



Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 10:35 AM EST

PDB ID : 9D19
EMDB ID : EMD-46425
Title : Ca²⁺ bound open-inactivated hSlo1 + beta2N-beta4 channel in detergent-conformation 3 of inactivating domain
Authors : Agarwal, S.; Nimigean, C.
Deposited on : 2024-08-07
Resolution : 2.88 Å(reported)
Based on initial model : 6v22

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

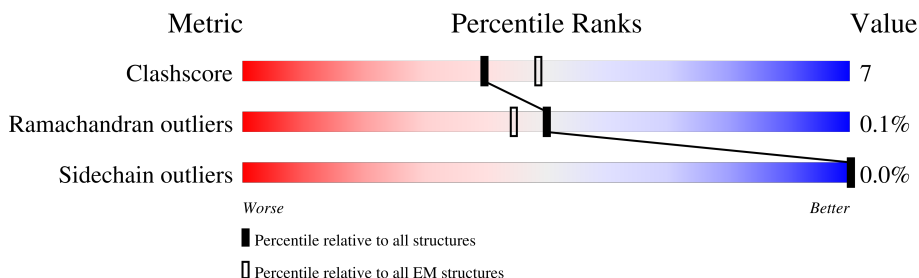
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1056	
1	B	1056	
1	C	1056	
1	D	1056	
2	E	239	
2	F	239	
2	G	239	
2	H	239	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLR	B	1105	-	-	X	-
6	CLR	D	1106	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 36018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Isoform 5 of Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	893	Total	C	N	O	S	0	0
			7116	4623	1159	1286	48		
1	B	893	Total	C	N	O	S	0	0
			7116	4623	1159	1286	48		
1	C	893	Total	C	N	O	S	0	0
			7116	4623	1159	1286	48		
1	D	893	Total	C	N	O	S	0	0
			7116	4623	1159	1286	48		

- Molecule 2 is a protein called Large-conductance Ca²⁺-activated K⁺ channel beta2 subunit, Calcium-activated potassium channel subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	214	Total	C	N	O	S	0	0
			1697	1085	287	312	13		
2	F	202	Total	C	N	O	S	0	0
			1599	1022	271	293	13		
2	G	202	Total	C	N	O	S	0	0
			1599	1022	271	293	13		
2	H	202	Total	C	N	O	S	0	0
			1599	1022	271	293	13		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	

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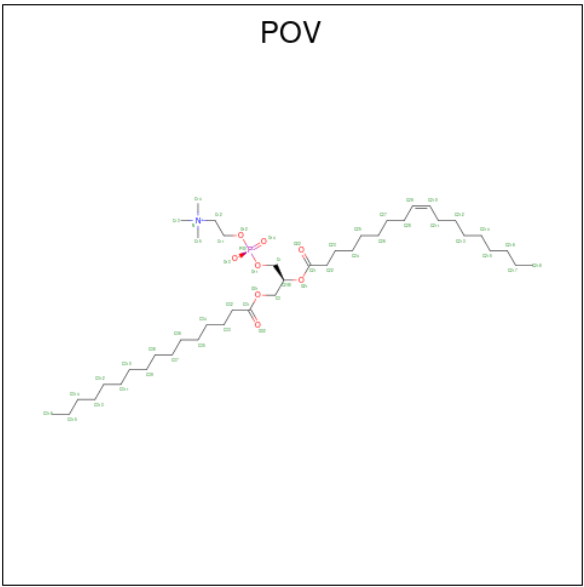
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Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
5	A	1	Total	C	O	P		0
			42	33	8	1		
5	A	1	Total	C	N	O	P	0
			37	27	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
5	A	1	Total	C	O	P		0
			42	33	8	1		
5	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
5	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
5	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
5	B	1	Total	C	O	P		0
			42	33	8	1		
5	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
5	C	1	Total	C	N	O	P	0
			37	27	1	8	1	
5	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
5	D	1	Total	C	N	O	P	0
			35	25	1	8	1	
5	D	1	Total	C	O	P		0
			42	33	8	1		
5	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
5	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
5	E	1	Total	C	O	P		0
			31	22	8	1		
5	F	1	Total	C	O	P		0
			31	22	8	1		
5	G	1	Total	C	O	P		0
			31	22	8	1		
5	H	1	Total	C	O	P		0
			31	22	8	1		

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	

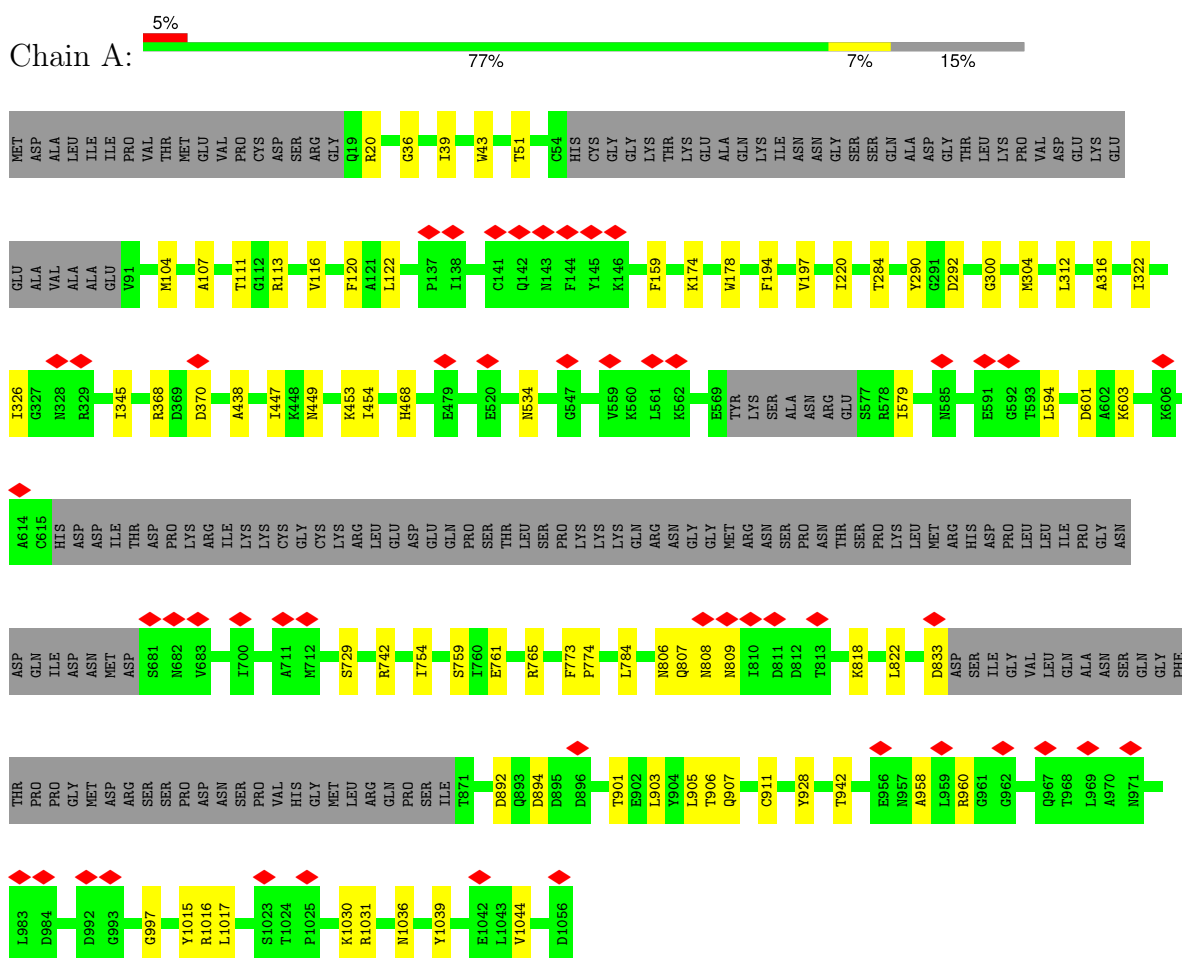
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	3	Total 3	K 3	0
7	C	1	Total 1	K 1	0

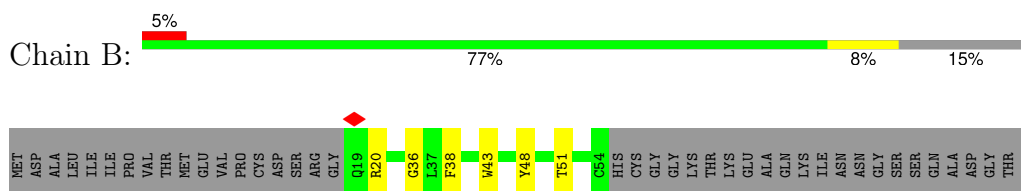
3 Residue-property plots [i](#)

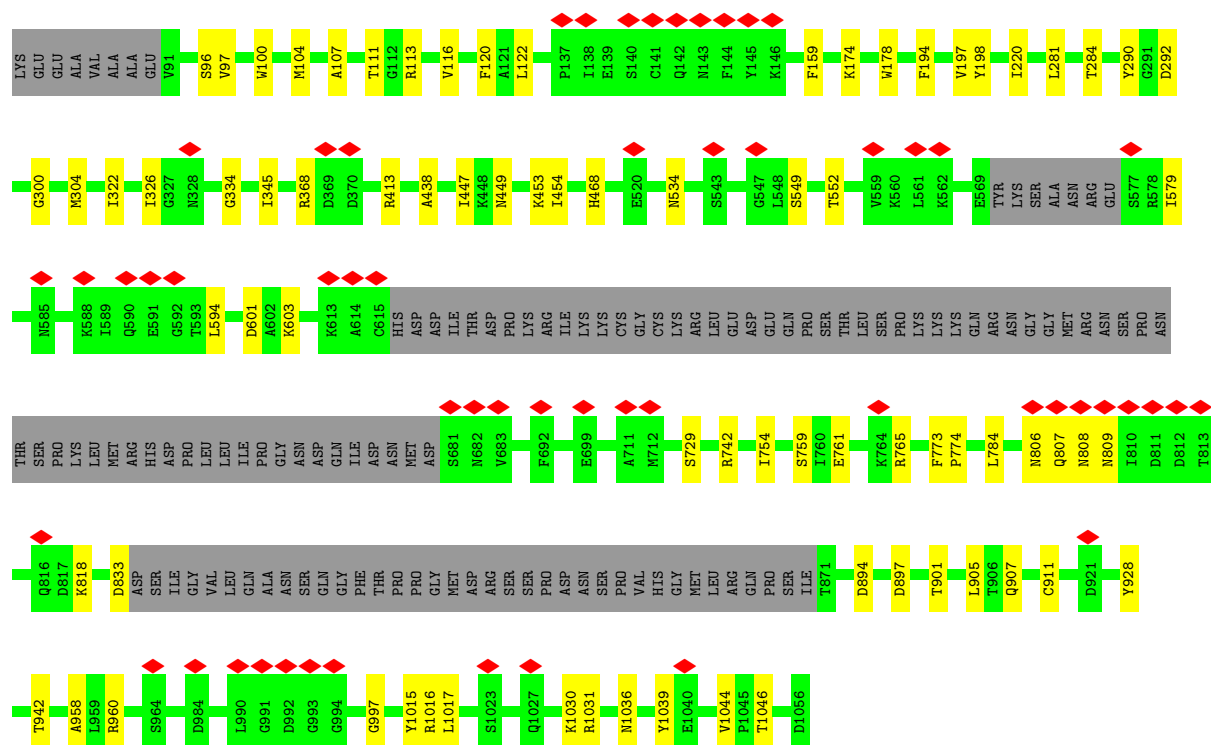
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

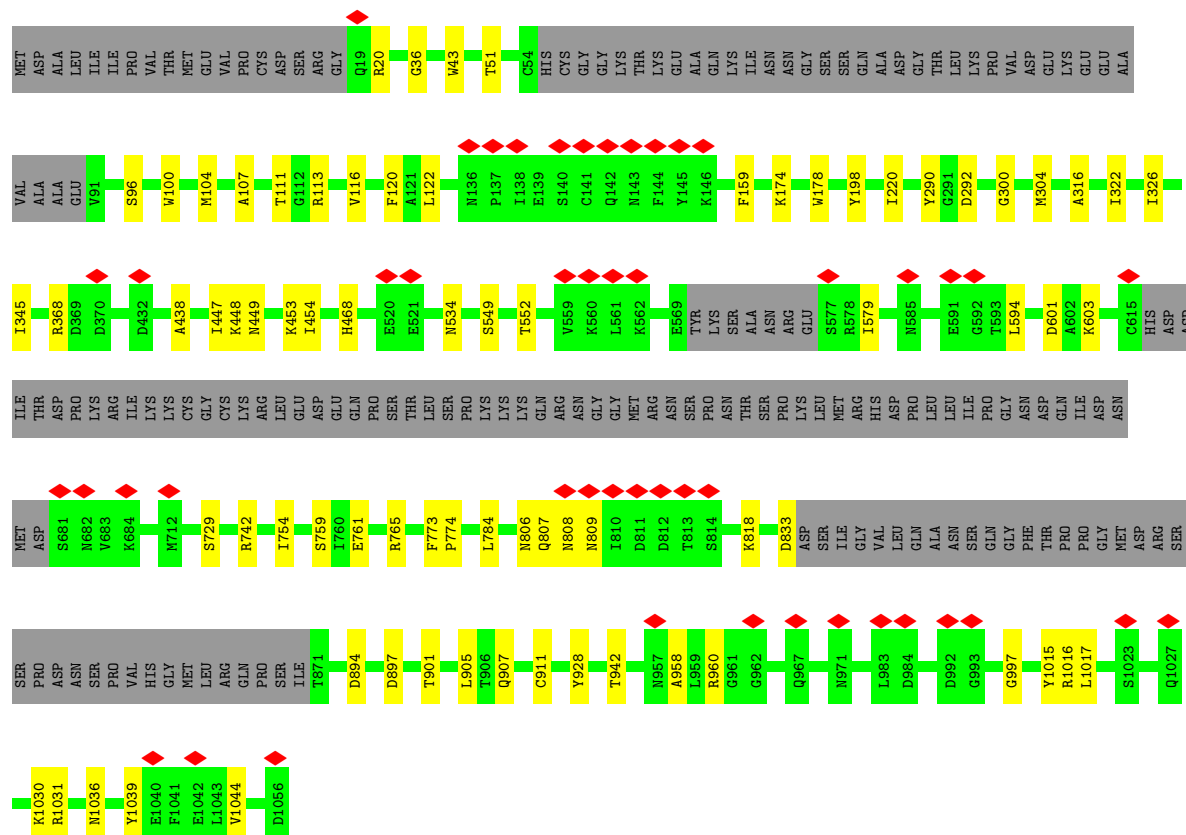
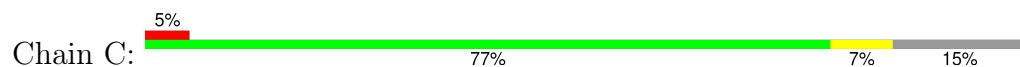


- Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

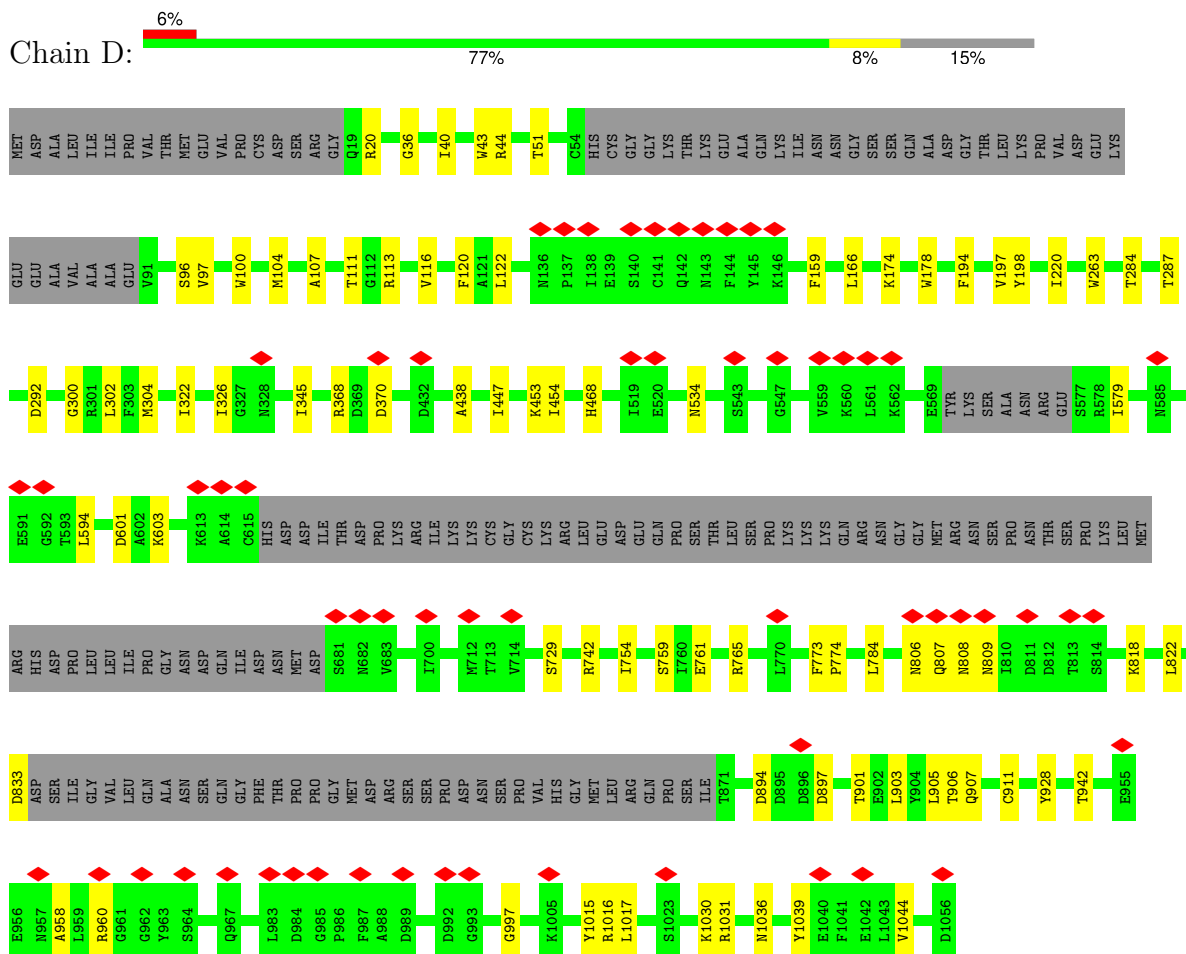




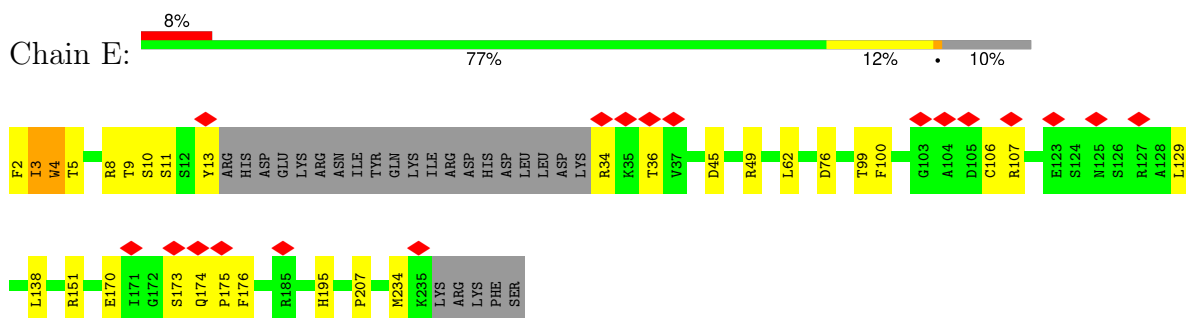
• Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1



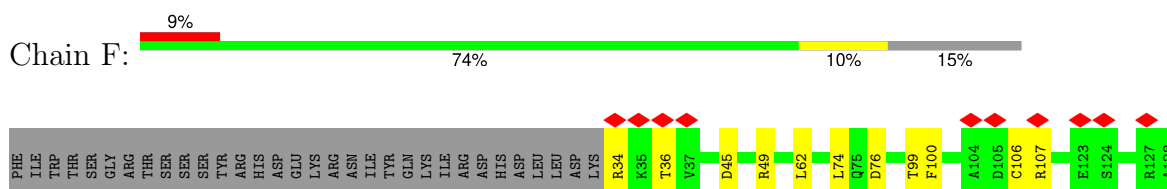
• Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

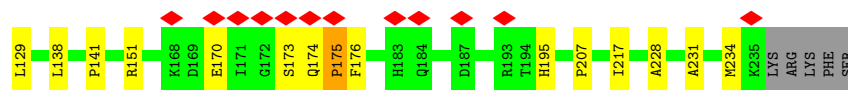


• Molecule 2: Large-conductance Ca²⁺-activated K⁺ channel beta2 subunit, Calcium-activated potassium channel subunit beta-4

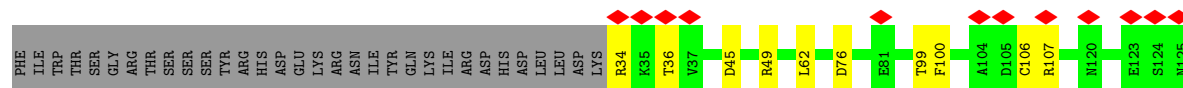
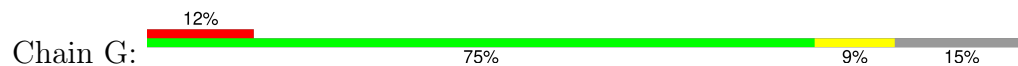


• Molecule 2: Large-conductance Ca²⁺-activated K⁺ channel beta2 subunit, Calcium-activated potassium channel subunit beta-4

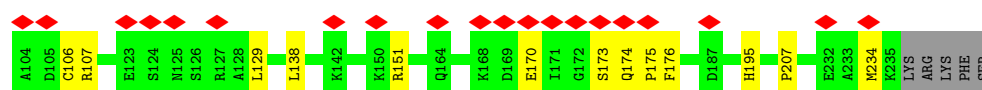
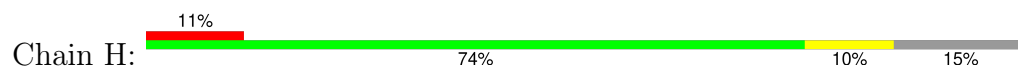




- Molecule 2: Large-conductance Ca^{2+} -activated K^{+} channel beta2 subunit, Calcium-activated potassium channel subunit beta-4



- Molecule 2: Large-conductance Ca^{2+} -activated K^{+} channel beta2 subunit, Calcium-activated potassium channel subunit beta-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	41832	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (\AA)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, POV, MG, K, CA

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	0.55	0/7281	0.76	0/9884
1	B	0.55	0/7281	0.76	0/9884
1	C	0.55	0/7281	0.76	0/9884
1	D	0.55	0/7281	0.76	0/9884
2	E	0.61	0/1736	0.88	0/2359
2	F	0.62	0/1635	0.88	0/2223
2	G	0.62	0/1635	0.88	0/2223
2	H	0.62	0/1635	0.88	0/2223
All	All	0.56	0/35765	0.79	0/48564

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7116	0	7111	91	0
1	B	7116	0	7111	109	0
1	C	7116	0	7111	90	0
1	D	7116	0	7111	122	0
2	E	1697	0	1672	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1599	0	1584	31	0
2	G	1599	0	1584	29	0
2	H	1599	0	1584	38	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	195	0	246	3	0
5	B	153	0	193	1	0
5	C	111	0	140	1	0
5	D	153	0	193	1	0
5	E	31	0	33	1	0
5	F	31	0	33	1	0
5	G	31	0	33	1	0
5	H	31	0	33	1	0
6	A	56	0	92	11	0
6	B	84	0	138	34	0
6	C	84	0	138	20	0
6	D	84	0	138	43	0
7	A	3	0	0	0	0
7	C	1	0	0	0	0
All	All	36018	0	36278	499	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 7.

All (499) 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:D:51:THR:HB	2:H:234:MET:CE	1.57	1.33
1:A:438:ALA:CB	1:B:818:LYS:HE2	1.74	1.18
1:B:51:THR:HB	2:F:234:MET:CE	1.72	1.18
1:B:438:ALA:CB	1:C:818:LYS:HE2	1.75	1.15
1:D:174:LYS:HG2	6:D:1106:CLR:H191	1.27	1.14
1:A:438:ALA:HB1	1:B:818:LYS:HE2	1.27	1.13
1:A:958:ALA:HB3	1:A:960:ARG:NH2	1.63	1.13
1:D:958:ALA:HB3	1:D:960:ARG:HH22	0.97	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:958:ALA:HB3	1:D:960:ARG:NH2	1.63	1.13
1:B:438:ALA:HB1	1:C:818:LYS:HE2	1.26	1.13
1:C:958:ALA:HB3	1:C:960:ARG:HH22	0.97	1.13
1:D:174:LYS:HG3	6:D:1106:CLR:H182	1.29	1.12
1:A:958:ALA:HB3	1:A:960:ARG:HH22	0.97	1.11
1:B:958:ALA:HB3	1:B:960:ARG:NH2	1.63	1.11
1:C:958:ALA:HB3	1:C:960:ARG:NH2	1.63	1.11
1:A:818:LYS:HE2	1:D:438:ALA:CB	1.78	1.11
1:B:958:ALA:HB3	1:B:960:ARG:HH22	0.97	1.10
1:B:958:ALA:CB	1:B:960:ARG:HH22	1.66	1.09
1:A:818:LYS:HE2	1:D:438:ALA:HB1	1.27	1.09
1:A:958:ALA:CB	1:A:960:ARG:HH22	1.66	1.08
1:C:958:ALA:CB	1:C:960:ARG:HH22	1.66	1.07
1:D:958:ALA:CB	1:D:960:ARG:HH22	1.66	1.07
1:D:174:LYS:HG2	6:D:1106:CLR:C19	1.85	1.05
1:B:100:TRP:CG	6:B:1105:CLR:H152	1.93	1.04
1:C:438:ALA:CB	1:D:818:LYS:HE2	1.86	1.04
1:D:51:THR:HB	2:H:234:MET:HE1	1.12	1.04
1:D:51:THR:CB	2:H:234:MET:CE	2.36	1.04
1:D:51:THR:CB	2:H:234:MET:HE1	1.89	1.03
6:B:1107:CLR:H212	6:B:1107:CLR:H183	1.40	1.02
1:C:438:ALA:HB1	1:D:818:LYS:HE2	1.40	1.02
6:C:1108:CLR:H212	6:C:1108:CLR:H183	1.40	1.02
6:D:1107:CLR:H212	6:D:1107:CLR:H183	1.40	0.99
1:A:438:ALA:HB1	1:B:818:LYS:CE	1.94	0.98
6:D:1105:CLR:H211	6:D:1105:CLR:H242	1.46	0.97
1:A:818:LYS:CE	1:D:438:ALA:HB1	1.93	0.97
1:D:174:LYS:CG	6:D:1106:CLR:H191	1.94	0.97
1:A:51:THR:HB	2:E:234:MET:CE	1.97	0.95
1:B:438:ALA:HB1	1:C:818:LYS:CE	1.96	0.94
1:D:174:LYS:HG3	6:D:1106:CLR:C18	1.98	0.92
1:D:96:SER:HB3	6:D:1105:CLR:H192	1.50	0.91
1:C:534:ASN:HD22	1:C:1036:ASN:HD22	1.20	0.90
1:C:174:LYS:HG3	6:C:1107:CLR:H182	1.55	0.89
1:A:534:ASN:HD22	1:A:1036:ASN:HD22	1.20	0.89
1:B:51:THR:HB	2:F:234:MET:HE1	1.53	0.89
1:B:534:ASN:HD22	1:B:1036:ASN:HD22	1.20	0.89
1:D:534:ASN:HD22	1:D:1036:ASN:HD22	1.20	0.88
1:B:174:LYS:HG3	6:B:1106:CLR:H182	1.55	0.87
6:D:1106:CLR:H21	2:H:40:LEU:HD21	1.58	0.85
1:C:51:THR:HB	2:G:234:MET:CE	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ALA:HB2	1:B:818:LYS:HE2	1.58	0.85
1:A:43:TRP:CD1	6:A:1105:CLR:H122	2.13	0.84
1:B:51:THR:HB	2:F:234:MET:HE2	1.59	0.84
2:E:106:CYS:SG	2:H:138:LEU:HD23	2.17	0.84
1:C:438:ALA:HB1	1:D:818:LYS:CE	2.07	0.83
1:A:51:THR:HB	2:E:234:MET:SD	2.18	0.83
2:E:10:SER:HA	2:E:13:TYR:CE2	2.12	0.83
2:E:8:ARG:O	2:E:9:THR:HG22	1.79	0.82
1:D:40:ILE:HA	6:D:1106:CLR:H212	1.60	0.82
1:D:174:LYS:CG	6:D:1106:CLR:C19	2.56	0.81
2:E:10:SER:HA	2:E:13:TYR:HE2	1.43	0.81
1:B:438:ALA:HB2	1:C:818:LYS:HE2	1.61	0.80
1:B:51:THR:CB	2:F:234:MET:CE	2.56	0.80
1:A:284:THR:HG1	1:B:290:TYR:HH	1.30	0.80
1:D:742:ARG:NH1	1:D:754:ILE:HD12	1.98	0.79
1:D:901:THR:HG23	1:D:905:LEU:HD23	1.64	0.79
5:F:301:POV:H37	5:F:301:POV:H24	1.65	0.79
1:A:818:LYS:CD	1:D:438:ALA:HB1	2.12	0.79
1:C:742:ARG:NH1	1:C:754:ILE:HD12	1.98	0.79
1:A:39:ILE:HG22	6:A:1105:CLR:H211	1.63	0.79
1:C:438:ALA:HB2	1:D:818:LYS:HE2	1.65	0.79
5:G:301:POV:H24	5:G:301:POV:H37	1.65	0.79
1:B:100:TRP:CD2	6:B:1105:CLR:H152	2.16	0.79
1:C:901:THR:HG23	1:C:905:LEU:HD23	1.64	0.79
1:A:901:THR:HG23	1:A:905:LEU:HD23	1.64	0.78
5:E:301:POV:H24	5:E:301:POV:H37	1.65	0.78
2:E:151:ARG:HH12	2:H:129:LEU:HD23	1.48	0.78
1:D:1017:LEU:HG	1:D:1031:ARG:CZ	2.14	0.78
1:A:742:ARG:NH1	1:A:754:ILE:HD12	1.98	0.77
5:H:301:POV:H24	5:H:301:POV:H37	1.65	0.77
1:B:1017:LEU:HG	1:B:1031:ARG:CZ	2.14	0.77
1:C:1017:LEU:HG	1:C:1031:ARG:CZ	2.14	0.77
1:B:742:ARG:NH1	1:B:754:ILE:HD12	1.98	0.77
1:A:1017:LEU:HG	1:A:1031:ARG:CZ	2.14	0.77
1:B:901:THR:HG23	1:B:905:LEU:HD23	1.64	0.77
2:F:129:LEU:HD23	2:G:151:ARG:HH12	1.49	0.77
1:A:818:LYS:HE2	1:D:438:ALA:HB2	1.65	0.77
1:A:438:ALA:HB1	1:B:818:LYS:CD	2.14	0.77
1:A:51:THR:CG2	2:E:234:MET:CE	2.64	0.76
1:D:1015:TYR:O	1:D:1031:ARG:HD3	1.87	0.75
1:B:1015:TYR:O	1:B:1031:ARG:HD3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:TRP:CD1	6:B:1105:CLR:H151	2.22	0.74
1:D:51:THR:CB	2:H:234:MET:HE2	2.15	0.74
1:A:51:THR:CG2	2:E:234:MET:HE1	2.18	0.74
1:A:51:THR:HB	2:E:234:MET:HE1	1.70	0.74
1:D:174:LYS:CG	6:D:1106:CLR:H182	2.14	0.74
1:B:96:SER:HB3	6:B:1105:CLR:H192	1.68	0.74
1:C:1015:TYR:O	1:C:1031:ARG:HD3	1.87	0.74
1:B:100:TRP:CD1	6:B:1105:CLR:C15	2.71	0.74
6:B:1105:CLR:C24	6:B:1105:CLR:H211	2.18	0.74
1:C:534:ASN:ND2	1:C:1036:ASN:HD22	1.86	0.74
1:A:1015:TYR:O	1:A:1031:ARG:HD3	1.87	0.73
1:D:534:ASN:ND2	1:D:1036:ASN:HD22	1.86	0.73
1:A:534:ASN:ND2	1:A:1036:ASN:HD22	1.86	0.73
1:B:534:ASN:ND2	1:B:1036:ASN:HD22	1.86	0.73
1:B:284:THR:HG1	1:C:290:TYR:HH	1.35	0.73
1:A:51:THR:CB	2:E:234:MET:CE	2.67	0.73
1:A:316:ALA:HB1	2:E:4:TRP:CH2	2.24	0.72
1:D:287:THR:HG21	2:E:2:PHE:CD2	2.25	0.72
1:A:818:LYS:CE	1:D:438:ALA:CB	2.62	0.71
1:D:345:ILE:HD11	1:D:928:TYR:CE1	2.26	0.71
1:A:345:ILE:HD11	1:A:928:TYR:CE1	2.26	0.71
1:B:438:ALA:HB1	1:C:818:LYS:CD	2.20	0.71
1:B:345:ILE:HD11	1:B:928:TYR:CE1	2.26	0.71
1:D:40:ILE:HG12	6:D:1106:CLR:C21	2.21	0.71
1:B:51:THR:CB	2:F:234:MET:HE1	2.18	0.70
1:C:51:THR:HB	2:G:234:MET:HE1	1.71	0.70
1:C:345:ILE:HD11	1:C:928:TYR:CE1	2.26	0.70
1:D:51:THR:CG2	2:H:234:MET:CE	2.70	0.70
6:B:1105:CLR:H211	6:B:1105:CLR:H242	1.74	0.69
1:C:438:ALA:HB1	1:D:818:LYS:CD	2.21	0.69
1:B:1017:LEU:HG	1:B:1031:ARG:NH2	2.08	0.69
1:A:1017:LEU:HG	1:A:1031:ARG:NH2	2.08	0.69
1:C:1017:LEU:HG	1:C:1031:ARG:NH2	2.08	0.68
1:D:1017:LEU:HG	1:D:1031:ARG:NH2	2.08	0.68
1:D:96:SER:HB3	6:D:1105:CLR:H22	1.76	0.68
1:A:51:THR:CB	2:E:234:MET:HE1	2.24	0.68
1:B:100:TRP:CG	6:B:1105:CLR:C15	2.72	0.67
1:A:174:LYS:HG3	6:A:1105:CLR:H182	1.75	0.67
1:C:549:SER:HG	1:C:552:THR:HG1	1.41	0.67
1:A:43:TRP:CG	6:A:1105:CLR:H122	2.30	0.67
1:D:40:ILE:HA	6:D:1106:CLR:C21	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:THR:CG2	2:E:2:PHE:CD2	2.77	0.66
1:D:300:GLY:O	1:D:304:MET:HG2	1.95	0.66
1:A:300:GLY:O	1:A:304:MET:HG2	1.95	0.66
1:C:300:GLY:O	1:C:304:MET:HG2	1.95	0.66
1:A:51:THR:HG22	2:E:234:MET:HE1	1.77	0.65
1:B:300:GLY:O	1:B:304:MET:HG2	1.95	0.65
1:B:549:SER:HG	1:B:552:THR:HG1	1.44	0.65
1:B:100:TRP:CD2	6:B:1105:CLR:C15	2.80	0.65
1:A:942:THR:HG22	1:A:942:THR:O	1.97	0.65
1:D:51:THR:HB	2:H:234:MET:SD	2.36	0.65
1:D:51:THR:CG2	2:H:234:MET:HE1	2.26	0.65
1:B:51:THR:CB	2:F:234:MET:HE2	2.26	0.65
1:A:438:ALA:CB	1:B:818:LYS:CE	2.60	0.64
1:B:51:THR:HB	2:F:234:MET:SD	2.36	0.64
1:D:942:THR:HG22	1:D:942:THR:O	1.97	0.64
1:D:287:THR:HG23	2:E:2:PHE:CE2	2.31	0.64
1:D:104:MET:SD	1:D:111:THR:OG1	2.56	0.64
1:A:51:THR:HG21	2:E:234:MET:HE2	1.79	0.64
1:B:104:MET:SD	1:B:111:THR:OG1	2.56	0.64
2:E:4:TRP:HE3	2:E:4:TRP:O	1.80	0.64
1:B:100:TRP:NE1	6:B:1105:CLR:H151	2.12	0.63
1:D:958:ALA:CB	1:D:960:ARG:NH2	2.41	0.63
1:A:104:MET:SD	1:A:111:THR:OG1	2.56	0.63
1:C:100:TRP:CH2	6:C:1106:CLR:H232	2.32	0.63
1:A:51:THR:CG2	2:E:234:MET:HE2	2.27	0.63
1:B:942:THR:HG22	1:B:942:THR:O	1.97	0.63
2:F:99:THR:HG21	2:F:107:ARG:HD2	1.81	0.63
1:C:942:THR:O	1:C:942:THR:HG22	1.97	0.63
1:D:100:TRP:CZ3	6:D:1105:CLR:H222	2.33	0.63
2:E:99:THR:HG21	2:E:107:ARG:HD2	1.81	0.62
1:D:97:VAL:HG23	6:D:1105:CLR:C18	2.29	0.62
2:G:99:THR:HG21	2:G:107:ARG:HD2	1.81	0.62
1:A:1016:ARG:HH22	1:A:1044:VAL:HG22	1.64	0.62
1:C:104:MET:SD	1:C:111:THR:OG1	2.56	0.61
1:D:1016:ARG:HH22	1:D:1044:VAL:HG22	1.64	0.61
1:B:907:GLN:OE1	1:B:1030:LYS:NZ	2.30	0.61
2:E:138:LEU:HD23	2:F:106:CYS:SG	2.40	0.61
2:H:99:THR:HG21	2:H:107:ARG:HD2	1.81	0.61
1:B:1016:ARG:HH22	1:B:1044:VAL:HG22	1.64	0.61
1:D:97:VAL:HG23	6:D:1105:CLR:H183	1.82	0.61
1:D:100:TRP:CD2	6:D:1105:CLR:H152	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:HIS:CE1	1:B:784:LEU:HD13	2.36	0.61
1:C:907:GLN:OE1	1:C:1030:LYS:NZ	2.30	0.61
1:C:1016:ARG:HH22	1:C:1044:VAL:HG22	1.64	0.61
1:A:958:ALA:CB	1:A:960:ARG:NH2	2.41	0.61
1:B:958:ALA:CB	1:B:960:ARG:NH2	2.41	0.61
1:A:39:ILE:CG2	6:A:1105:CLR:H211	2.30	0.60
1:B:1016:ARG:NH2	1:B:1044:VAL:HG22	2.17	0.60
1:D:1016:ARG:NH2	1:D:1044:VAL:HG22	2.17	0.60
1:A:1016:ARG:NH2	1:A:1044:VAL:HG22	2.17	0.60
1:C:958:ALA:CB	1:C:960:ARG:NH2	2.41	0.60
1:D:51:THR:CG2	2:H:234:MET:HE2	2.32	0.60
2:E:106:CYS:HB2	2:H:138:LEU:CD2	2.31	0.60
1:B:807:GLN:NE2	1:B:808:ASN:OD1	2.35	0.60
1:C:107:ALA:HB1	1:C:113:ARG:HG2	1.84	0.60
1:D:107:ALA:HB1	1:D:113:ARG:HG2	1.84	0.59
1:B:107:ALA:HB1	1:B:113:ARG:HG2	1.84	0.59
1:D:807:GLN:NE2	1:D:808:ASN:OD1	2.35	0.59
1:C:1016:ARG:NH2	1:C:1044:VAL:HG22	2.17	0.59
1:B:438:ALA:CB	1:C:818:LYS:CE	2.62	0.59
1:C:807:GLN:NE2	1:C:808:ASN:OD1	2.35	0.59
1:A:107:ALA:HB1	1:A:113:ARG:HG2	1.84	0.59
2:G:173:SER:O	2:G:174:GLN:HG3	2.03	0.59
1:A:807:GLN:NE2	1:A:808:ASN:OD1	2.35	0.59
1:C:51:THR:HB	2:G:234:MET:SD	2.43	0.58
2:H:173:SER:O	2:H:174:GLN:HG3	2.03	0.58
2:E:173:SER:O	2:E:174:GLN:HG3	2.03	0.58
1:D:287:THR:HG21	2:E:2:PHE:HD2	1.68	0.58
1:A:290:TYR:HH	1:D:284:THR:HG1	1.50	0.58
1:D:40:ILE:HG12	6:D:1106:CLR:H212	1.84	0.58
1:B:100:TRP:CE2	6:B:1105:CLR:C15	2.87	0.58
6:B:1107:CLR:H212	6:B:1107:CLR:C18	2.18	0.58
1:D:96:SER:CB	6:D:1105:CLR:H192	2.27	0.58
2:E:106:CYS:CB	2:H:138:LEU:CD2	2.82	0.58
1:B:468:HIS:CE1	1:C:784:LEU:HD13	2.39	0.58
6:D:1107:CLR:H183	6:D:1107:CLR:C21	2.19	0.57
2:F:173:SER:O	2:F:174:GLN:HG3	2.03	0.57
1:D:742:ARG:CZ	1:D:754:ILE:HD12	2.35	0.57
6:A:1106:CLR:H121	6:A:1106:CLR:H212	1.86	0.57
2:F:141:PRO:HG3	2:G:106:CYS:O	2.05	0.57
1:A:907:GLN:OE1	1:A:1030:LYS:NZ	2.30	0.57
2:E:10:SER:CA	2:E:13:TYR:HE2	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ARG:CZ	1:A:754:ILE:HD12	2.35	0.56
1:C:742:ARG:CZ	1:C:754:ILE:HD12	2.35	0.56
1:B:742:ARG:CZ	1:B:754:ILE:HD12	2.35	0.56
1:D:100:TRP:CG	6:D:1105:CLR:H152	2.41	0.56
1:D:51:THR:HG21	2:H:234:MET:HE2	1.86	0.56
2:F:129:LEU:HD23	2:G:151:ARG:NH1	2.20	0.56
1:B:51:THR:CG2	2:F:234:MET:HE2	2.36	0.56
1:D:100:TRP:CE2	6:D:1105:CLR:H152	2.41	0.55
2:E:100:PHE:CD2	2:E:151:ARG:HD2	2.42	0.55
1:C:1017:LEU:HA	1:C:1031:ARG:HG2	1.88	0.55
5:C:1109:POV:H13	2:F:74:LEU:HD11	1.89	0.55
2:H:100:PHE:CD2	2:H:151:ARG:HD2	2.42	0.55
1:B:1017:LEU:HA	1:B:1031:ARG:HG2	1.89	0.55
1:D:1017:LEU:HA	1:D:1031:ARG:HG2	1.89	0.55
2:E:2:PHE:HE1	2:E:5:THR:HG1	1.54	0.55
1:C:51:THR:CB	2:G:234:MET:CE	2.81	0.55
1:D:907:GLN:OE1	1:D:1030:LYS:NZ	2.30	0.55
6:D:1105:CLR:H211	6:D:1105:CLR:C24	2.18	0.55
1:C:51:THR:CB	2:G:234:MET:HE1	2.36	0.55
2:G:129:LEU:HD23	2:H:151:ARG:HH12	1.71	0.55
1:A:120:PHE:HD2	1:A:220:ILE:HD11	1.72	0.55
1:A:1017:LEU:HA	1:A:1031:ARG:HG2	1.88	0.55
1:B:120:PHE:HD2	1:B:220:ILE:HD11	1.72	0.55
2:F:100:PHE:CD2	2:F:151:ARG:HD2	2.42	0.55
2:G:62:LEU:HD13	2:G:207:PRO:HB2	1.89	0.54
1:D:833:ASP:OD1	1:D:833:ASP:N	2.36	0.54
1:C:120:PHE:HD2	1:C:220:ILE:HD11	1.72	0.54
1:C:174:LYS:HG3	6:C:1107:CLR:H8	1.89	0.54
2:G:100:PHE:CD2	2:G:151:ARG:HD2	2.42	0.54
2:H:62:LEU:HD13	2:H:207:PRO:HB2	1.89	0.54
1:A:833:ASP:OD1	1:A:833:ASP:N	2.36	0.54
1:B:174:LYS:HG3	6:B:1106:CLR:H8	1.89	0.54
1:D:287:THR:CG2	2:E:2:PHE:CE2	2.90	0.54
1:C:449:ASN:ND2	1:D:897:ASP:OD2	2.39	0.54
2:E:129:LEU:HD23	2:F:151:ARG:HH12	1.72	0.54
1:D:120:PHE:HD2	1:D:220:ILE:HD11	1.72	0.54
2:E:151:ARG:NH1	2:H:129:LEU:HD23	2.19	0.54
2:E:62:LEU:HD13	2:E:207:PRO:HB2	1.89	0.53
1:B:51:THR:CG2	2:F:234:MET:CE	2.86	0.53
1:C:468:HIS:CE1	1:D:784:LEU:HD13	2.44	0.53
1:D:759:SER:OG	1:D:761:GLU:OE1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:62:LEU:HD13	2:F:207:PRO:HB2	1.89	0.53
1:C:316:ALA:HA	2:E:8:ARG:NH1	2.24	0.53
1:C:438:ALA:CB	1:D:818:LYS:CE	2.70	0.53
1:D:594:LEU:HD12	1:D:594:LEU:O	2.09	0.53
1:A:594:LEU:HD12	1:A:594:LEU:O	2.09	0.52
1:B:759:SER:OG	1:B:761:GLU:OE1	2.27	0.52
1:C:594:LEU:HD12	1:C:594:LEU:O	2.09	0.52
2:E:4:TRP:HB3	2:E:8:ARG:HG2	1.91	0.52
1:A:742:ARG:HG3	1:A:773:PHE:CD1	2.45	0.52
1:A:759:SER:OG	1:A:761:GLU:OE1	2.27	0.52
1:C:100:TRP:CZ3	6:C:1106:CLR:H232	2.44	0.52
1:D:742:ARG:HG3	1:D:773:PHE:CD1	2.45	0.52
1:D:287:THR:HG23	2:E:2:PHE:HE2	1.73	0.52
1:D:100:TRP:CD1	6:D:1105:CLR:H152	2.44	0.52
1:B:594:LEU:HD12	1:B:594:LEU:O	2.09	0.52
2:E:9:THR:HG23	2:E:11:SER:OG	2.10	0.52
1:B:198:TYR:HE2	6:B:1107:CLR:H11	1.75	0.52
1:C:759:SER:OG	1:C:761:GLU:OE1	2.27	0.52
1:D:198:TYR:HE2	6:D:1107:CLR:H11	1.74	0.51
1:B:742:ARG:HG3	1:B:773:PHE:CD1	2.45	0.51
1:C:742:ARG:HG3	1:C:773:PHE:CD1	2.45	0.51
1:C:51:THR:CG2	2:G:234:MET:CE	2.87	0.51
1:D:287:THR:CG2	2:E:2:PHE:HD2	2.21	0.51
1:A:312:LEU:HD23	2:E:3:ILE:HD11	1.92	0.51
5:D:1108:POV:H28	5:D:1108:POV:H37	1.93	0.51
2:E:76:ASP:OD2	2:E:195:HIS:HB3	2.11	0.51
1:C:198:TYR:HE2	6:C:1108:CLR:H11	1.75	0.51
1:B:100:TRP:CD1	6:B:1105:CLR:H152	2.31	0.51
1:D:453:LYS:O	1:D:453:LYS:HG2	2.11	0.51
5:A:1110:POV:H28	5:A:1110:POV:H37	1.93	0.50
5:A:1113:POV:H37	5:A:1113:POV:H28	1.93	0.50
1:B:100:TRP:CE2	6:B:1105:CLR:C16	2.94	0.50
1:B:601:ASP:OD2	1:B:603:LYS:HG2	2.11	0.50
1:C:453:LYS:O	1:C:453:LYS:HG2	2.11	0.50
1:A:601:ASP:OD2	1:A:603:LYS:HG2	2.11	0.50
2:F:76:ASP:OD2	2:F:195:HIS:HB3	2.11	0.50
2:G:76:ASP:OD2	2:G:195:HIS:HB3	2.11	0.50
5:B:1110:POV:H37	5:B:1110:POV:H28	1.93	0.50
1:C:601:ASP:OD2	1:C:603:LYS:HG2	2.11	0.50
1:B:453:LYS:O	1:B:453:LYS:HG2	2.11	0.50
1:D:20:ARG:NH2	1:D:20:ARG:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:O	1:A:453:LYS:HG2	2.11	0.50
6:B:1107:CLR:H183	6:B:1107:CLR:C21	2.19	0.50
1:C:51:THR:CG2	2:G:234:MET:HE1	2.40	0.50
1:C:96:SER:HB3	6:C:1106:CLR:H192	1.93	0.50
1:C:833:ASP:OD1	1:C:833:ASP:N	2.36	0.50
1:A:174:LYS:HG2	6:A:1105:CLR:H191	1.92	0.49
5:A:1111:POV:H13	2:H:74:LEU:HD11	1.93	0.49
2:H:76:ASP:OD2	2:H:195:HIS:HB3	2.11	0.49
1:D:287:THR:HG23	2:E:2:PHE:CD2	2.45	0.49
1:D:601:ASP:OD2	1:D:603:LYS:HG2	2.11	0.49
1:A:20:ARG:NH2	1:A:20:ARG:HG3	2.26	0.49
1:B:20:ARG:NH2	1:B:20:ARG:HG3	2.26	0.49
1:C:20:ARG:NH2	1:C:20:ARG:HG3	2.26	0.49
1:D:174:LYS:HG3	6:D:1106:CLR:H191	1.90	0.49
6:D:1107:CLR:C21	6:D:1107:CLR:H121	2.43	0.49
6:B:1107:CLR:C21	6:B:1107:CLR:H121	2.43	0.49
6:C:1108:CLR:C21	6:C:1108:CLR:H121	2.43	0.49
1:D:40:ILE:CG1	6:D:1106:CLR:H211	2.42	0.49
1:D:263:TRP:HA	2:H:69:TRP:CH2	2.48	0.49
6:D:1107:CLR:H272	6:D:1107:CLR:H231	1.69	0.49
6:D:1106:CLR:H211	6:D:1106:CLR:H241	1.94	0.48
1:B:833:ASP:OD1	1:B:833:ASP:N	2.36	0.48
1:B:100:TRP:NE1	6:B:1105:CLR:C15	2.76	0.48
1:D:894:ASP:OD1	1:D:894:ASP:N	2.47	0.48
2:E:8:ARG:O	2:E:9:THR:CG2	2.56	0.48
2:E:106:CYS:CB	2:H:138:LEU:HD23	2.43	0.48
1:D:806:ASN:HA	1:D:809:ASN:HD21	1.79	0.48
1:D:40:ILE:CG1	6:D:1106:CLR:C21	2.90	0.47
1:A:894:ASP:OD1	1:A:894:ASP:N	2.47	0.47
2:E:170:GLU:OE1	2:E:173:SER:HB2	2.15	0.47
1:A:368:ARG:HG2	1:A:368:ARG:HH21	1.79	0.47
1:B:20:ARG:CG	1:B:20:ARG:HH21	2.28	0.47
1:B:368:ARG:HH21	1:B:368:ARG:HG2	1.79	0.47
1:C:20:ARG:CG	1:C:20:ARG:HH21	2.28	0.47
2:E:4:TRP:HB2	2:E:8:ARG:H	1.80	0.47
1:A:784:LEU:HD13	1:D:468:HIS:CE1	2.49	0.47
1:D:368:ARG:HG2	1:D:368:ARG:HH21	1.79	0.47
2:F:170:GLU:OE1	2:F:173:SER:HB2	2.15	0.47
1:B:894:ASP:OD1	1:B:894:ASP:N	2.47	0.47
6:D:1106:CLR:H21	2:H:40:LEU:CD2	2.37	0.47
1:A:806:ASN:HA	1:A:809:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:CG	6:D:1106:CLR:H193	2.43	0.47
2:G:138:LEU:HD23	2:H:106:CYS:SG	2.55	0.47
1:C:116:VAL:HG13	1:C:220:ILE:HB	1.97	0.47
1:C:368:ARG:HH21	1:C:368:ARG:HG2	1.79	0.47
2:E:2:PHE:O	2:E:4:TRP:N	2.47	0.47
2:G:170:GLU:OE1	2:G:173:SER:HB2	2.15	0.47
1:B:100:TRP:HB2	6:B:1105:CLR:H72	1.96	0.46
1:C:806:ASN:HA	1:C:809:ASN:HD21	1.79	0.46
1:D:116:VAL:HG13	1:D:220:ILE:HB	1.97	0.46
1:B:806:ASN:HA	1:B:809:ASN:HD21	1.79	0.46
1:D:579:ILE:O	1:D:579:ILE:HG22	2.16	0.46
1:D:20:ARG:HH21	1:D:20:ARG:CG	2.28	0.46
6:C:1108:CLR:C21	6:C:1108:CLR:C18	2.85	0.46
1:A:322:ILE:O	1:A:326:ILE:HG13	2.16	0.46
1:C:322:ILE:O	1:C:326:ILE:HG13	2.16	0.46
1:C:894:ASP:OD1	1:C:894:ASP:N	2.47	0.46
1:B:43:TRP:CD1	6:B:1106:CLR:H122	2.51	0.46
1:B:48:TYR:CE2	2:F:228:ALA:HB2	2.51	0.46
1:B:942:THR:O	1:B:942:THR:CG2	2.64	0.46
1:A:20:ARG:HH21	1:A:20:ARG:CG	2.28	0.46
1:B:116:VAL:HG13	1:B:220:ILE:HB	1.97	0.46
6:C:1106:CLR:C21	6:C:1106:CLR:H242	2.40	0.46
2:H:170:GLU:OE1	2:H:173:SER:HB2	2.15	0.46
1:D:174:LYS:HG3	6:D:1106:CLR:H8	1.99	0.45
1:B:174:LYS:HG3	6:B:1106:CLR:C18	2.38	0.45
1:C:43:TRP:CD1	6:C:1107:CLR:H122	2.51	0.45
6:C:1108:CLR:H212	6:C:1108:CLR:C18	2.18	0.45
1:D:942:THR:O	1:D:942:THR:CG2	2.64	0.45
1:A:116:VAL:HG13	1:A:220:ILE:HB	1.97	0.45
1:B:51:THR:HG21	2:F:231:ALA:HB1	1.98	0.45
1:B:322:ILE:O	1:B:326:ILE:HG13	2.16	0.45
1:B:579:ILE:O	1:B:579:ILE:HG22	2.16	0.45
1:C:942:THR:O	1:C:942:THR:CG2	2.64	0.45
2:E:106:CYS:SG	2:H:138:LEU:CD2	2.98	0.45
2:G:45:ASP:O	2:G:49:ARG:HG3	2.16	0.45
1:C:579:ILE:O	1:C:579:ILE:HG22	2.16	0.45
1:D:174:LYS:HB2	6:D:1106:CLR:H193	1.98	0.45
1:D:322:ILE:O	1:D:326:ILE:HG13	2.16	0.45
2:H:45:ASP:O	2:H:49:ARG:HG3	2.16	0.45
1:A:579:ILE:HG22	1:A:579:ILE:O	2.16	0.44
1:A:903:LEU:O	1:A:906:THR:OG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG23	6:B:1105:CLR:H222	1.99	0.44
2:F:45:ASP:O	2:F:49:ARG:HG3	2.16	0.44
1:B:742:ARG:HH12	1:B:754:ILE:HD12	1.81	0.44
2:E:45:ASP:O	2:E:49:ARG:HG3	2.16	0.44
2:E:176:PHE:O	2:E:176:PHE:CD1	2.70	0.44
2:H:176:PHE:O	2:H:176:PHE:CD1	2.70	0.44
1:A:292:ASP:OD1	1:A:292:ASP:N	2.51	0.44
1:A:892:ASP:OD2	1:A:1030:LYS:NZ	2.43	0.44
1:B:292:ASP:OD1	1:B:292:ASP:N	2.51	0.44
1:D:822:LEU:HD12	1:D:822:LEU:HA	1.85	0.44
1:A:818:LYS:HD3	1:D:438:ALA:HB1	1.97	0.44
2:F:62:LEU:HD12	2:F:62:LEU:HA	1.85	0.44
1:A:174:LYS:CG	6:A:1105:CLR:H191	2.48	0.44
1:C:292:ASP:OD1	1:C:292:ASP:N	2.51	0.44
1:D:292:ASP:N	1:D:292:ASP:OD1	2.51	0.44
2:F:176:PHE:O	2:F:176:PHE:CD1	2.70	0.44
2:G:176:PHE:CD1	2:G:176:PHE:O	2.70	0.44
1:C:438:ALA:HB1	1:D:818:LYS:HD3	1.97	0.44
1:C:742:ARG:HD2	1:C:774:PRO:HD2	2.00	0.44
1:D:742:ARG:HD2	1:D:774:PRO:HD2	1.99	0.43
1:C:174:LYS:CG	6:C:1107:CLR:H182	2.38	0.43
2:E:4:TRP:CB	2:E:8:ARG:HG2	2.48	0.43
1:A:942:THR:O	1:A:942:THR:CG2	2.64	0.43
1:B:447:ILE:HG22	1:B:454:ILE:HG21	2.00	0.43
6:B:1107:CLR:C18	6:B:1107:CLR:C21	2.86	0.43
1:C:174:LYS:HG2	6:C:1107:CLR:H191	2.00	0.43
1:B:742:ARG:HD2	1:B:774:PRO:HD2	2.00	0.43
1:D:911:CYS:SG	1:D:1031:ARG:O	2.77	0.43
6:C:1107:CLR:H162	6:C:1107:CLR:H222	1.51	0.43
1:D:36:GLY:HA3	1:D:178:TRP:CZ2	2.54	0.43
2:F:76:ASP:OD2	2:F:195:HIS:CD2	2.72	0.43
1:A:447:ILE:HG22	1:A:454:ILE:HG21	2.00	0.43
1:C:51:THR:CG2	2:G:234:MET:HE2	2.49	0.43
1:B:36:GLY:HA3	1:B:178:TRP:CZ2	2.54	0.43
1:D:96:SER:CB	6:D:1105:CLR:H22	2.47	0.43
2:G:76:ASP:OD2	2:G:195:HIS:CD2	2.72	0.43
1:A:449:ASN:ND2	1:B:897:ASP:OD2	2.43	0.43
1:B:174:LYS:HG2	6:B:1106:CLR:H191	2.01	0.43
2:E:10:SER:HA	2:E:13:TYR:CD2	2.51	0.43
1:A:438:ALA:HB1	1:B:818:LYS:HD3	1.95	0.43
1:A:742:ARG:HD2	1:A:774:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ARG:HG3	1:B:20:ARG:HH21	1.84	0.43
1:B:284:THR:OG1	1:C:290:TYR:OH	2.16	0.43
1:B:534:ASN:ND2	1:B:1036:ASN:ND2	2.63	0.42
1:B:911:CYS:SG	1:B:1031:ARG:O	2.77	0.42
1:C:36:GLY:HA3	1:C:178:TRP:CZ2	2.54	0.42
1:B:449:ASN:ND2	1:C:897:ASP:OD2	2.46	0.42
1:C:100:TRP:CE2	6:C:1106:CLR:H152	2.54	0.42
1:C:729:SER:O	1:C:765:ARG:NH2	2.53	0.42
1:D:447:ILE:HG22	1:D:454:ILE:HG21	2.00	0.42
1:A:20:ARG:HG3	1:A:20:ARG:HH21	1.84	0.42
1:A:729:SER:O	1:A:765:ARG:NH2	2.53	0.42
1:B:194:PHE:O	1:B:197:VAL:HG12	2.20	0.42
2:E:76:ASP:OD2	2:E:195:HIS:CD2	2.72	0.42
2:H:76:ASP:OD2	2:H:195:HIS:CD2	2.72	0.42
1:B:38:PHE:CE1	2:F:217:ILE:HG13	2.55	0.42
1:B:729:SER:O	1:B:765:ARG:NH2	2.53	0.42
6:C:1106:CLR:H231	6:C:1106:CLR:H263	1.65	0.42
6:C:1108:CLR:H182	6:C:1108:CLR:H8	1.78	0.42
1:A:194:PHE:O	1:A:197:VAL:HG12	2.20	0.42
1:C:447:ILE:HG22	1:C:454:ILE:HG21	2.00	0.42
1:A:36:GLY:HA3	1:A:178:TRP:CZ2	2.54	0.42
6:B:1105:CLR:H112	6:B:1105:CLR:H12	1.90	0.42
2:G:174:GLN:HA	2:G:175:PRO:HD2	1.90	0.42
1:B:1046:THR:O	1:B:1046:THR:OG1	2.38	0.42
1:A:911:CYS:SG	1:A:1031:ARG:O	2.77	0.42
6:A:1106:CLR:H121	6:A:1106:CLR:C21	2.49	0.42
6:B:1105:CLR:C22	6:B:1105:CLR:C18	2.97	0.42
1:C:911:CYS:SG	1:C:1031:ARG:O	2.77	0.42
1:D:166:LEU:HD23	1:D:166:LEU:HA	1.93	0.42
2:H:34:ARG:O	2:H:36:THR:N	2.53	0.42
2:H:62:LEU:HD12	2:H:62:LEU:HA	1.85	0.42
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.86	0.42
1:D:729:SER:O	1:D:765:ARG:NH2	2.53	0.42
2:H:173:SER:O	2:H:174:GLN:CG	2.68	0.42
6:C:1108:CLR:H183	6:C:1108:CLR:C21	2.19	0.42
2:F:174:GLN:HA	2:F:175:PRO:HD2	1.90	0.42
1:C:20:ARG:HG3	1:C:20:ARG:HH21	1.84	0.41
6:D:1107:CLR:H232	6:D:1107:CLR:H211	1.84	0.41
1:D:302:LEU:HD21	2:H:64:ILE:HD13	2.01	0.41
1:B:122:LEU:HD12	1:B:159:PHE:CD2	2.56	0.41
1:B:174:LYS:CG	6:B:1106:CLR:H182	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:TYR:CE2	6:B:1107:CLR:H11	2.55	0.41
6:B:1105:CLR:C22	6:B:1105:CLR:H181	2.51	0.41
6:D:1105:CLR:H183	6:D:1105:CLR:H20	1.68	0.41
6:A:1106:CLR:H272	6:A:1106:CLR:H231	1.85	0.41
1:C:122:LEU:HD12	1:C:159:PHE:CD2	2.56	0.41
1:C:448:LYS:HD3	1:C:448:LYS:HA	1.90	0.41
1:C:742:ARG:HH12	1:C:754:ILE:HD12	1.81	0.41
1:D:903:LEU:O	1:D:906:THR:OG1	2.31	0.41
2:E:62:LEU:HD12	2:E:62:LEU:HA	1.85	0.41
1:A:370:ASP:OD1	1:A:370:ASP:N	2.54	0.41
1:D:194:PHE:O	1:D:197:VAL:HG12	2.20	0.41
2:G:141:PRO:HG3	2:H:106:CYS:O	2.21	0.41
1:B:594:LEU:HD12	1:B:594:LEU:C	2.41	0.41
1:D:43:TRP:CD1	6:D:1106:CLR:H122	2.55	0.41
1:A:122:LEU:HD12	1:A:159:PHE:CD2	2.56	0.41
1:D:594:LEU:HD12	1:D:594:LEU:C	2.41	0.41
6:B:1105:CLR:H221	6:B:1105:CLR:H162	1.34	0.41
1:C:51:THR:HG21	2:G:234:MET:HE2	2.03	0.41
6:C:1106:CLR:H183	6:C:1106:CLR:H20	1.74	0.41
1:D:122:LEU:HD12	1:D:159:PHE:CD2	2.56	0.41
2:F:34:ARG:O	2:F:36:THR:N	2.53	0.41
2:G:34:ARG:O	2:G:36:THR:N	2.53	0.41
1:A:822:LEU:HD12	1:A:822:LEU:HA	1.85	0.41
1:A:997:GLY:HA3	1:A:1039:TYR:CG	2.56	0.41
1:B:334:GLY:O	1:B:413:ARG:NH2	2.42	0.41
6:B:1105:CLR:H182	6:B:1105:CLR:H8	1.75	0.41
1:C:51:THR:HG22	2:G:234:MET:HE1	2.03	0.40
1:C:997:GLY:HA3	1:C:1039:TYR:CG	2.56	0.40
2:E:173:SER:O	2:E:174:GLN:CG	2.68	0.40
2:G:173:SER:O	2:G:174:GLN:CG	2.68	0.40
1:D:997:GLY:HA3	1:D:1039:TYR:CG	2.56	0.40
6:D:1106:CLR:H183	6:D:1106:CLR:H20	1.75	0.40
1:A:174:LYS:HG3	6:A:1105:CLR:C18	2.49	0.40
2:E:34:ARG:O	2:E:36:THR:N	2.53	0.40
1:D:44:ARG:NH1	2:H:40:LEU:HD22	2.37	0.40
1:D:198:TYR:CE2	6:D:1107:CLR:H11	2.54	0.40
1:D:370:ASP:N	1:D:370:ASP:OD1	2.54	0.40
1:B:997:GLY:HA3	1:B:1039:TYR:CG	2.56	0.40
2:E:4:TRP:HB2	2:E:8:ARG:N	2.37	0.40
2:F:138:LEU:HD23	2:G:106:CYS:SG	2.61	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	883/1056 (84%)	857 (97%)	26 (3%)	0	100	100
1	B	883/1056 (84%)	856 (97%)	27 (3%)	0	100	100
1	C	883/1056 (84%)	857 (97%)	26 (3%)	0	100	100
1	D	883/1056 (84%)	857 (97%)	26 (3%)	0	100	100
2	E	210/239 (88%)	194 (92%)	14 (7%)	2 (1%)	13	36
2	F	200/239 (84%)	188 (94%)	11 (6%)	1 (0%)	25	53
2	G	200/239 (84%)	188 (94%)	11 (6%)	1 (0%)	25	53
2	H	200/239 (84%)	188 (94%)	11 (6%)	1 (0%)	25	53
All	All	4342/5180 (84%)	4185 (96%)	152 (4%)	5 (0%)	50	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	3	ILE
2	F	175	PRO
2	E	175	PRO
2	G	175	PRO
2	H	175	PRO

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	786/928 (85%)	786 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	786/928 (85%)	786 (100%)	0	100	100
1	C	786/928 (85%)	786 (100%)	0	100	100
1	D	786/928 (85%)	786 (100%)	0	100	100
2	E	193/218 (88%)	192 (100%)	1 (0%)	86	95
2	F	182/218 (84%)	182 (100%)	0	100	100
2	G	182/218 (84%)	182 (100%)	0	100	100
2	H	182/218 (84%)	182 (100%)	0	100	100
All	All	3883/4584 (85%)	3882 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	4	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	465	ASN
1	A	468	HIS
1	A	534	ASN
1	A	807	GLN
1	A	808	ASN
1	A	816	GLN
1	A	884	ASN
1	B	157	ASN
1	B	465	ASN
1	B	468	HIS
1	B	534	ASN
1	B	807	GLN
1	B	808	ASN
1	B	816	GLN
1	C	157	ASN
1	C	465	ASN
1	C	468	HIS
1	C	534	ASN
1	C	807	GLN
1	C	808	ASN

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Mol	Chain	Res	Type
1	C	816	GLN
1	C	884	ASN
1	D	157	ASN
1	D	465	ASN
1	D	468	HIS
1	D	534	ASN
1	D	807	GLN
1	D	808	ASN
1	D	816	GLN
1	D	884	ASN
2	G	195	HIS
2	H	195	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 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	POV	A	1110	-	41,41,51	1.02	2 (4%)	44,46,59	0.97	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLR	B	1105	-	31,31,31	0.85	2 (6%)	48,48,48	1.52	8 (16%)
5	POV	B	1110	-	41,41,51	1.02	2 (4%)	44,46,59	0.97	3 (6%)
6	CLR	D	1107	-	31,31,31	0.85	2 (6%)	48,48,48	1.52	9 (18%)
5	POV	A	1111	-	36,36,51	0.82	0	42,44,59	0.50	0
6	CLR	B	1107	-	31,31,31	0.84	2 (6%)	48,48,48	1.52	9 (18%)
6	CLR	C	1106	-	31,31,31	0.81	1 (3%)	48,48,48	1.58	9 (18%)
5	POV	B	1104	-	34,34,51	1.15	2 (5%)	40,42,59	2.53	8 (20%)
6	CLR	D	1105	-	31,31,31	0.84	2 (6%)	48,48,48	1.54	8 (16%)
5	POV	A	1113	-	41,41,51	1.02	2 (4%)	44,46,59	0.97	3 (6%)
5	POV	D	1104	-	34,34,51	1.15	2 (5%)	40,42,59	2.53	8 (20%)
6	CLR	A	1105	-	31,31,31	0.75	0	48,48,48	1.32	7 (14%)
6	CLR	D	1106	-	31,31,31	0.85	2 (6%)	48,48,48	1.62	6 (12%)
5	POV	A	1104	-	34,34,51	1.15	2 (5%)	40,42,59	2.53	8 (20%)
5	POV	C	1110	-	38,38,51	0.57	0	44,46,59	0.51	0
5	POV	D	1110	-	38,38,51	0.57	0	44,46,59	0.51	0
5	POV	C	1109	-	36,36,51	0.83	0	42,44,59	0.50	0
5	POV	C	1105	-	34,34,51	1.15	2 (5%)	40,42,59	2.53	8 (20%)
6	CLR	C	1107	-	31,31,31	0.38	0	48,48,48	0.49	0
6	CLR	C	1108	-	31,31,31	0.85	2 (6%)	48,48,48	1.52	9 (18%)
5	POV	D	1109	-	36,36,51	0.83	0	42,44,59	0.50	0
5	POV	A	1112	-	38,38,51	0.57	0	44,46,59	0.51	0
5	POV	G	301	-	30,30,51	1.19	2 (6%)	33,35,59	1.21	3 (9%)
5	POV	H	301	-	30,30,51	1.19	2 (6%)	33,35,59	1.21	3 (9%)
5	POV	D	1108	-	41,41,51	1.02	2 (4%)	44,46,59	0.97	3 (6%)
6	CLR	A	1106	-	31,31,31	0.80	0	48,48,48	1.06	4 (8%)
5	POV	B	1109	-	38,38,51	0.57	0	44,46,59	0.51	0
5	POV	E	301	-	30,30,51	1.19	2 (6%)	33,35,59	1.20	3 (9%)
6	CLR	B	1106	-	31,31,31	0.38	0	48,48,48	0.50	0
5	POV	F	301	-	30,30,51	1.18	2 (6%)	33,35,59	1.21	3 (9%)
5	POV	B	1108	-	36,36,51	0.83	0	42,44,59	0.49	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	POV	A	1110	-	-	15/45/45/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	B	1105	-	-	7/10/68/68	0/4/4/4
5	POV	B	1110	-	-	15/45/45/55	-
6	CLR	D	1107	-	-	7/10/68/68	0/4/4/4
5	POV	A	1111	-	-	7/40/40/55	-
6	CLR	B	1107	-	-	7/10/68/68	0/4/4/4
6	CLR	C	1106	-	-	9/10/68/68	0/4/4/4
5	POV	B	1104	-	-	19/38/38/55	-
6	CLR	D	1105	-	-	7/10/68/68	0/4/4/4
5	POV	A	1113	-	-	15/45/45/55	-
5	POV	D	1104	-	-	19/38/38/55	-
6	CLR	A	1105	-	-	6/10/68/68	0/4/4/4
6	CLR	D	1106	-	-	7/10/68/68	0/4/4/4
5	POV	A	1104	-	-	19/38/38/55	-
5	POV	C	1110	-	-	16/42/42/55	-
5	POV	D	1110	-	-	16/42/42/55	-
5	POV	C	1109	-	-	7/40/40/55	-
5	POV	C	1105	-	-	19/38/38/55	-
6	CLR	C	1107	-	-	7/10/68/68	0/4/4/4
6	CLR	C	1108	-	-	7/10/68/68	0/4/4/4
5	POV	D	1109	-	-	7/40/40/55	-
5	POV	A	1112	-	-	16/42/42/55	-
5	POV	G	301	-	-	15/34/34/55	-
5	POV	H	301	-	-	15/34/34/55	-
5	POV	D	1108	-	-	15/45/45/55	-
6	CLR	A	1106	-	-	3/10/68/68	0/4/4/4
5	POV	B	1109	-	-	16/42/42/55	-
5	POV	E	301	-	-	15/34/34/55	-
6	CLR	B	1106	-	-	7/10/68/68	0/4/4/4
5	POV	F	301	-	-	15/34/34/55	-
5	POV	B	1108	-	-	7/40/40/55	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1110	POV	O31-C31	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1113	POV	O31-C31	4.38	1.46	1.33
5	D	1108	POV	O31-C31	4.37	1.46	1.33
5	A	1110	POV	O31-C31	4.37	1.46	1.33
5	G	301	POV	O31-C31	4.31	1.45	1.33
5	E	301	POV	O31-C31	4.30	1.45	1.33
5	H	301	POV	O31-C31	4.30	1.45	1.33
5	F	301	POV	O31-C31	4.29	1.45	1.33
5	D	1104	POV	O31-C31	4.24	1.45	1.33
5	A	1104	POV	O31-C31	4.23	1.45	1.33
5	C	1105	POV	O31-C31	4.22	1.45	1.33
5	B	1104	POV	O31-C31	4.21	1.45	1.33
5	D	1104	POV	O21-C21	4.15	1.46	1.34
5	A	1104	POV	O21-C21	4.15	1.46	1.34
5	G	301	POV	O21-C21	4.14	1.46	1.34
5	H	301	POV	O21-C21	4.14	1.46	1.34
5	E	301	POV	O21-C21	4.13	1.46	1.34
5	B	1104	POV	O21-C21	4.13	1.45	1.34
5	C	1105	POV	O21-C21	4.13	1.45	1.34
5	F	301	POV	O21-C21	4.12	1.45	1.34
5	B	1110	POV	O21-C21	4.00	1.45	1.34
5	A	1110	POV	O21-C21	3.99	1.45	1.34
5	D	1108	POV	O21-C21	3.99	1.45	1.34
5	A	1113	POV	O21-C21	3.97	1.45	1.34
6	D	1107	CLR	C10-C9	-2.25	1.52	1.56
6	C	1108	CLR	C10-C9	-2.24	1.52	1.56
6	D	1106	CLR	C10-C9	-2.24	1.52	1.56
6	B	1107	CLR	C10-C9	-2.23	1.52	1.56
6	B	1105	CLR	C10-C9	-2.21	1.52	1.56
6	D	1105	CLR	C10-C9	-2.20	1.52	1.56
6	C	1106	CLR	C10-C9	-2.18	1.52	1.56
6	D	1106	CLR	C13-C14	-2.09	1.51	1.55
6	B	1105	CLR	C13-C14	-2.06	1.51	1.55
6	C	1108	CLR	C13-C14	-2.06	1.51	1.55
6	D	1105	CLR	C13-C14	-2.05	1.51	1.55
6	B	1107	CLR	C13-C14	-2.04	1.51	1.55
6	D	1107	CLR	C13-C14	-2.04	1.51	1.55

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1104	POV	C15-N-C13	-8.65	86.25	108.98
5	C	1105	POV	C15-N-C13	-8.65	86.25	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1104	POV	C15-N-C13	-8.65	86.26	108.98
5	B	1104	POV	C15-N-C13	-8.64	86.27	108.98
5	B	1104	POV	C15-N-C14	-8.52	86.61	108.98
5	D	1104	POV	C15-N-C14	-8.51	86.62	108.98
5	C	1105	POV	C15-N-C14	-8.51	86.63	108.98
5	A	1104	POV	C15-N-C14	-8.51	86.63	108.98
5	C	1105	POV	C15-N-C12	-5.90	86.47	109.91
5	A	1104	POV	C15-N-C12	-5.89	86.51	109.91
5	D	1104	POV	C15-N-C12	-5.88	86.53	109.91
5	B	1104	POV	C15-N-C12	-5.87	86.56	109.91
6	D	1106	CLR	C13-C17-C20	-4.94	111.86	119.50
6	C	1106	CLR	C13-C17-C20	-4.84	112.02	119.50
6	D	1105	CLR	C13-C17-C20	-4.83	112.04	119.50
6	B	1105	CLR	C13-C17-C20	-4.78	112.12	119.50
6	C	1108	CLR	C13-C17-C20	-4.56	112.46	119.50
6	B	1107	CLR	C13-C17-C20	-4.55	112.46	119.50
6	D	1107	CLR	C13-C17-C20	-4.54	112.48	119.50
6	D	1106	CLR	C13-C14-C8	-4.46	108.08	114.41
6	B	1105	CLR	C13-C14-C8	-4.26	108.37	114.41
6	A	1105	CLR	C13-C17-C20	-4.20	113.02	119.50
6	C	1106	CLR	C13-C14-C8	-4.14	108.54	114.41
5	C	1105	POV	C14-N-C13	4.06	119.63	108.98
5	A	1104	POV	C14-N-C13	4.06	119.63	108.98
6	D	1107	CLR	C13-C14-C8	-4.04	108.67	114.41
5	B	1104	POV	C14-N-C13	4.04	119.59	108.98
5	D	1104	POV	C14-N-C13	4.04	119.59	108.98
6	B	1107	CLR	C13-C14-C8	-4.03	108.69	114.41
6	D	1105	CLR	C13-C14-C8	-4.03	108.70	114.41
6	C	1108	CLR	C13-C14-C8	-4.01	108.72	114.41
5	G	301	POV	O21-C21-C22	3.98	120.08	111.48
5	H	301	POV	O21-C21-C22	3.98	120.08	111.48
5	F	301	POV	O21-C21-C22	3.97	120.07	111.48
5	E	301	POV	O21-C21-C22	3.96	120.06	111.48
6	D	1106	CLR	C17-C13-C14	3.73	104.38	100.10
5	B	1104	POV	O21-C21-C22	3.72	119.53	111.48
5	C	1105	POV	O21-C21-C22	3.72	119.52	111.48
5	D	1104	POV	O21-C21-C22	3.72	119.52	111.48
5	A	1104	POV	O21-C21-C22	3.72	119.52	111.48
6	B	1105	CLR	C17-C13-C14	3.33	103.92	100.10
6	D	1105	CLR	C17-C13-C14	3.27	103.85	100.10
6	C	1106	CLR	C4-C5-C10	3.23	120.56	116.42
6	A	1105	CLR	C16-C17-C20	3.23	117.07	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1106	CLR	C17-C13-C14	3.17	103.73	100.10
6	C	1108	CLR	C17-C13-C14	3.04	103.59	100.10
5	D	1108	POV	O21-C21-C22	3.04	118.06	111.48
6	B	1107	CLR	C17-C13-C14	3.03	103.58	100.10
5	A	1110	POV	O21-C21-C22	3.01	117.99	111.48
6	D	1107	CLR	C17-C13-C14	3.00	103.55	100.10
5	B	1110	POV	O21-C21-C22	3.00	117.98	111.48
5	A	1113	POV	O21-C21-C22	3.00	117.98	111.48
5	A	1110	POV	O31-C31-C32	2.79	120.36	111.83
5	A	1113	POV	O31-C31-C32	2.79	120.34	111.83
5	B	1110	POV	O31-C31-C32	2.79	120.33	111.83
5	D	1108	POV	O31-C31-C32	2.78	120.32	111.83
5	G	301	POV	O31-C31-C32	2.77	120.30	111.83
5	F	301	POV	O31-C31-C32	2.77	120.29	111.83
5	H	301	POV	O31-C31-C32	2.77	120.27	111.83
6	C	1108	CLR	C11-C12-C13	-2.76	108.08	112.74
6	B	1107	CLR	C11-C12-C13	-2.76	108.08	112.74
5	E	301	POV	O31-C31-C32	2.76	120.24	111.83
6	D	1107	CLR	C11-C12-C13	-2.75	108.09	112.74
5	C	1105	POV	O31-C31-C32	2.75	120.21	111.83
5	A	1104	POV	O31-C31-C32	2.74	120.18	111.83
5	B	1104	POV	O31-C31-C32	2.74	120.18	111.83
5	D	1104	POV	O31-C31-C32	2.73	120.15	111.83
6	A	1106	CLR	C11-C12-C13	-2.73	108.14	112.74
6	A	1106	CLR	C13-C17-C20	-2.73	115.29	119.50
6	D	1106	CLR	C11-C12-C13	-2.72	108.15	112.74
6	D	1105	CLR	C11-C12-C13	-2.69	108.20	112.74
6	C	1108	CLR	C4-C5-C10	2.68	119.85	116.42
6	D	1107	CLR	C4-C5-C10	2.67	119.84	116.42
6	B	1107	CLR	C4-C5-C10	2.67	119.84	116.42
6	D	1105	CLR	C4-C5-C10	2.66	119.83	116.42
6	A	1105	CLR	C13-C14-C8	-2.63	110.67	114.41
6	B	1105	CLR	C11-C12-C13	-2.54	108.45	112.74
6	C	1106	CLR	C11-C12-C13	-2.50	108.52	112.74
5	B	1104	POV	C13-N-C12	2.49	119.82	109.91
5	D	1104	POV	C13-N-C12	2.49	119.82	109.91
5	A	1104	POV	C13-N-C12	2.49	119.81	109.91
5	C	1105	POV	C13-N-C12	2.49	119.81	109.91
6	B	1105	CLR	C7-C8-C9	2.43	112.53	109.72
5	D	1104	POV	C14-N-C12	2.40	119.47	109.91
5	B	1104	POV	C14-N-C12	2.40	119.46	109.91
5	A	1104	POV	C14-N-C12	2.39	119.43	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1105	POV	C14-N-C12	2.39	119.42	109.91
6	D	1106	CLR	C4-C5-C10	2.38	119.47	116.42
6	A	1106	CLR	C9-C10-C5	2.37	113.12	109.65
6	C	1106	CLR	C10-C5-C6	-2.35	119.50	122.93
6	C	1106	CLR	C7-C8-C9	2.34	112.43	109.72
6	B	1107	CLR	C7-C8-C9	2.29	112.36	109.72
5	E	301	POV	C2-O21-C21	-2.25	112.42	117.80
5	H	301	POV	C2-O21-C21	-2.25	112.42	117.80
6	D	1107	CLR	C7-C8-C9	2.24	112.31	109.72
5	F	301	POV	C2-O21-C21	-2.24	112.43	117.80
6	D	1106	CLR	C10-C9-C8	-2.24	109.44	112.71
5	G	301	POV	C2-O21-C21	-2.24	112.44	117.80
5	A	1113	POV	C2-O21-C21	-2.23	112.45	117.80
6	C	1108	CLR	C7-C8-C9	2.23	112.30	109.72
6	D	1105	CLR	C7-C6-C5	-2.23	121.26	125.02
5	D	1108	POV	C2-O21-C21	-2.22	112.47	117.80
5	A	1110	POV	C2-O21-C21	-2.22	112.47	117.80
5	B	1110	POV	C2-O21-C21	-2.21	112.51	117.80
6	C	1108	CLR	C7-C6-C5	-2.21	121.29	125.02
6	B	1107	CLR	C7-C6-C5	-2.20	121.30	125.02
6	A	1105	CLR	C4-C5-C6	-2.20	117.59	120.57
6	D	1107	CLR	C7-C6-C5	-2.19	121.32	125.02
6	B	1105	CLR	C10-C9-C8	-2.18	109.52	112.71
6	C	1106	CLR	C7-C6-C5	-2.17	121.36	125.02
6	D	1105	CLR	C10-C5-C6	-2.15	119.78	122.93
6	A	1105	CLR	C22-C20-C17	2.12	114.73	110.33
6	A	1105	CLR	C4-C5-C10	2.11	119.13	116.42
6	D	1107	CLR	C10-C5-C6	-2.10	119.86	122.93
6	B	1107	CLR	C3-C4-C5	-2.10	108.71	112.05
6	B	1107	CLR	C10-C5-C6	-2.09	119.88	122.93
6	C	1108	CLR	C10-C5-C6	-2.09	119.88	122.93
6	D	1107	CLR	C3-C4-C5	-2.08	108.75	112.05
6	C	1108	CLR	C3-C4-C5	-2.07	108.76	112.05
6	A	1105	CLR	C21-C20-C17	-2.06	109.80	112.88
6	B	1105	CLR	C1-C10-C9	2.04	111.44	108.74
6	D	1105	CLR	C7-C8-C9	2.04	112.08	109.72
6	B	1105	CLR	C4-C5-C10	2.03	119.02	116.42
6	A	1106	CLR	C1-C10-C5	-2.02	105.27	108.74
6	C	1106	CLR	C3-C4-C5	-2.01	108.86	112.05

There are no chirality outliers.

All (362) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1104	POV	C1-O11-P-O12
5	A	1104	POV	C1-O11-P-O13
5	A	1104	POV	C11-O12-P-O11
5	A	1104	POV	C11-O12-P-O13
5	A	1104	POV	C11-O12-P-O14
5	A	1110	POV	C1-O11-P-O12
5	A	1110	POV	C1-O11-P-O13
5	A	1110	POV	C1-O11-P-O14
5	A	1110	POV	C11-O12-P-O11
5	A	1110	POV	C22-C21-O21-C2
5	A	1111	POV	C11-O12-P-O11
5	A	1112	POV	C1-O11-P-O13
5	A	1112	POV	C11-O12-P-O11
5	A	1112	POV	C11-O12-P-O14
5	A	1112	POV	O11-C1-C2-O21
5	A	1113	POV	C1-O11-P-O12
5	A	1113	POV	C1-O11-P-O13
5	A	1113	POV	C1-O11-P-O14
5	A	1113	POV	C11-O12-P-O11
5	A	1113	POV	C22-C21-O21-C2
5	B	1104	POV	C1-O11-P-O12
5	B	1104	POV	C1-O11-P-O13
5	B	1104	POV	C11-O12-P-O11
5	B	1104	POV	C11-O12-P-O13
5	B	1104	POV	C11-O12-P-O14
5	B	1108	POV	C11-O12-P-O11
5	B	1109	POV	C1-O11-P-O13
5	B	1109	POV	C11-O12-P-O11
5	B	1109	POV	C11-O12-P-O14
5	B	1109	POV	O11-C1-C2-O21
5	B	1110	POV	C1-O11-P-O12
5	B	1110	POV	C1-O11-P-O13
5	B	1110	POV	C1-O11-P-O14
5	B	1110	POV	C11-O12-P-O11
5	B	1110	POV	C22-C21-O21-C2
5	C	1105	POV	C1-O11-P-O12
5	C	1105	POV	C1-O11-P-O13
5	C	1105	POV	C11-O12-P-O11
5	C	1105	POV	C11-O12-P-O13
5	C	1105	POV	C11-O12-P-O14
5	C	1109	POV	C11-O12-P-O11
5	C	1110	POV	C1-O11-P-O13
5	C	1110	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
5	C	1110	POV	C11-O12-P-O14
5	C	1110	POV	O11-C1-C2-O21
5	D	1104	POV	C1-O11-P-O12
5	D	1104	POV	C1-O11-P-O13
5	D	1104	POV	C11-O12-P-O11
5	D	1104	POV	C11-O12-P-O13
5	D	1104	POV	C11-O12-P-O14
5	D	1108	POV	C1-O11-P-O12
5	D	1108	POV	C1-O11-P-O13
5	D	1108	POV	C1-O11-P-O14
5	D	1108	POV	C11-O12-P-O11
5	D	1108	POV	C22-C21-O21-C2
5	D	1109	POV	C11-O12-P-O11
5	D	1110	POV	C1-O11-P-O13
5	D	1110	POV	C11-O12-P-O11
5	D	1110	POV	C11-O12-P-O14
5	D	1110	POV	O11-C1-C2-O21
5	E	301	POV	C11-O12-P-O13
5	F	301	POV	C11-O12-P-O13
5	G	301	POV	C11-O12-P-O13
5	H	301	POV	C11-O12-P-O13
6	A	1105	CLR	C13-C17-C20-C21
6	A	1105	CLR	C13-C17-C20-C22
6	A	1105	CLR	C16-C17-C20-C22
6	D	1105	CLR	C13-C17-C20-C21
6	D	1105	CLR	C16-C17-C20-C22
6	C	1106	CLR	C20-C22-C23-C24
6	A	1105	CLR	C16-C17-C20-C21
6	D	1105	CLR	C16-C17-C20-C21
6	D	1105	CLR	C13-C17-C20-C22
5	A	1110	POV	O22-C21-O21-C2
5	A	1113	POV	O22-C21-O21-C2
5	B	1110	POV	O22-C21-O21-C2
5	D	1108	POV	O22-C21-O21-C2
6	B	1105	CLR	C21-C20-C22-C23
6	C	1106	CLR	C13-C17-C20-C22
5	A	1112	POV	C32-C31-O31-C3
5	B	1109	POV	C32-C31-O31-C3
5	C	1110	POV	C32-C31-O31-C3
5	D	1110	POV	C32-C31-O31-C3
6	D	1106	CLR	C13-C17-C20-C22
6	A	1106	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
6	C	1106	CLR	C13-C17-C20-C21
6	B	1106	CLR	C16-C17-C20-C21
6	C	1107	CLR	C16-C17-C20-C21
6	B	1105	CLR	C13-C17-C20-C22
6	B	1106	CLR	C13-C17-C20-C22
6	C	1107	CLR	C13-C17-C20-C22
6	B	1106	CLR	C17-C20-C22-C23
6	C	1107	CLR	C17-C20-C22-C23
6	A	1106	CLR	C22-C23-C24-C25
6	B	1106	CLR	C13-C17-C20-C21
6	C	1107	CLR	C13-C17-C20-C21
6	D	1106	CLR	C13-C17-C20-C21
6	C	1106	CLR	C22-C23-C24-C25
6	A	1105	CLR	C20-C22-C23-C24
6	B	1105	CLR	C22-C23-C24-C25
6	B	1107	CLR	C22-C23-C24-C25
6	C	1108	CLR	C22-C23-C24-C25
6	D	1107	CLR	C22-C23-C24-C25
5	A	1112	POV	O32-C31-O31-C3
5	B	1109	POV	O32-C31-O31-C3
5	C	1110	POV	O32-C31-O31-C3
5	D	1110	POV	O32-C31-O31-C3
6	B	1106	CLR	C21-C20-C22-C23
6	C	1107	CLR	C21-C20-C22-C23
6	B	1105	CLR	C16-C17-C20-C21
6	B	1105	CLR	C13-C17-C20-C21
5	A	1112	POV	C22-C21-O21-C2
5	B	1109	POV	C22-C21-O21-C2
5	C	1110	POV	C22-C21-O21-C2
5	D	1110	POV	C22-C21-O21-C2
5	A	1112	POV	O22-C21-O21-C2
5	B	1109	POV	O22-C21-O21-C2
5	C	1110	POV	O22-C21-O21-C2
5	D	1110	POV	O22-C21-O21-C2
5	A	1104	POV	C11-C12-N-C14
5	B	1104	POV	C11-C12-N-C14
5	C	1105	POV	C11-C12-N-C14
5	D	1104	POV	C11-C12-N-C14
6	B	1107	CLR	C21-C20-C22-C23
6	C	1108	CLR	C21-C20-C22-C23
6	D	1107	CLR	C21-C20-C22-C23
6	B	1106	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
6	C	1107	CLR	C16-C17-C20-C22
6	B	1107	CLR	C23-C24-C25-C26
6	C	1108	CLR	C23-C24-C25-C26
6	D	1107	CLR	C23-C24-C25-C26
5	A	1110	POV	C32-C33-C34-C35
5	A	1113	POV	C32-C33-C34-C35
5	B	1110	POV	C32-C33-C34-C35
5	D	1108	POV	C32-C33-C34-C35
5	A	1112	POV	C31-C32-C33-C34
5	B	1109	POV	C31-C32-C33-C34
5	C	1110	POV	C31-C32-C33-C34
5	D	1110	POV	C31-C32-C33-C34
5	D	1108	POV	C211-C212-C213-C214
5	A	1110	POV	C211-C212-C213-C214
5	A	1113	POV	C211-C212-C213-C214
5	B	1110	POV	C211-C212-C213-C214
5	B	1104	POV	C32-C31-O31-C3
5	C	1105	POV	C32-C31-O31-C3
6	D	1105	CLR	C20-C22-C23-C24
5	A	1104	POV	C31-C32-C33-C34
5	B	1104	POV	C31-C32-C33-C34
5	C	1105	POV	C31-C32-C33-C34
5	D	1104	POV	C31-C32-C33-C34
5	A	1104	POV	C32-C31-O31-C3
5	D	1104	POV	C32-C31-O31-C3
5	A	1104	POV	C22-C23-C24-C25
5	B	1104	POV	C22-C23-C24-C25
5	C	1105	POV	C22-C23-C24-C25
5	D	1104	POV	C22-C23-C24-C25
6	C	1106	CLR	C16-C17-C20-C21
5	A	1104	POV	O32-C31-O31-C3
5	B	1104	POV	O32-C31-O31-C3
5	C	1105	POV	O32-C31-O31-C3
5	D	1104	POV	O32-C31-O31-C3
6	D	1106	CLR	C16-C17-C20-C21
6	B	1105	CLR	C17-C20-C22-C23
5	A	1111	POV	C32-C33-C34-C35
5	B	1108	POV	C32-C33-C34-C35
5	C	1109	POV	C32-C33-C34-C35
5	D	1109	POV	C32-C33-C34-C35
6	C	1107	CLR	C20-C22-C23-C24
5	D	1108	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	1113	POV	C23-C24-C25-C26
5	A	1110	POV	C23-C24-C25-C26
5	B	1110	POV	C23-C24-C25-C26
6	B	1106	CLR	C20-C22-C23-C24
6	D	1106	CLR	C20-C22-C23-C24
5	A	1104	POV	C24-C25-C26-C27
5	B	1104	POV	C24-C25-C26-C27
5	C	1105	POV	C24-C25-C26-C27
5	D	1104	POV	C24-C25-C26-C27
5	E	301	POV	C22-C23-C24-C25
5	F	301	POV	C22-C23-C24-C25
5	G	301	POV	C22-C23-C24-C25
5	H	301	POV	C22-C23-C24-C25
6	B	1107	CLR	C23-C24-C25-C27
6	C	1108	CLR	C23-C24-C25-C27
6	D	1107	CLR	C23-C24-C25-C27
6	C	1106	CLR	C16-C17-C20-C22
6	D	1107	CLR	C20-C22-C23-C24
5	A	1111	POV	C2-C1-O11-P
5	B	1108	POV	C2-C1-O11-P
5	C	1109	POV	C2-C1-O11-P
5	D	1109	POV	C2-C1-O11-P
6	D	1106	CLR	C23-C24-C25-C27
6	B	1107	CLR	C20-C22-C23-C24
6	C	1108	CLR	C20-C22-C23-C24
6	B	1105	CLR	C16-C17-C20-C22
6	A	1106	CLR	C20-C22-C23-C24
5	A	1104	POV	C26-C27-C28-C29
5	B	1104	POV	C26-C27-C28-C29
5	C	1105	POV	C26-C27-C28-C29
5	D	1104	POV	C26-C27-C28-C29
6	D	1106	CLR	C16-C17-C20-C22
6	C	1106	CLR	C21-C20-C22-C23
5	D	1104	POV	C21-C22-C23-C24
5	A	1104	POV	C21-C22-C23-C24
5	B	1104	POV	C21-C22-C23-C24
5	C	1105	POV	C21-C22-C23-C24
5	E	301	POV	C31-C32-C33-C34
5	F	301	POV	C31-C32-C33-C34
5	G	301	POV	C31-C32-C33-C34
5	H	301	POV	C31-C32-C33-C34
6	C	1106	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
6	D	1106	CLR	C23-C24-C25-C26
6	A	1105	CLR	C22-C23-C24-C25
5	A	1104	POV	O11-C1-C2-C3
5	A	1112	POV	O11-C1-C2-C3
5	B	1104	POV	O11-C1-C2-C3
5	B	1109	POV	O11-C1-C2-C3
5	C	1105	POV	O11-C1-C2-C3
5	C	1110	POV	O11-C1-C2-C3
5	D	1104	POV	O11-C1-C2-C3
5	D	1110	POV	O11-C1-C2-C3
5	A	1111	POV	C22-C23-C24-C25
5	B	1108	POV	C22-C23-C24-C25
5	C	1109	POV	C22-C23-C24-C25
5	D	1109	POV	C22-C23-C24-C25
5	A	1104	POV	C1-C2-C3-O31
5	B	1104	POV	C1-C2-C3-O31
5	C	1105	POV	C1-C2-C3-O31
5	D	1104	POV	C1-C2-C3-O31
5	A	1104	POV	O21-C2-C3-O31
5	B	1104	POV	O21-C2-C3-O31
5	C	1105	POV	O21-C2-C3-O31
5	D	1104	POV	O21-C2-C3-O31
6	D	1105	CLR	C21-C20-C22-C23
5	B	1110	POV	C36-C37-C38-C39
5	A	1110	POV	C36-C37-C38-C39
5	A	1113	POV	C36-C37-C38-C39
5	D	1108	POV	C36-C37-C38-C39
6	D	1105	CLR	C23-C24-C25-C26
5	A	1104	POV	O11-C1-C2-O21
5	B	1104	POV	O11-C1-C2-O21
5	C	1105	POV	O11-C1-C2-O21
5	D	1104	POV	O11-C1-C2-O21
5	B	1110	POV	C34-C35-C36-C37
5	A	1110	POV	C34-C35-C36-C37
5	A	1113	POV	C34-C35-C36-C37
5	D	1108	POV	C34-C35-C36-C37
5	F	301	POV	C22-C21-O21-C2
5	A	1110	POV	C11-O12-P-O14
5	A	1111	POV	C11-O12-P-O13
5	A	1113	POV	C11-O12-P-O14
5	B	1108	POV	C11-O12-P-O13
5	B	1110	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
5	C	1109	POV	C11-O12-P-O13
5	D	1108	POV	C11-O12-P-O14
5	D	1109	POV	C11-O12-P-O13
5	E	301	POV	C1-O11-P-O14
5	E	301	POV	C11-O12-P-O11
5	E	301	POV	C11-O12-P-O14
5	F	301	POV	C1-O11-P-O14
5	F	301	POV	C11-O12-P-O11
5	F	301	POV	C11-O12-P-O14
5	G	301	POV	C1-O11-P-O14
5	G	301	POV	C11-O12-P-O11
5	G	301	POV	C11-O12-P-O14
5	H	301	POV	C1-O11-P-O14
5	H	301	POV	C11-O12-P-O11
5	H	301	POV	C11-O12-P-O14
5	E	301	POV	C22-C21-O21-C2
5	G	301	POV	C22-C21-O21-C2
5	H	301	POV	C22-C21-O21-C2
5	E	301	POV	C2-C1-O11-P
5	F	301	POV	C2-C1-O11-P
5	G	301	POV	C2-C1-O11-P
5	H	301	POV	C2-C1-O11-P
5	E	301	POV	O22-C21-O21-C2
5	F	301	POV	O22-C21-O21-C2
5	G	301	POV	O22-C21-O21-C2
5	H	301	POV	O22-C21-O21-C2
5	E	301	POV	O21-C21-C22-C23
5	F	301	POV	O21-C21-C22-C23
5	G	301	POV	O21-C21-C22-C23
5	H	301	POV	O21-C21-C22-C23
6	D	1107	CLR	C16-C17-C20-C22
6	B	1107	CLR	C16-C17-C20-C22
6	C	1108	CLR	C16-C17-C20-C22
5	A	1110	POV	C22-C23-C24-C25
5	A	1113	POV	C22-C23-C24-C25
5	B	1110	POV	C22-C23-C24-C25
5	D	1108	POV	C22-C23-C24-C25
5	A	1113	POV	C37-C38-C39-C310
5	B	1110	POV	C37-C38-C39-C310
5	A	1110	POV	C37-C38-C39-C310
5	A	1104	POV	C2-C1-O11-P
5	B	1104	POV	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
5	C	1105	POV	C2-C1-O11-P
5	D	1104	POV	C2-C1-O11-P
5	D	1108	POV	C37-C38-C39-C310
5	D	1108	POV	C310-C311-C312-C313
5	A	1110	POV	C310-C311-C312-C313
5	A	1113	POV	C310-C311-C312-C313
5	B	1110	POV	C310-C311-C312-C313
6	C	1106	CLR	C23-C24-C25-C26
5	G	301	POV	C32-C33-C34-C35
5	F	301	POV	C32-C33-C34-C35
5	E	301	POV	C32-C33-C34-C35
5	H	301	POV	C32-C33-C34-C35
5	D	1109	POV	C25-C26-C27-C28
5	A	1111	POV	C25-C26-C27-C28
5	B	1108	POV	C25-C26-C27-C28
5	C	1109	POV	C25-C26-C27-C28
5	G	301	POV	C32-C31-O31-C3
5	H	301	POV	C32-C31-O31-C3
5	E	301	POV	O32-C31-O31-C3
5	F	301	POV	O32-C31-O31-C3
5	G	301	POV	O32-C31-O31-C3
5	H	301	POV	O32-C31-O31-C3
5	E	301	POV	C32-C31-O31-C3
5	F	301	POV	C32-C31-O31-C3
5	G	301	POV	C26-C27-C28-C29
5	F	301	POV	C26-C27-C28-C29
5	H	301	POV	C26-C27-C28-C29
5	E	301	POV	C26-C27-C28-C29
5	C	1110	POV	C311-C310-C39-C38
5	A	1112	POV	O31-C31-C32-C33
5	B	1109	POV	O31-C31-C32-C33
5	C	1110	POV	O31-C31-C32-C33
5	D	1110	POV	O31-C31-C32-C33
5	A	1111	POV	C29-C210-C211-C212
5	D	1109	POV	C29-C210-C211-C212
5	A	1112	POV	C311-C310-C39-C38
5	B	1109	POV	C311-C310-C39-C38
5	D	1110	POV	C311-C310-C39-C38
5	B	1108	POV	C29-C210-C211-C212
5	C	1109	POV	C29-C210-C211-C212
6	C	1108	CLR	C16-C17-C20-C21
6	B	1107	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
6	D	1107	CLR	C16-C17-C20-C21
5	E	301	POV	C1-C2-O21-C21
5	F	301	POV	C1-C2-O21-C21
5	G	301	POV	C1-C2-O21-C21
5	H	301	POV	C1-C2-O21-C21
5	A	1112	POV	C11-C12-N-C13
5	B	1109	POV	C11-C12-N-C13
5	C	1110	POV	C11-C12-N-C13
5	D	1110	POV	C11-C12-N-C13
5	A	1112	POV	C11-C12-N-C14
5	A	1112	POV	C11-C12-N-C15
5	B	1109	POV	C11-C12-N-C14
5	B	1109	POV	C11-C12-N-C15
5	C	1110	POV	C11-C12-N-C14
5	C	1110	POV	C11-C12-N-C15
5	D	1110	POV	C11-C12-N-C14
5	D	1110	POV	C11-C12-N-C15
5	B	1109	POV	O32-C31-C32-C33
5	C	1110	POV	O32-C31-C32-C33
5	A	1112	POV	O32-C31-C32-C33
5	D	1110	POV	O32-C31-C32-C33
5	B	1104	POV	C25-C26-C27-C28
5	C	1105	POV	C25-C26-C27-C28
5	A	1104	POV	C25-C26-C27-C28
5	D	1104	POV	C25-C26-C27-C28

There are no ring outliers.

21 monomers are involved in 118 short contacts:

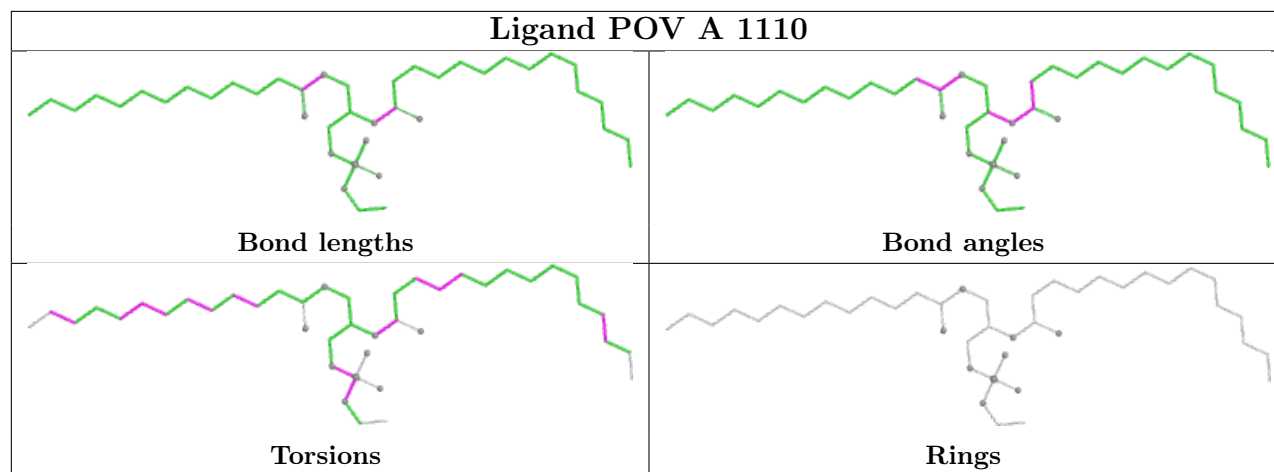
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1110	POV	1	0
6	B	1105	CLR	21	0
5	B	1110	POV	1	0
6	D	1107	CLR	7	0
5	A	1111	POV	1	0
6	B	1107	CLR	7	0
6	C	1106	CLR	7	0
6	D	1105	CLR	14	0
5	A	1113	POV	1	0
6	A	1105	CLR	8	0
6	D	1106	CLR	22	0
5	C	1109	POV	1	0

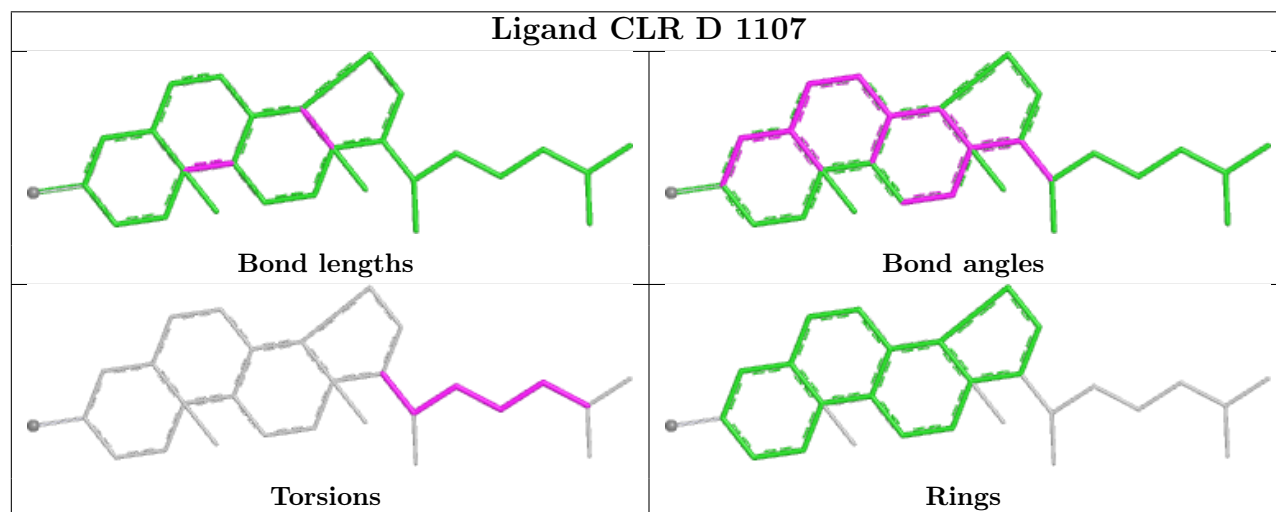
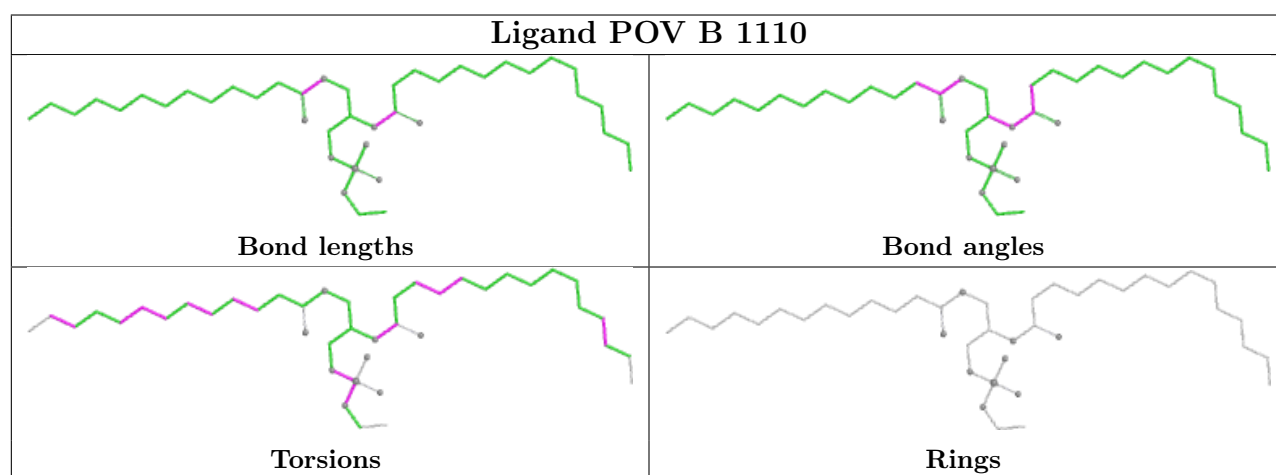
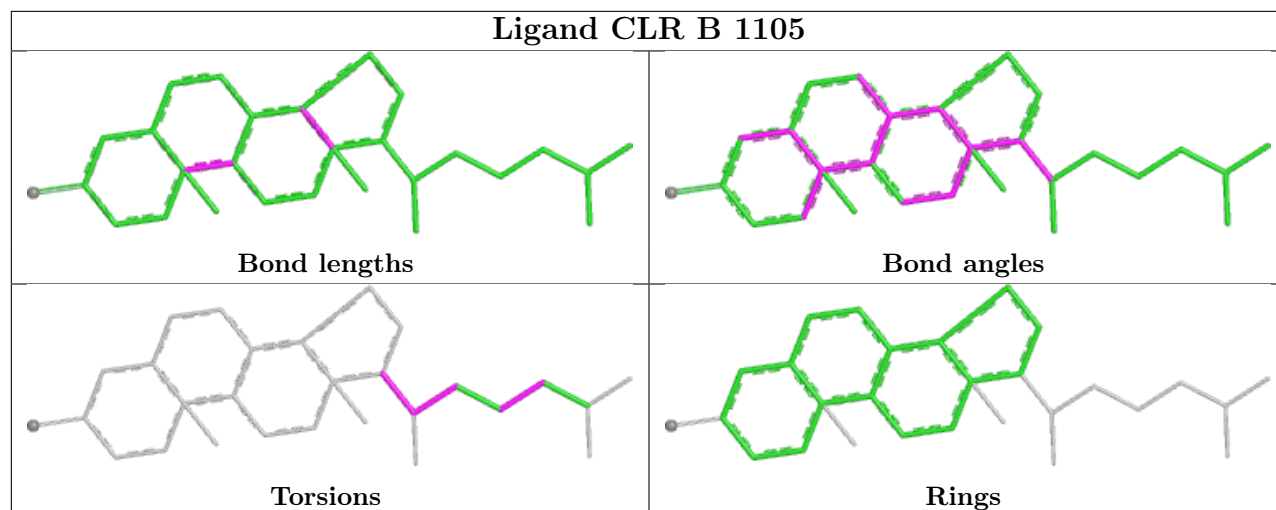
Continued on next page...

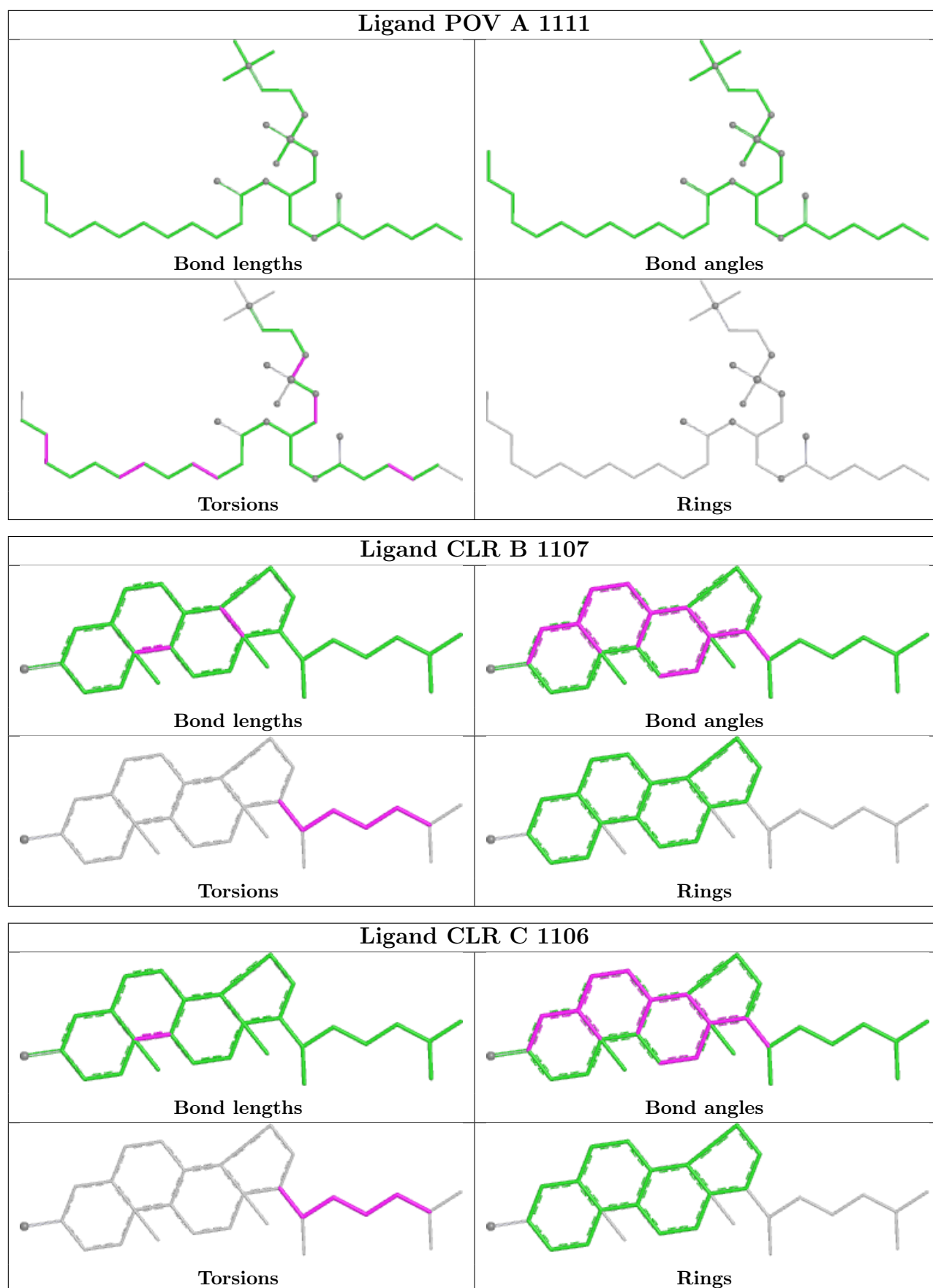
Continued from previous page...

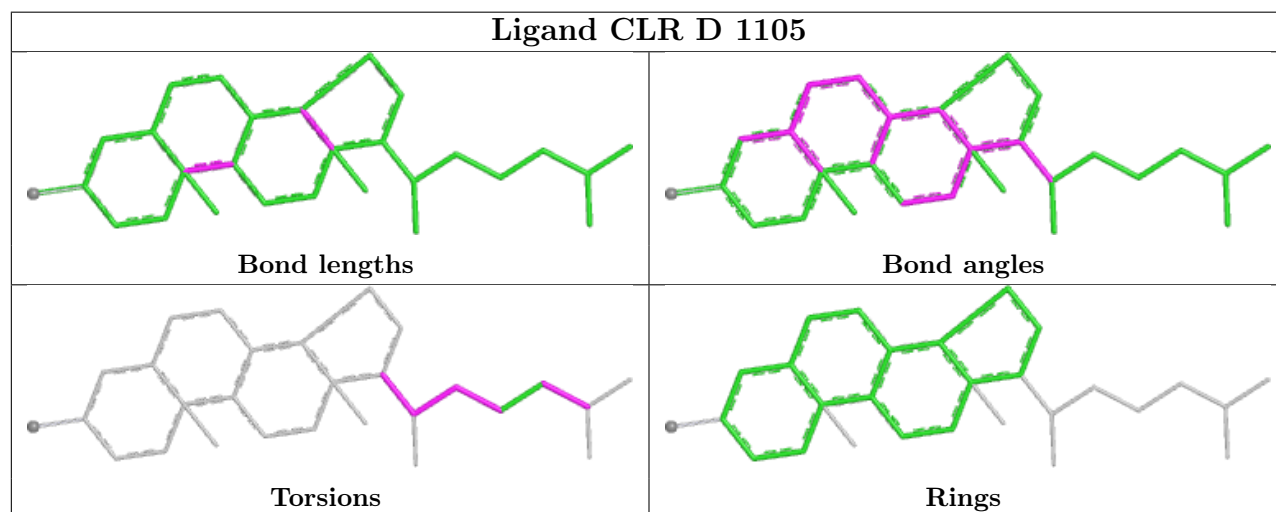
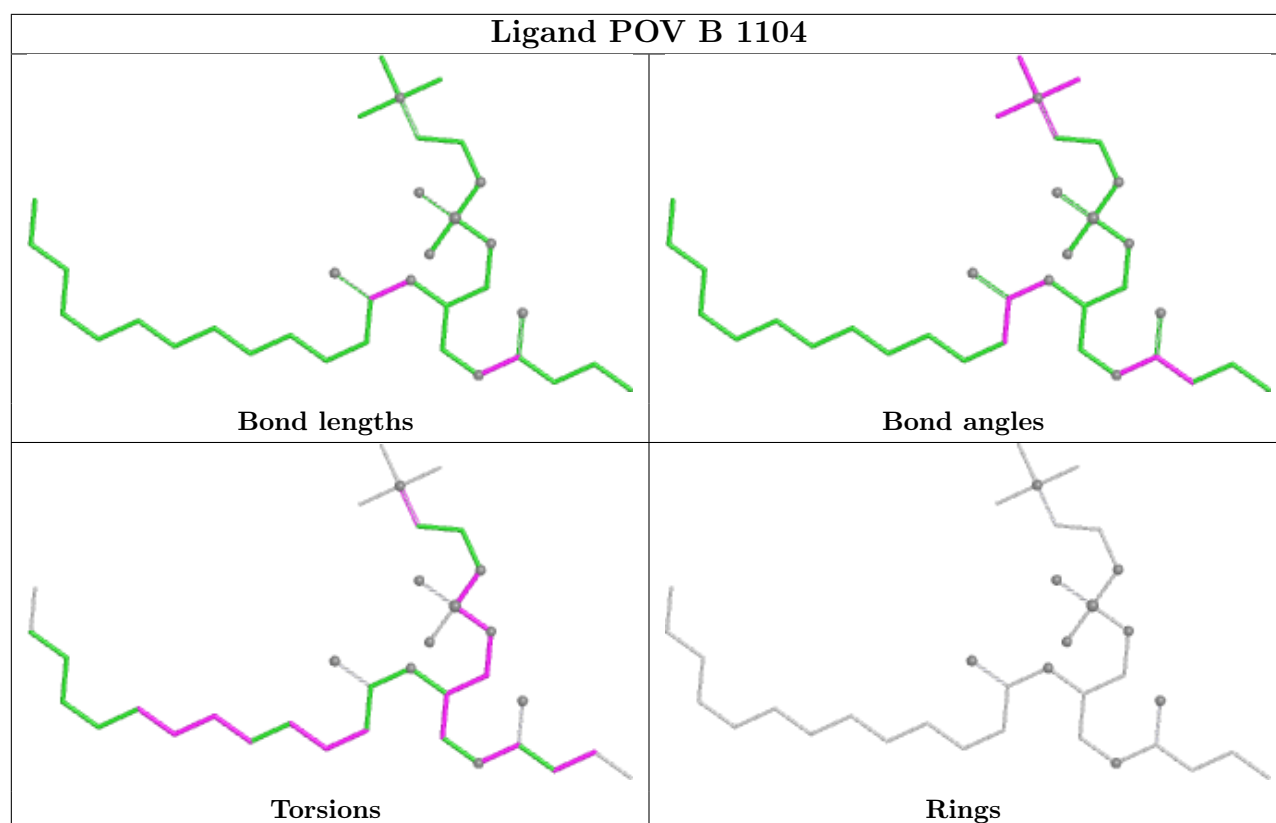
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1107	CLR	6	0
6	C	1108	CLR	7	0
5	G	301	POV	1	0
5	H	301	POV	1	0
5	D	1108	POV	1	0
6	A	1106	CLR	3	0
5	E	301	POV	1	0
6	B	1106	CLR	6	0
5	F	301	POV	1	0

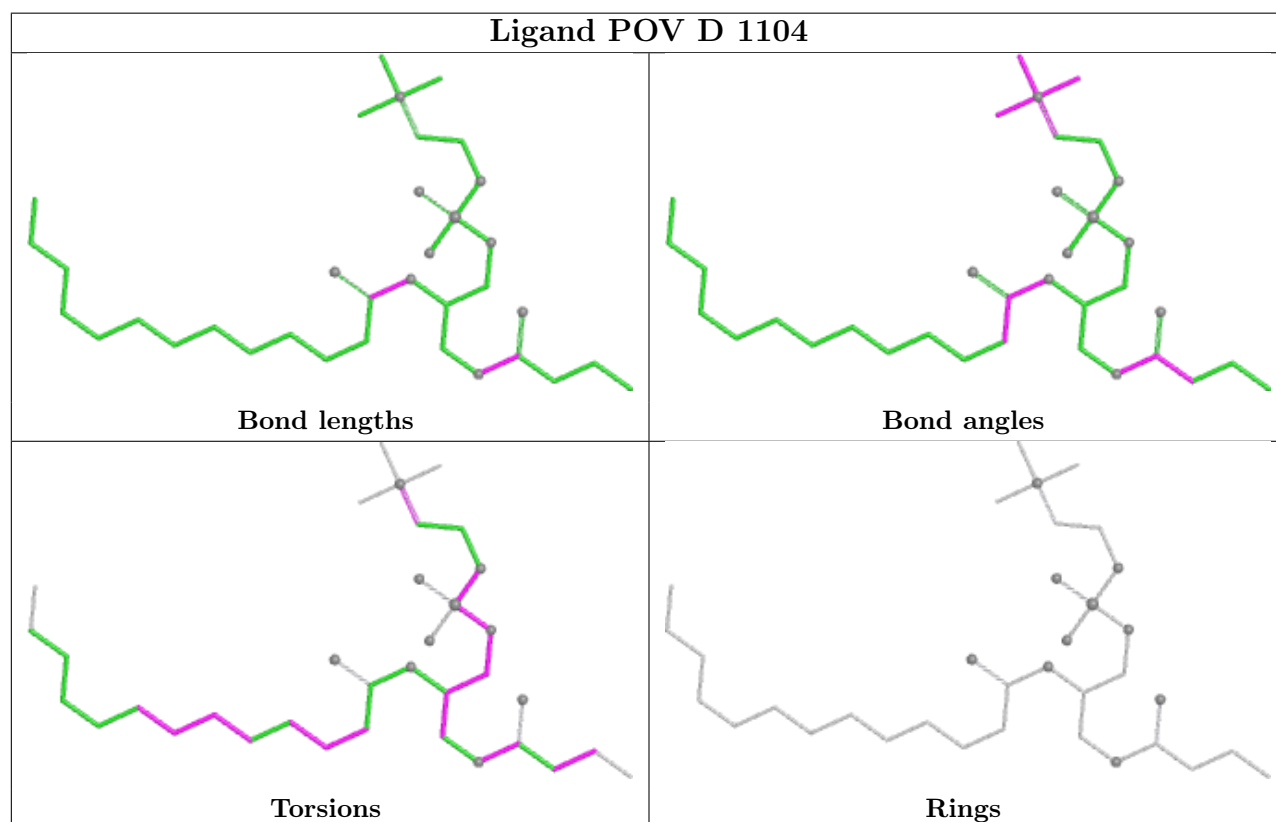
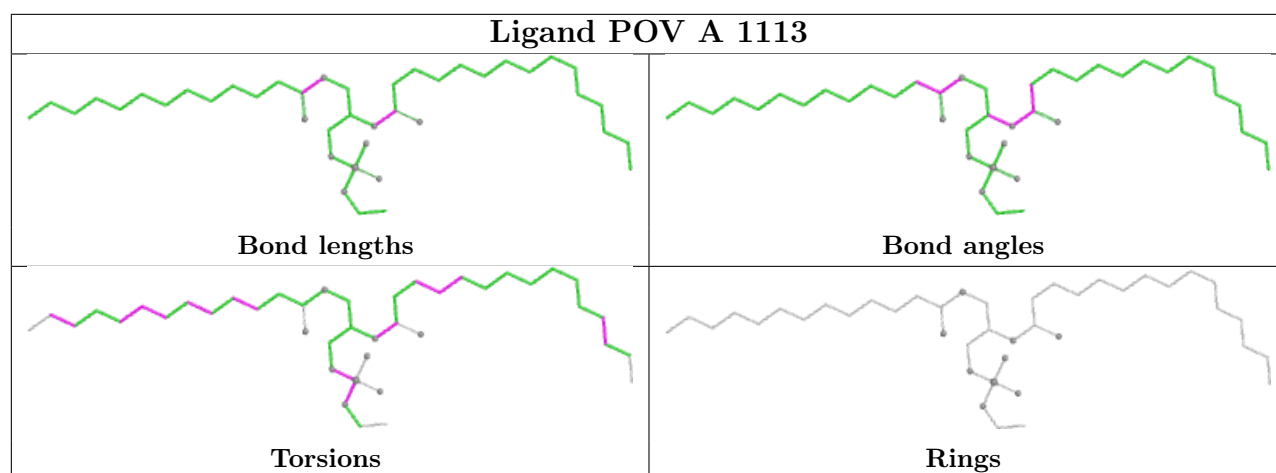
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

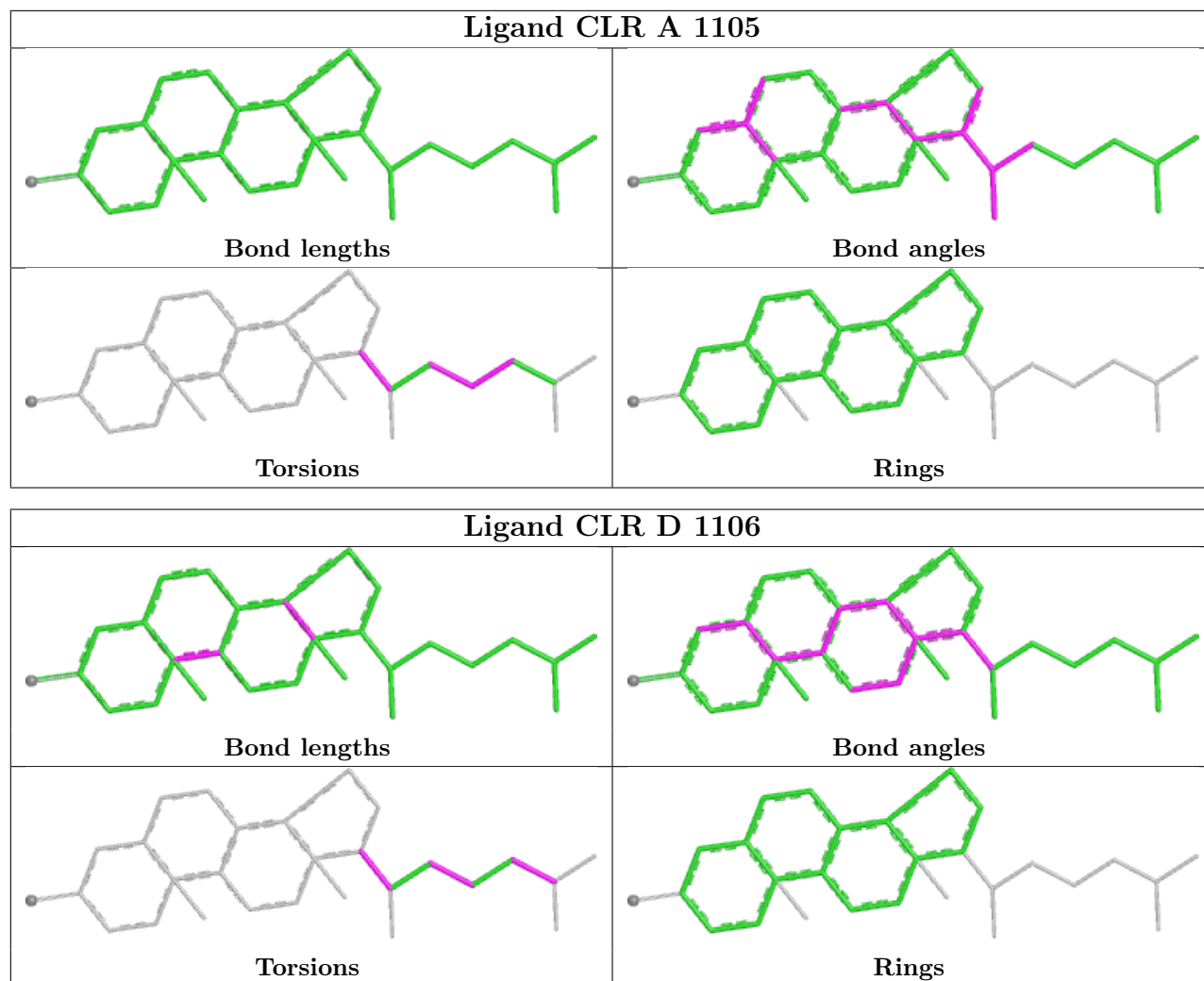


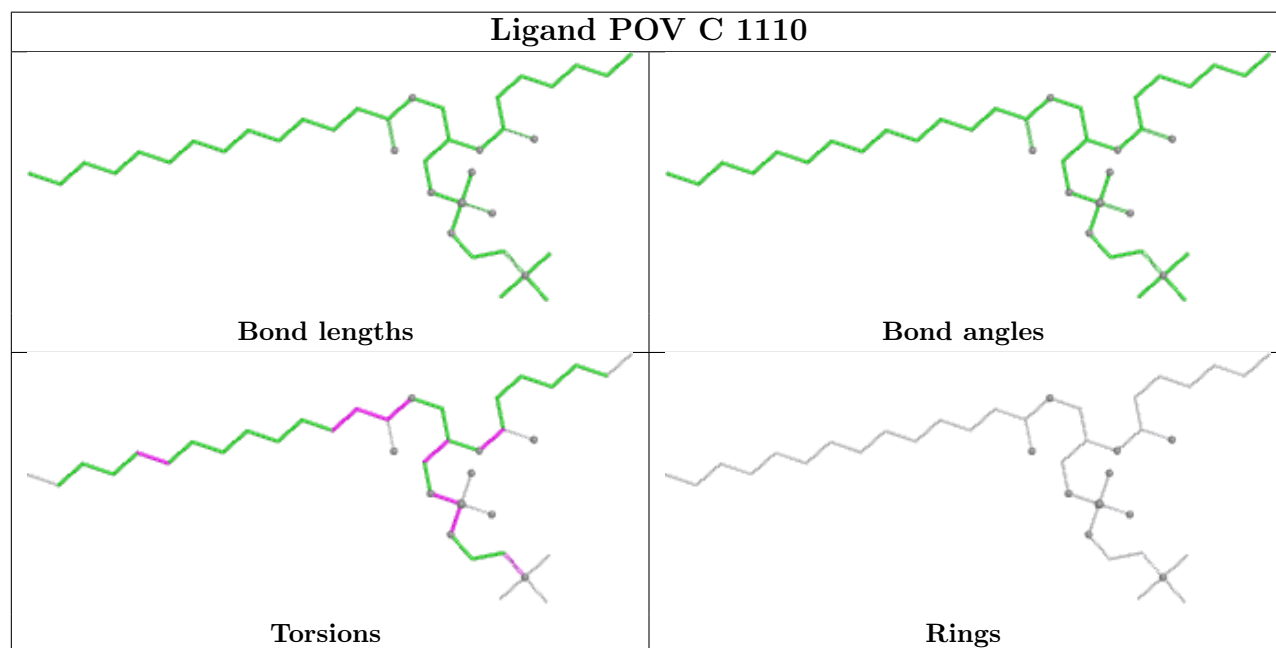
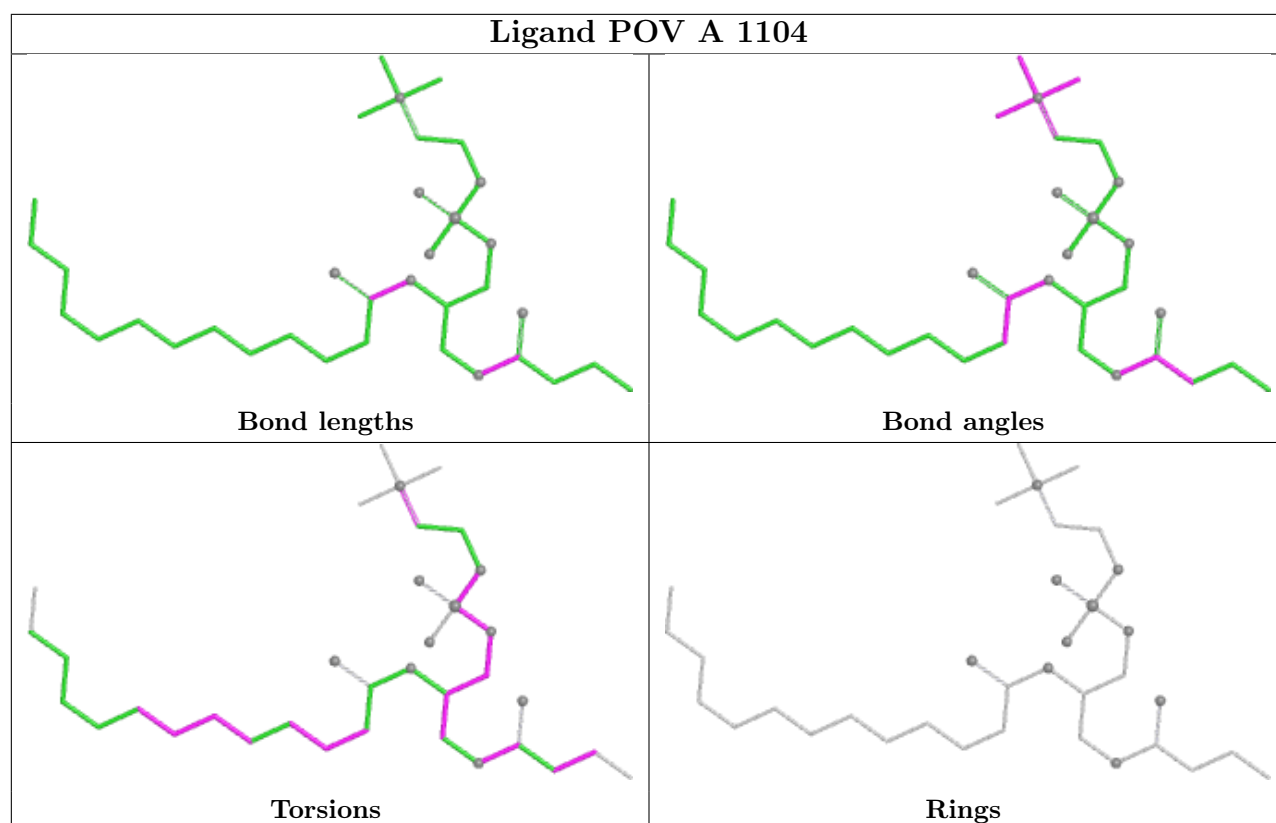


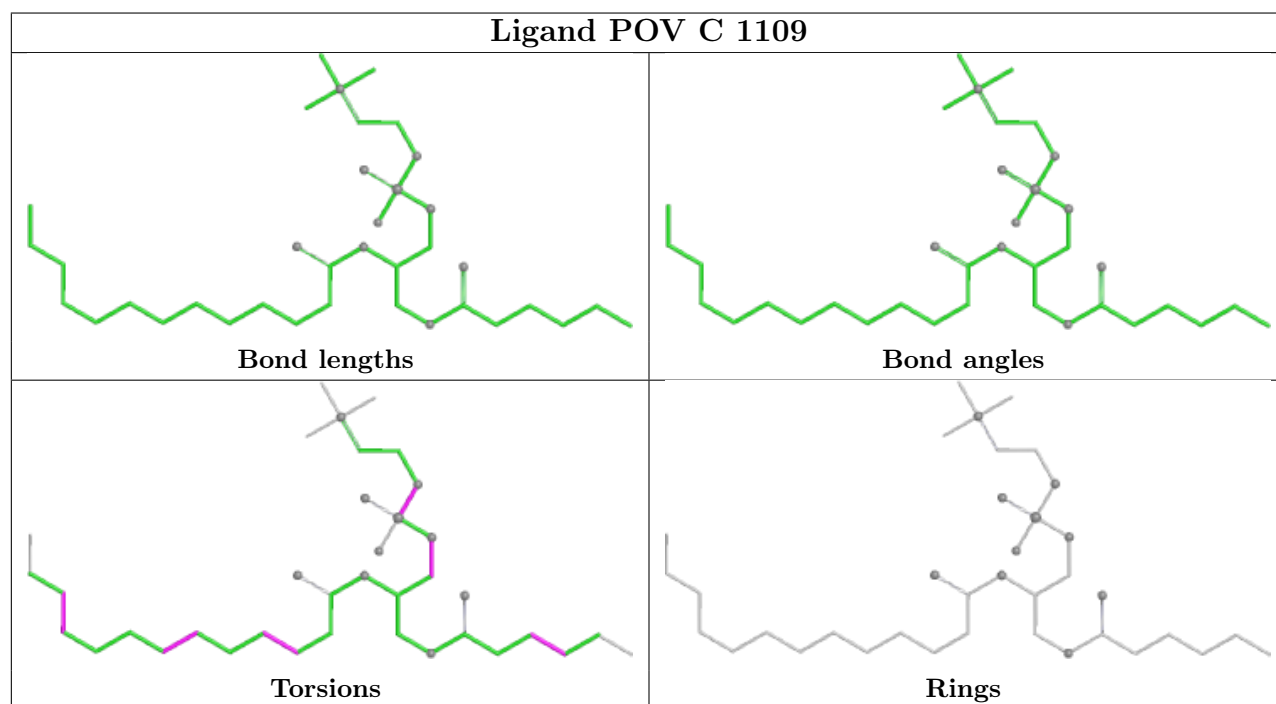
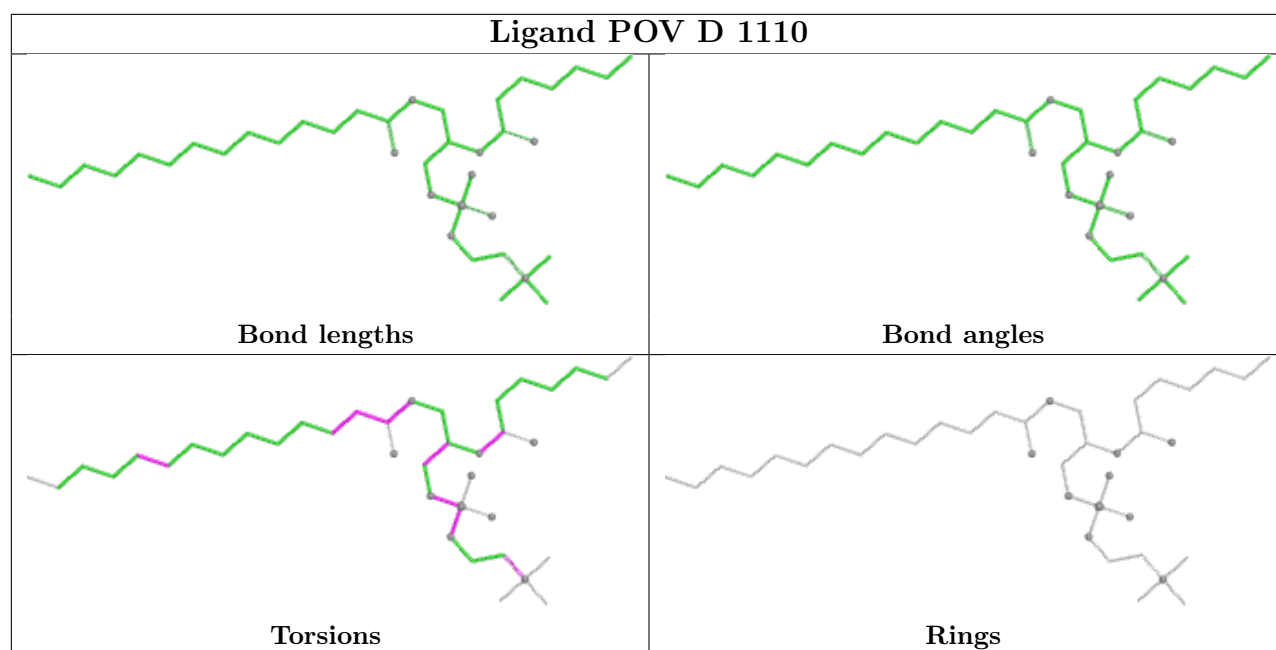


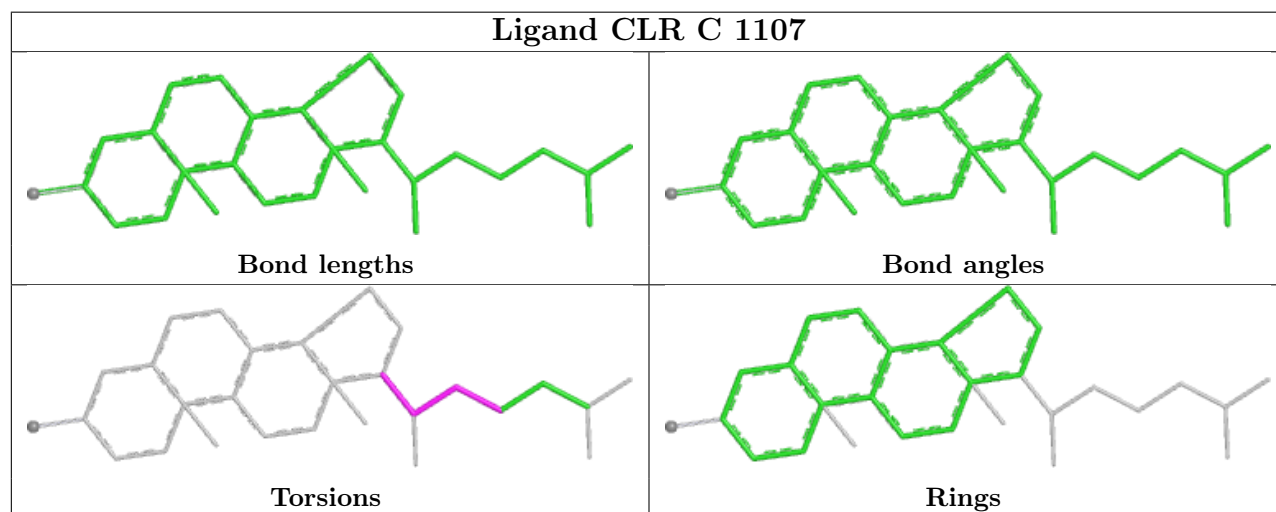
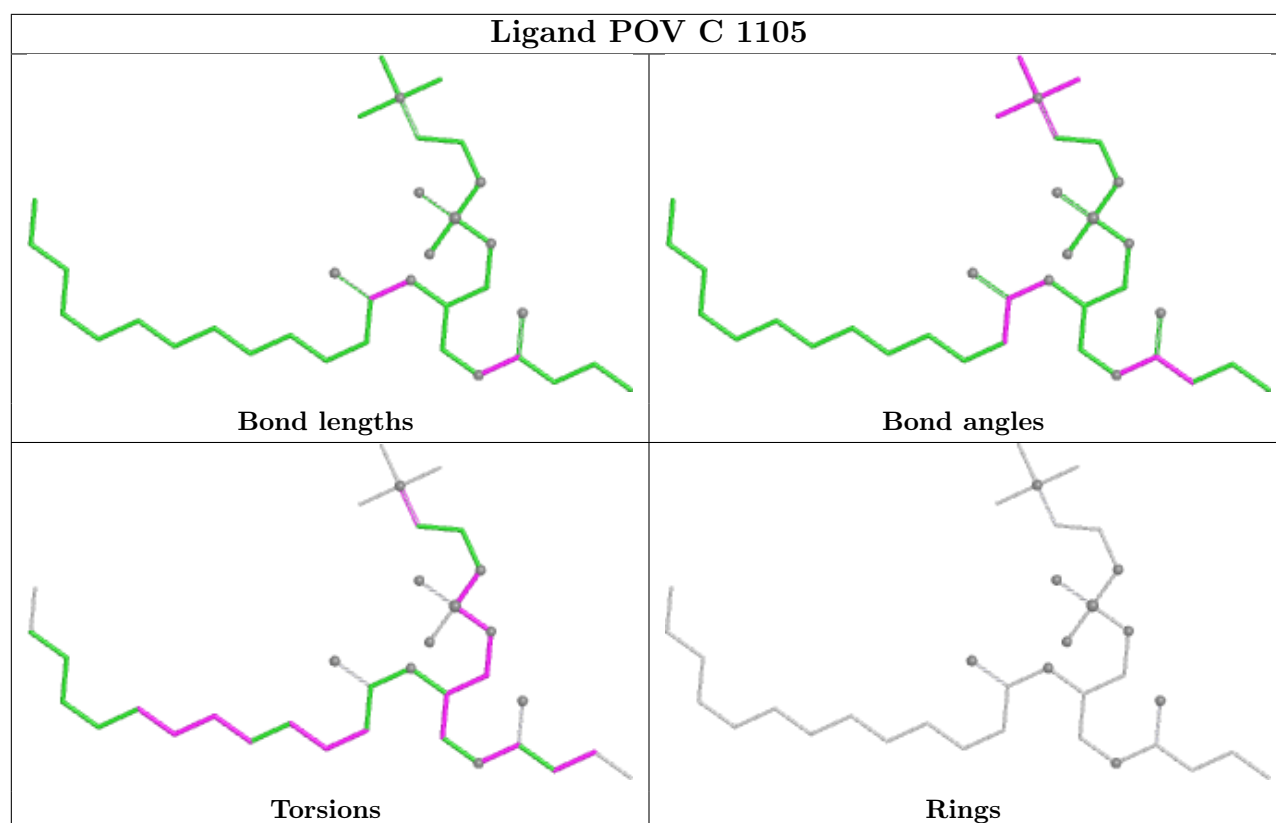


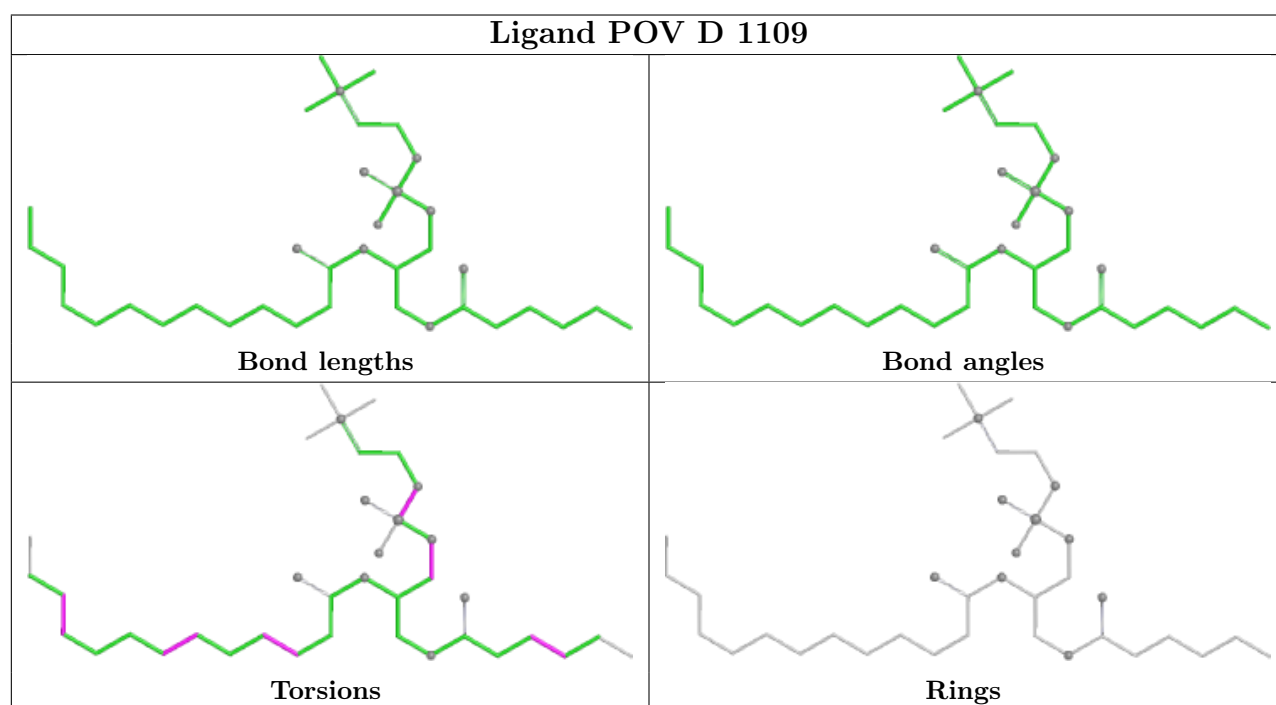
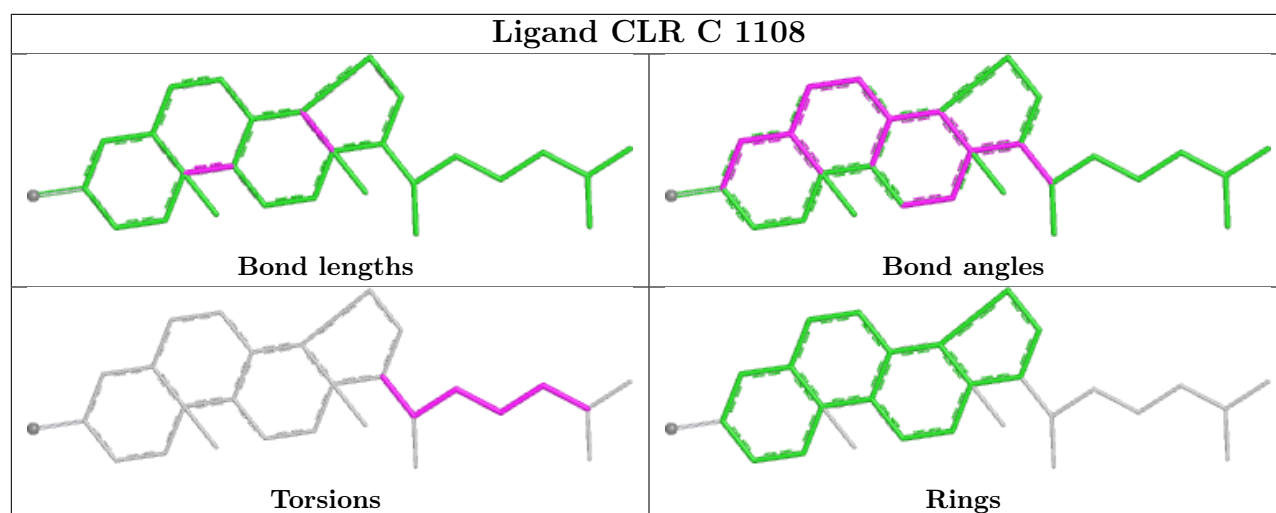


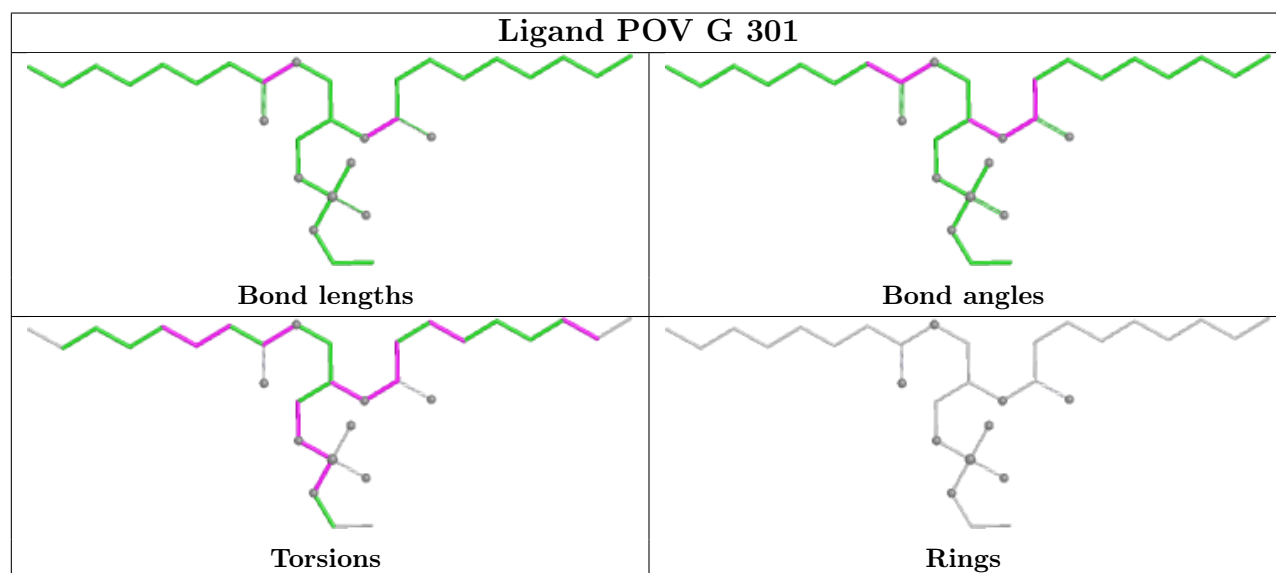
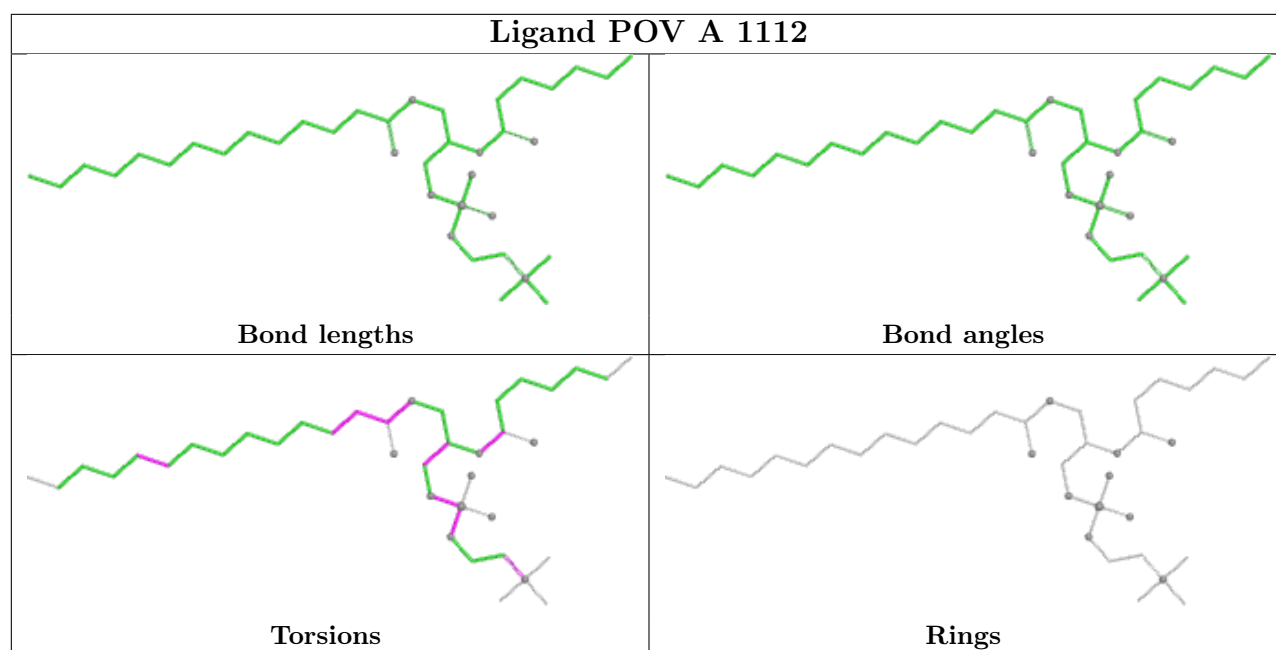


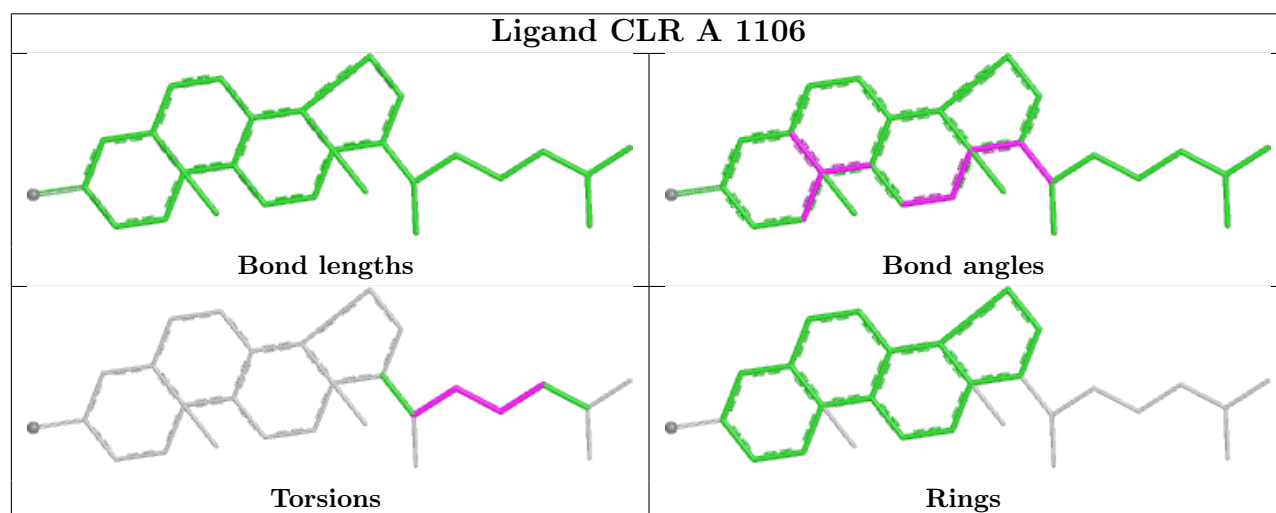
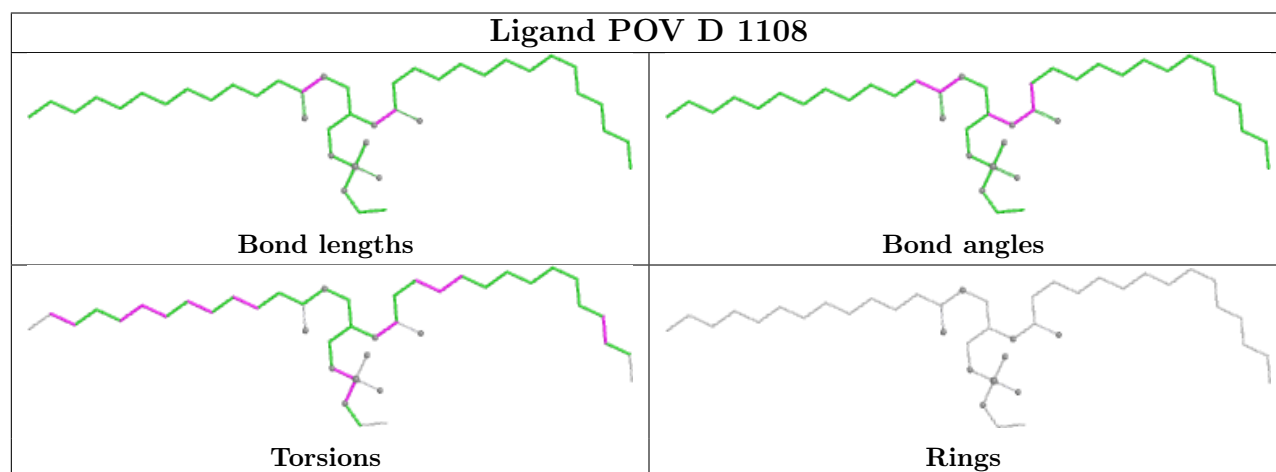
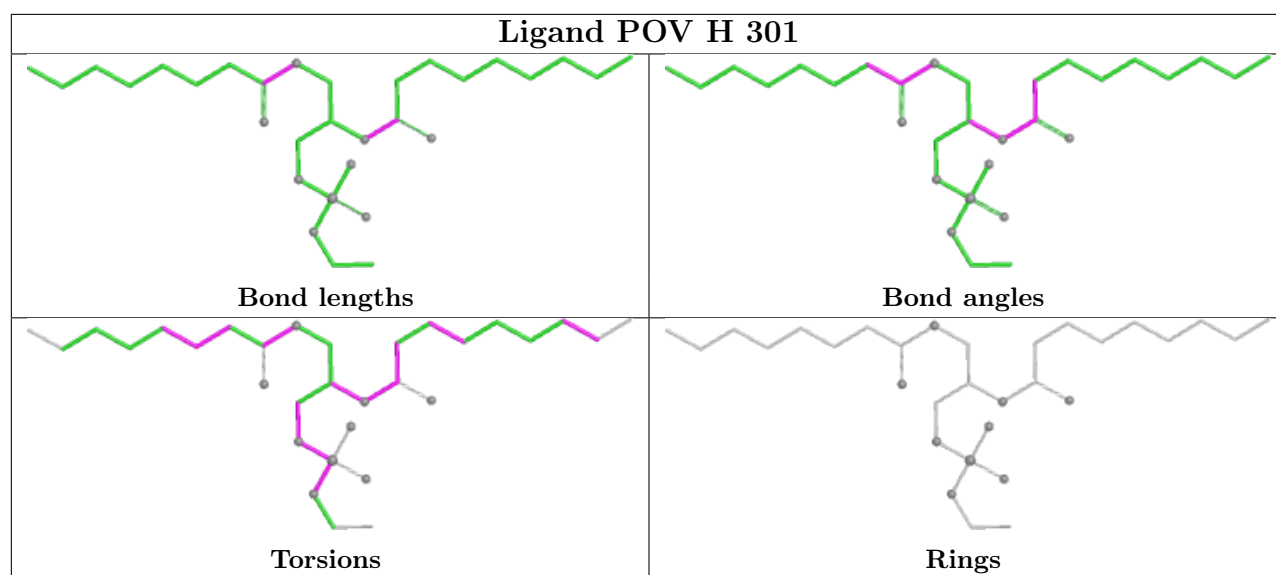


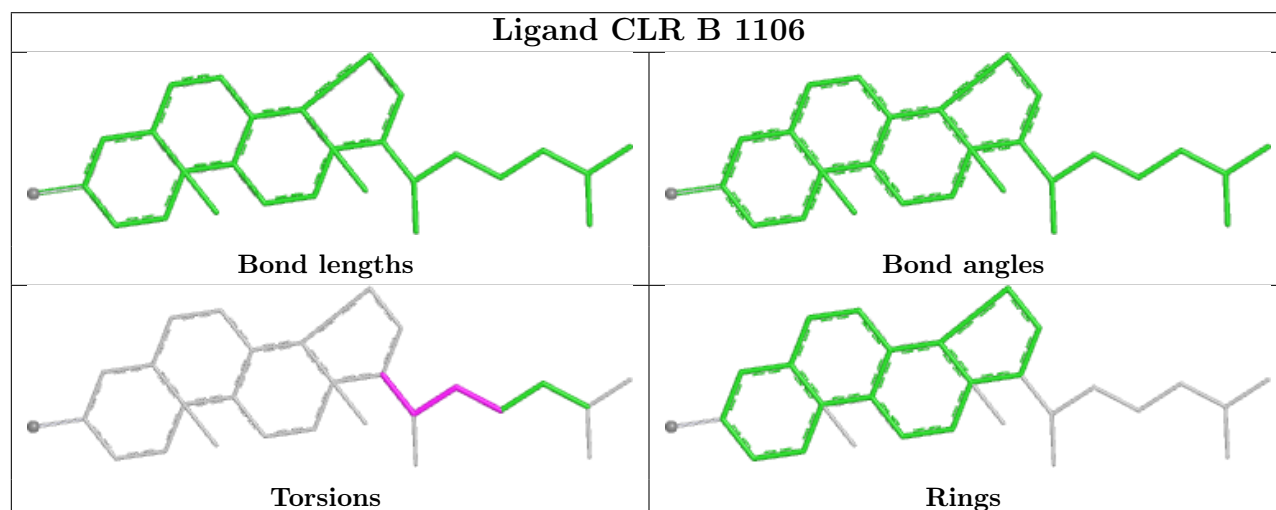
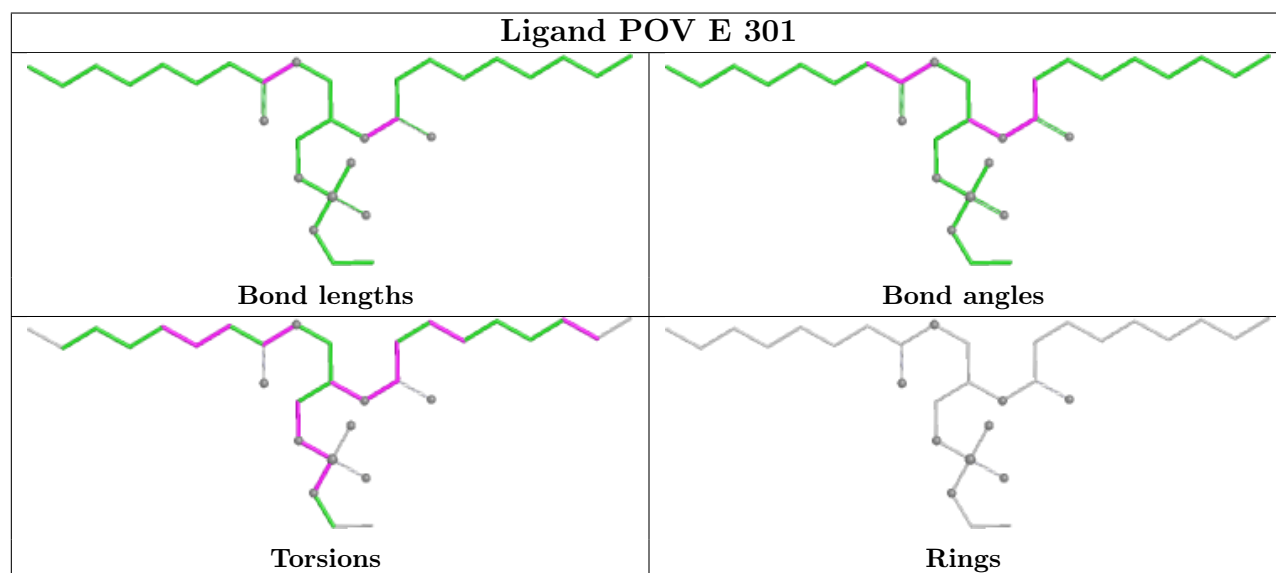
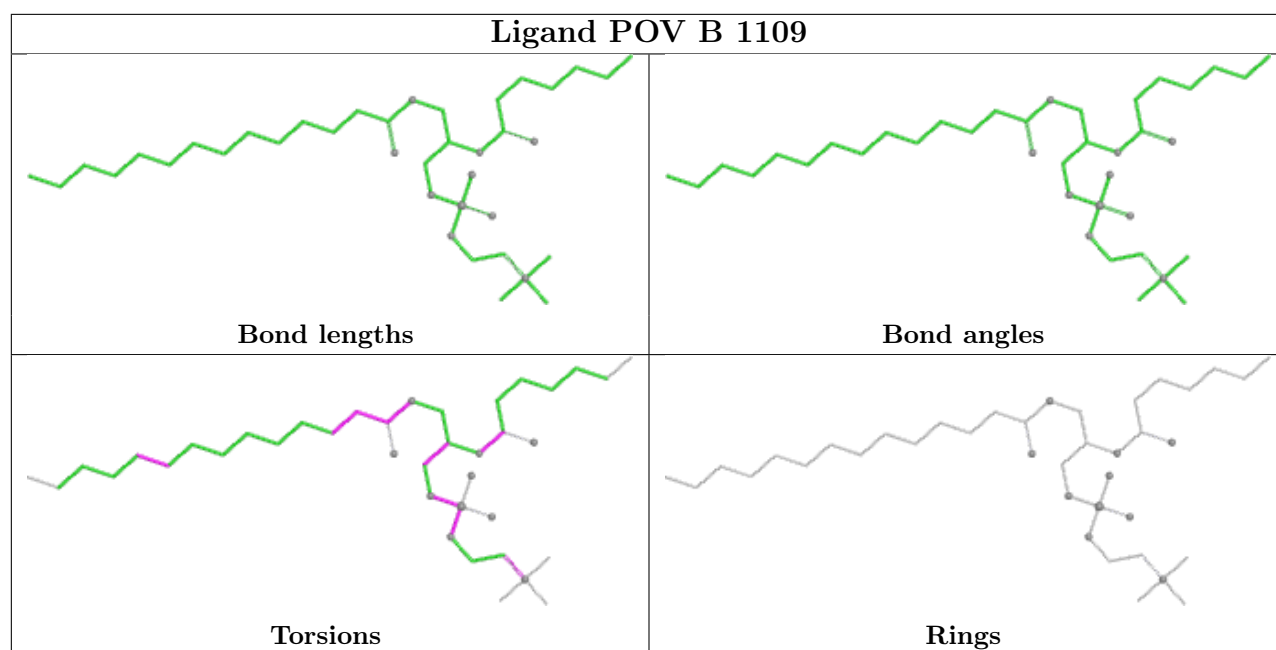


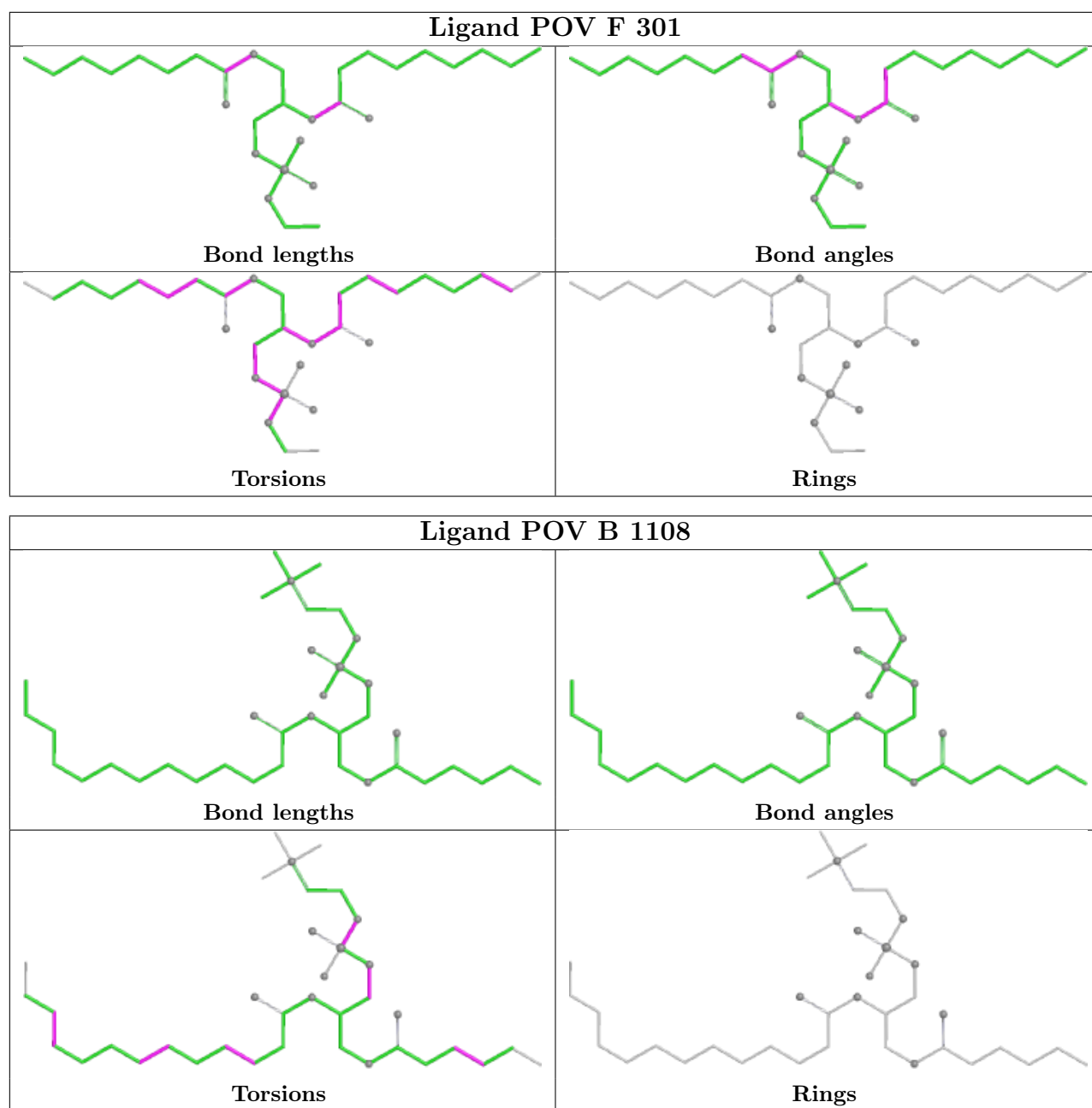












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

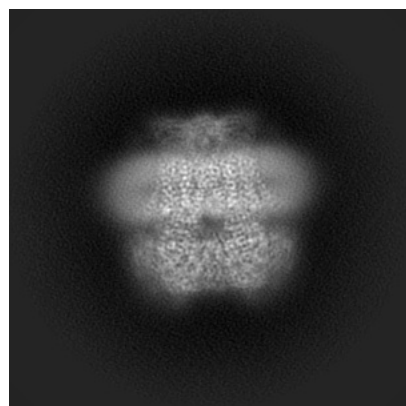
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46425. These allow visual inspection of the internal detail of the map and identification of artifacts.

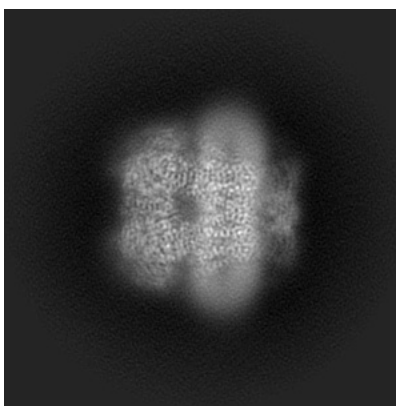
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

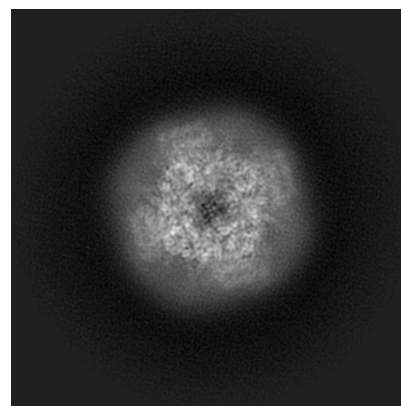
6.1.1 Primary map



X

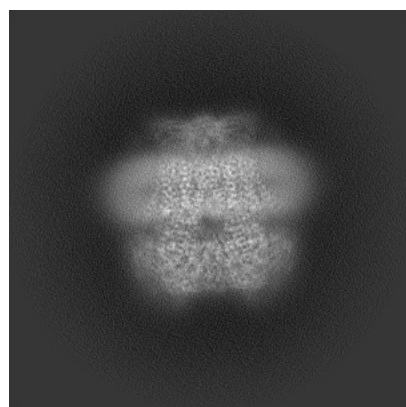


Y

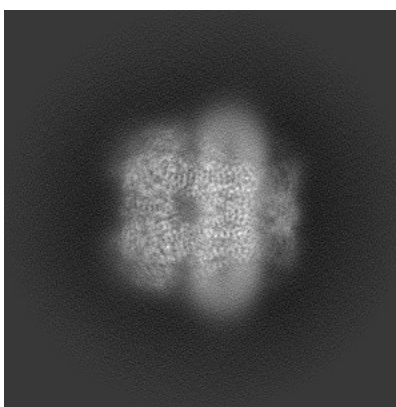


Z

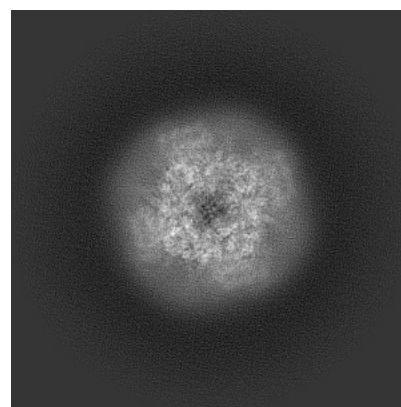
6.1.2 Raw map



X



Y

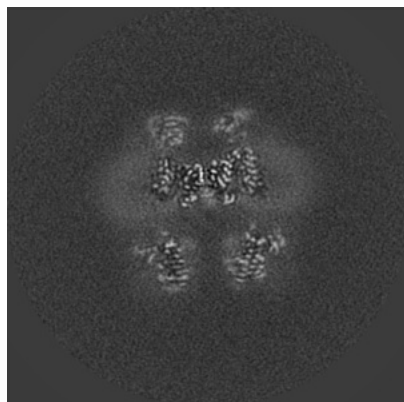


Z

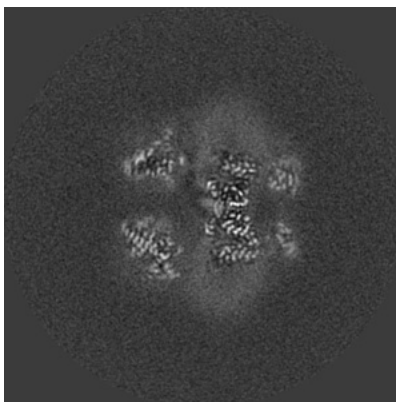
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

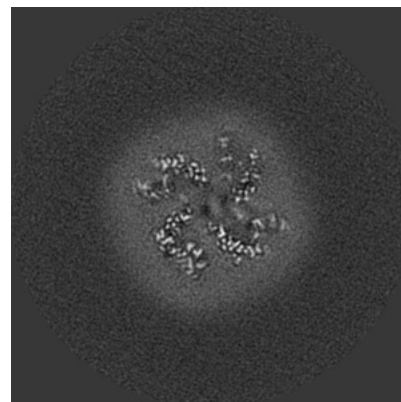
6.2.1 Primary map



X Index: 192

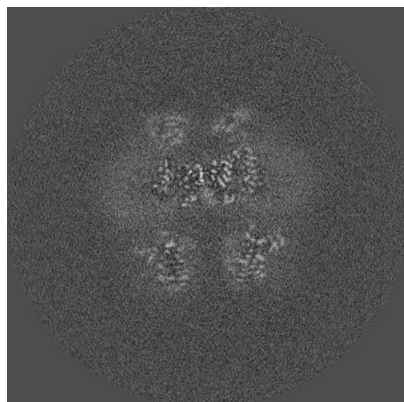


Y Index: 192

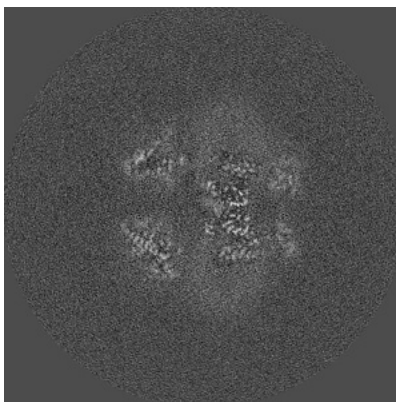


Z Index: 192

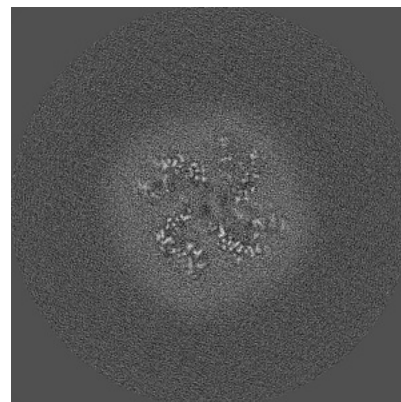
6.2.2 Raw map



X Index: 192



Y Index: 192

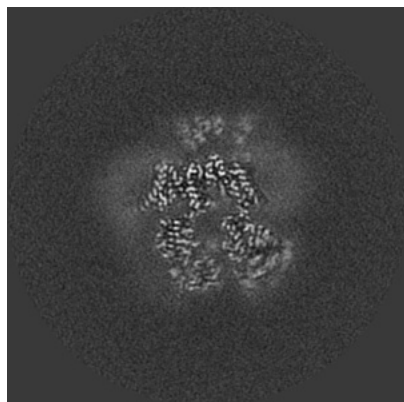


Z Index: 192

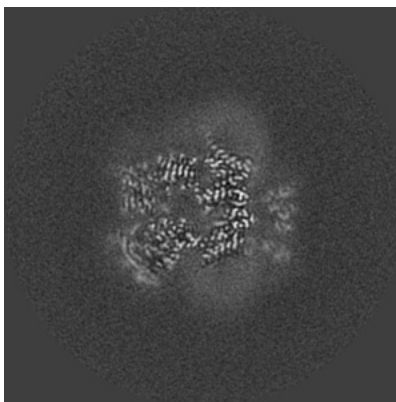
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

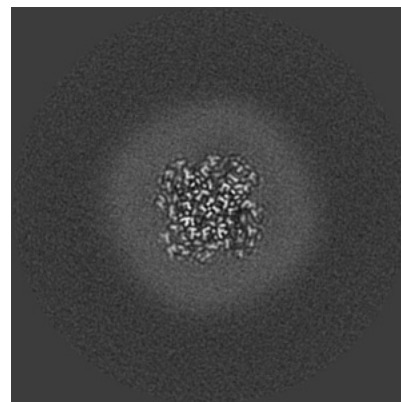
6.3.1 Primary map



X Index: 168

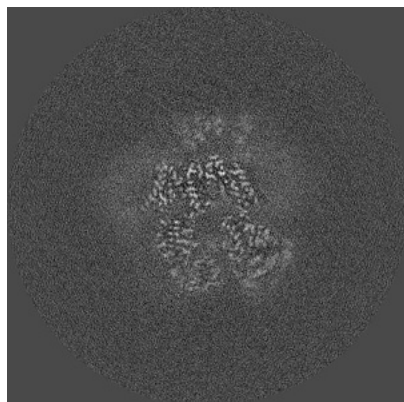


Y Index: 168

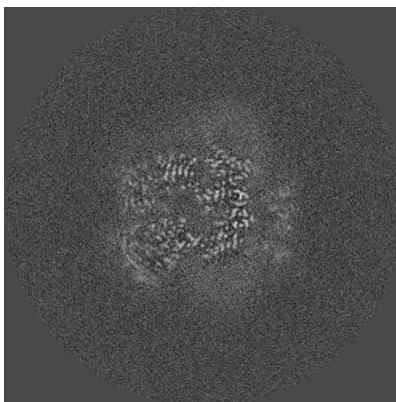


Z Index: 226

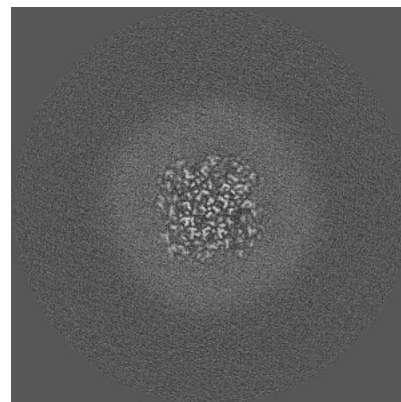
6.3.2 Raw map



X Index: 168



Y Index: 168

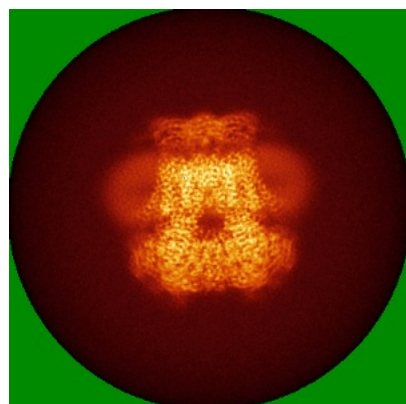


Z Index: 226

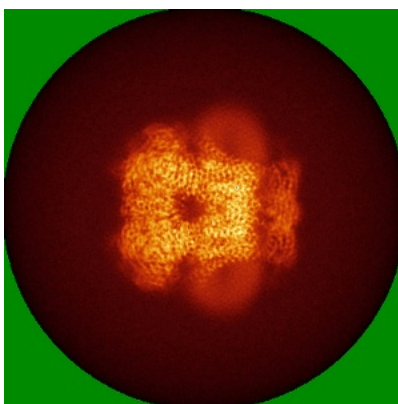
The images above show the largest variance slices of the map in three orthogonal directions.

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

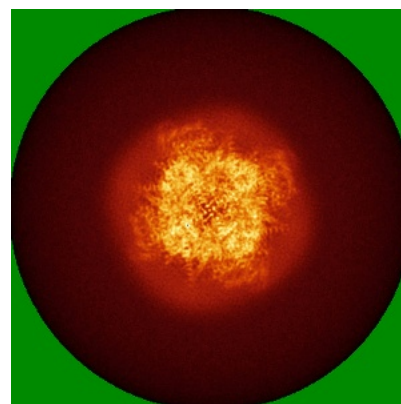
6.4.1 Primary map



X

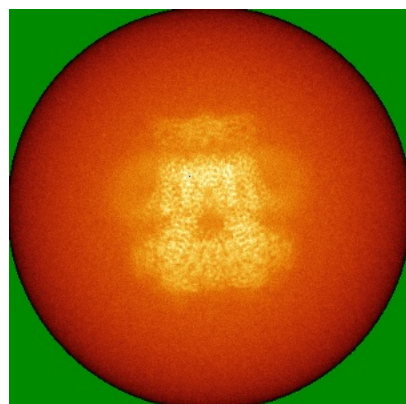


Y

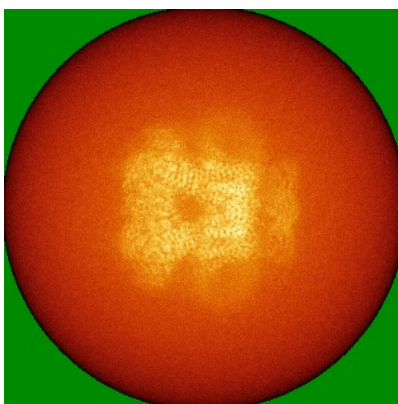


Z

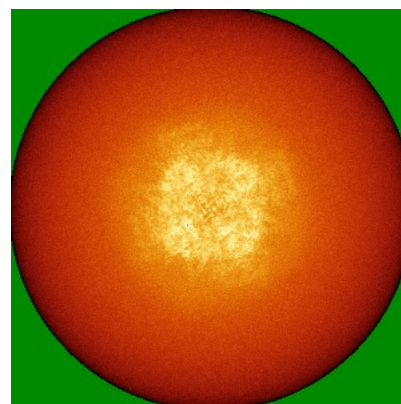
6.4.2 Raw map



X



Y

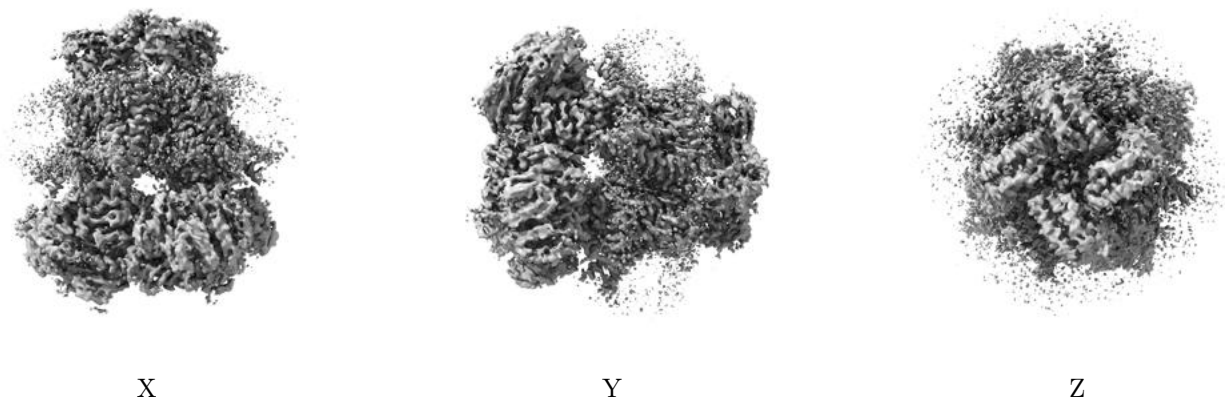


Z

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

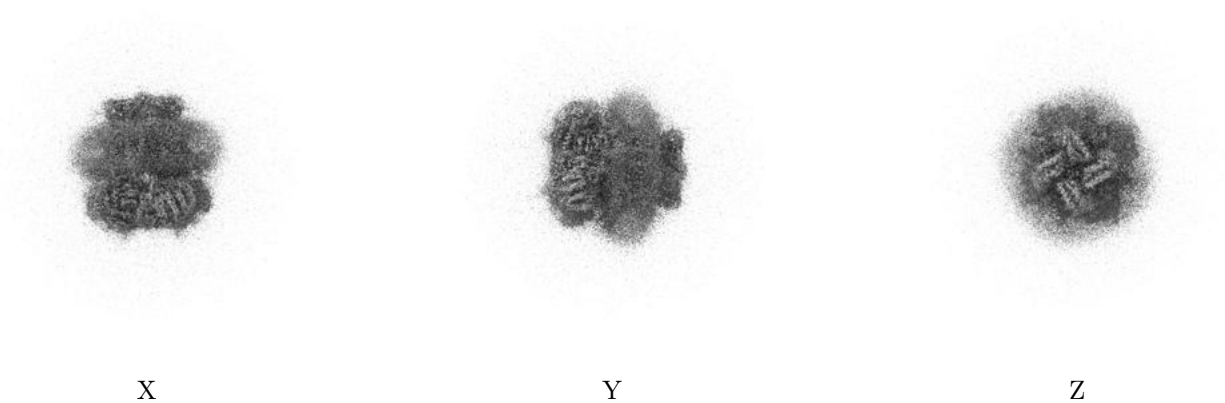
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

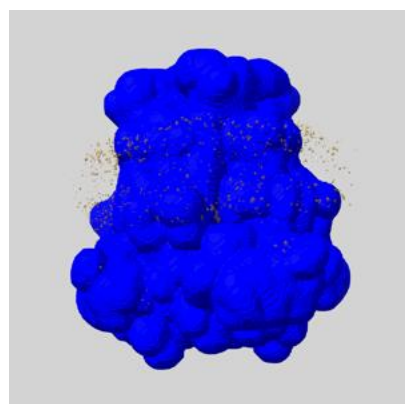
6.6 Mask visualisation [i](#)

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

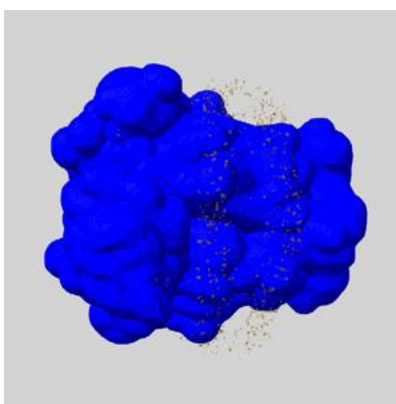
A mask typically either:

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

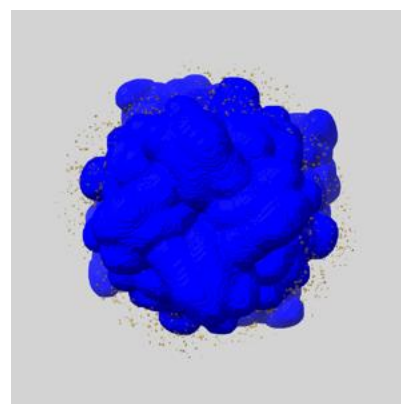
6.6.1 emd_46425_msk_1.map [i](#)



X



Y

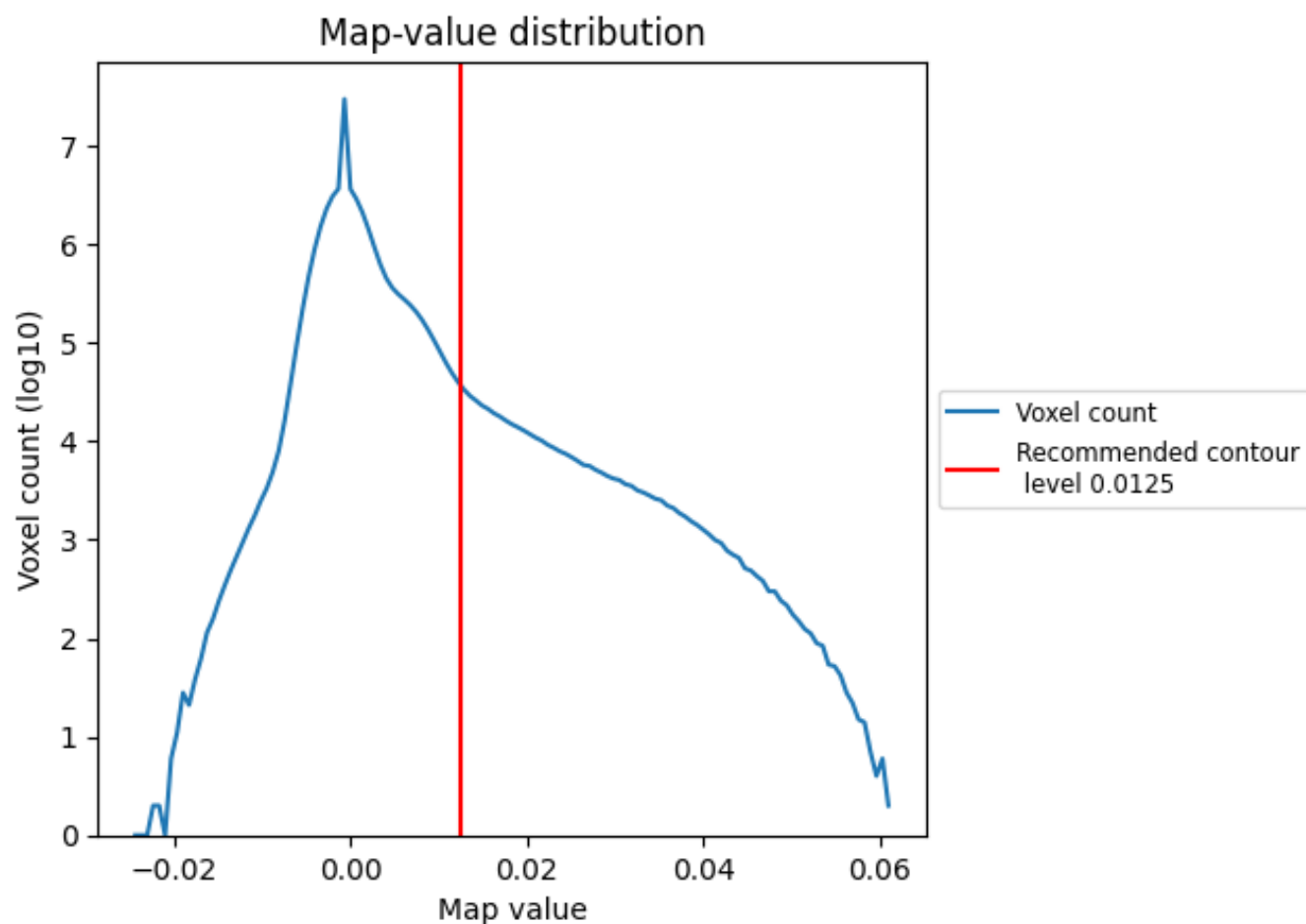


Z

7 Map analysis [i](#)

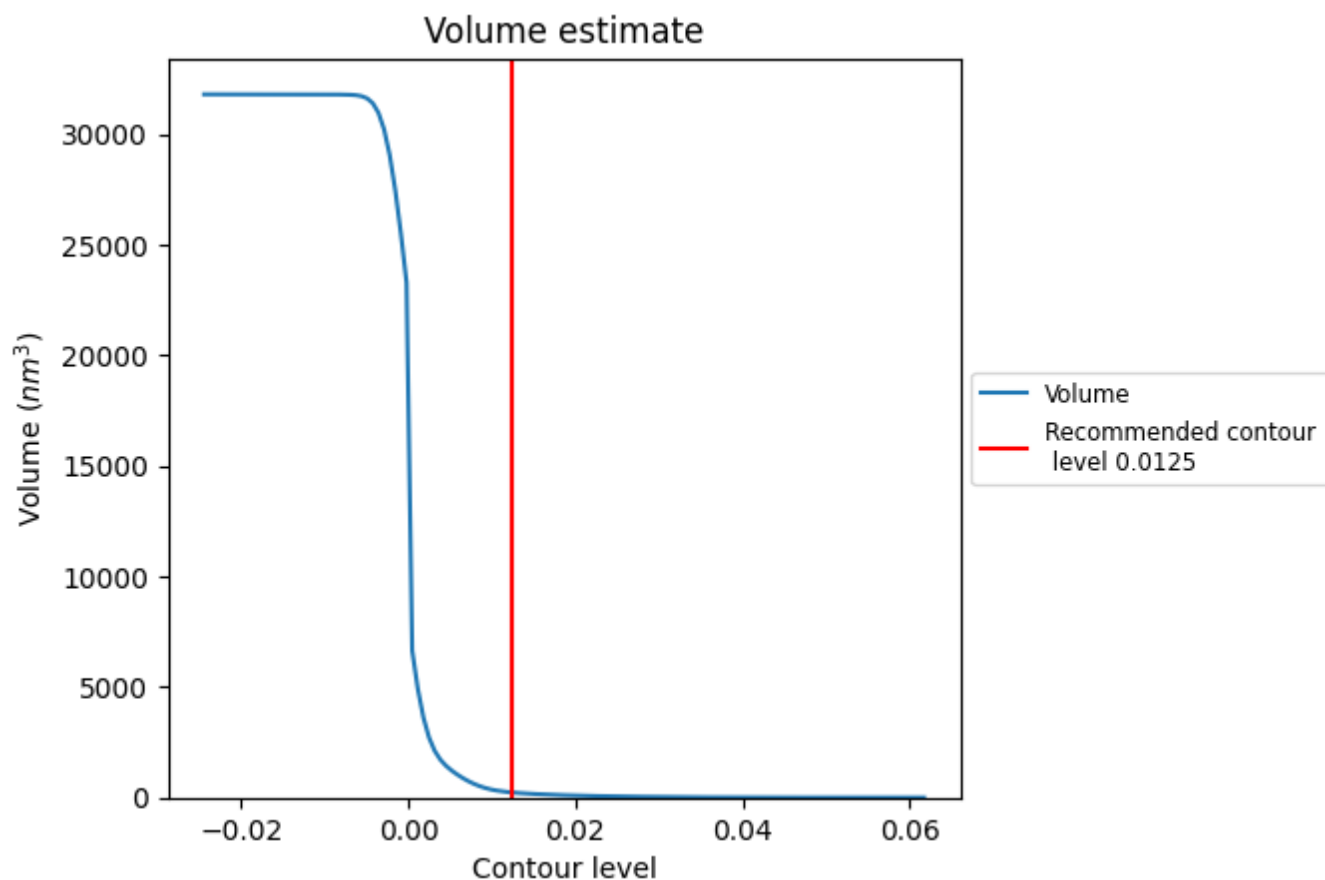
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

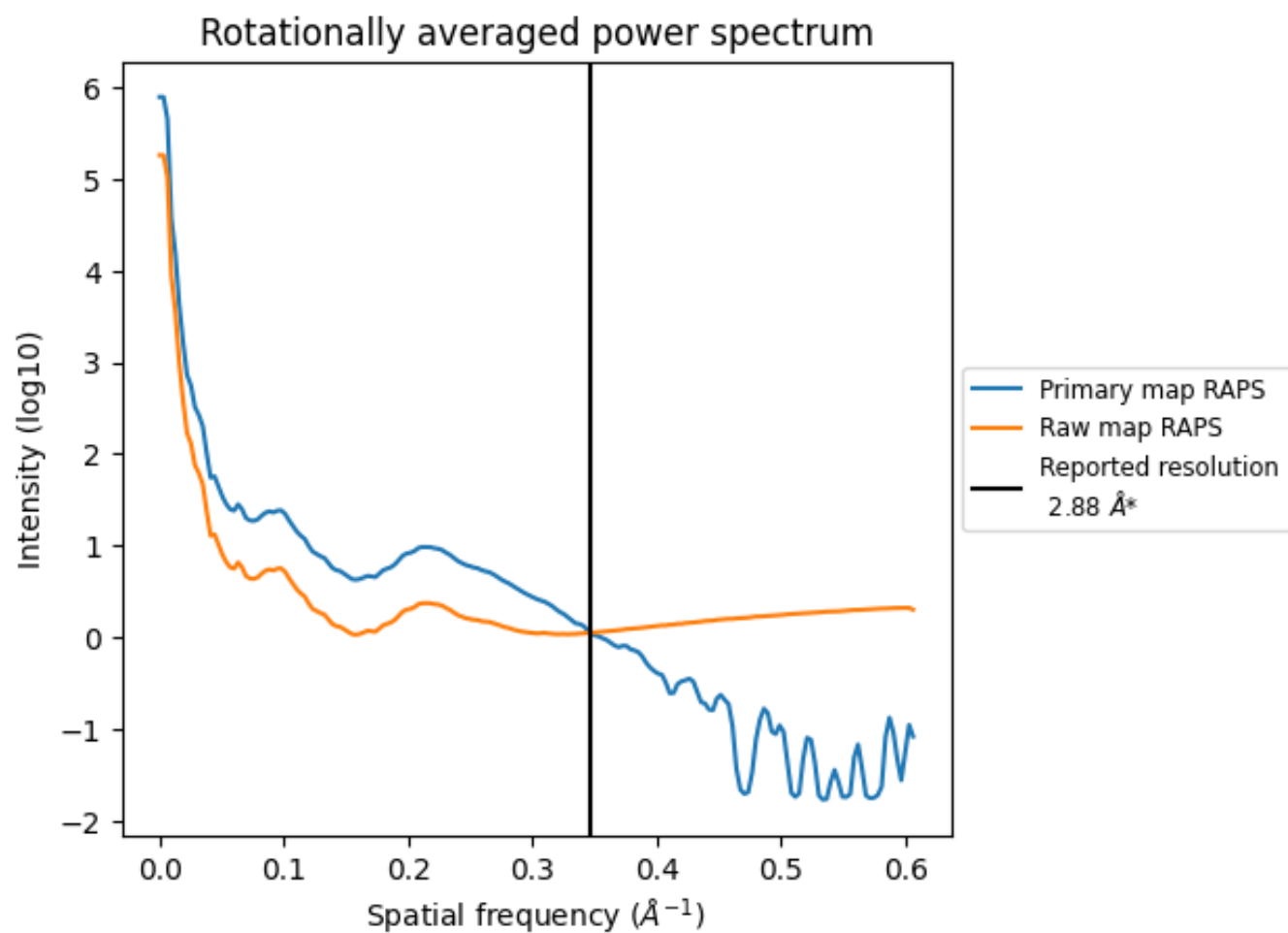
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; this corresponds to an approximate mass of 206 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

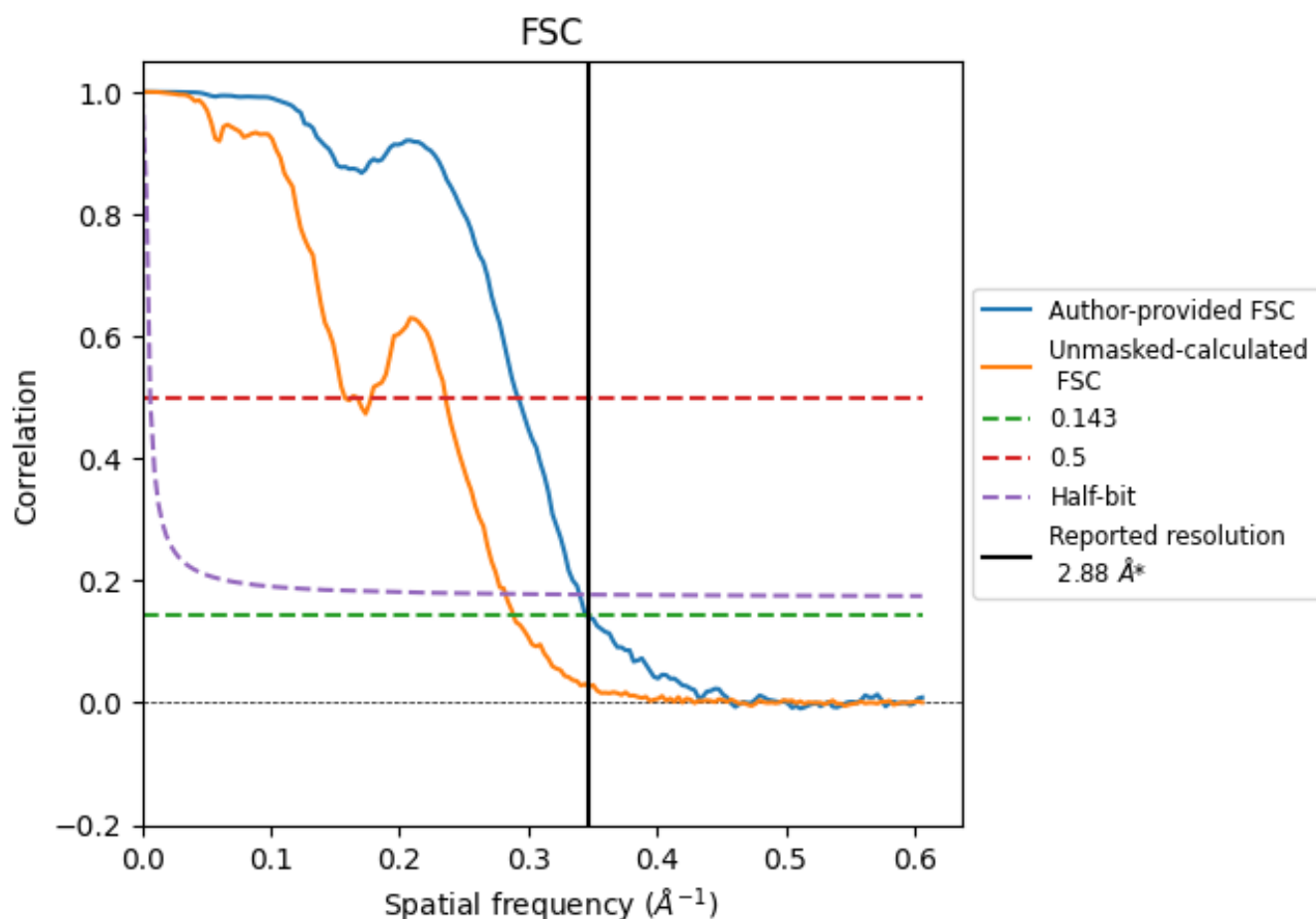


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.347 \AA^{-1}

8.2 Resolution estimates [i](#)

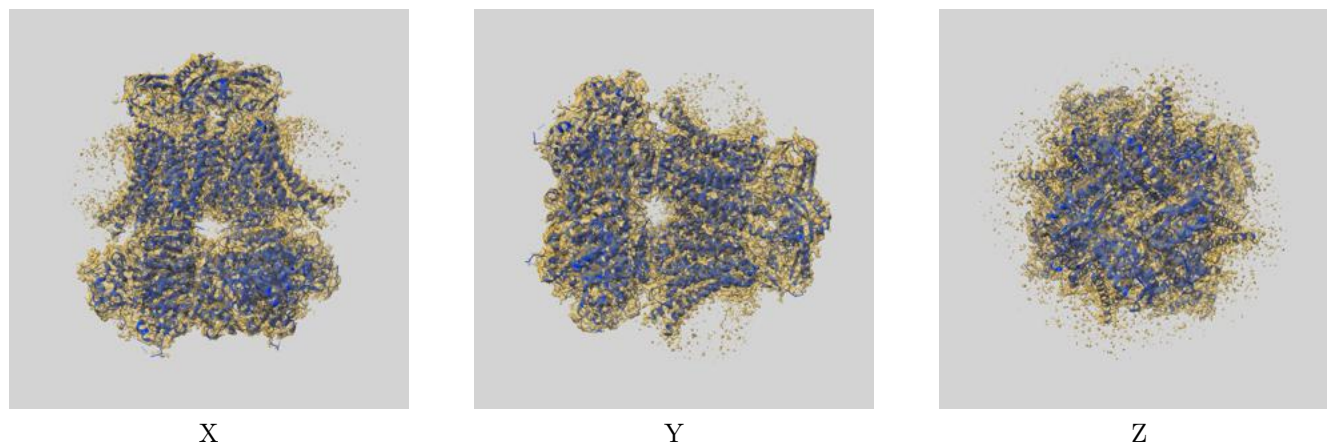
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.90	3.42	2.94
Unmasked-calculated*	3.47	6.35	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.88 by more than 10 %

9 Map-model fit [i](#)

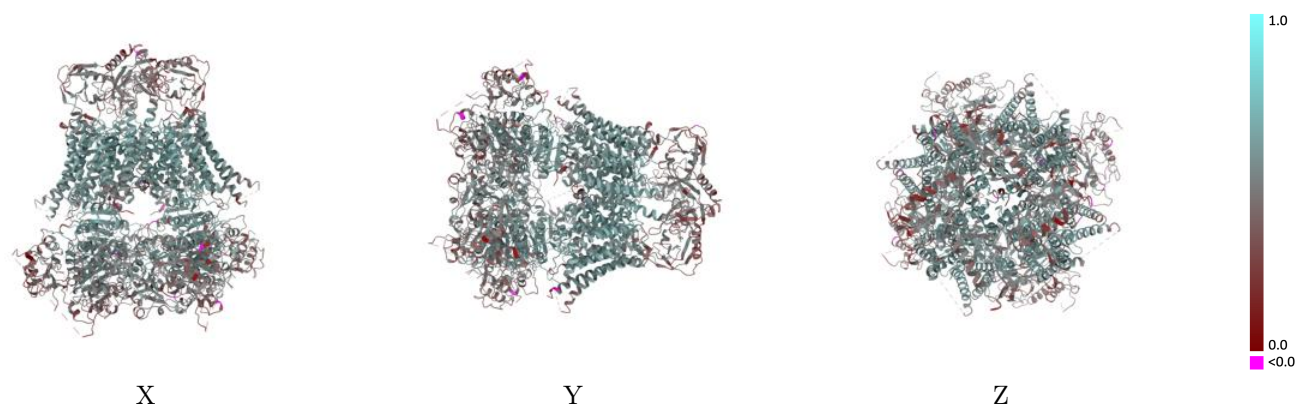
This section contains information regarding the fit between EMDB map EMD-46425 and PDB model 9D19. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



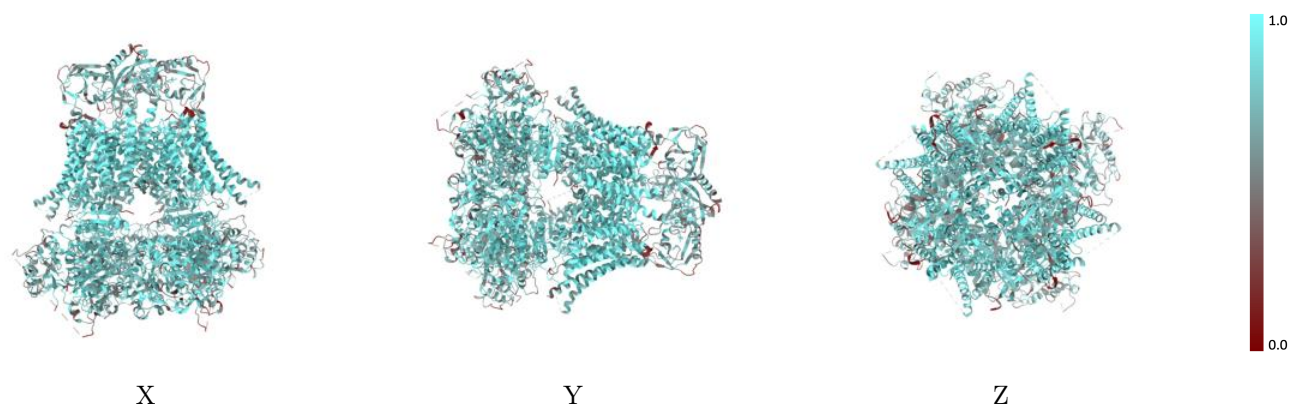
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



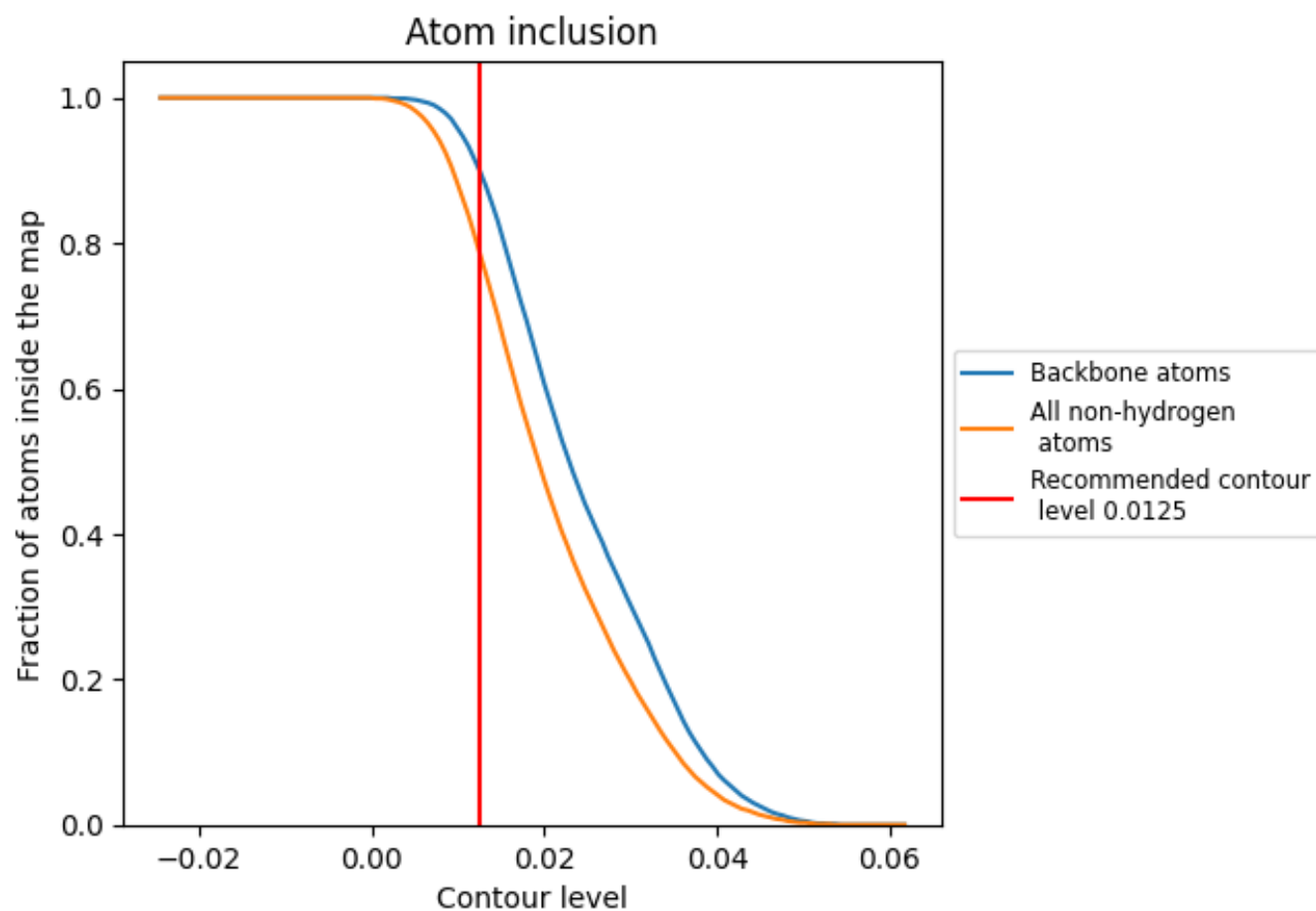
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7880	<div><div></div></div> 0.5010
A	<div><div></div></div> 0.8220	<div><div></div></div> 0.5320
B	<div><div></div></div> 0.8050	<div><div></div></div> 0.5110
C	<div><div></div></div> 0.8010	<div><div></div></div> 0.5070
D	<div><div></div></div> 0.8010	<div><div></div></div> 0.5090
E	<div><div></div></div> 0.7220	<div><div></div></div> 0.4680
F	<div><div></div></div> 0.7040	<div><div></div></div> 0.4240
G	<div><div></div></div> 0.7030	<div><div></div></div> 0.4440
H	<div><div></div></div> 0.6830	<div><div></div></div> 0.4310

1.0

0.0

<0.0