



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:02 PM UTC

PDB ID : 6S7T / pdb_00006s7t
EMDB ID : EMD-10112
Title : Cryo-EM structure of human oligosaccharyltransferase complex OST-B
Authors : Ramirez, A.S.; Kowal, J.; Locher, K.P.
Deposited on : 2019-07-05
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

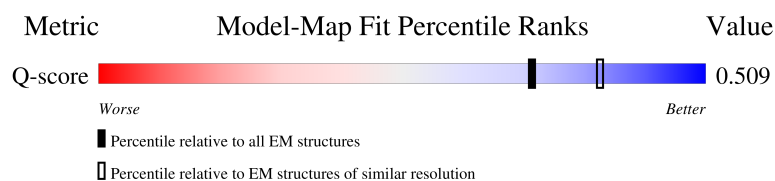
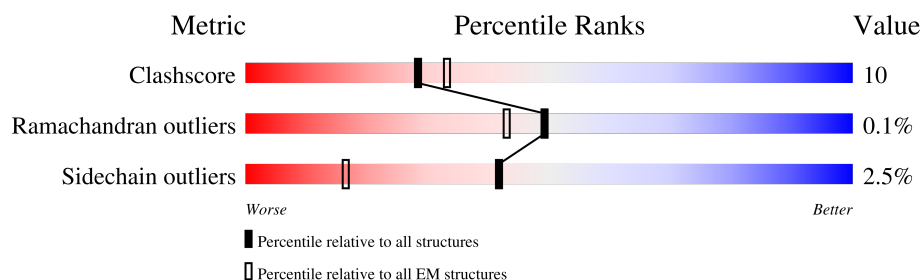
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



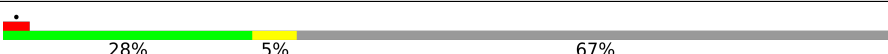
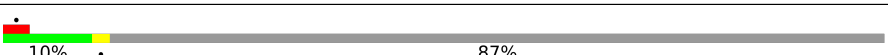
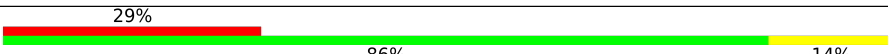
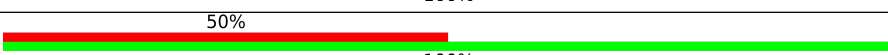
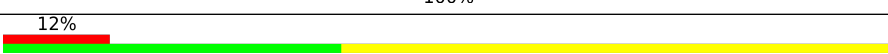
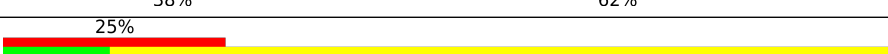
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	826	
2	B	37	
3	C	79	
4	D	113	

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Mol	Chain	Length	Quality of chain
5	E	607	
6	F	631	
7	G	456	
8	H	335	
9	I	292	
10	K	7	
11	J	2	
11	M	2	
12	L	8	
13	N	8	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 18445 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 Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	706	Total	C	N	O	S	0	0
			5739	3784	941	982	32		

- Molecule 2 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	33	Total	C	N	O	S	0	0
			258	174	39	43	2		

- Molecule 3 is a protein called Transmembrane protein 258.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	78	Total	C	N	O	S	0	0
			634	435	91	105	3		

- Molecule 4 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	103	Total	C	N	O	S	0	0
			817	544	128	141	4		

- Molecule 5 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	428	Total	C	N	O	S	0	0
			3461	2236	570	650	5		

- Molecule 6 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	250	Total	C	N	O	S	0	0
			1979	1291	328	356	4		

- Molecule 7 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	410	Total	C	N	O	S	0	0
			3233	2085	533	610	5		

- Molecule 8 is a protein called Magnesium transporter protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	112	Total	C	N	O	S	0	0
			872	573	144	145	10		

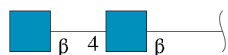
- Molecule 9 is a protein called Malectin.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	37	Total	C	N	O	S	0	0
			280	185	43	49	3		

- Molecule 10 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	7	Total	C	N	O	0	0
			40	23	8	9		

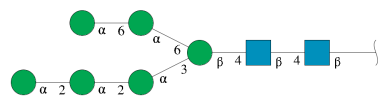
- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	J	2	Total	C	N	O	0	0
			28	16	2	10		
11	M	2	Total	C	N	O	0	0
			28	16	2	10		

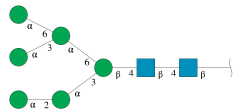
- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra

nose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



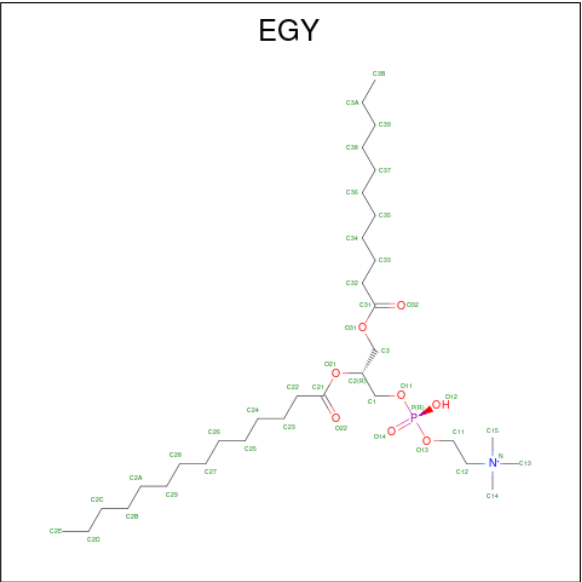
Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



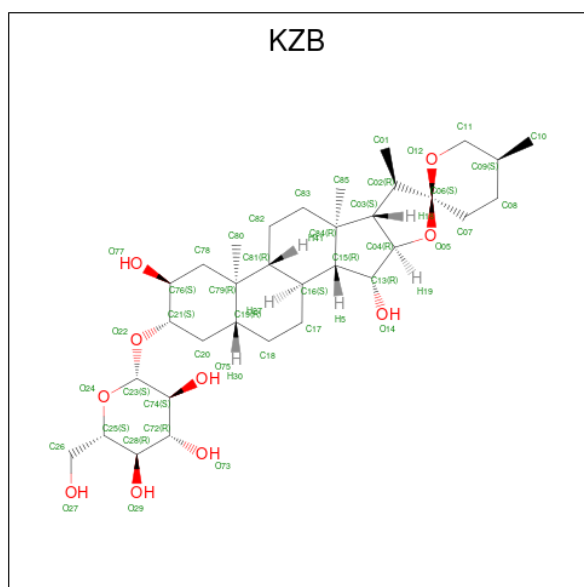
Mol	Chain	Residues	Atoms				AltConf	Trace
13	N	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 14 is (4R,7R)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(undecanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphadocosan-1-aminium (CCD ID: EGY) (formula: C₃₃H₆₇NO₈P).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
14	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	D	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	E	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	F	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 15 is (2 {S},3 {R},4 {R},5 {S},6 {S})-2-(hydroxymethyl)-6-[(1 {S},2 {R},3 {R},4 {R},5' {S},6 {S},7 {R},8 {S},9 {R},12 {R},13 {R},15 {S},16 {S},18 {R})-5',7,9,13-tetramethyl-3,15-bis(oxidanyl)spiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icosane-6,2'-oxane]-16-yl]oxy-oxane-3,4,5-triol (CCD ID: KZB) (formula: C₃₃H₅₄O₁₀).

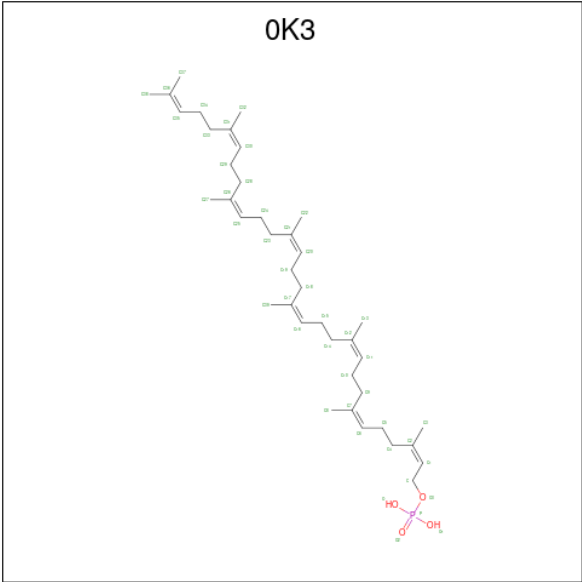


Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			32	27	5	
15	C	1	Total	C	O	0
			32	27	5	
15	C	1	Total	C	O	0
			32	27	5	
15	D	1	Total	C	O	0
			32	27	5	
15	D	1	Total	C	O	0
			32	27	5	
15	D	1	Total	C	O	0
			32	27	5	
15	E	1	Total	C	O	0
			32	27	5	
15	E	1	Total	C	O	0
			32	27	5	
15	F	1	Total	C	O	0
			32	27	5	
15	F	1	Total	C	O	0
			32	27	5	
15	F	1	Total	C	O	0
			32	27	5	
15	G	1	Total	C	O	0
			32	27	5	
15	G	1	Total	C	O	0
			32	27	5	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	E	1	Total	Mg	0
			1	1	

- Molecule 17 is (2Z,6Z,10Z,14Z,18Z,22Z,26Z)-3,7,11,15,19,23,27,31-octamethyldotriacont-2,6,10,14,18,22,26,30-octaen-1-yl dihydrogen phosphate (CCD ID: 0K3) (formula: C₄₀H₆₇O₄P).

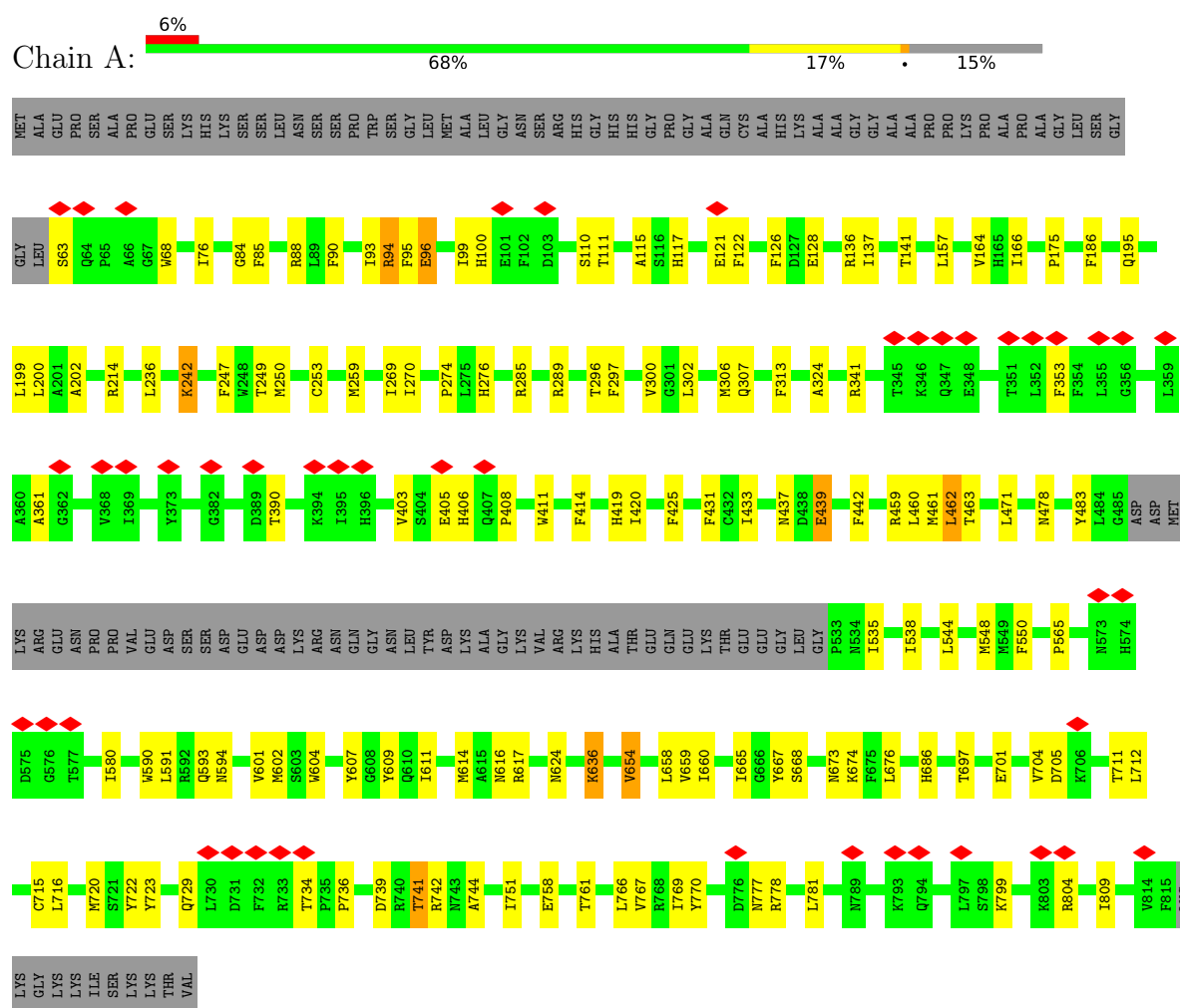


Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			45	40	4	1	

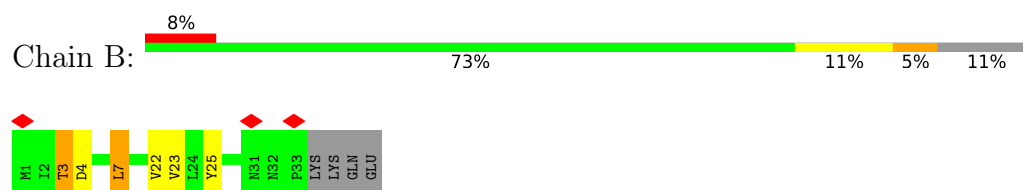
3 Residue-property plots

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

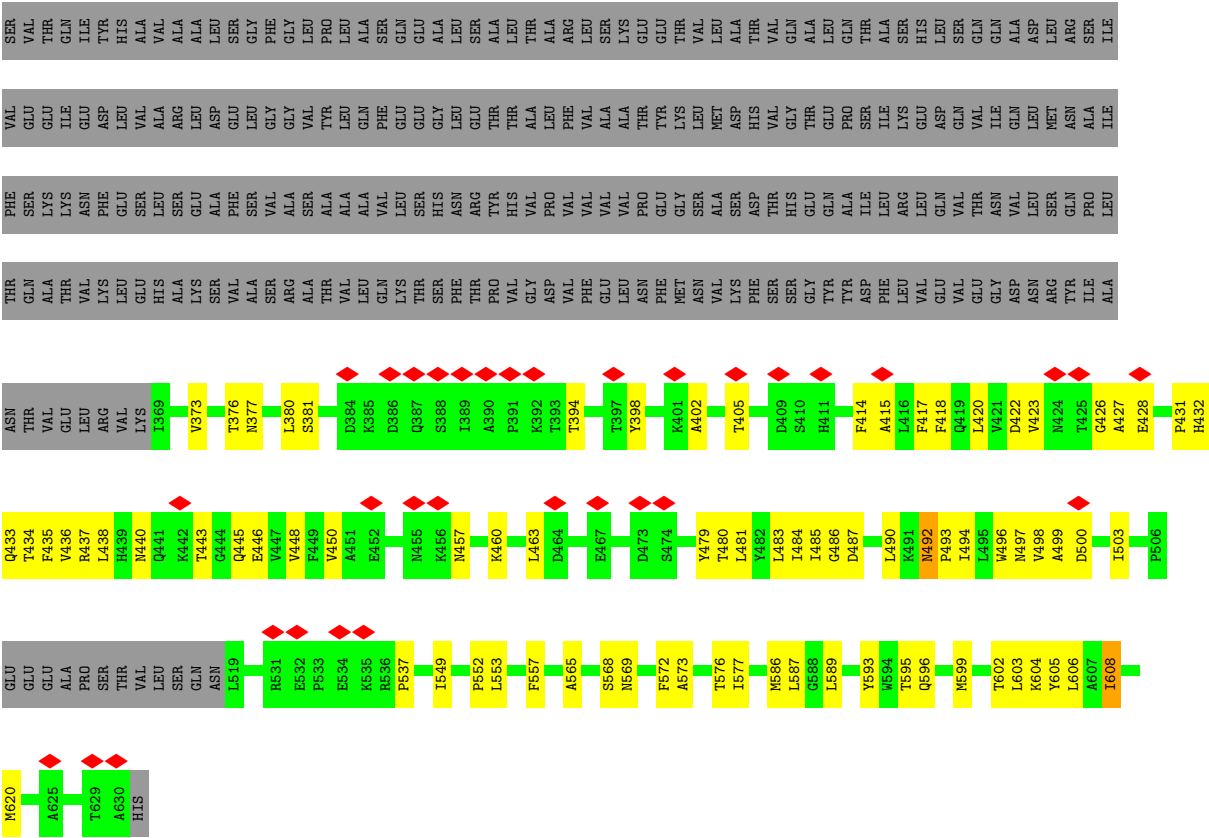
- Molecule 1: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3B



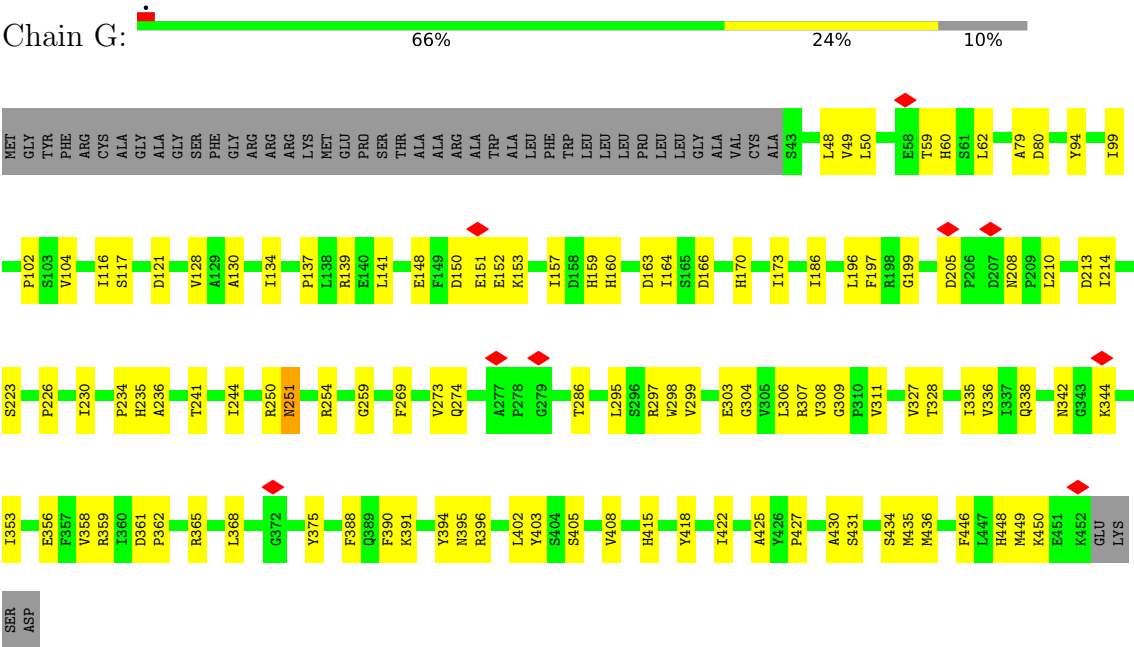
- Molecule 2: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4



- Chain F: 
- | Amino Acid | Frequency (%) |
|------------|---------------|
| MET | 5 |
| ALA | 27 |
| PRO | 27 |
| GLY | 27 |
| SER | 27 |
| THR | 27 |
| VAL | 27 |
| PHE | 27 |
| LEU | 27 |
| ALA | 27 |
| LEU | 27 |
| THR | 27 |
| ILE | 27 |
| ALA | 27 |
| SER | 27 |
| THR | 27 |
| TRP | 27 |
| ALA | 27 |
| SER | 27 |
| ALA | 27 |
| LEU | 27 |
| THR | 27 |
| PRO | 27 |
| THR | 27 |
| HIS | 27 |
| TYR | 27 |
| LEU | 27 |
| THR | 27 |
| LYS | 27 |
| HIS | 27 |
| GLN | 27 |
| ALA | 27 |
| ASP | 27 |
| SER | 27 |
| VAL | 27 |
| GLU | 27 |
| ARG | 27 |
| LEU | 27 |
| LYS | 27 |
| ALA | 27 |
| SER | 27 |
| CYS | 27 |
| ILE | 27 |
| ASP | 27 |
| LEU | 27 |
| ARG | 27 |
| PRO | 27 |
| PHE | 27 |
| SER | 27 |
| ASN | 27 |
| THR | 27 |
| LEU | 27 |
| ASN | 27 |
| THR | 27 |
| GLU | 27 |
| SER | 27 |
| ALA | 27 |
| VAL | 27 |
| ASP | 27 |
| SER | 27 |
| LEU | 27 |
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| TYR | 27 |
| ALA | 27 |
| ALA | 27 |
| GLN | 27 |
| SER | 27 |
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| PHE | 27 |
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| GLU | 27 |
| THR | 27 |
| LYS | 27 |
| ASP | 27 |
| SER | 27 |
| LEU | 27 |
| LEU | 27 |
| PHE | 27 |
| ALA | 27 |
| ALA | 27 |
| VAL | 27 |
| VAL | 27 |
| GLY | 27 |
| SER | 27 |
| LEU | 27 |
| ASP | 27 |



• Molecule 7: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit



• Molecule 8: Magnesium transporter protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	249725	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	322.56, 322.56, 322.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0K3, BMA, MG, MAN, KZB, NAG, EGY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/5916	0.42	0/8044
2	B	0.16	0/263	0.27	0/360
3	C	0.18	0/654	0.36	0/893
4	D	0.22	0/837	0.38	0/1135
5	E	0.24	0/3549	0.45	0/4833
6	F	0.21	0/2026	0.42	0/2760
7	G	0.22	0/3315	0.41	0/4502
8	H	0.15	0/897	0.40	0/1212
9	I	0.20	0/289	0.59	0/396
10	K	0.07	0/39	0.19	0/53
All	All	0.22	0/17785	0.42	0/24188

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

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	5739	0	5682	105	0
2	B	258	0	272	5	0
3	C	634	0	647	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	817	0	829	20	0
5	E	3461	0	3421	79	0
6	F	1979	0	2005	71	0
7	G	3233	0	3174	74	0
8	H	872	0	865	12	0
9	I	280	0	278	5	0
10	K	40	0	40	1	0
11	J	28	0	25	0	0
11	M	28	0	25	0	0
12	L	94	0	79	0	0
13	N	94	0	79	2	0
14	A	253	0	0	8	0
14	C	43	0	0	3	0
14	D	43	0	0	2	0
14	E	43	0	0	0	0
14	F	43	0	0	0	0
15	A	32	0	0	2	0
15	C	64	0	0	1	0
15	D	96	0	0	0	0
15	E	64	0	0	6	0
15	F	96	0	0	0	0
15	G	64	0	0	0	0
16	A	1	0	0	0	0
16	E	1	0	0	0	0
17	A	45	0	66	3	0
All	All	18445	0	17487	342	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 10.

All (342) 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)
5:E:440:LEU:HB3	15:E:702:KZB:C10	1.70	1.20
1:A:361:ALA:CB	14:A:918:EGY:C37	2.32	1.06
1:A:361:ALA:HB1	14:A:918:EGY:C37	1.89	1.01
5:E:440:LEU:CB	15:E:702:KZB:C10	2.48	0.90
14:A:915:EGY:C25	15:A:919:KZB:C01	2.55	0.85
1:A:93:ILE:HD11	2:B:7:LEU:HD13	1.59	0.83
14:C:101:EGY:C14	5:E:290:ASP:OD2	2.28	0.81
5:E:291:VAL:HG21	5:E:305:LEU:HD13	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:414:PHE:HB3	6:F:463:LEU:HB3	1.64	0.79
6:F:595:THR:HG22	6:F:596:GLN:HG3	1.65	0.78
7:G:390:PHE:O	7:G:405:SER:HA	1.84	0.77
6:F:496:TRP:CZ3	6:F:498:VAL:HA	2.21	0.76
6:F:572:PHE:HD1	6:F:577:ILE:HD11	1.49	0.75
1:A:361:ALA:HB3	14:A:918:EGY:C37	2.15	0.75
6:F:437:ARG:NH2	6:F:446:GLU:OE1	2.19	0.75
1:A:809:ILE:HD11	7:G:79:ALA:HB3	1.68	0.74
5:E:440:LEU:HD13	15:E:702:KZB:C10	2.17	0.74
3:C:11:SER:H	9:I:264:TYR:HE1	1.35	0.74
7:G:353:ILE:HG23	7:G:368:LEU:HB2	1.70	0.73
1:A:63:SER:HB2	1:A:68:TRP:HE1	1.54	0.73
1:A:425:PHE:CE1	1:A:471:LEU:HD12	2.24	0.73
1:A:405:GLU:HB3	1:A:459:ARG:HB2	1.71	0.72
5:E:404:PHE:HZ	5:E:434:LEU:HD21	1.54	0.72
5:E:440:LEU:CD1	15:E:702:KZB:C10	2.68	0.72
7:G:297:ARG:NH1	7:G:303:GLU:OE1	2.18	0.71
6:F:434:THR:HG22	6:F:485:ILE:HG13	1.73	0.70
8:H:237:ASN:HD21	8:H:269:THR:HG21	1.57	0.70
14:C:101:EGY:C14	5:E:290:ASP:CG	2.65	0.69
1:A:200:LEU:HD13	2:B:22:VAL:HG11	1.74	0.69
6:F:437:ARG:HD3	6:F:484:ILE:HD11	1.75	0.69
6:F:568:SER:HB3	7:G:450:LYS:HB2	1.74	0.69
5:E:417:VAL:HG13	5:E:419:GLN:H	1.57	0.69
7:G:48:LEU:HD12	7:G:94:TYR:CD2	2.28	0.68
6:F:422:ASP:OD1	6:F:423:VAL:N	2.27	0.68
1:A:195:GLN:NE2	2:B:25:TYR:OH	2.25	0.68
6:F:417:PHE:HD1	6:F:460:LYS:HG3	1.59	0.67
1:A:259:MET:HG2	1:A:269:ILE:HD12	1.76	0.67
5:E:290:ASP:O	5:E:334:TYR:HA	1.95	0.67
1:A:274:PRO:HG3	1:A:324:ALA:HA	1.78	0.66
5:E:282:THR:HG22	5:E:359:VAL:O	1.95	0.66
6:F:427:ALA:O	6:F:428:GLU:HG2	1.96	0.66
14:A:915:EGY:C12	15:A:919:KZB:O77	2.45	0.65
1:A:460:LEU:HD21	17:A:921:OK3:H16	1.77	0.65
15:E:702:KZB:C01	15:E:703:KZB:O14	2.43	0.65
7:G:251:ASN:OD1	7:G:251:ASN:N	2.30	0.65
6:F:481:LEU:HB3	6:F:498:VAL:HG12	1.79	0.65
7:G:210:LEU:HD11	7:G:250:ARG:HE	1.62	0.65
1:A:723:TYR:HA	1:A:751:ILE:HD11	1.79	0.64
5:E:48:LYS:HG2	5:E:134:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:381:ILE:HG21	5:E:409:ILE:HD11	1.81	0.63
7:G:327:VAL:HG12	7:G:328:THR:HG23	1.81	0.63
1:A:668:SER:O	1:A:673:ASN:ND2	2.28	0.62
5:E:188:LEU:HD12	5:E:203:PHE:HE1	1.64	0.62
7:G:134:ILE:HG21	7:G:139:ARG:HG3	1.81	0.62
1:A:777:ASN:C	1:A:777:ASN:HD22	2.07	0.62
7:G:205:ASP:HB3	7:G:208:ASN:HB2	1.82	0.62
14:C:101:EGY:C14	5:E:290:ASP:OD1	2.48	0.62
5:E:384:ASP:HB3	5:E:425:VAL:HG22	1.80	0.62
1:A:616:ASN:O	1:A:617:ARG:NH1	2.33	0.61
14:D:201:EGY:C2E	6:F:606:LEU:HD21	2.30	0.61
6:F:422:ASP:HB3	6:F:426:GLY:HA2	1.82	0.61
1:A:722:TYR:OH	1:A:739:ASP:OD2	2.18	0.61
6:F:569:ASN:O	7:G:448:HIS:ND1	2.34	0.61
6:F:576:THR:HG22	6:F:620:MET:HG3	1.82	0.61
1:A:90:PHE:O	1:A:94:ARG:HD2	2.01	0.60
6:F:433:GLN:OE1	7:G:159:HIS:HD2	1.85	0.60
5:E:368:LEU:HD21	5:E:370:VAL:HG23	1.83	0.60
1:A:307:GLN:HE22	4:D:111:PHE:HB2	1.67	0.59
5:E:181:ASN:ND2	5:E:219:GLU:OE1	2.33	0.59
6:F:496:TRP:HZ3	6:F:498:VAL:HA	1.67	0.59
7:G:311:VAL:HG12	7:G:335:ILE:HG13	1.84	0.59
7:G:359:ARG:HB2	7:G:388:PHE:CE1	2.37	0.59
3:C:79:VAL:HG11	5:E:401:LEU:HD21	1.84	0.59
6:F:565:ALA:HA	7:G:449:MET:HE1	1.83	0.59
6:F:417:PHE:CD1	6:F:460:LYS:HG3	2.37	0.59
5:E:376:GLU:HB2	5:E:404:PHE:CE2	2.38	0.58
7:G:186:ILE:HG21	7:G:214:ILE:HD12	1.84	0.58
1:A:289:ARG:HG2	4:D:85:PHE:HE1	1.68	0.58
6:F:433:GLN:HG3	6:F:435:PHE:CD2	2.38	0.58
1:A:403:VAL:HB	1:A:406:HIS:HD2	1.68	0.58
5:E:36:VAL:HG13	5:E:171:GLN:HB3	1.86	0.58
6:F:432:HIS:H	6:F:487:ASP:HB3	1.68	0.58
6:F:493:PRO:HB2	7:G:160:HIS:CD2	2.38	0.58
1:A:95:PHE:O	1:A:96:GLU:HG3	2.04	0.58
7:G:139:ARG:HH11	7:G:151:GLU:HA	1.68	0.58
1:A:425:PHE:HE1	1:A:471:LEU:HD12	1.66	0.57
5:E:160:HIS:CE1	5:E:200:TYR:HE2	2.22	0.57
5:E:50:THR:HG23	5:E:132:GLU:HG2	1.87	0.57
1:A:607:TYR:CZ	1:A:660:ILE:HD12	2.39	0.57
6:F:440:ASN:HB2	6:F:479:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:380:LEU:HD11	6:F:498:VAL:HG22	1.86	0.57
6:F:376:THR:HG22	6:F:377:ASN:ND2	2.20	0.57
1:A:115:ALA:HB2	1:A:166:ILE:HD12	1.87	0.57
1:A:659:VAL:HG11	1:A:720:MET:HG2	1.86	0.57
6:F:573:ALA:HB3	6:F:576:THR:HG23	1.86	0.57
1:A:414:PHE:HA	1:A:461:MET:HE1	1.86	0.57
15:E:702:KZB:C01	15:E:703:KZB:C13	2.83	0.57
5:E:171:GLN:HG3	5:E:203:PHE:HB2	1.86	0.56
5:E:198:LEU:HD13	5:E:200:TYR:HE1	1.70	0.56
5:E:191:PRO:HB3	5:E:200:TYR:HA	1.88	0.56
7:G:50:LEU:HD12	7:G:99:ILE:HG12	1.86	0.56
1:A:614:MET:HB3	5:E:297:ILE:HD11	1.88	0.55
5:E:225:LEU:HD21	5:E:277:ILE:HG12	1.88	0.55
1:A:483:TYR:OH	8:H:286:LEU:O	2.21	0.55
8:H:305:ALA:O	8:H:309:LEU:HB2	2.05	0.55
1:A:590:TRP:NE1	1:A:594:ASN:HD22	2.05	0.55
3:C:44:THR:O	3:C:48:ARG:HG3	2.07	0.55
1:A:247:PHE:N	4:D:96:ASP:OD2	2.39	0.55
1:A:157:LEU:HD23	1:A:164:VAL:HG11	1.88	0.55
5:E:157:GLU:HG2	5:E:215:LYS:HG2	1.88	0.55
7:G:368:LEU:HB3	7:G:375:TYR:HB3	1.89	0.54
5:E:344:ASN:HB2	5:E:349:TYR:CD1	2.43	0.54
1:A:270:ILE:O	1:A:274:PRO:HD2	2.07	0.54
5:E:188:LEU:HD12	5:E:203:PHE:CE1	2.43	0.54
4:D:77:ILE:HG13	4:D:90:PRO:HB3	1.90	0.54
6:F:487:ASP:OD1	6:F:490:LEU:HG	2.08	0.54
1:A:361:ALA:HB1	14:A:918:EGY:C39	2.37	0.54
1:A:95:PHE:C	1:A:96:GLU:HG3	2.32	0.53
1:A:437:ASN:ND2	1:A:439:GLU:OE1	2.42	0.53
5:E:365:ILE:HB	5:E:416:LEU:HB2	1.90	0.53
6:F:398:TYR:HE1	6:F:494:ILE:HG23	1.73	0.53
7:G:244:ILE:HG21	7:G:295:LEU:HD21	1.91	0.53
1:A:777:ASN:O	7:G:250:ARG:HG2	2.08	0.53
1:A:758:GLU:OE2	1:A:761:THR:OG1	2.21	0.53
5:E:247:ASN:OD1	5:E:247:ASN:N	2.41	0.53
7:G:173:ILE:HG23	7:G:197:PHE:HB3	1.90	0.53
7:G:230:ILE:HD11	7:G:234:PRO:HD3	1.90	0.53
6:F:381:SER:HB2	6:F:415:ALA:HB3	1.91	0.52
7:G:223:SER:OG	7:G:235:HIS:O	2.28	0.52
5:E:371:LYS:HG2	5:E:410:VAL:HG12	1.91	0.52
6:F:486:GLY:HA2	6:F:490:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:402:ALA:HB3	6:F:499:ALA:HB2	1.92	0.52
5:E:436:LEU:HA	5:E:439:PRO:HD2	1.91	0.52
1:A:601:VAL:HG21	1:A:611:ILE:HG21	1.90	0.52
14:D:201:EGY:C2E	6:F:606:LEU:CD2	2.88	0.52
6:F:380:LEU:HD21	6:F:498:VAL:HG21	1.92	0.52
7:G:309:GLY:HA3	7:G:336:VAL:HG13	1.92	0.52
5:E:74:GLU:OE1	5:E:74:GLU:N	2.34	0.52
7:G:307:ARG:NH1	7:G:338:GLN:OE1	2.21	0.52
6:F:492:ASN:OD1	6:F:492:ASN:N	2.43	0.51
1:A:697:THR:HG22	1:A:701:GLU:H	1.73	0.51
6:F:373:VAL:HG12	6:F:492:ASN:OD1	2.10	0.51
7:G:166:ASP:OD2	7:G:170:HIS:N	2.40	0.51
7:G:415:HIS:HA	7:G:418:TYR:CE2	2.45	0.51
5:E:291:VAL:HG23	13:N:2:NAG:H81	1.93	0.51
6:F:485:ILE:CG2	6:F:494:ILE:HB	2.40	0.51
6:F:440:ASN:HB2	6:F:479:TYR:HE1	1.75	0.51
6:F:438:LEU:HD23	6:F:481:LEU:HA	1.93	0.51
6:F:553:LEU:O	6:F:557:PHE:HD1	1.92	0.51
7:G:390:PHE:HE1	7:G:408:VAL:HG21	1.76	0.51
1:A:408:PRO:HG3	8:H:239:ILE:HD12	1.92	0.51
7:G:102:PRO:HB3	7:G:130:ALA:HA	1.93	0.51
1:A:431:PHE:CE1	1:A:478:ASN:ND2	2.78	0.51
1:A:110:SER:HB2	1:A:122:PHE:HE1	1.75	0.50
1:A:778:ARG:NH2	7:G:121:ASP:OD1	2.44	0.50
7:G:163:ASP:OD1	7:G:164:ILE:N	2.44	0.50
1:A:419:HIS:HB3	1:A:550:PHE:HD1	1.76	0.50
1:A:591:LEU:HD21	1:A:601:VAL:HG11	1.92	0.50
3:C:53:GLU:OE1	5:E:458:ARG:NH2	2.43	0.50
6:F:485:ILE:HG23	6:F:494:ILE:HB	1.94	0.50
4:D:52:PRO:HG3	7:G:425:ALA:HB2	1.94	0.49
6:F:398:TYR:HD1	6:F:496:TRP:CD1	2.29	0.49
1:A:137:ILE:O	1:A:141:THR:OG1	2.20	0.49
5:E:36:VAL:O	5:E:171:GLN:HA	2.12	0.49
7:G:152:GLU:HG3	7:G:153:LYS:HG2	1.95	0.49
1:A:715:CYS:SG	1:A:716:LEU:N	2.86	0.49
1:A:214:ARG:HG3	1:A:462:LEU:HD13	1.95	0.49
1:A:674:LYS:HD2	10:K:5:THR:HB	1.94	0.49
5:E:395:GLU:O	5:E:408:VAL:HB	2.12	0.49
1:A:302:LEU:HD11	1:A:306:MET:HE3	1.94	0.48
1:A:544:LEU:HD13	2:B:23:VAL:HG21	1.94	0.48
1:A:431:PHE:CD1	1:A:478:ASN:ND2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:PRO:HB3	7:G:422:ILE:HD11	1.94	0.48
4:D:33:TYR:HH	7:G:434:SER:HG	1.60	0.48
1:A:742:ARG:O	1:A:744:ALA:N	2.45	0.48
7:G:356:GLU:HG2	7:G:365:ARG:HG2	1.94	0.48
9:I:267:ASP:OD1	9:I:268:ASN:N	2.43	0.48
5:E:368:LEU:HD23	5:E:369:THR:N	2.28	0.48
6:F:435:PHE:HB3	6:F:448:VAL:CG1	2.44	0.48
5:E:191:PRO:HG3	5:E:200:TYR:CE1	2.48	0.48
7:G:59:THR:HG23	7:G:60:HIS:ND1	2.29	0.48
1:A:799:LYS:HG3	1:A:804:ARG:NH2	2.29	0.48
5:E:84:LEU:HG	5:E:133:THR:HG22	1.95	0.48
7:G:236:ALA:O	7:G:241:THR:OG1	2.32	0.47
1:A:136:ARG:NH2	1:A:624:ASN:OD1	2.45	0.47
1:A:544:LEU:O	1:A:548:MET:HG2	2.14	0.47
6:F:373:VAL:HB	6:F:490:LEU:HD22	1.96	0.47
1:A:100:HIS:ND1	1:A:565:PRO:HB3	2.29	0.47
1:A:313:PHE:HZ	4:D:54:ASN:OD1	1.97	0.47
3:C:31:PHE:CE1	15:C:103:KZB:C13	2.97	0.47
1:A:249:THR:HG21	1:A:296:THR:HB	1.95	0.47
1:A:705:ASP:OD1	1:A:744:ALA:HB1	2.14	0.47
5:E:73:LEU:HD11	5:E:81:LEU:HD22	1.96	0.47
5:E:146:ILE:HD12	5:E:255:ALA:HB1	1.96	0.47
6:F:443:THR:HG23	6:F:445:GLN:H	1.80	0.47
5:E:355:PHE:HD1	5:E:424:ILE:HD13	1.80	0.47
6:F:599:MET:HE3	6:F:603:LEU:HG	1.97	0.47
7:G:358:VAL:HG12	7:G:362:PRO:HA	1.97	0.47
1:A:781:LEU:HD11	7:G:148:GLU:HB2	1.97	0.47
6:F:405:THR:HG22	6:F:500:ASP:HB2	1.97	0.47
6:F:433:GLN:HG3	6:F:435:PHE:CE2	2.49	0.47
7:G:213:ASP:OD1	7:G:213:ASP:N	2.47	0.47
1:A:712:LEU:HD12	1:A:712:LEU:O	2.14	0.47
5:E:198:LEU:HD13	5:E:200:TYR:CE1	2.48	0.47
6:F:438:LEU:HA	6:F:480:THR:O	2.14	0.47
6:F:497:ASN:OD1	6:F:497:ASN:N	2.46	0.46
3:C:43:SER:HB3	3:C:48:ARG:HG2	1.98	0.46
1:A:604:TRP:CE3	1:A:604:TRP:HA	2.50	0.46
4:D:105:HIS:HB3	7:G:436:MET:HE2	1.98	0.46
1:A:276:HIS:CD2	1:A:442:PHE:HB2	2.51	0.46
1:A:729:GLN:HB2	1:A:736:PRO:HA	1.98	0.46
6:F:420:LEU:HD13	6:F:485:ILE:HD11	1.98	0.46
1:A:111:THR:HG22	1:A:166:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:549:ILE:O	6:F:552:PRO:HD2	2.16	0.45
6:F:380:LEU:HB2	6:F:394:THR:HG23	1.97	0.45
1:A:419:HIS:CD2	1:A:420:ILE:HG23	2.51	0.45
1:A:665:ILE:HD11	1:A:766:LEU:HD12	1.98	0.45
1:A:777:ASN:C	1:A:777:ASN:ND2	2.73	0.45
5:E:75:PRO:HA	5:E:78:GLU:CD	2.41	0.45
5:E:373:ILE:HD13	5:E:408:VAL:HG22	1.97	0.45
6:F:377:ASN:O	6:F:418:PHE:HA	2.17	0.45
6:F:428:GLU:OE1	6:F:457:ASN:ND2	2.49	0.45
1:A:593:GLN:HE22	5:E:329:HIS:HB3	1.81	0.45
3:C:73:LEU:HD11	5:E:239:TRP:CG	2.51	0.45
7:G:48:LEU:HD23	7:G:49:VAL:N	2.32	0.45
5:E:291:VAL:HG21	5:E:305:LEU:CD1	2.39	0.45
5:E:392:ALA:HB3	5:E:410:VAL:HG23	1.97	0.45
7:G:391:LYS:HE2	7:G:403:TYR:OH	2.17	0.45
1:A:535:ILE:O	1:A:538:ILE:HG22	2.16	0.45
6:F:398:TYR:CE1	6:F:494:ILE:HG23	2.50	0.45
4:D:88:ILE:HG22	4:D:92:ARG:HD3	1.97	0.45
1:A:285:ARG:NH1	14:A:916:EGY:O14	2.45	0.45
5:E:299:ASN:HD22	13:N:1:NAG:H83	1.82	0.45
1:A:658:LEU:CD2	1:A:769:ILE:HG12	2.47	0.44
1:A:660:ILE:HG12	1:A:767:VAL:HG22	1.99	0.44
7:G:415:HIS:HA	7:G:418:TYR:HE2	1.82	0.44
1:A:117:HIS:O	1:A:121:GLU:HG3	2.18	0.44
1:A:126:PHE:CD2	1:A:126:PHE:O	2.70	0.44
3:C:59:VAL:HG11	9:I:285:THR:HG21	1.98	0.44
6:F:422:ASP:H	6:F:426:GLY:HA3	1.82	0.44
7:G:157:ILE:HD11	7:G:226:PRO:HG3	1.99	0.44
1:A:460:LEU:O	1:A:463:THR:HG22	2.18	0.44
5:E:283:ILE:H	5:E:358:HIS:HD2	1.64	0.44
6:F:493:PRO:HB2	7:G:160:HIS:NE2	2.33	0.44
1:A:439:GLU:CD	1:A:439:GLU:H	2.26	0.44
5:E:145:GLN:HB3	5:E:258:LYS:HD3	1.99	0.44
6:F:398:TYR:CD1	6:F:496:TRP:CD1	3.04	0.44
6:F:604:LYS:O	6:F:608:ILE:HG22	2.17	0.44
3:C:3:LEU:HD11	5:E:425:VAL:HG11	2.00	0.44
7:G:359:ARG:HB2	7:G:388:PHE:CD1	2.51	0.44
7:G:394:TYR:HB3	7:G:402:LEU:HB2	2.00	0.44
1:A:186:PHE:HB2	1:A:202:ALA:HB2	1.99	0.44
1:A:242:LYS:NZ	1:A:242:LYS:HB2	2.33	0.44
5:E:173:MET:HE3	5:E:175:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TRP:CD2	8:H:272:VAL:HG21	2.53	0.43
7:G:199:GLY:HA3	7:G:259:GLY:O	2.18	0.43
3:C:12:PRO:HG2	5:E:435:MET:HE1	2.00	0.43
5:E:249:ASP:OD1	5:E:329:HIS:HD2	2.01	0.43
5:E:351:LEU:O	5:E:425:VAL:HA	2.18	0.43
7:G:62:LEU:HD23	7:G:269:PHE:HD2	1.83	0.43
1:A:84:GLY:O	1:A:88:ARG:NH2	2.47	0.43
7:G:116:ILE:HG21	7:G:141:LEU:HD11	2.00	0.43
8:H:258:HIS:CE1	8:H:263:ALA:HB3	2.53	0.43
1:A:76:ILE:HG21	1:A:199:LEU:HD13	2.01	0.43
1:A:676:LEU:HD12	1:A:676:LEU:HA	1.88	0.43
7:G:395:ASN:O	7:G:396:ARG:NH1	2.43	0.43
1:A:602:MET:HB2	1:A:654:VAL:HG21	2.00	0.43
1:A:723:TYR:CA	1:A:751:ILE:HD11	2.47	0.43
5:E:368:LEU:CD2	5:E:370:VAL:HG23	2.48	0.43
5:E:417:VAL:HG22	5:E:418:GLU:H	1.83	0.43
4:D:63:CYS:HA	7:G:435:MET:HE1	2.01	0.43
7:G:361:ASP:OD1	7:G:361:ASP:N	2.50	0.43
4:D:77:ILE:HD13	7:G:446:PHE:HZ	1.84	0.43
14:A:915:EGY:O12	4:D:92:ARG:NH2	2.52	0.43
7:G:273:VAL:HG13	7:G:286:THR:HG22	2.01	0.43
1:A:253:CYS:SG	1:A:297:PHE:HA	2.58	0.42
5:E:225:LEU:CD1	5:E:250:LEU:HD13	2.48	0.42
7:G:254:ARG:NH1	7:G:298:TRP:O	2.51	0.42
1:A:433:ILE:HG21	8:H:220:ALA:HB2	2.01	0.42
3:C:35:TRP:CH2	9:I:289:LEU:HD21	2.54	0.42
6:F:435:PHE:HB3	6:F:448:VAL:HG13	2.00	0.42
1:A:250:MET:HE1	1:A:300:VAL:HG11	2.02	0.42
4:D:44:TYR:CE2	7:G:427:PRO:HG2	2.54	0.42
6:F:431:PRO:HG2	6:F:485:ILE:HD11	2.02	0.42
7:G:295:LEU:O	7:G:299:VAL:HG13	2.19	0.42
1:A:96:GLU:HG2	5:E:299:ASN:HB2	2.01	0.42
4:D:41:GLN:HE21	4:D:41:GLN:HB2	1.70	0.42
1:A:723:TYR:HD1	1:A:751:ILE:HG13	1.84	0.42
1:A:439:GLU:OE2	1:A:439:GLU:N	2.53	0.42
3:C:69:LEU:HD13	5:E:439:PRO:HG3	2.02	0.42
1:A:720:MET:HG3	1:A:770:TYR:CE1	2.55	0.42
5:E:198:LEU:HD12	5:E:198:LEU:O	2.19	0.42
6:F:436:VAL:HG22	6:F:483:LEU:CD1	2.49	0.42
7:G:164:ILE:HD12	7:G:274:GLN:NE2	2.34	0.42
1:A:636:LYS:HZ3	1:A:686:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:LEU:HD12	5:E:127:ILE:HD11	2.01	0.41
7:G:196:LEU:HD11	7:G:273:VAL:HG12	2.03	0.41
7:G:254:ARG:NH2	7:G:304:GLY:O	2.52	0.41
7:G:427:PRO:O	7:G:430:ALA:HB3	2.20	0.41
8:H:275:PHE:HE1	8:H:316:TRP:HE3	1.68	0.41
5:E:49:VAL:HG22	5:E:133:THR:OG1	2.21	0.41
6:F:589:LEU:HD11	6:F:605:TYR:HB3	2.01	0.41
1:A:667:TYR:O	1:A:741:THR:HG21	2.20	0.41
4:D:71:VAL:O	4:D:75:ILE:HG13	2.20	0.41
5:E:74:GLU:O	5:E:78:GLU:HG3	2.21	0.41
7:G:139:ARG:HH11	7:G:150:ASP:C	2.29	0.41
1:A:431:PHE:HZ	8:H:287:CYS:CB	2.34	0.41
4:D:48:VAL:HG13	6:F:537:PRO:CG	2.51	0.41
5:E:215:LYS:NZ	5:E:215:LYS:HB3	2.35	0.41
5:E:281:LYS:HA	5:E:315:GLU:HA	2.03	0.41
5:E:391:ARG:NH1	5:E:409:ILE:HG23	2.36	0.41
6:F:593:TYR:CD1	6:F:602:THR:HG21	2.56	0.41
1:A:85:PHE:CD1	1:A:175:PRO:HB2	2.55	0.41
1:A:607:TYR:CE1	1:A:660:ILE:HD12	2.56	0.41
6:F:463:LEU:HD21	6:F:503:ILE:HD11	2.02	0.41
4:D:11:ARG:HA	4:D:11:ARG:HD3	1.82	0.41
6:F:481:LEU:O	6:F:497:ASN:HA	2.21	0.41
7:G:80:ASP:OD1	7:G:80:ASP:N	2.54	0.41
8:H:275:PHE:HD1	8:H:313:PHE:HD1	1.69	0.41
8:H:291:THR:O	8:H:293:ASP:N	2.54	0.41
4:D:41:GLN:NE2	7:G:431:SER:OG	2.54	0.41
5:E:238:HIS:NE2	5:E:375:PRO:HG3	2.36	0.41
5:E:369:THR:HG22	5:E:412:TYR:HD1	1.86	0.41
9:I:262:ASN:OD1	9:I:262:ASN:N	2.53	0.41
1:A:96:GLU:HG2	5:E:299:ASN:CB	2.51	0.40
4:D:48:VAL:HG13	6:F:537:PRO:HG2	2.04	0.40
2:B:3:THR:HG22	2:B:4:ASP:H	1.86	0.40
7:G:308:VAL:HG13	7:G:335:ILE:HD11	2.04	0.40
1:A:778:ARG:NH1	7:G:117:SER:HB3	2.35	0.40
5:E:174:ARG:HG3	5:E:199:ASP:OD1	2.21	0.40
5:E:227:ILE:HG23	5:E:248:VAL:HG13	2.03	0.40
6:F:603:LEU:HD23	6:F:603:LEU:HA	1.97	0.40
1:A:63:SER:HB2	1:A:68:TRP:NE1	2.30	0.40
17:A:921:0K3:H8	17:A:921:0K3:H11	1.77	0.40
8:H:244:TYR:CZ	8:H:267:ALA:HB2	2.56	0.40
1:A:341:ARG:HA	1:A:353:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:TYR:OH	1:A:624:ASN:HB2	2.20	0.40
17:A:921:OK3:H61	17:A:921:OK3:H51	2.02	0.40
5:E:266:TYR:OH	5:E:278:ARG:NE	2.49	0.40
6:F:586:MET:HE3	6:F:586:MET:HB2	1.99	0.40
7:G:104:VAL:HG13	7:G:137:PRO:HG2	2.03	0.40
7:G:306:LEU:HB3	7:G:402:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	702/826 (85%)	674 (96%)	28 (4%)	0	100	100
2	B	31/37 (84%)	31 (100%)	0	0	100	100
3	C	76/79 (96%)	73 (96%)	3 (4%)	0	100	100
4	D	101/113 (89%)	97 (96%)	4 (4%)	0	100	100
5	E	424/607 (70%)	390 (92%)	33 (8%)	1 (0%)	43	74
6	F	246/631 (39%)	233 (95%)	13 (5%)	0	100	100
7	G	408/456 (90%)	384 (94%)	23 (6%)	1 (0%)	43	74
8	H	108/335 (32%)	99 (92%)	9 (8%)	0	100	100
9	I	35/292 (12%)	28 (80%)	7 (20%)	0	100	100
10	K	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	2136/3383 (63%)	2013 (94%)	121 (6%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	194	SER

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Mol	Chain	Res	Type
7	G	342	ASN

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	611/703 (87%)	595 (97%)	16 (3%)	40	62
2	B	29/33 (88%)	27 (93%)	2 (7%)	14	39
3	C	69/70 (99%)	65 (94%)	4 (6%)	18	44
4	D	90/98 (92%)	88 (98%)	2 (2%)	45	65
5	E	386/537 (72%)	371 (96%)	15 (4%)	28	54
6	F	216/541 (40%)	212 (98%)	4 (2%)	50	68
7	G	357/390 (92%)	354 (99%)	3 (1%)	73	77
8	H	91/286 (32%)	90 (99%)	1 (1%)	65	74
9	I	33/243 (14%)	32 (97%)	1 (3%)	36	60
10	K	2/2 (100%)	2 (100%)	0	100	100
All	All	1884/2903 (65%)	1836 (98%)	48 (2%)	42	63

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	96	GLU
1	A	99	ILE
1	A	128	GLU
1	A	236	LEU
1	A	242	LYS
1	A	390	THR
1	A	439	GLU
1	A	462	LEU
1	A	580	ILE
1	A	636	LYS
1	A	654	VAL

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Mol	Chain	Res	Type
1	A	704	VAL
1	A	711	THR
1	A	734	THR
1	A	741	THR
2	B	3	THR
2	B	7	LEU
3	C	26	LEU
3	C	33	THR
3	C	38	VAL
3	C	73	LEU
4	D	48	VAL
4	D	68	ILE
5	E	36	VAL
5	E	49	VAL
5	E	88	VAL
5	E	147	THR
5	E	247	ASN
5	E	257	LEU
5	E	284	LEU
5	E	310	ASP
5	E	314	MET
5	E	315	GLU
5	E	336	LEU
5	E	373	ILE
5	E	376	GLU
5	E	434	LEU
5	E	436	LEU
6	F	450	VAL
6	F	492	ASN
6	F	587	LEU
6	F	608	ILE
7	G	128	VAL
7	G	251	ASN
7	G	344	LYS
8	H	309	LEU
9	I	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	A	195	GLN

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Mol	Chain	Res	Type
1	A	231	GLN
1	A	307	GLN
1	A	406	HIS
1	A	435	ASN
1	A	593	GLN
1	A	594	ASN
1	A	623	ASN
1	A	755	HIS
4	D	41	GLN
5	E	160	HIS
5	E	190	ASN
5	E	238	HIS
5	E	252	HIS
5	E	329	HIS
5	E	358	HIS
5	E	380	ASN
5	E	420	HIS
6	F	377	ASN
6	F	412	GLN
6	F	441	GLN
6	F	528	HIS
6	F	583	HIS
6	F	601	GLN
6	F	623	GLN
7	G	159	HIS
7	G	395	ASN
7	G	401	HIS
7	G	415	HIS
8	H	237	ASN
8	H	246	HIS

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 ⓘ

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	J	1	11,1	14,14,15	0.20	0	17,19,21	0.48	0
11	NAG	J	2	11	14,14,15	0.17	0	17,19,21	0.54	0
12	NAG	L	1	1,12	14,14,15	0.36	0	17,19,21	0.41	0
12	NAG	L	2	12	14,14,15	0.19	0	17,19,21	0.45	0
12	BMA	L	3	12	11,11,12	0.57	0	15,15,17	0.74	0
12	MAN	L	4	12	11,11,12	0.75	1 (9%)	15,15,17	1.09	2 (13%)
12	MAN	L	5	12	11,11,12	0.68	1 (9%)	15,15,17	0.95	2 (13%)
12	MAN	L	6	12	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
12	MAN	L	7	12	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
12	MAN	L	8	12	11,11,12	0.71	0	15,15,17	1.10	2 (13%)
11	NAG	M	1	11,1	14,14,15	0.15	0	17,19,21	0.42	0
11	NAG	M	2	11	14,14,15	0.22	0	17,19,21	0.61	0
13	NAG	N	1	13,5	14,14,15	0.36	0	17,19,21	0.55	0
13	NAG	N	2	13	14,14,15	0.43	0	17,19,21	0.39	0
13	BMA	N	3	13	11,11,12	0.58	0	15,15,17	0.75	0
13	MAN	N	4	13	11,11,12	0.67	0	15,15,17	0.94	2 (13%)
13	MAN	N	5	13	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
13	MAN	N	6	13	11,11,12	0.81	1 (9%)	15,15,17	0.98	2 (13%)
13	MAN	N	7	13	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
13	MAN	N	8	13	11,11,12	0.62	0	15,15,17	1.02	2 (13%)

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
11	NAG	J	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	L	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	L	2	12	-	2/6/23/26	0/1/1/1
12	BMA	L	3	12	-	2/2/19/22	0/1/1/1
12	MAN	L	4	12	-	2/2/19/22	0/1/1/1
12	MAN	L	5	12	-	2/2/19/22	0/1/1/1
12	MAN	L	6	12	-	1/2/19/22	0/1/1/1
12	MAN	L	7	12	-	0/2/19/22	1/1/1/1
12	MAN	L	8	12	-	2/2/19/22	1/1/1/1
11	NAG	M	1	11,1	-	4/6/23/26	0/1/1/1
11	NAG	M	2	11	-	4/6/23/26	0/1/1/1
13	NAG	N	1	13,5	-	2/6/23/26	0/1/1/1
13	NAG	N	2	13	-	2/6/23/26	0/1/1/1
13	BMA	N	3	13	-	1/2/19/22	0/1/1/1
13	MAN	N	4	13	-	0/2/19/22	0/1/1/1
13	MAN	N	5	13	-	0/2/19/22	0/1/1/1
13	MAN	N	6	13	-	0/2/19/22	0/1/1/1
13	MAN	N	7	13	-	2/2/19/22	0/1/1/1
13	MAN	N	8	13	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	6	MAN	O5-C1	-2.35	1.39	1.43
12	L	4	MAN	O5-C1	-2.18	1.40	1.43
12	L	5	MAN	O5-C1	-2.04	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	8	MAN	C1-O5-C5	3.02	116.23	112.19
12	L	7	MAN	C1-O5-C5	2.92	116.10	112.19
12	L	4	MAN	C1-O5-C5	2.77	115.90	112.19
13	N	6	MAN	O2-C2-C3	-2.55	104.87	110.15
12	L	4	MAN	O2-C2-C3	-2.43	105.12	110.15
13	N	8	MAN	C1-O5-C5	2.42	115.43	112.19
13	N	7	MAN	O2-C2-C3	-2.42	105.15	110.15
12	L	8	MAN	O2-C2-C3	-2.41	105.15	110.15
12	L	7	MAN	O2-C2-C3	-2.40	105.19	110.15
12	L	6	MAN	C1-O5-C5	2.40	115.40	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	8	MAN	O2-C2-C3	-2.36	105.27	110.15
12	L	6	MAN	O2-C2-C3	-2.32	105.35	110.15
13	N	7	MAN	C1-O5-C5	2.31	115.29	112.19
12	L	5	MAN	C1-O5-C5	2.31	115.28	112.19
13	N	5	MAN	C1-O5-C5	2.31	115.28	112.19
13	N	5	MAN	O2-C2-C3	-2.28	105.43	110.15
13	N	6	MAN	C1-O5-C5	2.27	115.22	112.19
12	L	5	MAN	O2-C2-C3	-2.20	105.59	110.15
13	N	4	MAN	C1-O5-C5	2.18	115.10	112.19
13	N	4	MAN	O2-C2-C3	-2.09	105.82	110.15

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	2	NAG	O5-C5-C6-O6
12	L	4	MAN	O5-C5-C6-O6
12	L	5	MAN	O5-C5-C6-O6
12	L	8	MAN	O5-C5-C6-O6
11	M	2	NAG	O5-C5-C6-O6
11	M	2	NAG	C4-C5-C6-O6
12	L	4	MAN	C4-C5-C6-O6
12	L	5	MAN	C4-C5-C6-O6
11	M	1	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
11	J	2	NAG	C4-C5-C6-O6
12	L	2	NAG	C4-C5-C6-O6
12	L	8	MAN	C4-C5-C6-O6
11	J	1	NAG	C8-C7-N2-C2
11	J	1	NAG	O7-C7-N2-C2
11	M	1	NAG	C8-C7-N2-C2
11	M	1	NAG	O7-C7-N2-C2
13	N	1	NAG	C8-C7-N2-C2
13	N	1	NAG	O7-C7-N2-C2
11	M	1	NAG	C4-C5-C6-O6
13	N	7	MAN	O5-C5-C6-O6
13	N	2	NAG	O5-C5-C6-O6
12	L	3	BMA	C4-C5-C6-O6
12	L	3	BMA	O5-C5-C6-O6
11	M	2	NAG	C1-C2-N2-C7
12	L	1	NAG	C4-C5-C6-O6
13	N	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	M	2	NAG	C3-C2-N2-C7
13	N	7	MAN	C4-C5-C6-O6
12	L	1	NAG	O5-C5-C6-O6
13	N	2	NAG	C4-C5-C6-O6
12	L	6	MAN	C4-C5-C6-O6

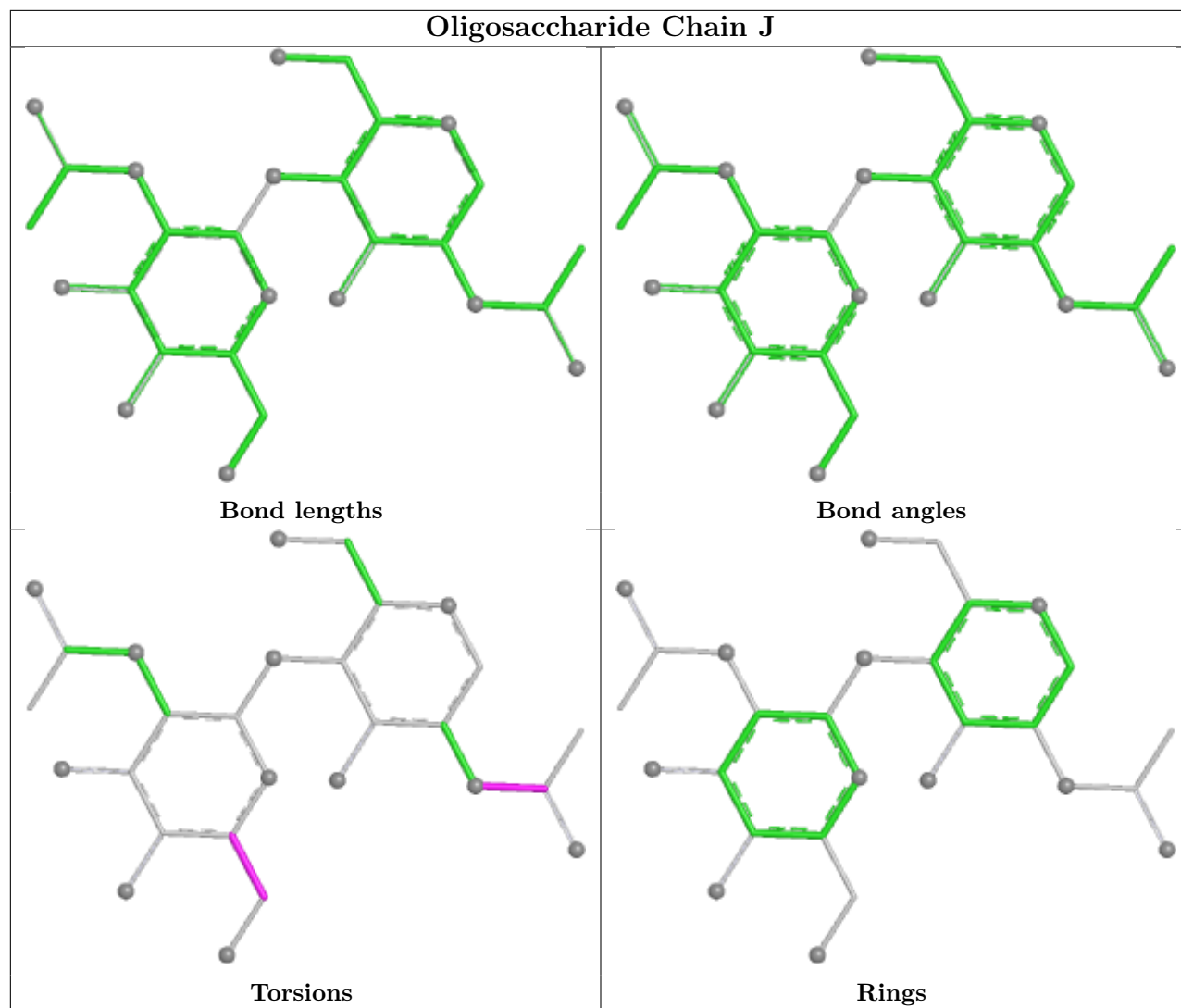
All (2) ring outliers are listed below:

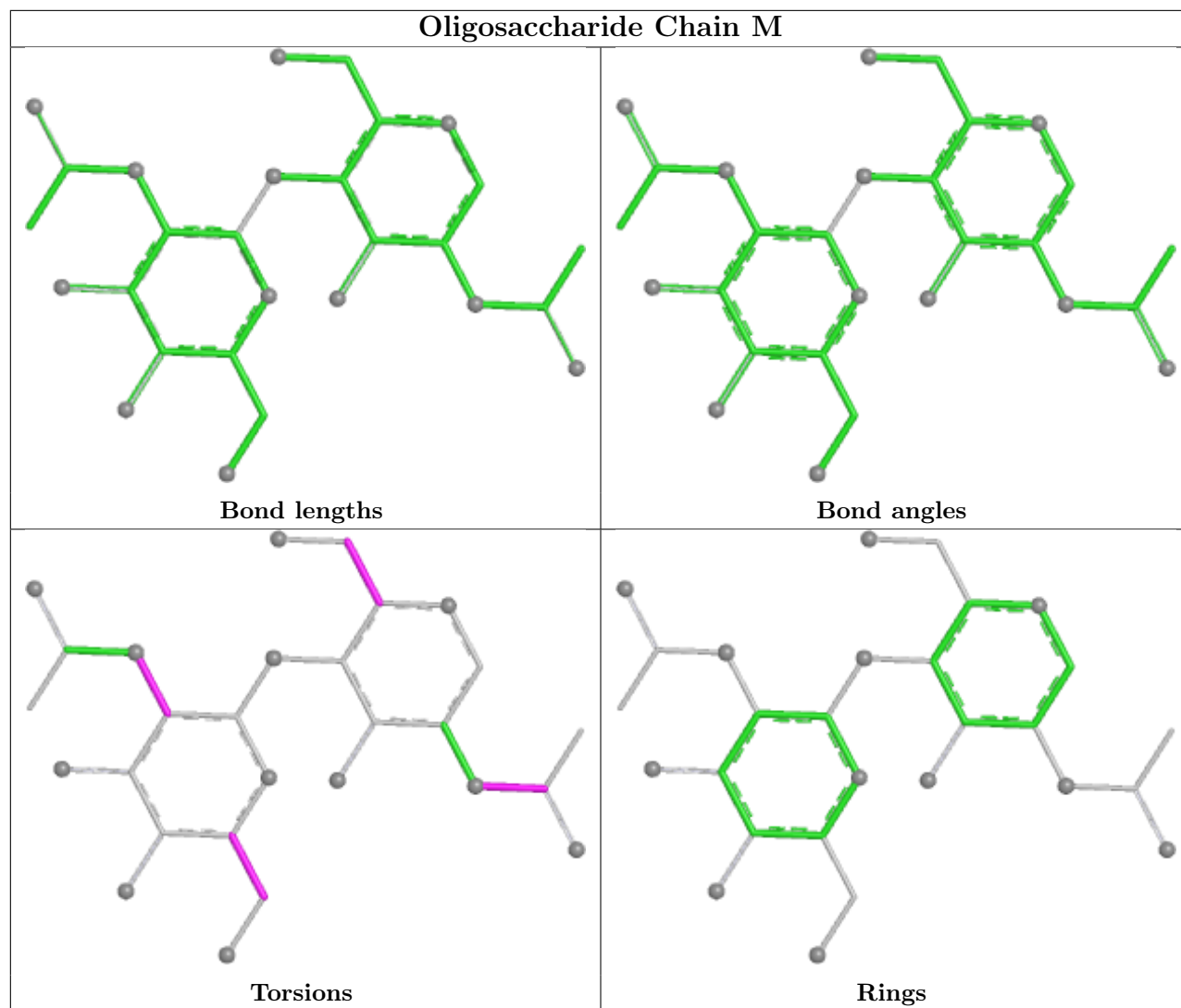
Mol	Chain	Res	Type	Atoms
12	L	7	MAN	C1-C2-C3-C4-C5-O5
12	L	8	MAN	C1-C2-C3-C4-C5-O5

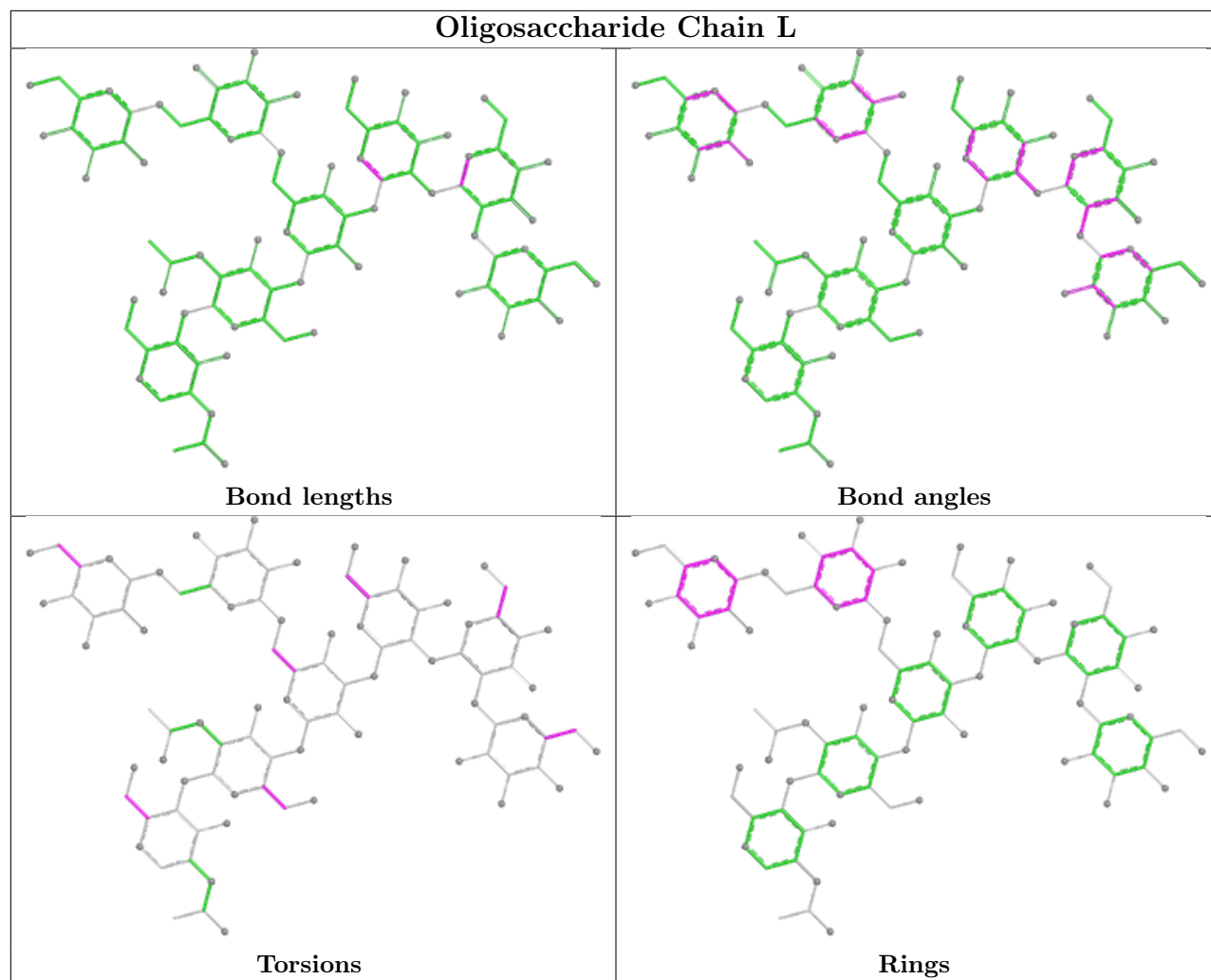
2 monomers are involved in 2 short contacts:

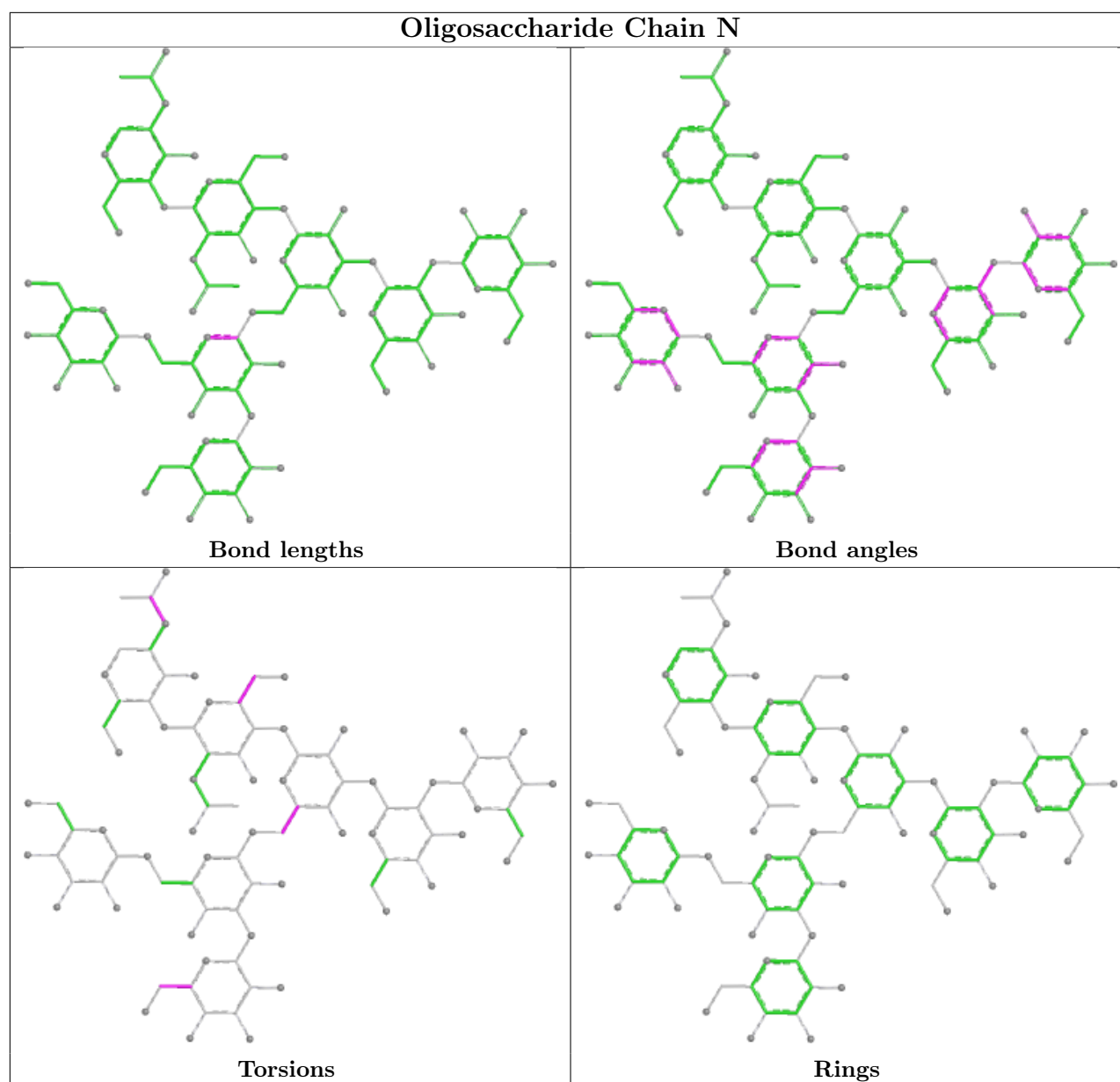
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N	2	NAG	1	0
13	N	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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
14	EGY	A	914	-	37,37,42	1.45	6 (16%)	43,45,50	1.13	2 (4%)
15	KZB	C	103	-	37,37,49	0.69	0	58,62,80	2.05	12 (20%)
15	KZB	D	203	-	37,37,49	0.69	0	58,62,80	1.98	14 (24%)
15	KZB	F	703	-	37,37,49	0.70	1 (2%)	58,62,80	1.95	12 (20%)
15	KZB	D	204	-	37,37,49	0.94	1 (2%)	58,62,80	2.10	15 (25%)
14	EGY	A	917	-	42,42,42	1.39	6 (14%)	48,50,50	1.09	3 (6%)
15	KZB	C	102	-	37,37,49	0.64	0	58,62,80	1.97	11 (18%)
15	KZB	E	703	-	37,37,49	0.73	1 (2%)	58,62,80	1.92	13 (22%)
15	KZB	G	502	-	37,37,49	0.68	1 (2%)	58,62,80	1.98	14 (24%)
14	EGY	F	701	-	42,42,42	1.39	6 (14%)	48,50,50	1.11	3 (6%)
14	EGY	A	918	-	42,42,42	1.39	6 (14%)	48,50,50	1.08	2 (4%)
15	KZB	A	919	-	37,37,49	0.71	0	58,62,80	2.00	15 (25%)
14	EGY	E	701	-	42,42,42	1.37	7 (16%)	48,50,50	1.06	2 (4%)
14	EGY	D	201	-	42,42,42	1.38	6 (14%)	48,50,50	1.11	2 (4%)
15	KZB	D	202	-	37,37,49	0.63	0	58,62,80	2.17	16 (27%)
14	EGY	A	913	-	42,42,42	1.39	6 (14%)	48,50,50	1.08	2 (4%)
15	KZB	F	702	-	37,37,49	0.70	1 (2%)	58,62,80	2.01	16 (27%)
14	EGY	A	915	-	42,42,42	1.38	6 (14%)	48,50,50	1.11	2 (4%)
15	KZB	G	501	-	37,37,49	0.76	1 (2%)	58,62,80	2.22	19 (32%)
17	0K3	A	921	-	44,44,44	1.98	6 (13%)	52,54,54	2.51	18 (34%)
15	KZB	F	704	-	37,37,49	0.66	1 (2%)	58,62,80	1.99	11 (18%)
15	KZB	E	702	-	37,37,49	0.73	0	58,62,80	1.89	11 (18%)
14	EGY	A	916	-	42,42,42	1.38	6 (14%)	48,50,50	1.10	2 (4%)
14	EGY	C	101	-	42,42,42	1.38	6 (14%)	48,50,50	1.11	2 (4%)

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
14	EGY	A	914	-	-	22/41/41/46	-
15	KZB	C	103	-	-	-	0/6/6/7
15	KZB	D	203	-	-	-	0/6/6/7
15	KZB	F	703	-	-	-	0/6/6/7
15	KZB	D	204	-	-	-	0/6/6/7
14	EGY	A	917	-	-	24/46/46/46	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	KZB	C	102	-	-	-	0/6/6/7
15	KZB	E	703	-	-	-	0/6/6/7
15	KZB	G	502	-	-	-	0/6/6/7
14	EGY	F	701	-	-	20/46/46/46	-
14	EGY	A	918	-	-	27/46/46/46	-
15	KZB	A	919	-	-	-	0/6/6/7
14	EGY	E	701	-	-	27/46/46/46	-
14	EGY	D	201	-	-	21/46/46/46	-
15	KZB	D	202	-	-	-	0/6/6/7
14	EGY	A	913	-	-	19/46/46/46	-
15	KZB	F	702	-	-	-	0/6/6/7
14	EGY	A	915	-	-	26/46/46/46	-
15	KZB	G	501	-	-	-	0/6/6/7
17	0K3	A	921	-	-	17/49/49/49	-
15	KZB	F	704	-	-	-	0/6/6/7
15	KZB	E	702	-	-	-	0/6/6/7
14	EGY	A	916	-	-	22/46/46/46	-
14	EGY	C	101	-	-	27/46/46/46	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	921	0K3	C1-C2	8.91	1.53	1.33
14	E	701	EGY	O21-C21	3.69	1.44	1.34
14	A	917	EGY	O21-C21	3.56	1.44	1.34
14	A	913	EGY	O21-C21	3.53	1.44	1.34
14	F	701	EGY	O21-C21	3.53	1.44	1.34
14	A	918	EGY	O21-C21	3.52	1.44	1.34
14	A	915	EGY	O21-C21	3.50	1.44	1.34
14	A	914	EGY	O21-C21	3.49	1.44	1.34
14	A	916	EGY	O21-C21	3.49	1.44	1.34
14	D	201	EGY	O21-C21	3.44	1.44	1.34
14	C	101	EGY	O21-C21	3.44	1.44	1.34
14	A	918	EGY	O31-C31	3.40	1.43	1.33
14	F	701	EGY	O31-C31	3.38	1.43	1.33
14	A	913	EGY	O31-C31	3.37	1.43	1.33
14	D	201	EGY	O31-C31	3.36	1.43	1.33
14	A	916	EGY	O31-C31	3.34	1.43	1.33
14	A	917	EGY	O31-C31	3.34	1.43	1.33
14	C	101	EGY	O31-C31	3.32	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	915	EGY	O31-C31	3.31	1.43	1.33
14	A	914	EGY	O31-C31	3.28	1.42	1.33
14	E	701	EGY	O31-C31	3.22	1.42	1.33
14	D	201	EGY	O21-C2	-2.80	1.40	1.46
14	C	101	EGY	O21-C2	-2.75	1.40	1.46
17	A	921	0K3	P-O	2.73	1.64	1.54
14	A	915	EGY	O21-C2	-2.72	1.40	1.46
14	A	914	EGY	O21-C2	-2.71	1.40	1.46
14	A	918	EGY	O21-C2	-2.70	1.40	1.46
14	A	917	EGY	O21-C2	-2.70	1.40	1.46
14	A	913	EGY	O21-C2	-2.70	1.40	1.46
14	A	916	EGY	O21-C2	-2.68	1.40	1.46
14	F	701	EGY	O21-C2	-2.67	1.40	1.46
17	A	921	0K3	C9-C7	2.48	1.56	1.51
15	D	204	KZB	C84-C03	-2.37	1.51	1.56
17	A	921	0K3	P-O1	-2.31	1.46	1.54
15	G	501	KZB	C84-C03	-2.28	1.51	1.56
17	A	921	0K3	C23-C21	2.28	1.56	1.51
14	E	701	EGY	O21-C2	-2.27	1.41	1.46
14	A	913	EGY	P-O13	2.24	1.68	1.59
14	A	918	EGY	P-O13	2.23	1.68	1.59
14	A	916	EGY	P-O13	2.22	1.68	1.59
14	A	917	EGY	P-O13	2.22	1.68	1.59
14	A	917	EGY	P-O11	2.22	1.68	1.59
14	A	914	EGY	P-O13	2.22	1.68	1.59
14	A	913	EGY	P-O11	2.21	1.68	1.59
14	C	101	EGY	P-O13	2.21	1.68	1.59
14	A	915	EGY	P-O13	2.21	1.68	1.59
14	A	918	EGY	P-O11	2.20	1.68	1.59
14	D	201	EGY	P-O11	2.19	1.68	1.59
14	E	701	EGY	P-O13	2.19	1.68	1.59
14	E	701	EGY	P-O11	2.18	1.67	1.59
14	D	201	EGY	P-O13	2.17	1.67	1.59
14	A	916	EGY	P-O11	2.17	1.67	1.59
14	F	701	EGY	P-O11	2.16	1.67	1.59
14	C	101	EGY	P-O11	2.16	1.67	1.59
14	A	914	EGY	P-O11	2.15	1.67	1.59
14	A	915	EGY	P-O11	2.15	1.67	1.59
14	F	701	EGY	P-O13	2.15	1.67	1.59
14	A	913	EGY	C22-C21	2.15	1.56	1.50
14	C	101	EGY	C22-C21	2.12	1.56	1.50
14	D	201	EGY	C22-C21	2.12	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	917	EGY	C22-C21	2.11	1.56	1.50
14	A	916	EGY	C22-C21	2.10	1.56	1.50
14	A	918	EGY	C22-C21	2.10	1.56	1.50
14	A	915	EGY	C22-C21	2.09	1.56	1.50
14	E	701	EGY	C22-C21	2.08	1.56	1.50
15	G	502	KZB	C84-C03	-2.08	1.52	1.56
15	F	702	KZB	C84-C03	-2.07	1.52	1.56
14	A	914	EGY	C22-C21	2.07	1.56	1.50
14	F	701	EGY	C22-C21	2.06	1.56	1.50
15	F	703	KZB	C84-C03	-2.05	1.52	1.56
15	F	704	KZB	C84-C03	-2.04	1.52	1.56
14	E	701	EGY	C13-N	-2.04	1.44	1.50
17	A	921	0K3	C-C1	2.03	1.54	1.49
15	E	703	KZB	C84-C03	-2.00	1.52	1.56

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	921	0K3	C-C1-C2	-10.51	108.98	126.20
15	F	704	KZB	O05-C04-C13	8.74	127.89	110.20
15	G	502	KZB	O05-C04-C13	8.63	127.67	110.20
15	D	203	KZB	O05-C04-C13	8.55	127.50	110.20
15	F	702	KZB	O05-C04-C13	8.54	127.49	110.20
15	A	919	KZB	O05-C04-C13	8.50	127.40	110.20
15	D	202	KZB	O05-C04-C13	8.43	127.26	110.20
15	E	702	KZB	O05-C04-C13	8.35	127.11	110.20
15	E	703	KZB	O05-C04-C13	8.33	127.07	110.20
15	D	204	KZB	O05-C04-C13	8.18	126.75	110.20
15	C	102	KZB	O05-C04-C13	8.12	126.63	110.20
15	C	103	KZB	O05-C04-C13	8.09	126.57	110.20
15	G	501	KZB	O05-C04-C13	7.95	126.30	110.20
15	F	703	KZB	O05-C04-C13	7.87	126.12	110.20
15	D	202	KZB	C79-C81-C16	-6.19	106.14	112.43
15	C	102	KZB	C19-C20-C21	-6.10	107.14	114.40
15	C	103	KZB	C79-C81-C16	-6.03	106.31	112.43
17	A	921	0K3	C3-C2-C1	-5.31	109.99	123.63
15	D	204	KZB	C01-C02-C06	-5.27	106.44	114.94
15	D	202	KZB	C17-C16-C81	-5.22	104.26	110.52
17	A	921	0K3	C4-C2-C1	-5.06	109.81	121.17
15	G	502	KZB	C79-C81-C16	-4.82	107.53	112.43
15	F	704	KZB	C19-C20-C21	-4.78	108.71	114.40
15	E	702	KZB	C19-C20-C21	-4.70	108.81	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	103	KZB	C17-C16-C81	-4.66	104.93	110.52
15	G	501	KZB	O12-C11-C09	-4.57	106.30	112.17
15	D	204	KZB	C02-C03-C04	-4.44	97.15	104.28
15	G	502	KZB	C17-C16-C81	-4.41	105.23	110.52
15	E	703	KZB	C19-C20-C21	-4.24	109.36	114.40
15	F	703	KZB	C19-C20-C21	-4.21	109.39	114.40
15	C	103	KZB	C02-C03-C04	-4.21	97.52	104.28
15	G	501	KZB	C19-C20-C21	-4.20	109.41	114.40
15	A	919	KZB	C79-C81-C16	-4.18	108.18	112.43
15	G	501	KZB	O12-C06-C07	4.13	114.36	110.76
14	F	701	EGY	O21-C21-C22	4.11	120.37	111.48
15	A	919	KZB	C84-C15-C16	-4.11	108.18	113.90
15	F	704	KZB	C17-C16-C81	-4.07	105.64	110.52
14	A	915	EGY	O21-C21-C22	4.07	120.29	111.48
15	E	703	KZB	C84-C15-C16	-4.04	108.26	113.90
14	A	916	EGY	O21-C21-C22	4.03	120.19	111.48
14	C	101	EGY	O21-C21-C22	4.00	120.13	111.48
14	A	918	EGY	O21-C21-C22	3.98	120.10	111.48
14	D	201	EGY	O21-C21-C22	3.97	120.07	111.48
14	A	917	EGY	O21-C21-C22	3.93	119.99	111.48
14	A	914	EGY	O21-C21-C22	3.93	119.98	111.48
14	E	701	EGY	O21-C21-C22	3.92	119.96	111.48
14	A	913	EGY	O21-C21-C22	3.92	119.95	111.48
15	D	204	KZB	C19-C20-C21	-3.87	109.80	114.40
15	G	502	KZB	C19-C20-C21	-3.83	109.85	114.40
15	A	919	KZB	C19-C20-C21	-3.82	109.85	114.40
15	D	203	KZB	C82-C81-C79	-3.77	109.66	113.91
15	G	501	KZB	C08-C09-C11	-3.75	104.04	108.59
15	G	501	KZB	C82-C81-C79	-3.75	109.69	113.91
15	F	702	KZB	C79-C81-C16	-3.74	108.63	112.43
15	C	103	KZB	C84-C03-C02	3.74	131.55	120.50
15	F	702	KZB	C07-C06-C02	-3.74	108.89	115.66
15	D	203	KZB	C17-C16-C81	-3.73	106.05	110.52
15	G	501	KZB	C02-C03-C04	-3.70	98.33	104.28
15	D	203	KZB	C79-C81-C16	-3.69	108.68	112.43
15	C	103	KZB	C19-C20-C21	-3.69	110.02	114.40
15	G	501	KZB	C84-C15-C16	-3.66	108.79	113.90
17	A	921	OK3	C19-C20-C21	-3.64	119.30	127.62
15	F	702	KZB	C17-C16-C81	-3.61	106.19	110.52
15	G	501	KZB	C17-C16-C81	-3.61	106.19	110.52
15	F	703	KZB	C17-C16-C81	-3.61	106.19	110.52
15	E	702	KZB	C84-C15-C16	-3.61	108.87	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	703	KZB	C79-C81-C16	-3.60	108.77	112.43
15	F	702	KZB	C19-C20-C21	-3.56	110.16	114.40
15	A	919	KZB	C17-C16-C81	-3.52	106.30	110.52
15	D	203	KZB	C19-C20-C21	-3.46	110.28	114.40
15	C	102	KZB	C84-C03-C02	3.44	130.67	120.50
15	C	102	KZB	C02-C03-C04	-3.40	98.81	104.28
15	F	704	KZB	C84-C15-C16	-3.39	109.17	113.90
15	D	203	KZB	C79-C78-C76	-3.39	108.59	114.17
15	G	501	KZB	C07-C08-C09	-3.38	104.93	111.67
15	C	102	KZB	C17-C16-C81	-3.37	106.49	110.52
15	D	202	KZB	C18-C17-C16	-3.34	106.83	112.16
15	F	704	KZB	C82-C81-C79	-3.32	110.17	113.91
15	F	702	KZB	O12-C11-C09	-3.30	107.93	112.17
15	D	202	KZB	C19-C20-C21	-3.30	110.47	114.40
15	F	703	KZB	C82-C81-C79	-3.30	110.19	113.91
15	G	501	KZB	C07-C06-C02	-3.27	109.74	115.66
15	F	703	KZB	C84-C03-C02	3.26	130.12	120.50
15	F	702	KZB	C82-C81-C79	-3.25	110.25	113.91
15	A	919	KZB	C84-C03-C02	3.23	130.05	120.50
15	F	703	KZB	C02-C03-C04	-3.23	99.09	104.28
15	D	203	KZB	C84-C15-C16	-3.23	109.40	113.90
15	E	703	KZB	C84-C03-C02	3.20	129.96	120.50
15	F	704	KZB	C79-C81-C16	-3.20	109.18	112.43
15	E	703	KZB	C02-C03-C04	-3.18	99.17	104.28
15	A	919	KZB	C82-C83-C84	-3.17	107.39	112.74
17	A	921	OK3	C8-C7-C9	3.16	120.71	115.23
15	E	702	KZB	C84-C03-C02	3.16	129.83	120.50
15	D	202	KZB	O12-C11-C09	-3.14	108.14	112.17
15	C	102	KZB	C18-C17-C16	-3.13	107.17	112.16
15	F	702	KZB	C84-C03-C02	3.12	129.73	120.50
15	F	704	KZB	C84-C03-C02	3.12	129.72	120.50
17	A	921	OK3	C24-C25-C26	-3.11	120.51	127.62
15	D	202	KZB	C84-C03-C02	3.10	129.67	120.50
15	F	703	KZB	C20-C19-C79	-3.10	109.36	112.66
15	D	203	KZB	C84-C03-C02	3.10	129.66	120.50
15	G	501	KZB	C79-C81-C16	-3.09	109.29	112.43
17	A	921	OK3	C3-C2-C4	-3.09	109.86	115.23
15	D	204	KZB	C78-C79-C19	3.07	110.16	107.23
15	G	502	KZB	C82-C81-C79	-3.05	110.48	113.91
15	D	204	KZB	C15-C16-C81	-3.04	103.81	109.17
15	G	502	KZB	C84-C03-C02	3.00	129.38	120.50
15	D	203	KZB	C18-C17-C16	-2.98	107.40	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	921	OK3	C5-C6-C7	-2.98	120.80	127.62
17	A	921	OK3	C22-C21-C23	2.98	120.40	115.23
15	D	204	KZB	C07-C06-C02	-2.98	110.26	115.66
15	D	202	KZB	C80-C79-C81	-2.98	107.18	111.18
15	A	919	KZB	C07-C06-C02	-2.96	110.30	115.66
15	F	703	KZB	C84-C15-C16	-2.95	109.79	113.90
15	C	102	KZB	C20-C19-C79	-2.94	109.53	112.66
15	C	103	KZB	C79-C78-C76	-2.91	109.39	114.17
15	E	702	KZB	C02-C03-C04	-2.89	99.63	104.28
15	E	703	KZB	C82-C81-C79	-2.86	110.69	113.91
15	D	204	KZB	C82-C83-C84	-2.85	107.93	112.74
17	A	921	OK3	C39-C17-C18	2.84	120.17	115.23
15	D	204	KZB	C84-C03-C02	2.84	128.90	120.50
15	G	501	KZB	C84-C03-C02	2.84	128.89	120.50
17	A	921	OK3	C29-C30-C31	-2.82	121.16	127.62
17	A	921	OK3	C32-C31-C33	2.82	120.13	115.23
15	F	703	KZB	C18-C17-C16	-2.82	107.66	112.16
14	F	701	EGY	O31-C31-C32	2.82	120.43	111.83
15	A	919	KZB	C79-C78-C76	-2.81	109.54	114.17
15	F	704	KZB	C08-C07-C06	-2.79	107.56	111.93
14	A	914	EGY	O31-C31-C32	2.79	120.33	111.83
15	F	702	KZB	C84-C15-C16	-2.79	110.02	113.90
15	D	202	KZB	C83-C84-C03	2.78	119.31	115.36
15	G	502	KZB	C20-C19-C79	-2.77	109.72	112.66
17	A	921	OK3	C10-C11-C12	-2.77	121.29	127.62
15	F	704	KZB	C18-C17-C16	-2.76	107.75	112.16
15	F	703	KZB	O12-C11-C09	-2.76	108.62	112.17
15	G	502	KZB	C18-C17-C16	-2.76	107.75	112.16
14	D	201	EGY	O31-C31-C32	2.76	120.24	111.83
14	C	101	EGY	O31-C31-C32	2.74	120.19	111.83
15	G	502	KZB	C84-C15-C16	-2.73	110.09	113.90
15	D	204	KZB	O12-C11-C09	-2.72	108.67	112.17
15	D	203	KZB	C02-C03-C04	-2.72	99.90	104.28
14	A	917	EGY	O31-C31-C32	2.72	120.13	111.83
15	D	202	KZB	C79-C78-C76	-2.71	109.71	114.17
15	E	702	KZB	O12-C11-C09	-2.69	108.71	112.17
14	A	916	EGY	O31-C31-C32	2.69	120.02	111.83
15	E	703	KZB	O12-C11-C09	-2.68	108.73	112.17
14	A	915	EGY	O31-C31-C32	2.67	119.99	111.83
14	A	913	EGY	O31-C31-C32	2.66	119.96	111.83
17	A	921	OK3	C27-C26-C28	2.66	119.84	115.23
15	E	703	KZB	C20-C19-C79	-2.65	109.84	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	921	OK3	C13-C12-C14	2.64	119.81	115.23
17	A	921	OK3	C15-C16-C17	-2.63	121.61	127.62
14	A	918	EGY	O31-C31-C32	2.62	119.83	111.83
15	A	919	KZB	O12-C11-C09	-2.61	108.81	112.17
15	D	203	KZB	C07-C06-C02	-2.61	110.93	115.66
15	D	202	KZB	C07-C06-C02	-2.60	110.95	115.66
15	F	702	KZB	C07-C08-C09	-2.59	106.50	111.67
15	F	702	KZB	O12-C06-C07	2.57	113.00	110.76
15	C	103	KZB	C82-C83-C84	-2.56	108.43	112.74
15	D	202	KZB	C20-C19-C79	-2.55	109.94	112.66
15	D	203	KZB	C80-C79-C81	-2.53	107.78	111.18
17	A	921	OK3	O1-P-O2	-2.51	101.05	110.83
15	D	202	KZB	C84-C15-C16	-2.49	110.42	113.90
15	C	102	KZB	C08-C07-C06	-2.48	108.05	111.93
15	D	204	KZB	C84-C15-C16	-2.47	110.45	113.90
15	C	103	KZB	C08-C07-C06	-2.47	108.06	111.93
15	A	919	KZB	C20-C19-C79	-2.47	110.03	112.66
15	G	501	KZB	C20-C19-C79	-2.45	110.05	112.66
15	E	702	KZB	C78-C79-C19	2.44	109.56	107.23
15	F	702	KZB	C79-C78-C76	-2.44	110.16	114.17
15	F	704	KZB	C20-C19-C79	-2.42	110.08	112.66
15	E	702	KZB	C82-C81-C79	-2.42	111.19	113.91
15	E	702	KZB	C07-C06-C02	-2.41	111.29	115.66
15	F	704	KZB	C83-C84-C15	-2.40	103.42	108.11
15	E	702	KZB	C82-C83-C84	-2.39	108.70	112.74
15	A	919	KZB	C82-C81-C79	-2.39	111.22	113.91
14	E	701	EGY	O31-C31-C32	2.39	119.12	111.83
15	E	703	KZB	C07-C06-C02	-2.39	111.33	115.66
15	D	204	KZB	C17-C18-C19	-2.37	107.24	111.84
15	E	703	KZB	C82-C83-C84	-2.37	108.74	112.74
15	A	919	KZB	C83-C84-C03	2.36	118.72	115.36
15	F	702	KZB	C20-C19-C79	-2.34	110.17	112.66
15	G	502	KZB	C79-C78-C76	-2.33	110.34	114.17
15	C	103	KZB	C83-C84-C03	2.33	118.67	115.36
15	G	502	KZB	C02-C03-C04	-2.32	100.54	104.28
15	A	919	KZB	C18-C17-C16	-2.32	108.46	112.16
15	G	501	KZB	C06-C02-C03	-2.30	99.98	103.37
15	C	103	KZB	O12-C11-C09	-2.30	109.22	112.17
15	G	501	KZB	C08-C07-C06	-2.29	108.34	111.93
15	E	703	KZB	C17-C16-C81	-2.29	107.78	110.52
15	C	103	KZB	C18-C17-C16	-2.29	108.51	112.16
15	D	204	KZB	C83-C84-C03	2.28	118.61	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	F	702	KZB	C18-C17-C16	-2.28	108.53	112.16
15	G	502	KZB	C08-C07-C06	-2.26	108.39	111.93
15	F	702	KZB	C10-C09-C08	-2.25	107.16	112.08
15	D	204	KZB	C82-C81-C79	-2.25	111.38	113.91
15	D	202	KZB	C02-C03-C04	-2.22	100.71	104.28
15	D	202	KZB	C83-C84-C15	-2.21	103.79	108.11
15	C	102	KZB	C84-C15-C16	-2.21	110.82	113.90
15	G	501	KZB	C18-C17-C16	-2.20	108.65	112.16
15	D	203	KZB	C20-C19-C79	-2.20	110.32	112.66
15	E	703	KZB	C18-C17-C16	-2.19	108.66	112.16
15	G	502	KZB	C82-C83-C84	-2.19	109.04	112.74
17	A	921	OK3	C37-C36-C38	2.19	119.62	114.59
15	D	203	KZB	O12-C11-C09	-2.18	109.37	112.17
15	F	702	KZB	C02-C03-C04	-2.18	100.78	104.28
15	D	202	KZB	C82-C81-C79	-2.18	111.46	113.91
15	C	102	KZB	C17-C18-C19	-2.15	107.66	111.84
15	C	102	KZB	C82-C81-C79	-2.14	111.50	113.91
15	D	204	KZB	C17-C16-C15	-2.11	109.31	112.29
15	G	501	KZB	C79-C78-C76	-2.10	110.72	114.17
15	E	703	KZB	C79-C78-C76	-2.08	110.75	114.17
15	G	501	KZB	C11-O12-C06	2.08	117.27	113.69
15	A	919	KZB	C07-C08-C09	-2.03	107.61	111.67
14	F	701	EGY	C11-C12-N	-2.02	109.35	115.82
15	E	702	KZB	C15-C16-C81	-2.02	105.61	109.17
15	G	502	KZB	C07-C06-C02	-2.01	112.02	115.66
15	F	703	KZB	C80-C79-C81	-2.01	108.48	111.18
14	A	917	EGY	C11-C12-N	-2.00	109.39	115.82

There are no chirality outliers.

All (252) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	913	EGY	C11-O13-P-O14
14	A	913	EGY	C11-O13-P-O11
14	A	914	EGY	C11-O13-P-O14
14	A	914	EGY	C11-O13-P-O11
14	A	914	EGY	C1-O11-P-O12
14	A	914	EGY	C1-O11-P-O14
14	A	914	EGY	C1-O11-P-O13
14	A	914	EGY	C2-C3-O31-C31
14	A	915	EGY	C11-O13-P-O12
14	A	915	EGY	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
14	A	915	EGY	C11-O13-P-O11
14	A	915	EGY	C1-O11-P-O12
14	A	915	EGY	C1-O11-P-O13
14	A	916	EGY	C11-O13-P-O12
14	A	916	EGY	C11-O13-P-O14
14	A	916	EGY	C11-O13-P-O11
14	A	916	EGY	C1-O11-P-O14
14	A	916	EGY	C1-O11-P-O13
14	A	916	EGY	O13-C11-C12-N
14	A	917	EGY	C11-O13-P-O14
14	A	917	EGY	C11-O13-P-O11
14	A	917	EGY	C1-O11-P-O12
14	A	917	EGY	C1-O11-P-O14
14	A	917	EGY	C1-O11-P-O13
14	A	918	EGY	C11-O13-P-O14
14	A	918	EGY	C1-O11-P-O12
14	A	918	EGY	C12-C11-O13-P
14	A	918	EGY	O13-C11-C12-N
14	C	101	EGY	C11-O13-P-O12
14	C	101	EGY	C11-O13-P-O11
14	C	101	EGY	C1-O11-P-O12
14	C	101	EGY	C1-O11-P-O13
14	D	201	EGY	C11-O13-P-O12
14	D	201	EGY	C11-O13-P-O14
14	D	201	EGY	C11-O13-P-O11
14	D	201	EGY	C1-O11-P-O12
14	D	201	EGY	O13-C11-C12-N
14	E	701	EGY	C11-O13-P-O12
14	E	701	EGY	C11-O13-P-O11
14	E	701	EGY	C1-O11-P-O12
14	E	701	EGY	C1-O11-P-O14
14	E	701	EGY	C1-O11-P-O13
14	E	701	EGY	C22-C21-O21-C2
14	F	701	EGY	C11-O13-P-O12
14	F	701	EGY	C11-O13-P-O11
14	F	701	EGY	C12-C11-O13-P
14	F	701	EGY	C22-C21-O21-C2
17	A	921	0K3	C-O3-P-O2
17	A	921	0K3	C-O3-P-O
17	A	921	0K3	C-O3-P-O1
17	A	921	0K3	C-C1-C2-C3
17	A	921	0K3	C-C1-C2-C4

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Mol	Chain	Res	Type	Atoms
17	A	921	0K3	C31-C33-C34-C35
14	A	913	EGY	O32-C31-O31-C3
14	A	915	EGY	O32-C31-O31-C3
14	A	913	EGY	C32-C31-O31-C3
14	A	915	EGY	C32-C31-O31-C3
14	C	101	EGY	O32-C31-O31-C3
14	F	701	EGY	O32-C31-O31-C3
14	E	701	EGY	O22-C21-O21-C2
14	F	701	EGY	O22-C21-O21-C2
14	C	101	EGY	C32-C31-O31-C3
14	F	701	EGY	C32-C31-O31-C3
17	A	921	0K3	C8-C7-C9-C10
17	A	921	0K3	C6-C7-C9-C10
14	A	915	EGY	C22-C21-O21-C2
17	A	921	0K3	C2-C4-C5-C6
17	A	921	0K3	C21-C23-C24-C25
14	A	914	EGY	C32-C31-O31-C3
14	A	915	EGY	O22-C21-O21-C2
14	E	701	EGY	C11-C12-N-C15
14	A	915	EGY	C32-C33-C34-C35
14	D	201	EGY	C25-C26-C27-C28
14	C	101	EGY	C21-C22-C23-C24
14	A	918	EGY	C31-C32-C33-C34
14	D	201	EGY	C22-C21-O21-C2
14	A	914	EGY	C21-C22-C23-C24
14	E	701	EGY	C11-C12-N-C14
14	A	918	EGY	C21-C22-C23-C24
14	E	701	EGY	C31-C32-C33-C34
14	C	101	EGY	C22-C21-O21-C2
14	A	914	EGY	O32-C31-O31-C3
14	A	913	EGY	C31-C32-C33-C34
14	C	101	EGY	O22-C21-O21-C2
14	D	201	EGY	O22-C21-O21-C2
14	A	917	EGY	C32-C31-O31-C3
14	E	701	EGY	C11-C12-N-C13
14	C	101	EGY	C32-C33-C34-C35
14	A	914	EGY	C36-C37-C38-C39
14	F	701	EGY	C32-C33-C34-C35
14	A	913	EGY	C36-C37-C38-C39
14	A	916	EGY	C32-C31-O31-C3
14	A	914	EGY	C35-C36-C37-C38
14	E	701	EGY	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
14	A	915	EGY	C35-C36-C37-C38
14	A	916	EGY	C34-C35-C36-C37
14	A	917	EGY	C34-C35-C36-C37
14	A	917	EGY	O32-C31-O31-C3
14	A	913	EGY	C29-C2A-C2B-C2C
17	A	921	0K3	C11-C10-C9-C7
14	A	915	EGY	C23-C24-C25-C26
14	C	101	EGY	C33-C34-C35-C36
14	A	918	EGY	C34-C35-C36-C37
14	A	916	EGY	C22-C21-O21-C2
14	A	917	EGY	C22-C21-O21-C2
14	F	701	EGY	C38-C39-C3A-C3B
14	A	913	EGY	C35-C36-C37-C38
14	E	701	EGY	C26-C27-C28-C29
14	C	101	EGY	C26-C27-C28-C29
14	D	201	EGY	C35-C36-C37-C38
14	A	916	EGY	O32-C31-O31-C3
14	A	914	EGY	C25-C26-C27-C28
14	A	917	EGY	C23-C24-C25-C26
14	A	917	EGY	C2A-C2B-C2C-C2D
14	E	701	EGY	C28-C29-C2A-C2B
14	A	918	EGY	C22-C21-O21-C2
14	C	101	EGY	C37-C38-C39-C3A
14	A	918	EGY	C32-C33-C34-C35
14	A	914	EGY	C31-C32-C33-C34
14	A	916	EGY	O22-C21-O21-C2
17	A	921	0K3	C12-C14-C15-C16
14	F	701	EGY	C37-C38-C39-C3A
14	E	701	EGY	C21-C22-C23-C24
14	A	913	EGY	C26-C27-C28-C29
14	A	918	EGY	C22-C23-C24-C25
14	E	701	EGY	C2A-C2B-C2C-C2D
14	A	915	EGY	C31-C32-C33-C34
14	A	916	EGY	O11-C1-C2-C3
14	A	917	EGY	O22-C21-O21-C2
14	C	101	EGY	C1-C2-C3-O31
14	A	918	EGY	C26-C27-C28-C29
14	C	101	EGY	C24-C25-C26-C27
14	A	917	EGY	C29-C2A-C2B-C2C
14	A	918	EGY	O22-C21-O21-C2
14	C	101	EGY	C34-C35-C36-C37
14	A	913	EGY	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
14	C	101	EGY	C36-C37-C38-C39
14	A	916	EGY	C1-C2-O21-C21
14	D	201	EGY	C29-C2A-C2B-C2C
14	A	918	EGY	C27-C28-C29-C2A
14	E	701	EGY	C33-C34-C35-C36
14	D	201	EGY	C22-C23-C24-C25
14	C	101	EGY	C25-C26-C27-C28
14	A	916	EGY	C2B-C2C-C2D-C2E
14	A	918	EGY	C38-C39-C3A-C3B
14	A	917	EGY	C36-C37-C38-C39
14	A	918	EGY	C28-C29-C2A-C2B
14	D	201	EGY	C34-C35-C36-C37
14	A	913	EGY	C38-C39-C3A-C3B
14	A	914	EGY	C38-C39-C3A-C3B
14	A	918	EGY	C24-C25-C26-C27
17	A	921	0K3	C27-C26-C28-C29
14	A	915	EGY	C2B-C2C-C2D-C2E
17	A	921	0K3	C13-C12-C14-C15
17	A	921	0K3	C25-C26-C28-C29
14	A	918	EGY	C23-C24-C25-C26
14	F	701	EGY	C1-C2-C3-O31
14	E	701	EGY	C36-C37-C38-C39
17	A	921	0K3	C11-C12-C14-C15
14	A	916	EGY	C33-C34-C35-C36
14	F	701	EGY	C27-C28-C29-C2A
14	A	916	EGY	C38-C39-C3A-C3B
14	A	914	EGY	C23-C24-C25-C26
14	A	914	EGY	O21-C2-C3-O31
14	E	701	EGY	O21-C2-C3-O31
14	C	101	EGY	C38-C39-C3A-C3B
14	D	201	EGY	C38-C39-C3A-C3B
14	A	915	EGY	C26-C27-C28-C29
14	A	913	EGY	C27-C28-C29-C2A
14	A	915	EGY	C29-C2A-C2B-C2C
14	A	915	EGY	C2A-C2B-C2C-C2D
14	A	918	EGY	C37-C38-C39-C3A
14	F	701	EGY	C2B-C2C-C2D-C2E
14	A	918	EGY	C1-C2-O21-C21
14	F	701	EGY	C3-C2-O21-C21
14	F	701	EGY	O21-C2-C3-O31
14	A	917	EGY	C24-C25-C26-C27
14	F	701	EGY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
14	D	201	EGY	C36-C37-C38-C39
14	A	913	EGY	O13-C11-C12-N
14	A	915	EGY	O13-C11-C12-N
14	E	701	EGY	O13-C11-C12-N
14	F	701	EGY	O13-C11-C12-N
14	D	201	EGY	C2A-C2B-C2C-C2D
14	A	917	EGY	C28-C29-C2A-C2B
14	A	914	EGY	C32-C33-C34-C35
14	E	701	EGY	C24-C25-C26-C27
14	C	101	EGY	C27-C28-C29-C2A
14	A	916	EGY	O11-C1-C2-O21
14	A	913	EGY	C33-C34-C35-C36
14	A	915	EGY	C24-C25-C26-C27
14	C	101	EGY	O21-C2-C3-O31
14	A	916	EGY	C2A-C2B-C2C-C2D
14	A	914	EGY	C1-C2-C3-O31
14	A	913	EGY	C2A-C2B-C2C-C2D
14	A	915	EGY	C27-C28-C29-C2A
14	D	201	EGY	C33-C34-C35-C36
14	A	913	EGY	C11-O13-P-O12
14	A	916	EGY	C1-O11-P-O12
14	A	918	EGY	C1-O11-P-O13
14	C	101	EGY	C11-O13-P-O14
14	C	101	EGY	C1-O11-P-O14
14	D	201	EGY	C1-O11-P-O14
14	D	201	EGY	C1-O11-P-O13
14	F	701	EGY	C11-O13-P-O14
14	A	918	EGY	C33-C34-C35-C36
14	A	914	EGY	C1-C2-O21-C21
14	A	914	EGY	C22-C23-C24-C25
14	C	101	EGY	C2B-C2C-C2D-C2E
14	E	701	EGY	C25-C26-C27-C28
14	C	101	EGY	C29-C2A-C2B-C2C
14	E	701	EGY	C32-C33-C34-C35
14	A	917	EGY	O11-C1-C2-O21
14	A	917	EGY	C35-C36-C37-C38
14	E	701	EGY	C23-C24-C25-C26
14	A	916	EGY	O21-C2-C3-O31
14	A	916	EGY	C36-C37-C38-C39
14	A	917	EGY	C25-C26-C27-C28
14	A	913	EGY	C34-C35-C36-C37
14	E	701	EGY	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
14	D	201	EGY	C23-C24-C25-C26
14	A	914	EGY	C2-C1-O11-P
14	A	916	EGY	C35-C36-C37-C38
14	A	917	EGY	C33-C34-C35-C36
14	A	917	EGY	C27-C28-C29-C2A
14	A	918	EGY	C35-C36-C37-C38
14	A	915	EGY	C22-C23-C24-C25
14	F	701	EGY	C24-C25-C26-C27
17	A	921	0K3	C1-C2-C4-C5
14	D	201	EGY	C2B-C2C-C2D-C2E
14	D	201	EGY	C37-C38-C39-C3A
14	A	913	EGY	C11-C12-N-C13
14	A	915	EGY	C38-C39-C3A-C3B
14	A	917	EGY	C12-C11-O13-P
14	F	701	EGY	C35-C36-C37-C38
14	C	101	EGY	O31-C31-C32-C33
14	A	917	EGY	C37-C38-C39-C3A
14	A	918	EGY	O21-C21-C22-C23
14	A	918	EGY	O31-C31-C32-C33
14	A	914	EGY	O11-C1-C2-C3
14	A	915	EGY	O11-C1-C2-C3
14	A	917	EGY	C38-C39-C3A-C3B
14	A	915	EGY	C1-C2-O21-C21
14	A	915	EGY	C3-C2-O21-C21
14	E	701	EGY	C1-C2-O21-C21
14	A	915	EGY	C11-C12-N-C13
14	A	918	EGY	C11-C12-N-C13
14	C	101	EGY	O32-C31-C32-C33
14	A	913	EGY	C11-C12-N-C14
14	E	701	EGY	C35-C36-C37-C38
14	A	918	EGY	O32-C31-C32-C33
14	A	918	EGY	O22-C21-C22-C23

There are no ring outliers.

10 monomers are involved in 23 short contacts:

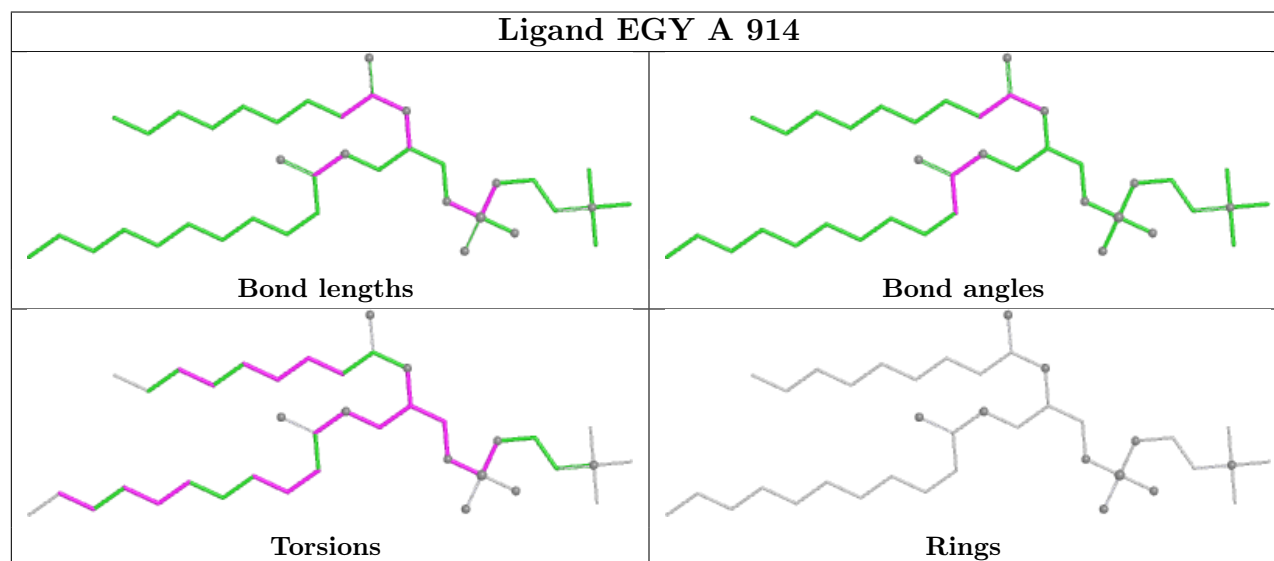
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	103	KZB	1	0
15	E	703	KZB	2	0
14	A	918	EGY	4	0
15	A	919	KZB	2	0
14	D	201	EGY	2	0

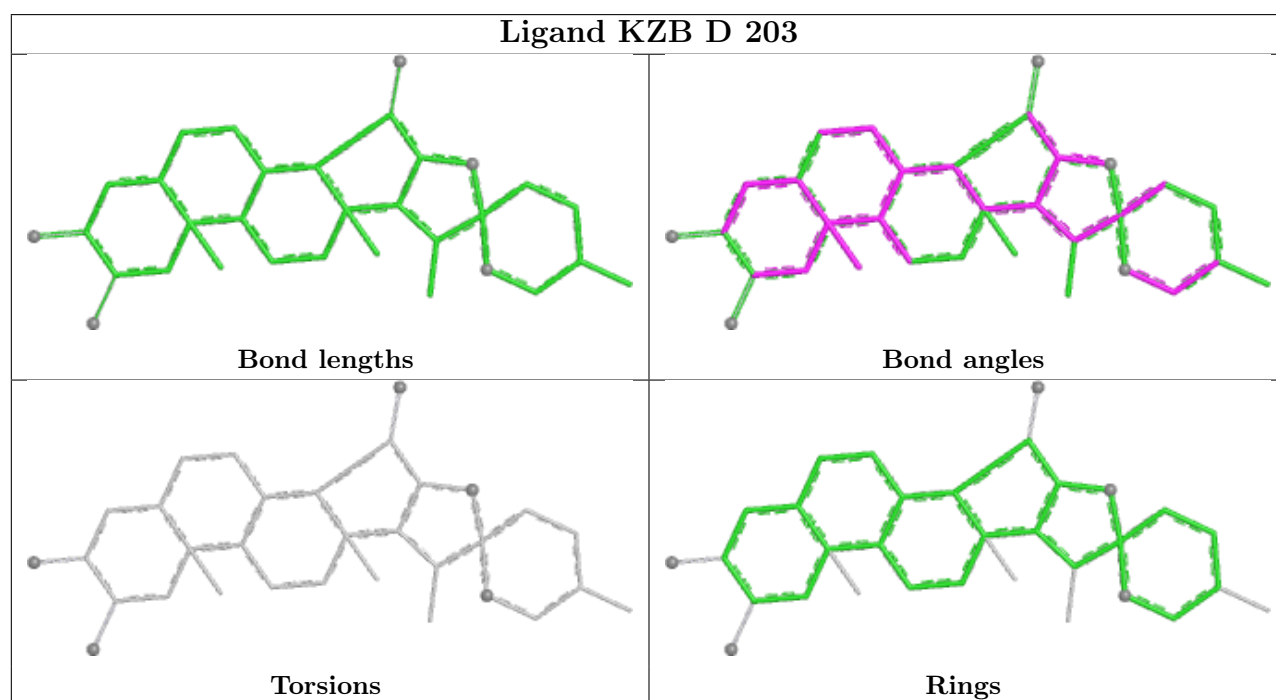
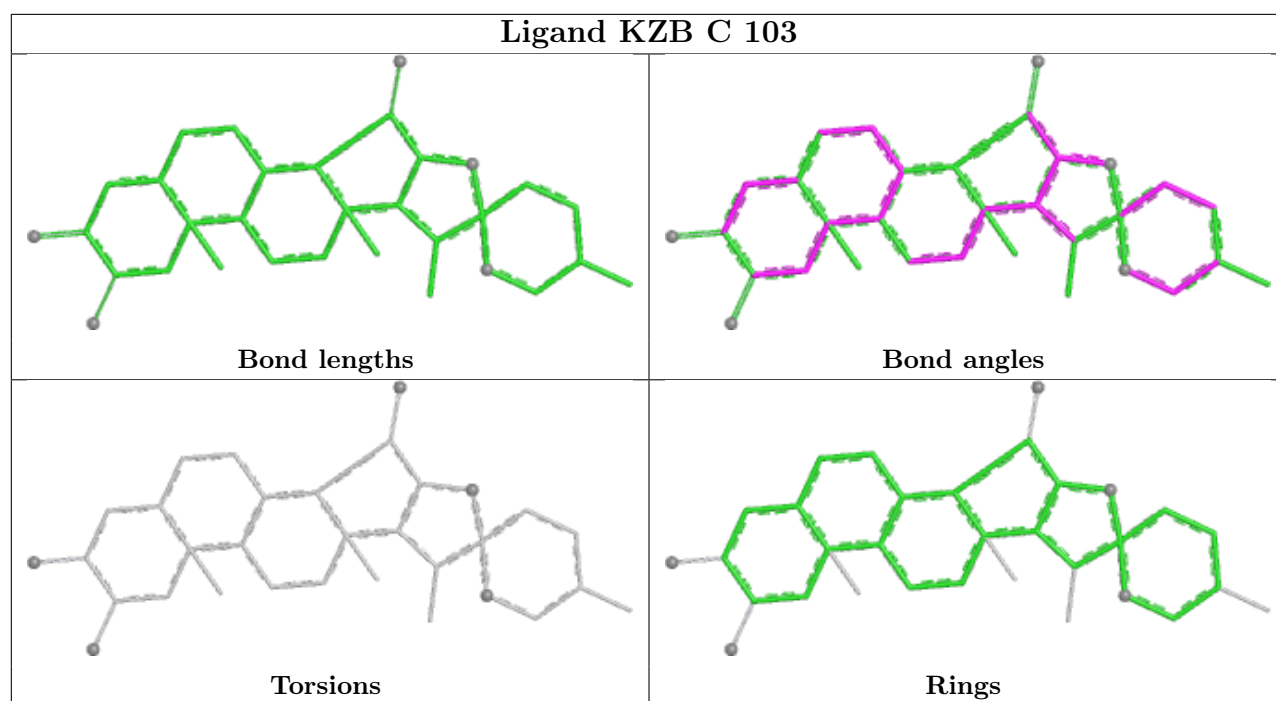
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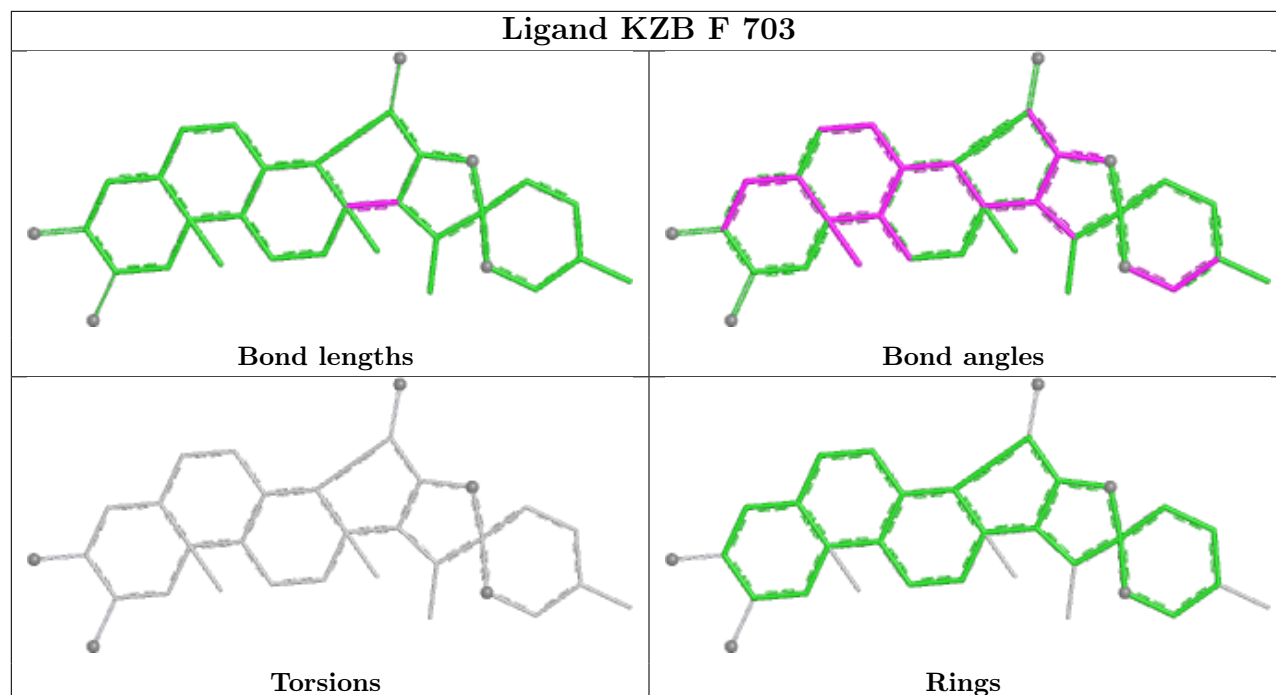
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	915	EGY	3	0
17	A	921	OK3	3	0
15	E	702	KZB	6	0
14	A	916	EGY	1	0
14	C	101	EGY	3	0

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

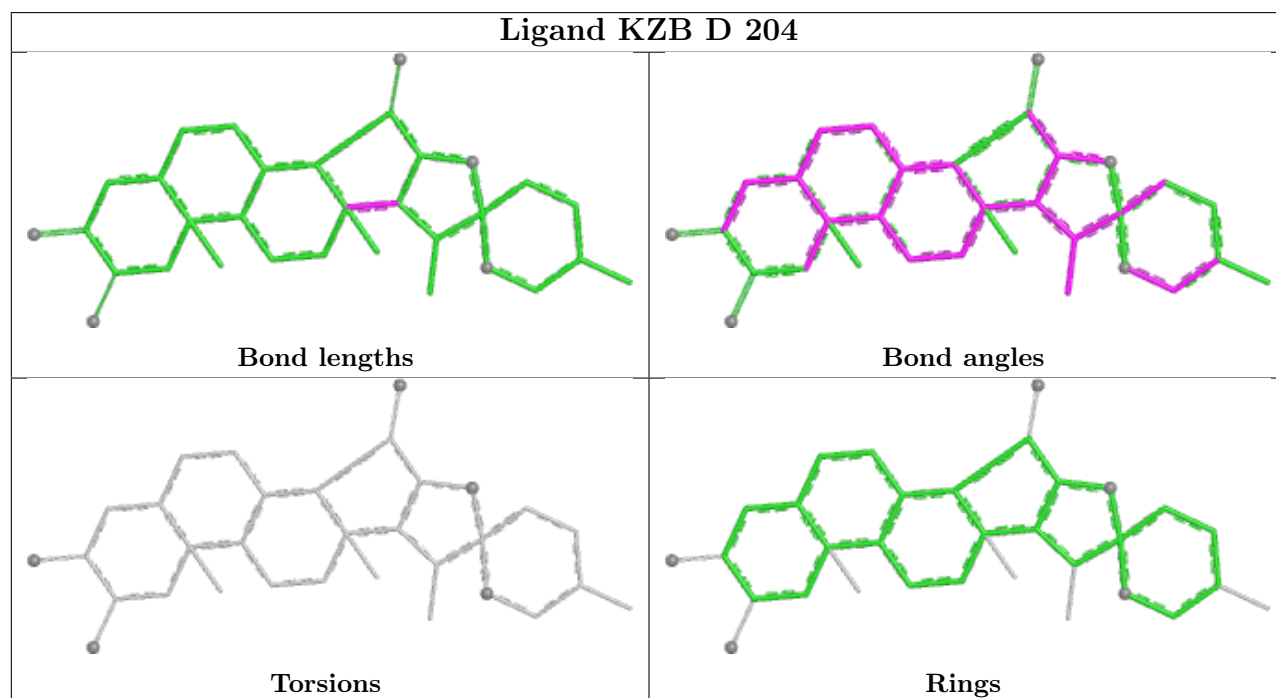


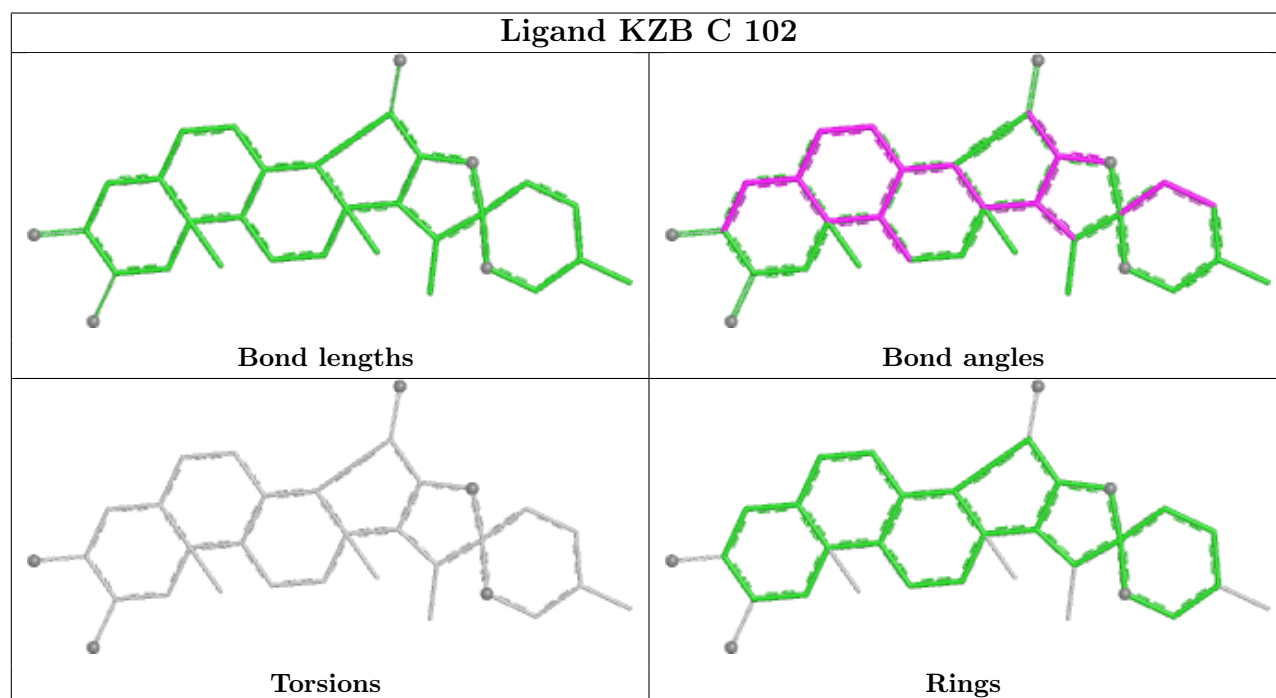
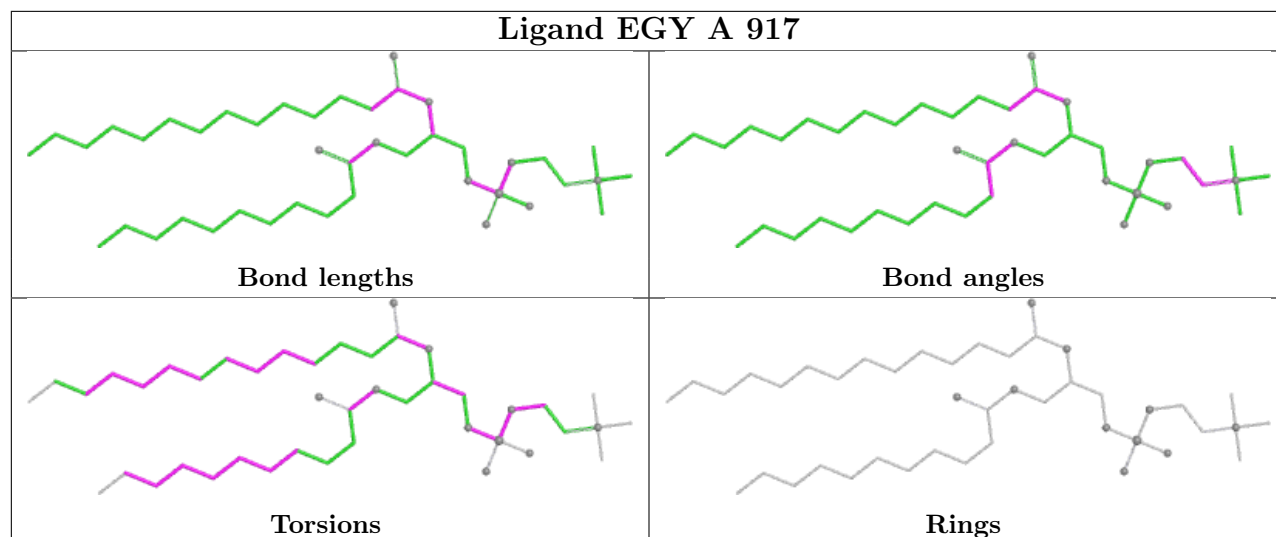


Ligand KZB F 703

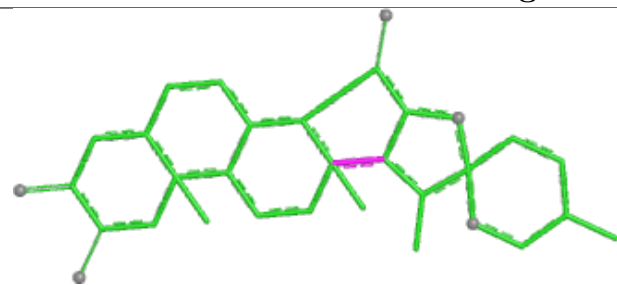


Ligand KZB D 204

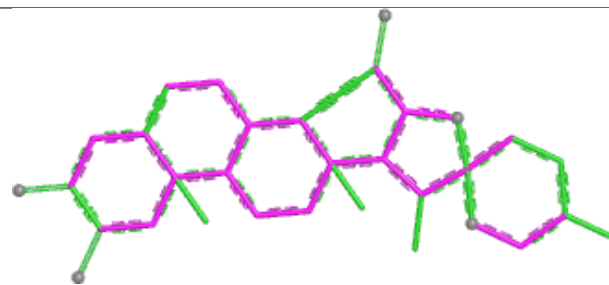




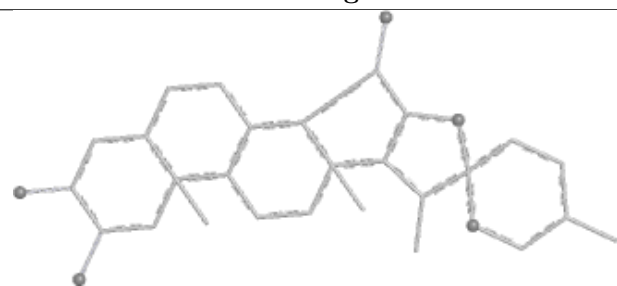
Ligand KZB E 703



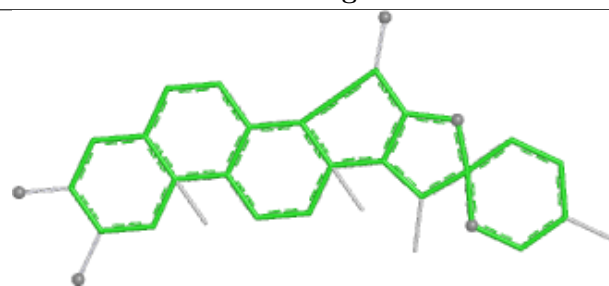
Bond lengths



Bond angles

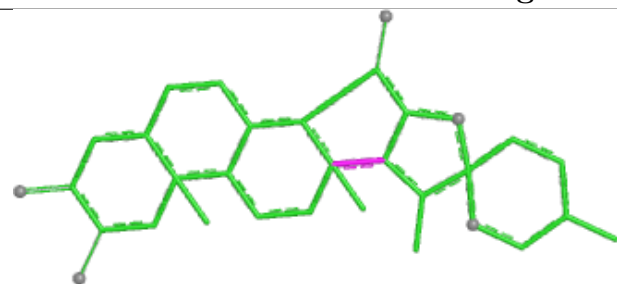


Torsions

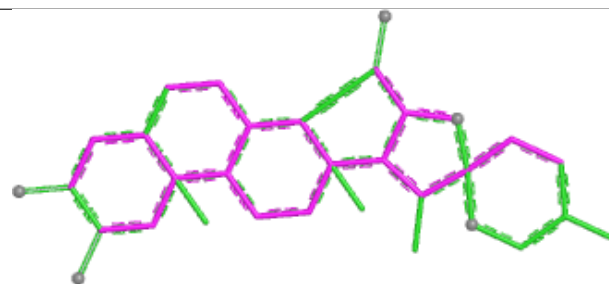


Rings

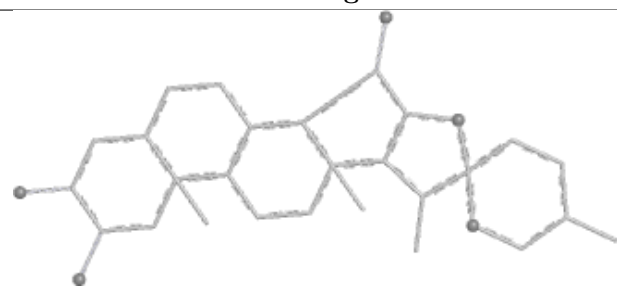
Ligand KZB G 502



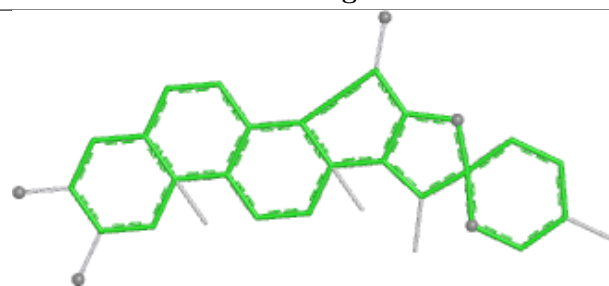
Bond lengths



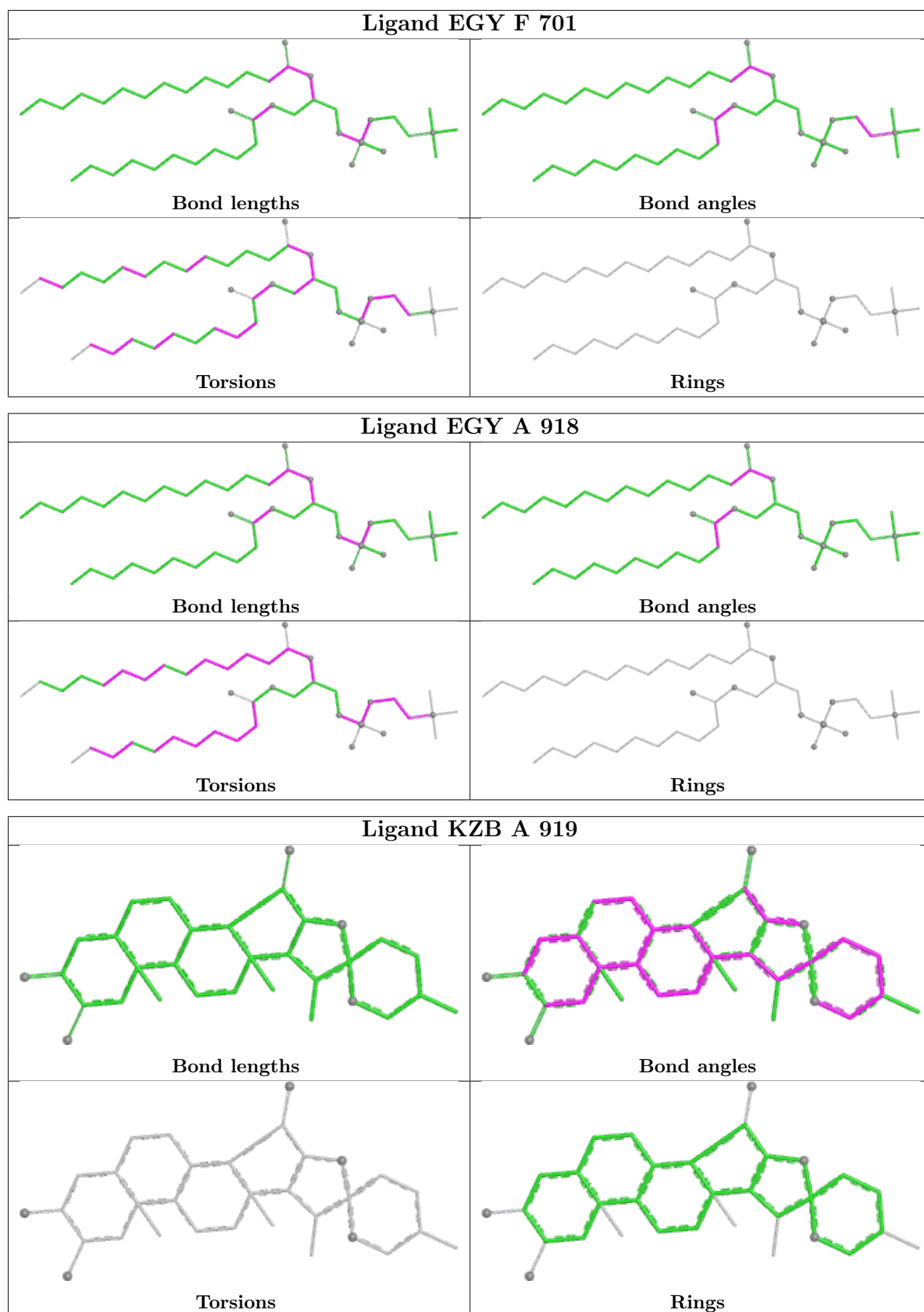
Bond angles

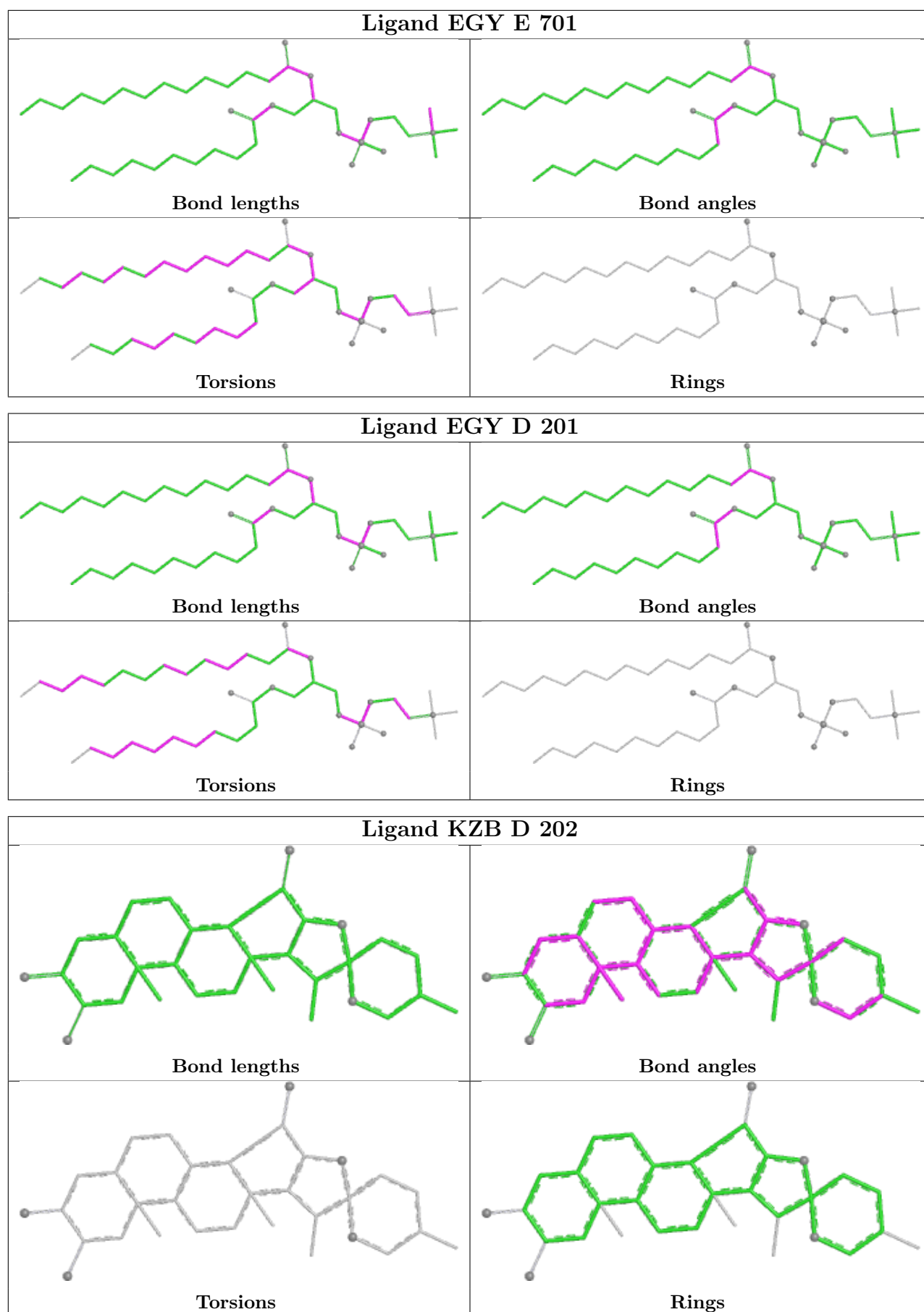


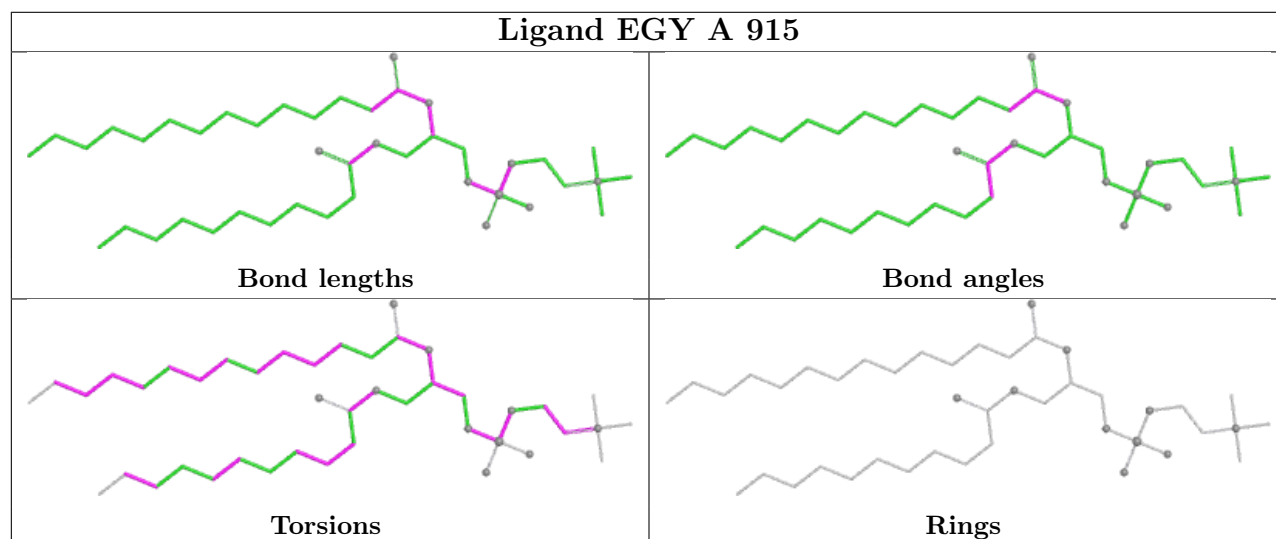
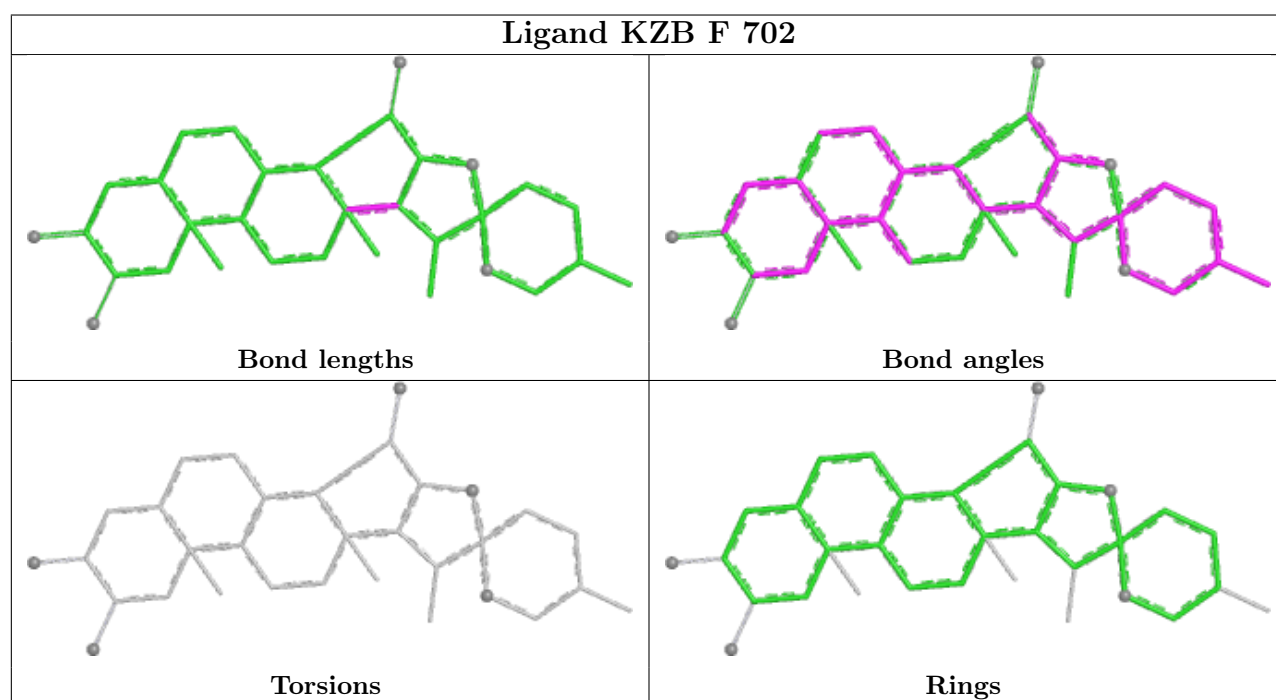
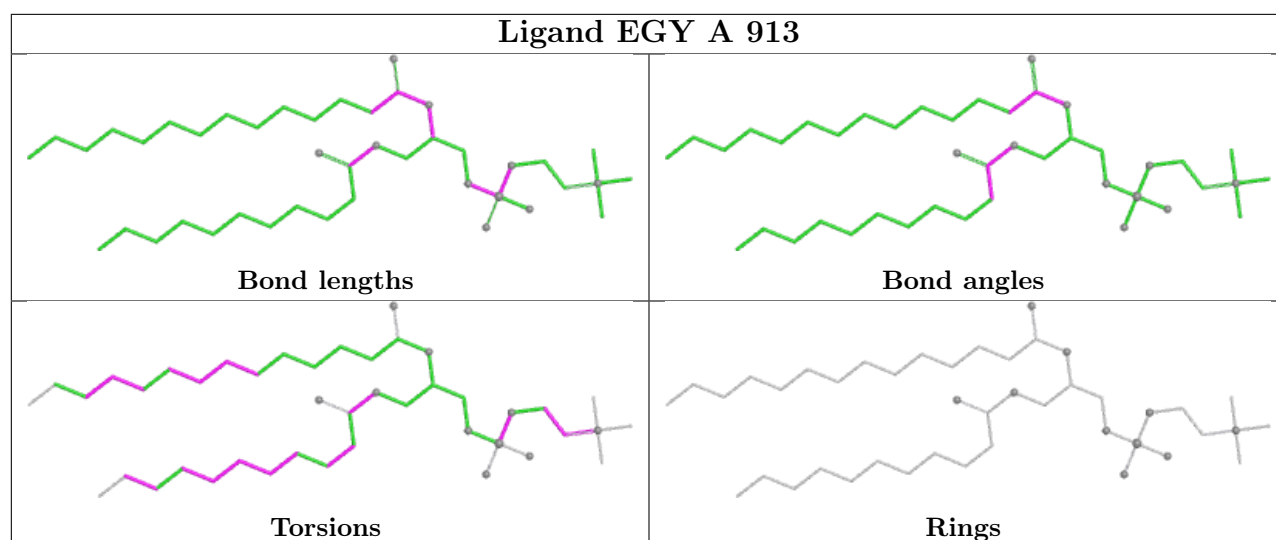
Torsions

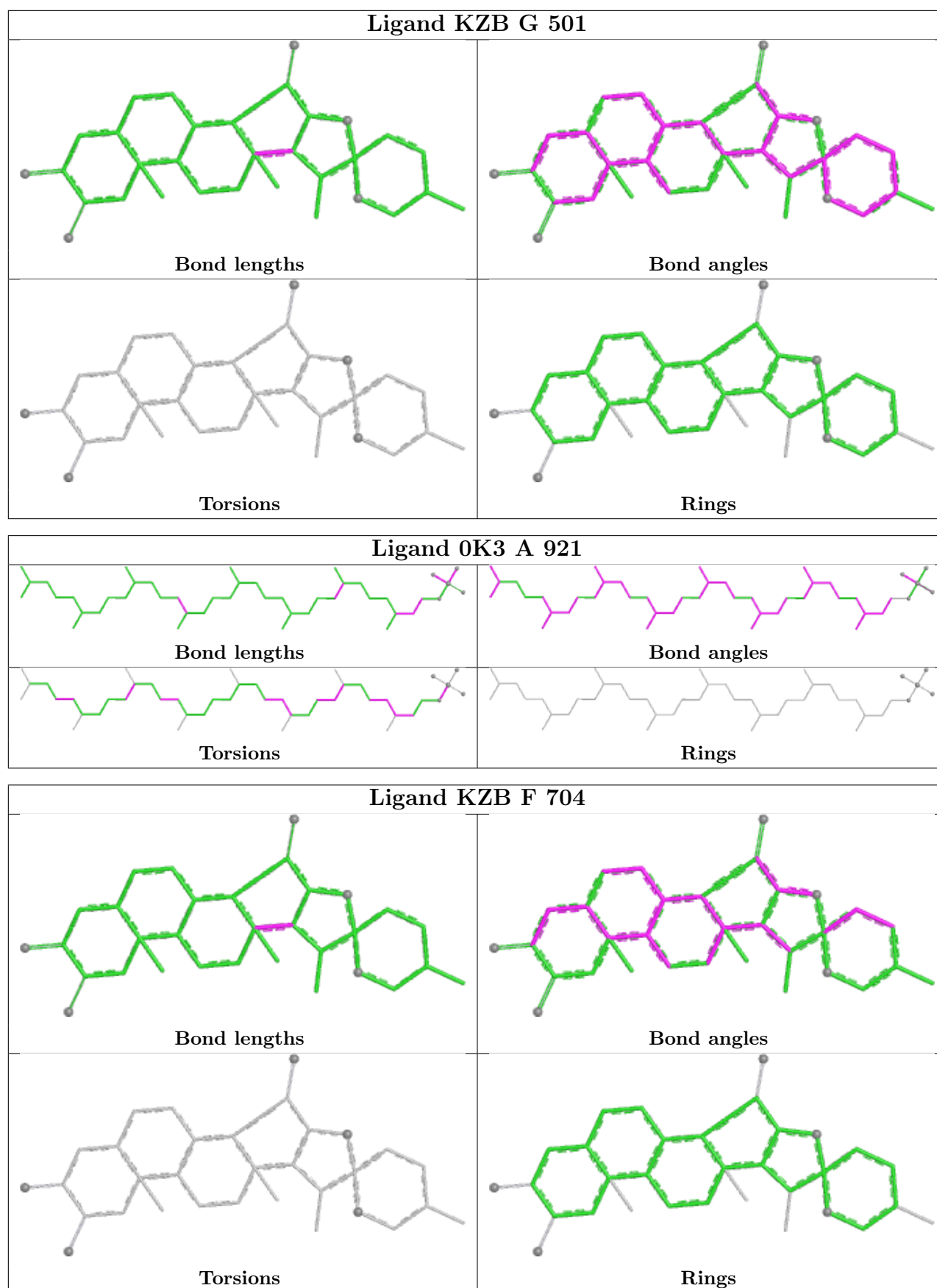


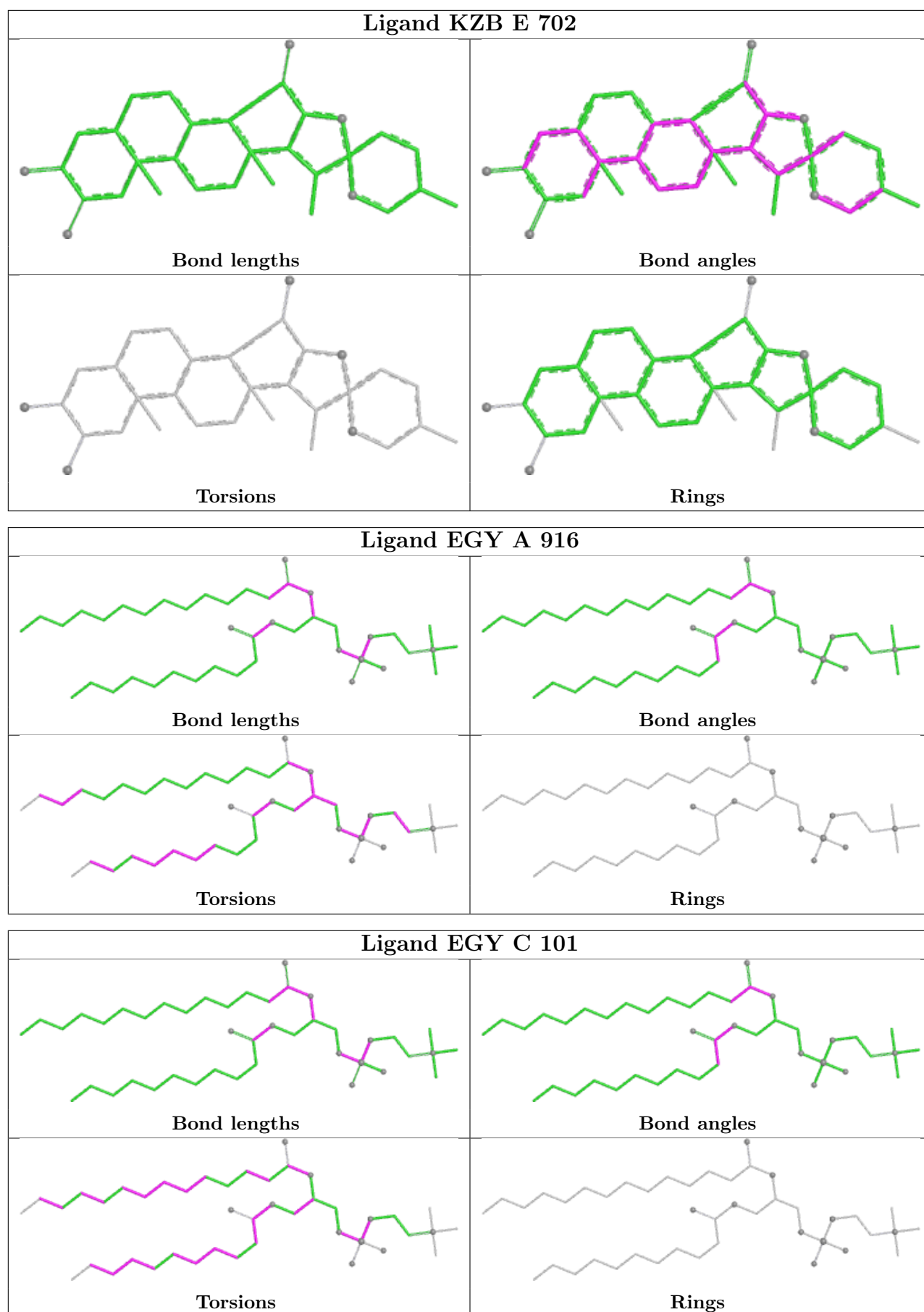
Rings











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.

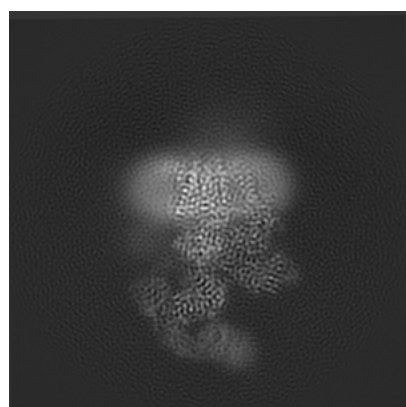
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10112. These allow visual inspection of the internal detail of the map and identification of artifacts.

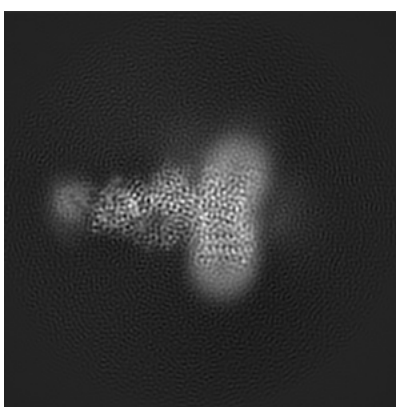
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

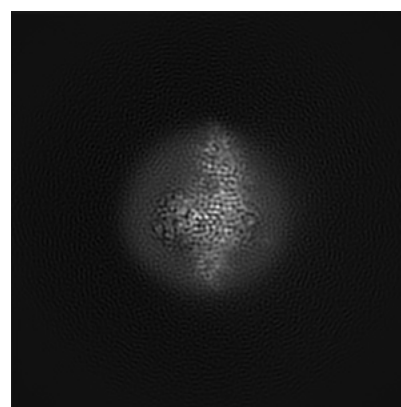
6.1.1 Primary map



X



Y

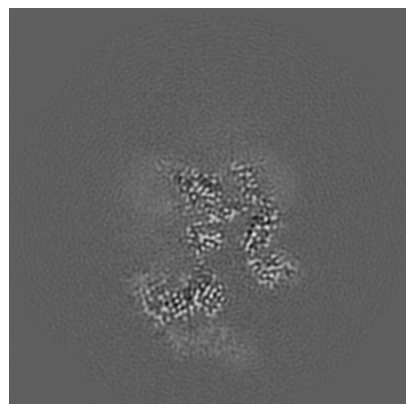


Z

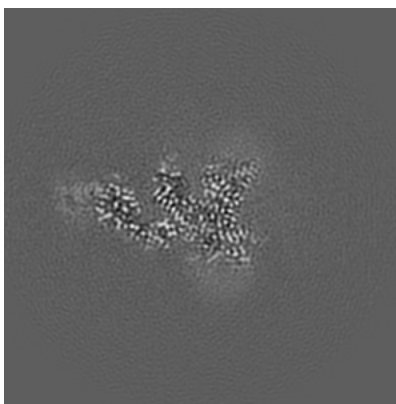
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

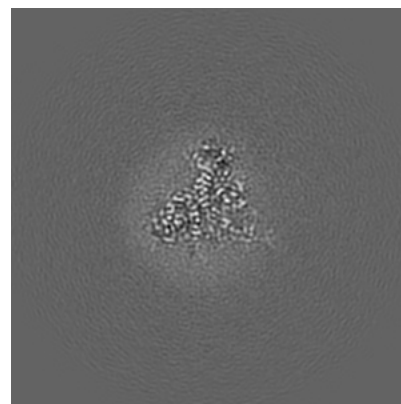
6.2.1 Primary map



X Index: 192



Y Index: 192

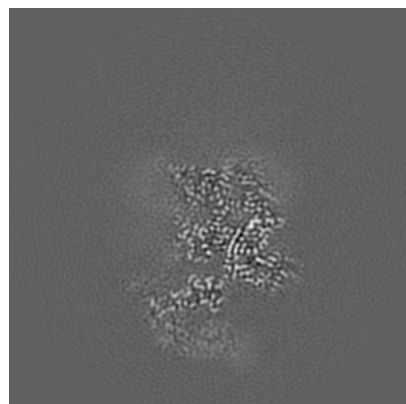


Z Index: 192

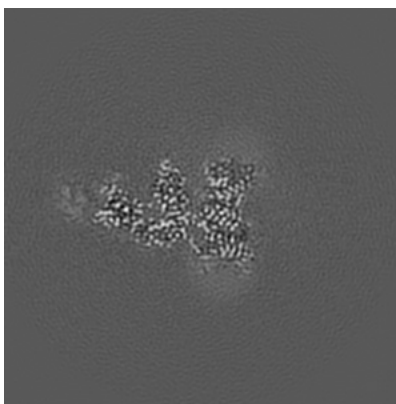
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

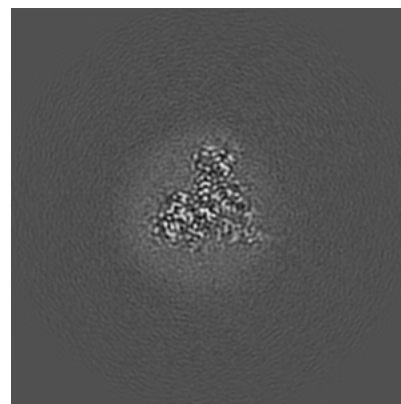
6.3.1 Primary map



X Index: 201



Y Index: 186

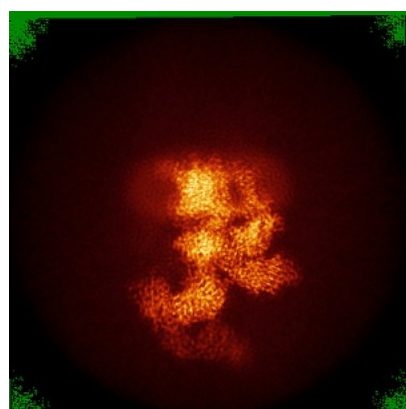


Z Index: 194

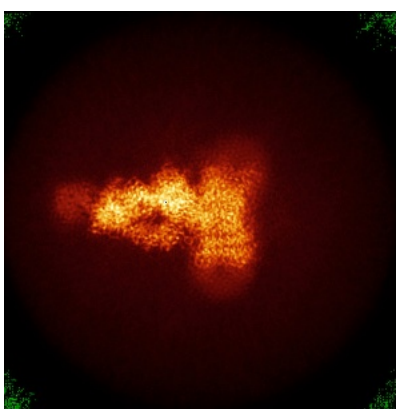
The images above show the largest variance slices of the map in three orthogonal directions.

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

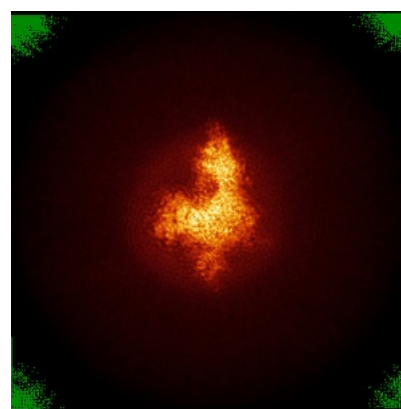
6.4.1 Primary map



X



Y

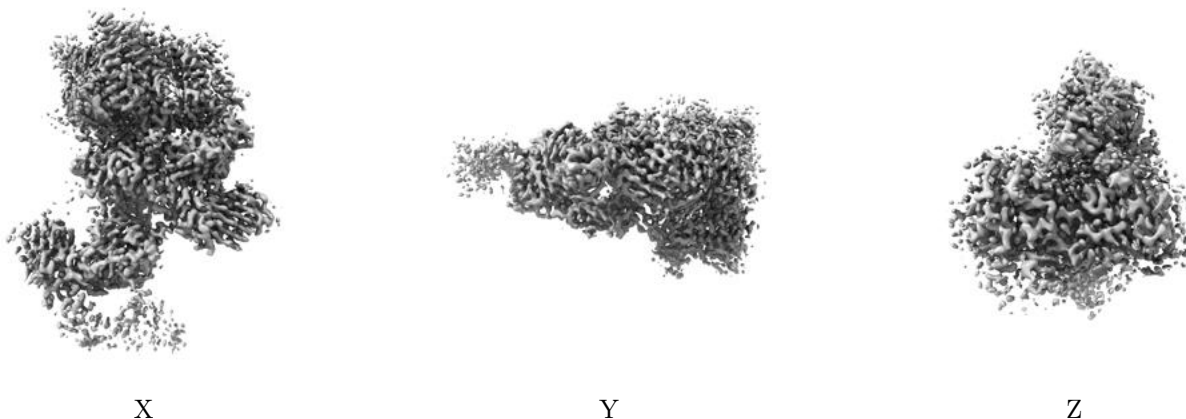


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

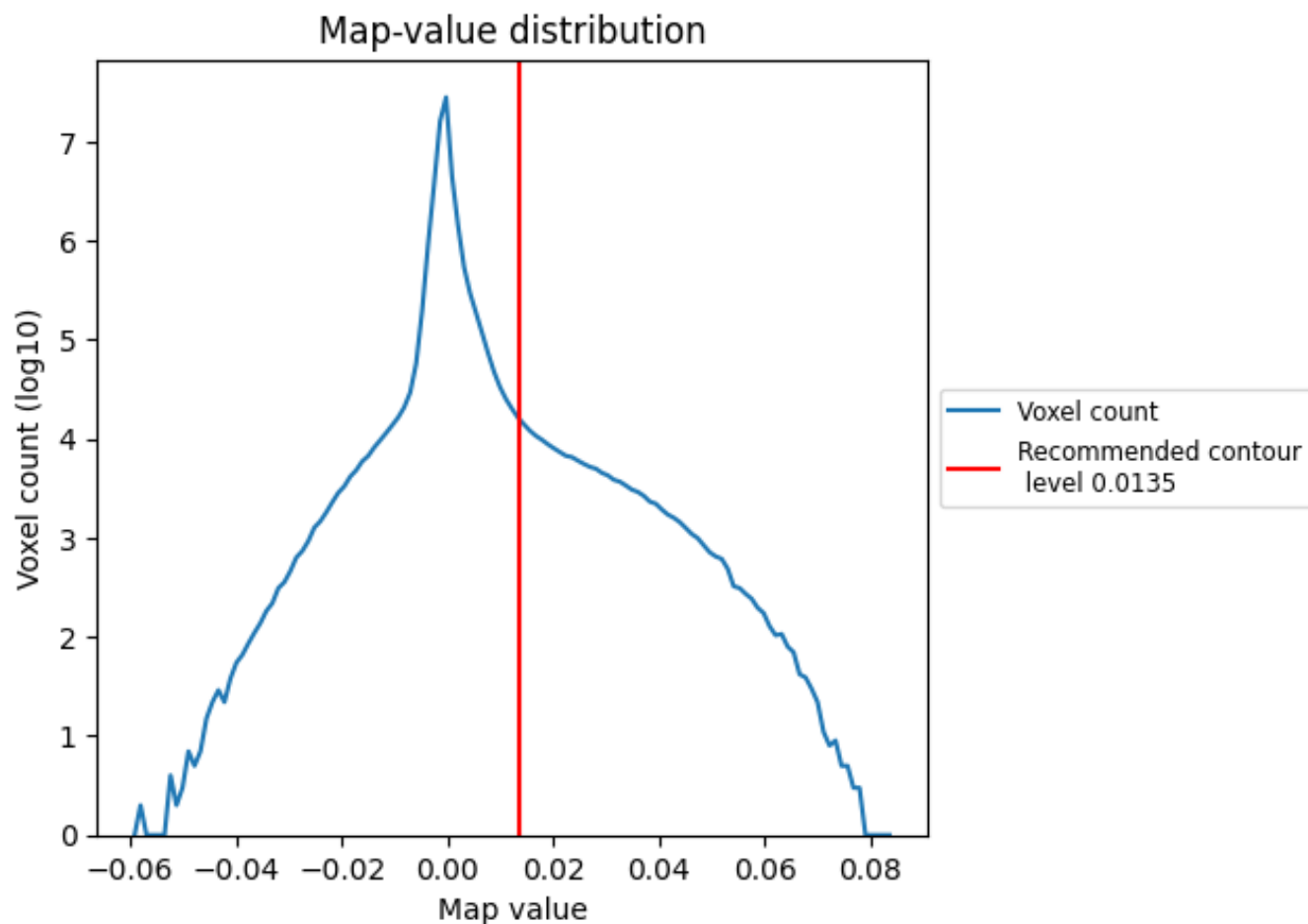
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

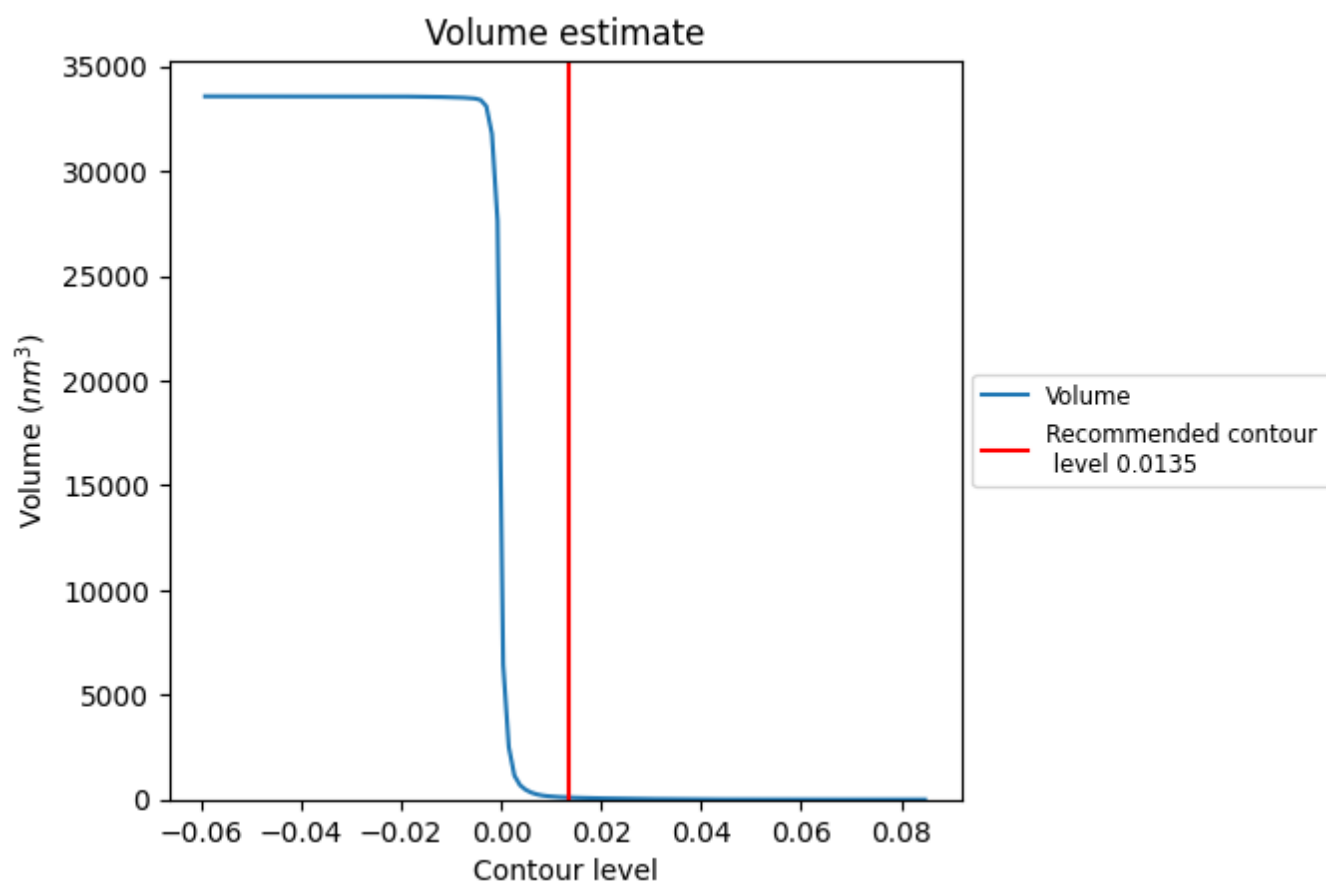
This section contains the results of statistical analysis of the map.

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.

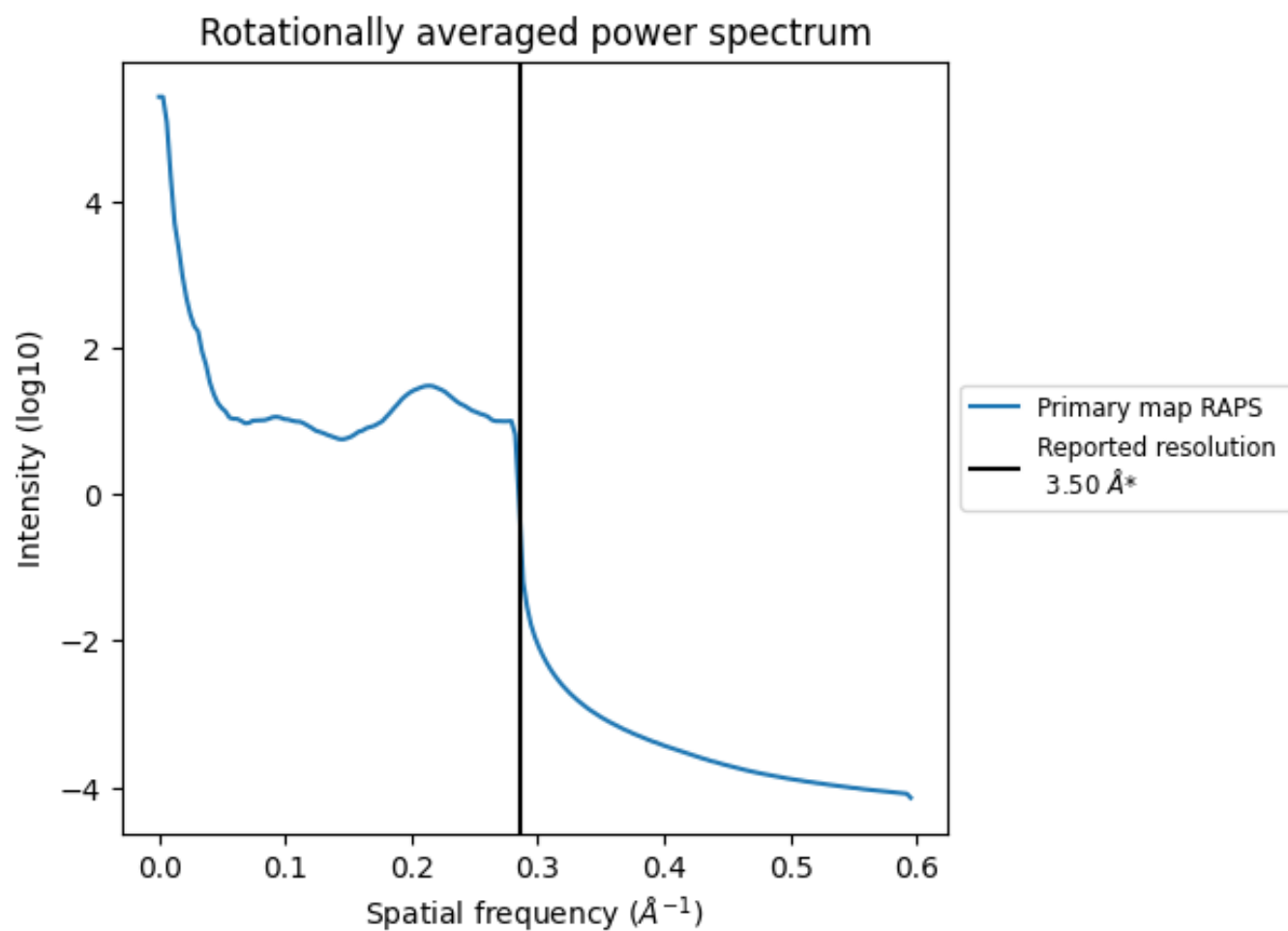
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

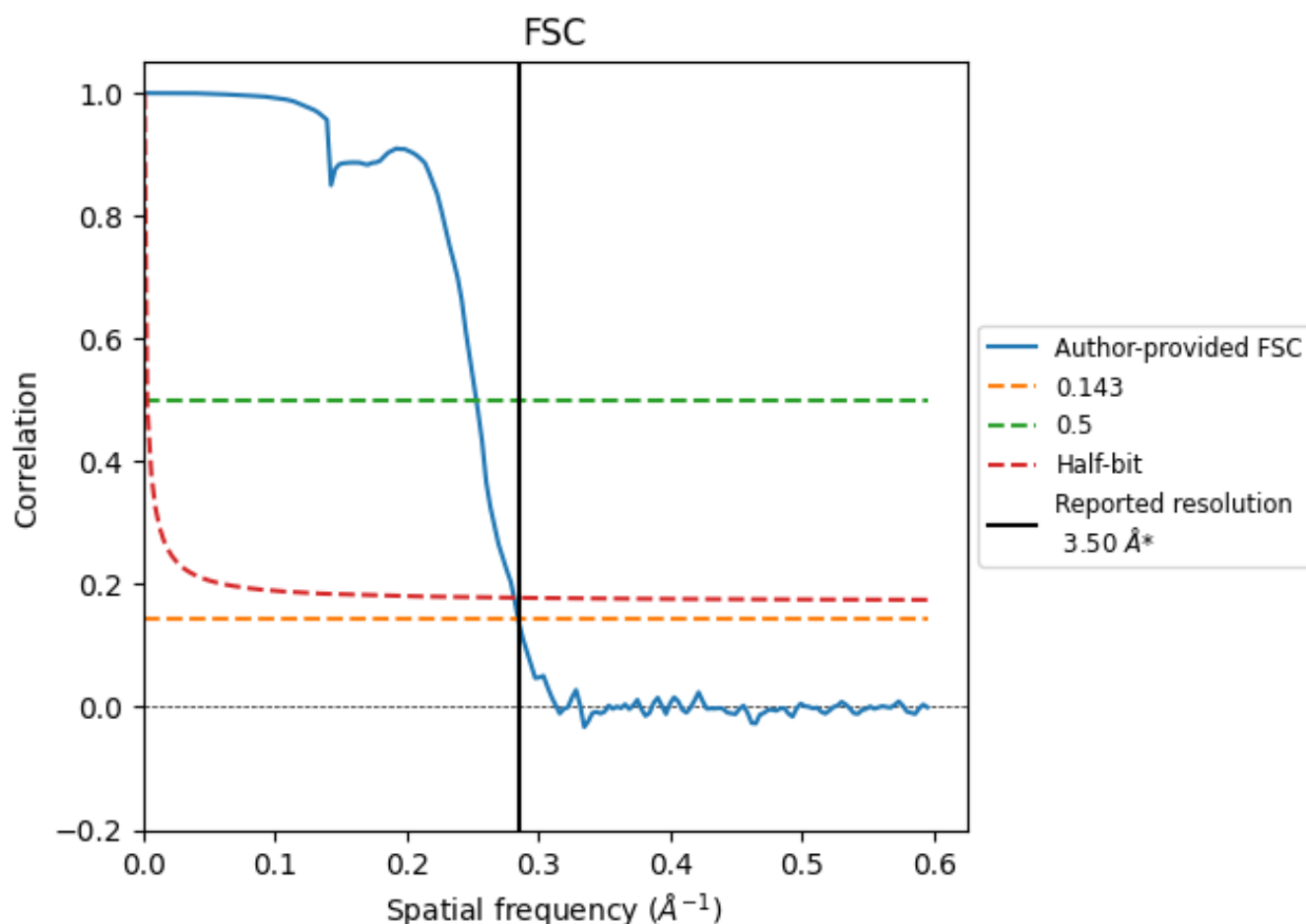


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.95	3.55
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

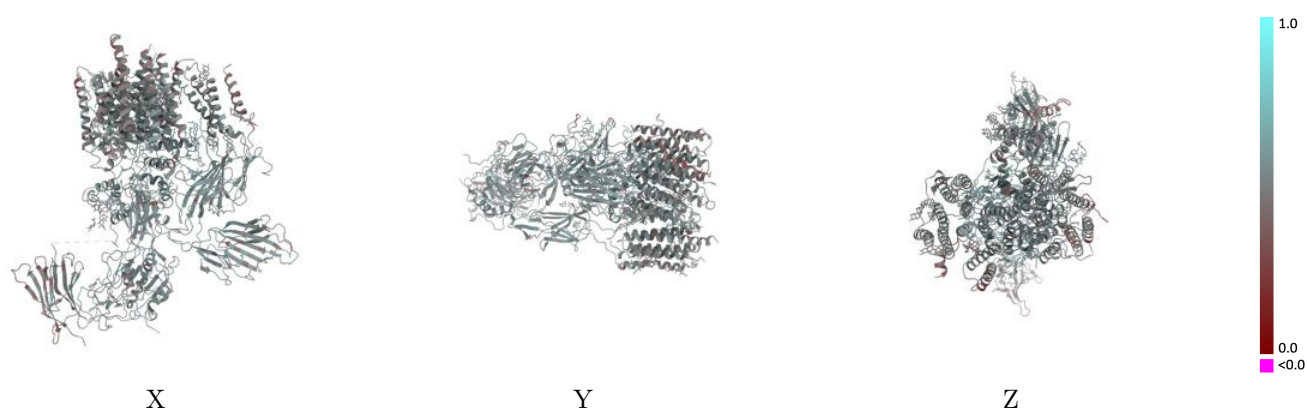
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10112 and PDB model 6S7T. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

This section was not generated.

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

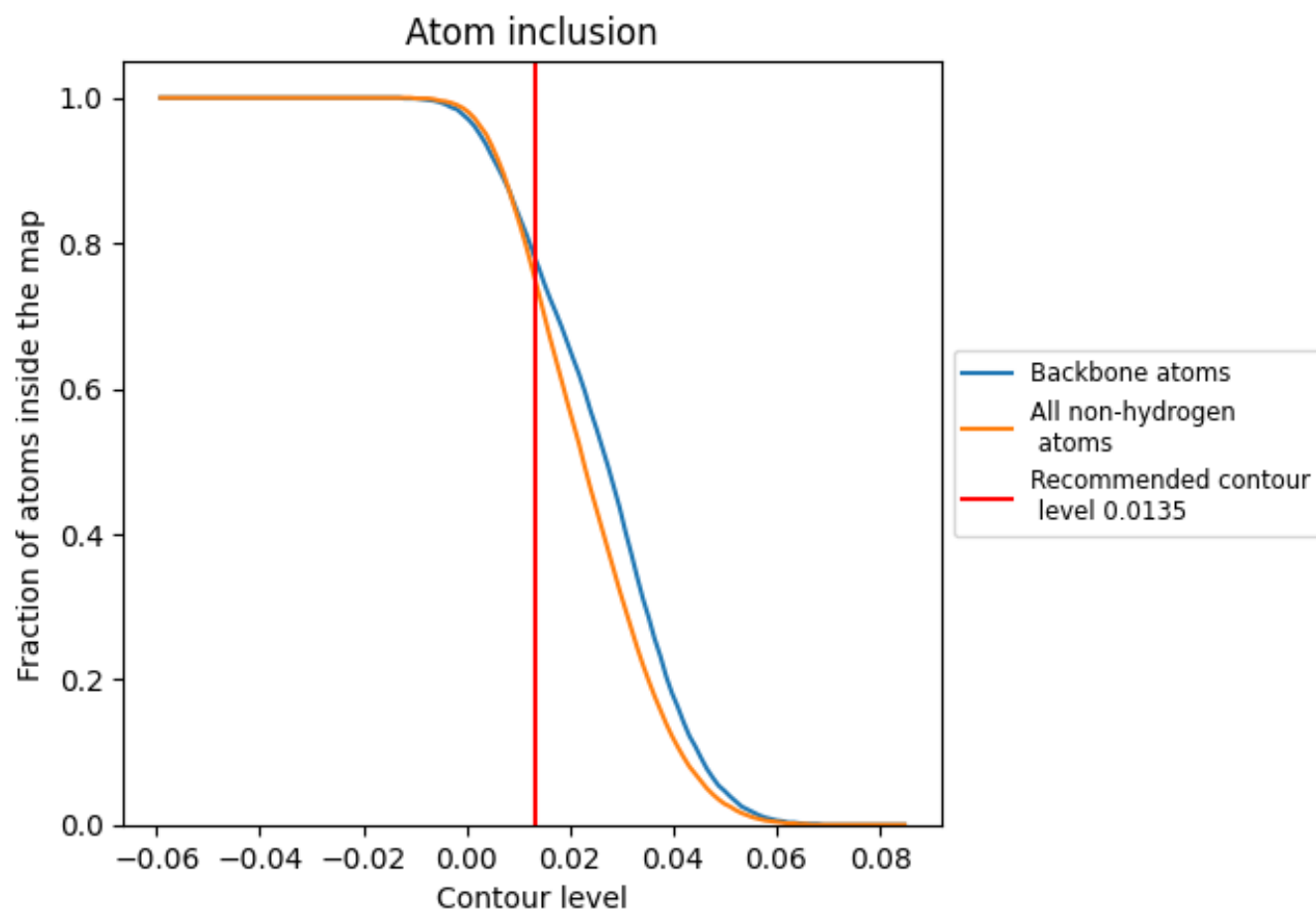


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.5090
A	0.7570	0.5190
B	0.6950	0.4880
C	0.7300	0.5040
D	0.7530	0.4930
E	0.7770	0.5230
F	0.6690	0.4690
G	0.7880	0.5240
H	0.6640	0.4630
I	0.4760	0.4330
J	0.7140	0.5160
K	0.5750	0.5460
L	0.6600	0.5060
M	0.4290	0.4950
N	0.6920	0.5500

