



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:46 PM UTC

PDB ID : 8TKF / pdb\_00008tkf  
EMDB ID : EMD-41349  
Title : Human Type 3 IP3 Receptor - Activated State (+IP3/ATP/JD Ca2+)  
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.  
Deposited on : 2023-07-25  
Resolution : 3.20 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:

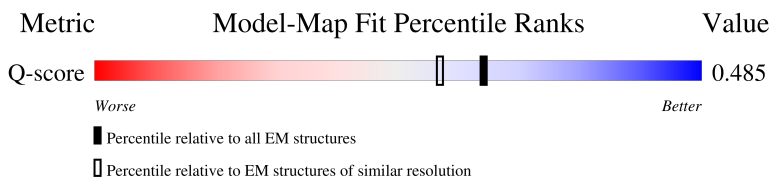
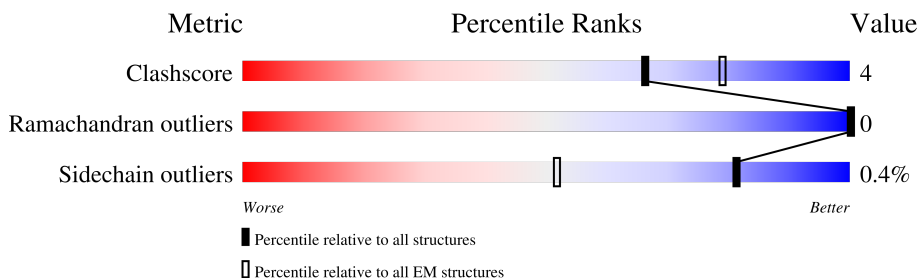
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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	<div> <div>5%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	B	2671	<div> <div>5%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	C	2671	<div> <div>5%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	D	2671	<div> <div>6%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 148344 atoms, of which 74244 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.

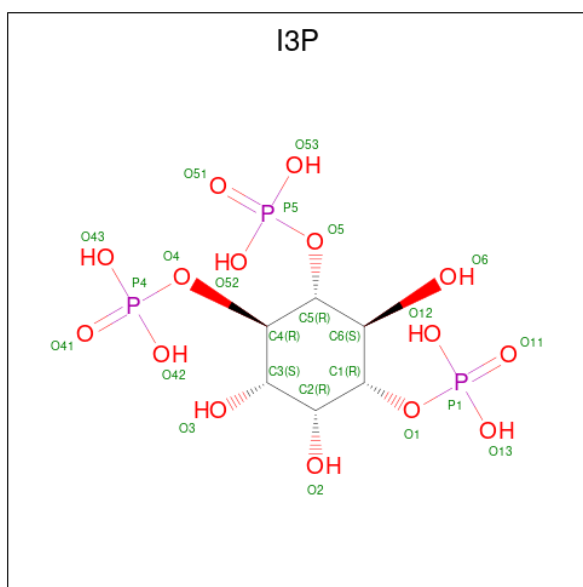
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		
1	B	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		
1	C	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		
1	D	2272	Total	C	H	N	O	S	0	0
			36472	11639	18244	3114	3363	112		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: 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).

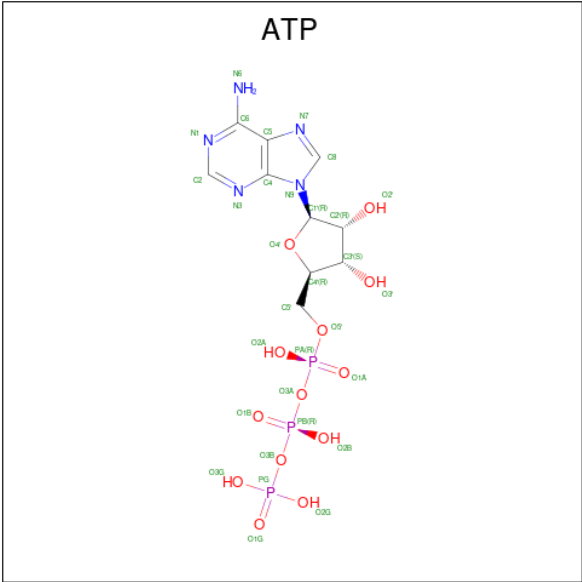


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

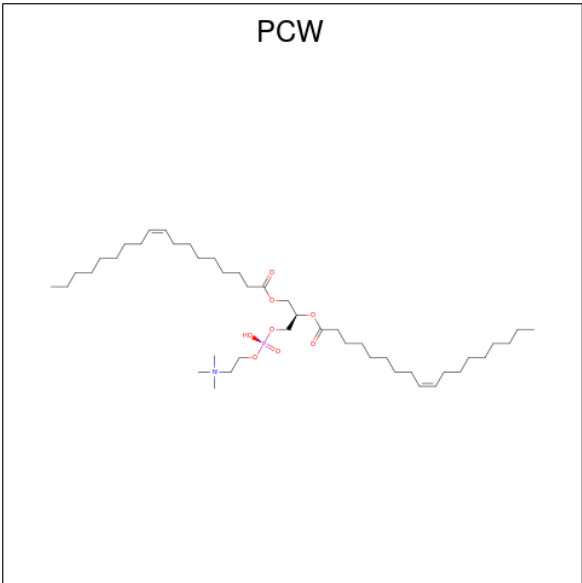
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



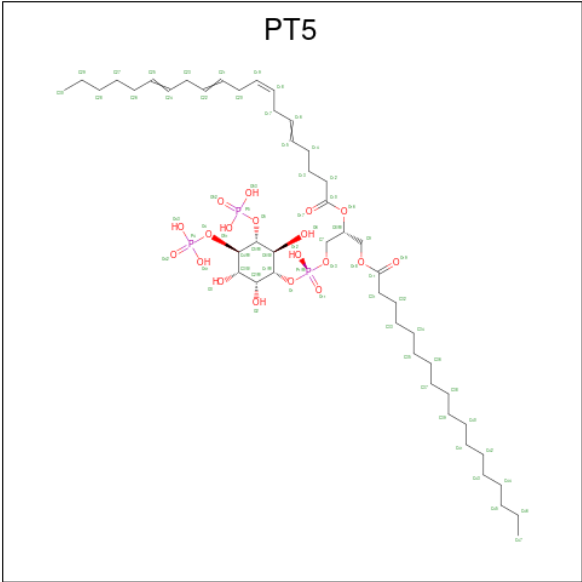
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C<sub>44</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	A	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			101	33	58	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			105	35	60	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			114	37	67	1	8	1	
6	D	1	Total	C	H	N	O	P	0
			98	31	57	1	8	1	

- Molecule 7 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: C<sub>47</sub>H<sub>85</sub>O<sub>19</sub>P<sub>3</sub>).

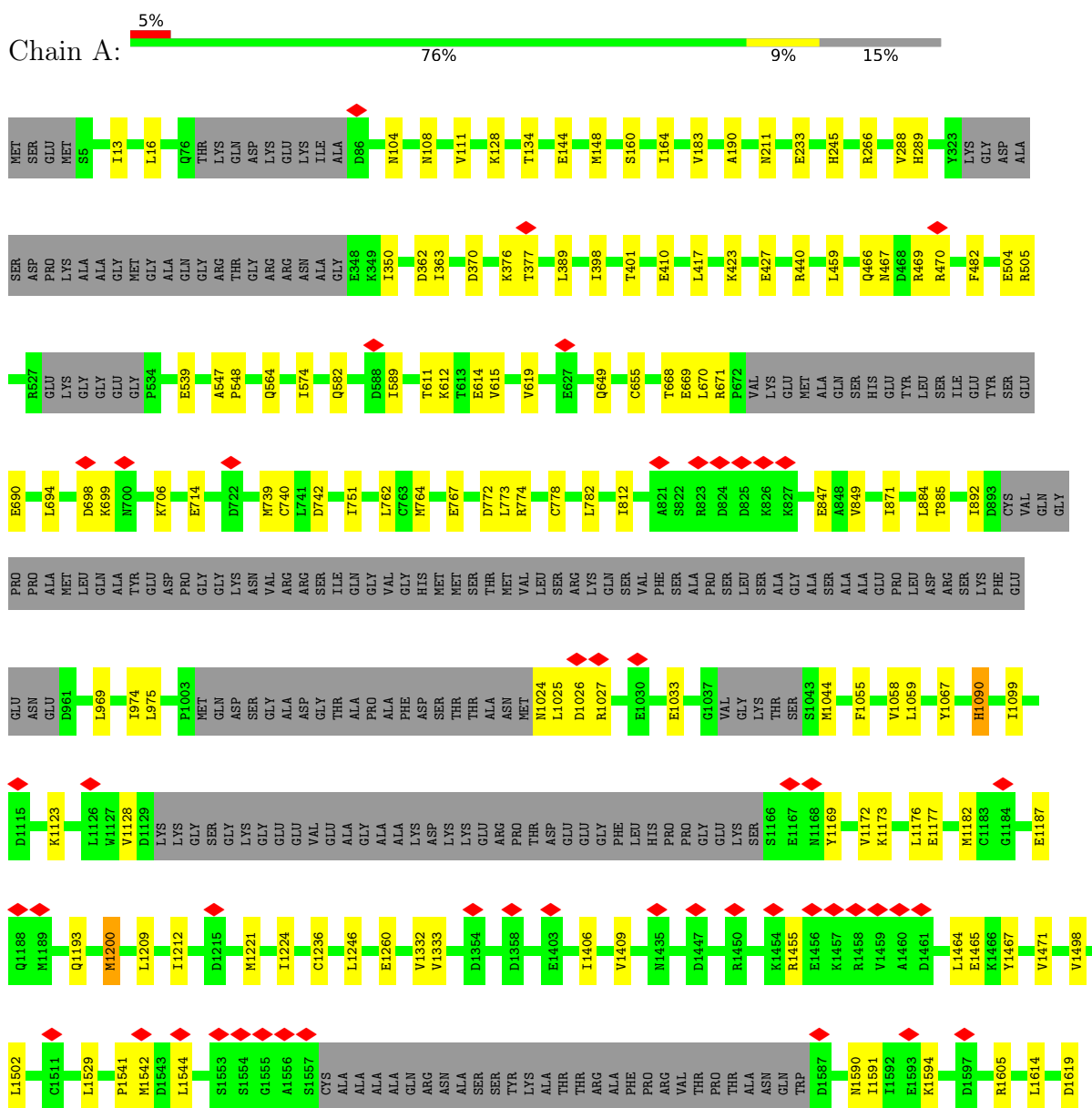


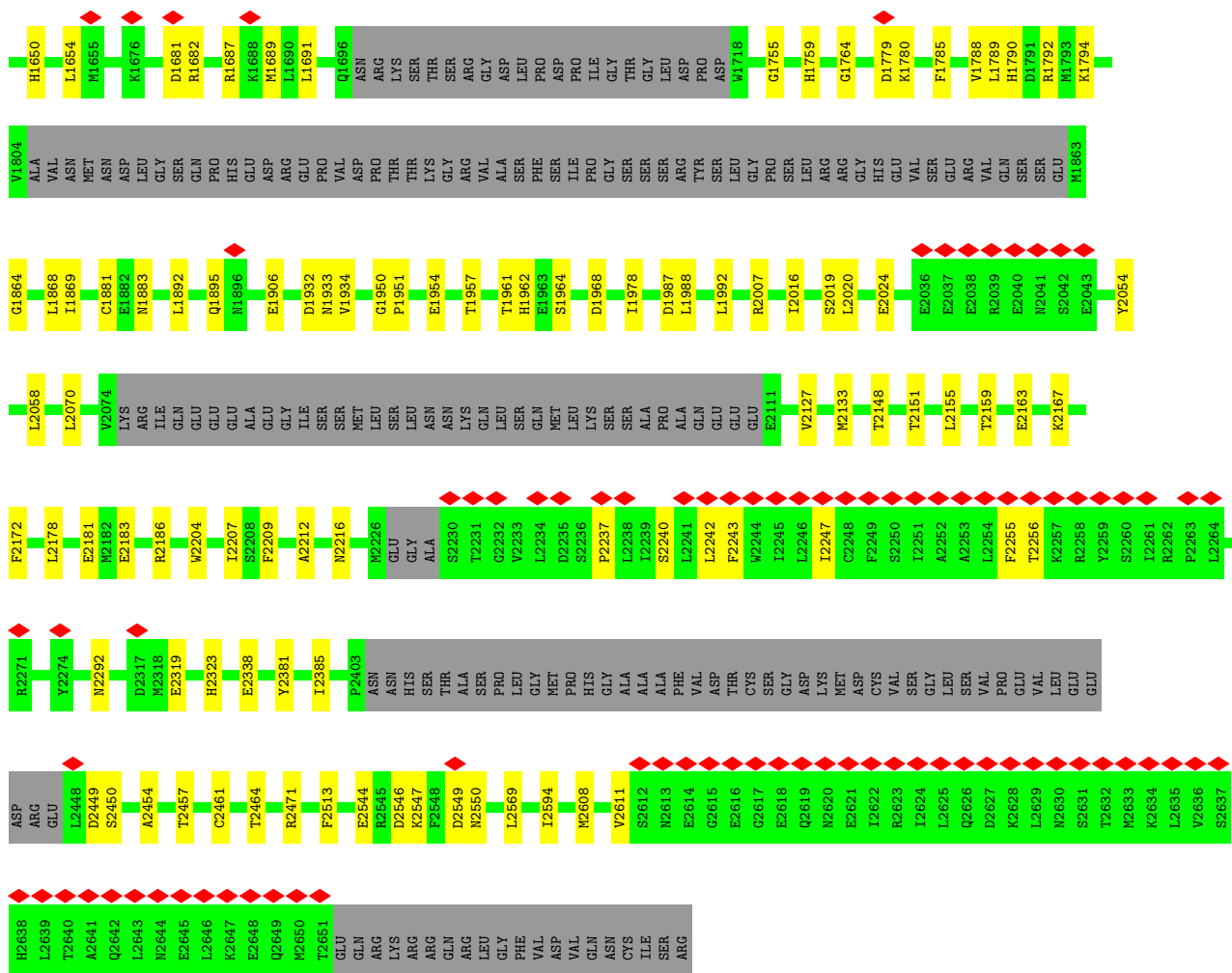
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	O	P	0
			118	42	54	19	3	
7	B	1	Total	C	H	O	P	0
			118	42	54	19	3	
7	C	1	Total	C	H	O	P	0
			118	42	54	19	3	
7	D	1	Total	C	H	O	P	0
			118	42	54	19	3	

### 3 Residue-property plots

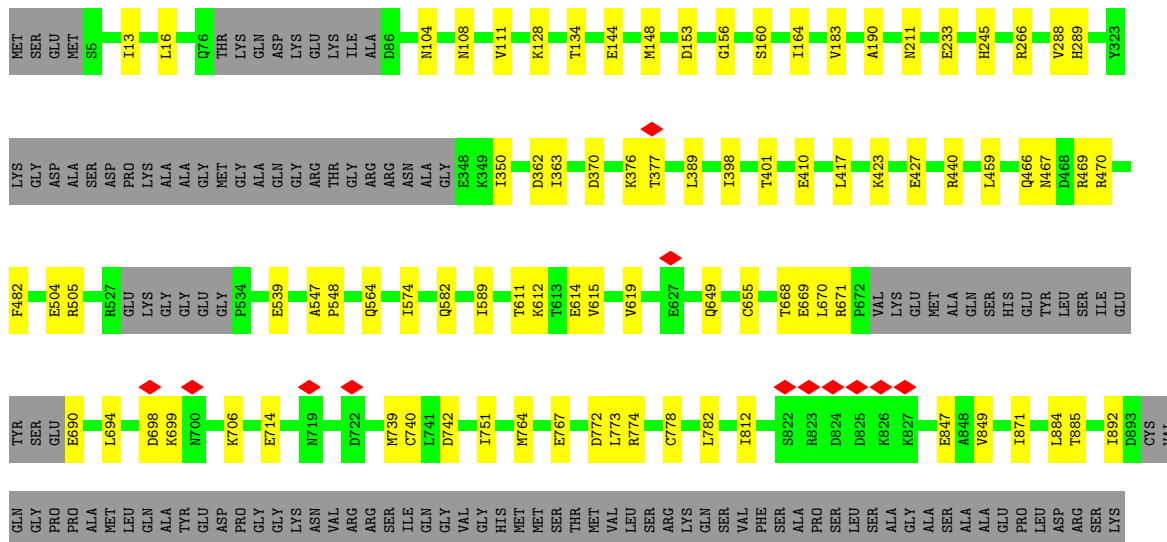
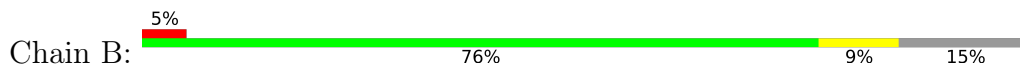
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

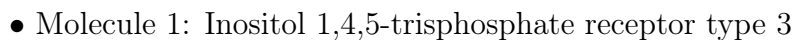
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

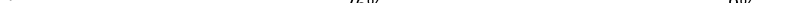




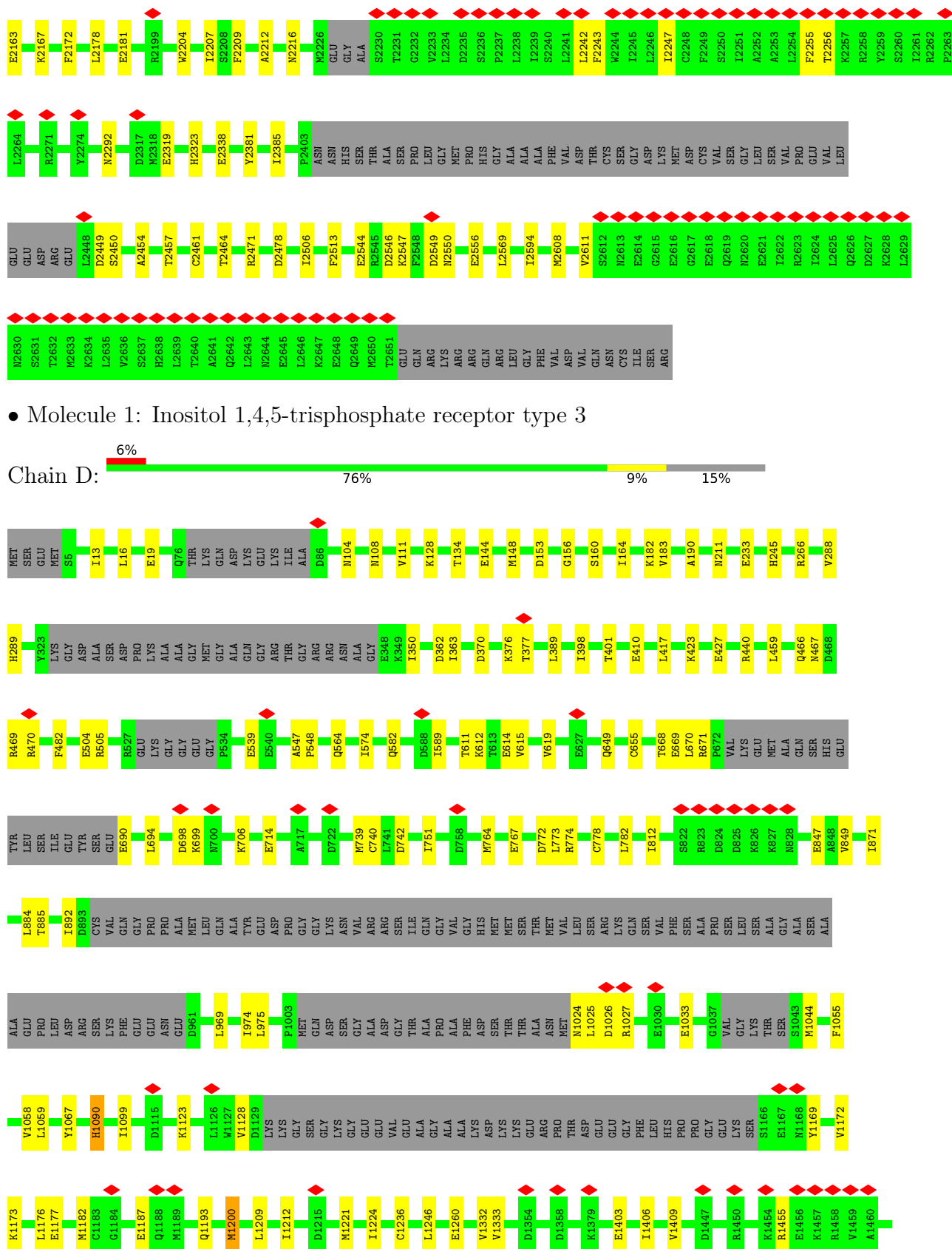
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

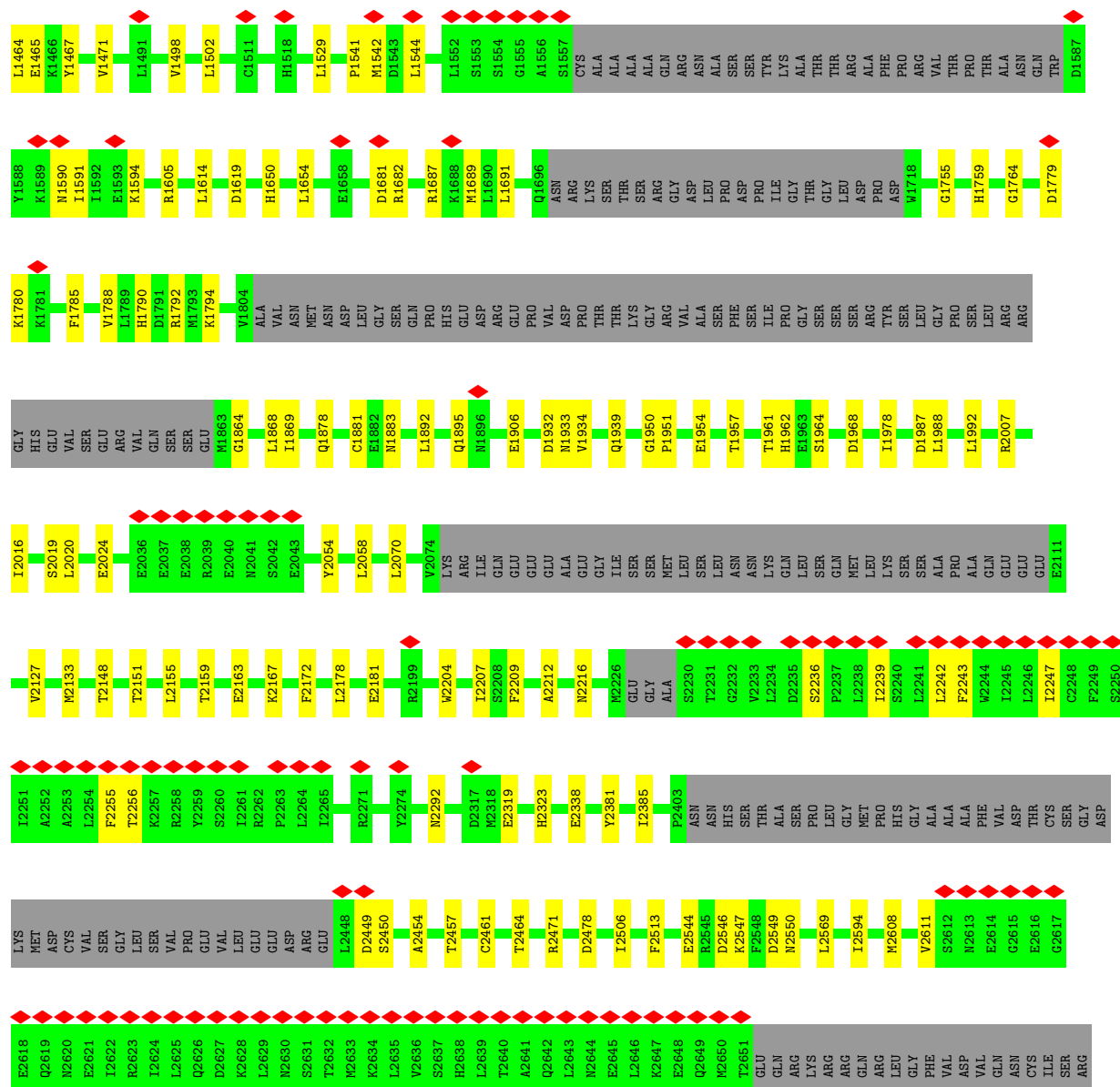




Chain C:  5% 76% 9% 15%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	228188	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	107.065	Depositor
Minimum map value	-41.251	Depositor
Average map value	0.126	Depositor
Map value standard deviation	1.558	Depositor
Recommended contour level	6	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: PT5, ZN, I3P, CA, 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	0.10	1/18566 (0.0%)	0.22	2/25094 (0.0%)
1	B	0.10	1/18566 (0.0%)	0.22	2/25094 (0.0%)
1	C	0.10	1/18566 (0.0%)	0.22	2/25094 (0.0%)
1	D	0.10	1/18566 (0.0%)	0.22	2/25094 (0.0%)
All	All	0.10	4/74264 (0.0%)	0.22	8/100376 (0.0%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1090	HIS	CE1-NE2	-5.15	1.27	1.32
1	A	1090	HIS	CE1-NE2	-5.10	1.27	1.32
1	B	1090	HIS	CE1-NE2	-5.08	1.27	1.32
1	C	1090	HIS	CE1-NE2	-5.05	1.27	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	HIS	ND1-CG-CD2	-6.47	99.63	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1090	HIS	ND1-CG-CD2	-6.47	99.63	106.10
1	B	1090	HIS	ND1-CG-CD2	-6.46	99.64	106.10
1	C	1090	HIS	ND1-CG-CD2	-6.45	99.65	106.10
1	D	1090	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
1	B	1090	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	A	1090	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
1	C	1090	HIS	CE1-NE2-CD2	-5.21	103.79	109.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1090	HIS	Sidechain
1	B	1090	HIS	Sidechain
1	C	1090	HIS	Sidechain
1	D	1090	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	18228	18244	18243	148	0
1	B	18228	18244	18243	144	0
1	C	18228	18244	18243	147	0
1	D	18228	18244	18243	150	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	1	0
3	B	24	9	9	1	0
3	C	24	9	9	1	0
3	D	24	9	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
6	A	176	242	242	1	0
6	B	176	242	242	1	0
6	C	176	242	242	1	0
6	D	176	242	242	1	0
7	A	64	54	64	3	0
7	B	64	54	64	3	0
7	C	64	54	64	3	0
7	D	64	54	64	3	0
All	All	74100	74244	74280	583	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 (583) 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:1182:MET:SD	1:B:1193:GLN:NE2	2.60	0.75
1:D:1182:MET:SD	1:D:1193:GLN:NE2	2.60	0.75
1:C:1182:MET:SD	1:C:1193:GLN:NE2	2.60	0.74
1:A:1182:MET:SD	1:A:1193:GLN:NE2	2.60	0.74
1:C:2255:PHE:O	1:C:2256:THR:OG1	2.06	0.73
1:A:2255:PHE:O	1:A:2256:THR:OG1	2.06	0.73
1:B:2255:PHE:O	1:B:2256:THR:OG1	2.06	0.72
1:B:164:ILE:HD11	1:B:183:VAL:HG21	1.73	0.71
1:D:350:ILE:HD11	1:D:401:THR:HG21	1.73	0.71
1:C:164:ILE:HD11	1:C:183:VAL:HG21	1.73	0.70
1:A:164:ILE:HD11	1:A:183:VAL:HG21	1.73	0.70
1:D:164:ILE:HD11	1:D:183:VAL:HG21	1.73	0.70
1:D:2255:PHE:O	1:D:2256:THR:OG1	2.06	0.70
1:A:350:ILE:HD11	1:A:401:THR:HG21	1.73	0.70
1:B:1790:HIS:NE2	1:B:1906:GLU:OE2	2.25	0.69
1:D:1790:HIS:NE2	1:D:1906:GLU:OE2	2.25	0.69
1:A:1790:HIS:NE2	1:A:1906:GLU:OE2	2.26	0.69
1:A:614:GLU:N	1:A:614:GLU:OE1	2.26	0.69
1:B:350:ILE:HD11	1:B:401:THR:HG21	1.73	0.69
1:C:1790:HIS:NE2	1:C:1906:GLU:OE2	2.26	0.68
1:A:892:ILE:HG21	1:A:1058:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:GLU:OE1	1:B:614:GLU:N	2.26	0.68
1:C:614:GLU:N	1:C:614:GLU:OE1	2.26	0.68
1:D:614:GLU:OE1	1:D:614:GLU:N	2.26	0.68
1:C:350:ILE:HD11	1:C:401:THR:HG21	1.73	0.68
1:C:892:ILE:HG21	1:C:1058:VAL:HG13	1.76	0.68
1:C:1962:HIS:ND1	1:C:1964:SER:OG	2.24	0.67
1:D:892:ILE:HG21	1:D:1058:VAL:HG13	1.76	0.67
1:B:892:ILE:HG21	1:B:1058:VAL:HG13	1.76	0.67
1:D:1221:MET:SD	1:D:1224:ILE:HD11	2.38	0.64
1:A:1221:MET:SD	1:A:1224:ILE:HD11	2.38	0.64
1:C:772:ASP:OD1	1:C:773:LEU:N	2.31	0.64
1:A:772:ASP:OD1	1:A:773:LEU:N	2.31	0.64
1:C:1221:MET:SD	1:C:1224:ILE:HD11	2.38	0.64
1:B:128:LYS:O	1:B:440:ARG:NH1	2.31	0.64
1:B:1221:MET:SD	1:B:1224:ILE:HD11	2.38	0.64
1:D:1962:HIS:CE1	1:D:1964:SER:HG	2.15	0.63
1:B:2024:GLU:OE1	1:B:2024:GLU:N	2.32	0.63
1:B:772:ASP:OD1	1:B:773:LEU:N	2.31	0.63
1:A:1794:LYS:NZ	1:A:1906:GLU:OE1	2.32	0.63
1:A:128:LYS:O	1:A:440:ARG:NH1	2.31	0.63
1:C:128:LYS:O	1:C:440:ARG:NH1	2.31	0.63
1:C:2024:GLU:N	1:C:2024:GLU:OE1	2.32	0.63
1:D:128:LYS:O	1:D:440:ARG:NH1	2.31	0.63
1:D:1794:LYS:NZ	1:D:1906:GLU:OE1	2.32	0.63
1:A:2381:TYR:CZ	1:A:2385:ILE:HD11	2.34	0.63
1:B:2381:TYR:CZ	1:B:2385:ILE:HD11	2.34	0.63
1:C:2381:TYR:CZ	1:C:2385:ILE:HD11	2.34	0.62
1:D:2381:TYR:CZ	1:D:2385:ILE:HD11	2.34	0.62
1:C:1794:LYS:NZ	1:C:1906:GLU:OE1	2.32	0.62
1:B:1794:LYS:NZ	1:B:1906:GLU:OE1	2.32	0.62
1:B:1619:ASP:OD2	1:B:1687:ARG:NH2	2.33	0.62
1:D:2024:GLU:OE1	1:D:2024:GLU:N	2.32	0.62
1:A:2024:GLU:N	1:A:2024:GLU:OE1	2.32	0.62
1:A:370:ASP:OD2	1:A:423:LYS:NZ	2.26	0.62
1:D:772:ASP:OD1	1:D:773:LEU:N	2.31	0.62
1:C:1619:ASP:OD2	1:C:1687:ARG:NH2	2.33	0.62
1:B:847:GLU:N	1:B:847:GLU:OE1	2.33	0.62
1:A:410:GLU:N	1:A:410:GLU:OE1	2.33	0.62
1:A:1619:ASP:OD2	1:A:1687:ARG:NH2	2.33	0.62
1:D:410:GLU:N	1:D:410:GLU:OE1	2.33	0.62
1:B:410:GLU:N	1:B:410:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:GLU:N	1:C:847:GLU:OE1	2.33	0.61
1:D:847:GLU:OE1	1:D:847:GLU:N	2.33	0.61
1:A:847:GLU:N	1:A:847:GLU:OE1	2.33	0.61
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.33	0.61
1:B:1033:GLU:OE2	1:B:1605:ARG:NH1	2.34	0.60
1:C:1033:GLU:OE2	1:C:1605:ARG:NH1	2.34	0.60
1:D:1033:GLU:OE2	1:D:1605:ARG:NH1	2.34	0.60
1:A:1033:GLU:OE2	1:A:1605:ARG:NH1	2.34	0.60
1:C:410:GLU:OE1	1:C:410:GLU:N	2.33	0.60
1:D:370:ASP:OD2	1:D:423:LYS:NZ	2.26	0.60
1:B:2242:LEU:HD13	7:B:2701:PT5:H37	1.83	0.59
1:A:885:THR:HG23	1:A:975:LEU:CD2	2.32	0.59
1:A:2243:PHE:CE2	1:A:2247:ILE:HD11	2.38	0.59
1:D:885:THR:HG23	1:D:975:LEU:CD2	2.32	0.59
1:B:2243:PHE:CE2	1:B:2247:ILE:HD11	2.38	0.59
1:A:1962:HIS:ND1	1:A:1964:SER:OG	2.24	0.58
1:B:885:THR:HG23	1:B:975:LEU:CD2	2.32	0.58
1:C:885:THR:HG23	1:C:975:LEU:CD2	2.32	0.58
1:B:1542:MET:SD	1:B:1542:MET:N	2.76	0.58
1:D:1187:GLU:OE1	1:D:1187:GLU:N	2.36	0.58
1:C:1542:MET:N	1:C:1542:MET:SD	2.76	0.58
1:D:1542:MET:SD	1:D:1542:MET:N	2.76	0.58
1:B:767:GLU:OE1	1:B:774:ARG:NH1	2.36	0.58
1:A:1542:MET:SD	1:A:1542:MET:N	2.76	0.58
1:A:767:GLU:OE1	1:A:774:ARG:NH1	2.36	0.58
6:C:2708:PCW:H19	1:D:2242:LEU:HD11	1.86	0.58
1:D:767:GLU:OE1	1:D:774:ARG:NH1	2.36	0.58
1:C:2243:PHE:CE2	1:C:2247:ILE:HD11	2.38	0.57
1:D:2243:PHE:CE2	1:D:2247:ILE:HD11	2.38	0.57
1:D:2209:PHE:CE1	7:D:2701:PT5:H19	2.38	0.57
1:A:164:ILE:O	1:A:164:ILE:HG23	2.04	0.57
1:B:1962:HIS:ND1	1:B:1964:SER:OG	2.25	0.57
1:B:164:ILE:HG23	1:B:164:ILE:O	2.04	0.57
1:B:1934:VAL:HG11	1:B:1988:LEU:HD13	1.87	0.57
1:A:1187:GLU:N	1:A:1187:GLU:OE1	2.36	0.56
1:C:164:ILE:HG23	1:C:164:ILE:O	2.04	0.56
1:D:164:ILE:HG23	1:D:164:ILE:O	2.04	0.56
1:A:1590:ASN:OD1	1:A:1594:LYS:NZ	2.37	0.56
1:B:1455:ARG:NH1	1:B:1465:GLU:OE2	2.39	0.56
1:C:767:GLU:OE1	1:C:774:ARG:NH1	2.36	0.56
1:D:1209:LEU:O	1:D:1212:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:LEU:O	1:B:1212:ILE:HG22	2.05	0.56
1:C:1187:GLU:N	1:C:1187:GLU:OE1	2.36	0.56
1:C:2319:GLU:O	1:C:2323:HIS:ND1	2.38	0.56
1:D:969:LEU:HD11	1:D:1067:TYR:HE2	1.70	0.56
1:D:1934:VAL:HG11	1:D:1988:LEU:HD13	1.87	0.56
6:B:2708:PCW:H19	1:C:2242:LEU:HD11	1.87	0.56
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.87	0.56
1:B:1590:ASN:OD1	1:B:1594:LYS:NZ	2.37	0.56
1:C:1934:VAL:HG11	1:C:1988:LEU:HD13	1.87	0.56
1:D:1590:ASN:OD1	1:D:1594:LYS:NZ	2.37	0.56
1:C:2209:PHE:CE1	7:C:2701:PT5:H19	2.41	0.56
1:D:2319:GLU:O	1:D:2323:HIS:ND1	2.38	0.56
1:A:969:LEU:HD11	1:A:1067:TYR:HE2	1.70	0.56
1:B:969:LEU:HD11	1:B:1067:TYR:HE2	1.70	0.56
1:C:1209:LEU:O	1:C:1212:ILE:HG22	2.05	0.56
1:D:376:LYS:O	1:D:377:THR:OG1	2.21	0.56
1:D:466:GLN:OE1	1:D:469:ARG:NH2	2.39	0.56
1:A:1455:ARG:NH1	1:A:1465:GLU:OE2	2.39	0.55
1:A:2155:LEU:HD22	1:A:2178:LEU:HD11	1.88	0.55
1:D:2155:LEU:HD22	1:D:2178:LEU:HD11	1.88	0.55
1:A:1209:LEU:O	1:A:1212:ILE:HG22	2.05	0.55
1:B:1962:HIS:CE1	1:B:1964:SER:HG	2.17	0.55
1:C:144:GLU:OE1	1:C:211:ASN:ND2	2.40	0.55
1:A:2242:LEU:HD13	7:A:3009:PT5:H37	1.87	0.55
1:C:389:LEU:HB2	1:C:398:ILE:HD12	1.89	0.55
1:C:1455:ARG:NH1	1:C:1465:GLU:OE2	2.39	0.55
1:C:2155:LEU:HD22	1:C:2178:LEU:HD11	1.88	0.55
1:A:690:GLU:OE1	1:A:690:GLU:N	2.40	0.55
1:C:1406:ILE:HG23	1:C:1409:VAL:H	1.72	0.55
1:B:2155:LEU:HD22	1:B:2178:LEU:HD11	1.88	0.55
1:B:2449:ASP:OD1	1:B:2450:SER:N	2.40	0.55
1:C:370:ASP:OD2	1:C:423:LYS:NZ	2.26	0.55
1:C:466:GLN:OE1	1:C:469:ARG:NH2	2.39	0.55
1:A:1406:ILE:HG23	1:A:1409:VAL:H	1.72	0.55
1:D:1406:ILE:HG23	1:D:1409:VAL:H	1.72	0.55
1:D:2449:ASP:OD1	1:D:2450:SER:N	2.40	0.55
1:B:389:LEU:HB2	1:B:398:ILE:HD12	1.89	0.55
1:B:1187:GLU:N	1:B:1187:GLU:OE1	2.36	0.55
1:C:690:GLU:OE1	1:C:690:GLU:N	2.40	0.55
1:C:969:LEU:HD11	1:C:1067:TYR:HE2	1.70	0.55
1:D:690:GLU:N	1:D:690:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2319:GLU:O	1:A:2323:HIS:ND1	2.38	0.54
1:B:564:GLN:HB3	1:B:574:ILE:HD12	1.89	0.54
1:A:706:LYS:NZ	1:A:714:GLU:OE1	2.30	0.54
1:A:1895:GLN:OE1	1:A:1895:GLN:N	2.41	0.54
1:B:466:GLN:OE1	1:B:469:ARG:NH2	2.39	0.54
1:C:1590:ASN:OD1	1:C:1594:LYS:NZ	2.37	0.54
1:D:1455:ARG:NH1	1:D:1465:GLU:OE2	2.39	0.54
1:A:1173:LYS:NZ	1:A:1177:GLU:OE2	2.40	0.54
1:B:1406:ILE:HG23	1:B:1409:VAL:H	1.72	0.54
1:B:1895:GLN:N	1:B:1895:GLN:OE1	2.41	0.54
1:C:1895:GLN:N	1:C:1895:GLN:OE1	2.41	0.54
1:A:144:GLU:OE1	1:A:211:ASN:ND2	2.40	0.54
1:A:2449:ASP:OD1	1:A:2450:SER:N	2.40	0.54
1:C:1173:LYS:NZ	1:C:1177:GLU:OE2	2.40	0.54
1:A:466:GLN:OE1	1:A:469:ARG:NH2	2.39	0.54
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.89	0.54
1:C:2242:LEU:HD13	7:C:2701:PT5:H37	1.90	0.54
1:D:144:GLU:OE1	1:D:211:ASN:ND2	2.40	0.54
1:D:389:LEU:HB2	1:D:398:ILE:HD12	1.89	0.54
1:B:690:GLU:N	1:B:690:GLU:OE1	2.40	0.54
1:D:564:GLN:HB3	1:D:574:ILE:HD12	1.89	0.54
1:D:2544:GLU:N	1:D:2544:GLU:OE1	2.41	0.54
1:A:2163:GLU:OE1	1:A:2163:GLU:N	2.40	0.54
1:B:2544:GLU:N	1:B:2544:GLU:OE1	2.41	0.54
1:D:1895:GLN:OE1	1:D:1895:GLN:N	2.41	0.54
1:C:1957:THR:OG1	1:C:2007:ARG:NH2	2.41	0.54
1:B:144:GLU:OE1	1:B:211:ASN:ND2	2.40	0.53
1:B:1173:LYS:NZ	1:B:1177:GLU:OE2	2.40	0.53
1:C:2544:GLU:N	1:C:2544:GLU:OE1	2.41	0.53
1:A:389:LEU:HB2	1:A:398:ILE:HD12	1.89	0.53
1:B:669:GLU:OE2	1:B:671:ARG:NH2	2.40	0.53
1:B:1957:THR:OG1	1:B:2007:ARG:NH2	2.41	0.53
1:B:2319:GLU:O	1:B:2323:HIS:ND1	2.38	0.53
1:D:1957:THR:OG1	1:D:2007:ARG:NH2	2.41	0.53
1:C:2449:ASP:OD1	1:C:2450:SER:N	2.40	0.53
1:D:2163:GLU:OE1	1:D:2163:GLU:N	2.40	0.53
1:A:1957:THR:OG1	1:A:2007:ARG:NH2	2.41	0.53
1:C:649:GLN:NE2	1:C:739:MET:O	2.42	0.53
1:C:1128:VAL:O	1:C:1169:TYR:OH	2.27	0.53
1:D:669:GLU:OE2	1:D:671:ARG:NH2	2.41	0.53
1:B:1957:THR:O	1:B:1961:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:GLN:HB3	1:C:574:ILE:HD12	1.89	0.53
1:A:1128:VAL:O	1:A:1169:TYR:OH	2.27	0.53
1:A:2148:THR:OG1	1:A:2151:THR:OG1	2.24	0.53
1:B:649:GLN:NE2	1:B:739:MET:O	2.42	0.53
1:D:1173:LYS:NZ	1:D:1177:GLU:OE2	2.40	0.53
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.41	0.53
1:B:2163:GLU:N	1:B:2163:GLU:OE1	2.40	0.53
1:A:1260:GLU:OE1	1:A:1260:GLU:N	2.41	0.53
1:C:266:ARG:NH2	3:C:2703:I3P:O42	2.42	0.53
1:A:2209:PHE:CE1	7:A:3009:PT5:H19	2.44	0.52
1:D:1128:VAL:O	1:D:1169:TYR:OH	2.27	0.52
1:D:1260:GLU:OE1	1:D:1260:GLU:N	2.41	0.52
1:A:649:GLN:NE2	1:A:739:MET:O	2.42	0.52
1:A:1957:THR:O	1:A:1961:THR:HG22	2.09	0.52
1:A:266:ARG:NH2	3:A:3002:I3P:O42	2.42	0.52
1:B:2212:ALA:O	1:B:2216:ASN:ND2	2.41	0.52
1:D:649:GLN:NE2	1:D:739:MET:O	2.42	0.52
1:C:1968:ASP:OD1	1:C:2019:SER:OG	2.28	0.52
1:D:1957:THR:O	1:D:1961:THR:HG22	2.09	0.52
1:C:669:GLU:OE2	1:C:671:ARG:NH2	2.41	0.52
1:D:266:ARG:NH2	3:D:2703:I3P:O42	2.42	0.52
1:B:1968:ASP:OD1	1:B:2019:SER:OG	2.28	0.52
1:D:2209:PHE:CZ	7:D:2701:PT5:H19	2.45	0.52
1:C:1957:THR:O	1:C:1961:THR:HG22	2.09	0.51
1:C:670:LEU:HD23	1:C:670:LEU:H	1.75	0.51
1:D:2242:LEU:HD13	7:D:2701:PT5:H37	1.91	0.51
1:A:2549:ASP:OD1	1:A:2550:ASN:N	2.43	0.51
1:B:2127:VAL:HG22	1:B:2133:MET:HG2	1.93	0.51
1:C:2212:ALA:O	1:C:2216:ASN:ND2	2.41	0.51
1:B:370:ASP:OD2	1:B:423:LYS:NZ	2.26	0.51
1:A:1681:ASP:OD1	1:A:1682:ARG:N	2.44	0.51
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.28	0.51
1:D:1968:ASP:OD1	1:D:2019:SER:OG	2.28	0.51
1:B:670:LEU:H	1:B:670:LEU:HD23	1.75	0.51
1:B:1128:VAL:O	1:B:1169:TYR:OH	2.27	0.51
1:C:245:HIS:NE2	1:C:427:GLU:OE1	2.42	0.51
1:C:1541:PRO:HD2	1:C:1544:LEU:HD23	1.93	0.51
1:B:1541:PRO:HD2	1:B:1544:LEU:HD23	1.93	0.51
1:C:2127:VAL:HG22	1:C:2133:MET:HG2	1.93	0.51
1:D:670:LEU:HD23	1:D:670:LEU:H	1.76	0.51
1:B:2148:THR:OG1	1:B:2151:THR:OG1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2163:GLU:OE1	1:C:2163:GLU:N	2.40	0.50
1:D:1681:ASP:OD1	1:D:1682:ARG:N	2.44	0.50
1:D:2127:VAL:HG22	1:D:2133:MET:HG2	1.93	0.50
1:D:1962:HIS:ND1	1:D:1964:SER:OG	2.24	0.50
1:B:1260:GLU:OE1	1:B:1260:GLU:N	2.41	0.50
1:D:1541:PRO:HD2	1:D:1544:LEU:HD23	1.93	0.50
1:A:2471:ARG:NH2	1:D:2478:ASP:OD1	2.45	0.50
1:C:2549:ASP:OD1	1:C:2550:ASN:N	2.43	0.50
1:B:245:HIS:NE2	1:B:427:GLU:OE1	2.42	0.50
1:A:504:GLU:OE1	1:A:504:GLU:N	2.44	0.50
1:A:670:LEU:HD23	1:A:670:LEU:H	1.75	0.50
1:C:1260:GLU:OE1	1:C:1260:GLU:N	2.41	0.50
1:A:1541:PRO:HD2	1:A:1544:LEU:HD23	1.93	0.49
1:A:2127:VAL:HG22	1:A:2133:MET:HG2	1.93	0.49
1:B:615:VAL:O	1:B:619:VAL:HG23	2.12	0.49
1:D:2148:THR:OG1	1:D:2151:THR:OG1	2.24	0.49
1:A:2338:GLU:OE1	1:A:2338:GLU:N	2.45	0.49
1:B:539:GLU:OE1	1:B:539:GLU:N	2.44	0.49
1:D:245:HIS:NE2	1:D:427:GLU:OE1	2.42	0.49
1:C:482:PHE:O	1:C:505:ARG:NH1	2.44	0.49
1:C:615:VAL:O	1:C:619:VAL:HG23	2.12	0.49
1:B:266:ARG:NH2	3:B:2703:I3P:O42	2.42	0.49
1:C:539:GLU:OE1	1:C:539:GLU:N	2.44	0.49
1:D:706:LYS:NZ	1:D:714:GLU:OE1	2.30	0.49
1:A:362:ASP:OD1	1:A:363:ILE:N	2.45	0.49
1:A:669:GLU:OE2	1:A:671:ARG:NH2	2.41	0.49
1:D:615:VAL:O	1:D:619:VAL:HG23	2.12	0.49
1:A:539:GLU:N	1:A:539:GLU:OE1	2.44	0.49
1:D:362:ASP:OD1	1:D:363:ILE:N	2.46	0.49
1:D:2016:ILE:HG22	1:D:2020:LEU:HD12	1.95	0.49
1:B:2549:ASP:OD1	1:B:2550:ASN:N	2.43	0.49
1:A:2148:THR:HG1	1:A:2151:THR:HG1	1.57	0.49
1:B:1236:CYS:HB3	1:B:1246:LEU:HD12	1.95	0.49
1:D:2338:GLU:OE1	1:D:2338:GLU:N	2.45	0.49
1:B:504:GLU:OE1	1:B:504:GLU:N	2.44	0.48
1:A:589:ILE:HG22	1:A:589:ILE:O	2.13	0.48
1:B:668:THR:HG22	1:B:694:LEU:CD1	2.43	0.48
1:D:2212:ALA:O	1:D:2216:ASN:ND2	2.41	0.48
1:A:615:VAL:O	1:A:619:VAL:HG23	2.12	0.48
1:A:2513:PHE:CD2	1:D:2506:ILE:HG21	2.48	0.48
1:C:376:LYS:O	1:C:377:THR:OG1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:589:ILE:HG22	1:C:589:ILE:O	2.13	0.48
1:C:2454:ALA:HB1	1:C:2464:THR:HG21	1.95	0.48
1:C:104:ASN:O	1:C:108:ASN:ND2	2.38	0.48
1:C:1236:CYS:HB3	1:C:1246:LEU:HD12	1.95	0.48
1:A:245:HIS:NE2	1:A:427:GLU:OE1	2.42	0.48
1:A:2212:ALA:O	1:A:2216:ASN:ND2	2.41	0.48
1:A:1236:CYS:HB3	1:A:1246:LEU:HD12	1.95	0.48
1:A:2016:ILE:HG22	1:A:2020:LEU:HD12	1.95	0.48
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.47	0.48
1:D:2454:ALA:HB1	1:D:2464:THR:HG21	1.95	0.48
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.47	0.48
1:C:2209:PHE:CZ	7:C:2701:PT5:H19	2.48	0.48
1:D:668:THR:HG22	1:D:694:LEU:CD1	2.43	0.48
1:C:1779:ASP:OD1	1:C:1780:LYS:N	2.47	0.48
1:C:2338:GLU:OE1	1:C:2338:GLU:N	2.45	0.48
1:D:504:GLU:OE1	1:D:504:GLU:N	2.44	0.48
1:A:668:THR:HG22	1:A:694:LEU:CD1	2.43	0.47
1:A:2454:ALA:HB1	1:A:2464:THR:HG21	1.95	0.47
1:D:589:ILE:HG22	1:D:589:ILE:O	2.13	0.47
1:A:148:MET:HE2	1:A:190:ALA:HB1	1.97	0.47
1:B:2016:ILE:HG22	1:B:2020:LEU:HD12	1.95	0.47
1:B:2454:ALA:HB1	1:B:2464:THR:HG21	1.95	0.47
1:C:668:THR:HG22	1:C:694:LEU:CD1	2.43	0.47
1:A:467:ASN:OD1	1:A:470:ARG:NH2	2.47	0.47
1:A:2209:PHE:CZ	7:A:3009:PT5:H19	2.49	0.47
1:C:467:ASN:OD1	1:C:470:ARG:NH2	2.47	0.47
1:D:1779:ASP:OD1	1:D:1780:LYS:N	2.47	0.47
1:D:2255:PHE:C	1:D:2256:THR:HG1	2.12	0.47
1:B:467:ASN:OD1	1:B:470:ARG:NH2	2.47	0.47
1:B:2209:PHE:CE1	7:B:2701:PT5:H19	2.50	0.47
1:D:104:ASN:O	1:D:108:ASN:ND2	2.38	0.47
1:D:148:MET:HE2	1:D:190:ALA:HB1	1.97	0.47
1:D:1403:GLU:OE1	1:D:1403:GLU:N	2.44	0.47
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.47	0.47
1:A:2242:LEU:HD11	6:D:2708:PCW:H19	1.96	0.47
1:B:376:LYS:O	1:B:377:THR:OG1	2.21	0.47
1:C:2478:ASP:OD1	1:D:2471:ARG:NH2	2.47	0.47
1:D:611:THR:OG1	1:D:612:LYS:N	2.48	0.47
1:D:1236:CYS:HB3	1:D:1246:LEU:HD12	1.95	0.47
1:C:1044:MET:SD	1:C:1044:MET:N	2.82	0.47
1:D:2549:ASP:OD1	1:D:2550:ASN:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:MET:HE2	1:B:190:ALA:HB1	1.97	0.47
1:C:611:THR:OG1	1:C:612:LYS:N	2.48	0.47
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.47	0.47
1:C:2016:ILE:HG22	1:C:2020:LEU:HD12	1.95	0.47
1:D:467:ASN:OD1	1:D:470:ARG:NH2	2.47	0.47
1:D:539:GLU:OE1	1:D:539:GLU:N	2.44	0.47
1:A:1209:LEU:O	1:A:1209:LEU:HD23	2.15	0.47
1:B:611:THR:OG1	1:B:612:LYS:N	2.48	0.47
1:B:1024:ASN:OD1	1:B:1025:LEU:N	2.46	0.47
1:A:1614:LEU:HD13	1:A:1614:LEU:O	2.15	0.47
1:C:1209:LEU:O	1:C:1209:LEU:HD23	2.15	0.47
1:A:111:VAL:O	1:A:111:VAL:HG12	2.15	0.47
1:B:589:ILE:O	1:B:589:ILE:HG22	2.13	0.47
1:B:1681:ASP:OD1	1:B:1682:ARG:N	2.44	0.47
1:B:2338:GLU:OE1	1:B:2338:GLU:N	2.45	0.47
1:C:148:MET:HE2	1:C:190:ALA:HB1	1.97	0.47
1:D:1954:GLU:OE1	1:D:1954:GLU:N	2.44	0.47
1:A:871:ILE:HD13	1:A:974:ILE:HG23	1.97	0.46
1:A:1779:ASP:OD1	1:A:1780:LYS:N	2.47	0.46
1:B:233:GLU:OE1	1:B:233:GLU:N	2.48	0.46
1:B:1779:ASP:OD1	1:B:1780:LYS:N	2.47	0.46
1:C:362:ASP:OD1	1:C:363:ILE:N	2.46	0.46
1:C:504:GLU:OE1	1:C:504:GLU:N	2.44	0.46
1:C:706:LYS:NZ	1:C:714:GLU:OE1	2.30	0.46
1:C:1026:ASP:OD1	1:C:1027:ARG:N	2.48	0.46
1:C:1024:ASN:OD1	1:C:1025:LEU:N	2.46	0.46
1:D:871:ILE:HD13	1:D:974:ILE:HG23	1.97	0.46
1:A:233:GLU:N	1:A:233:GLU:OE1	2.49	0.46
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.44	0.46
1:D:1209:LEU:O	1:D:1209:LEU:HD23	2.15	0.46
1:A:698:ASP:OD1	1:A:699:LYS:N	2.47	0.46
6:A:3007:PCW:H19	1:B:2242:LEU:HD11	1.97	0.46
1:B:871:ILE:HD13	1:B:974:ILE:HG23	1.97	0.46
1:A:1026:ASP:OD1	1:A:1027:ARG:N	2.48	0.46
1:B:1209:LEU:O	1:B:1209:LEU:HD23	2.15	0.46
1:B:1332:VAL:HG23	1:B:1333:VAL:HG23	1.98	0.46
1:C:1502:LEU:HD22	1:C:1529:LEU:CD2	2.46	0.46
1:D:1026:ASP:OD1	1:D:1027:ARG:N	2.48	0.46
1:A:1502:LEU:HD22	1:A:1529:LEU:CD2	2.46	0.46
1:B:582:GLN:NE2	1:B:614:GLU:OE2	2.49	0.46
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:ILE:HD13	1:C:974:ILE:HG23	1.97	0.46
1:C:1954:GLU:OE1	1:C:1954:GLU:N	2.44	0.46
1:D:233:GLU:OE1	1:D:233:GLU:N	2.49	0.46
1:D:1332:VAL:HG23	1:D:1333:VAL:HG23	1.98	0.46
1:B:111:VAL:HG12	1:B:111:VAL:O	2.15	0.46
1:B:482:PHE:O	1:B:505:ARG:NH1	2.44	0.46
1:C:849:VAL:O	1:C:849:VAL:HG13	2.16	0.46
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.31	0.46
1:B:1026:ASP:OD1	1:B:1027:ARG:N	2.48	0.46
1:B:1502:LEU:HD22	1:B:1529:LEU:CD2	2.46	0.46
1:C:1614:LEU:HD13	1:C:1614:LEU:O	2.15	0.46
1:C:2178:LEU:HD13	1:C:2569:LEU:HD22	1.98	0.46
1:D:111:VAL:HG12	1:D:111:VAL:O	2.15	0.46
1:D:849:VAL:HG13	1:D:849:VAL:O	2.16	0.46
1:D:1502:LEU:HD22	1:D:1529:LEU:CD2	2.46	0.46
1:A:2204:TRP:HE3	1:A:2207:ILE:HD11	1.81	0.46
1:B:698:ASP:OD1	1:B:699:LYS:N	2.47	0.46
1:C:1403:GLU:OE1	1:C:1403:GLU:N	2.44	0.46
1:D:1614:LEU:HD13	1:D:1614:LEU:O	2.15	0.46
1:A:849:VAL:O	1:A:849:VAL:HG13	2.16	0.46
1:A:1467:TYR:O	1:A:1471:VAL:HG22	2.16	0.46
1:A:1978:ILE:N	1:A:1978:ILE:HD12	2.31	0.46
1:B:1614:LEU:HD13	1:B:1614:LEU:O	2.15	0.46
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.31	0.46
1:D:2204:TRP:HE3	1:D:2207:ILE:HD11	1.81	0.46
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.31	0.45
1:B:1978:ILE:HD12	1:B:1978:ILE:N	2.31	0.45
1:B:2178:LEU:HD13	1:B:2569:LEU:HD22	1.98	0.45
1:C:13:ILE:N	1:C:13:ILE:HD12	2.32	0.45
1:C:111:VAL:HG12	1:C:111:VAL:O	2.15	0.45
1:C:153:ASP:OD2	1:C:156:GLY:N	2.46	0.45
1:A:13:ILE:N	1:A:13:ILE:HD12	2.32	0.45
1:A:104:ASN:O	1:A:108:ASN:ND2	2.38	0.45
1:A:482:PHE:O	1:A:505:ARG:NH1	2.44	0.45
1:A:1332:VAL:HG23	1:A:1333:VAL:HG23	1.98	0.45
1:C:233:GLU:N	1:C:233:GLU:OE1	2.49	0.45
1:B:362:ASP:OD1	1:B:363:ILE:N	2.45	0.45
1:B:2204:TRP:HE3	1:B:2207:ILE:HD11	1.81	0.45
1:C:134:THR:HG22	1:C:160:SER:OG	2.16	0.45
1:C:1332:VAL:HG23	1:C:1333:VAL:HG23	1.98	0.45
1:D:1467:TYR:O	1:D:1471:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:CB	1:A:398:ILE:HD12	2.46	0.45
1:B:134:THR:HG22	1:B:160:SER:OG	2.16	0.45
1:D:13:ILE:N	1:D:13:ILE:HD12	2.32	0.45
1:B:849:VAL:HG13	1:B:849:VAL:O	2.16	0.45
1:D:389:LEU:CB	1:D:398:ILE:HD12	2.46	0.45
1:B:1687:ARG:O	1:B:1691:LEU:HD23	2.17	0.45
1:A:134:THR:HG22	1:A:160:SER:OG	2.16	0.45
1:B:13:ILE:HD12	1:B:13:ILE:N	2.32	0.45
1:C:389:LEU:CB	1:C:398:ILE:HD12	2.46	0.45
1:D:1687:ARG:O	1:D:1691:LEU:HD23	2.17	0.45
1:A:782:LEU:O	1:A:782:LEU:HD23	2.17	0.45
1:C:698:ASP:OD1	1:C:699:LYS:N	2.47	0.45
1:D:1978:ILE:HD12	1:D:1978:ILE:N	2.31	0.45
1:B:782:LEU:HD23	1:B:782:LEU:O	2.17	0.45
1:C:1978:ILE:N	1:C:1978:ILE:HD12	2.31	0.45
1:D:482:PHE:O	1:D:505:ARG:NH1	2.44	0.45
1:D:1024:ASN:OD1	1:D:1025:LEU:N	2.46	0.45
1:B:389:LEU:CB	1:B:398:ILE:HD12	2.46	0.45
1:C:1687:ARG:O	1:C:1691:LEU:HD23	2.17	0.45
1:A:376:LYS:O	1:A:377:THR:OG1	2.21	0.44
1:B:1467:TYR:O	1:B:1471:VAL:HG22	2.16	0.44
1:B:2172:PHE:HZ	1:B:2594:ILE:HG23	1.82	0.44
1:B:2478:ASP:OD1	1:C:2471:ARG:NH2	2.49	0.44
1:C:782:LEU:HD23	1:C:782:LEU:O	2.17	0.44
1:D:782:LEU:O	1:D:782:LEU:HD23	2.17	0.44
1:A:1881:CYS:SG	1:A:1892:LEU:HD12	2.58	0.44
1:A:2178:LEU:HD13	1:A:2569:LEU:HD22	1.98	0.44
1:C:582:GLN:NE2	1:C:614:GLU:OE2	2.49	0.44
1:A:1498:VAL:O	1:A:1502:LEU:HD23	2.18	0.44
1:A:1792:ARG:HH21	1:A:1869:ILE:HD13	1.82	0.44
1:B:1881:CYS:SG	1:B:1892:LEU:HD12	2.58	0.44
1:D:134:THR:HG22	1:D:160:SER:OG	2.16	0.44
1:B:2381:TYR:CE2	1:B:2385:ILE:HD11	2.53	0.44
1:C:1467:TYR:O	1:C:1471:VAL:HG22	2.16	0.44
1:C:1881:CYS:SG	1:C:1892:LEU:HD12	2.58	0.44
1:C:2204:TRP:HE3	1:C:2207:ILE:HD11	1.81	0.44
1:D:582:GLN:NE2	1:D:614:GLU:OE2	2.49	0.44
1:A:582:GLN:NE2	1:A:614:GLU:OE2	2.49	0.44
1:D:1934:VAL:HG23	1:D:1992:LEU:HD11	1.99	0.44
1:D:2178:LEU:HD13	1:D:2569:LEU:HD22	1.98	0.44
1:D:2381:TYR:CE2	1:D:2385:ILE:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1934:VAL:HG23	1:A:1992:LEU:HD11	1.99	0.44
1:A:1954:GLU:OE1	1:A:1954:GLU:N	2.44	0.44
1:A:2172:PHE:HZ	1:A:2594:ILE:HG23	1.82	0.44
1:B:871:ILE:HD11	1:B:884:LEU:CD2	2.48	0.44
1:B:1934:VAL:HG23	1:B:1992:LEU:HD11	1.99	0.44
1:C:1934:VAL:HG23	1:C:1992:LEU:HD11	1.99	0.44
1:D:871:ILE:HD11	1:D:884:LEU:CD2	2.48	0.44
1:A:1687:ARG:O	1:A:1691:LEU:HD23	2.17	0.44
1:C:871:ILE:HD11	1:C:884:LEU:CD2	2.48	0.44
1:C:2381:TYR:CE2	1:C:2385:ILE:HD11	2.53	0.44
1:A:2381:TYR:CE2	1:A:2385:ILE:HD11	2.53	0.44
1:C:1792:ARG:HH21	1:C:1869:ILE:HD13	1.82	0.44
1:D:2546:ASP:OD1	1:D:2547:LYS:N	2.51	0.44
1:C:1055:PHE:CE2	1:C:1059:LEU:HD11	2.53	0.44
1:D:1498:VAL:O	1:D:1502:LEU:HD23	2.18	0.44
1:B:104:ASN:O	1:B:108:ASN:ND2	2.38	0.43
1:B:288:VAL:C	1:B:289:HIS:HD1	2.27	0.43
1:B:1055:PHE:CE2	1:B:1059:LEU:HD11	2.53	0.43
1:B:2054:TYR:CE2	1:B:2058:LEU:HD11	2.54	0.43
1:C:2172:PHE:HZ	1:C:2594:ILE:HG23	1.82	0.43
1:A:288:VAL:C	1:A:289:HIS:HD1	2.27	0.43
1:A:2546:ASP:OD1	1:A:2547:LYS:N	2.51	0.43
1:C:2546:ASP:OD1	1:C:2547:LYS:N	2.51	0.43
1:D:1055:PHE:CE2	1:D:1059:LEU:HD11	2.53	0.43
1:A:2183:GLU:OE2	1:A:2186:ARG:NH2	2.50	0.43
1:D:2054:TYR:CE2	1:D:2058:LEU:HD11	2.54	0.43
1:D:2172:PHE:HZ	1:D:2594:ILE:HG23	1.82	0.43
1:D:1792:ARG:HH21	1:D:1869:ILE:HD13	1.82	0.43
1:D:1881:CYS:SG	1:D:1892:LEU:HD12	2.58	0.43
1:A:1055:PHE:CE2	1:A:1059:LEU:HD11	2.53	0.43
1:C:288:VAL:C	1:C:289:HIS:HD1	2.27	0.43
1:C:1498:VAL:O	1:C:1502:LEU:HD23	2.18	0.43
1:C:2457:THR:O	1:C:2461:CYS:SG	2.77	0.43
1:D:153:ASP:OD2	1:D:156:GLY:N	2.46	0.43
1:D:2457:THR:O	1:D:2461:CYS:SG	2.77	0.43
1:B:2546:ASP:OD1	1:B:2547:LYS:N	2.51	0.43
1:C:871:ILE:HD11	1:C:884:LEU:HD23	2.01	0.43
1:A:871:ILE:HD11	1:A:884:LEU:CD2	2.48	0.43
1:B:1792:ARG:HH21	1:B:1869:ILE:HD13	1.82	0.43
1:D:288:VAL:C	1:D:289:HIS:HD1	2.27	0.43
1:D:698:ASP:OD1	1:D:699:LYS:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2159:THR:HG21	1:D:2167:LYS:HB3	2.01	0.43
1:A:1962:HIS:CE1	1:A:1964:SER:HG	2.24	0.43
1:A:2151:THR:OG1	1:A:2181:GLU:OE2	2.37	0.43
1:B:16:LEU:HD12	1:B:16:LEU:N	2.34	0.43
1:C:2054:TYR:CE2	1:C:2058:LEU:HD11	2.54	0.43
1:A:1200:MET:HE2	1:A:1200:MET:HA	2.01	0.43
1:A:1987:ASP:OD1	1:A:1988:LEU:N	2.52	0.43
1:A:2054:TYR:CE2	1:A:2058:LEU:HD11	2.54	0.43
1:B:1200:MET:HA	1:B:1200:MET:HE2	2.01	0.43
1:B:1498:VAL:O	1:B:1502:LEU:HD23	2.18	0.43
1:C:16:LEU:N	1:C:16:LEU:HD12	2.34	0.43
1:D:871:ILE:HD11	1:D:884:LEU:HD23	2.01	0.43
1:B:2159:THR:HG21	1:B:2167:LYS:HB3	2.01	0.42
1:B:2457:THR:O	1:B:2461:CYS:SG	2.77	0.42
1:C:2155:LEU:CD2	1:C:2178:LEU:HD11	2.49	0.42
1:C:2159:THR:HG21	1:C:2167:LYS:HB3	2.01	0.42
1:D:1172:VAL:O	1:D:1176:LEU:HD23	2.19	0.42
1:A:417:LEU:N	1:A:417:LEU:HD12	2.34	0.42
1:A:1172:VAL:O	1:A:1176:LEU:HD23	2.20	0.42
1:B:871:ILE:HD11	1:B:884:LEU:HD23	2.01	0.42
1:C:417:LEU:HD12	1:C:417:LEU:N	2.34	0.42
1:D:1987:ASP:OD1	1:D:1988:LEU:N	2.52	0.42
1:A:2457:THR:O	1:A:2461:CYS:SG	2.77	0.42
1:B:1172:VAL:O	1:B:1176:LEU:HD23	2.19	0.42
1:B:2151:THR:OG1	1:B:2181:GLU:OE2	2.37	0.42
1:D:1785:PHE:O	1:D:1788:VAL:HG12	2.20	0.42
1:A:1785:PHE:O	1:A:1788:VAL:HG12	2.20	0.42
1:A:2159:THR:HG21	1:A:2167:LYS:HB3	2.01	0.42
1:C:619:VAL:HG21	1:C:655:CYS:SG	2.60	0.42
1:D:2155:LEU:CD2	1:D:2178:LEU:HD11	2.49	0.42
1:D:2608:MET:HA	1:D:2611:VAL:HG12	2.01	0.42
1:A:871:ILE:HD11	1:A:884:LEU:HD23	2.01	0.42
1:B:1650:HIS:ND1	1:B:1654:LEU:HD23	2.35	0.42
1:C:764:MET:HE3	1:C:778:CYS:SG	2.60	0.42
1:C:1172:VAL:O	1:C:1176:LEU:HD23	2.20	0.42
1:C:1987:ASP:OD1	1:C:1988:LEU:N	2.52	0.42
1:D:16:LEU:HD12	1:D:16:LEU:N	2.34	0.42
1:D:1200:MET:HA	1:D:1200:MET:HE2	2.01	0.42
1:B:417:LEU:N	1:B:417:LEU:HD12	2.34	0.42
1:B:764:MET:HE3	1:B:778:CYS:SG	2.60	0.42
1:A:16:LEU:N	1:A:16:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:OD2	1:B:156:GLY:N	2.46	0.42
1:D:417:LEU:N	1:D:417:LEU:HD12	2.34	0.42
1:A:611:THR:OG1	1:A:612:LYS:N	2.48	0.42
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.52	0.42
1:C:1200:MET:HE2	1:C:1200:MET:HA	2.01	0.42
1:D:547:ALA:N	1:D:548:PRO:HD2	2.35	0.42
1:D:619:VAL:HG21	1:D:655:CYS:SG	2.60	0.42
1:A:1864:GLY:O	1:A:1868:LEU:HD13	2.20	0.42
1:C:2506:ILE:HG21	1:D:2513:PHE:CD2	2.54	0.42
1:D:2151:THR:OG1	1:D:2181:GLU:OE2	2.37	0.42
1:A:619:VAL:HG21	1:A:655:CYS:SG	2.60	0.41
1:A:812:ILE:HD12	1:A:812:ILE:N	2.35	0.41
1:B:1785:PHE:O	1:B:1788:VAL:HG12	2.20	0.41
1:B:2155:LEU:CD2	1:B:2178:LEU:HD11	2.49	0.41
1:B:2183:GLU:OE2	1:B:2186:ARG:NH2	2.50	0.41
1:C:1785:PHE:O	1:C:1788:VAL:HG12	2.20	0.41
1:D:1864:GLY:O	1:D:1868:LEU:HD13	2.20	0.41
1:A:740:CYS:SG	1:A:751:ILE:HD12	2.60	0.41
1:B:812:ILE:N	1:B:812:ILE:HD12	2.35	0.41
1:C:1650:HIS:ND1	1:C:1654:LEU:HD23	2.35	0.41
1:C:2608:MET:HA	1:C:2611:VAL:HG12	2.01	0.41
1:D:19:GLU:CD	1:D:182:LYS:HZ1	2.28	0.41
1:A:1650:HIS:ND1	1:A:1654:LEU:HD23	2.35	0.41
1:B:1864:GLY:O	1:B:1868:LEU:HD13	2.20	0.41
1:B:2562:GLU:OE2	1:B:2609:SER:OG	2.39	0.41
1:C:547:ALA:N	1:C:548:PRO:HD2	2.35	0.41
1:C:2151:THR:OG1	1:C:2181:GLU:OE2	2.37	0.41
1:B:547:ALA:N	1:B:548:PRO:HD2	2.35	0.41
1:B:611:THR:O	1:B:615:VAL:HG23	2.21	0.41
1:B:619:VAL:HG21	1:B:655:CYS:SG	2.60	0.41
1:C:1864:GLY:O	1:C:1868:LEU:HD13	2.20	0.41
1:D:764:MET:HE3	1:D:778:CYS:SG	2.60	0.41
1:D:1650:HIS:ND1	1:D:1654:LEU:HD23	2.35	0.41
1:A:2608:MET:HA	1:A:2611:VAL:HG12	2.01	0.41
1:B:2608:MET:HA	1:B:2611:VAL:HG12	2.01	0.41
1:D:740:CYS:SG	1:D:751:ILE:HD12	2.60	0.41
1:A:1024:ASN:OD1	1:A:1025:LEU:N	2.46	0.41
1:C:812:ILE:HD12	1:C:812:ILE:N	2.35	0.41
1:A:547:ALA:N	1:A:548:PRO:HD2	2.35	0.41
1:A:2155:LEU:CD2	1:A:2178:LEU:HD11	2.49	0.41
1:B:2506:ILE:HG21	1:C:2513:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:740:CYS:SG	1:C:751:ILE:HD12	2.60	0.41
1:A:611:THR:O	1:A:615:VAL:HG23	2.21	0.41
1:A:764:MET:HE3	1:A:778:CYS:SG	2.60	0.41
1:B:740:CYS:SG	1:B:751:ILE:HD12	2.60	0.41
1:A:1764:GLY:O	1:A:1883:ASN:ND2	2.54	0.41
1:A:1785:PHE:CE2	1:A:1789:LEU:HD11	2.56	0.41
1:A:2237:PRO:O	1:A:2240:SER:OG	2.30	0.41
1:B:706:LYS:NZ	1:B:714:GLU:OE1	2.30	0.41
1:B:1764:GLY:O	1:B:1883:ASN:ND2	2.54	0.41
1:B:1954:GLU:OE1	1:B:1954:GLU:N	2.44	0.41
1:C:611:THR:O	1:C:615:VAL:HG23	2.21	0.41
1:C:2556:GLU:OE1	1:C:2556:GLU:N	2.48	0.41
1:D:1099:ILE:HD11	1:D:1591:ILE:HG21	2.03	0.41
1:A:1755:GLY:O	1:A:1759:HIS:ND1	2.54	0.41
1:A:2016:ILE:CG2	1:A:2020:LEU:HD12	2.51	0.41
1:D:812:ILE:N	1:D:812:ILE:HD12	2.35	0.41
1:D:1764:GLY:O	1:D:1883:ASN:ND2	2.54	0.41
1:D:1878:GLN:OE1	1:D:1939:GLN:NE2	2.51	0.41
1:C:1764:GLY:O	1:C:1883:ASN:ND2	2.54	0.40
1:B:2209:PHE:CZ	7:B:2701:PT5:H19	2.56	0.40
1:C:2016:ILE:CG2	1:C:2020:LEU:HD12	2.51	0.40
1:D:1755:GLY:O	1:D:1759:HIS:ND1	2.54	0.40
1:A:1099:ILE:HD11	1:A:1591:ILE:HG21	2.03	0.40
1:B:2236:SER:O	1:B:2239:ILE:HG22	2.22	0.40
1:A:762:LEU:O	1:A:762:LEU:HD23	2.21	0.40
1:C:1110:ILE:HG12	1:C:1182:MET:HE2	2.04	0.40
1:C:762:LEU:HD23	1:C:762:LEU:O	2.21	0.40
1:D:611:THR:O	1:D:615:VAL:HG23	2.21	0.40
1:D:2236:SER:O	1:D:2239:ILE:HG22	2.22	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	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
1	B	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
1	C	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
1	D	2242/2671 (84%)	2198 (98%)	44 (2%)	0	100	100
All	All	8968/10684 (84%)	8792 (98%)	176 (2%)	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	2023/2385 (85%)	2014 (100%)	9 (0%)	84	86
1	B	2023/2385 (85%)	2014 (100%)	9 (0%)	84	86
1	C	2023/2385 (85%)	2014 (100%)	9 (0%)	84	86
1	D	2023/2385 (85%)	2014 (100%)	9 (0%)	84	86
All	All	8092/9540 (85%)	8056 (100%)	36 (0%)	81	86

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	LEU
1	A	742	ASP
1	A	1044	MET
1	A	1123	LYS
1	A	1200	MET
1	A	1464	LEU
1	A	1689	MET
1	A	2070	LEU
1	A	2292	ASN
1	B	459	LEU
1	B	742	ASP
1	B	1044	MET
1	B	1123	LYS

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Mol	Chain	Res	Type
1	B	1200	MET
1	B	1464	LEU
1	B	1689	MET
1	B	2070	LEU
1	B	2292	ASN
1	C	459	LEU
1	C	742	ASP
1	C	1044	MET
1	C	1123	LYS
1	C	1200	MET
1	C	1464	LEU
1	C	1689	MET
1	C	2070	LEU
1	C	2292	ASN
1	D	459	LEU
1	D	742	ASP
1	D	1044	MET
1	D	1123	LYS
1	D	1200	MET
1	D	1464	LEU
1	D	1689	MET
1	D	2070	LEU
1	D	2292	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	301	ASN
1	A	399	GLN
1	A	551	HIS
1	A	582	GLN
1	A	754	GLN
1	A	1270	ASN
1	A	1271	ASN
1	A	1293	HIS
1	A	1359	HIS
1	A	1773	HIS
1	A	1797	GLN
1	A	1884	HIS
1	A	2063	HIS
1	A	2161	GLN

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Mol	Chain	Res	Type
1	A	2550	ASN
1	B	68	GLN
1	B	103	GLN
1	B	399	GLN
1	B	551	HIS
1	B	582	GLN
1	B	704	HIS
1	B	710	GLN
1	B	754	GLN
1	B	1106	ASN
1	B	1193	GLN
1	B	1270	ASN
1	B	1271	ASN
1	B	1293	HIS
1	B	1359	HIS
1	B	1435	ASN
1	B	1773	HIS
1	B	1797	GLN
1	B	2063	HIS
1	B	2161	GLN
1	B	2550	ASN
1	C	68	GLN
1	C	301	ASN
1	C	399	GLN
1	C	551	HIS
1	C	582	GLN
1	C	600	HIS
1	C	710	GLN
1	C	754	GLN
1	C	1106	ASN
1	C	1193	GLN
1	C	1270	ASN
1	C	1271	ASN
1	C	1293	HIS
1	C	1359	HIS
1	C	1435	ASN
1	C	1611	GLN
1	C	1773	HIS
1	C	1797	GLN
1	C	1884	HIS
1	C	2063	HIS
1	C	2161	GLN

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Mol	Chain	Res	Type
1	C	2550	ASN
1	D	68	GLN
1	D	399	GLN
1	D	551	HIS
1	D	562	HIS
1	D	582	GLN
1	D	710	GLN
1	D	754	GLN
1	D	785	HIS
1	D	1106	ASN
1	D	1193	GLN
1	D	1270	ASN
1	D	1271	ASN
1	D	1293	HIS
1	D	1359	HIS
1	D	1435	ASN
1	D	1518	HIS
1	D	1611	GLN
1	D	1773	HIS
1	D	1797	GLN
1	D	1884	HIS
1	D	2063	HIS
1	D	2161	GLN
1	D	2510	ASN
1	D	2550	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	ATP	D	2705	-	32,33,33	0.26	0	48,52,52	0.68	0
6	PCW	D	2706	-	42,42,53	0.54	0	48,50,61	0.50	0
3	I3P	D	2703	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
6	PCW	C	2708	-	46,46,53	0.52	0	52,54,61	0.46	0
6	PCW	D	2707	-	44,44,53	0.53	0	50,52,61	0.50	0
7	PT5	C	2701	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
6	PCW	D	2709	-	40,40,53	0.55	0	46,48,61	0.49	0
6	PCW	B	2708	-	46,46,53	0.52	0	52,54,61	0.46	0
3	I3P	C	2703	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
6	PCW	A	3006	-	44,44,53	0.53	0	50,52,61	0.50	0
7	PT5	A	3009	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
6	PCW	C	2707	-	44,44,53	0.53	0	50,52,61	0.50	0
6	PCW	B	2707	-	44,44,53	0.53	0	50,52,61	0.50	0
6	PCW	C	2706	-	42,42,53	0.54	0	48,50,61	0.50	0
3	I3P	B	2703	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
5	ATP	C	2705	-	32,33,33	0.26	0	48,52,52	0.68	0
7	PT5	B	2701	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
6	PCW	A	3007	-	46,46,53	0.52	0	52,54,61	0.46	0
5	ATP	B	2705	-	32,33,33	0.26	0	48,52,52	0.68	0
3	I3P	A	3002	-	24,24,24	2.18	3 (12%)	39,39,39	0.89	0
6	PCW	A	3008	-	40,40,53	0.55	0	46,48,61	0.49	0
6	PCW	C	2709	-	40,40,53	0.55	0	46,48,61	0.49	0
5	ATP	A	3004	-	32,33,33	0.26	0	48,52,52	0.68	0
6	PCW	B	2709	-	40,40,53	0.55	0	46,48,61	0.49	0
6	PCW	B	2706	-	42,42,53	0.54	0	48,50,61	0.50	0
7	PT5	D	2701	-	64,64,69	1.51	7 (10%)	79,82,87	1.13	6 (7%)
6	PCW	A	3005	-	42,42,53	0.54	0	48,50,61	0.50	0
6	PCW	D	2708	-	46,46,53	0.52	0	52,54,61	0.46	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	ATP	D	2705	-	-	2/22/38/38	0/3/3/3
6	PCW	D	2706	-	-	11/46/46/57	-
3	I3P	D	2703	-	-	2/15/39/39	0/1/1/1
6	PCW	C	2708	-	-	11/50/50/57	-
6	PCW	D	2707	-	-	8/48/48/57	-
7	PT5	C	2701	-	-	23/61/85/90	0/1/1/1
6	PCW	D	2709	-	-	14/44/44/57	-
6	PCW	B	2708	-	-	11/50/50/57	-
3	I3P	C	2703	-	-	2/15/39/39	0/1/1/1
6	PCW	A	3006	-	-	8/48/48/57	-
7	PT5	A	3009	-	-	23/61/85/90	0/1/1/1
6	PCW	C	2707	-	-	8/48/48/57	-
6	PCW	B	2707	-	-	8/48/48/57	-
6	PCW	C	2706	-	-	11/46/46/57	-
3	I3P	B	2703	-	-	2/15/39/39	0/1/1/1
5	ATP	C	2705	-	-	2/22/38/38	0/3/3/3
7	PT5	B	2701	-	-	23/61/85/90	0/1/1/1
6	PCW	A	3007	-	-	11/50/50/57	-
5	ATP	B	2705	-	-	2/22/38/38	0/3/3/3
3	I3P	A	3002	-	-	2/15/39/39	0/1/1/1
6	PCW	A	3008	-	-	14/44/44/57	-
6	PCW	C	2709	-	-	14/44/44/57	-
5	ATP	A	3004	-	-	2/22/38/38	0/3/3/3
6	PCW	B	2709	-	-	14/44/44/57	-
6	PCW	B	2706	-	-	11/46/46/57	-
7	PT5	D	2701	-	-	23/61/85/90	0/1/1/1
6	PCW	A	3005	-	-	11/46/46/57	-
6	PCW	D	2708	-	-	12/50/50/57	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2703	I3P	P4-O4	6.06	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	2703	I3P	P4-O4	6.06	1.70	1.59
3	D	2703	I3P	P4-O4	6.05	1.70	1.59
3	A	3002	I3P	P5-O5	5.93	1.69	1.59
3	C	2703	I3P	P5-O5	5.93	1.69	1.59
3	D	2703	I3P	P5-O5	5.93	1.69	1.59
3	B	2703	I3P	P5-O5	5.92	1.69	1.59
3	D	2703	I3P	P1-O1	5.68	1.69	1.59
3	A	3002	I3P	P1-O1	5.68	1.69	1.59
3	C	2703	I3P	P1-O1	5.68	1.69	1.59
3	B	2703	I3P	P1-O1	5.68	1.69	1.59
7	C	2701	PT5	P5-O5	4.81	1.68	1.59
7	A	3009	PT5	P5-O5	4.81	1.68	1.59
7	B	2701	PT5	P5-O5	4.81	1.68	1.59
7	D	2701	PT5	P5-O5	4.81	1.68	1.59
7	D	2701	PT5	O18-C11	3.93	1.44	1.33
7	B	2701	PT5	O18-C11	3.93	1.44	1.33
7	A	3009	PT5	O18-C11	3.93	1.44	1.33
7	C	2701	PT5	O18-C11	3.92	1.44	1.33
7	A	3009	PT5	O16-C10	3.84	1.45	1.34
7	B	2701	PT5	O16-C10	3.84	1.45	1.34
7	D	2701	PT5	O16-C10	3.84	1.45	1.34
7	C	2701	PT5	O16-C10	3.84	1.45	1.34
7	D	2701	PT5	P4-O4	3.63	1.65	1.59
7	A	3009	PT5	P4-O4	3.63	1.65	1.59
7	C	2701	PT5	P4-O4	3.63	1.65	1.59
7	B	2701	PT5	P4-O4	3.63	1.65	1.59
7	D	2701	PT5	C12-C10	3.02	1.59	1.50
7	C	2701	PT5	C12-C10	3.02	1.59	1.50
7	B	2701	PT5	C12-C10	3.02	1.59	1.50
7	A	3009	PT5	C12-C10	3.01	1.59	1.50
7	D	2701	PT5	O16-C8	-2.60	1.40	1.46
7	C	2701	PT5	O16-C8	-2.60	1.40	1.46
7	A	3009	PT5	O16-C8	-2.60	1.40	1.46
7	B	2701	PT5	O16-C8	-2.60	1.40	1.46
7	C	2701	PT5	C31-C11	2.28	1.57	1.50
7	B	2701	PT5	C31-C11	2.28	1.57	1.50
7	A	3009	PT5	C31-C11	2.28	1.57	1.50
7	D	2701	PT5	C31-C11	2.28	1.57	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3009	PT5	O16-C10-C12	3.76	119.61	111.48
7	D	2701	PT5	O16-C10-C12	3.76	119.61	111.48
7	B	2701	PT5	O16-C10-C12	3.76	119.61	111.48
7	C	2701	PT5	O16-C10-C12	3.76	119.61	111.48
7	B	2701	PT5	C17-C16-C15	-3.74	92.03	123.57
7	A	3009	PT5	C17-C16-C15	-3.74	92.03	123.57
7	D	2701	PT5	C17-C16-C15	-3.74	92.03	123.57
7	C	2701	PT5	C17-C16-C15	-3.74	92.04	123.57
7	C	2701	PT5	C23-C22-C21	-3.43	94.62	123.57
7	B	2701	PT5	C23-C22-C21	-3.43	94.62	123.57
7	A	3009	PT5	C23-C22-C21	-3.43	94.62	123.57
7	D	2701	PT5	C23-C22-C21	-3.43	94.62	123.57
7	B	2701	PT5	C20-C19-C18	3.29	151.38	123.57
7	D	2701	PT5	C20-C19-C18	3.29	151.38	123.57
7	A	3009	PT5	C20-C19-C18	3.29	151.38	123.57
7	C	2701	PT5	C20-C19-C18	3.29	151.37	123.57
7	D	2701	PT5	O18-C11-C31	2.53	119.54	111.83
7	C	2701	PT5	O18-C11-C31	2.53	119.54	111.83
7	A	3009	PT5	O18-C11-C31	2.53	119.54	111.83
7	B	2701	PT5	O18-C11-C31	2.53	119.54	111.83
7	C	2701	PT5	C12-C13-C14	-2.05	108.87	113.35
7	B	2701	PT5	C12-C13-C14	-2.05	108.88	113.35
7	A	3009	PT5	C12-C13-C14	-2.05	108.88	113.35
7	D	2701	PT5	C12-C13-C14	-2.05	108.88	113.35

There are no chirality outliers.

All (285) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	PB-O3B-PG-O3G
5	B	2705	ATP	PB-O3B-PG-O3G
5	C	2705	ATP	PB-O3B-PG-O3G
5	D	2705	ATP	PB-O3B-PG-O3G
6	A	3005	PCW	C1-O3P-P-O2P
6	A	3005	PCW	C4-O4P-P-O1P
6	A	3005	PCW	C4-O4P-P-O3P
6	A	3006	PCW	C1-O3P-P-O1P
6	A	3006	PCW	C1-O3P-P-O2P
6	A	3006	PCW	C1-O3P-P-O4P
6	A	3007	PCW	C1-O3P-P-O2P
6	A	3007	PCW	C1-O3P-P-O4P
6	A	3008	PCW	C2-C1-O3P-P
6	A	3008	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
6	A	3008	PCW	C1-O3P-P-O4P
6	B	2706	PCW	C1-O3P-P-O2P
6	B	2706	PCW	C4-O4P-P-O1P
6	B	2706	PCW	C4-O4P-P-O3P
6	B	2707	PCW	C1-O3P-P-O1P
6	B	2707	PCW	C1-O3P-P-O2P
6	B	2707	PCW	C1-O3P-P-O4P
6	B	2708	PCW	C1-O3P-P-O2P
6	B	2708	PCW	C1-O3P-P-O4P
6	B	2709	PCW	C2-C1-O3P-P
6	B	2709	PCW	C1-O3P-P-O1P
6	B	2709	PCW	C1-O3P-P-O4P
6	C	2706	PCW	C1-O3P-P-O2P
6	C	2706	PCW	C4-O4P-P-O1P
6	C	2706	PCW	C4-O4P-P-O3P
6	C	2707	PCW	C1-O3P-P-O1P
6	C	2707	PCW	C1-O3P-P-O2P
6	C	2707	PCW	C1-O3P-P-O4P
6	C	2708	PCW	C1-O3P-P-O2P
6	C	2708	PCW	C1-O3P-P-O4P
6	C	2709	PCW	C2-C1-O3P-P
6	C	2709	PCW	C1-O3P-P-O1P
6	C	2709	PCW	C1-O3P-P-O4P
6	D	2706	PCW	C1-O3P-P-O2P
6	D	2706	PCW	C4-O4P-P-O1P
6	D	2706	PCW	C4-O4P-P-O3P
6	D	2707	PCW	C1-O3P-P-O1P
6	D	2707	PCW	C1-O3P-P-O2P
6	D	2707	PCW	C1-O3P-P-O4P
6	D	2708	PCW	C1-O3P-P-O2P
6	D	2708	PCW	C1-O3P-P-O4P
6	D	2709	PCW	C2-C1-O3P-P
6	D	2709	PCW	C1-O3P-P-O1P
6	D	2709	PCW	C1-O3P-P-O4P
7	A	3009	PT5	O16-C8-C9-O18
7	A	3009	PT5	C12-C10-O16-C8
7	A	3009	PT5	C18-C19-C20-C21
7	A	3009	PT5	C22-C23-C24-C25
7	B	2701	PT5	O16-C8-C9-O18
7	B	2701	PT5	C12-C10-O16-C8
7	B	2701	PT5	C18-C19-C20-C21
7	B	2701	PT5	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
7	C	2701	PT5	O16-C8-C9-O18
7	C	2701	PT5	C12-C10-O16-C8
7	C	2701	PT5	C18-C19-C20-C21
7	C	2701	PT5	C22-C23-C24-C25
7	D	2701	PT5	O16-C8-C9-O18
7	D	2701	PT5	C12-C10-O16-C8
7	D	2701	PT5	C18-C19-C20-C21
7	D	2701	PT5	C22-C23-C24-C25
6	A	3007	PCW	C12-C11-O3-C3
6	B	2708	PCW	C12-C11-O3-C3
6	C	2708	PCW	C12-C11-O3-C3
6	D	2708	PCW	C12-C11-O3-C3
6	A	3007	PCW	O11-C11-O3-C3
6	B	2708	PCW	O11-C11-O3-C3
6	C	2708	PCW	O11-C11-O3-C3
6	D	2708	PCW	O11-C11-O3-C3
7	A	3009	PT5	O17-C10-O16-C8
7	B	2701	PT5	O17-C10-O16-C8
7	C	2701	PT5	O17-C10-O16-C8
7	D	2701	PT5	O17-C10-O16-C8
7	A	3009	PT5	C11-C31-C32-C33
7	B	2701	PT5	C11-C31-C32-C33
7	C	2701	PT5	C11-C31-C32-C33
7	D	2701	PT5	C11-C31-C32-C33
6	A	3007	PCW	C34-C35-C36-C37
6	B	2708	PCW	C34-C35-C36-C37
6	C	2708	PCW	C34-C35-C36-C37
6	D	2708	PCW	C34-C35-C36-C37
7	A	3009	PT5	C32-C33-C34-C35
7	B	2701	PT5	C32-C33-C34-C35
7	C	2701	PT5	C32-C33-C34-C35
7	D	2701	PT5	C32-C33-C34-C35
7	C	2701	PT5	C38-C39-C40-C41
7	A	3009	PT5	C38-C39-C40-C41
7	B	2701	PT5	C38-C39-C40-C41
7	D	2701	PT5	C38-C39-C40-C41
6	A	3007	PCW	C14-C15-C16-C17
6	B	2708	PCW	C14-C15-C16-C17
6	C	2708	PCW	C14-C15-C16-C17
6	D	2708	PCW	C14-C15-C16-C17
6	A	3005	PCW	C32-C31-O2-C2
6	B	2706	PCW	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
6	C	2706	PCW	C32-C31-O2-C2
6	D	2706	PCW	C32-C31-O2-C2
6	A	3005	PCW	O31-C31-O2-C2
6	B	2706	PCW	O31-C31-O2-C2
6	C	2706	PCW	O31-C31-O2-C2
6	D	2706	PCW	O31-C31-O2-C2
6	A	3008	PCW	O3P-C1-C2-C3
6	B	2709	PCW	O3P-C1-C2-C3
6	C	2709	PCW	O3P-C1-C2-C3
6	D	2709	PCW	O3P-C1-C2-C3
7	A	3009	PT5	C36-C37-C38-C39
7	B	2701	PT5	C36-C37-C38-C39
7	C	2701	PT5	C36-C37-C38-C39
7	D	2701	PT5	C36-C37-C38-C39
7	A	3009	PT5	C10-C12-C13-C14
7	B	2701	PT5	C10-C12-C13-C14
7	C	2701	PT5	C10-C12-C13-C14
7	D	2701	PT5	C10-C12-C13-C14
7	A	3009	PT5	C7-C8-C9-O18
7	B	2701	PT5	C7-C8-C9-O18
7	C	2701	PT5	C7-C8-C9-O18
7	D	2701	PT5	C7-C8-C9-O18
7	A	3009	PT5	C31-C11-O18-C9
7	B	2701	PT5	C31-C11-O18-C9
7	C	2701	PT5	C31-C11-O18-C9
7	D	2701	PT5	C31-C11-O18-C9
7	A	3009	PT5	C13-C14-C15-C16
7	B	2701	PT5	C13-C14-C15-C16
7	C	2701	PT5	C13-C14-C15-C16
7	D	2701	PT5	C13-C14-C15-C16
6	A	3006	PCW	O3P-C1-C2-O2
6	A	3008	PCW	O3P-C1-C2-O2
6	B	2707	PCW	O3P-C1-C2-O2
6	B	2709	PCW	O3P-C1-C2-O2
6	C	2707	PCW	O3P-C1-C2-O2
6	C	2709	PCW	O3P-C1-C2-O2
6	D	2707	PCW	O3P-C1-C2-O2
6	D	2709	PCW	O3P-C1-C2-O2
6	A	3007	PCW	C2-C1-O3P-P
6	B	2708	PCW	C2-C1-O3P-P
6	C	2708	PCW	C2-C1-O3P-P
6	D	2708	PCW	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
6	A	3006	PCW	C36-C37-C38-C39
6	B	2707	PCW	C36-C37-C38-C39
6	C	2707	PCW	C36-C37-C38-C39
6	D	2707	PCW	C36-C37-C38-C39
6	A	3006	PCW	O3P-C1-C2-C3
6	B	2707	PCW	O3P-C1-C2-C3
6	C	2707	PCW	O3P-C1-C2-C3
6	D	2707	PCW	O3P-C1-C2-C3
6	A	3005	PCW	C17-C18-C19-C20
6	B	2706	PCW	C17-C18-C19-C20
6	C	2706	PCW	C17-C18-C19-C20
6	D	2706	PCW	C17-C18-C19-C20
6	A	3008	PCW	C32-C31-O2-C2
6	B	2709	PCW	C32-C31-O2-C2
6	C	2709	PCW	C32-C31-O2-C2
6	D	2709	PCW	C32-C31-O2-C2
7	A	3009	PT5	O19-C11-O18-C9
7	B	2701	PT5	O19-C11-O18-C9
7	C	2701	PT5	O19-C11-O18-C9
7	D	2701	PT5	O19-C11-O18-C9
6	C	2706	PCW	C15-C16-C17-C18
6	A	3005	PCW	C15-C16-C17-C18
6	B	2706	PCW	C15-C16-C17-C18
6	D	2706	PCW	C15-C16-C17-C18
6	A	3005	PCW	C22-C23-C24-C25
6	B	2706	PCW	C22-C23-C24-C25
6	C	2706	PCW	C22-C23-C24-C25
6	D	2706	PCW	C22-C23-C24-C25
6	A	3008	PCW	O4P-C4-C5-N
6	B	2709	PCW	O4P-C4-C5-N
6	C	2709	PCW	O4P-C4-C5-N
6	D	2709	PCW	O4P-C4-C5-N
6	A	3008	PCW	O31-C31-O2-C2
6	B	2709	PCW	O31-C31-O2-C2
6	C	2709	PCW	O31-C31-O2-C2
6	D	2709	PCW	O31-C31-O2-C2
6	A	3007	PCW	C13-C14-C15-C16
6	B	2708	PCW	C13-C14-C15-C16
6	C	2708	PCW	C13-C14-C15-C16
6	D	2708	PCW	C13-C14-C15-C16
6	A	3005	PCW	C1-O3P-P-O1P
6	A	3005	PCW	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
6	A	3006	PCW	C4-O4P-P-O3P
6	A	3007	PCW	C1-O3P-P-O1P
6	A	3008	PCW	C1-O3P-P-O2P
6	B	2706	PCW	C1-O3P-P-O1P
6	B	2706	PCW	C1-O3P-P-O4P
6	B	2707	PCW	C4-O4P-P-O3P
6	B	2708	PCW	C1-O3P-P-O1P
6	B	2709	PCW	C1-O3P-P-O2P
6	C	2706	PCW	C1-O3P-P-O1P
6	C	2706	PCW	C1-O3P-P-O4P
6	C	2707	PCW	C4-O4P-P-O3P
6	C	2708	PCW	C1-O3P-P-O1P
6	C	2709	PCW	C1-O3P-P-O2P
6	D	2706	PCW	C1-O3P-P-O1P
6	D	2706	PCW	C1-O3P-P-O4P
6	D	2707	PCW	C4-O4P-P-O3P
6	D	2708	PCW	C1-O3P-P-O1P
6	D	2709	PCW	C1-O3P-P-O2P
7	A	3009	PT5	C8-C7-O13-P1
7	B	2701	PT5	C8-C7-O13-P1
7	C	2701	PT5	C8-C7-O13-P1
7	D	2701	PT5	C8-C7-O13-P1
6	A	3005	PCW	C32-C33-C34-C35
6	B	2706	PCW	C32-C33-C34-C35
6	C	2706	PCW	C32-C33-C34-C35
6	D	2706	PCW	C32-C33-C34-C35
7	A	3009	PT5	O13-C7-C8-C9
7	B	2701	PT5	O13-C7-C8-C9
7	C	2701	PT5	O13-C7-C8-C9
7	D	2701	PT5	O13-C7-C8-C9
7	A	3009	PT5	C40-C41-C42-C43
7	B	2701	PT5	C40-C41-C42-C43
7	C	2701	PT5	C40-C41-C42-C43
7	D	2701	PT5	C40-C41-C42-C43
6	A	3008	PCW	O2-C2-C3-O3
6	B	2709	PCW	O2-C2-C3-O3
6	C	2709	PCW	O2-C2-C3-O3
6	D	2709	PCW	O2-C2-C3-O3
6	A	3006	PCW	C35-C36-C37-C38
6	B	2707	PCW	C35-C36-C37-C38
6	C	2707	PCW	C35-C36-C37-C38
6	D	2707	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
7	A	3009	PT5	C15-C16-C17-C18
7	A	3009	PT5	C16-C17-C18-C19
7	B	2701	PT5	C15-C16-C17-C18
7	B	2701	PT5	C16-C17-C18-C19
7	C	2701	PT5	C15-C16-C17-C18
7	C	2701	PT5	C16-C17-C18-C19
7	D	2701	PT5	C15-C16-C17-C18
7	D	2701	PT5	C16-C17-C18-C19
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	2703	I3P	C5-O5-P5-O51
7	A	3009	PT5	C31-C32-C33-C34
7	B	2701	PT5	C31-C32-C33-C34
7	C	2701	PT5	C31-C32-C33-C34
7	D	2701	PT5	C31-C32-C33-C34
7	A	3009	PT5	O13-C7-C8-O16
7	B	2701	PT5	O13-C7-C8-O16
7	C	2701	PT5	O13-C7-C8-O16
7	D	2701	PT5	O13-C7-C8-O16
7	A	3009	PT5	C24-C25-C26-C27
7	B	2701	PT5	C24-C25-C26-C27
7	C	2701	PT5	C24-C25-C26-C27
7	D	2701	PT5	C24-C25-C26-C27
5	A	3004	ATP	PB-O3B-PG-O1G
5	B	2705	ATP	PB-O3B-PG-O1G
5	C	2705	ATP	PB-O3B-PG-O1G
5	D	2705	ATP	PB-O3B-PG-O1G
6	A	3007	PCW	C17-C18-C19-C20
6	B	2708	PCW	C17-C18-C19-C20
6	C	2708	PCW	C17-C18-C19-C20
6	D	2708	PCW	C17-C18-C19-C20
6	A	3008	PCW	C1-C2-C3-O3
6	B	2709	PCW	C1-C2-C3-O3
6	C	2709	PCW	C1-C2-C3-O3
6	D	2709	PCW	C1-C2-C3-O3
6	A	3008	PCW	C5-C4-O4P-P
6	B	2709	PCW	C5-C4-O4P-P
6	C	2709	PCW	C5-C4-O4P-P
6	D	2709	PCW	C5-C4-O4P-P
6	A	3007	PCW	C20-C21-C22-C23
6	B	2708	PCW	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
6	C	2708	PCW	C20-C21-C22-C23
6	D	2708	PCW	C20-C21-C22-C23
6	A	3008	PCW	C37-C38-C39-C40
6	B	2709	PCW	C37-C38-C39-C40
6	C	2709	PCW	C37-C38-C39-C40
6	D	2709	PCW	C37-C38-C39-C40
7	A	3009	PT5	C1-O1-P1-O11
7	B	2701	PT5	C1-O1-P1-O11
7	C	2701	PT5	C1-O1-P1-O11
7	D	2701	PT5	C1-O1-P1-O11
3	A	3002	I3P	C5-O5-P5-O52
3	B	2703	I3P	C5-O5-P5-O52
3	C	2703	I3P	C5-O5-P5-O52
3	D	2703	I3P	C5-O5-P5-O52
6	A	3008	PCW	C32-C33-C34-C35
6	B	2709	PCW	C32-C33-C34-C35
6	C	2709	PCW	C32-C33-C34-C35
6	D	2709	PCW	C32-C33-C34-C35
6	D	2708	PCW	O2-C2-C3-O3

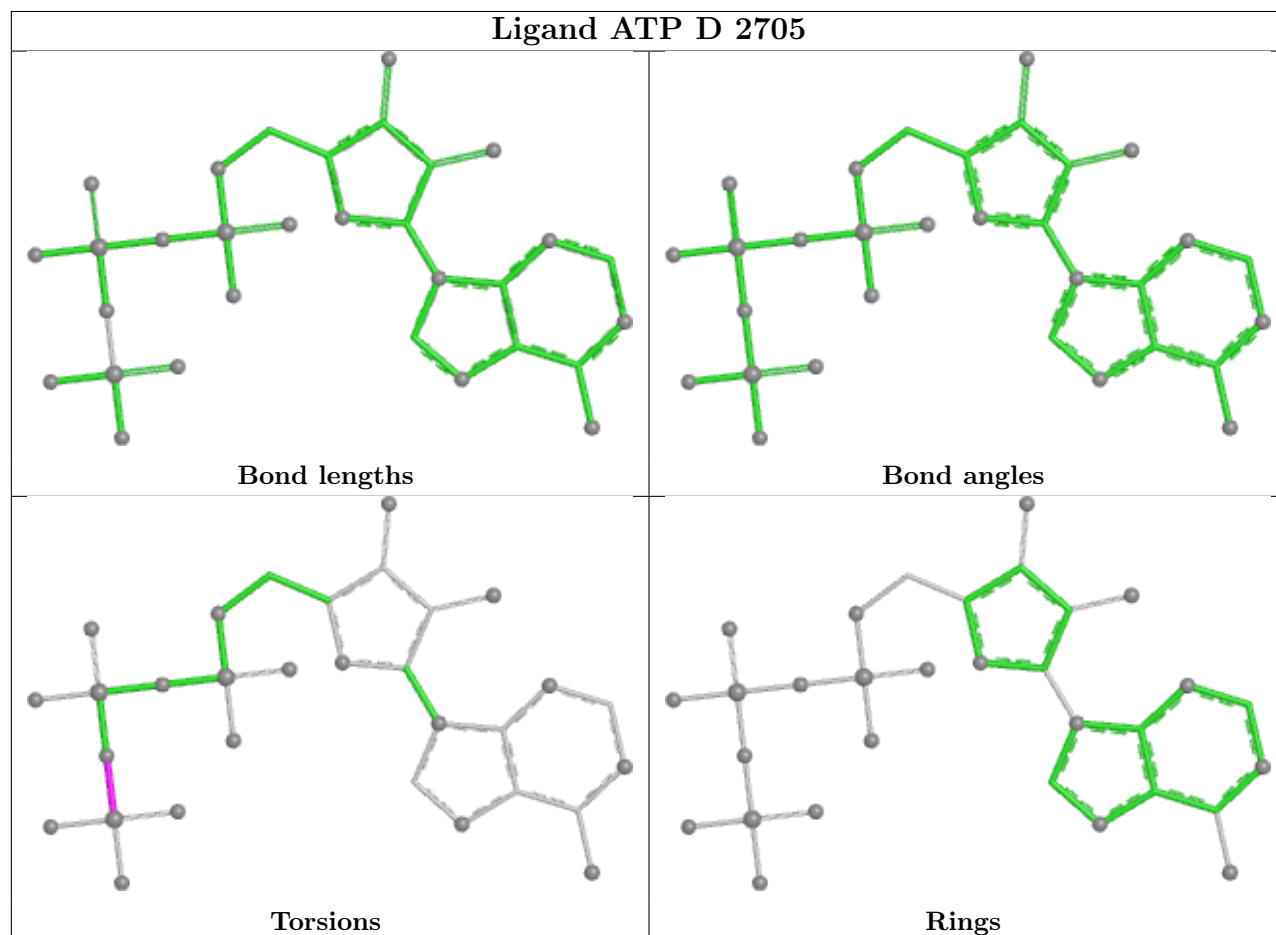
There are no ring outliers.

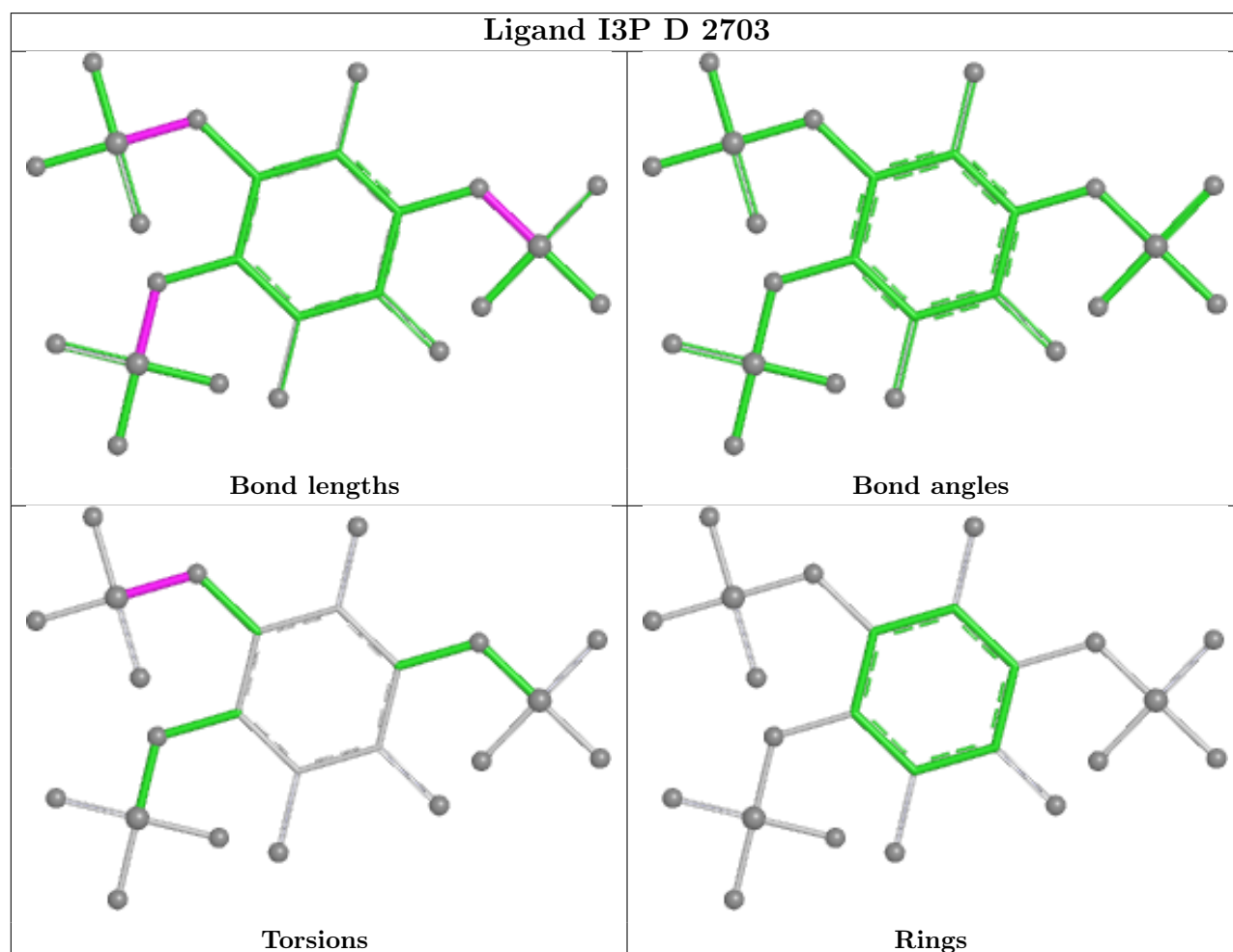
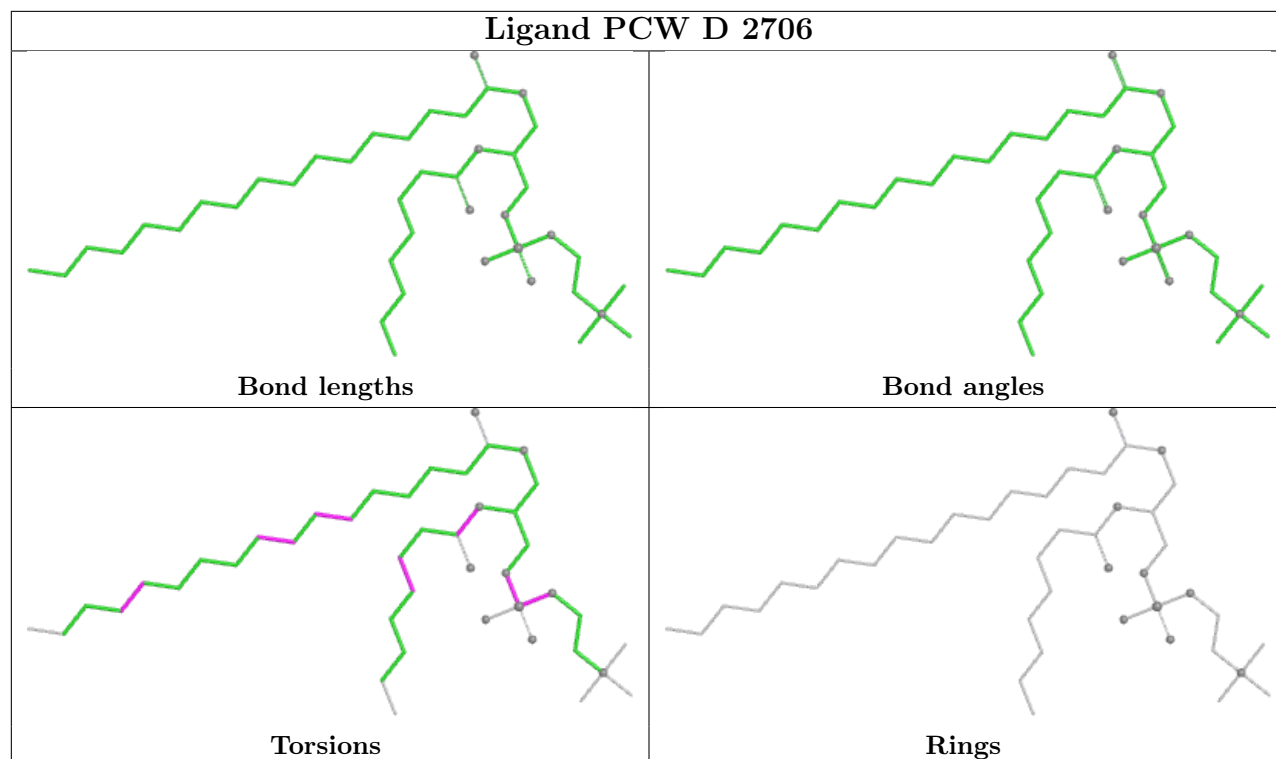
12 monomers are involved in 20 short contacts:

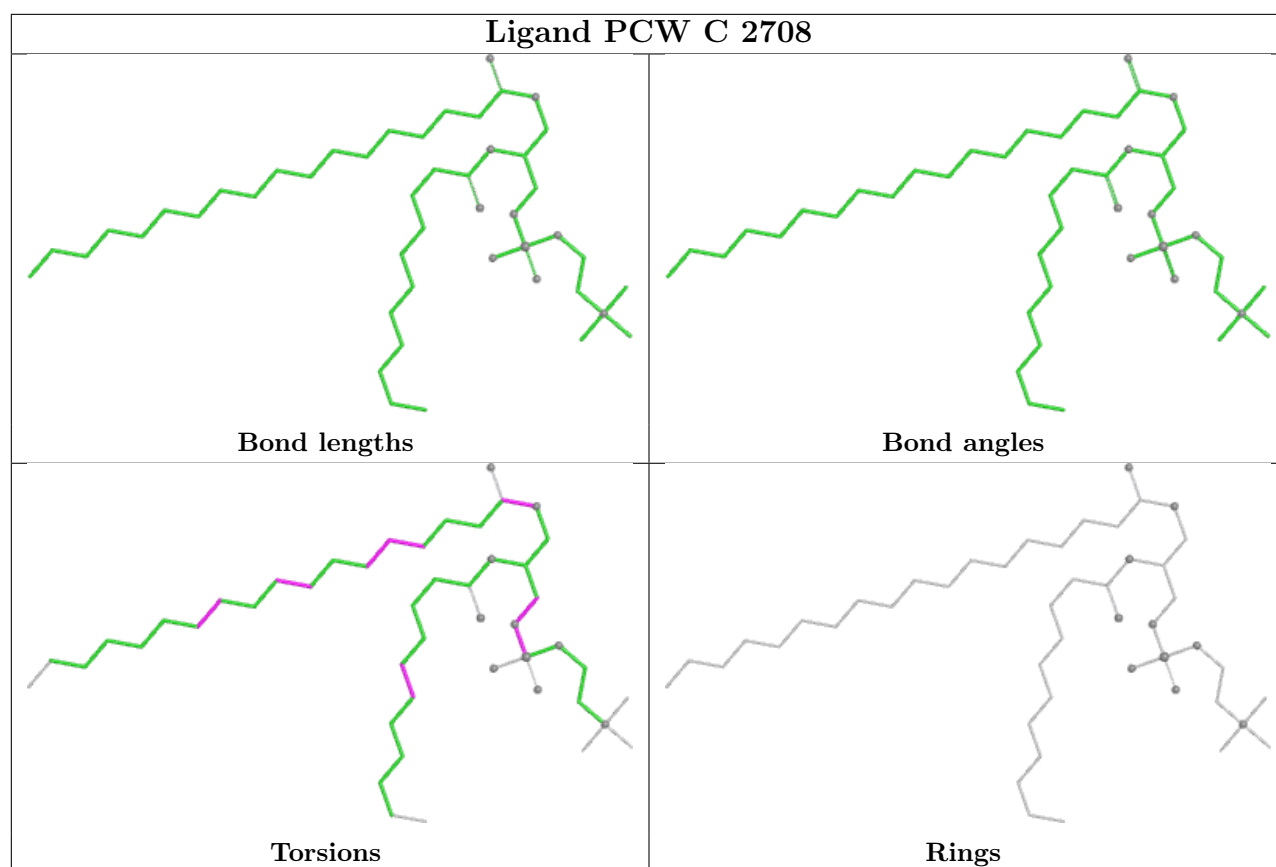
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2703	I3P	1	0
6	C	2708	PCW	1	0
7	C	2701	PT5	3	0
6	B	2708	PCW	1	0
3	C	2703	I3P	1	0
7	A	3009	PT5	3	0
3	B	2703	I3P	1	0
7	B	2701	PT5	3	0
6	A	3007	PCW	1	0
3	A	3002	I3P	1	0
7	D	2701	PT5	3	0
6	D	2708	PCW	1	0

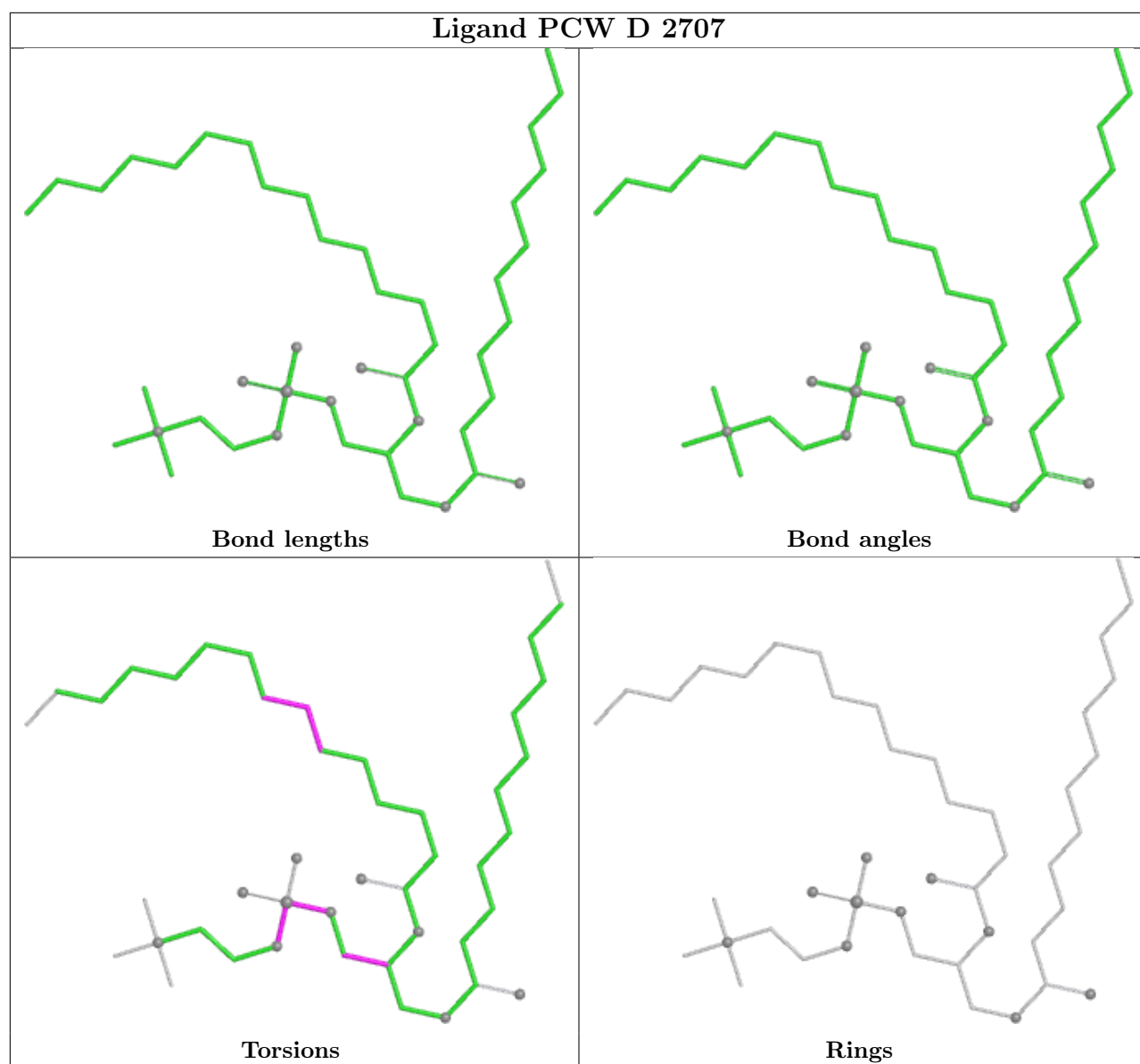
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

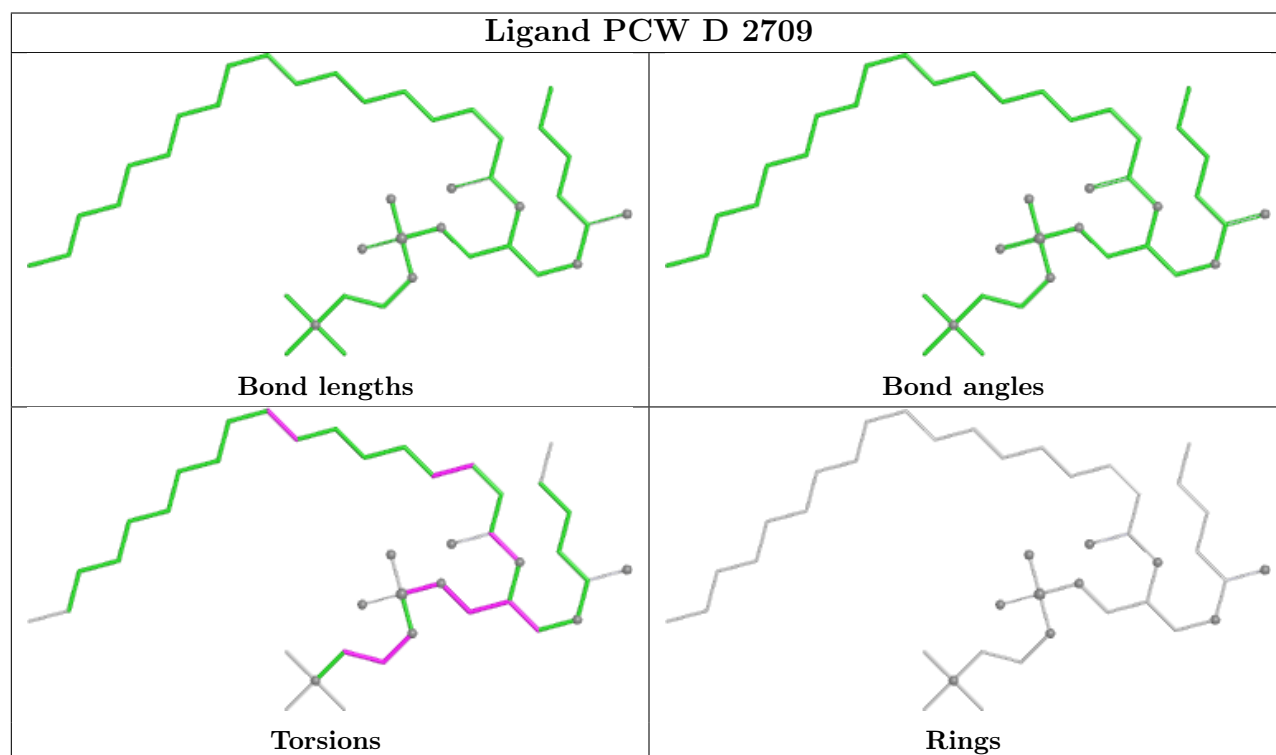
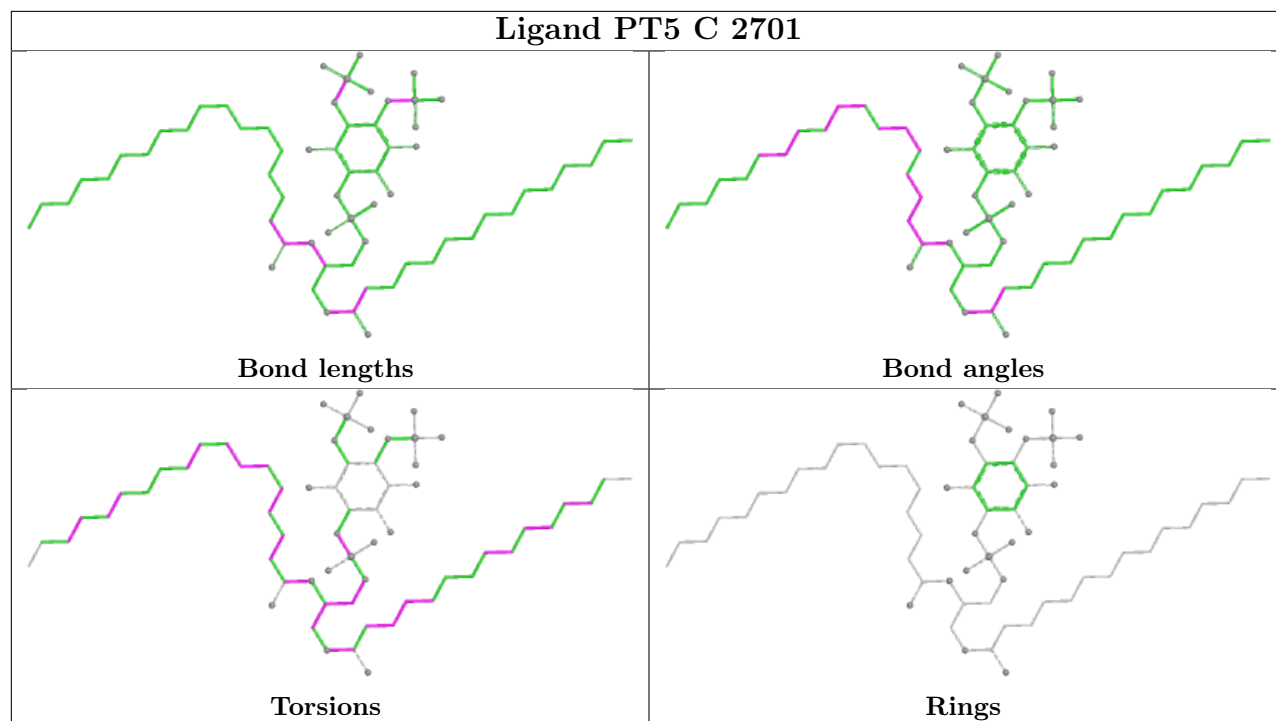
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

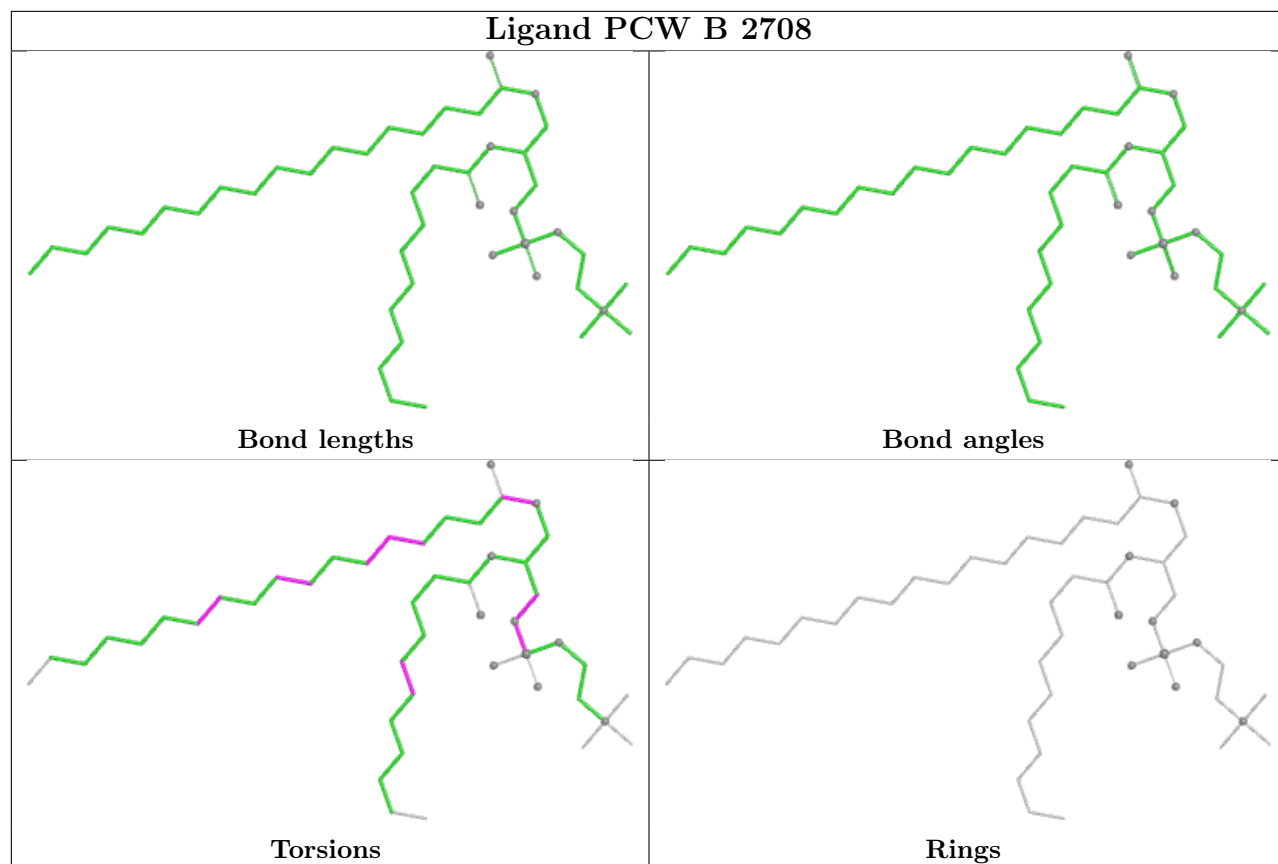


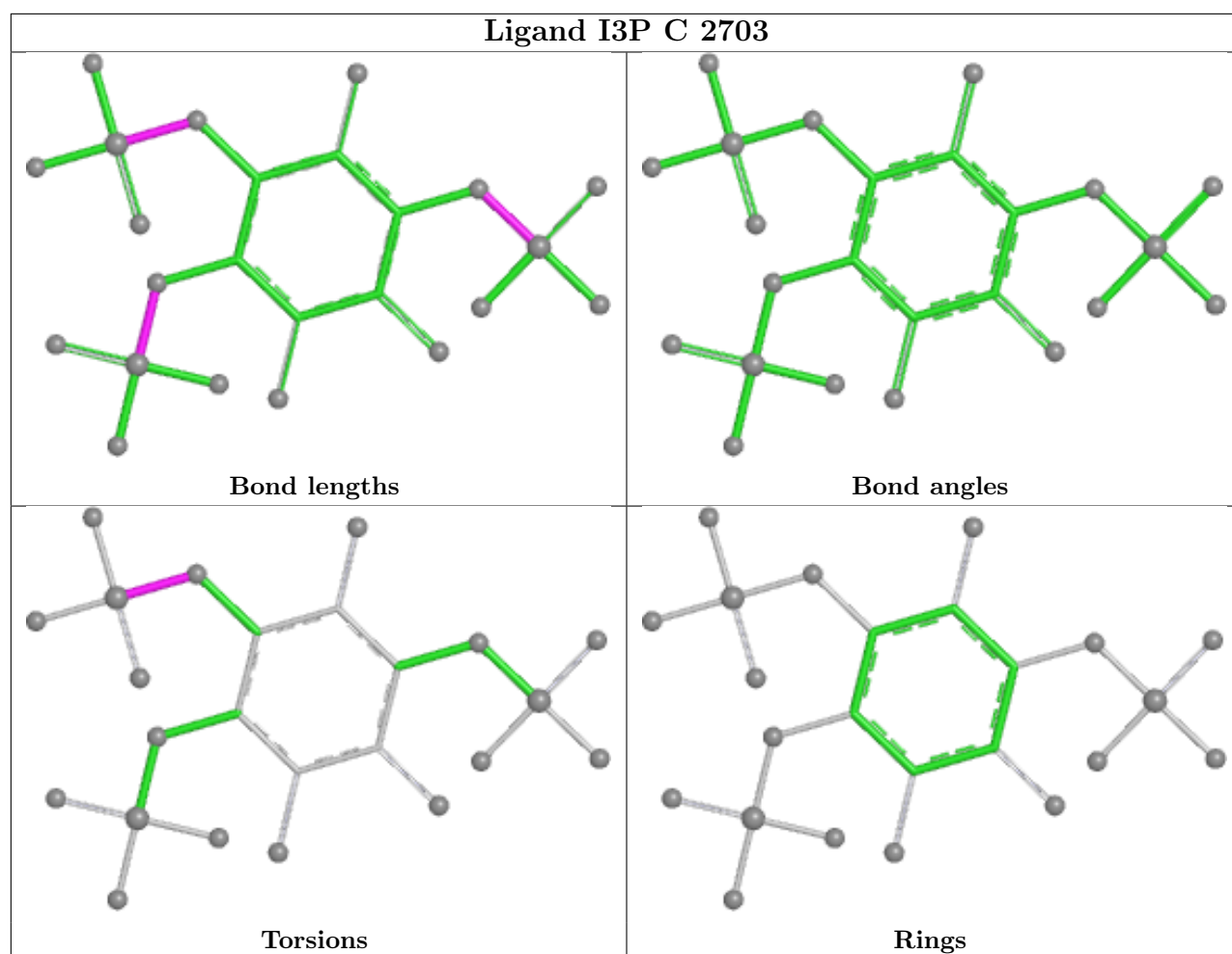


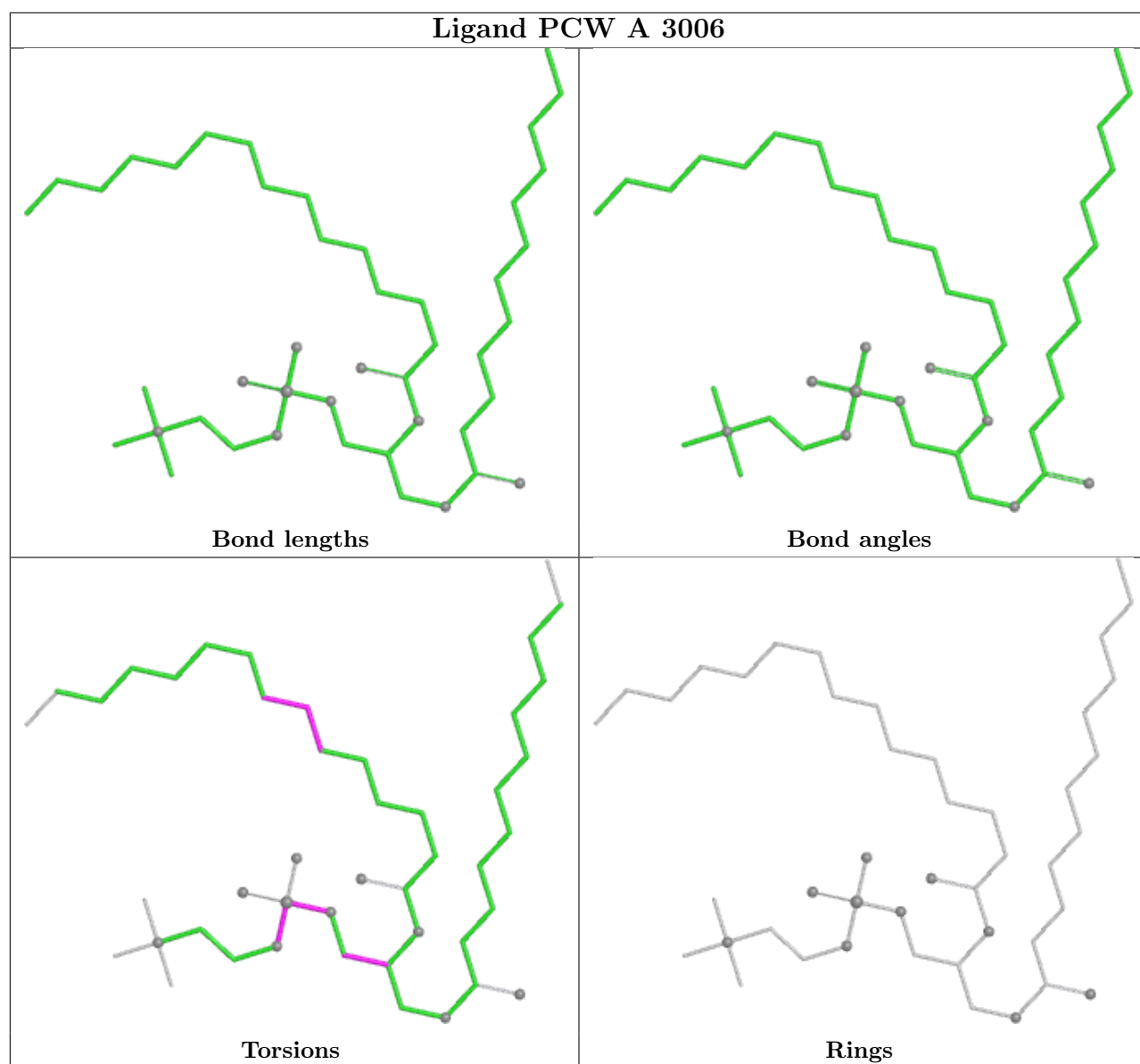


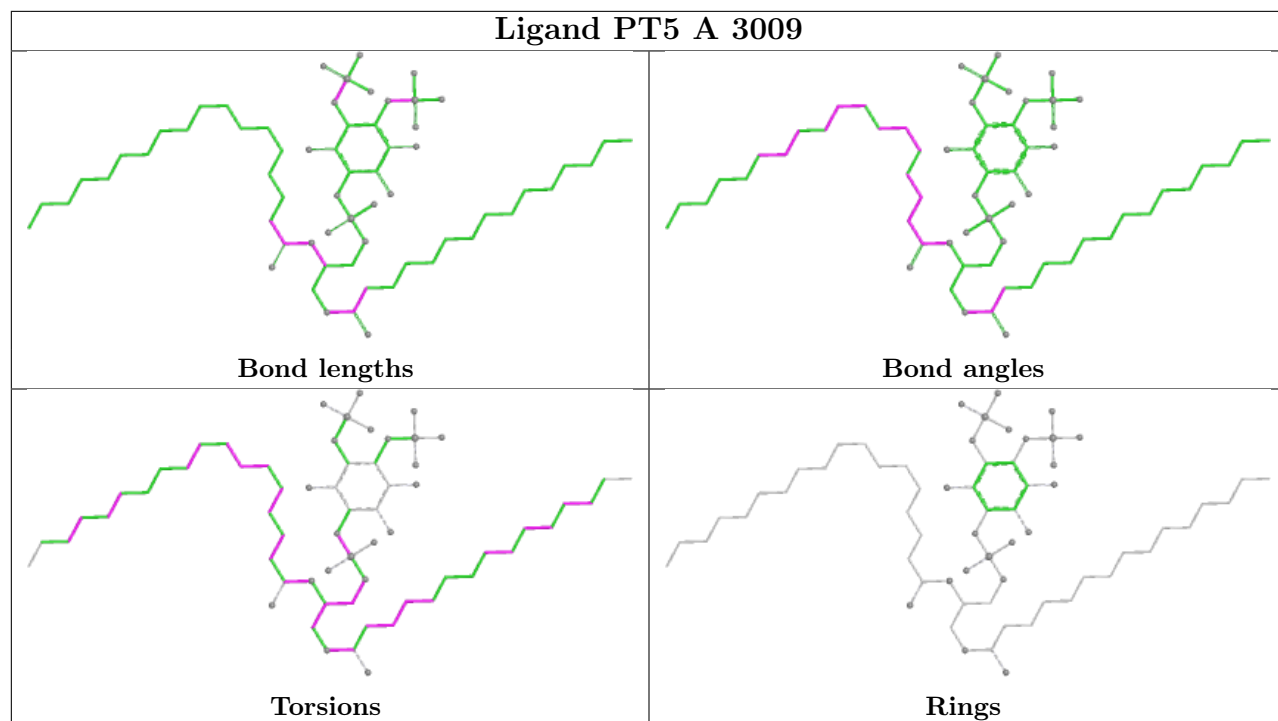


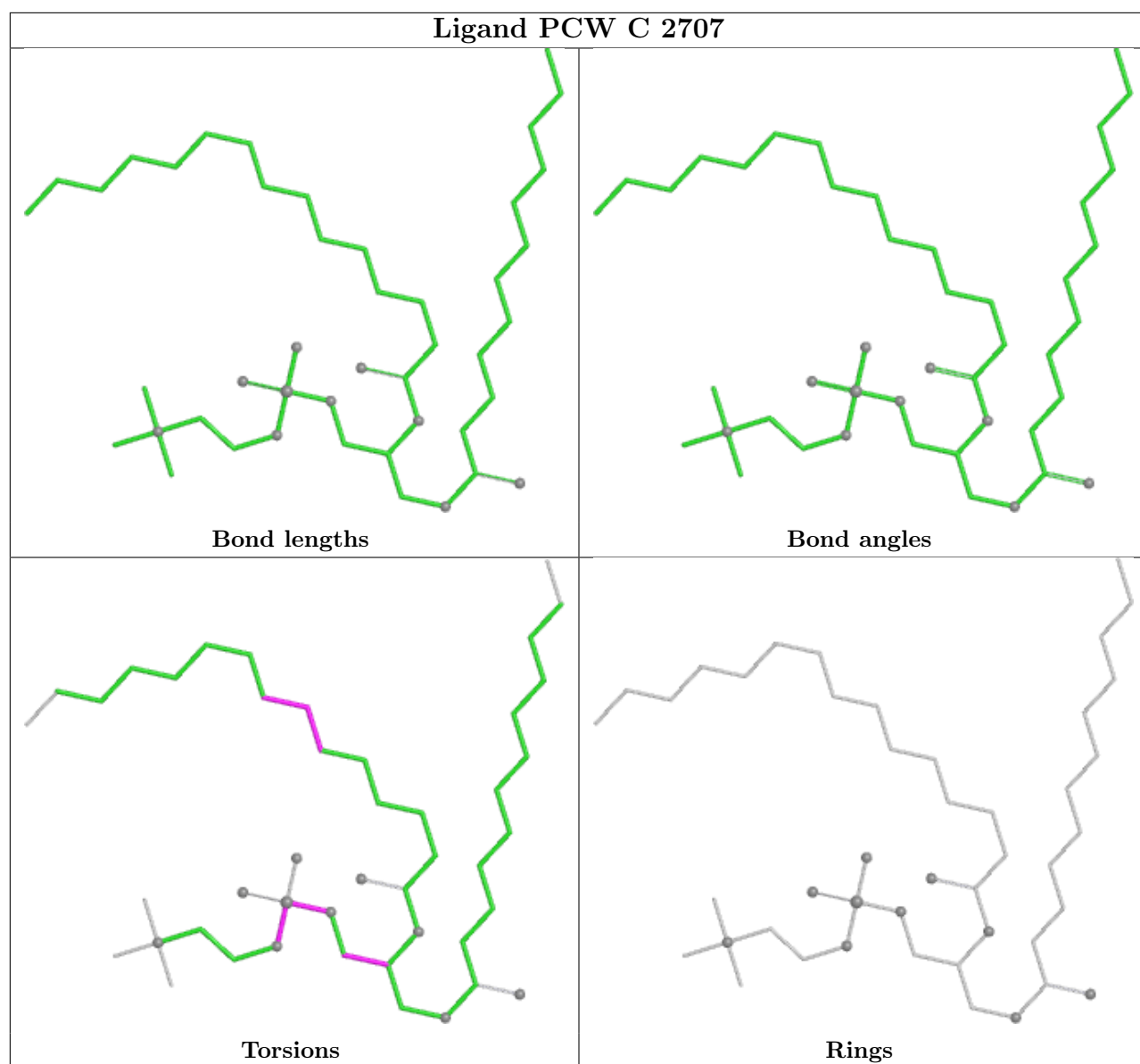


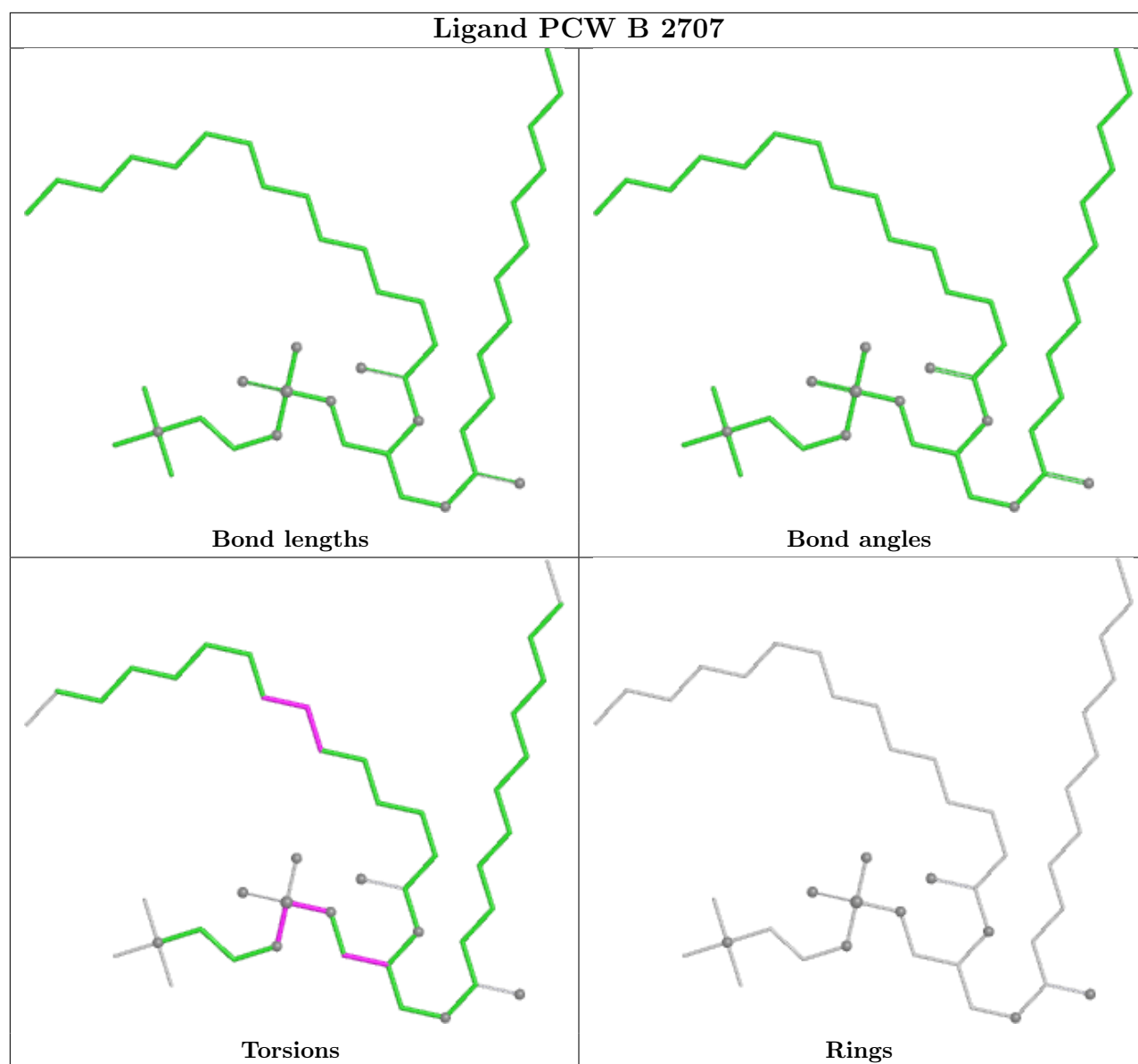


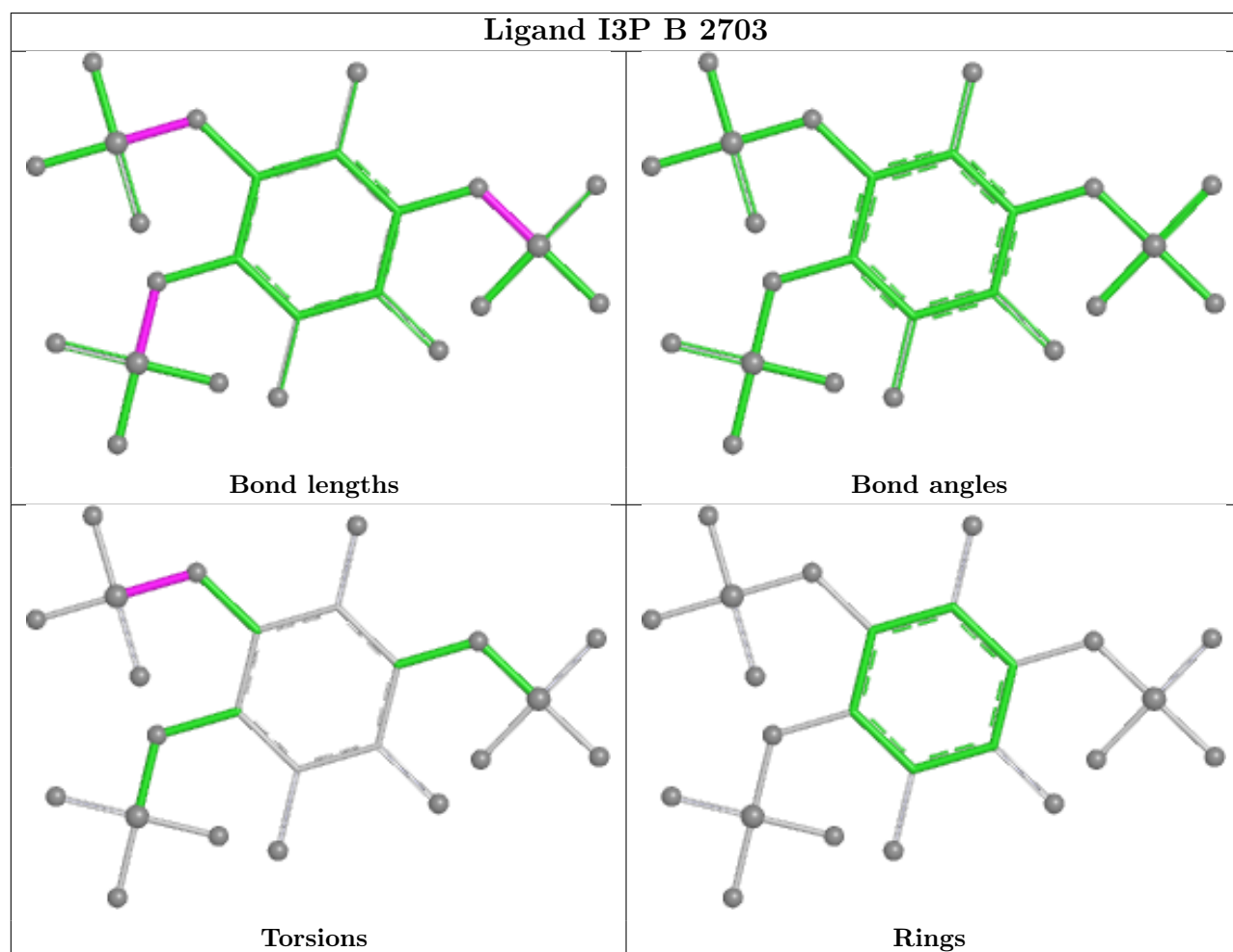
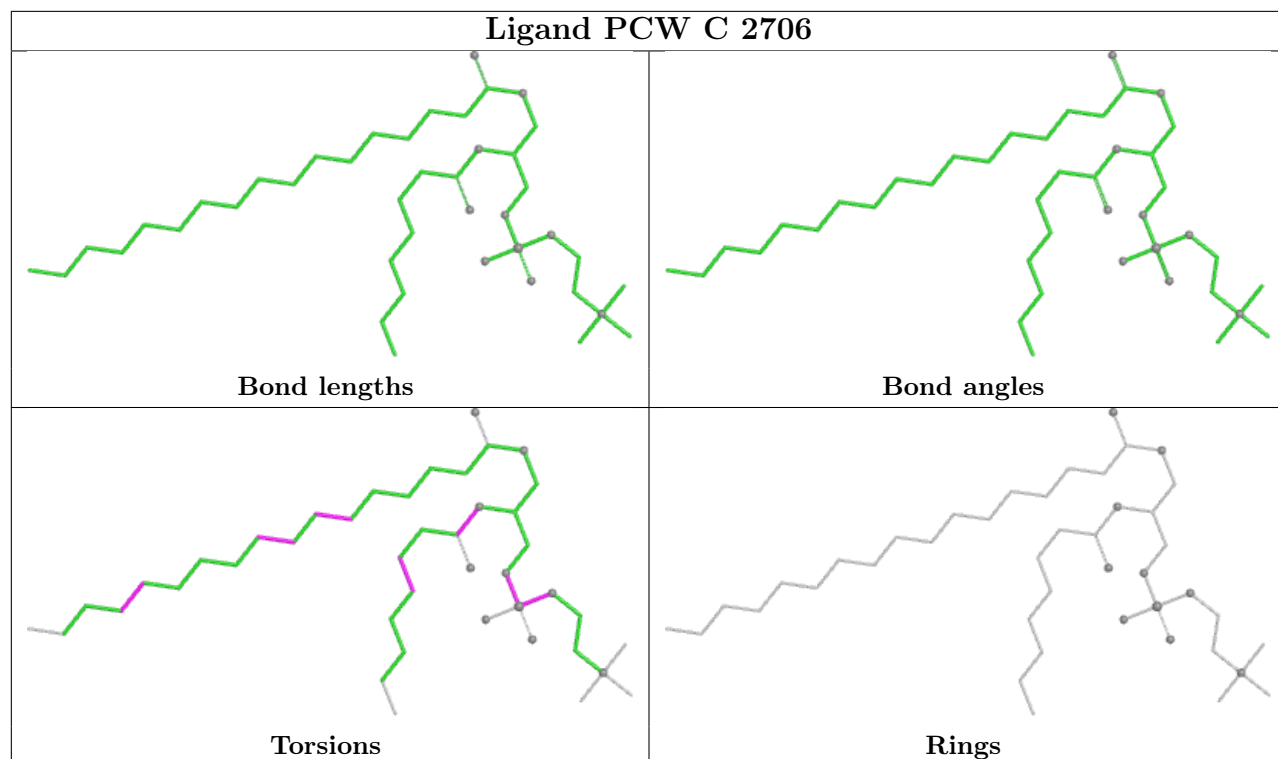


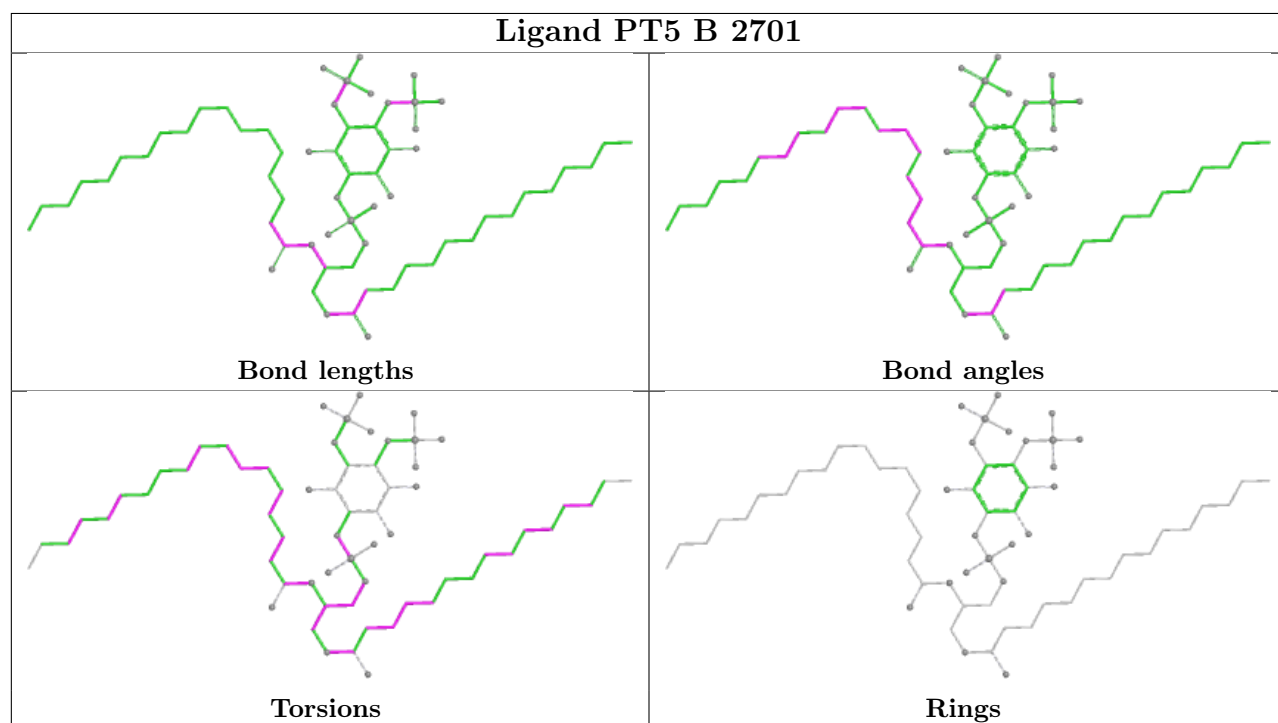
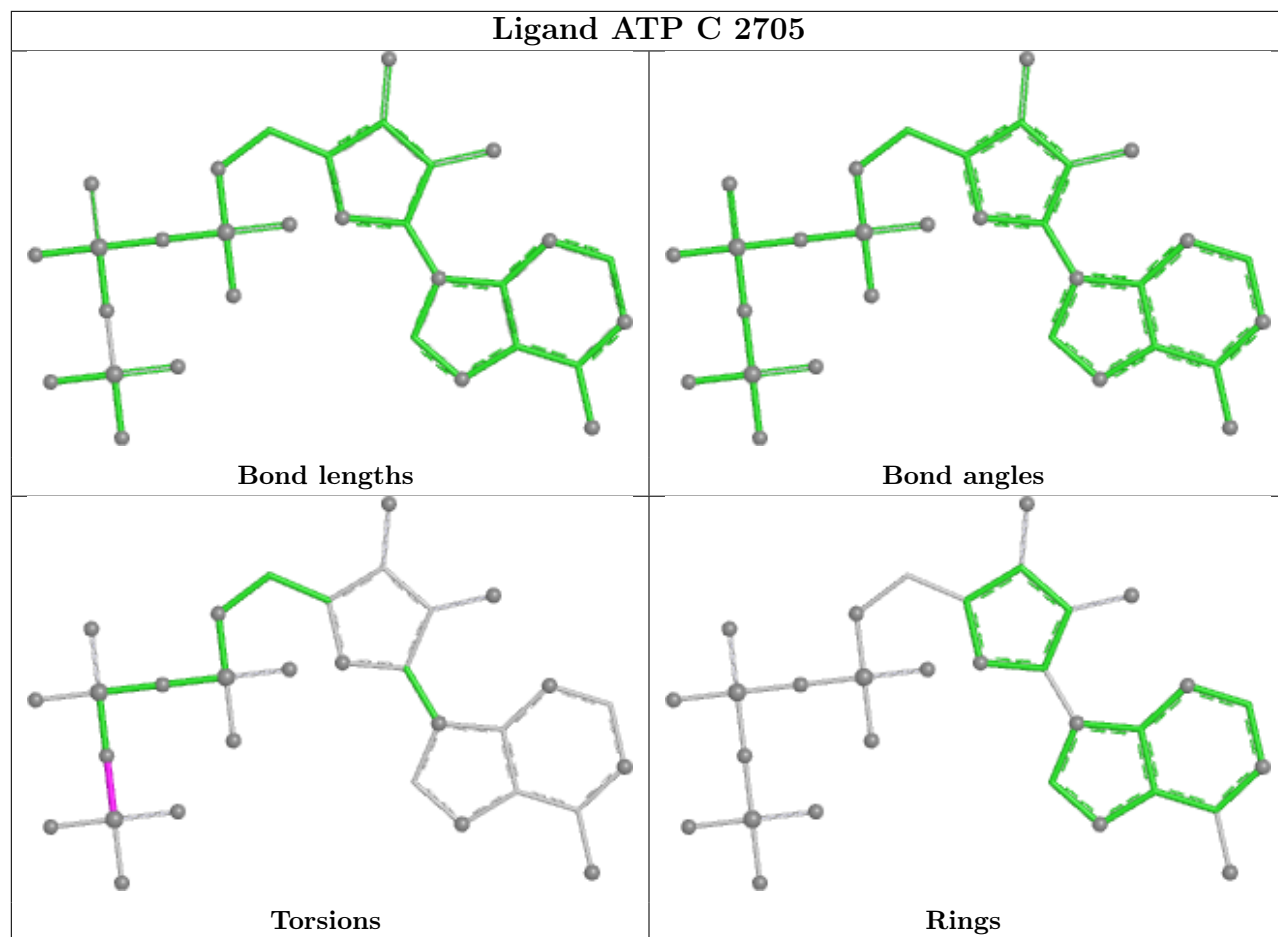




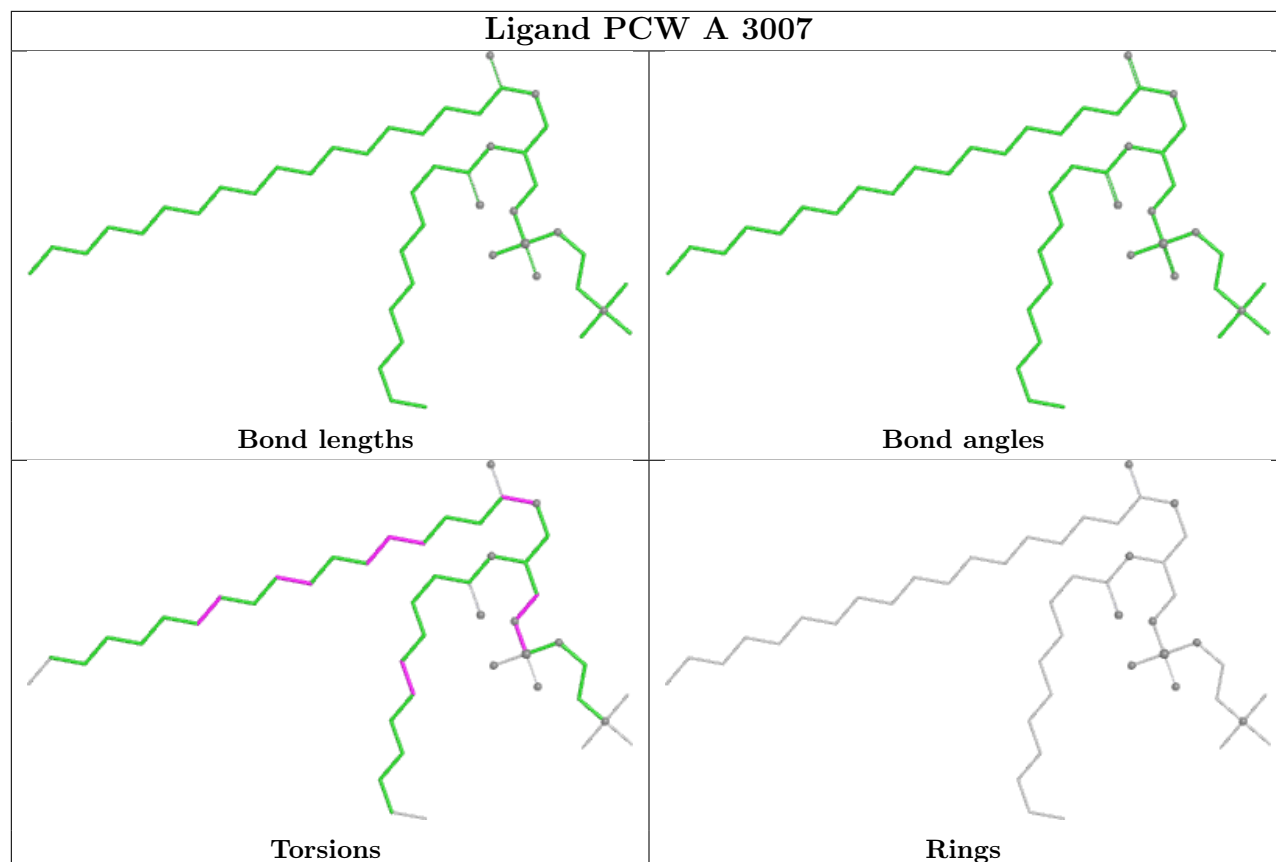




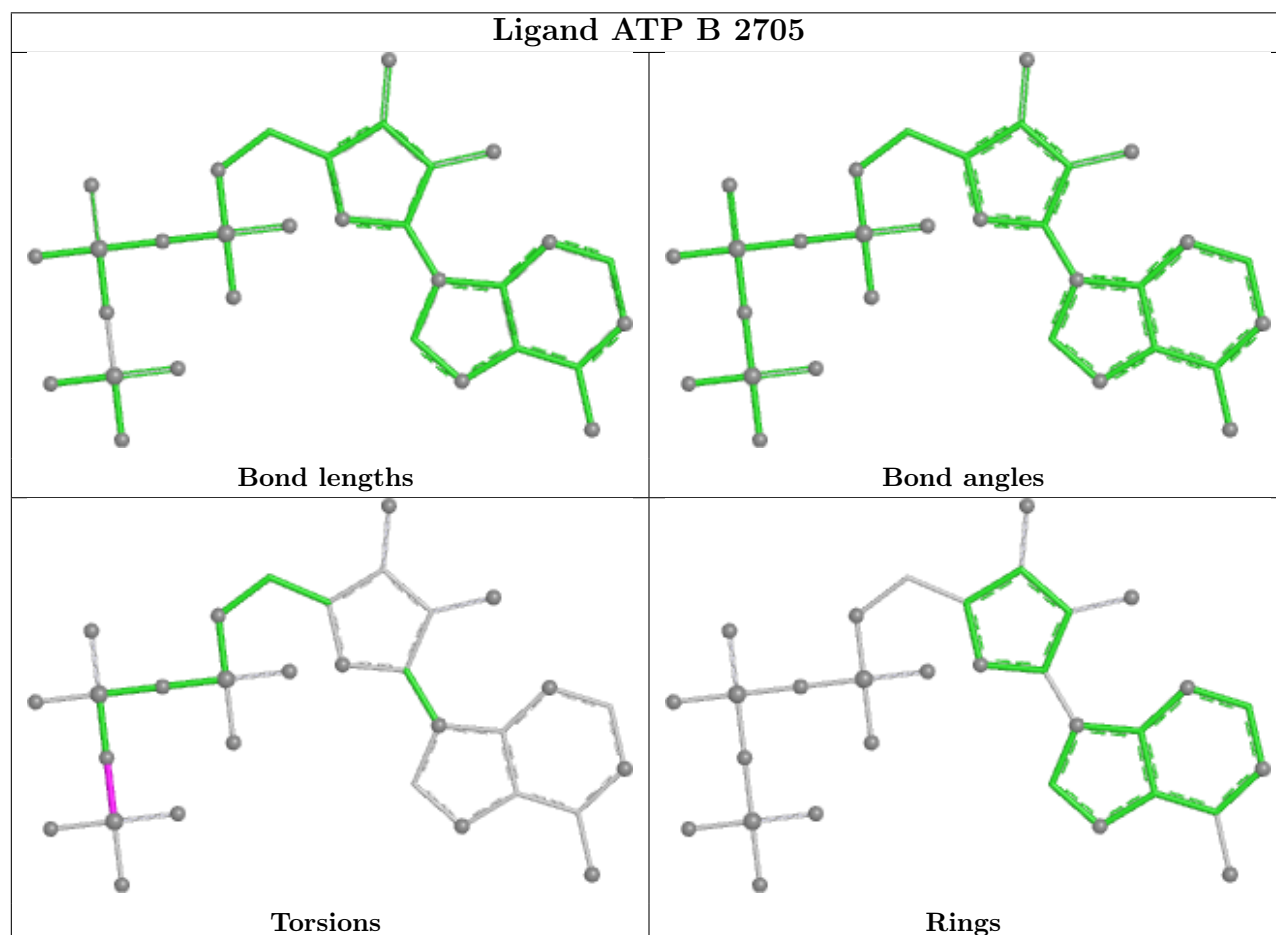


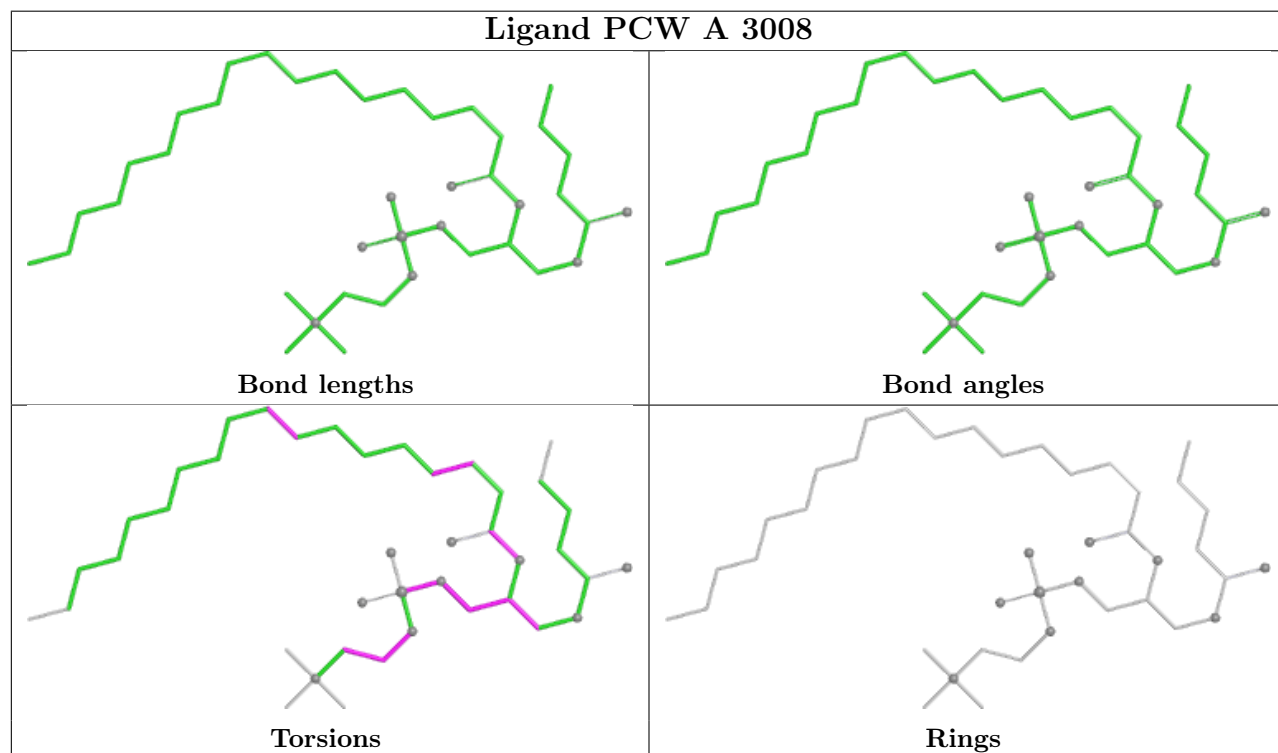
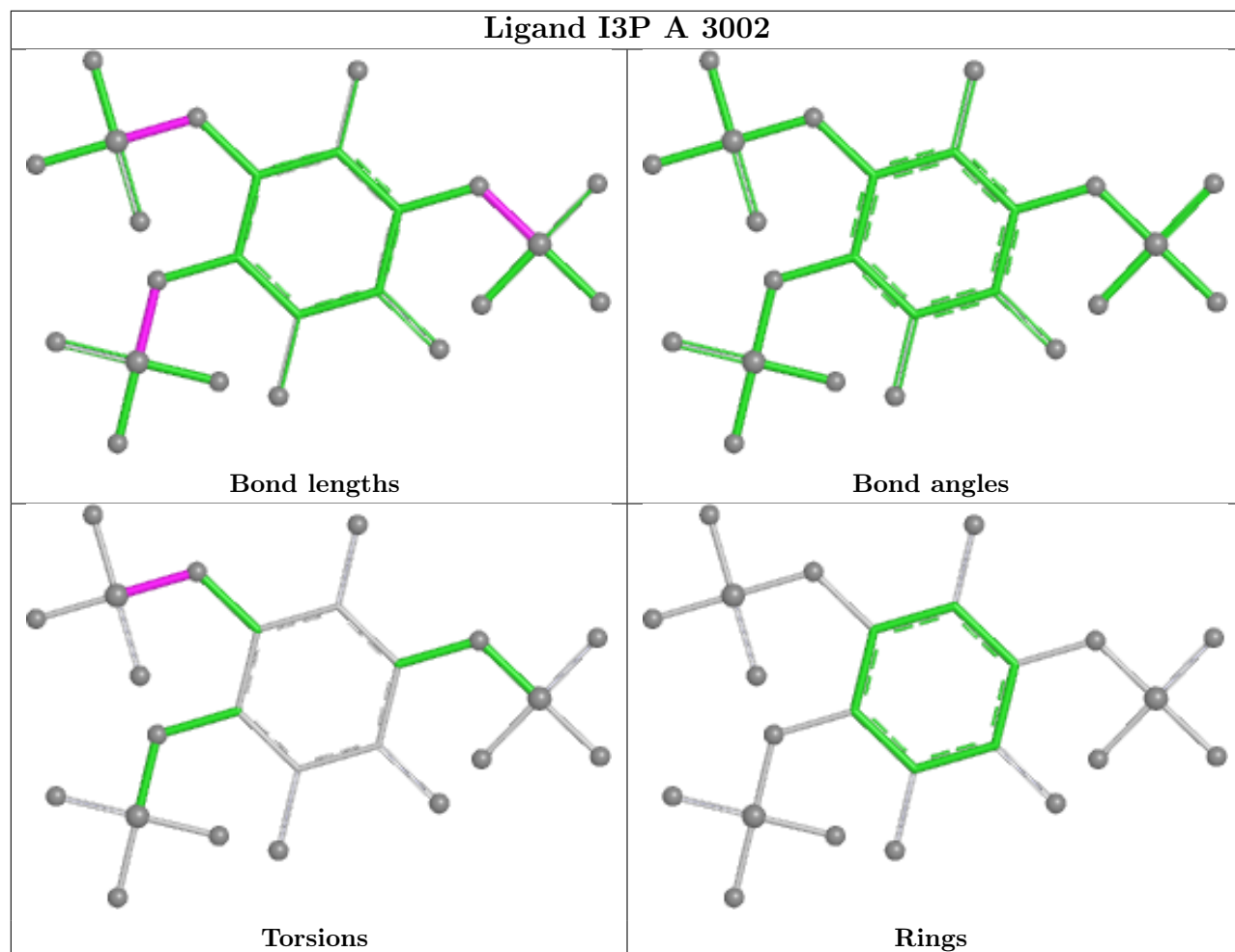


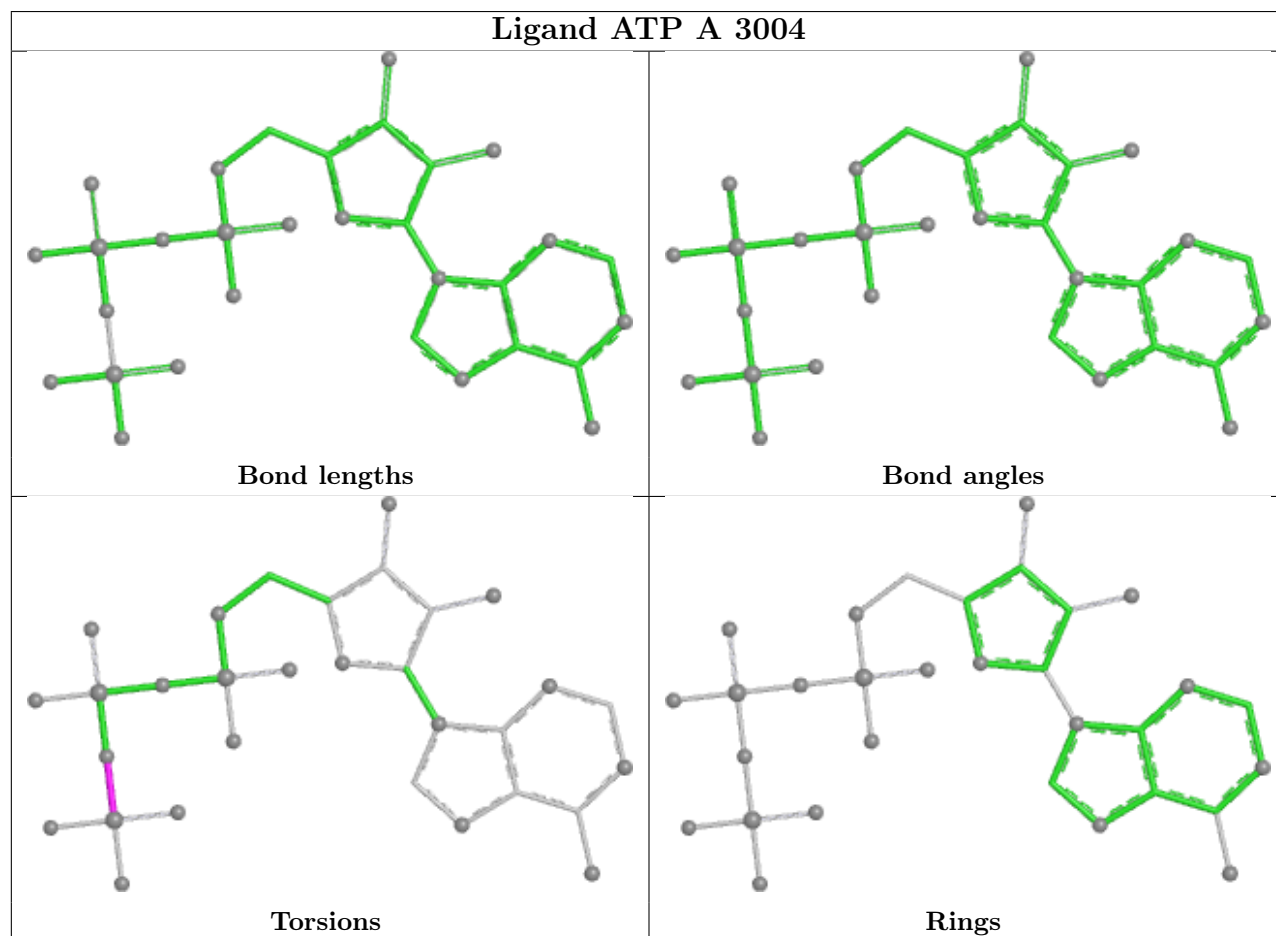
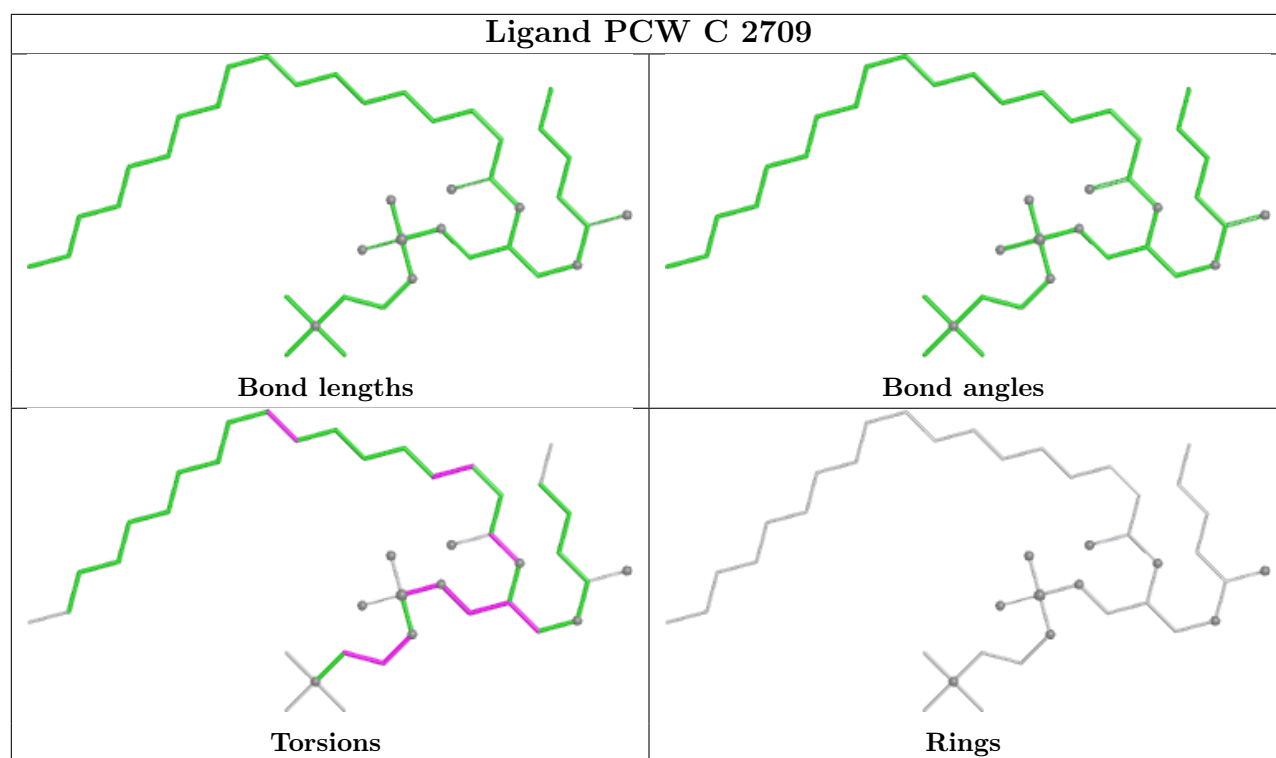
## Ligand PCW A 3007

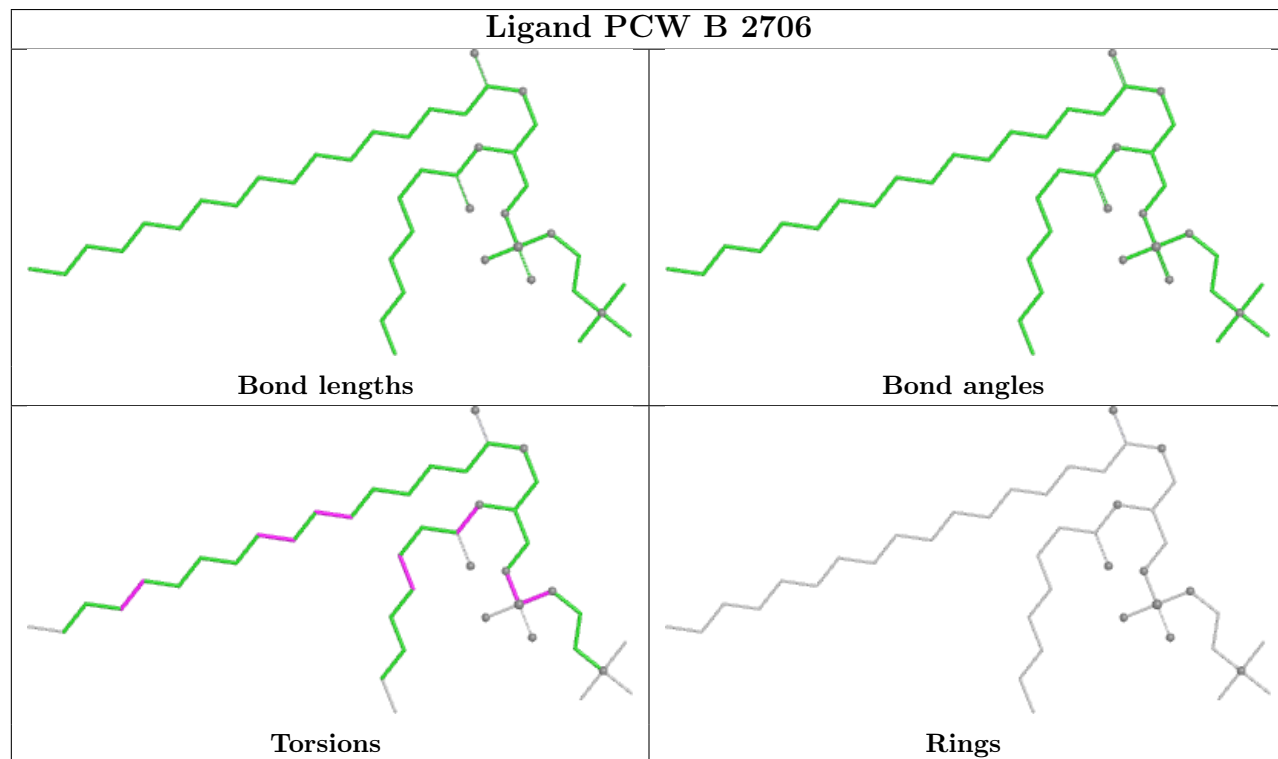
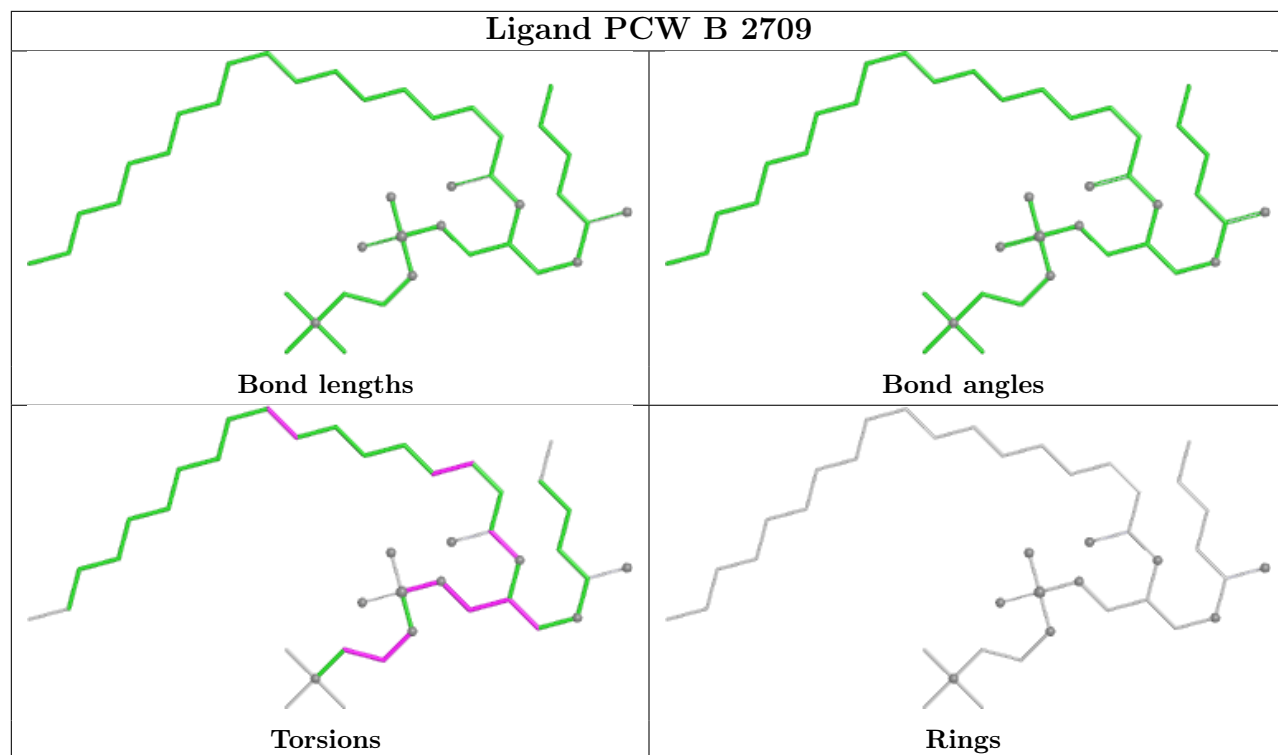


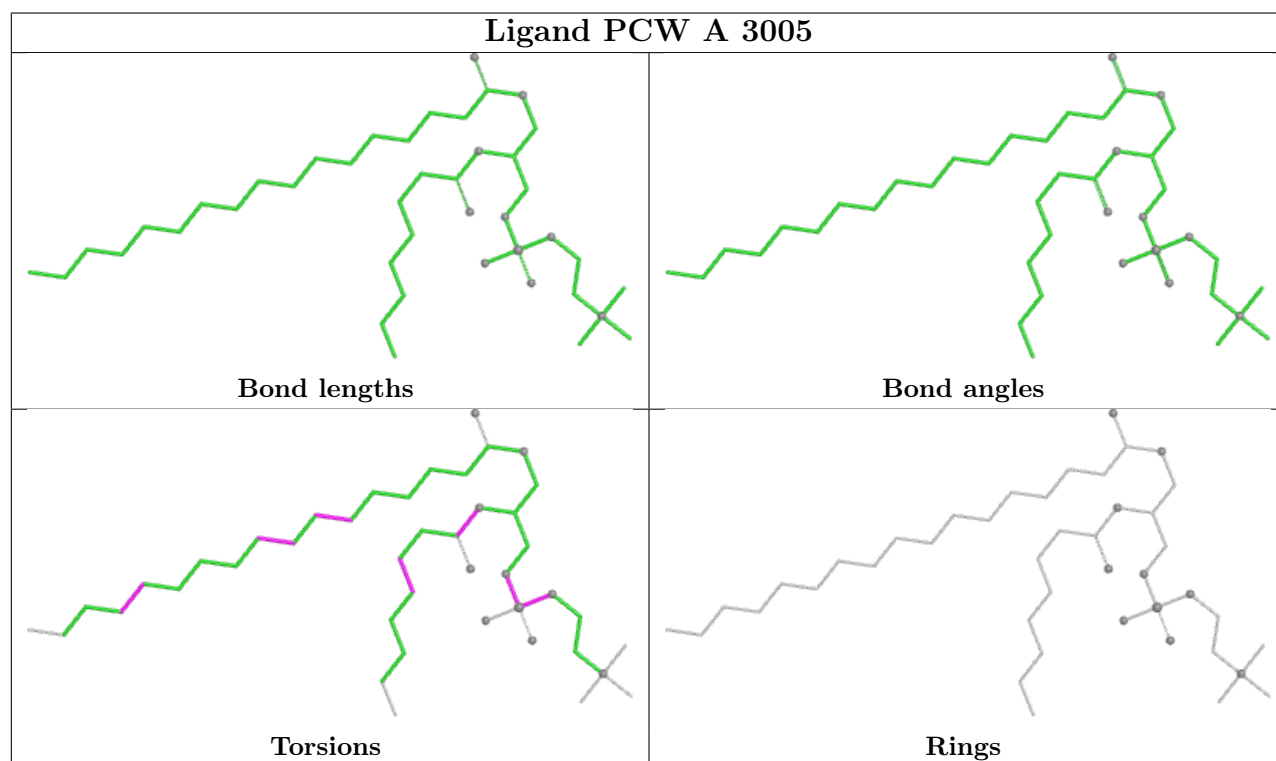
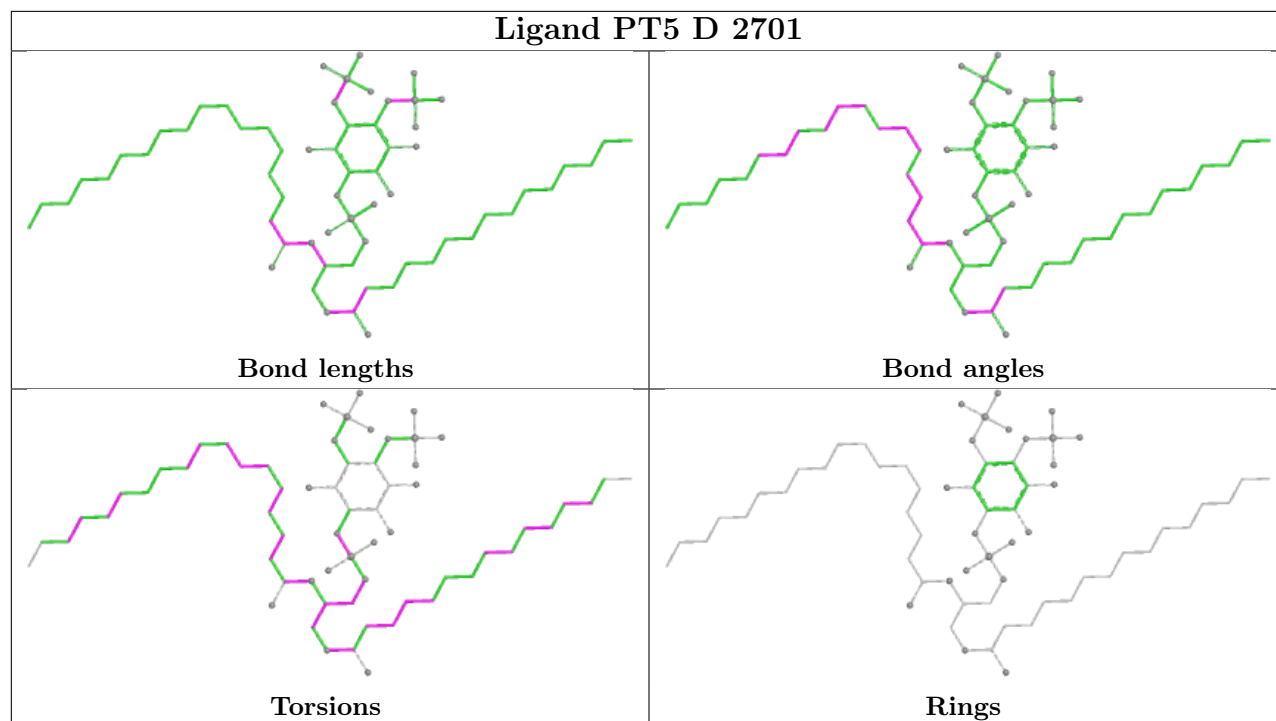
## Ligand ATP B 2705

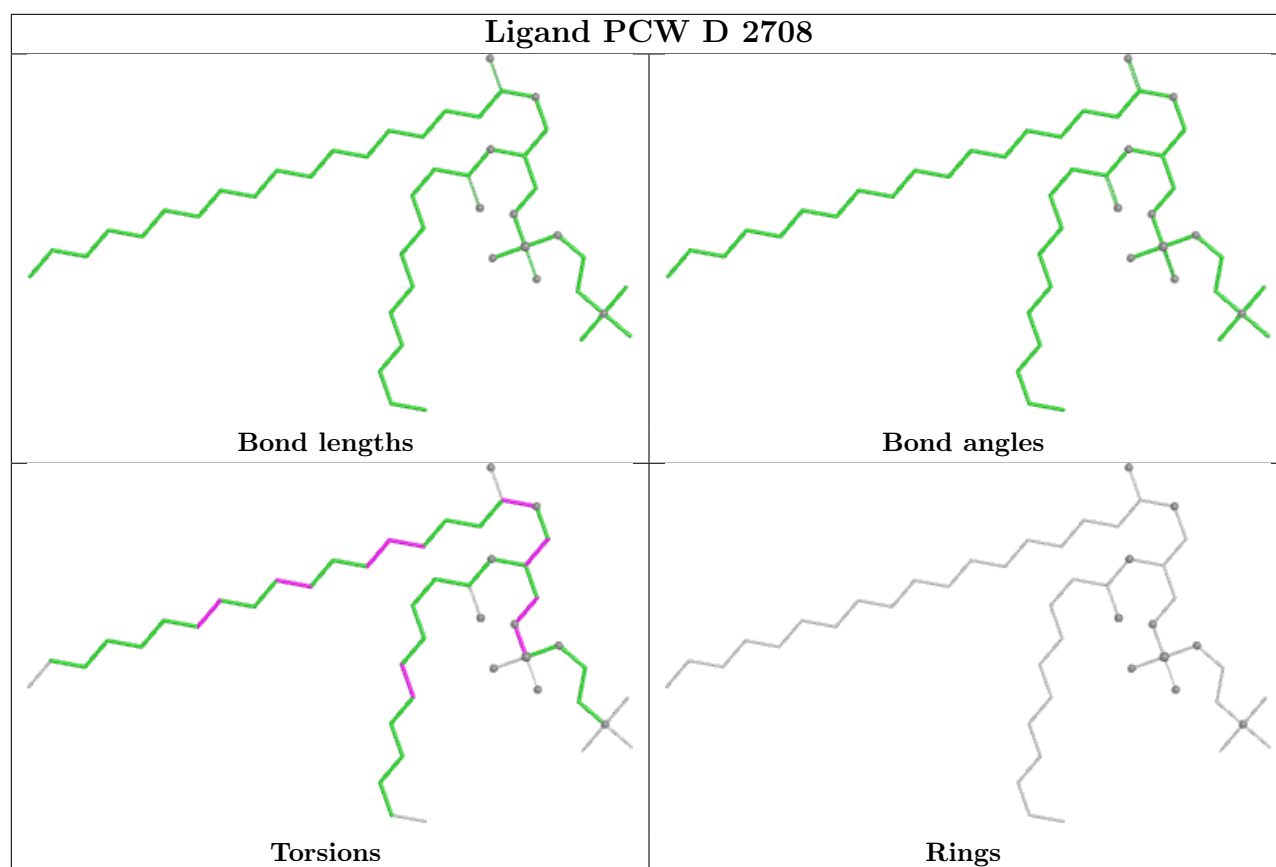












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

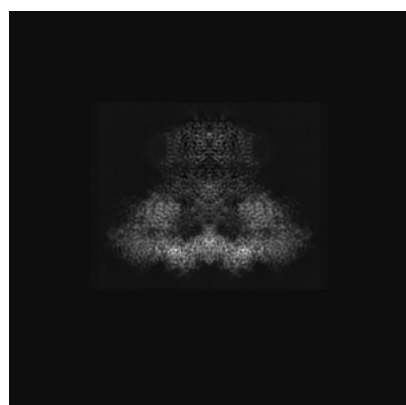
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41349. These allow visual inspection of the internal detail of the map and identification of artifacts.

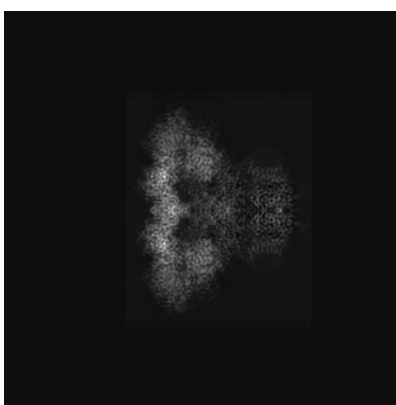
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

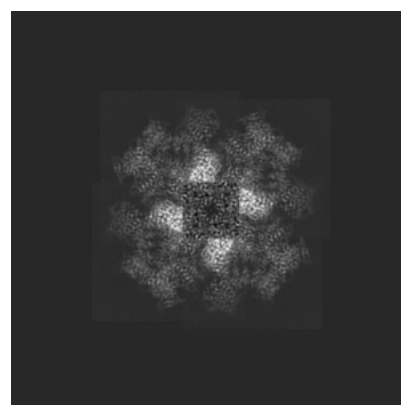
#### 6.1.1 Primary map



X



Y



Z

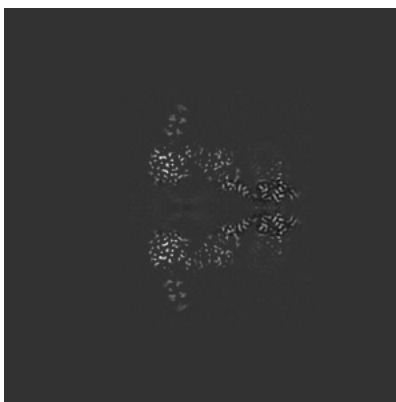
The images above show the map projected in three orthogonal directions.

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

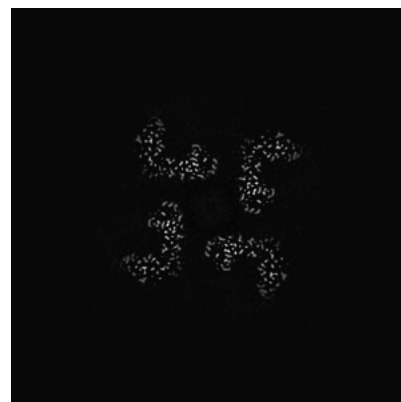
#### 6.2.1 Primary map



X Index: 336



Y Index: 336

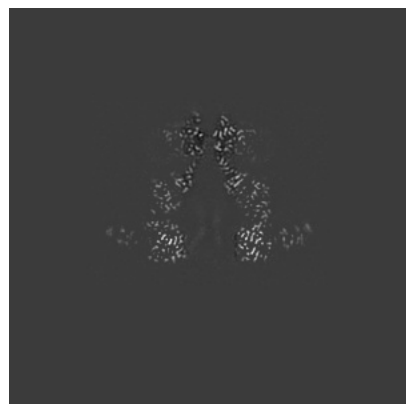


Z Index: 336

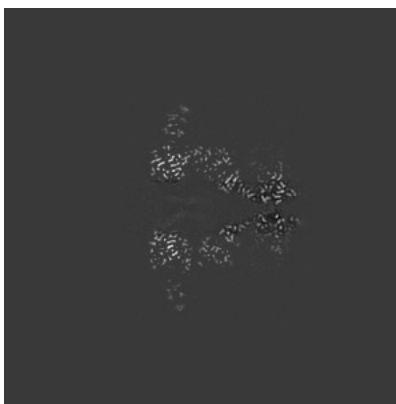
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 333



Y Index: 339

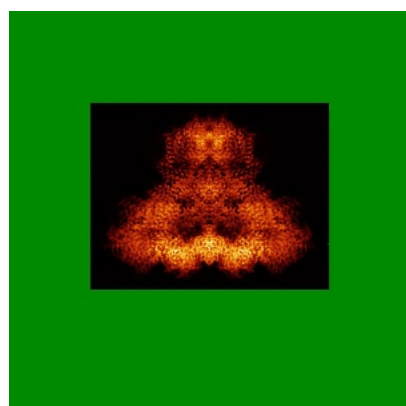


Z Index: 269

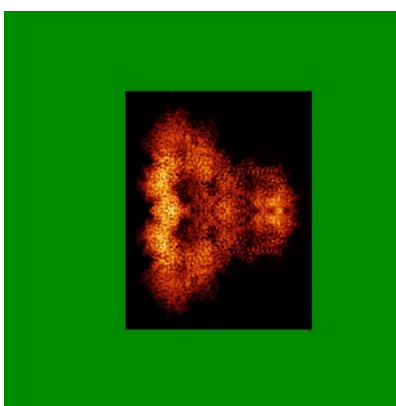
The images above show the largest variance slices of the map in three orthogonal directions.

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

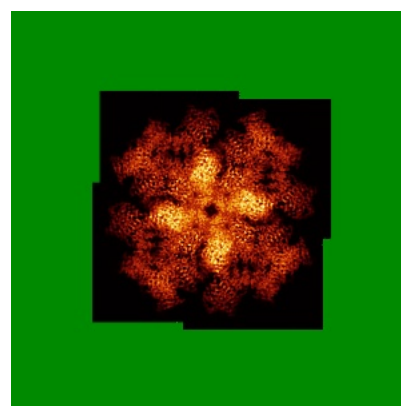
### 6.4.1 Primary map



X



Y

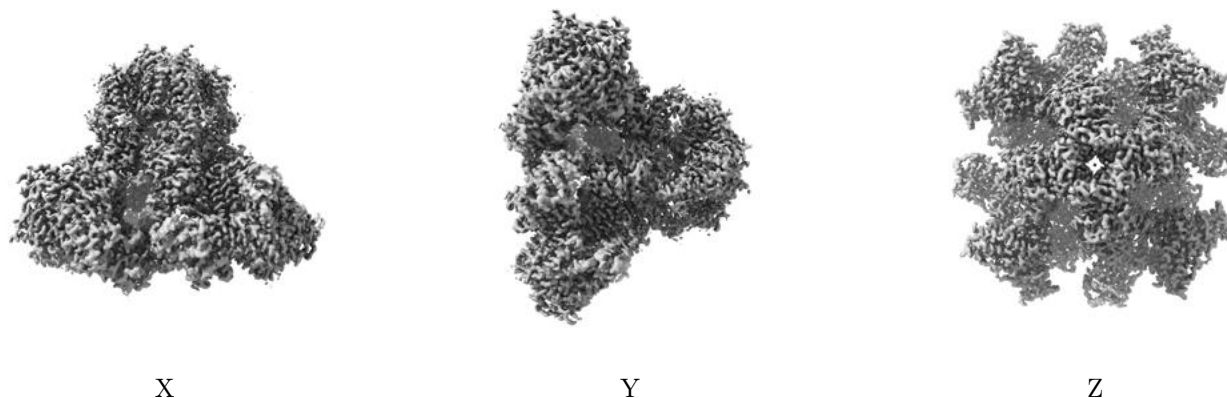


Z

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.

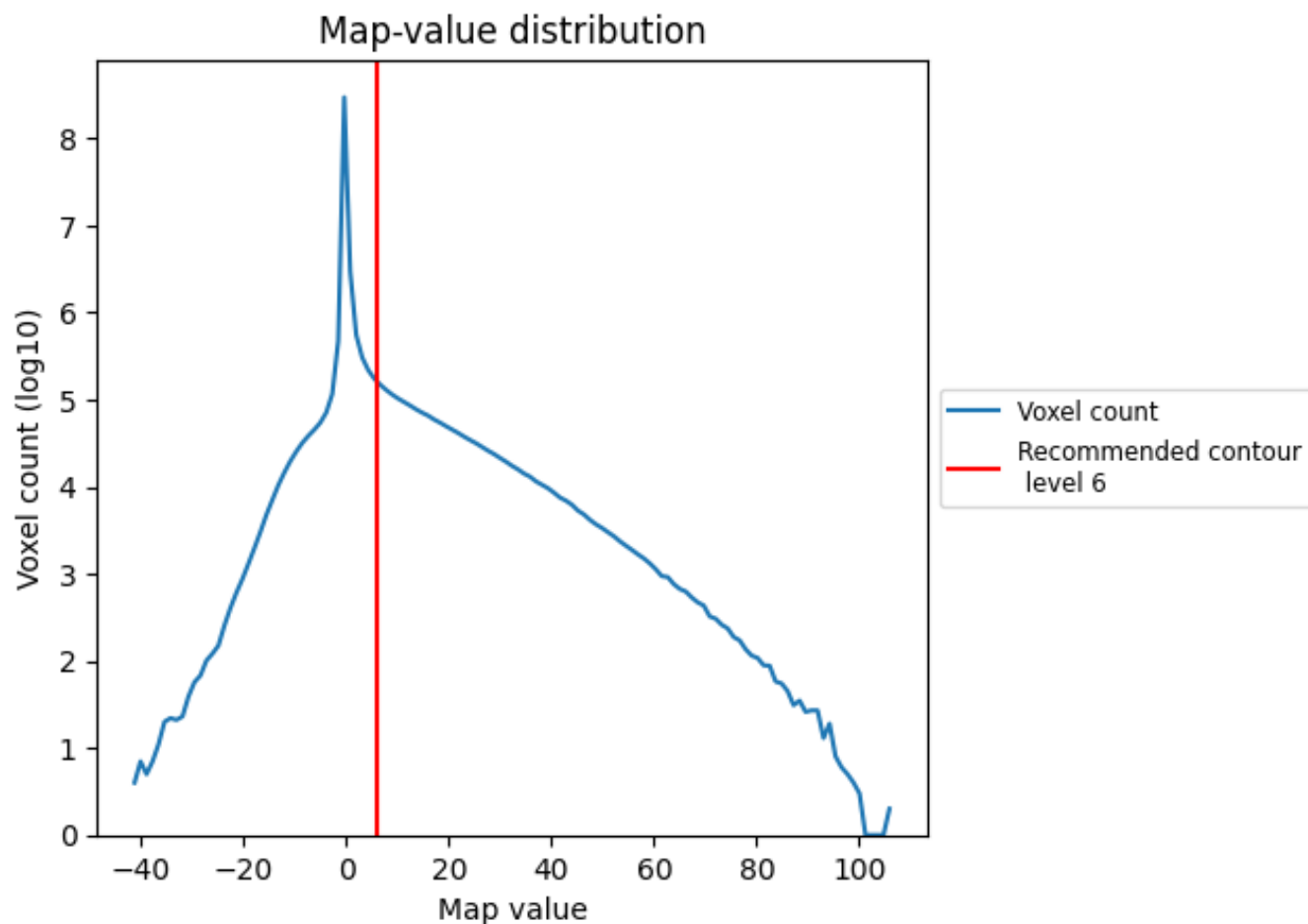
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

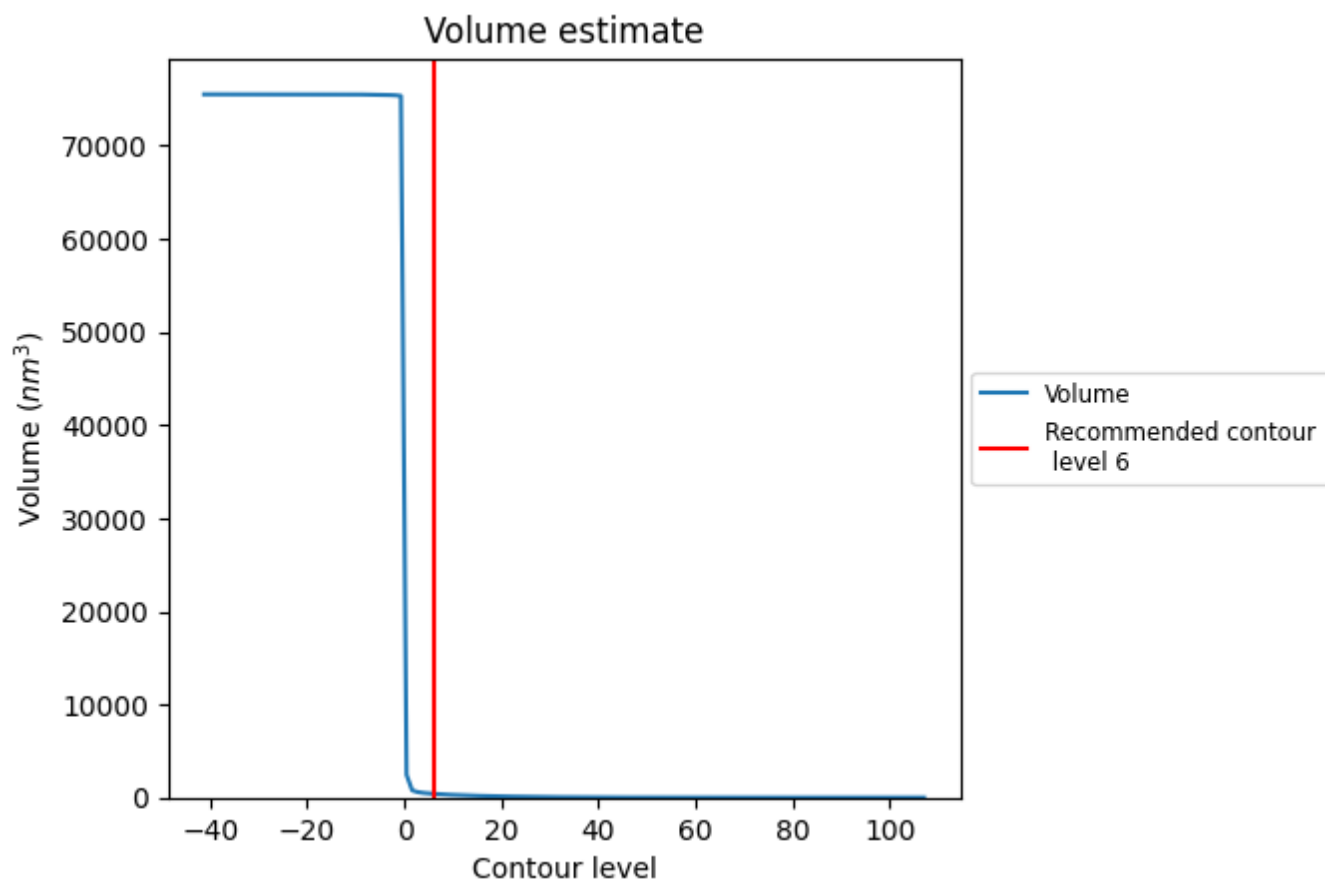
This section contains the results of statistical analysis of the map.

### 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.

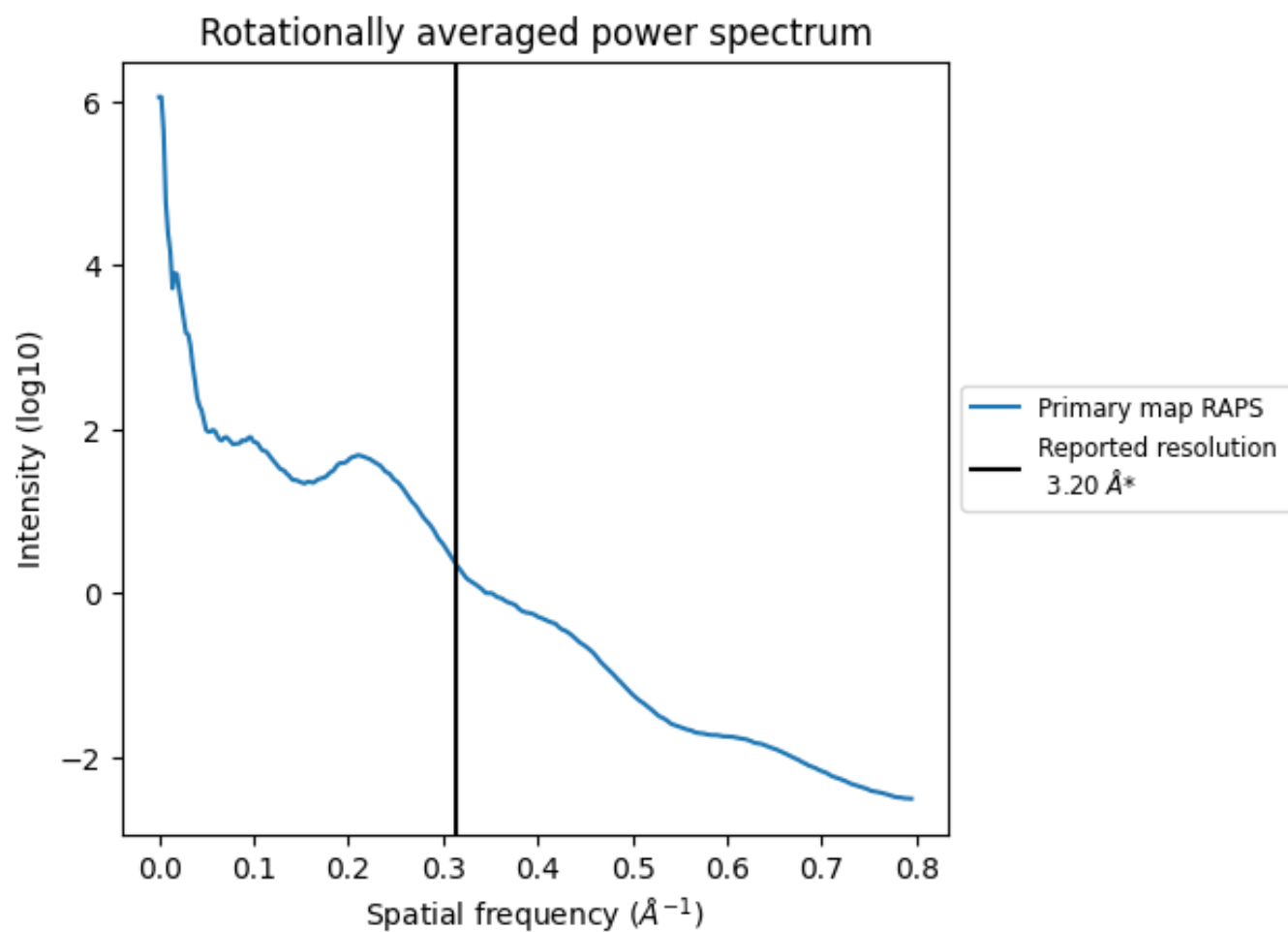
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404  $\text{nm}^3$ ; this corresponds to an approximate mass of 365 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 0.312 Å<sup>-1</sup>

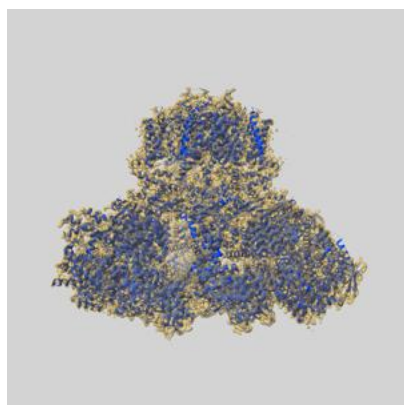
## 8 Fourier-Shell correlation

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

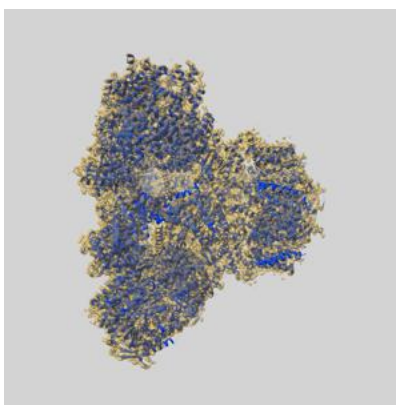
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41349 and PDB model 8TKF. Per-residue inclusion information can be found in section 3 on page 8.

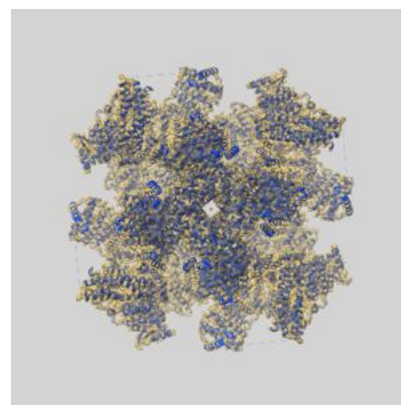
### 9.1 Map-model overlay [i](#)



X



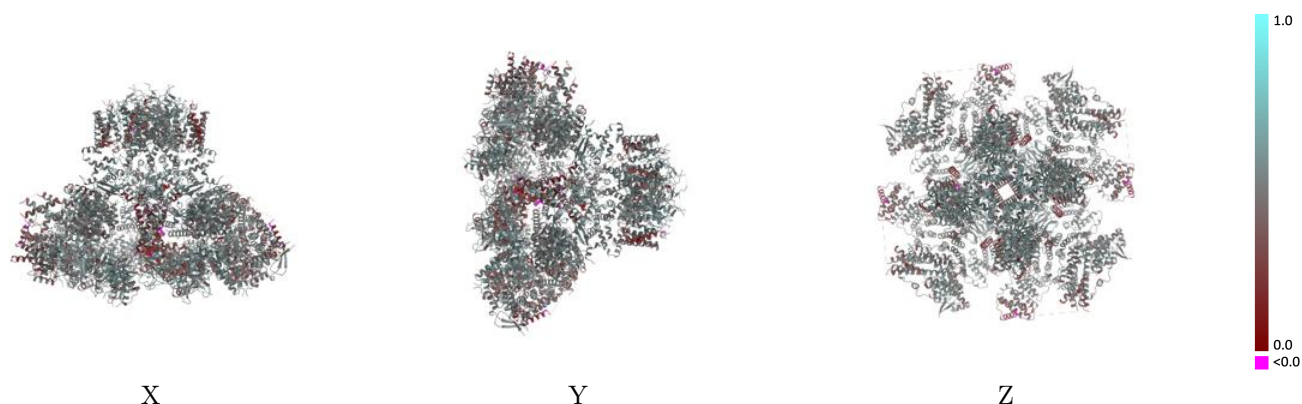
Y



Z

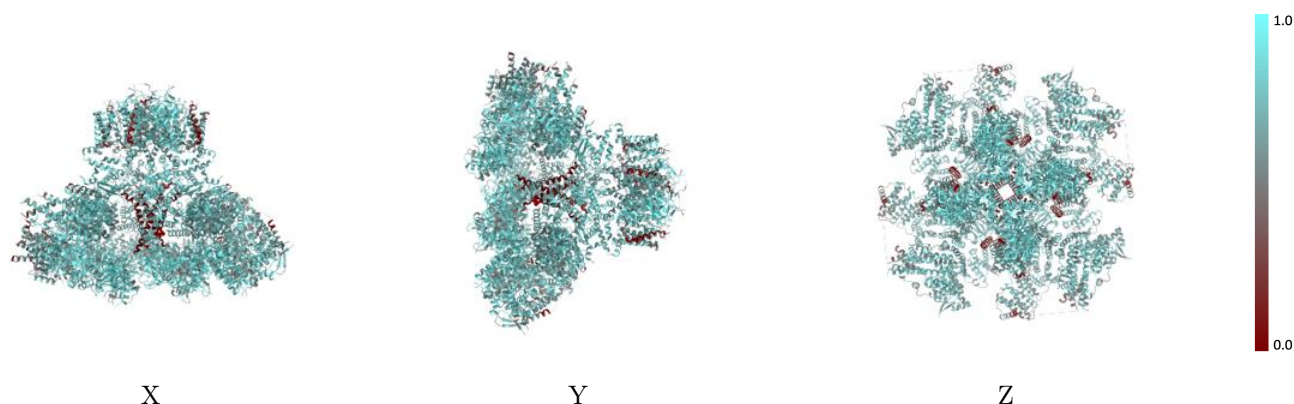
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



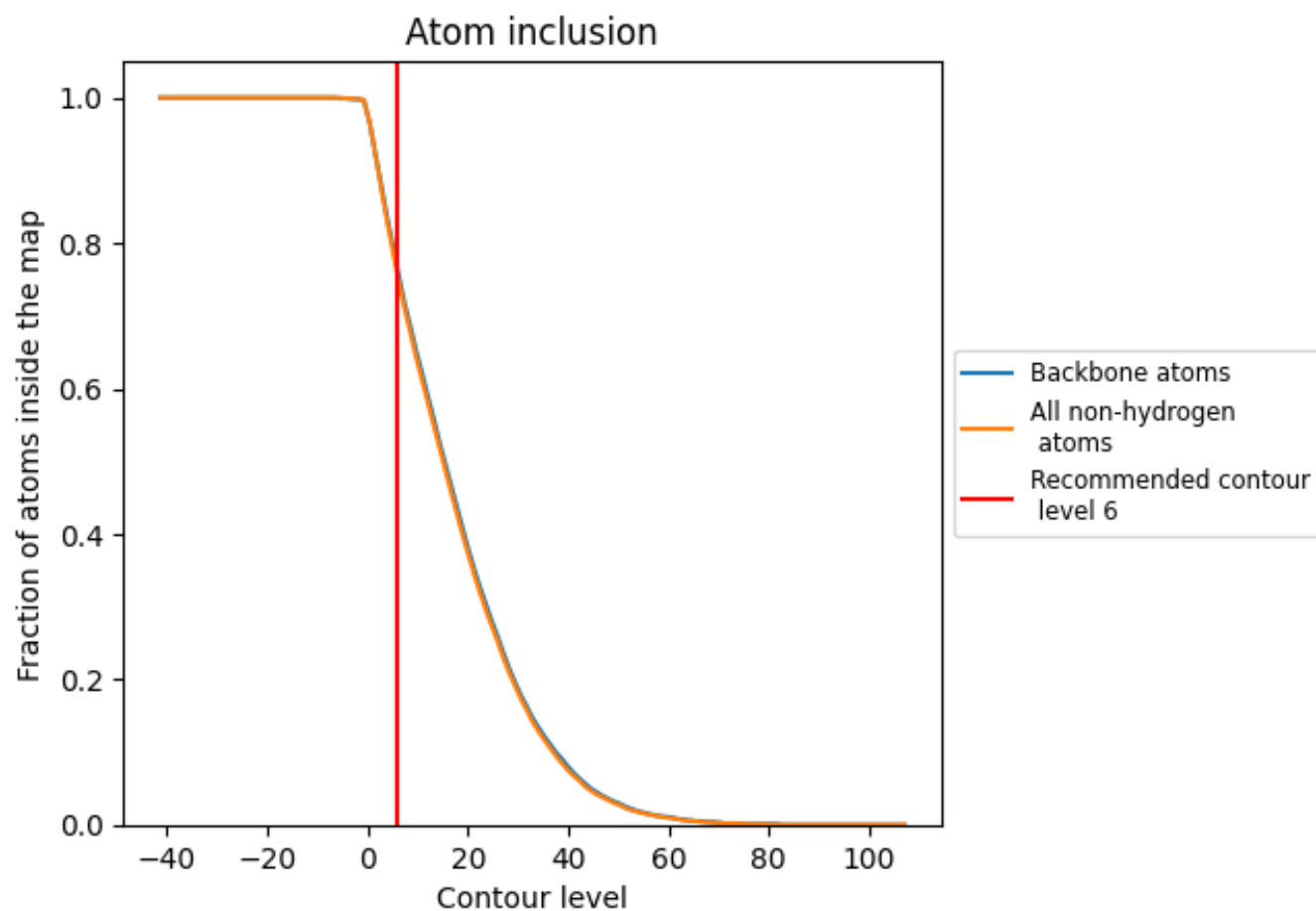
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7550	<div><div></div></div> 0.4850
A	<div><div></div></div> 0.7630	<div><div></div></div> 0.4850
B	<div><div></div></div> 0.7590	<div><div></div></div> 0.4850
C	<div><div></div></div> 0.7590	<div><div></div></div> 0.4860
D	<div><div></div></div> 0.7590	<div><div></div></div> 0.4850

