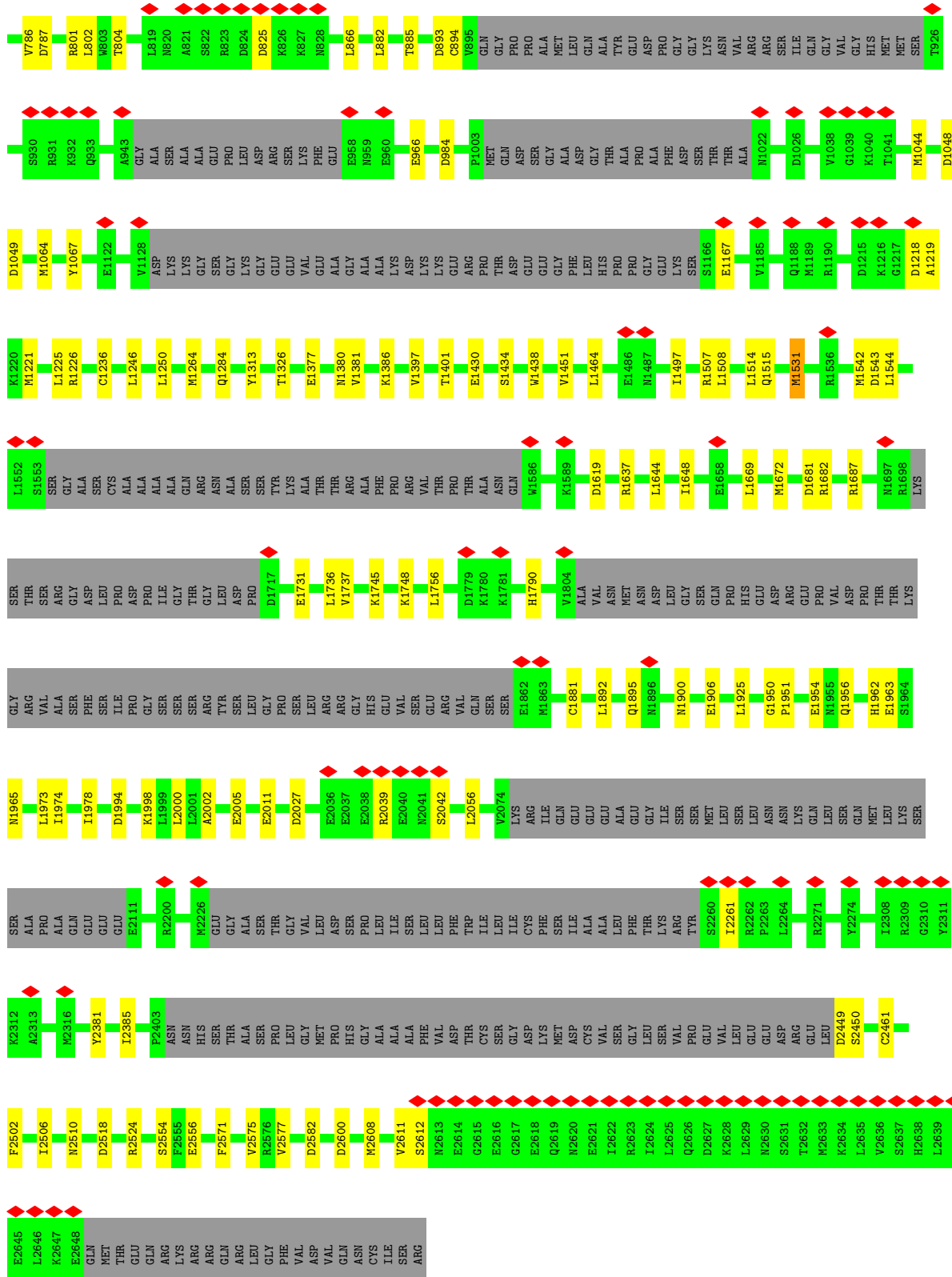






• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D: 79% 6% 15%



LEU	D2449	S2450	C2461	F2502	I2506	N2510	D2518	R2524	I2533	T2537	S2554	F2555	E2556	F2571	V2575	R2576	V2577	D2582	D2600	N2608	S2612	N2613	E2614	G2615	E2616	G2617	E2618	Q2619	N2620	E2621	I2622	R2623	I2624	L2625	Q2626	D2627	R2628	L2629	N2630	S2631	T2632	N2633	R2634	L2635
V2636	S2637	H2638	L2639	T2640	A2641	Q2642	L2643	N2644	E2645	L2646	K2647	E2648	GLN	MET	THR	GLU	GLN	ARG	LYS	ARG	ARG	GLN	ARG	LEU	GLY	PHE	VAL	ASP	VAL	VAL	GLN	ASN	CYS	ILE	SER	ARG								

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	767556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	139.562	Depositor
Minimum map value	-52.157	Depositor
Average map value	0.159	Depositor
Map value standard deviation	1.900	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	422.68802, 422.68802, 422.68802	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.629, 0.629, 0.629	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P, ZN, ATP, PCW

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	0.24	0/18521	0.44	0/25031
1	B	0.24	0/18521	0.44	0/25031
1	C	0.24	0/18521	0.44	0/25031
1	D	0.24	0/18521	0.44	0/25031
All	All	0.24	0/74084	0.44	0/100124

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1962	HIS	Sidechain
1	B	1962	HIS	Sidechain
1	C	1962	HIS	Sidechain
1	D	1962	HIS	Sidechain

## 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	18187	18207	18211	95	0
1	B	18187	18208	18211	96	0
1	C	18187	18207	18211	95	0
1	D	18187	18208	18211	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0
3	B	24	9	9	0	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	31	12	12	0	0
4	B	31	12	12	0	0
4	C	31	12	12	0	0
4	D	31	12	12	0	0
5	A	323	447	449	5	0
5	B	231	323	325	5	0
5	C	323	448	449	7	0
5	D	231	328	325	7	0
All	All	74080	74460	74476	384	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 3.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2608:MET:O	1:B:2612:SER:OG	1.98	0.82
1:A:2608:MET:O	1:A:2612:SER:OG	1.98	0.82
1:B:1430:GLU:O	1:B:1434:SER:OG	1.98	0.81
1:D:1430:GLU:O	1:D:1434:SER:OG	1.98	0.81
1:C:2608:MET:O	1:C:2612:SER:OG	1.98	0.80
1:C:1430:GLU:O	1:C:1434:SER:OG	1.98	0.80
1:D:2608:MET:O	1:D:2612:SER:OG	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:GLU:O	1:A:1434:SER:OG	1.98	0.80
1:B:2518:ASP:OD1	1:C:2524:ARG:NH1	2.16	0.79
1:B:2554:SER:OG	1:B:2556:GLU:OE1	2.02	0.77
1:C:2554:SER:OG	1:C:2556:GLU:OE1	2.02	0.76
1:A:743:ARG:NE	1:A:787:ASP:OD1	2.20	0.75
1:B:743:ARG:NE	1:B:787:ASP:OD1	2.20	0.74
1:C:743:ARG:NE	1:C:787:ASP:OD1	2.20	0.74
1:D:743:ARG:NE	1:D:787:ASP:OD1	2.20	0.73
1:D:2554:SER:OG	1:D:2556:GLU:OE1	2.02	0.73
1:C:446:ASN:OD1	1:C:512:GLN:NE2	2.23	0.72
1:C:2039:ARG:NH1	1:C:2042:SER:O	2.23	0.72
1:B:446:ASN:OD1	1:B:512:GLN:NE2	2.23	0.71
1:A:2039:ARG:NH1	1:A:2042:SER:O	2.23	0.71
1:D:2039:ARG:NH1	1:D:2042:SER:O	2.23	0.71
1:B:2039:ARG:NH1	1:B:2042:SER:O	2.23	0.71
1:A:446:ASN:OD1	1:A:512:GLN:NE2	2.23	0.71
1:D:446:ASN:OD1	1:D:512:GLN:NE2	2.23	0.70
1:D:2506:ILE:O	1:D:2510:ASN:ND2	2.25	0.70
1:A:2554:SER:OG	1:A:2556:GLU:OE1	2.02	0.70
1:A:2506:ILE:O	1:A:2510:ASN:ND2	2.25	0.70
1:C:2506:ILE:O	1:C:2510:ASN:ND2	2.25	0.69
1:B:2506:ILE:O	1:B:2510:ASN:ND2	2.25	0.69
1:B:320:ASN:ND2	1:B:350:ILE:O	2.26	0.69
1:D:320:ASN:ND2	1:D:350:ILE:O	2.26	0.69
1:C:320:ASN:ND2	1:C:350:ILE:O	2.26	0.69
1:A:320:ASN:ND2	1:A:350:ILE:O	2.26	0.68
1:A:2518:ASP:OD1	1:B:2524:ARG:NH1	2.28	0.65
1:A:606:LEU:CD1	1:A:648:THR:HG21	2.28	0.63
1:D:606:LEU:CD1	1:D:648:THR:HG21	2.28	0.63
1:C:606:LEU:CD1	1:C:648:THR:HG21	2.28	0.63
1:C:1895:GLN:O	1:C:1900:ASN:ND2	2.32	0.63
1:C:623:ARG:NH2	1:C:661:ASN:OD1	2.32	0.63
1:B:1895:GLN:O	1:B:1900:ASN:ND2	2.32	0.63
1:D:1895:GLN:O	1:D:1900:ASN:ND2	2.32	0.63
1:B:606:LEU:CD1	1:B:648:THR:HG21	2.28	0.63
1:B:623:ARG:NH2	1:B:661:ASN:OD1	2.32	0.62
1:A:1895:GLN:O	1:A:1900:ASN:ND2	2.32	0.62
1:A:623:ARG:NH2	1:A:661:ASN:OD1	2.31	0.62
1:D:623:ARG:NH2	1:D:661:ASN:OD1	2.31	0.62
1:A:2524:ARG:NH1	1:D:2518:ASP:OD1	2.29	0.61
1:C:2502:PHE:CD1	5:C:2709:PCW:C48	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1542:MET:N	1:C:1542:MET:SD	2.74	0.60
1:D:772:ASP:OD1	1:D:773:LEU:N	2.35	0.60
1:D:1542:MET:SD	1:D:1542:MET:N	2.75	0.60
1:A:772:ASP:OD1	1:A:773:LEU:N	2.35	0.59
1:A:1542:MET:SD	1:A:1542:MET:N	2.75	0.59
1:D:2502:PHE:CD1	5:D:2701:PCW:C48	2.84	0.59
1:C:2518:ASP:OD1	1:D:2524:ARG:NH1	2.31	0.59
1:B:1542:MET:SD	1:B:1542:MET:N	2.74	0.59
1:C:772:ASP:OD1	1:C:773:LEU:N	2.35	0.59
1:D:1313:TYR:OH	1:D:1377:GLU:OE1	2.19	0.59
1:B:772:ASP:OD1	1:B:773:LEU:N	2.35	0.59
1:C:1956:GLN:NE2	1:C:2002:ALA:O	2.36	0.59
1:D:1956:GLN:NE2	1:D:2002:ALA:O	2.36	0.59
1:A:1956:GLN:NE2	1:A:2002:ALA:O	2.36	0.58
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.85	0.57
1:D:564:GLN:HB3	1:D:574:ILE:HD12	1.85	0.57
1:B:564:GLN:HB3	1:B:574:ILE:HD12	1.85	0.57
1:B:1956:GLN:NE2	1:B:2002:ALA:O	2.36	0.57
1:B:144:GLU:OE1	1:B:211:ASN:ND2	2.37	0.57
1:C:564:GLN:HB3	1:C:574:ILE:HD12	1.85	0.57
1:A:1064:MET:SD	1:A:1637:ARG:NH1	2.78	0.57
1:B:1221:MET:SD	1:B:1225:LEU:HD13	2.45	0.57
1:C:144:GLU:OE1	1:C:211:ASN:ND2	2.38	0.56
1:A:1221:MET:SD	1:A:1225:LEU:HD13	2.45	0.56
1:A:1737:VAL:CG1	1:A:1756:LEU:HD23	2.36	0.56
1:C:1221:MET:SD	1:C:1225:LEU:HD13	2.45	0.56
1:A:1994:ASP:OD2	1:A:1998:LYS:NZ	2.38	0.56
1:B:1737:VAL:CG1	1:B:1756:LEU:HD23	2.36	0.56
1:D:2011:GLU:N	1:D:2011:GLU:OE1	2.39	0.56
1:D:1221:MET:SD	1:D:1225:LEU:HD13	2.45	0.56
1:D:1064:MET:SD	1:D:1637:ARG:NH1	2.78	0.56
1:D:1737:VAL:CG1	1:D:1756:LEU:HD23	2.36	0.56
1:D:144:GLU:OE1	1:D:211:ASN:ND2	2.37	0.55
1:A:144:GLU:OE1	1:A:211:ASN:ND2	2.37	0.55
1:A:2011:GLU:OE1	1:A:2011:GLU:N	2.39	0.55
1:C:1737:VAL:CG1	1:C:1756:LEU:HD23	2.36	0.55
1:B:1994:ASP:OD2	1:B:1998:LYS:NZ	2.38	0.55
1:A:2381:TYR:CZ	1:A:2385:ILE:HD11	2.42	0.54
1:B:2381:TYR:CZ	1:B:2385:ILE:HD11	2.42	0.54
1:C:1619:ASP:OD2	1:C:1687:ARG:NH2	2.40	0.54
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.40	0.54
1:A:467:ASN:OD1	1:A:468:ASP:N	2.41	0.54
1:C:467:ASN:OD1	1:C:468:ASP:N	2.41	0.54
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.41	0.54
1:D:482:PHE:O	1:D:505:ARG:NH1	2.41	0.54
1:B:1619:ASP:OD2	1:B:1687:ARG:NH2	2.40	0.54
1:C:245:HIS:NE2	1:C:427:GLU:OE1	2.39	0.54
1:D:2381:TYR:CZ	1:D:2385:ILE:HD11	2.42	0.54
1:A:1048:ASP:OD1	1:A:1049:ASP:N	2.41	0.54
1:A:1619:ASP:OD2	1:A:1687:ARG:NH2	2.40	0.54
1:C:2381:TYR:CZ	1:C:2385:ILE:HD11	2.42	0.54
1:D:245:HIS:NE2	1:D:427:GLU:OE1	2.39	0.54
1:B:1064:MET:SD	1:B:1637:ARG:NH1	2.78	0.54
1:D:467:ASN:OD1	1:D:468:ASP:N	2.41	0.54
5:A:3010:PCW:H83	5:A:3010:PCW:O4P	2.08	0.53
1:B:467:ASN:OD1	1:B:468:ASP:N	2.41	0.53
5:D:2702:PCW:O4P	5:D:2702:PCW:H83	2.08	0.53
1:B:2011:GLU:OE1	1:B:2011:GLU:N	2.39	0.53
1:C:1064:MET:SD	1:C:1637:ARG:NH1	2.78	0.53
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.41	0.53
5:B:2701:PCW:H83	5:B:2701:PCW:O4P	2.08	0.53
1:B:255:ASP:OD1	1:B:256:GLU:N	2.41	0.53
1:C:1167:GLU:OE1	1:C:1167:GLU:N	2.42	0.53
1:A:255:ASP:OD1	1:A:256:GLU:N	2.41	0.53
1:D:1167:GLU:N	1:D:1167:GLU:OE1	2.42	0.53
1:A:1313:TYR:OH	1:A:1377:GLU:OE1	2.19	0.53
5:C:2701:PCW:O4P	5:C:2701:PCW:H83	2.08	0.53
1:B:245:HIS:NE2	1:B:427:GLU:OE1	2.39	0.53
1:B:1167:GLU:N	1:B:1167:GLU:OE1	2.42	0.53
1:B:2502:PHE:CD1	5:B:2708:PCW:C48	2.92	0.53
1:C:2011:GLU:N	1:C:2011:GLU:OE1	2.39	0.53
1:A:606:LEU:HD12	1:A:648:THR:HG21	1.91	0.52
1:D:606:LEU:HD12	1:D:648:THR:HG21	1.91	0.52
1:D:255:ASP:OD1	1:D:256:GLU:N	2.41	0.52
1:A:1167:GLU:N	1:A:1167:GLU:OE1	2.42	0.52
1:A:482:PHE:O	1:A:505:ARG:NH1	2.41	0.52
1:B:606:LEU:HD12	1:B:648:THR:HG21	1.91	0.52
1:C:606:LEU:HD12	1:C:648:THR:HG21	1.91	0.52
1:C:1313:TYR:OH	1:C:1377:GLU:OE1	2.19	0.52
1:C:482:PHE:O	1:C:505:ARG:NH1	2.41	0.51
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.43	0.51
1:C:1543:ASP:OD1	1:C:1544:LEU:N	2.43	0.51
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.43	0.51
1:D:1954:GLU:OE1	1:D:1954:GLU:N	2.42	0.51
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.43	0.51
1:C:2502:PHE:HD1	5:C:2709:PCW:H483	1.74	0.51
1:D:164:ILE:HG23	1:D:164:ILE:O	2.11	0.51
1:B:1954:GLU:OE1	1:B:1954:GLU:N	2.42	0.51
1:B:1543:ASP:OD1	1:B:1544:LEU:N	2.43	0.51
1:C:255:ASP:OD1	1:C:256:GLU:N	2.41	0.51
1:B:893:ASP:OD1	1:B:894:CYS:N	2.44	0.51
1:D:1543:ASP:OD1	1:D:1544:LEU:N	2.43	0.50
1:A:164:ILE:O	1:A:164:ILE:HG23	2.11	0.50
1:A:1464:LEU:O	1:A:1464:LEU:HD23	2.12	0.50
1:B:1326:THR:HG21	1:B:1386:LYS:HG2	1.93	0.50
1:D:2502:PHE:HD1	5:D:2701:PCW:H483	1.75	0.50
1:C:164:ILE:HG23	1:C:164:ILE:O	2.11	0.50
1:A:1543:ASP:OD1	1:A:1544:LEU:N	2.43	0.50
1:C:1464:LEU:O	1:C:1464:LEU:HD23	2.12	0.50
1:A:1326:THR:HG21	1:A:1386:LYS:HG2	1.93	0.50
1:B:966:GLU:OE2	1:B:1067:TYR:OH	2.23	0.50
1:C:1326:THR:HG21	1:C:1386:LYS:HG2	1.93	0.50
1:A:893:ASP:OD1	1:A:894:CYS:N	2.44	0.49
1:B:649:GLN:NE2	1:B:738:ARG:O	2.41	0.49
1:A:1954:GLU:N	1:A:1954:GLU:OE1	2.42	0.49
1:D:1994:ASP:OD2	1:D:1998:LYS:NZ	2.38	0.49
1:A:245:HIS:NE2	1:A:427:GLU:OE1	2.39	0.49
1:B:1326:THR:HG21	1:B:1386:LYS:CG	2.43	0.49
1:B:1464:LEU:HD23	1:B:1464:LEU:O	2.12	0.49
1:B:2449:ASP:OD1	1:B:2450:SER:N	2.46	0.49
1:C:649:GLN:NE2	1:C:738:ARG:O	2.41	0.49
1:D:1326:THR:HG21	1:D:1386:LYS:HG2	1.93	0.49
1:C:1954:GLU:OE1	1:C:1954:GLU:N	2.42	0.49
1:B:164:ILE:HG23	1:B:164:ILE:O	2.11	0.49
1:B:482:PHE:O	1:B:505:ARG:NH1	2.41	0.49
1:D:1464:LEU:HD23	1:D:1464:LEU:O	2.12	0.49
1:D:2262:ARG:NH1	5:D:2702:PCW:O1P	2.44	0.48
1:A:2449:ASP:OD1	1:A:2450:SER:N	2.46	0.48
1:C:1963:GLU:O	1:C:1965:ASN:ND2	2.46	0.48
1:D:1326:THR:HG21	1:D:1386:LYS:CG	2.43	0.48
1:D:1963:GLU:O	1:D:1965:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1326:THR:HG21	1:A:1386:LYS:CG	2.43	0.48
1:A:1963:GLU:O	1:A:1965:ASN:ND2	2.46	0.48
1:D:893:ASP:OD1	1:D:894:CYS:N	2.44	0.48
1:C:1326:THR:HG21	1:C:1386:LYS:CG	2.43	0.48
1:B:1963:GLU:O	1:B:1965:ASN:ND2	2.47	0.48
1:C:2449:ASP:OD1	1:C:2450:SER:N	2.46	0.48
1:A:2502:PHE:CD1	5:A:3008:PCW:C48	2.97	0.48
1:D:2449:ASP:OD1	1:D:2450:SER:N	2.46	0.48
1:D:2533:ILE:O	1:D:2537:THR:OG1	2.26	0.48
1:B:1438:TRP:CE3	1:B:1497:ILE:HG21	2.49	0.47
1:A:1438:TRP:CE3	1:A:1497:ILE:HG21	2.49	0.47
1:C:231:LEU:HD23	1:C:231:LEU:H	1.79	0.47
1:C:1438:TRP:CE3	1:C:1497:ILE:HG21	2.49	0.47
1:D:649:GLN:NE2	1:D:738:ARG:O	2.41	0.47
1:C:893:ASP:OD1	1:C:894:CYS:N	2.44	0.47
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.47	0.47
1:D:1438:TRP:CE3	1:D:1497:ILE:HG21	2.49	0.47
1:B:786:VAL:HG21	1:B:866:LEU:HD11	1.97	0.47
1:B:231:LEU:HD23	1:B:231:LEU:H	1.80	0.47
1:B:1978:ILE:HD12	1:B:1978:ILE:N	2.30	0.47
1:D:882:LEU:O	1:D:885:THR:HG22	2.15	0.47
1:D:1284:GLN:N	1:D:1284:GLN:OE1	2.48	0.47
1:A:966:GLU:OE2	1:A:1067:TYR:OH	2.23	0.47
1:C:1531:MET:SD	1:C:1531:MET:N	2.88	0.47
1:C:1978:ILE:N	1:C:1978:ILE:HD12	2.30	0.47
1:C:2261:ILE:HG22	1:C:2261:ILE:O	2.15	0.47
1:A:1284:GLN:OE1	1:A:1284:GLN:N	2.48	0.46
1:B:1284:GLN:N	1:B:1284:GLN:OE1	2.48	0.46
1:B:1681:ASP:OD1	1:B:1682:ARG:N	2.47	0.46
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.15	0.46
1:D:19:GLU:OE1	1:D:182:LYS:NZ	2.43	0.46
1:A:1978:ILE:N	1:A:1978:ILE:HD12	2.30	0.46
1:C:1284:GLN:OE1	1:C:1284:GLN:N	2.48	0.46
1:A:2262:ARG:NH1	5:A:3010:PCW:O1P	2.46	0.46
1:B:802:LEU:CD2	1:B:804:THR:HG22	2.45	0.46
1:C:882:LEU:O	1:C:885:THR:HG22	2.15	0.46
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.15	0.46
1:A:557:TYR:CD2	1:A:589:ILE:HG22	2.51	0.46
1:A:1531:MET:N	1:A:1531:MET:SD	2.88	0.46
1:A:1681:ASP:OD1	1:A:1682:ARG:N	2.47	0.46
1:D:1380:ASN:OD1	1:D:1381:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1380:ASN:OD1	1:A:1381:VAL:N	2.49	0.46
1:D:1681:ASP:OD1	1:D:1682:ARG:N	2.47	0.46
1:A:2261:ILE:HG22	1:A:2261:ILE:O	2.15	0.46
1:D:802:LEU:CD2	1:D:804:THR:HG22	2.45	0.46
1:D:1531:MET:SD	1:D:1531:MET:N	2.88	0.46
1:D:786:VAL:HG21	1:D:866:LEU:HD11	1.97	0.46
1:A:786:VAL:HG21	1:A:866:LEU:HD11	1.97	0.46
1:C:802:LEU:CD2	1:C:804:THR:HG22	2.45	0.46
1:A:231:LEU:HD23	1:A:231:LEU:H	1.79	0.46
1:A:882:LEU:O	1:A:885:THR:HG22	2.15	0.46
1:C:786:VAL:HG21	1:C:866:LEU:HD11	1.97	0.46
1:D:231:LEU:H	1:D:231:LEU:HD23	1.79	0.46
1:D:782:LEU:O	1:D:782:LEU:HD23	2.16	0.46
1:D:557:TYR:CD2	1:D:589:ILE:HG22	2.51	0.46
1:D:1978:ILE:HD12	1:D:1978:ILE:N	2.30	0.46
1:B:782:LEU:HD23	1:B:782:LEU:O	2.16	0.45
1:A:305:ARG:NH1	1:A:365:SER:OG	2.50	0.45
1:A:802:LEU:CD2	1:A:804:THR:HG22	2.45	0.45
1:A:2511:LEU:HD21	1:B:2362:VAL:HG23	1.98	0.45
1:B:882:LEU:O	1:B:885:THR:HG22	2.15	0.45
1:B:1531:MET:SD	1:B:1531:MET:N	2.88	0.45
1:C:557:TYR:CD2	1:C:589:ILE:HG22	2.51	0.45
1:C:1380:ASN:OD1	1:C:1381:VAL:N	2.49	0.45
1:D:305:ARG:NH1	1:D:365:SER:OG	2.50	0.45
1:A:782:LEU:O	1:A:782:LEU:HD23	2.16	0.45
1:C:305:ARG:NH1	1:C:365:SER:OG	2.50	0.45
1:D:2502:PHE:CD1	5:D:2701:PCW:H483	2.51	0.45
1:B:557:TYR:CD2	1:B:589:ILE:HG22	2.51	0.45
1:B:1380:ASN:OD1	1:B:1381:VAL:N	2.49	0.45
1:B:305:ARG:NH1	1:B:365:SER:OG	2.50	0.45
1:B:2571:PHE:O	1:B:2575:VAL:HG23	2.17	0.45
1:A:740:CYS:SG	1:A:751:ILE:HD12	2.56	0.45
1:A:2571:PHE:O	1:A:2575:VAL:HG23	2.17	0.45
1:C:740:CYS:SG	1:C:751:ILE:HD12	2.56	0.45
1:D:740:CYS:SG	1:D:751:ILE:HD12	2.56	0.45
1:D:2571:PHE:O	1:D:2575:VAL:HG23	2.17	0.44
1:C:782:LEU:HD23	1:C:782:LEU:O	2.16	0.44
1:C:1994:ASP:OD2	1:C:1998:LYS:NZ	2.38	0.44
1:B:740:CYS:SG	1:B:751:ILE:HD12	2.56	0.44
1:B:1313:TYR:OH	1:B:1377:GLU:OE1	2.19	0.44
1:A:1397:VAL:O	1:A:1401:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2502:PHE:HD1	5:B:2708:PCW:H483	1.82	0.44
1:C:2502:PHE:CD1	5:C:2709:PCW:H483	2.50	0.44
1:A:2204:TRP:O	1:A:2292:ASN:ND2	2.48	0.44
1:A:19:GLU:OE1	1:A:182:LYS:NZ	2.43	0.44
1:C:746:LEU:HD23	1:C:746:LEU:O	2.18	0.44
1:D:1397:VAL:O	1:D:1401:THR:HG22	2.18	0.44
1:D:1451:VAL:HG22	1:D:1464:LEU:HD22	2.00	0.44
1:B:1397:VAL:O	1:B:1401:THR:HG22	2.18	0.43
1:C:2571:PHE:O	1:C:2575:VAL:HG23	2.17	0.43
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.33	0.43
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.33	0.43
1:C:1250:LEU:HD11	1:C:1264:MET:SD	2.58	0.43
1:D:510:ARG:NH2	1:D:567:TYR:OH	2.49	0.43
5:A:3006:PCW:H83	5:A:3006:PCW:O4P	2.18	0.43
1:A:1250:LEU:HD11	1:A:1264:MET:SD	2.58	0.43
1:B:746:LEU:O	1:B:746:LEU:HD23	2.18	0.43
1:D:746:LEU:O	1:D:746:LEU:HD23	2.18	0.43
1:B:1250:LEU:HD11	1:B:1264:MET:SD	2.58	0.43
1:D:1250:LEU:HD11	1:D:1264:MET:SD	2.58	0.43
1:C:1397:VAL:O	1:C:1401:THR:HG22	2.18	0.43
1:C:1451:VAL:HG22	1:C:1464:LEU:HD22	2.00	0.43
5:C:2707:PCW:H83	5:C:2707:PCW:O4P	2.18	0.43
1:D:1644:LEU:HD23	1:D:1731:GLU:HG3	2.01	0.43
1:D:2502:PHE:CD1	5:D:2701:PCW:C47	3.02	0.43
1:A:1644:LEU:HD23	1:A:1731:GLU:HG3	2.01	0.43
1:C:1644:LEU:HD23	1:C:1731:GLU:HG3	2.01	0.43
1:A:1451:VAL:HG22	1:A:1464:LEU:HD22	2.00	0.43
1:B:760:ILE:HG21	1:B:781:MET:HB2	2.01	0.43
1:C:760:ILE:HG21	1:C:781:MET:HB2	2.01	0.43
1:D:966:GLU:OE2	1:D:1067:TYR:OH	2.23	0.43
1:D:1127:TRP:O	1:D:1169:TYR:OH	2.36	0.43
1:A:649:GLN:NE2	1:A:738:ARG:O	2.41	0.43
1:B:2000:LEU:HD13	1:B:2056:LEU:HD21	2.01	0.43
1:B:2502:PHE:CD1	5:B:2708:PCW:H483	2.54	0.43
1:A:746:LEU:HD23	1:A:746:LEU:O	2.18	0.42
1:A:203:ASP:OD1	1:A:204:ASN:N	2.52	0.42
1:A:2000:LEU:HD13	1:A:2056:LEU:HD21	2.01	0.42
1:B:1236:CYS:SG	1:B:1246:LEU:HD12	2.59	0.42
1:B:1451:VAL:HG22	1:B:1464:LEU:HD22	2.00	0.42
5:B:2707:PCW:O4P	5:B:2707:PCW:H83	2.18	0.42
1:C:1236:CYS:SG	1:C:1246:LEU:HD12	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1236:CYS:SG	1:D:1246:LEU:HD12	2.59	0.42
1:A:2506:ILE:HB	5:A:3008:PCW:H482	2.01	0.42
1:A:2577:VAL:HG12	1:A:2577:VAL:O	2.20	0.42
1:B:1644:LEU:HD23	1:B:1731:GLU:HG3	2.01	0.42
1:C:1669:LEU:HD23	1:C:1672:MET:HE3	2.02	0.42
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.33	0.42
5:D:2708:PCW:H83	5:D:2708:PCW:O4P	2.19	0.42
1:D:203:ASP:OD1	1:D:204:ASN:N	2.52	0.42
1:D:760:ILE:HG21	1:D:781:MET:HB2	2.01	0.42
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.33	0.42
1:D:2577:VAL:O	1:D:2577:VAL:HG12	2.20	0.42
1:A:1236:CYS:SG	1:A:1246:LEU:HD12	2.59	0.42
1:A:1881:CYS:SG	1:A:1892:LEU:HD12	2.60	0.42
1:B:203:ASP:OD1	1:B:204:ASN:N	2.52	0.42
1:B:1790:HIS:NE2	1:B:1906:GLU:OE2	2.53	0.42
1:B:2577:VAL:HG12	1:B:2577:VAL:O	2.20	0.42
1:C:203:ASP:OD1	1:C:204:ASN:N	2.52	0.42
1:A:12:ASP:OD1	1:A:227:PHE:N	2.53	0.42
1:A:760:ILE:HG21	1:A:781:MET:HB2	2.01	0.42
1:A:1974:ILE:HD12	1:A:2000:LEU:HD12	2.02	0.42
1:D:398:ILE:HD13	1:D:419:THR:HG22	2.02	0.42
1:A:368:GLU:OE1	1:A:390:ARG:NH2	2.53	0.42
1:C:503:ARG:NH2	1:C:566:ASP:O	2.53	0.42
1:C:398:ILE:HD13	1:C:419:THR:HG22	2.02	0.42
1:D:1881:CYS:SG	1:D:1892:LEU:HD12	2.60	0.42
1:B:503:ARG:NH2	1:B:566:ASP:O	2.53	0.41
1:C:1974:ILE:HD12	1:C:2000:LEU:HD12	2.02	0.41
1:D:1326:THR:HG21	1:D:1386:LYS:HD3	2.01	0.41
1:D:1790:HIS:NE2	1:D:1906:GLU:OE2	2.53	0.41
1:D:1974:ILE:HD12	1:D:2000:LEU:HD12	2.02	0.41
1:A:1326:THR:HG21	1:A:1386:LYS:HD3	2.01	0.41
1:A:1790:HIS:NE2	1:A:1906:GLU:OE2	2.53	0.41
1:C:12:ASP:OD1	1:C:227:PHE:N	2.53	0.41
1:C:966:GLU:OE2	1:C:1067:TYR:OH	2.23	0.41
1:C:2000:LEU:HD13	1:C:2056:LEU:HD21	2.01	0.41
1:C:2502:PHE:CD1	5:C:2709:PCW:C47	3.01	0.41
1:D:2000:LEU:HD13	1:D:2056:LEU:HD21	2.01	0.41
1:B:368:GLU:OE1	1:B:390:ARG:NH2	2.53	0.41
1:C:19:GLU:OE1	1:C:182:LYS:NZ	2.43	0.41
1:C:1326:THR:HG21	1:C:1386:LYS:HD3	2.02	0.41
1:D:1669:LEU:HD23	1:D:1672:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:ASP:O	1:A:1219:ALA:HB3	2.21	0.41
1:C:368:GLU:OE1	1:C:390:ARG:NH2	2.53	0.41
1:C:1790:HIS:NE2	1:C:1906:GLU:OE2	2.53	0.41
1:B:1508:LEU:HD21	1:B:1514:LEU:HD11	2.03	0.41
1:B:1881:CYS:SG	1:B:1892:LEU:HD12	2.60	0.41
1:C:1881:CYS:SG	1:C:1892:LEU:HD12	2.60	0.41
1:C:2577:VAL:HG12	1:C:2577:VAL:O	2.20	0.41
1:D:1508:LEU:HD21	1:D:1514:LEU:HD11	2.03	0.41
1:A:510:ARG:NH2	1:A:567:TYR:OH	2.49	0.41
1:B:1218:ASP:O	1:B:1219:ALA:HB3	2.21	0.41
1:A:1508:LEU:HD21	1:A:1514:LEU:HD11	2.03	0.41
1:B:1925:LEU:HD21	1:B:1973:LEU:HD23	2.03	0.41
1:C:1218:ASP:O	1:C:1219:ALA:HB3	2.21	0.41
1:B:398:ILE:HD13	1:B:419:THR:HG22	2.02	0.41
1:B:1974:ILE:HD12	1:B:2000:LEU:HD12	2.02	0.41
1:C:1451:VAL:CG2	1:C:1464:LEU:HD22	2.51	0.41
1:C:1925:LEU:HD21	1:C:1973:LEU:HD23	2.03	0.41
1:C:2002:ALA:HA	1:C:2005:GLU:HG3	2.03	0.41
1:C:2611:VAL:O	1:C:2611:VAL:HG12	2.20	0.41
1:D:368:GLU:OE1	1:D:390:ARG:NH2	2.53	0.41
1:B:2611:VAL:O	1:B:2611:VAL:HG12	2.20	0.41
1:C:1508:LEU:HD21	1:C:1514:LEU:HD11	2.03	0.41
1:D:503:ARG:NH2	1:D:566:ASP:O	2.53	0.41
1:D:1925:LEU:HD21	1:D:1973:LEU:HD23	2.03	0.41
1:B:1326:THR:HG21	1:B:1386:LYS:HD3	2.01	0.40
1:C:2502:PHE:CG	5:C:2709:PCW:C47	2.68	0.40
1:D:2276:LEU:HD12	1:D:2276:LEU:N	2.36	0.40
1:A:1285:HIS:NE2	1:A:1289:LEU:HD11	2.36	0.40
1:D:266:ARG:NH2	3:D:2704:I3P:O43	2.55	0.40
1:D:1451:VAL:CG2	1:D:1464:LEU:HD22	2.51	0.40
1:A:503:ARG:NH2	1:A:566:ASP:O	2.53	0.40
1:A:2002:ALA:HA	1:A:2005:GLU:HG3	2.03	0.40
1:A:2276:LEU:HD12	1:A:2276:LEU:N	2.37	0.40
1:B:581:MET:O	1:B:585:ILE:HG12	2.22	0.40
1:B:2002:ALA:HA	1:B:2005:GLU:HG3	2.03	0.40
1:D:2002:ALA:HA	1:D:2005:GLU:HG3	2.03	0.40
1:A:1785:PHE:CE2	1:A:1789:LEU:HD11	2.57	0.40
1:B:1740:LEU:O	1:B:1744:THR:HG22	2.22	0.40
1:B:1785:PHE:CE2	1:B:1789:LEU:HD11	2.57	0.40
1:C:266:ARG:NH2	3:C:2703:I3P:O43	2.55	0.40
1:A:398:ILE:HD13	1:A:419:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:GLN:NE2	1:A:1906:GLU:O	2.55	0.40
1:A:1925:LEU:HD21	1:A:1973:LEU:HD23	2.03	0.40
1:B:1285:HIS:NE2	1:B:1289:LEU:HD11	2.36	0.40
1:B:1451:VAL:CG2	1:B:1464:LEU:HD22	2.51	0.40
1:B:1797:GLN:NE2	1:B:1906:GLU:O	2.55	0.40
1:B:1965:ASN:OD1	1:B:2015:ARG:NH2	2.55	0.40
1:B:2276:LEU:N	1:B:2276:LEU:HD12	2.37	0.40
1:C:1648:ILE:HG23	1:C:1736:LEU:HD22	2.04	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	2238/2671 (84%)	2195 (98%)	43 (2%)	0	100	100
1	B	2238/2671 (84%)	2195 (98%)	43 (2%)	0	100	100
1	C	2238/2671 (84%)	2194 (98%)	44 (2%)	0	100	100
1	D	2238/2671 (84%)	2193 (98%)	45 (2%)	0	100	100
All	All	8952/10684 (84%)	8777 (98%)	175 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	2021/2385 (85%)	2007 (99%)	14 (1%)	84	94
1	B	2021/2385 (85%)	2007 (99%)	14 (1%)	84	94
1	C	2021/2385 (85%)	2007 (99%)	14 (1%)	84	94
1	D	2021/2385 (85%)	2007 (99%)	14 (1%)	84	94
All	All	8084/9540 (85%)	8028 (99%)	56 (1%)	84	94

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	567	TYR
1	A	825	ASP
1	A	1044	MET
1	A	1226	ARG
1	A	1507	ARG
1	A	1515	GLN
1	A	1531	MET
1	A	1745	LYS
1	A	1748	LYS
1	A	2027	ASP
1	A	2461	CYS
1	A	2582	ASP
1	A	2600	ASP
1	B	198	ASN
1	B	567	TYR
1	B	825	ASP
1	B	1044	MET
1	B	1226	ARG
1	B	1507	ARG
1	B	1515	GLN
1	B	1531	MET
1	B	1745	LYS
1	B	1748	LYS
1	B	2027	ASP
1	B	2461	CYS
1	B	2582	ASP
1	B	2600	ASP
1	C	198	ASN
1	C	567	TYR
1	C	825	ASP
1	C	1044	MET
1	C	1226	ARG

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Mol	Chain	Res	Type
1	C	1507	ARG
1	C	1515	GLN
1	C	1531	MET
1	C	1745	LYS
1	C	1748	LYS
1	C	2027	ASP
1	C	2461	CYS
1	C	2582	ASP
1	C	2600	ASP
1	D	198	ASN
1	D	567	TYR
1	D	825	ASP
1	D	1044	MET
1	D	1226	ARG
1	D	1507	ARG
1	D	1515	GLN
1	D	1531	MET
1	D	1745	LYS
1	D	1748	LYS
1	D	2027	ASP
1	D	2461	CYS
1	D	2582	ASP
1	D	2600	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	GLN
1	A	1518	HIS
1	B	512	GLN
1	B	1518	HIS
1	C	512	GLN
1	C	1518	HIS
1	D	512	GLN
1	D	1518	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	$\# Z  > 2$
5	PCW	B	2701	-	50,50,53	0.50	0	56,58,61	0.52	0
5	PCW	C	2707	-	40,40,53	0.55	0	46,48,61	0.56	0
5	PCW	D	2706	-	42,42,53	0.53	0	48,50,61	0.48	0
5	PCW	A	3009	-	45,45,53	0.52	0	50,53,61	0.48	0
5	PCW	A	3004	-	42,42,53	0.53	0	48,50,61	0.48	0
5	PCW	C	2710	-	45,45,53	0.52	0	50,53,61	0.48	0
5	PCW	D	2708	-	40,40,53	0.55	0	46,48,61	0.56	0
3	I3P	D	2704	-	24,24,24	2.07	3 (12%)	36,39,39	0.90	0
5	PCW	B	2706	-	47,47,53	0.51	0	52,55,61	0.52	1 (1%)
4	ATP	B	2704	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
5	PCW	C	2708	-	45,45,53	0.52	0	50,53,61	0.48	0
5	PCW	B	2705	-	42,42,53	0.53	0	48,50,61	0.48	0
4	ATP	D	2705	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
5	PCW	C	2709	-	47,47,53	0.52	0	52,55,61	0.50	0
5	PCW	B	2708	-	47,47,53	0.52	0	52,55,61	0.50	0
5	PCW	A	3008	-	47,47,53	0.52	0	52,55,61	0.50	0
5	PCW	C	2701	-	50,50,53	0.50	0	56,58,61	0.52	0
4	ATP	C	2704	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
5	PCW	D	2707	-	47,47,53	0.51	0	52,55,61	0.52	1 (1%)
3	I3P	B	2703	-	24,24,24	2.07	3 (12%)	36,39,39	0.90	0
5	PCW	D	2702	-	50,50,53	0.50	0	56,58,61	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PCW	A	3005	-	47,47,53	0.51	0	52,55,61	0.52	1 (1%)
5	PCW	A	3007	-	45,45,53	0.52	0	50,53,61	0.48	0
3	I3P	C	2703	-	24,24,24	2.07	3 (12%)	36,39,39	0.90	0
5	PCW	A	3010	-	50,50,53	0.50	0	56,58,61	0.52	0
5	PCW	A	3006	-	40,40,53	0.55	0	46,48,61	0.56	0
4	ATP	A	3003	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
5	PCW	C	2705	-	42,42,53	0.53	0	48,50,61	0.48	0
5	PCW	C	2706	-	47,47,53	0.51	0	52,55,61	0.52	1 (1%)
3	I3P	A	3002	-	24,24,24	2.07	3 (12%)	36,39,39	0.90	0
5	PCW	B	2707	-	40,40,53	0.55	0	46,48,61	0.56	0
5	PCW	D	2701	-	47,47,53	0.52	0	52,55,61	0.50	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
5	PCW	B	2701	-	-	18/54/54/57	-
5	PCW	C	2707	-	-	17/44/44/57	-
5	PCW	D	2706	-	-	11/46/46/57	-
5	PCW	A	3009	-	-	15/49/49/57	-
5	PCW	A	3004	-	-	11/46/46/57	-
5	PCW	C	2710	-	-	15/49/49/57	-
5	PCW	D	2708	-	-	17/44/44/57	-
3	I3P	D	2704	-	-	3/15/39/39	0/1/1/1
5	PCW	B	2706	-	-	19/51/51/57	-
4	ATP	B	2704	-	-	9/18/38/38	0/3/3/3
5	PCW	C	2708	-	-	15/49/49/57	-
5	PCW	B	2705	-	-	11/46/46/57	-
4	ATP	D	2705	-	-	9/18/38/38	0/3/3/3
5	PCW	C	2709	-	-	14/51/51/57	-
5	PCW	B	2708	-	-	14/51/51/57	-
5	PCW	A	3008	-	-	14/51/51/57	-
5	PCW	C	2701	-	-	18/54/54/57	-
4	ATP	C	2704	-	-	9/18/38/38	0/3/3/3
5	PCW	D	2707	-	-	19/51/51/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3P	B	2703	-	-	3/15/39/39	0/1/1/1
5	PCW	D	2702	-	-	18/54/54/57	-
5	PCW	A	3005	-	-	19/51/51/57	-
5	PCW	A	3007	-	-	15/49/49/57	-
3	I3P	C	2703	-	-	3/15/39/39	0/1/1/1
5	PCW	A	3010	-	-	18/54/54/57	-
5	PCW	A	3006	-	-	17/44/44/57	-
4	ATP	A	3003	-	-	9/18/38/38	0/3/3/3
5	PCW	C	2705	-	-	11/46/46/57	-
5	PCW	C	2706	-	-	19/51/51/57	-
3	I3P	A	3002	-	-	3/15/39/39	0/1/1/1
5	PCW	B	2707	-	-	17/44/44/57	-
5	PCW	D	2701	-	-	14/51/51/57	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2703	I3P	P4-O4	5.76	1.70	1.59
3	D	2704	I3P	P4-O4	5.76	1.70	1.59
3	C	2703	I3P	P4-O4	5.76	1.70	1.59
3	A	3002	I3P	P4-O4	5.76	1.70	1.59
3	A	3002	I3P	P5-O5	5.61	1.69	1.59
3	C	2703	I3P	P5-O5	5.61	1.69	1.59
3	B	2703	I3P	P5-O5	5.61	1.69	1.59
3	D	2704	I3P	P5-O5	5.61	1.69	1.59
3	B	2703	I3P	P1-O1	5.41	1.69	1.59
3	A	3002	I3P	P1-O1	5.40	1.69	1.59
3	C	2703	I3P	P1-O1	5.40	1.69	1.59
3	D	2704	I3P	P1-O1	5.40	1.69	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2705	ATP	C5-C6-N6	2.30	123.85	120.35
4	B	2704	ATP	C5-C6-N6	2.30	123.85	120.35
4	C	2704	ATP	C5-C6-N6	2.30	123.85	120.35
4	A	3003	ATP	C5-C6-N6	2.30	123.84	120.35
4	B	2704	ATP	PB-O3B-PG	2.05	139.85	132.83
4	C	2704	ATP	PB-O3B-PG	2.05	139.85	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3003	ATP	PB-O3B-PG	2.05	139.85	132.83
4	D	2705	ATP	PB-O3B-PG	2.05	139.85	132.83
5	C	2706	PCW	C3-C2-C1	2.01	116.53	111.79
5	D	2707	PCW	C3-C2-C1	2.01	116.53	111.79
5	B	2706	PCW	C3-C2-C1	2.00	116.53	111.79
5	A	3005	PCW	C3-C2-C1	2.00	116.53	111.79

There are no chirality outliers.

All (424) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	I3P	C5-O5-P5-O51
3	B	2703	I3P	C5-O5-P5-O51
3	C	2703	I3P	C5-O5-P5-O51
3	D	2704	I3P	C5-O5-P5-O51
4	A	3003	ATP	PB-O3B-PG-O3G
4	A	3003	ATP	C5'-O5'-PA-O1A
4	A	3003	ATP	C5'-O5'-PA-O2A
4	B	2704	ATP	PB-O3B-PG-O3G
4	B	2704	ATP	C5'-O5'-PA-O1A
4	B	2704	ATP	C5'-O5'-PA-O2A
4	C	2704	ATP	PB-O3B-PG-O3G
4	C	2704	ATP	C5'-O5'-PA-O1A
4	C	2704	ATP	C5'-O5'-PA-O2A
4	D	2705	ATP	PB-O3B-PG-O3G
4	D	2705	ATP	C5'-O5'-PA-O1A
4	D	2705	ATP	C5'-O5'-PA-O2A
5	A	3004	PCW	O4P-C4-C5-N
5	A	3006	PCW	O4P-C4-C5-N
5	A	3007	PCW	O3P-C1-C2-O2
5	A	3007	PCW	C32-C31-O2-C2
5	A	3007	PCW	C1-O3P-P-O1P
5	A	3007	PCW	C1-O3P-P-O2P
5	A	3007	PCW	C4-O4P-P-O2P
5	A	3008	PCW	O4P-C4-C5-N
5	A	3008	PCW	C32-C31-O2-C2
5	A	3008	PCW	C4-O4P-P-O2P
5	A	3009	PCW	O3P-C1-C2-O2
5	A	3009	PCW	C32-C31-O2-C2
5	A	3009	PCW	C1-O3P-P-O1P
5	A	3009	PCW	C1-O3P-P-O2P
5	A	3009	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
5	A	3010	PCW	O4P-C4-C5-N
5	A	3010	PCW	C1-O3P-P-O1P
5	A	3010	PCW	C1-O3P-P-O2P
5	B	2701	PCW	O4P-C4-C5-N
5	B	2701	PCW	C1-O3P-P-O1P
5	B	2701	PCW	C1-O3P-P-O2P
5	B	2705	PCW	O4P-C4-C5-N
5	B	2707	PCW	O4P-C4-C5-N
5	B	2708	PCW	O4P-C4-C5-N
5	B	2708	PCW	C32-C31-O2-C2
5	B	2708	PCW	C4-O4P-P-O2P
5	C	2701	PCW	O4P-C4-C5-N
5	C	2701	PCW	C1-O3P-P-O1P
5	C	2701	PCW	C1-O3P-P-O2P
5	C	2705	PCW	O4P-C4-C5-N
5	C	2707	PCW	O4P-C4-C5-N
5	C	2708	PCW	O3P-C1-C2-O2
5	C	2708	PCW	C32-C31-O2-C2
5	C	2708	PCW	C1-O3P-P-O1P
5	C	2708	PCW	C1-O3P-P-O2P
5	C	2708	PCW	C4-O4P-P-O2P
5	C	2709	PCW	O4P-C4-C5-N
5	C	2709	PCW	C32-C31-O2-C2
5	C	2709	PCW	C4-O4P-P-O2P
5	C	2710	PCW	O3P-C1-C2-O2
5	C	2710	PCW	C32-C31-O2-C2
5	C	2710	PCW	C1-O3P-P-O1P
5	C	2710	PCW	C1-O3P-P-O2P
5	C	2710	PCW	C4-O4P-P-O2P
5	D	2701	PCW	O4P-C4-C5-N
5	D	2701	PCW	C32-C31-O2-C2
5	D	2701	PCW	C4-O4P-P-O2P
5	D	2702	PCW	O4P-C4-C5-N
5	D	2702	PCW	C1-O3P-P-O1P
5	D	2702	PCW	C1-O3P-P-O2P
5	D	2706	PCW	O4P-C4-C5-N
5	D	2708	PCW	O4P-C4-C5-N
5	A	3004	PCW	O11-C11-O3-C3
5	A	3005	PCW	O11-C11-O3-C3
5	B	2705	PCW	O11-C11-O3-C3
5	B	2706	PCW	O11-C11-O3-C3
5	C	2705	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
5	C	2706	PCW	O11-C11-O3-C3
5	D	2706	PCW	O11-C11-O3-C3
5	D	2707	PCW	O11-C11-O3-C3
5	A	3007	PCW	O31-C31-O2-C2
5	A	3009	PCW	O31-C31-O2-C2
5	C	2708	PCW	O31-C31-O2-C2
5	C	2710	PCW	O31-C31-O2-C2
5	A	3004	PCW	C12-C11-O3-C3
5	A	3005	PCW	C12-C11-O3-C3
5	B	2705	PCW	C12-C11-O3-C3
5	B	2706	PCW	C12-C11-O3-C3
5	C	2705	PCW	C12-C11-O3-C3
5	C	2706	PCW	C12-C11-O3-C3
5	D	2706	PCW	C12-C11-O3-C3
5	D	2707	PCW	C12-C11-O3-C3
5	A	3008	PCW	O31-C31-O2-C2
5	B	2708	PCW	O31-C31-O2-C2
5	C	2709	PCW	O31-C31-O2-C2
5	D	2701	PCW	O31-C31-O2-C2
5	A	3008	PCW	C15-C16-C17-C18
5	B	2708	PCW	C15-C16-C17-C18
5	C	2709	PCW	C15-C16-C17-C18
5	D	2701	PCW	C15-C16-C17-C18
4	A	3003	ATP	C3'-C4'-C5'-O5'
4	B	2704	ATP	C3'-C4'-C5'-O5'
4	C	2704	ATP	C3'-C4'-C5'-O5'
4	D	2705	ATP	C3'-C4'-C5'-O5'
4	A	3003	ATP	O4'-C4'-C5'-O5'
4	B	2704	ATP	O4'-C4'-C5'-O5'
4	C	2704	ATP	O4'-C4'-C5'-O5'
4	D	2705	ATP	O4'-C4'-C5'-O5'
5	A	3006	PCW	C1-O3P-P-O4P
5	A	3007	PCW	C1-O3P-P-O4P
5	A	3009	PCW	C1-O3P-P-O4P
5	A	3010	PCW	C1-O3P-P-O4P
5	A	3010	PCW	C4-O4P-P-O3P
5	B	2701	PCW	C1-O3P-P-O4P
5	B	2701	PCW	C4-O4P-P-O3P
5	B	2707	PCW	C1-O3P-P-O4P
5	C	2701	PCW	C1-O3P-P-O4P
5	C	2701	PCW	C4-O4P-P-O3P
5	C	2707	PCW	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
5	C	2708	PCW	C1-O3P-P-O4P
5	C	2710	PCW	C1-O3P-P-O4P
5	D	2702	PCW	C1-O3P-P-O4P
5	D	2702	PCW	C4-O4P-P-O3P
5	D	2708	PCW	C1-O3P-P-O4P
5	A	3007	PCW	C12-C11-O3-C3
5	A	3009	PCW	C12-C11-O3-C3
5	C	2708	PCW	C12-C11-O3-C3
5	C	2710	PCW	C12-C11-O3-C3
5	A	3005	PCW	C33-C34-C35-C36
5	B	2706	PCW	C33-C34-C35-C36
5	D	2707	PCW	C33-C34-C35-C36
5	C	2706	PCW	C33-C34-C35-C36
5	A	3007	PCW	O11-C11-O3-C3
5	A	3009	PCW	O11-C11-O3-C3
5	C	2708	PCW	O11-C11-O3-C3
5	C	2710	PCW	O11-C11-O3-C3
5	A	3005	PCW	C42-C43-C44-C45
5	B	2706	PCW	C42-C43-C44-C45
5	C	2706	PCW	C42-C43-C44-C45
5	D	2707	PCW	C42-C43-C44-C45
5	A	3008	PCW	C43-C44-C45-C46
5	B	2708	PCW	C43-C44-C45-C46
5	C	2709	PCW	C43-C44-C45-C46
5	D	2701	PCW	C43-C44-C45-C46
5	A	3004	PCW	C20-C21-C22-C23
5	B	2705	PCW	C20-C21-C22-C23
5	C	2705	PCW	C20-C21-C22-C23
5	D	2706	PCW	C20-C21-C22-C23
5	A	3006	PCW	C44-C45-C46-C47
5	B	2707	PCW	C44-C45-C46-C47
5	C	2707	PCW	C44-C45-C46-C47
5	D	2708	PCW	C44-C45-C46-C47
5	A	3005	PCW	C32-C31-O2-C2
5	A	3006	PCW	C32-C31-O2-C2
5	B	2706	PCW	C32-C31-O2-C2
5	B	2707	PCW	C32-C31-O2-C2
5	C	2706	PCW	C32-C31-O2-C2
5	C	2707	PCW	C32-C31-O2-C2
5	D	2707	PCW	C32-C31-O2-C2
5	D	2708	PCW	C32-C31-O2-C2
5	A	3006	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
5	B	2707	PCW	O31-C31-O2-C2
5	C	2707	PCW	O31-C31-O2-C2
5	D	2708	PCW	O31-C31-O2-C2
5	A	3005	PCW	O31-C31-O2-C2
5	B	2706	PCW	O31-C31-O2-C2
5	C	2706	PCW	O31-C31-O2-C2
5	D	2707	PCW	O31-C31-O2-C2
5	A	3007	PCW	C4-O4P-P-O3P
5	A	3009	PCW	C4-O4P-P-O3P
5	C	2708	PCW	C4-O4P-P-O3P
5	C	2710	PCW	C4-O4P-P-O3P
5	A	3010	PCW	C37-C38-C39-C40
5	B	2701	PCW	C37-C38-C39-C40
5	C	2701	PCW	C37-C38-C39-C40
5	D	2702	PCW	C37-C38-C39-C40
5	A	3006	PCW	C39-C40-C41-C42
5	B	2707	PCW	C39-C40-C41-C42
5	C	2707	PCW	C39-C40-C41-C42
5	D	2708	PCW	C39-C40-C41-C42
5	A	3005	PCW	O3P-C1-C2-C3
5	A	3006	PCW	O3P-C1-C2-C3
5	A	3007	PCW	O3P-C1-C2-C3
5	A	3008	PCW	O3P-C1-C2-C3
5	A	3009	PCW	O3P-C1-C2-C3
5	B	2706	PCW	O3P-C1-C2-C3
5	B	2707	PCW	O3P-C1-C2-C3
5	B	2708	PCW	O3P-C1-C2-C3
5	C	2706	PCW	O3P-C1-C2-C3
5	C	2707	PCW	O3P-C1-C2-C3
5	C	2708	PCW	O3P-C1-C2-C3
5	C	2709	PCW	O3P-C1-C2-C3
5	C	2710	PCW	O3P-C1-C2-C3
5	D	2701	PCW	O3P-C1-C2-C3
5	D	2707	PCW	O3P-C1-C2-C3
5	D	2708	PCW	O3P-C1-C2-C3
5	A	3010	PCW	C32-C31-O2-C2
5	B	2701	PCW	C32-C31-O2-C2
5	C	2701	PCW	C32-C31-O2-C2
5	D	2702	PCW	C32-C31-O2-C2
5	A	3006	PCW	C2-C1-O3P-P
5	B	2707	PCW	C2-C1-O3P-P
5	C	2707	PCW	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
5	D	2708	PCW	C2-C1-O3P-P
5	A	3004	PCW	O3P-C1-C2-O2
5	B	2705	PCW	O3P-C1-C2-O2
5	C	2705	PCW	O3P-C1-C2-O2
5	D	2706	PCW	O3P-C1-C2-O2
5	A	3008	PCW	C45-C46-C47-C48
5	B	2708	PCW	C45-C46-C47-C48
5	C	2709	PCW	C45-C46-C47-C48
5	D	2701	PCW	C45-C46-C47-C48
5	A	3005	PCW	O2-C2-C3-O3
5	A	3006	PCW	O2-C2-C3-O3
5	A	3010	PCW	O2-C2-C3-O3
5	B	2701	PCW	O2-C2-C3-O3
5	B	2706	PCW	O2-C2-C3-O3
5	B	2707	PCW	O2-C2-C3-O3
5	C	2701	PCW	O2-C2-C3-O3
5	C	2706	PCW	O2-C2-C3-O3
5	C	2707	PCW	O2-C2-C3-O3
5	D	2702	PCW	O2-C2-C3-O3
5	D	2707	PCW	O2-C2-C3-O3
5	D	2708	PCW	O2-C2-C3-O3
5	A	3010	PCW	C31-C32-C33-C34
5	B	2701	PCW	C31-C32-C33-C34
5	C	2701	PCW	C31-C32-C33-C34
5	D	2702	PCW	C31-C32-C33-C34
5	A	3010	PCW	O31-C31-O2-C2
5	B	2701	PCW	O31-C31-O2-C2
5	C	2701	PCW	O31-C31-O2-C2
5	D	2702	PCW	O31-C31-O2-C2
5	A	3007	PCW	C19-C20-C21-C22
5	A	3009	PCW	C19-C20-C21-C22
5	C	2708	PCW	C19-C20-C21-C22
5	C	2710	PCW	C19-C20-C21-C22
5	A	3010	PCW	C36-C37-C38-C39
5	B	2701	PCW	C36-C37-C38-C39
5	C	2701	PCW	C36-C37-C38-C39
5	D	2702	PCW	C36-C37-C38-C39
5	A	3005	PCW	O3P-C1-C2-O2
5	B	2706	PCW	O3P-C1-C2-O2
5	C	2706	PCW	O3P-C1-C2-O2
5	D	2707	PCW	O3P-C1-C2-O2
4	A	3003	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	B	2704	ATP	PB-O3B-PG-O2G
4	C	2704	ATP	PB-O3B-PG-O2G
4	D	2705	ATP	PB-O3B-PG-O2G
5	A	3004	PCW	O2-C2-C3-O3
5	B	2705	PCW	O2-C2-C3-O3
5	C	2705	PCW	O2-C2-C3-O3
5	D	2706	PCW	O2-C2-C3-O3
3	A	3002	I3P	C4-O4-P4-O42
3	B	2703	I3P	C4-O4-P4-O42
3	C	2703	I3P	C4-O4-P4-O42
3	D	2704	I3P	C4-O4-P4-O42
4	A	3003	ATP	C5'-O5'-PA-O3A
4	B	2704	ATP	C5'-O5'-PA-O3A
4	C	2704	ATP	C5'-O5'-PA-O3A
4	D	2705	ATP	C5'-O5'-PA-O3A
5	A	3006	PCW	C1-O3P-P-O2P
5	A	3007	PCW	C4-O4P-P-O1P
5	A	3009	PCW	C4-O4P-P-O1P
5	A	3010	PCW	C4-O4P-P-O2P
5	B	2701	PCW	C4-O4P-P-O2P
5	B	2707	PCW	C1-O3P-P-O2P
5	C	2701	PCW	C4-O4P-P-O2P
5	C	2707	PCW	C1-O3P-P-O2P
5	C	2708	PCW	C4-O4P-P-O1P
5	C	2710	PCW	C4-O4P-P-O1P
5	D	2702	PCW	C4-O4P-P-O2P
5	D	2708	PCW	C1-O3P-P-O2P
5	A	3005	PCW	C4-C5-N-C8
5	B	2706	PCW	C4-C5-N-C8
5	C	2706	PCW	C4-C5-N-C8
5	D	2707	PCW	C4-C5-N-C8
5	A	3007	PCW	O4P-C4-C5-N
5	A	3009	PCW	O4P-C4-C5-N
5	C	2708	PCW	O4P-C4-C5-N
5	C	2710	PCW	O4P-C4-C5-N
5	A	3008	PCW	C13-C14-C15-C16
5	B	2708	PCW	C13-C14-C15-C16
5	C	2709	PCW	C13-C14-C15-C16
5	D	2701	PCW	C13-C14-C15-C16
5	A	3006	PCW	C31-C32-C33-C34
5	B	2707	PCW	C31-C32-C33-C34
5	C	2707	PCW	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
5	D	2708	PCW	C31-C32-C33-C34
5	A	3005	PCW	O2-C31-C32-C33
5	B	2706	PCW	O2-C31-C32-C33
5	C	2706	PCW	O2-C31-C32-C33
5	D	2707	PCW	O2-C31-C32-C33
5	A	3006	PCW	O3P-C1-C2-O2
5	A	3008	PCW	O3P-C1-C2-O2
5	B	2707	PCW	O3P-C1-C2-O2
5	B	2708	PCW	O3P-C1-C2-O2
5	C	2707	PCW	O3P-C1-C2-O2
5	C	2709	PCW	O3P-C1-C2-O2
5	D	2701	PCW	O3P-C1-C2-O2
5	D	2708	PCW	O3P-C1-C2-O2
5	A	3004	PCW	C1-O3P-P-O4P
5	A	3005	PCW	C4-O4P-P-O3P
5	B	2705	PCW	C1-O3P-P-O4P
5	B	2706	PCW	C4-O4P-P-O3P
5	C	2705	PCW	C1-O3P-P-O4P
5	C	2706	PCW	C4-O4P-P-O3P
5	D	2706	PCW	C1-O3P-P-O4P
5	D	2707	PCW	C4-O4P-P-O3P
5	A	3005	PCW	C1-C2-C3-O3
5	A	3006	PCW	C1-C2-C3-O3
5	A	3010	PCW	C1-C2-C3-O3
5	B	2701	PCW	C1-C2-C3-O3
5	B	2706	PCW	C1-C2-C3-O3
5	B	2707	PCW	C1-C2-C3-O3
5	C	2701	PCW	C1-C2-C3-O3
5	C	2706	PCW	C1-C2-C3-O3
5	C	2707	PCW	C1-C2-C3-O3
5	D	2702	PCW	C1-C2-C3-O3
5	D	2707	PCW	C1-C2-C3-O3
5	D	2708	PCW	C1-C2-C3-O3
5	A	3010	PCW	O3P-C1-C2-O2
5	B	2701	PCW	O3P-C1-C2-O2
5	C	2701	PCW	O3P-C1-C2-O2
5	D	2702	PCW	O3P-C1-C2-O2
5	A	3005	PCW	C14-C15-C16-C17
5	B	2706	PCW	C14-C15-C16-C17
5	C	2706	PCW	C14-C15-C16-C17
5	D	2707	PCW	C14-C15-C16-C17
5	A	3007	PCW	C3-C2-O2-C31

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Mol	Chain	Res	Type	Atoms
5	A	3009	PCW	C3-C2-O2-C31
5	A	3010	PCW	C3-C2-O2-C31
5	B	2701	PCW	C3-C2-O2-C31
5	C	2701	PCW	C3-C2-O2-C31
5	C	2708	PCW	C3-C2-O2-C31
5	C	2710	PCW	C3-C2-O2-C31
5	D	2702	PCW	C3-C2-O2-C31
5	A	3004	PCW	O3P-C1-C2-C3
5	B	2705	PCW	O3P-C1-C2-C3
5	C	2705	PCW	O3P-C1-C2-C3
5	D	2706	PCW	O3P-C1-C2-C3
5	A	3006	PCW	C32-C33-C34-C35
5	B	2707	PCW	C32-C33-C34-C35
5	C	2707	PCW	C32-C33-C34-C35
5	D	2708	PCW	C32-C33-C34-C35
4	A	3003	ATP	PB-O3B-PG-O1G
4	B	2704	ATP	PB-O3B-PG-O1G
4	C	2704	ATP	PB-O3B-PG-O1G
4	D	2705	ATP	PB-O3B-PG-O1G
5	A	3005	PCW	C4-C5-N-C6
5	A	3005	PCW	C4-C5-N-C7
5	B	2706	PCW	C4-C5-N-C6
5	B	2706	PCW	C4-C5-N-C7
5	C	2706	PCW	C4-C5-N-C6
5	C	2706	PCW	C4-C5-N-C7
5	D	2707	PCW	C4-C5-N-C6
5	D	2707	PCW	C4-C5-N-C7
5	A	3005	PCW	C16-C17-C18-C19
5	B	2706	PCW	C16-C17-C18-C19
5	C	2706	PCW	C16-C17-C18-C19
5	D	2707	PCW	C16-C17-C18-C19
5	A	3008	PCW	C39-C40-C41-C42
5	B	2708	PCW	C39-C40-C41-C42
5	C	2709	PCW	C39-C40-C41-C42
5	D	2701	PCW	C39-C40-C41-C42
5	A	3004	PCW	C1-C2-C3-O3
5	B	2705	PCW	C1-C2-C3-O3
5	C	2705	PCW	C1-C2-C3-O3
5	D	2706	PCW	C1-C2-C3-O3
5	A	3008	PCW	C32-C33-C34-C35
5	B	2708	PCW	C32-C33-C34-C35
5	C	2709	PCW	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
5	D	2701	PCW	C32-C33-C34-C35
5	A	3010	PCW	O3P-C1-C2-C3
5	B	2701	PCW	O3P-C1-C2-C3
5	C	2701	PCW	O3P-C1-C2-C3
5	D	2702	PCW	O3P-C1-C2-C3
5	D	2708	PCW	C42-C43-C44-C45
3	A	3002	I3P	C4-O4-P4-O43
3	B	2703	I3P	C4-O4-P4-O43
3	C	2703	I3P	C4-O4-P4-O43
3	D	2704	I3P	C4-O4-P4-O43
5	A	3006	PCW	C42-C43-C44-C45
5	B	2707	PCW	C42-C43-C44-C45
5	C	2707	PCW	C42-C43-C44-C45
4	A	3003	ATP	PG-O3B-PB-O2B
4	B	2704	ATP	PG-O3B-PB-O2B
4	C	2704	ATP	PG-O3B-PB-O2B
4	D	2705	ATP	PG-O3B-PB-O2B
5	A	3006	PCW	C35-C36-C37-C38
5	B	2707	PCW	C35-C36-C37-C38
5	C	2707	PCW	C35-C36-C37-C38
5	D	2708	PCW	C35-C36-C37-C38
5	A	3010	PCW	O11-C11-O3-C3
5	B	2701	PCW	O11-C11-O3-C3
5	C	2701	PCW	O11-C11-O3-C3
5	D	2702	PCW	O11-C11-O3-C3
5	A	3010	PCW	C12-C11-O3-C3
5	B	2701	PCW	C12-C11-O3-C3
5	C	2701	PCW	C12-C11-O3-C3
5	D	2702	PCW	C12-C11-O3-C3
5	A	3005	PCW	C37-C38-C39-C40
5	A	3008	PCW	C17-C18-C19-C20
5	B	2706	PCW	C37-C38-C39-C40
5	B	2708	PCW	C17-C18-C19-C20
5	C	2706	PCW	C37-C38-C39-C40
5	C	2709	PCW	C17-C18-C19-C20
5	D	2701	PCW	C17-C18-C19-C20
5	D	2707	PCW	C37-C38-C39-C40
5	A	3005	PCW	C4-O4P-P-O2P
5	A	3008	PCW	C4-O4P-P-O1P
5	B	2706	PCW	C4-O4P-P-O2P
5	B	2708	PCW	C4-O4P-P-O1P
5	C	2706	PCW	C4-O4P-P-O2P

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	2709	PCW	C4-O4P-P-O1P
5	D	2701	PCW	C4-O4P-P-O1P
5	D	2707	PCW	C4-O4P-P-O2P
5	A	3006	PCW	C5-C4-O4P-P
5	B	2707	PCW	C5-C4-O4P-P
5	C	2707	PCW	C5-C4-O4P-P
5	D	2708	PCW	C5-C4-O4P-P
5	A	3004	PCW	O3-C11-C12-C13
5	B	2705	PCW	O3-C11-C12-C13
5	C	2705	PCW	O3-C11-C12-C13
5	D	2706	PCW	O3-C11-C12-C13
5	A	3004	PCW	O11-C11-C12-C13
5	B	2705	PCW	O11-C11-C12-C13
5	C	2705	PCW	O11-C11-C12-C13
5	D	2706	PCW	O11-C11-C12-C13

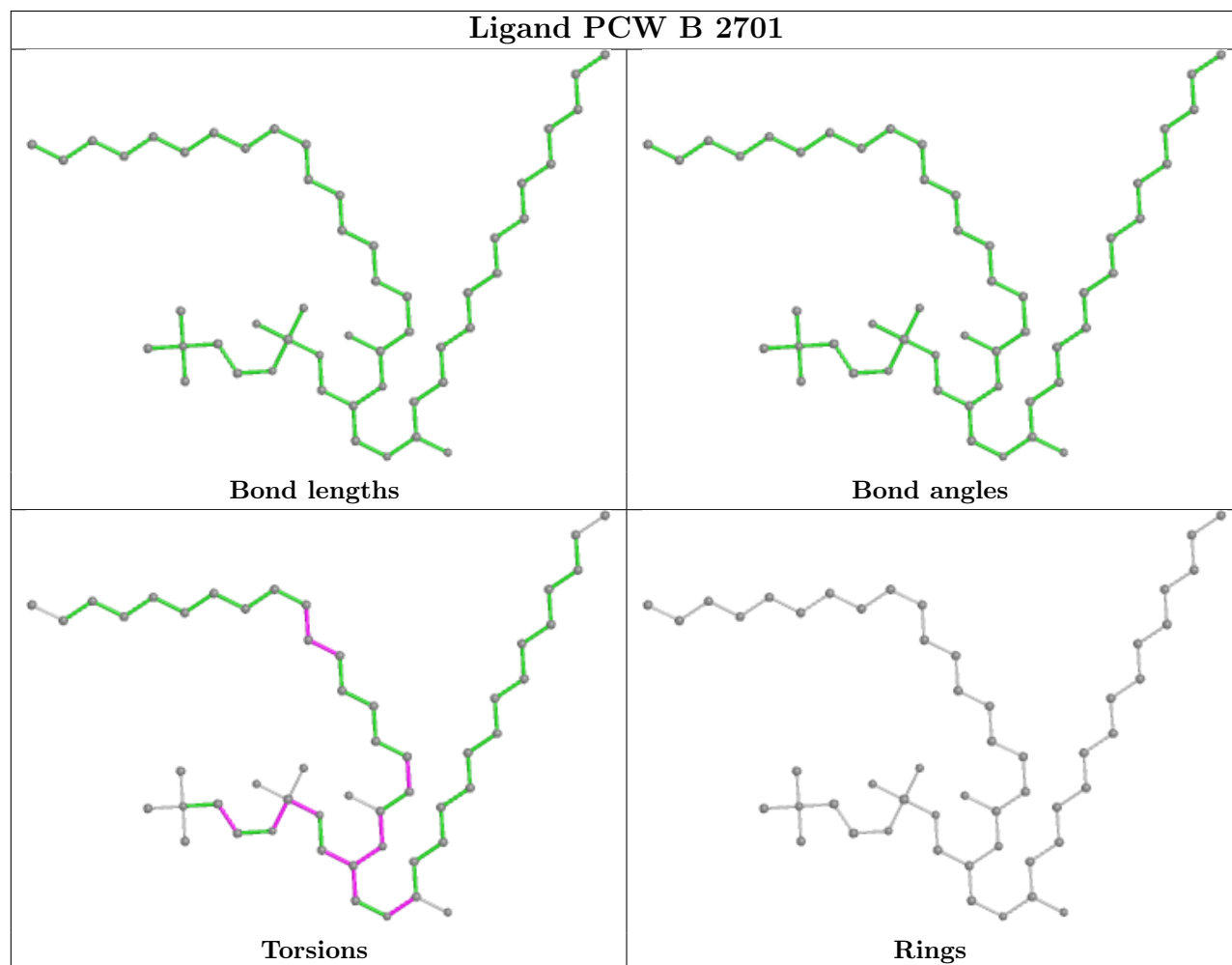
There are no ring outliers.

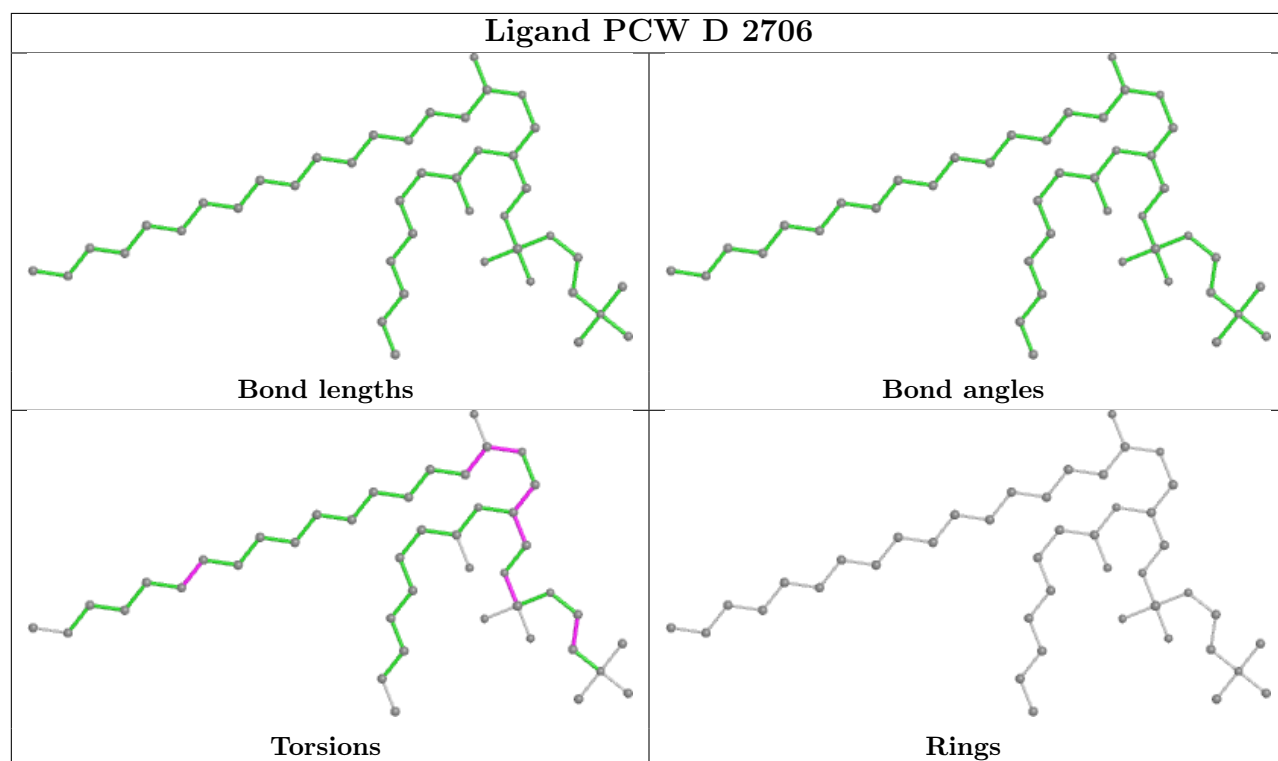
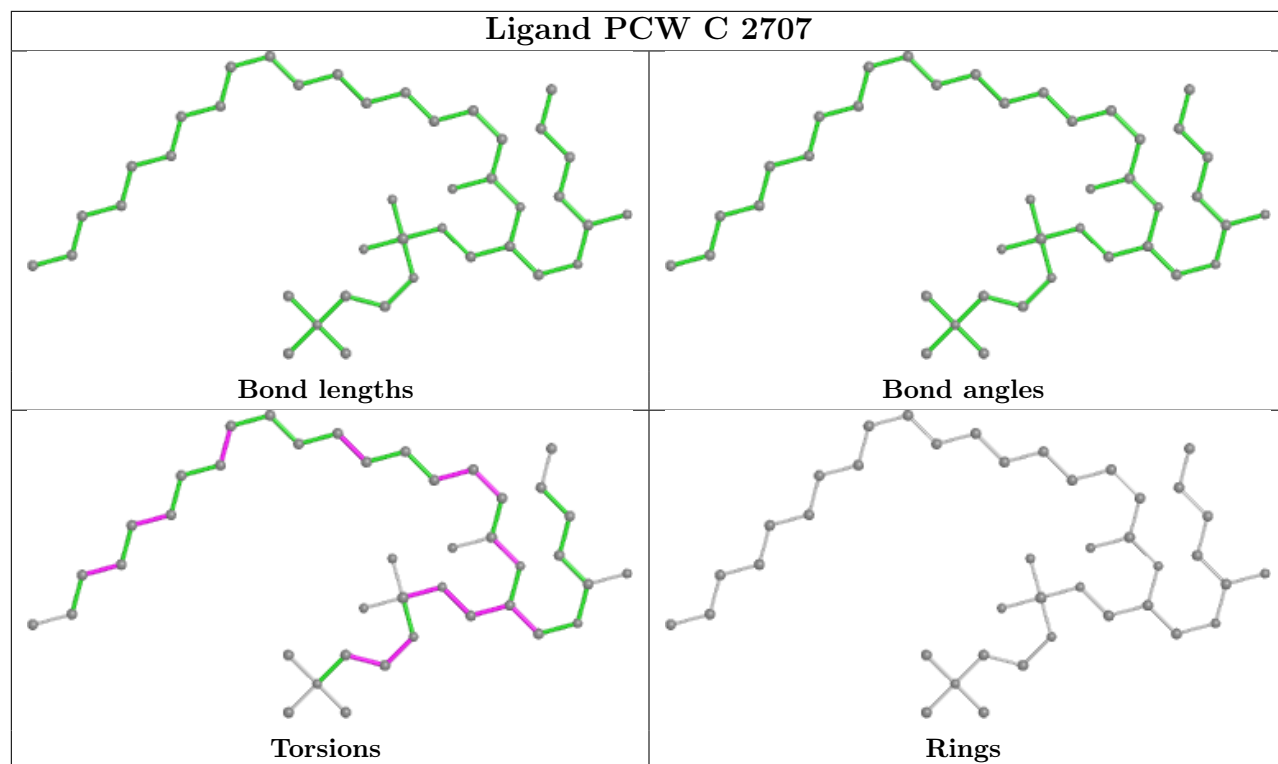
14 monomers are involved in 26 short contacts:

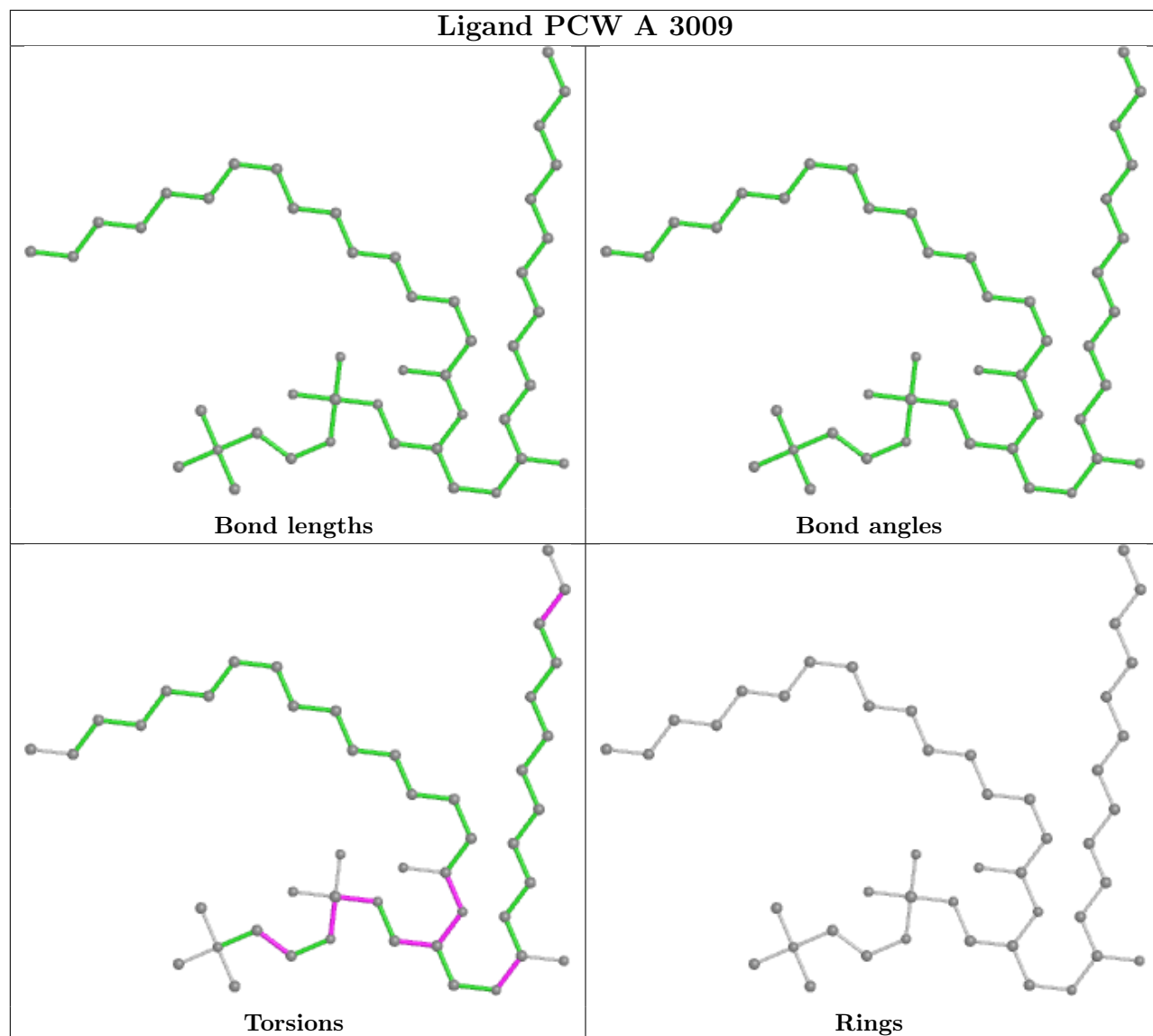
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2701	PCW	1	0
5	C	2707	PCW	1	0
5	D	2708	PCW	1	0
3	D	2704	I3P	1	0
5	C	2709	PCW	5	0
5	B	2708	PCW	3	0
5	A	3008	PCW	2	0
5	C	2701	PCW	1	0
5	D	2702	PCW	2	0
3	C	2703	I3P	1	0
5	A	3010	PCW	2	0
5	A	3006	PCW	1	0
5	B	2707	PCW	1	0
5	D	2701	PCW	4	0

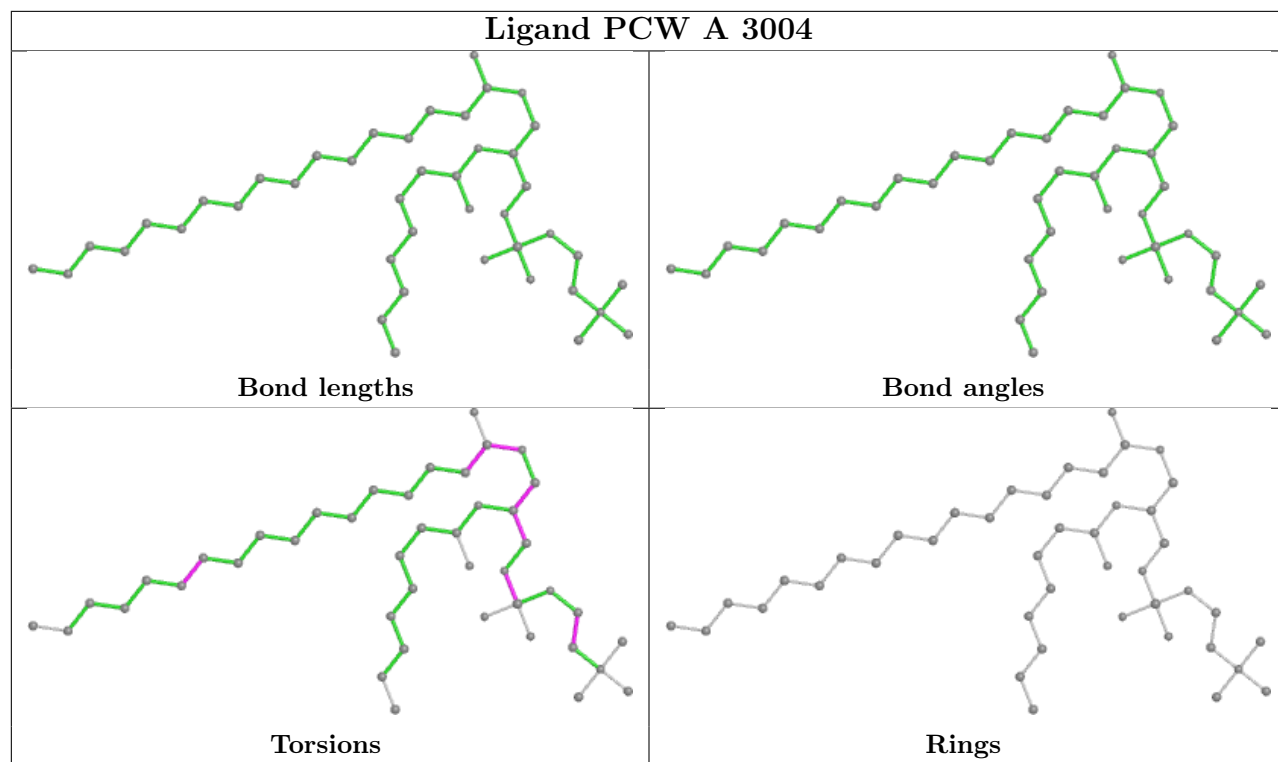
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

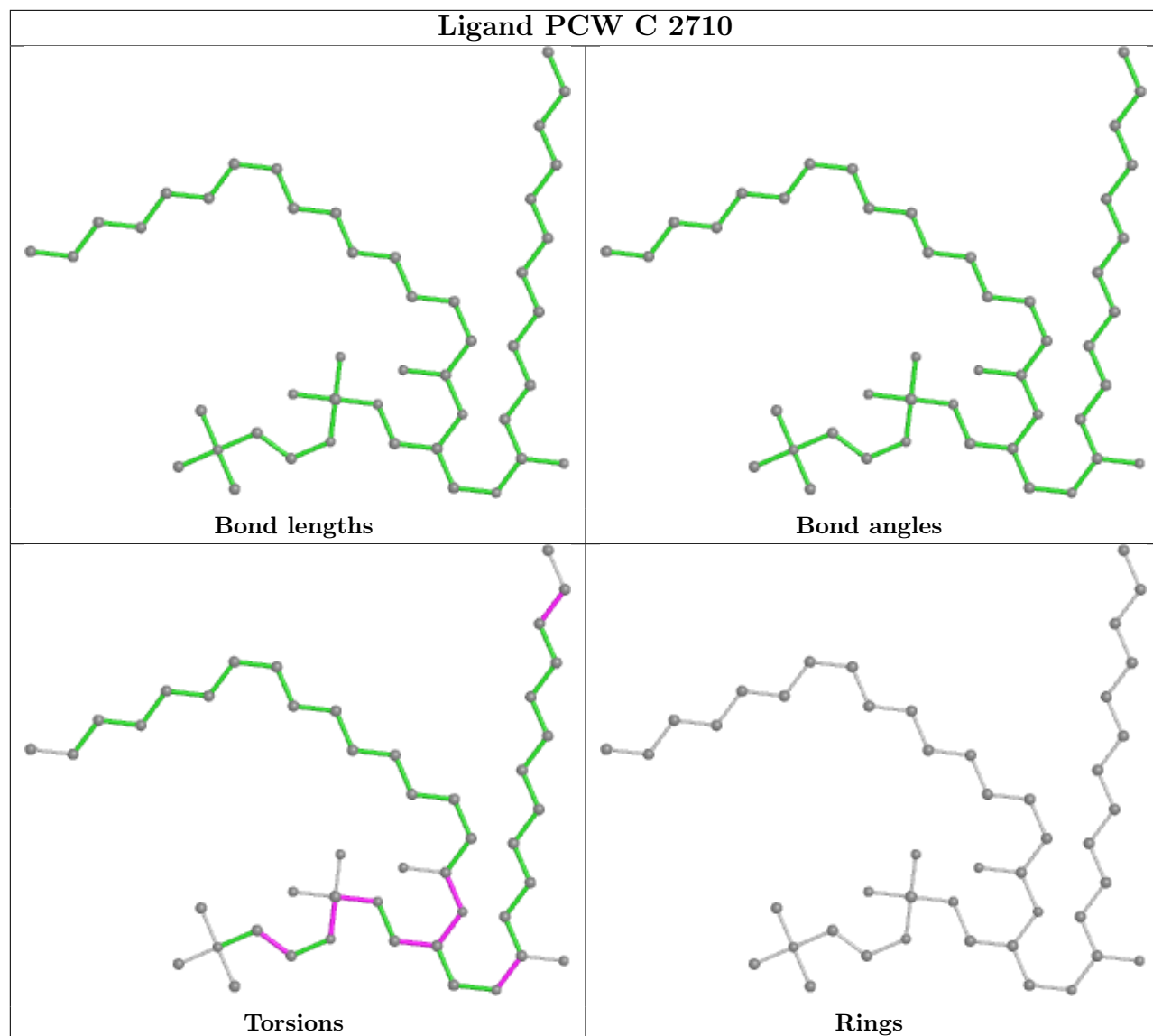
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

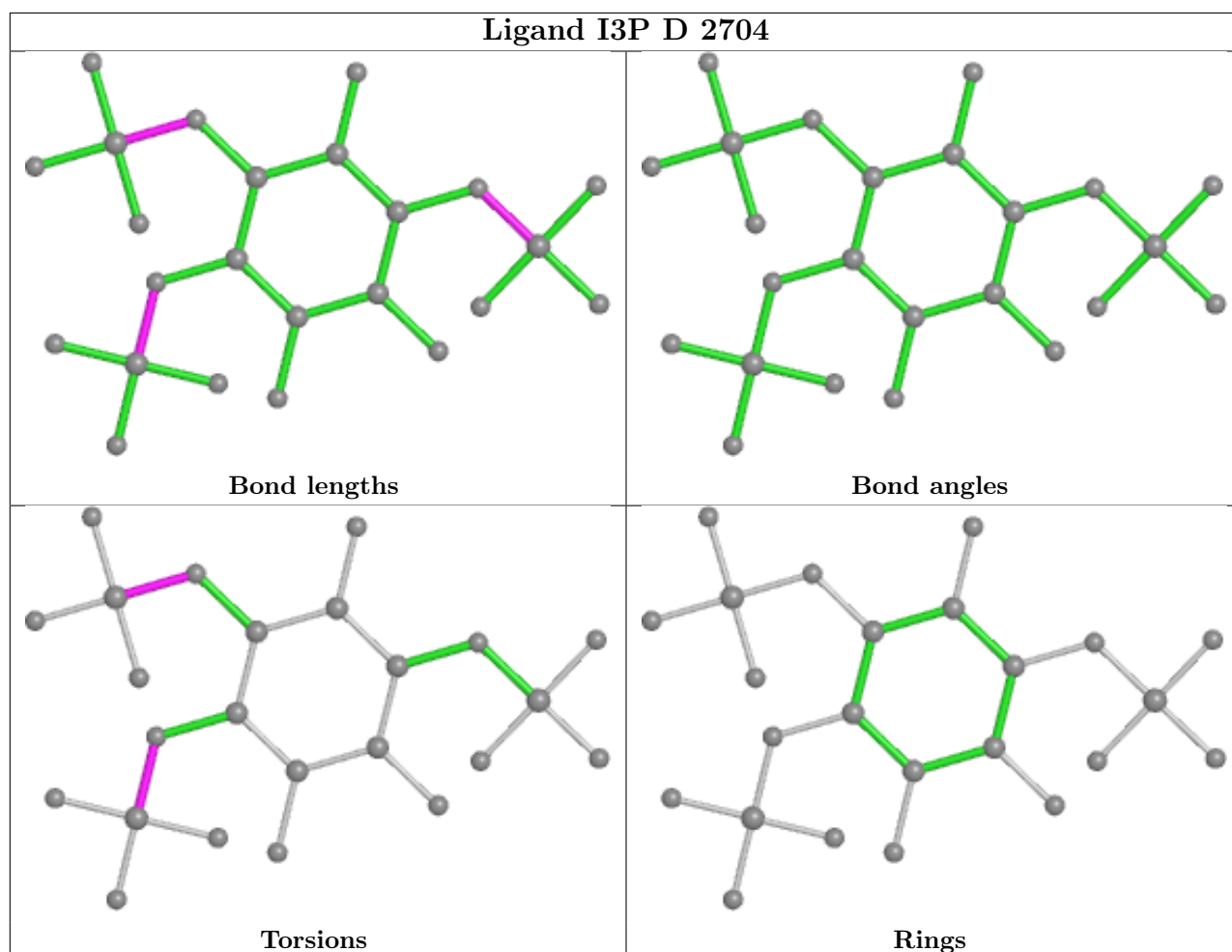
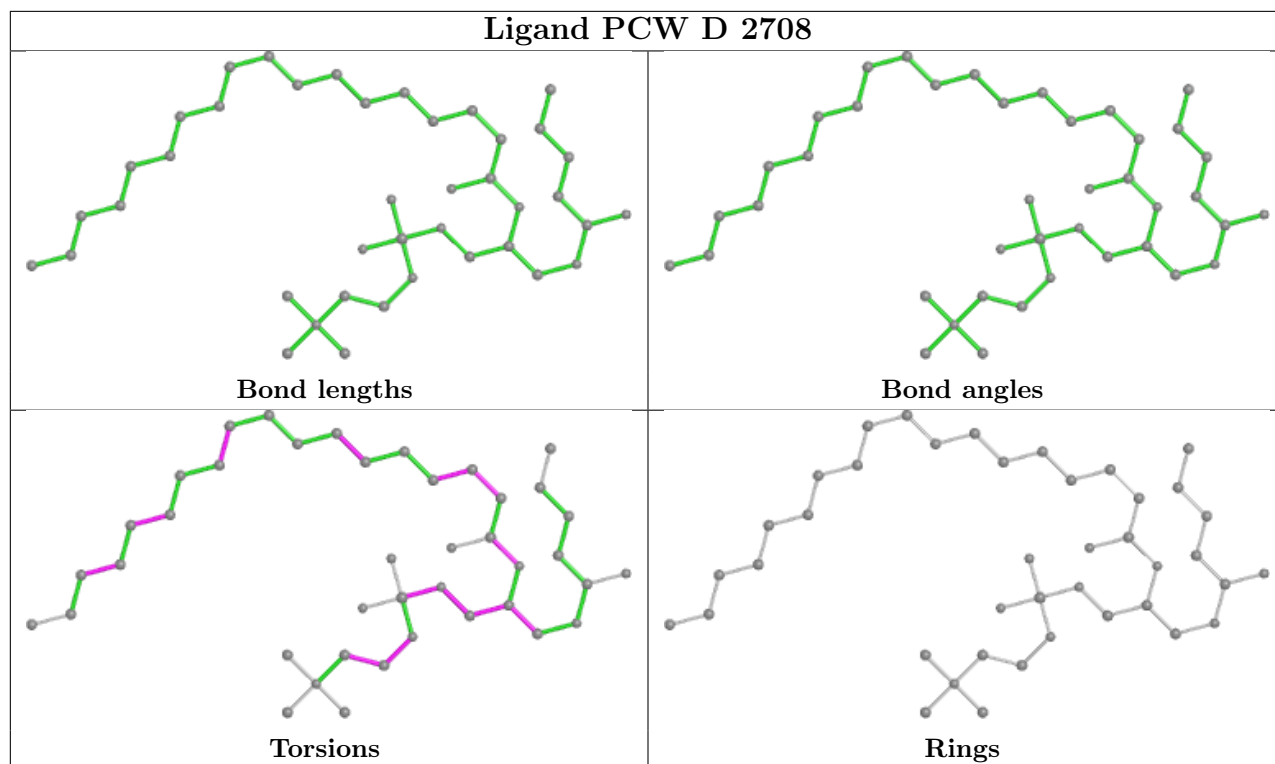


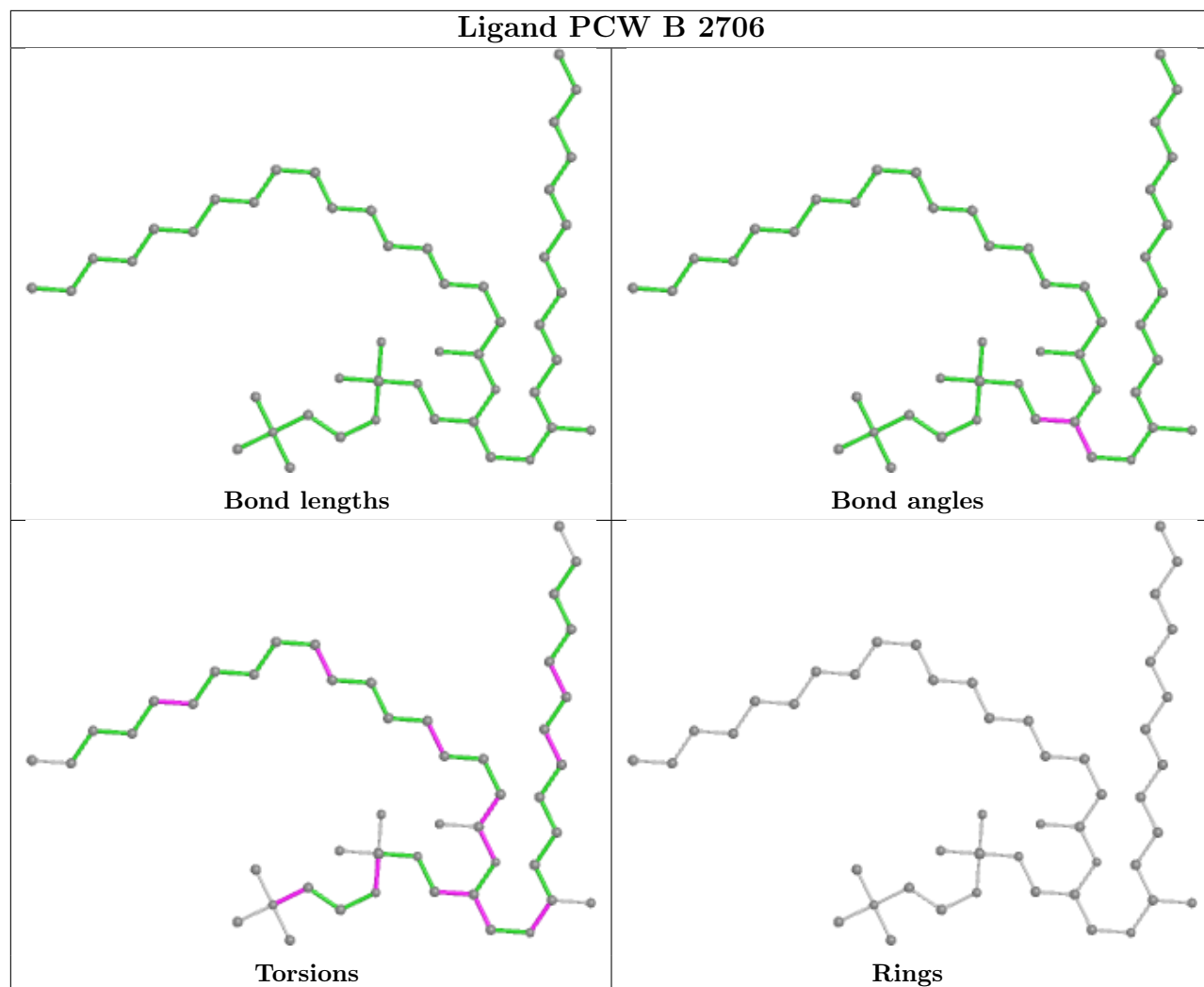




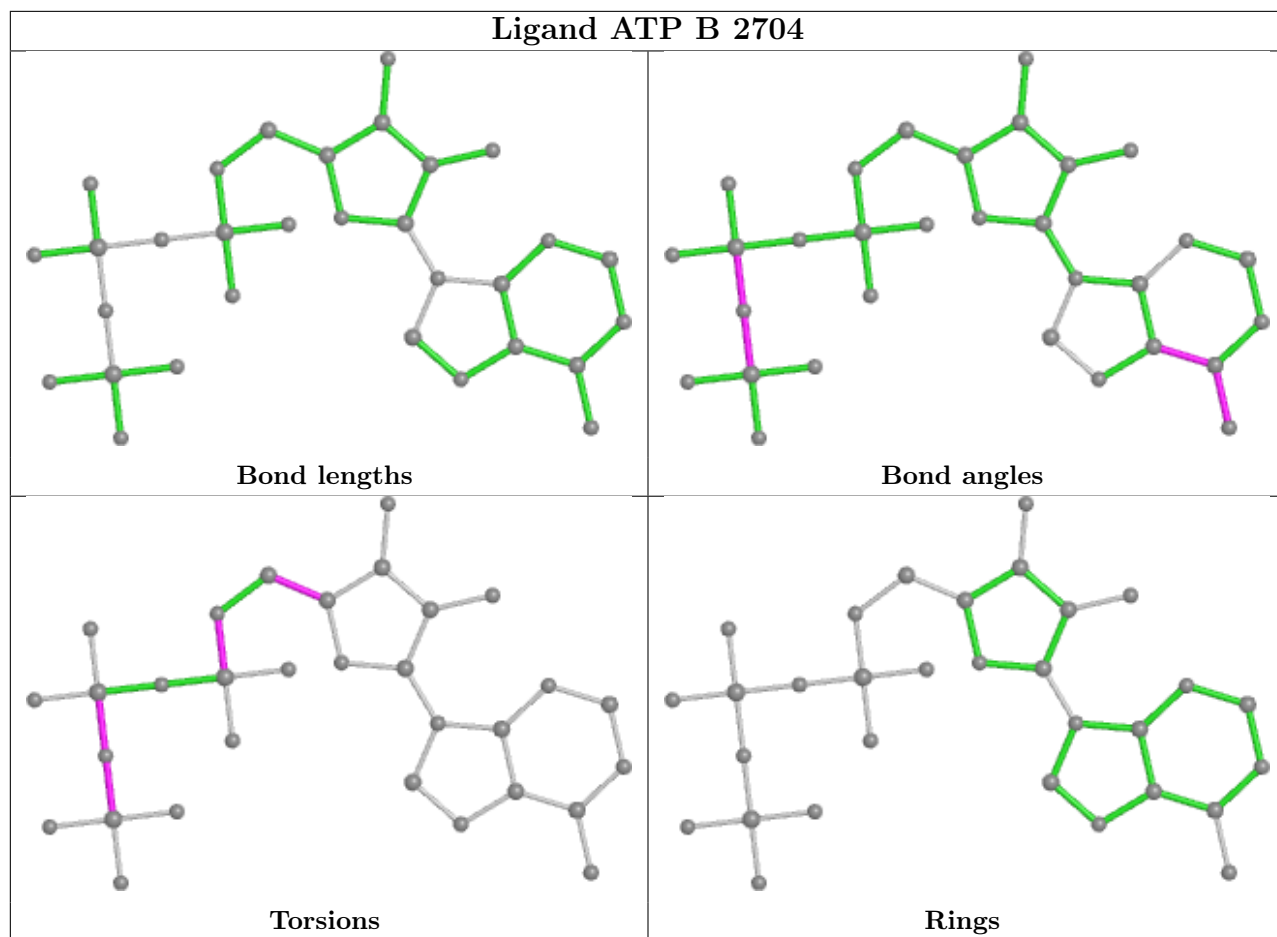


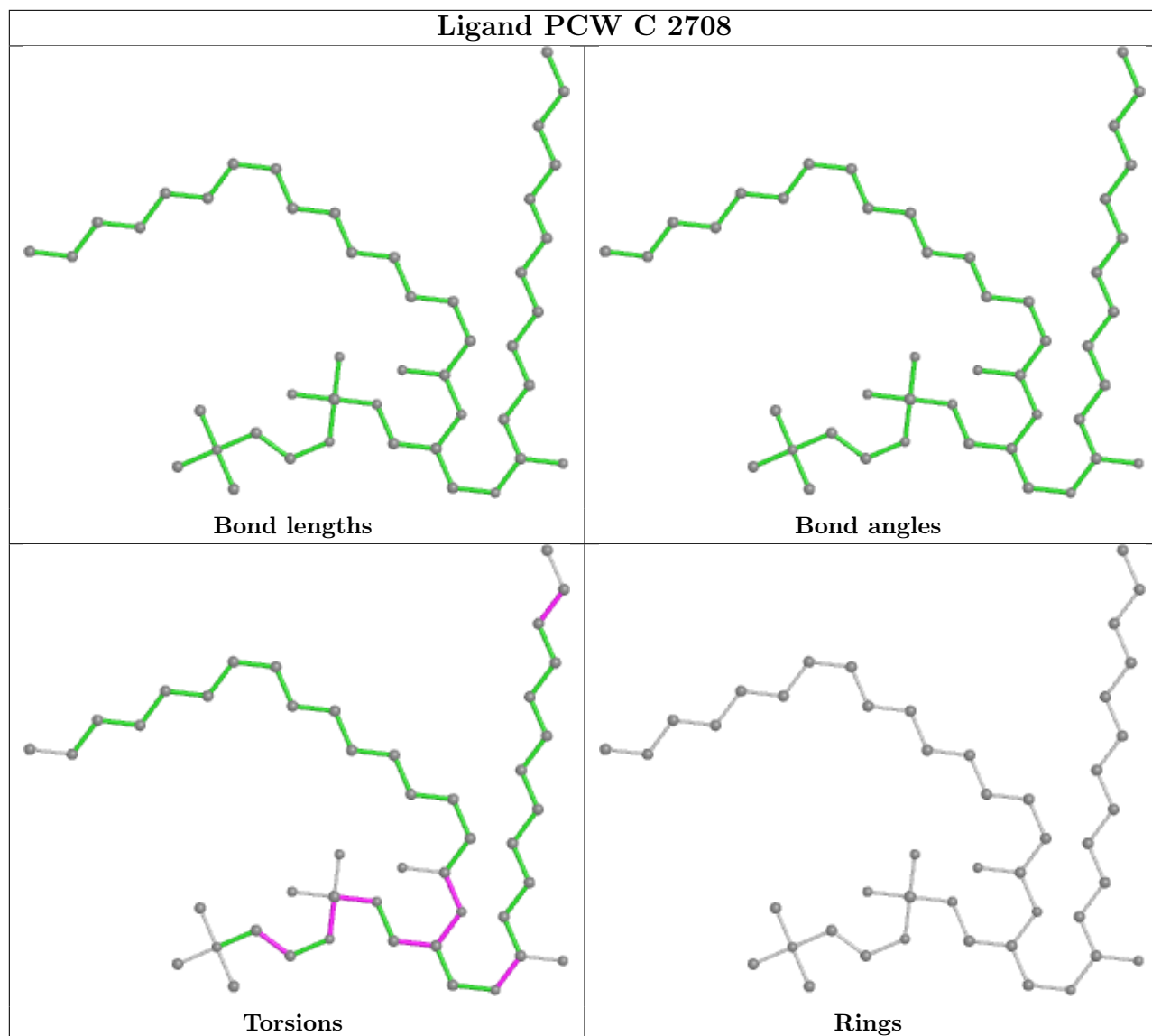


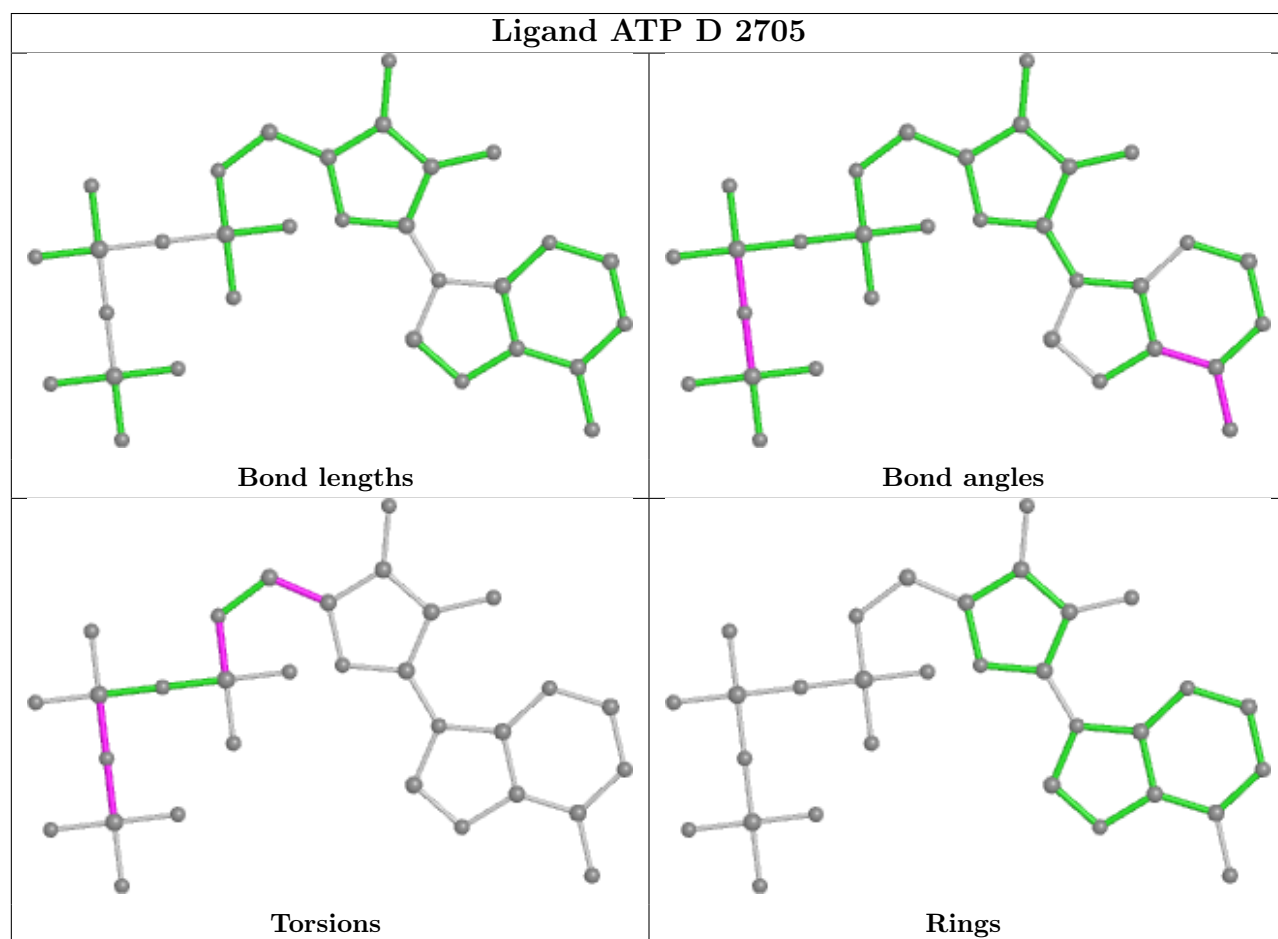
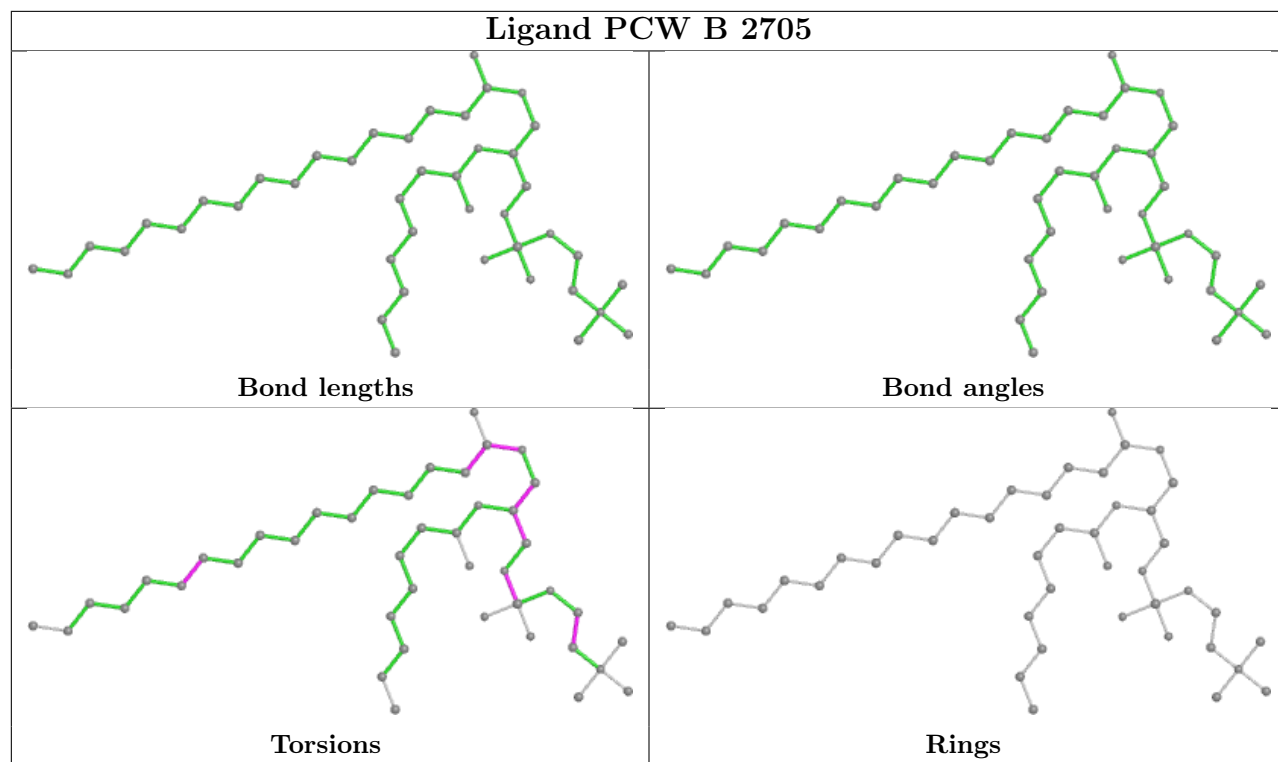


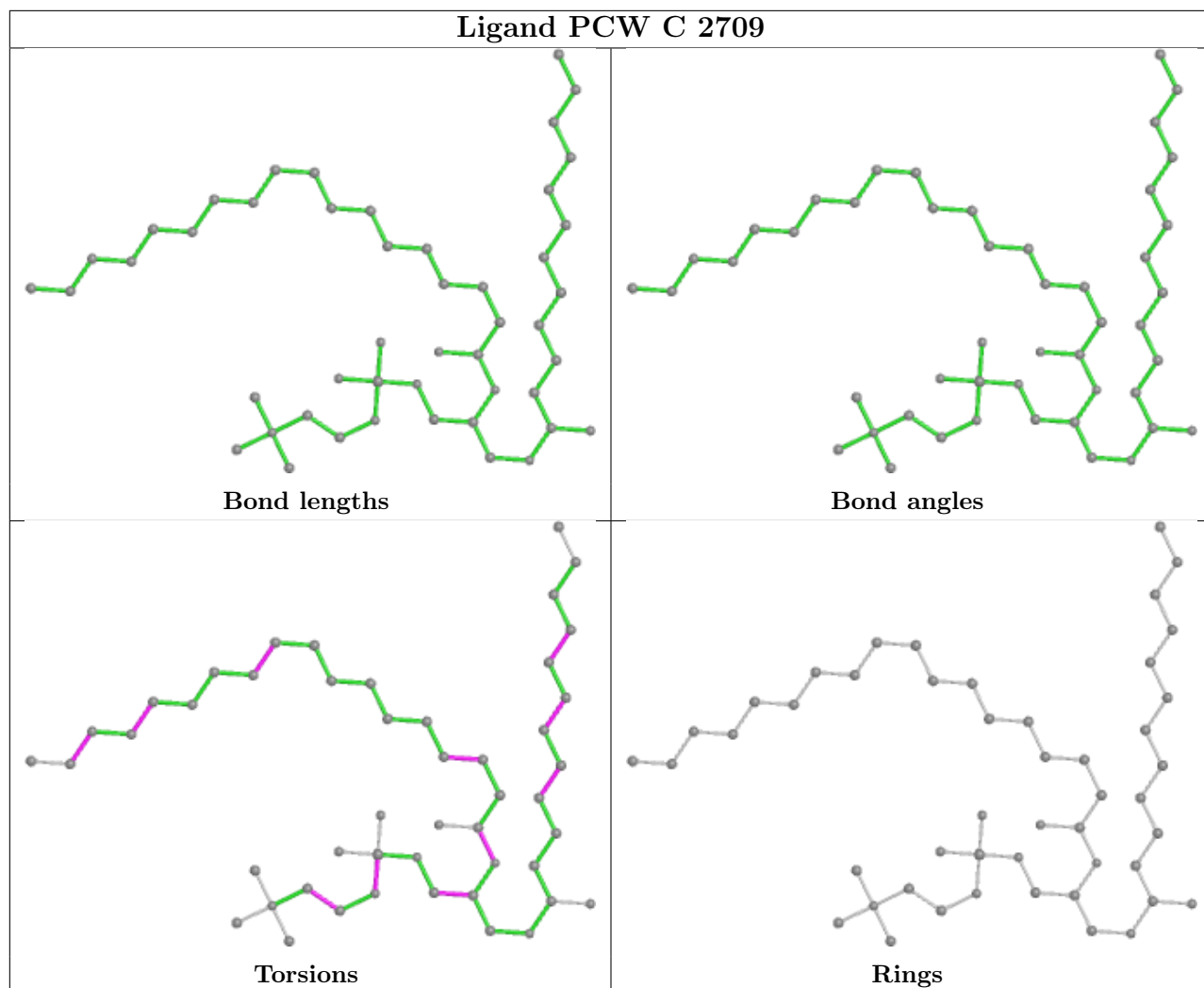


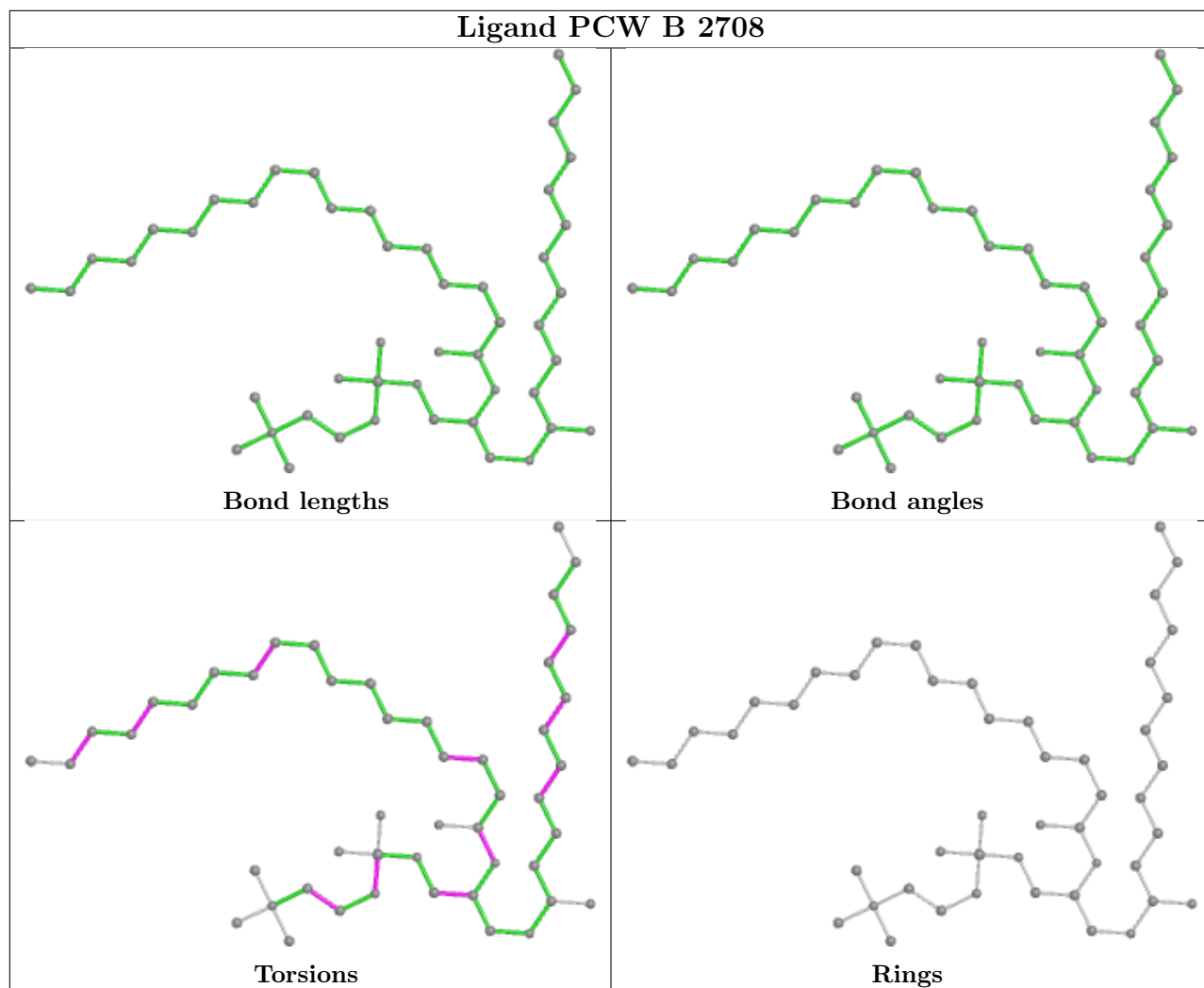


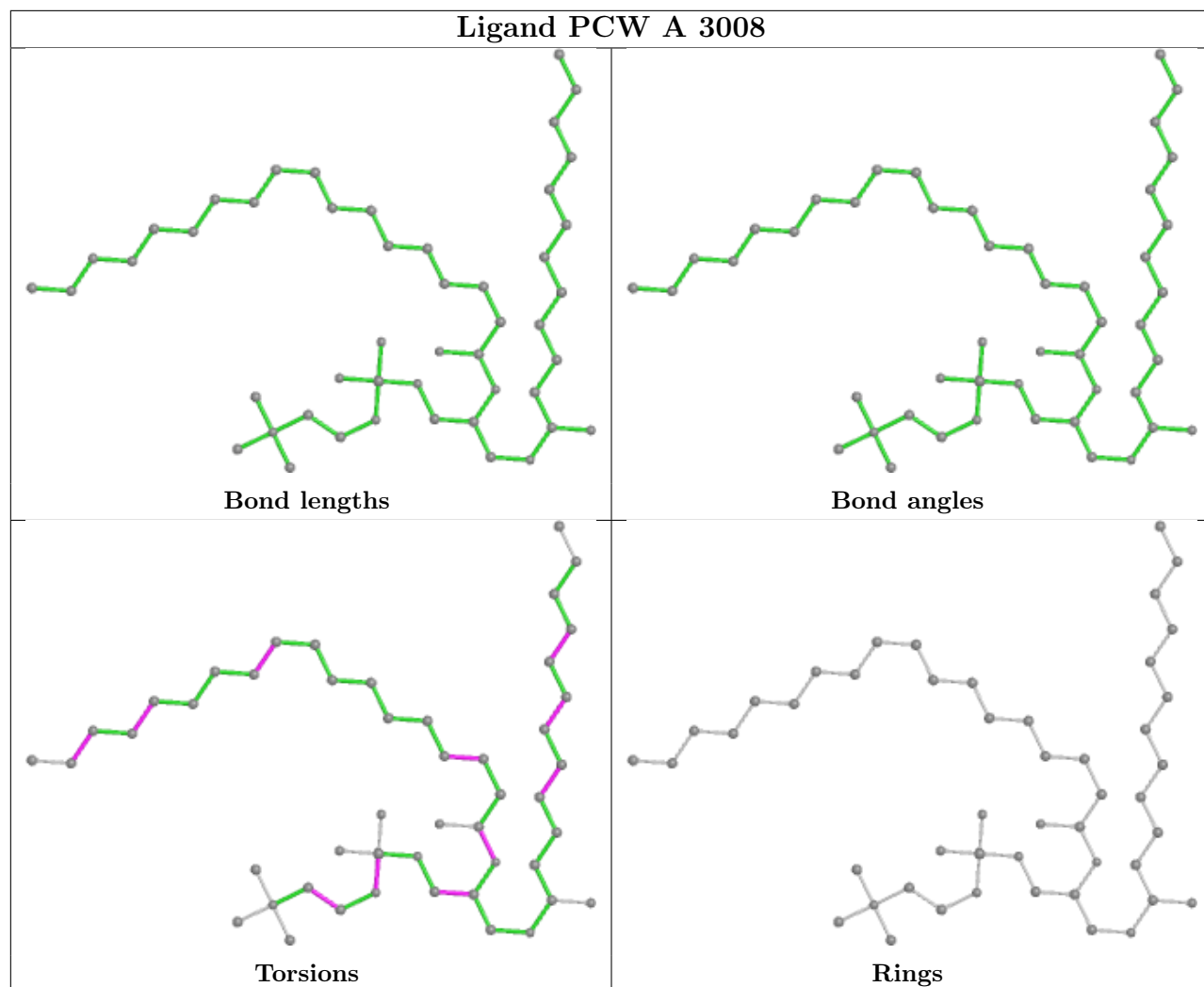


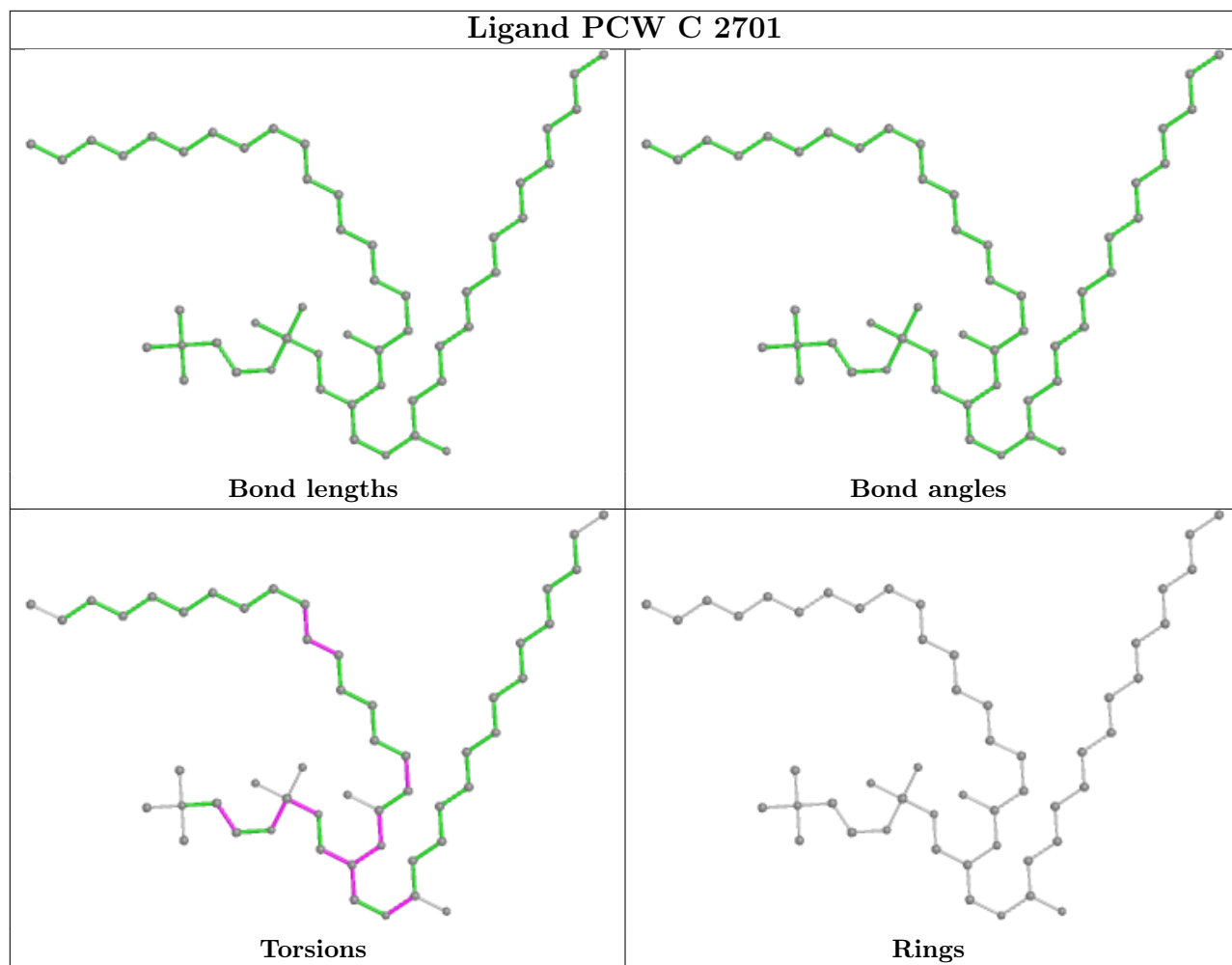


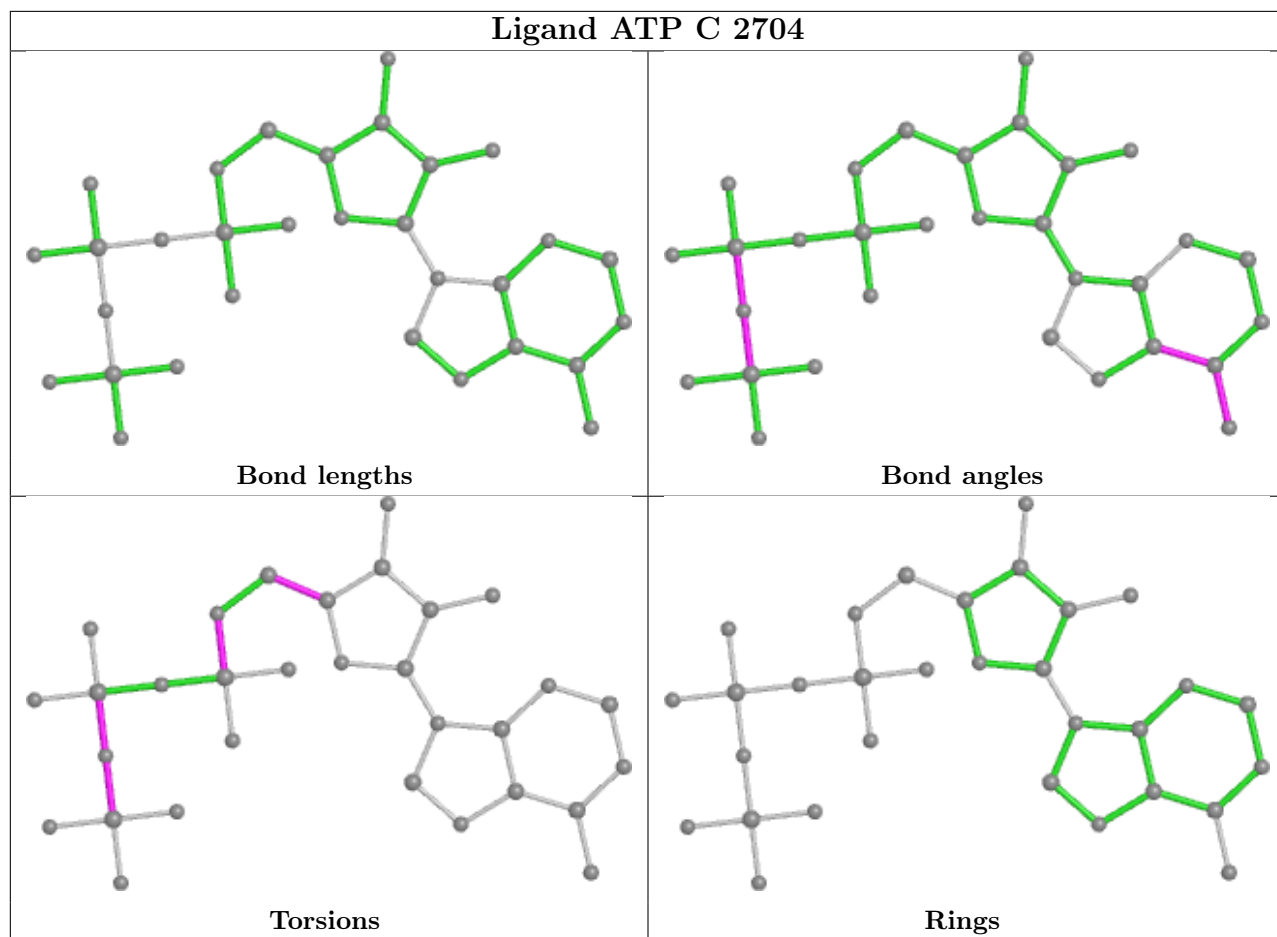




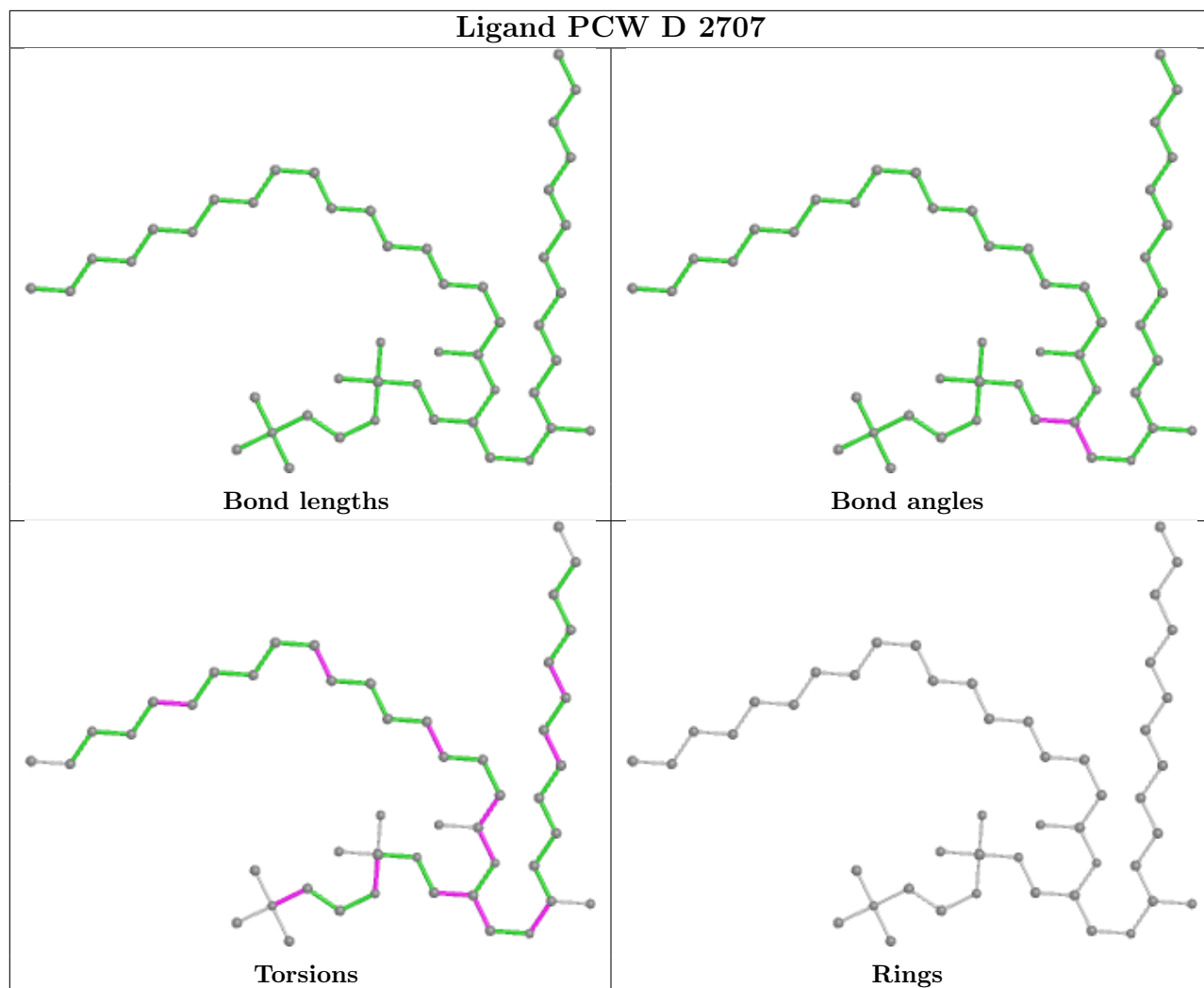


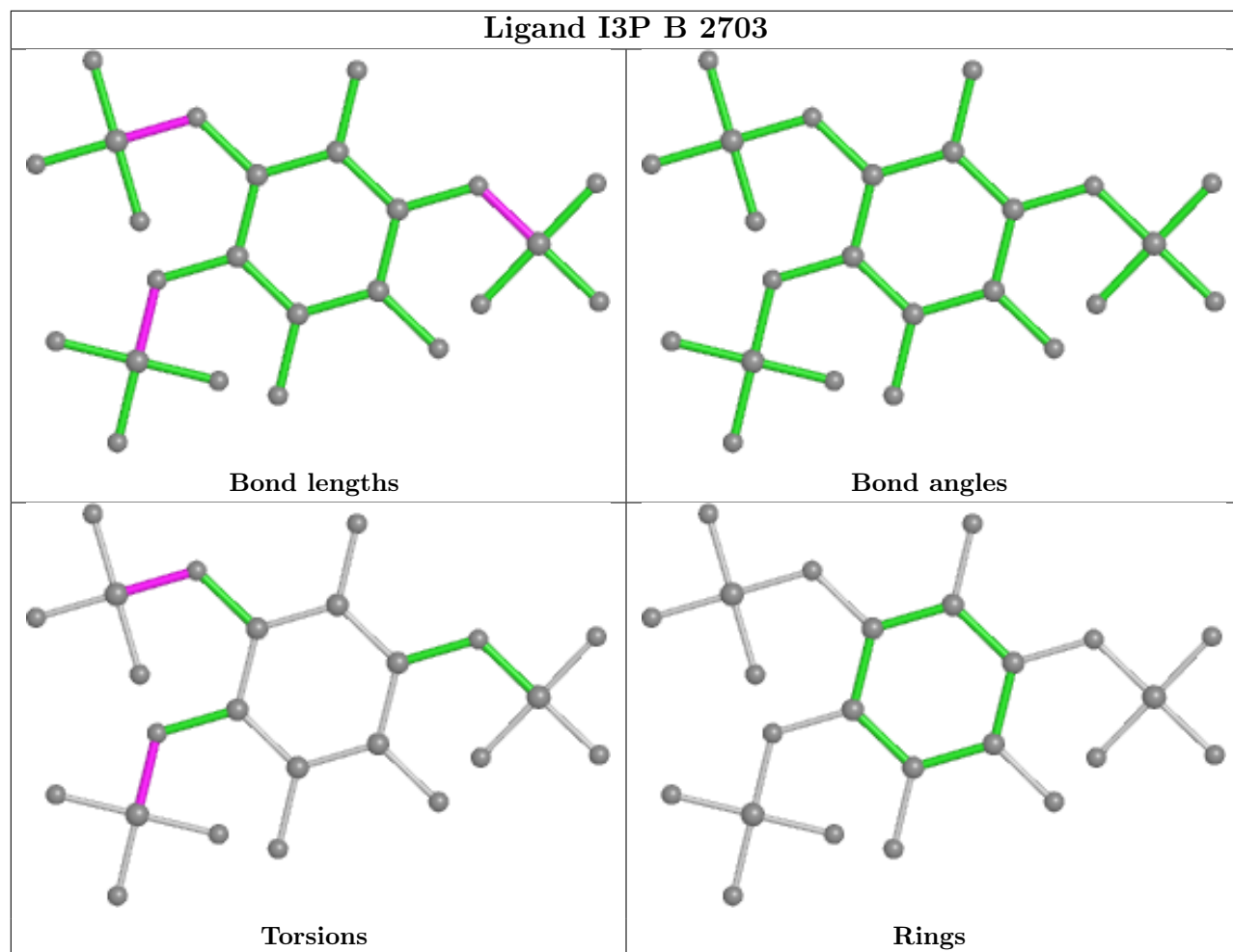


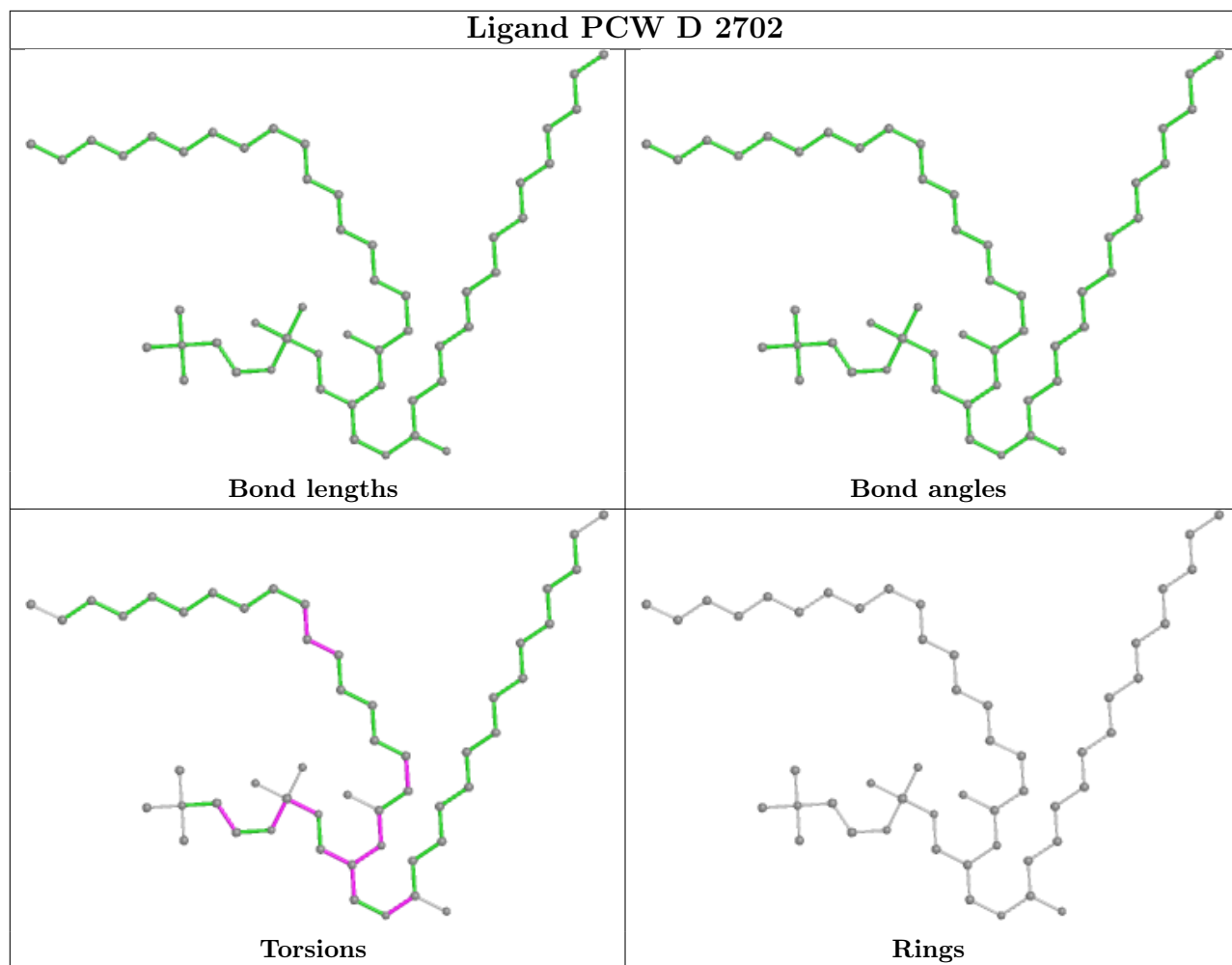


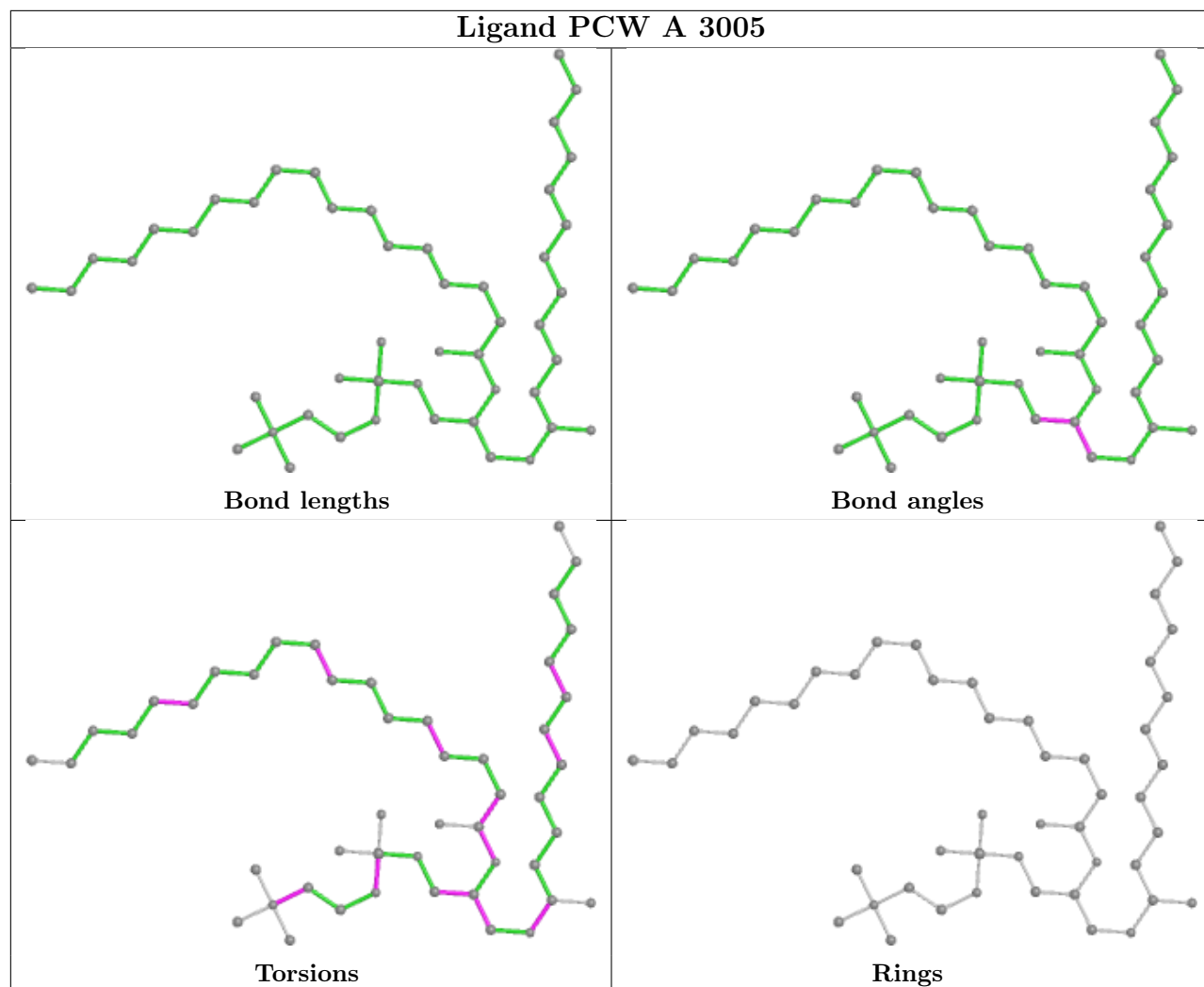


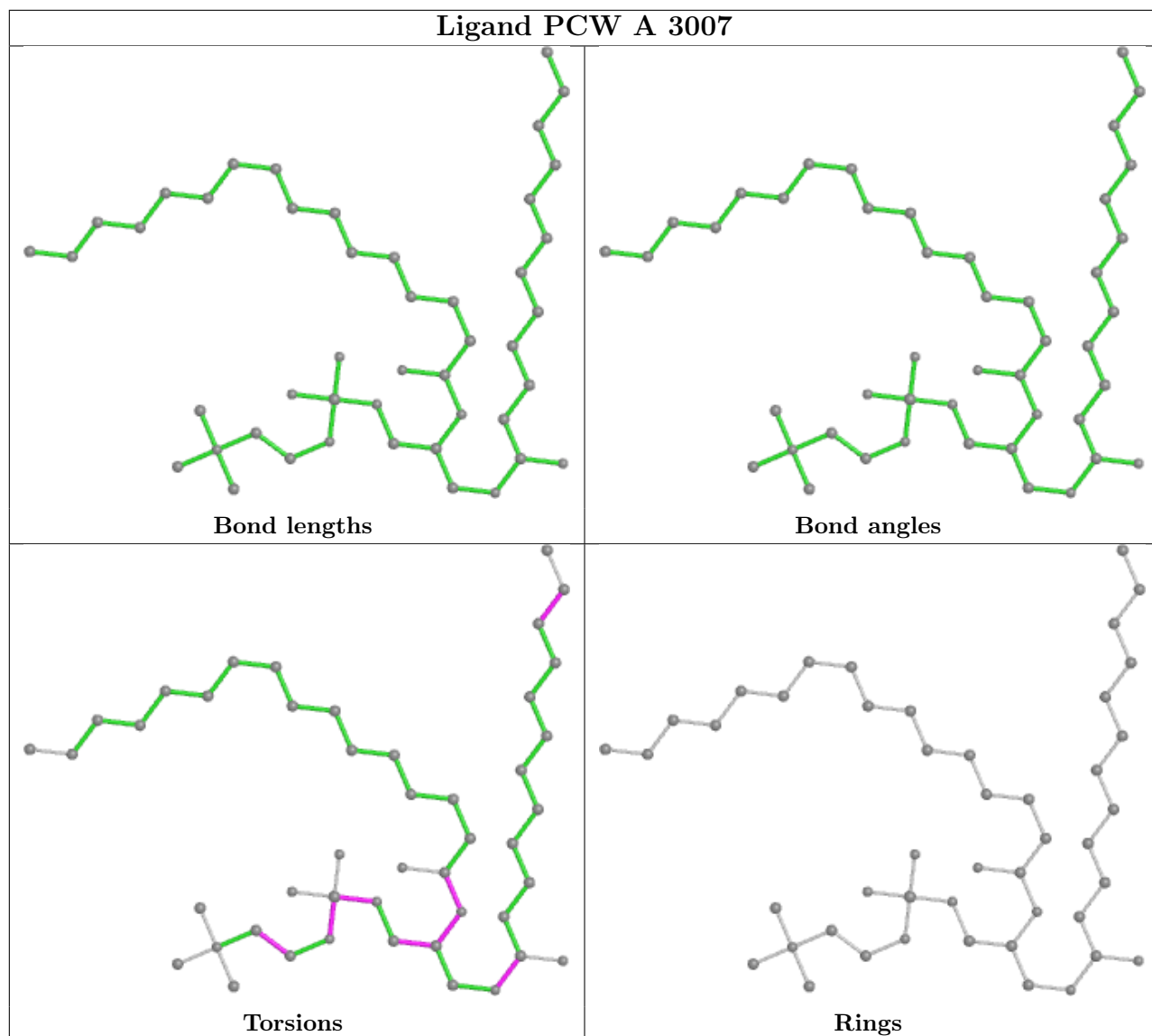


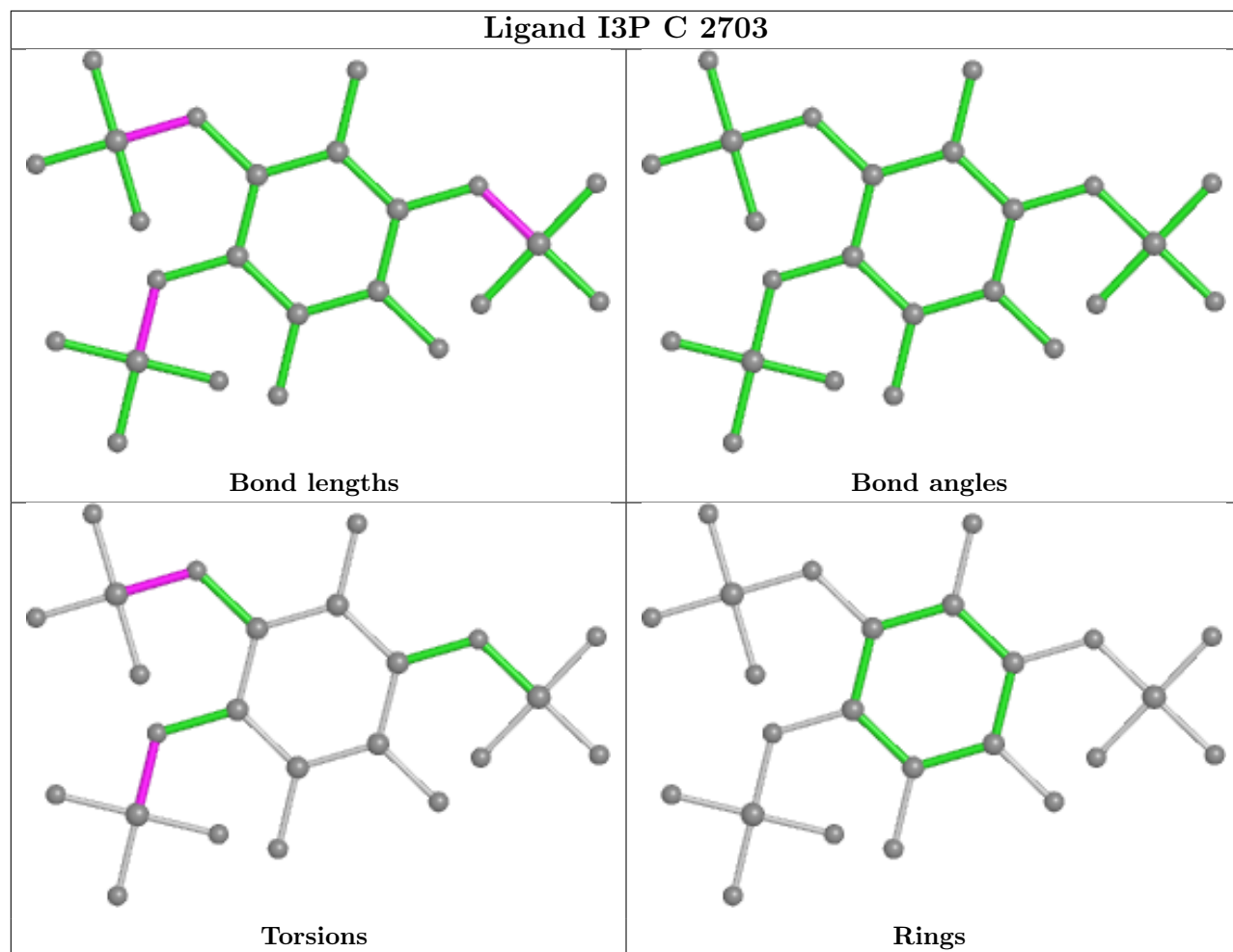


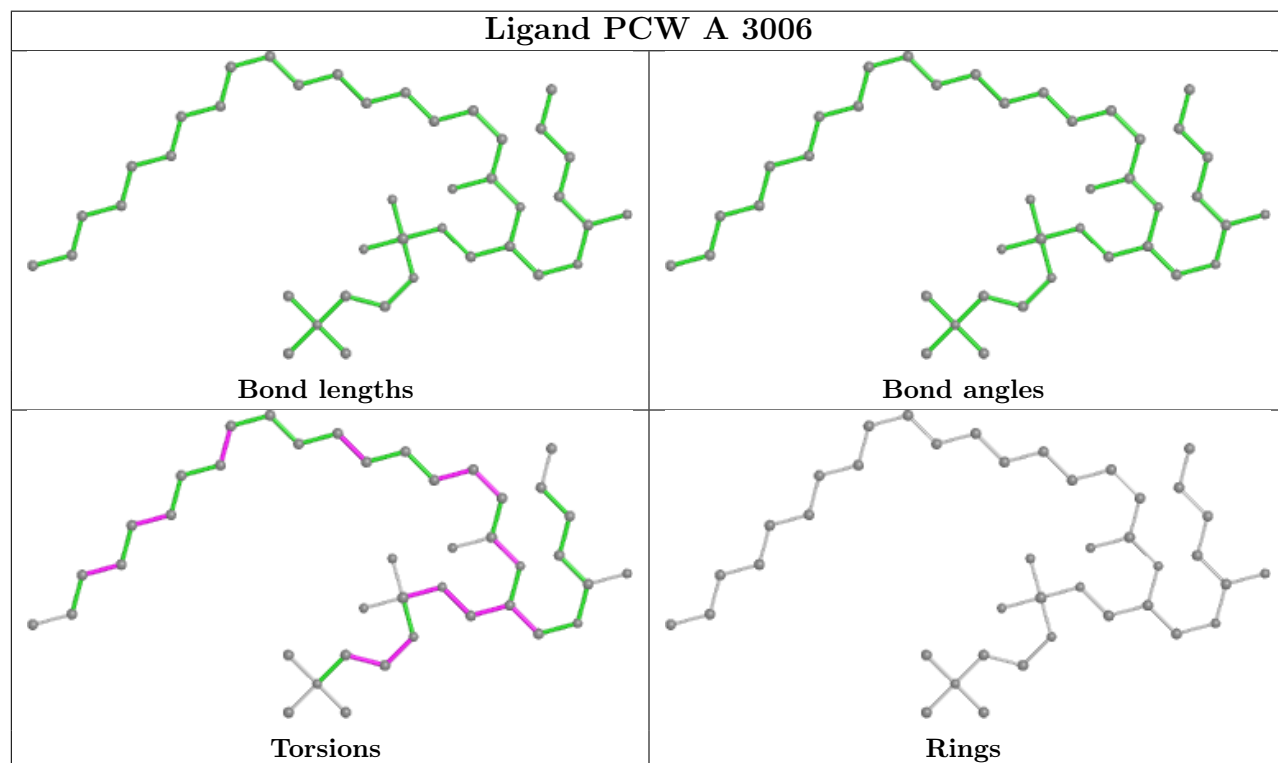
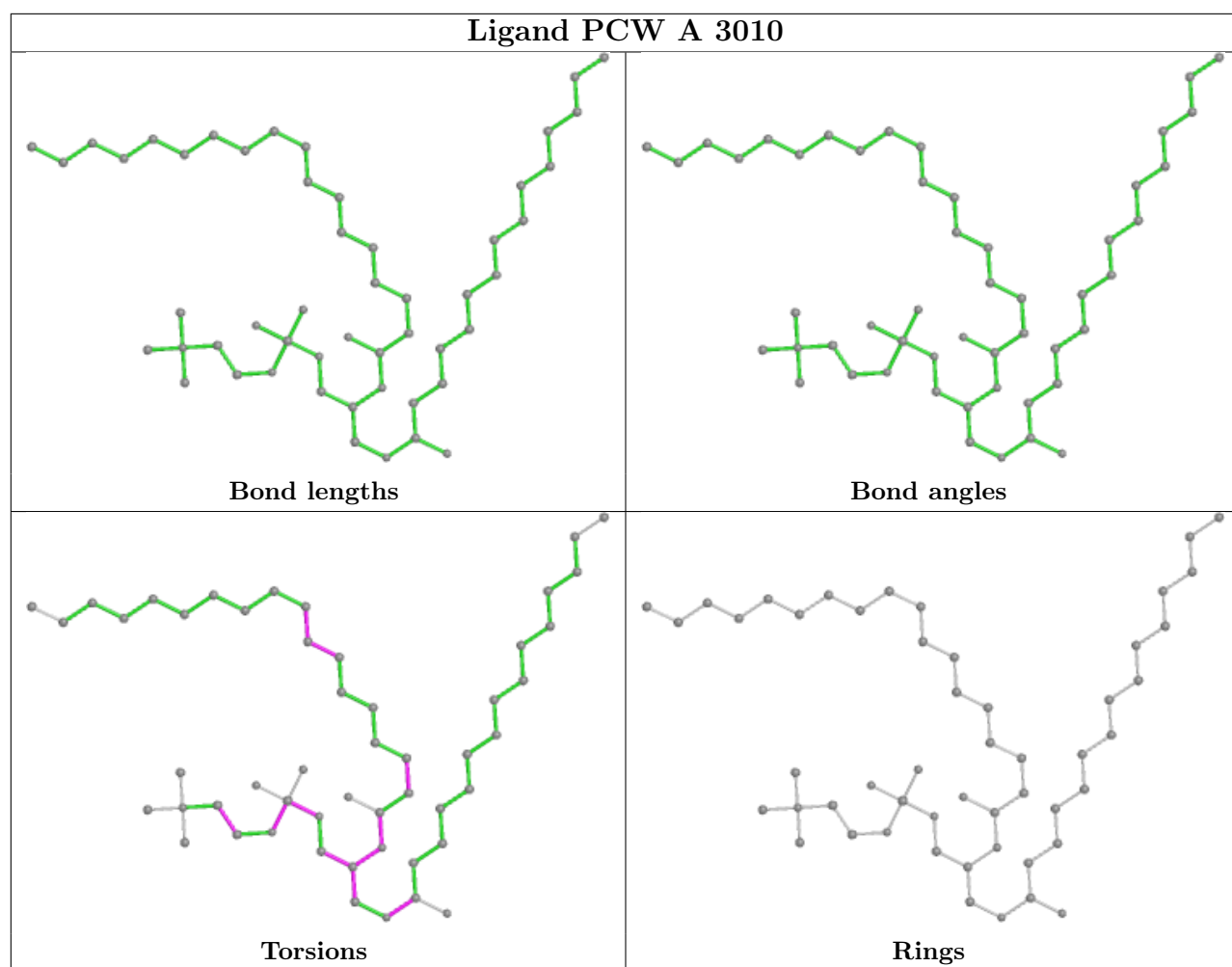


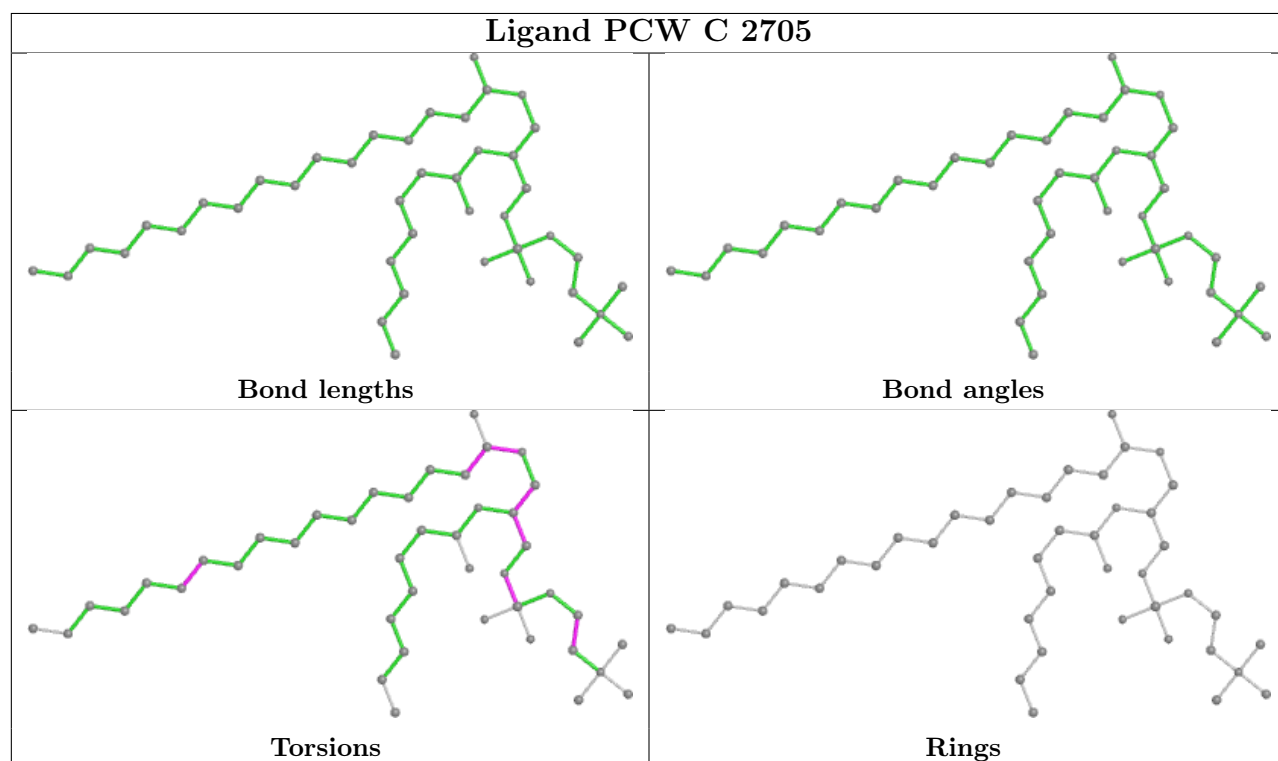
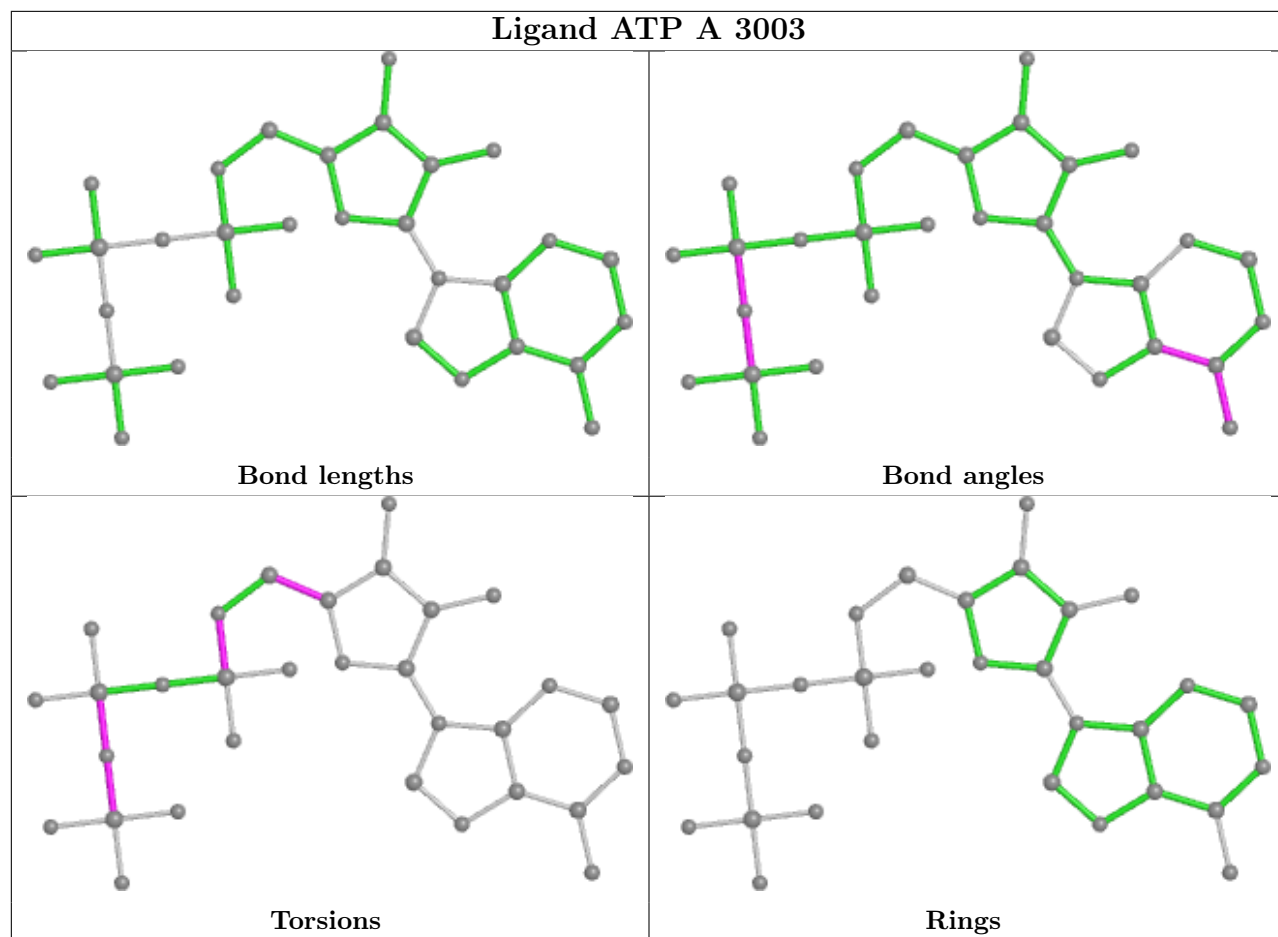




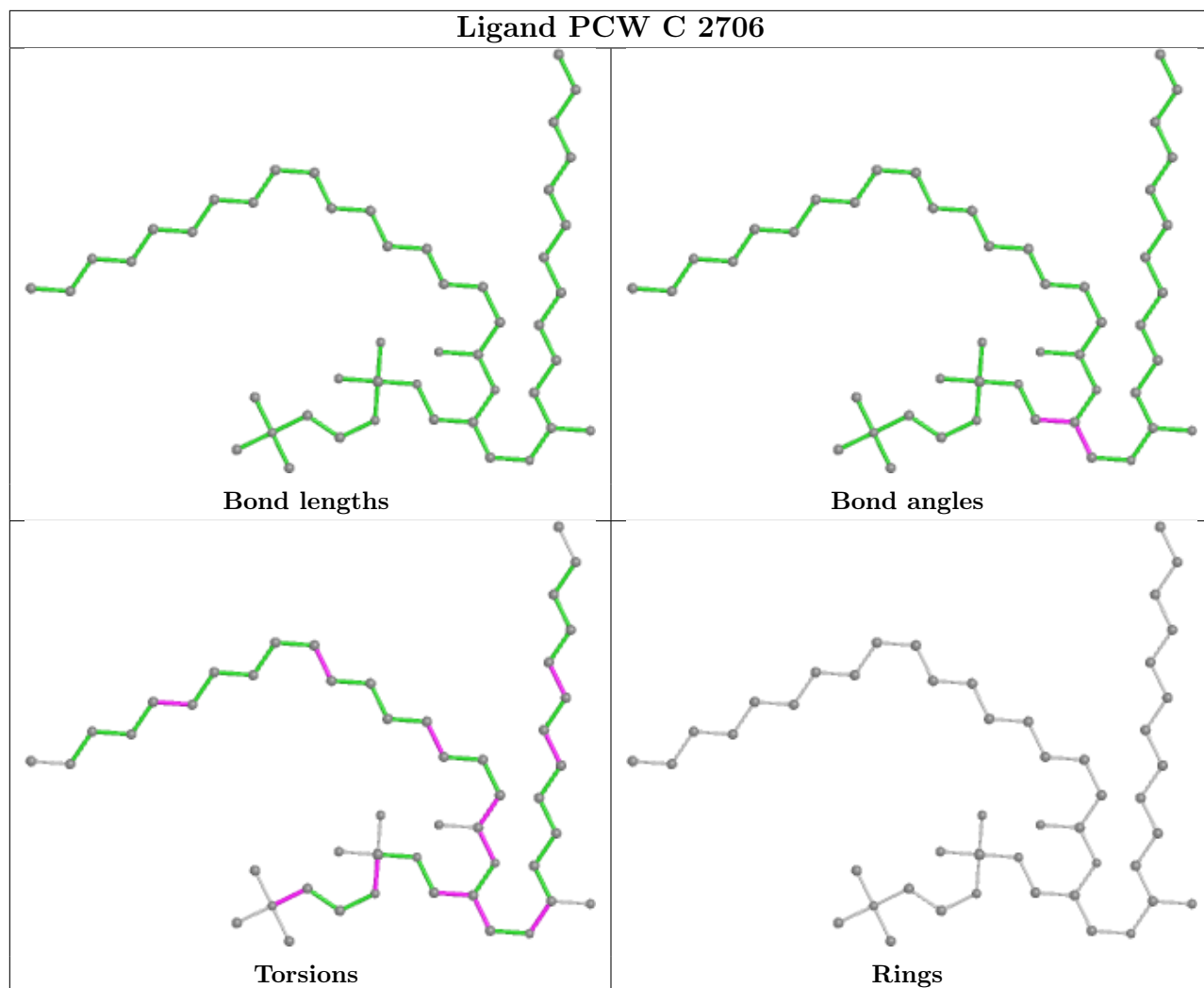


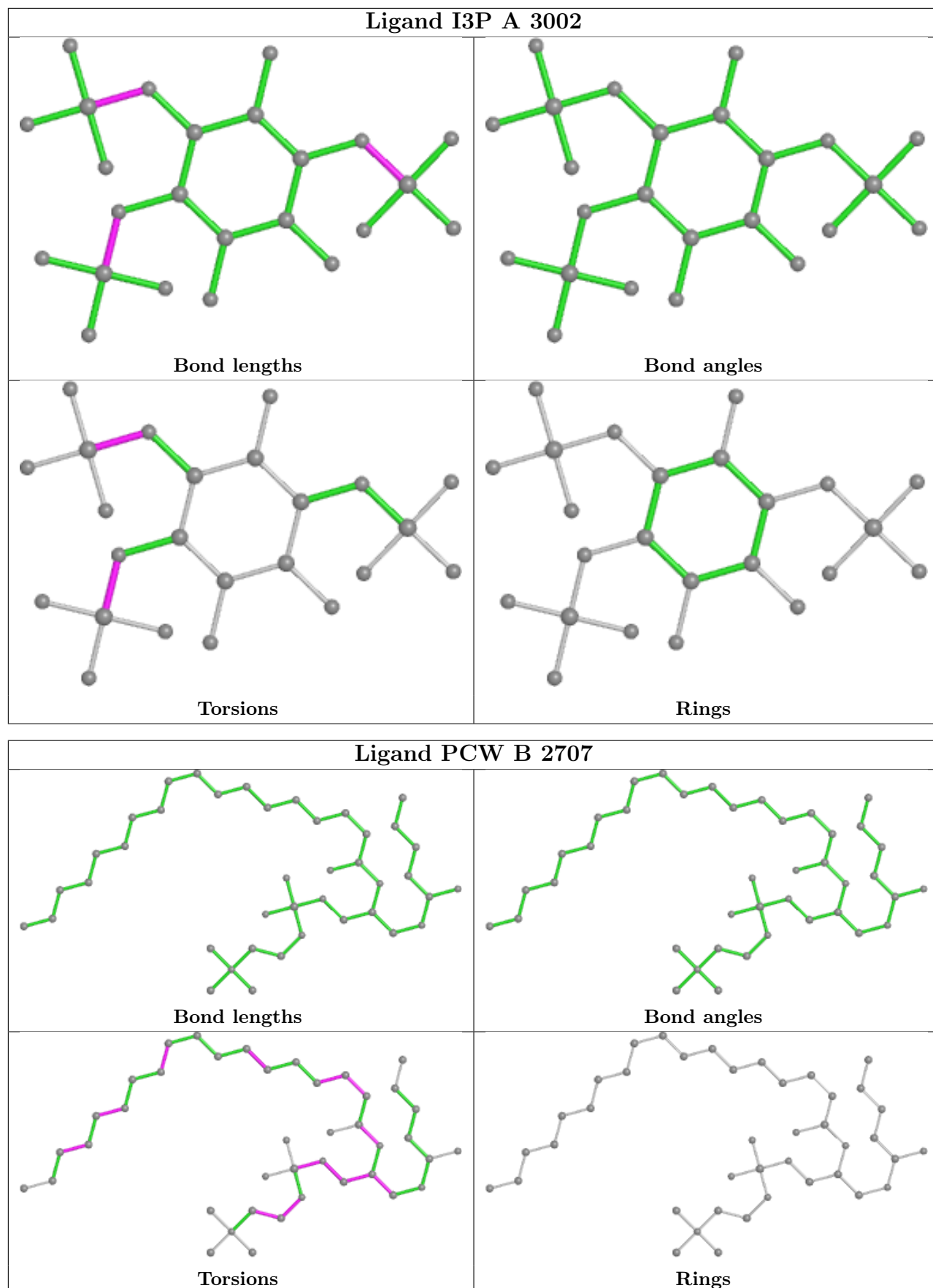


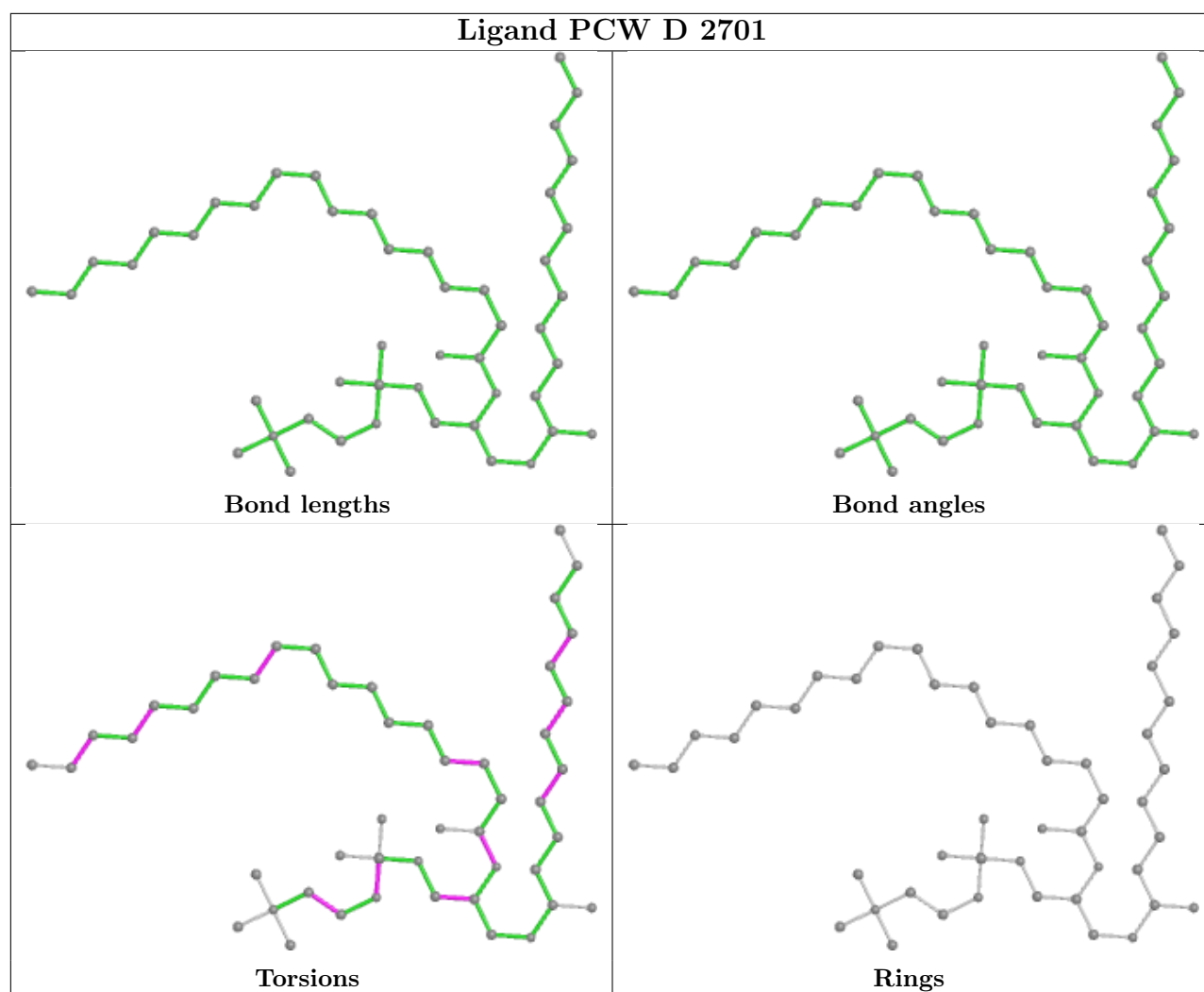












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

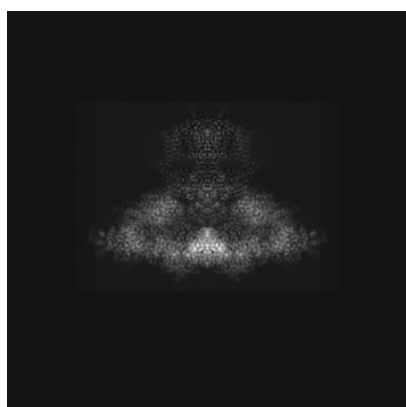
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41323. These allow visual inspection of the internal detail of the map and identification of artifacts.

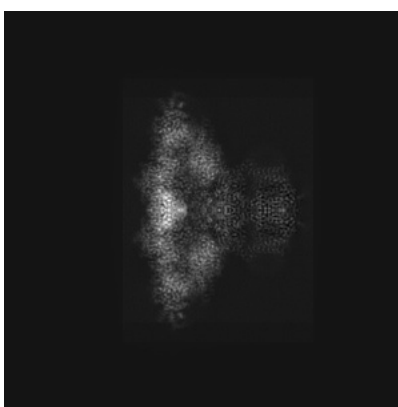
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

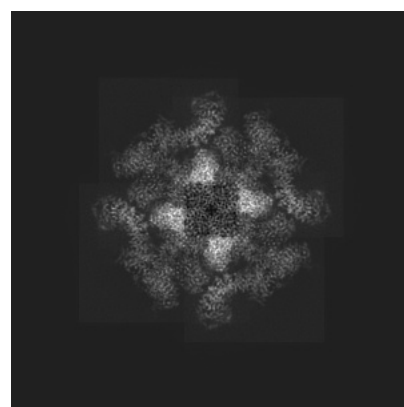
#### 6.1.1 Primary map



X



Y



Z

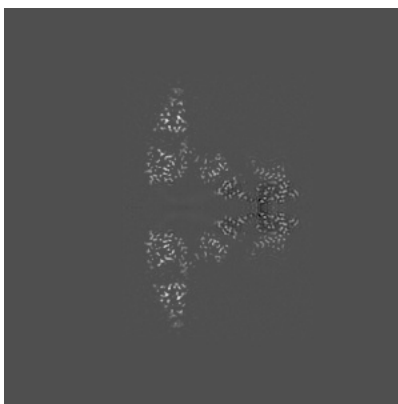
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

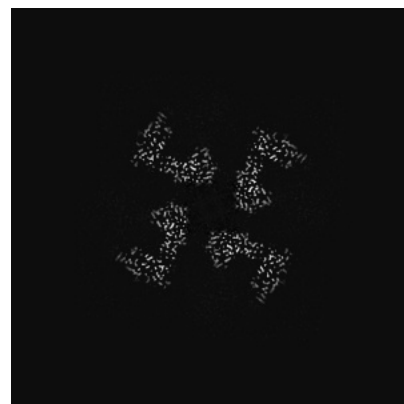
#### 6.2.1 Primary map



X Index: 336



Y Index: 336



Z Index: 336

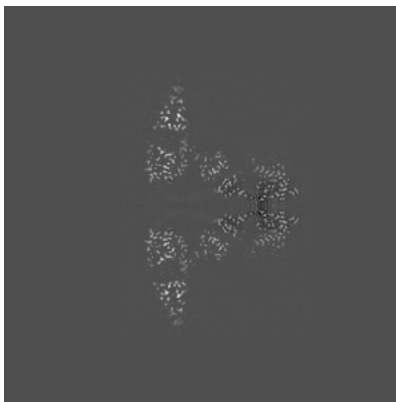
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 336



Y Index: 336

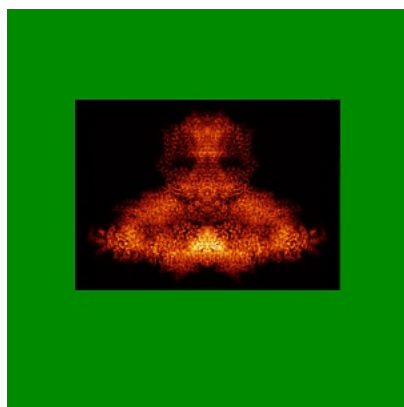


Z Index: 277

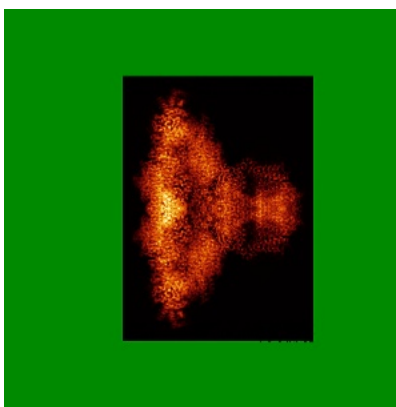
The images above show the largest variance slices of the map in three orthogonal directions.

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

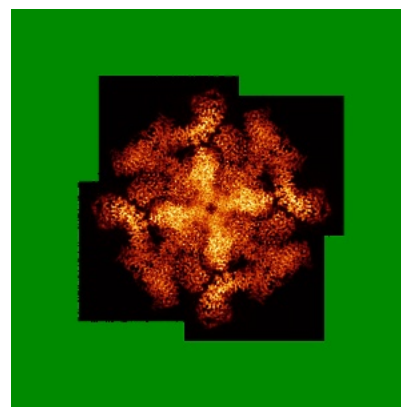
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

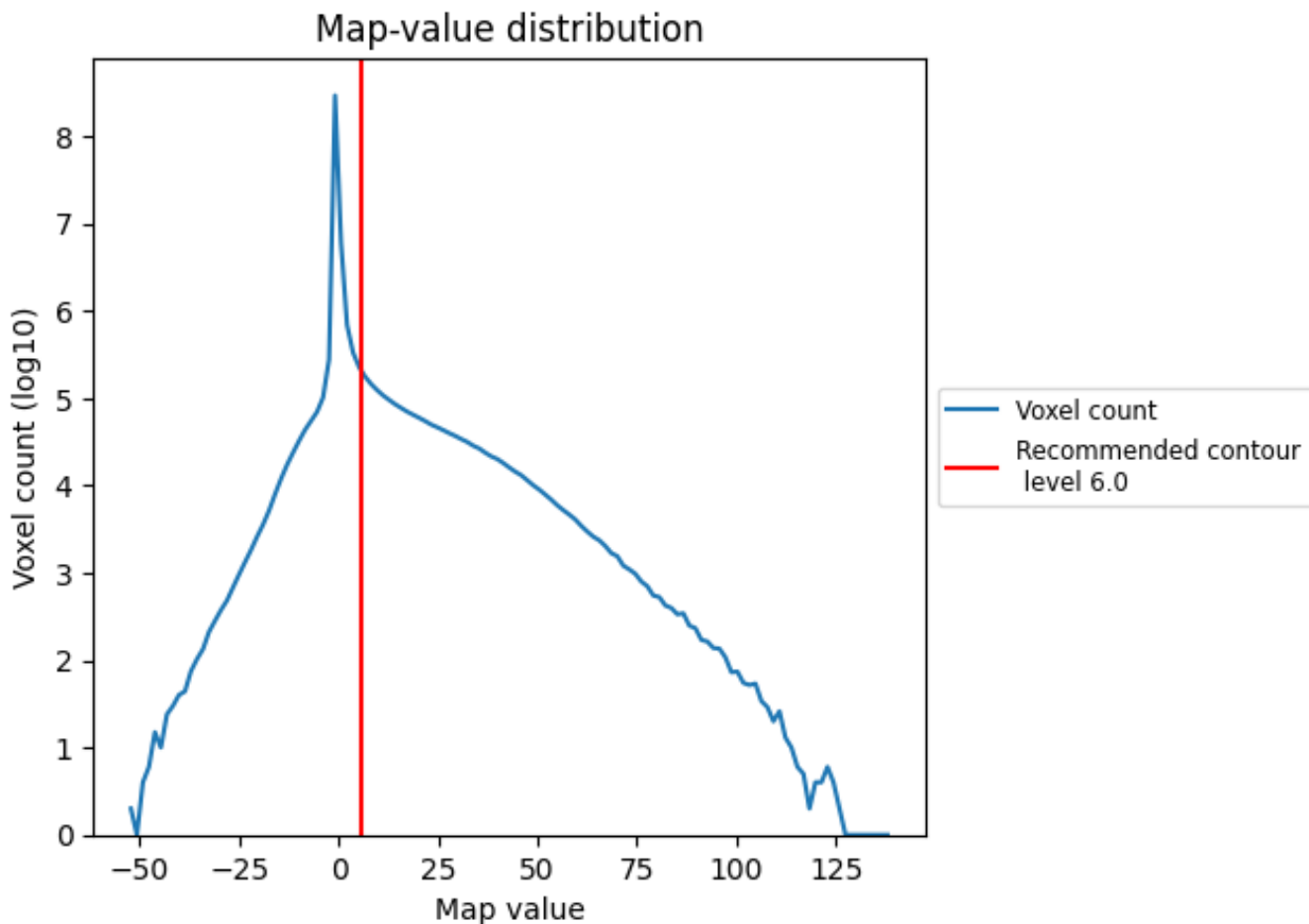
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

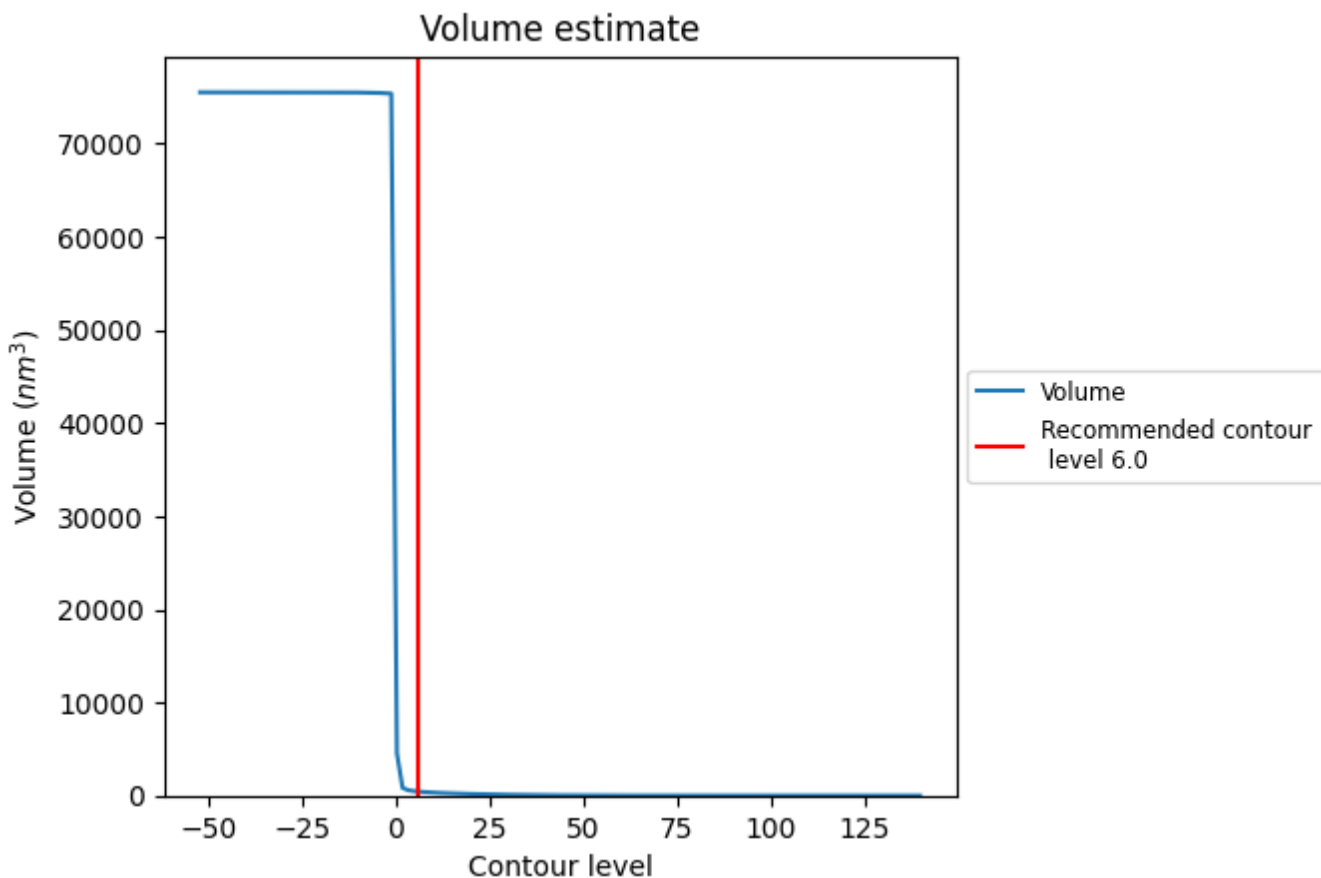
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

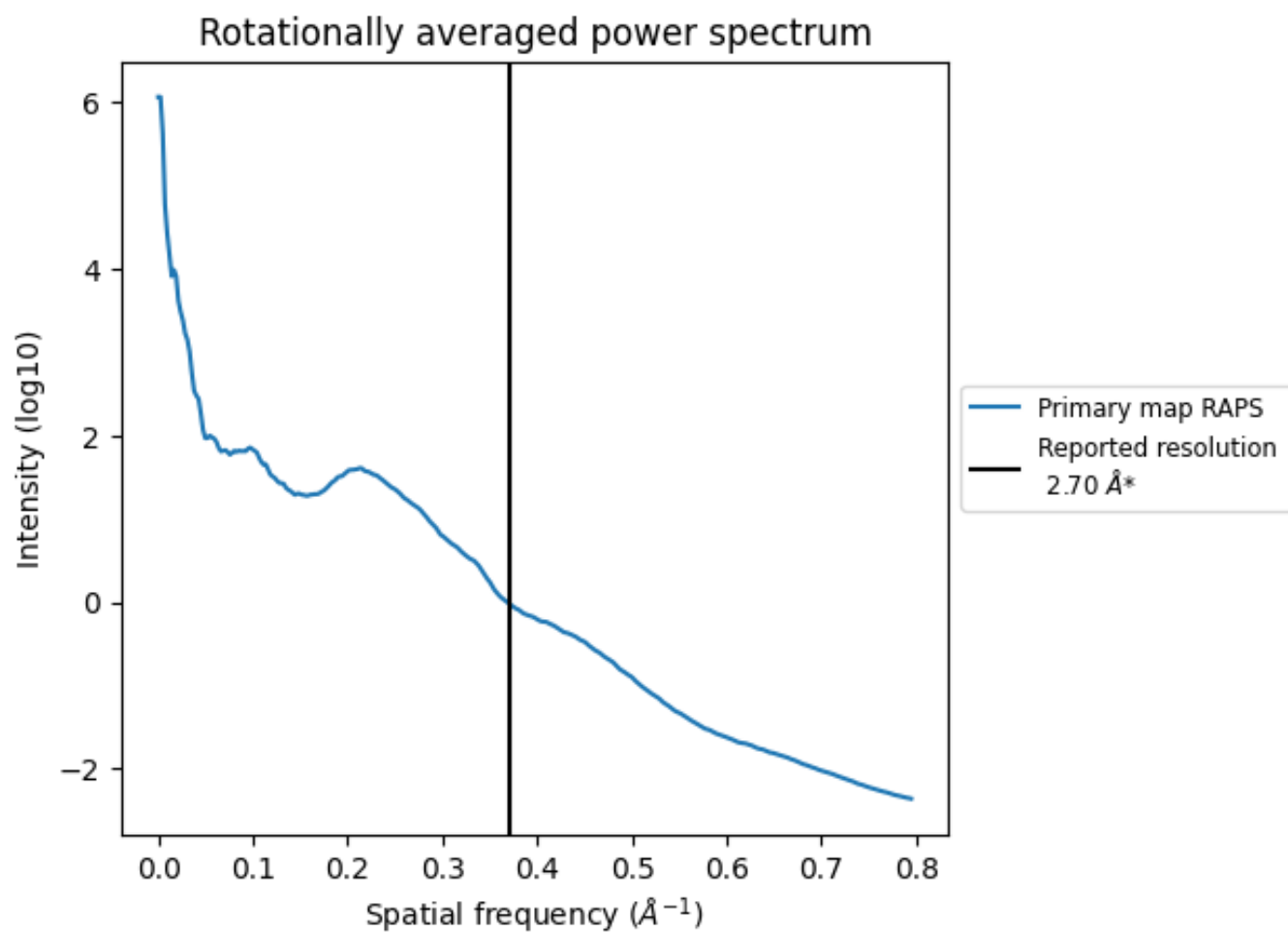


The volume at the recommended contour level is 429  $\text{nm}^3$ ; this corresponds to an approximate mass of 388 kDa.

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



### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

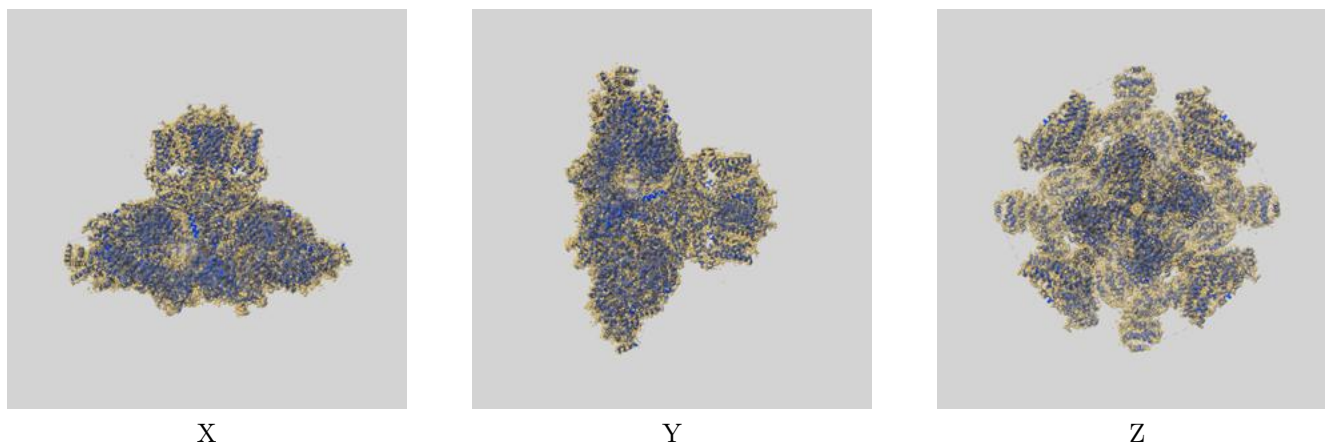
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

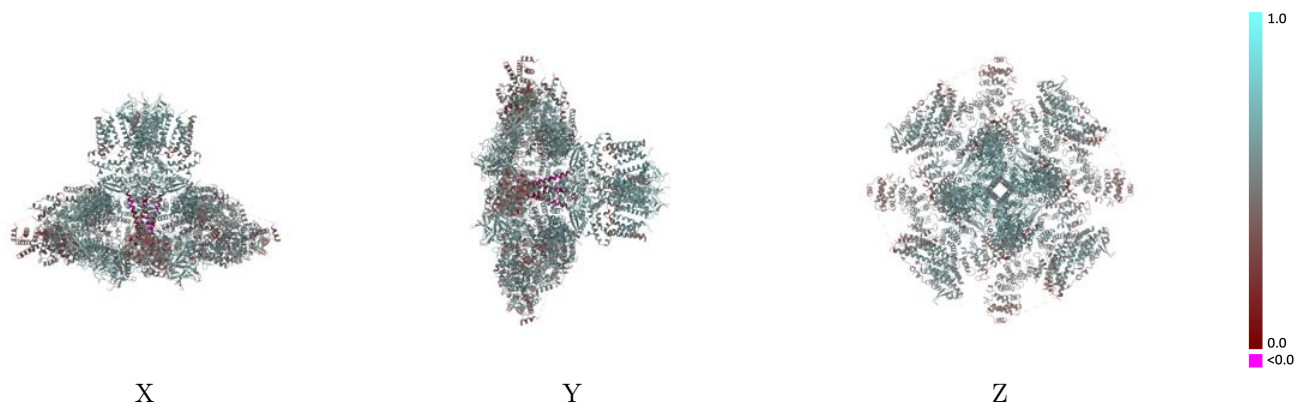
This section contains information regarding the fit between EMDB map EMD-41323 and PDB model 8TK8. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



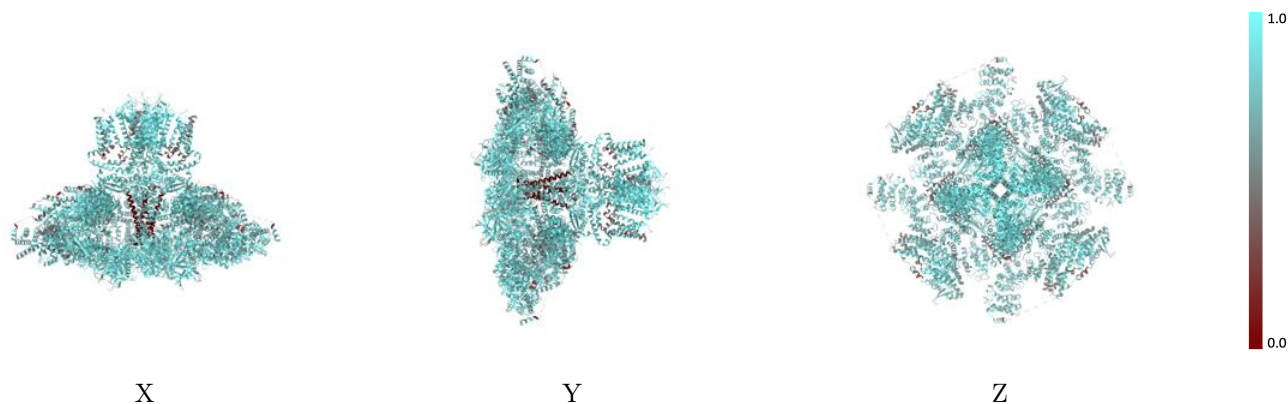
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



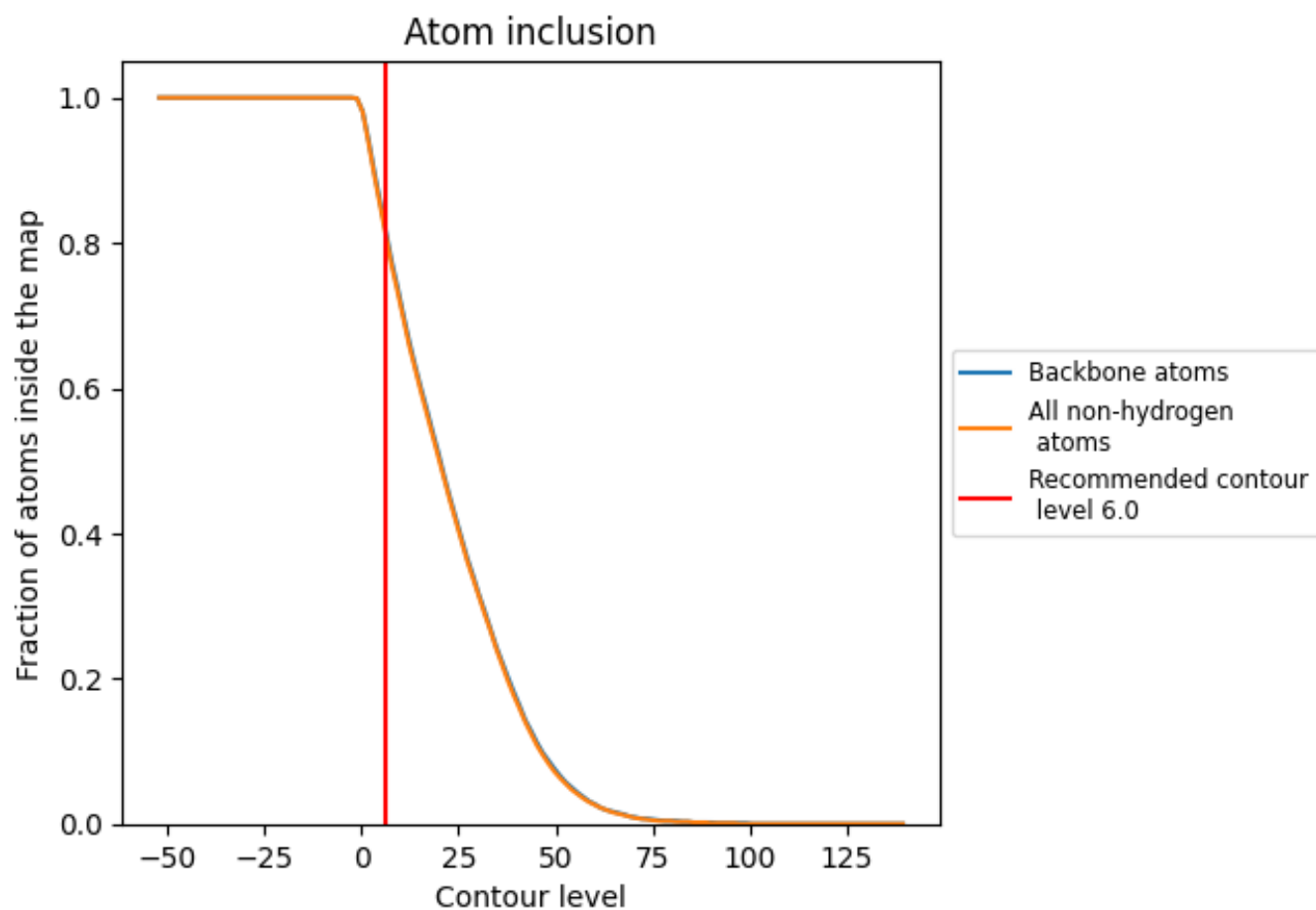
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.5240
A	 0.8220	 0.5230
B	 0.8170	 0.5220
C	 0.8230	 0.5290
D	 0.8200	 0.5240

