



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 01:44 PM UTC

PDB ID : 7MJO / pdb_00007mjo
EMDB ID : EMD-23880
Title : Vascular KATP channel: Kir6.1 SUR2B quatrefoil-like conformation 1
Authors : Sung, M.W.; Shyng, S.L.
Deposited on : 2021-04-20
Resolution : 4.00 Å(reported)
Based on initial model : 6BAA

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:

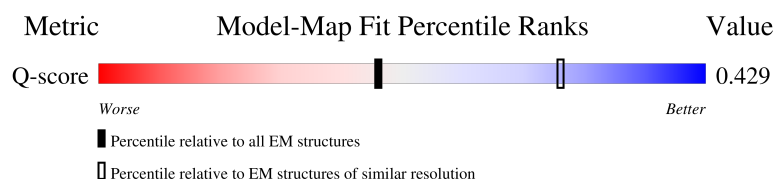
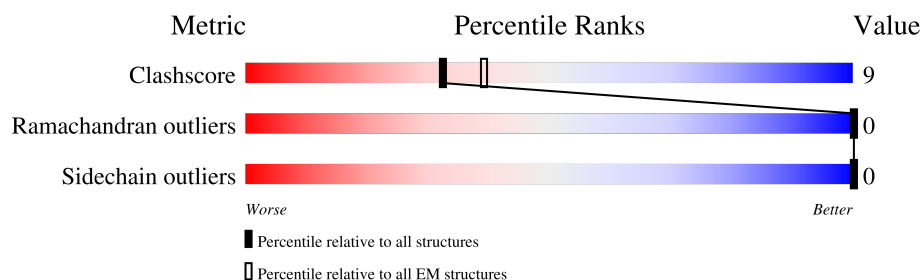
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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	7587 (3.50 - 4.50)

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	424	 64% 17% 19%
1	B	424	 64% 15% 21%
1	C	424	 66% 13% 21%
1	D	424	 65% 14% 21%

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Mol	Chain	Length	Quality of chain
2	E	1545	23% 83% 8% 8%
2	G	1545	12% 87%
3	F	2	50% 50%
3	N	2	100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19977 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 ATP-sensitive inward rectifier potassium channel 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	345	Total	C	N	O	S	0	0
			2448	1571	439	425	13		
1	B	337	Total	C	N	O	S	0	0
			2426	1552	433	426	15		
1	C	337	Total	C	N	O	S	0	0
			2407	1548	430	415	14		
1	D	337	Total	C	N	O	S	0	0
			2423	1555	429	426	13		

- Molecule 2 is a protein called Isoform SUR2B of ATP-binding cassette sub-family C member 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1420	Total	C	N	O	S	0	0
			8338	5228	1549	1546	15		
2	G	205	Total	C	N	O	S	0	0
			1261	799	231	226	5		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

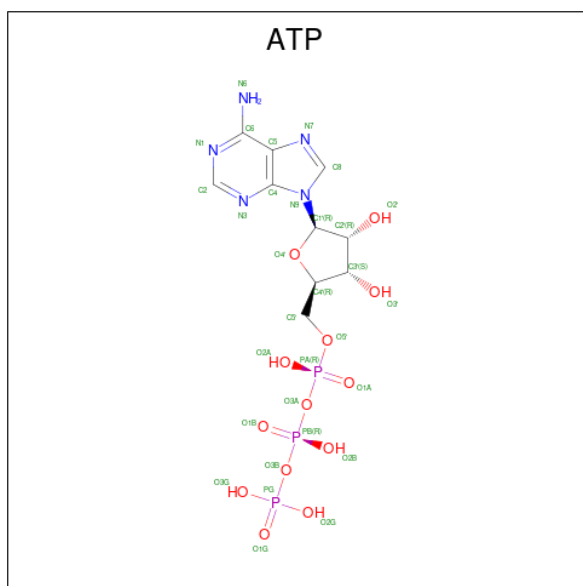


Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

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

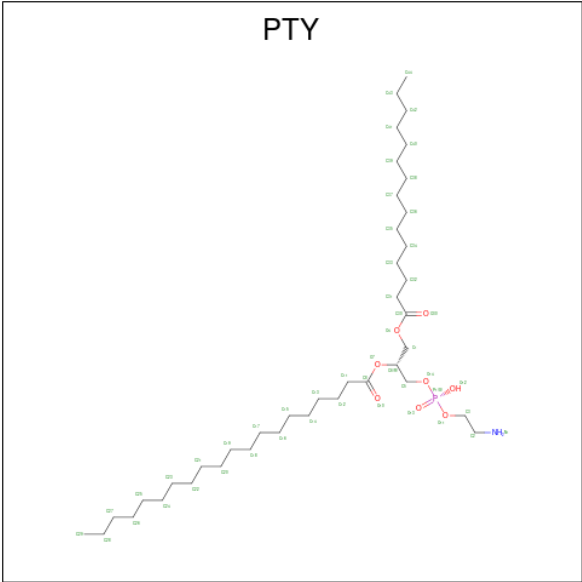
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	K	0
			2	2	

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



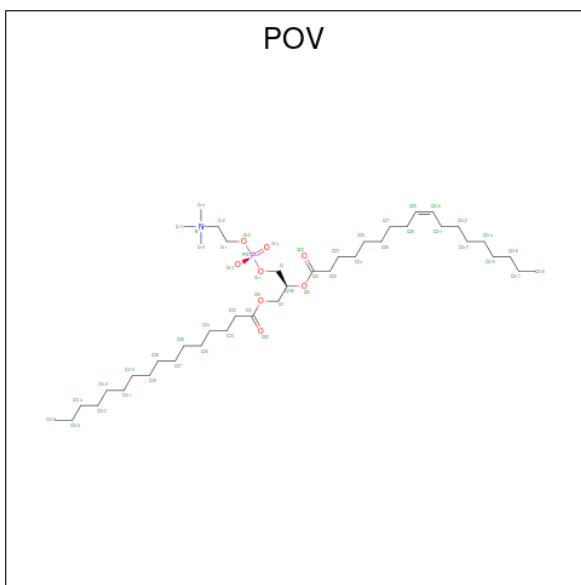
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



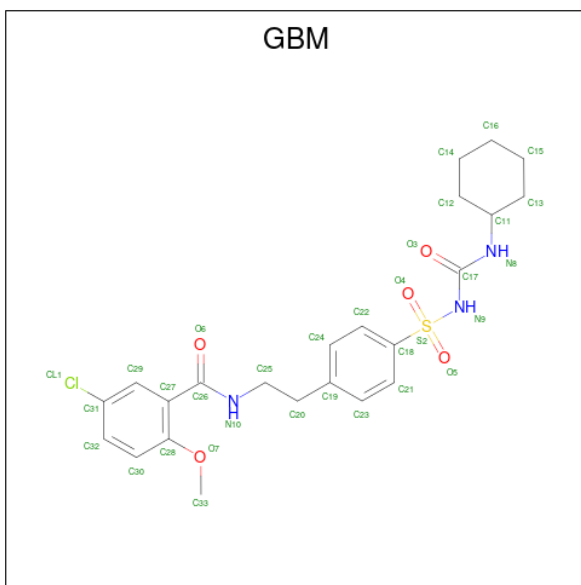
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	D	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	E	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	D	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 8 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxy benzamide (CCD ID: GBM) (formula: $C_{23}H_{28}ClN_3O_5S$) (labeled as "Ligand of Interest" by depositor).

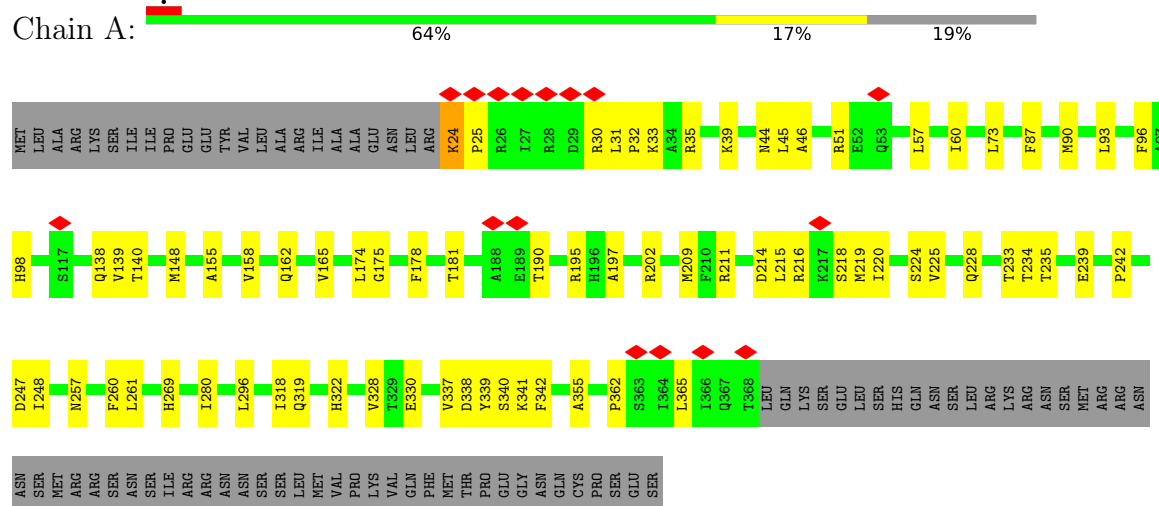


Mol	Chain	Residues	Atoms						AltConf
8	E	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	

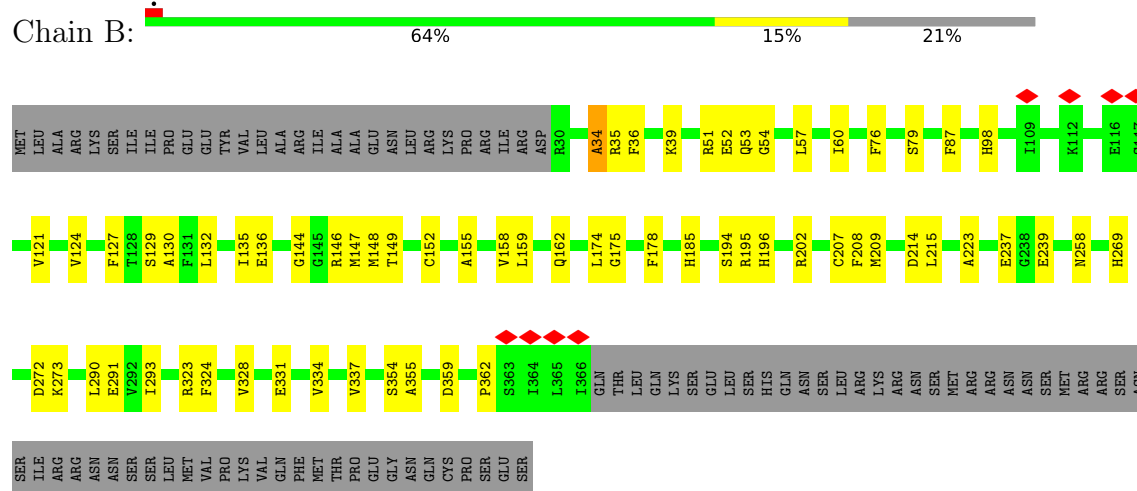
3 Residue-property plots

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: ATP-sensitive inward rectifier potassium channel 8

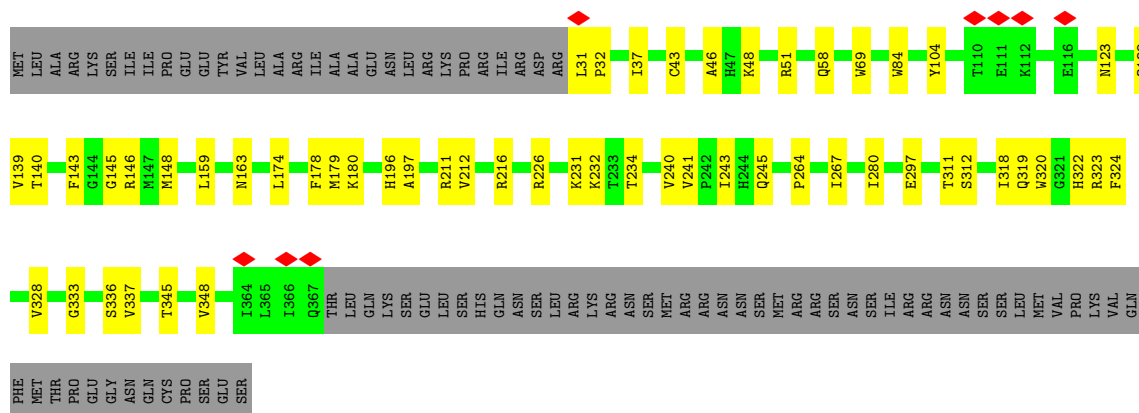


- Molecule 1: ATP-sensitive inward rectifier potassium channel 8



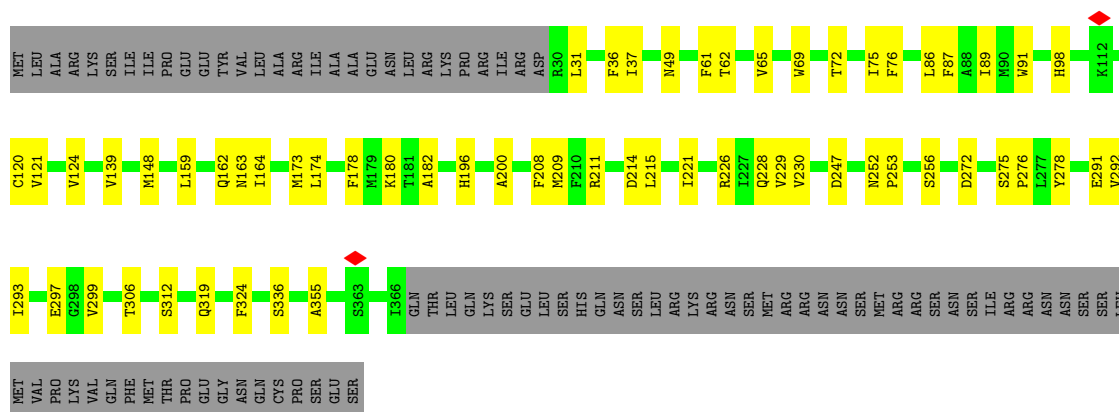
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8





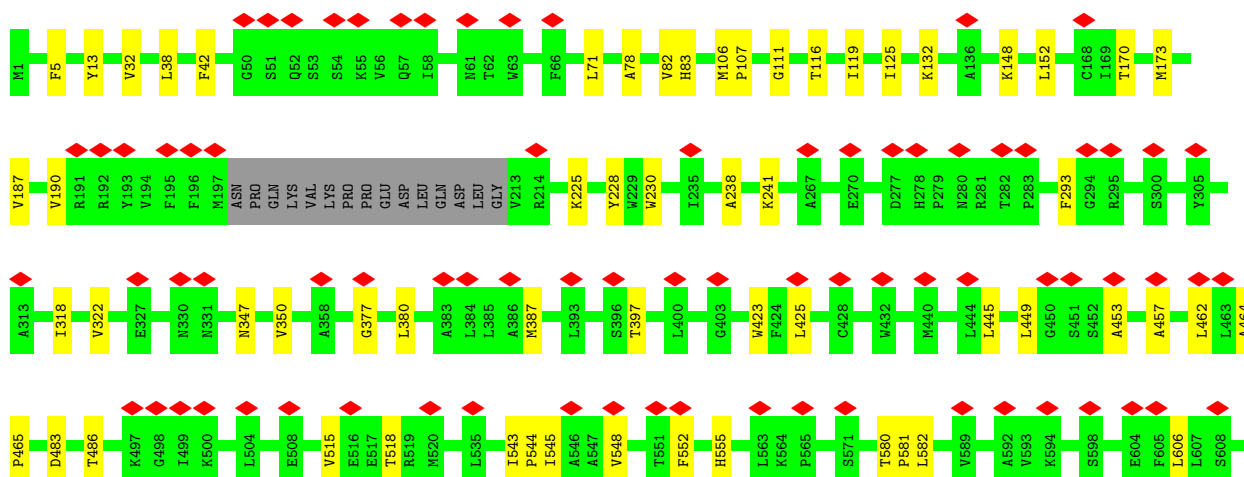
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8

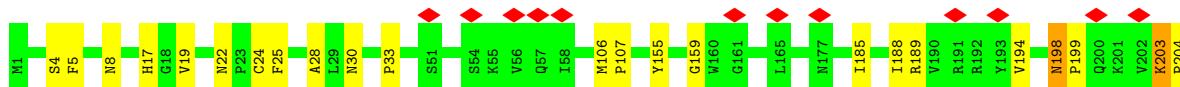
Chain D: 65% 14% 21%



- Molecule 2: Isoform SUR2B of ATP-binding cassette sub-family C member 9

Chain E: 23% 83% 8% 8%







PRO
GLU
CYS
LYS
CYS
THR
ASP
ASP
ARG
LEU
TRP
GLU
ALA
LEU
GLU
ILE
ALA
GLN
LEU
LYS
ASN
MET
VAL
VAL
LYS
SER
SER
LEU
PRO
GLY
GLY
LEU
ASP
ALA
THR
THR
THR
GLU
GLY
GLY
ASN
GLU
PHE
SER
SER
VAL
GLY
GLN
ARG
GLN
LEU
PHE
CYS
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ALA
ALA
PHE
VAL
ARG
LYS
SER
SER

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VAL
PHE
ALA
PHE
SER
VAL
ARG
ALA
ASP
MET

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

50%

50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.366	Depositor
Minimum map value	-10.130	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	122.322, 161.994, 155.382	wwPDB
Map dimensions	74, 98, 94	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.653, 1.653, 1.653	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, POV, K, ATP, NAG, GBM

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	0/2499	0.48	3/3419 (0.1%)
1	B	0.25	0/2476	0.44	1/3377 (0.0%)
1	C	0.27	0/2456	0.42	0/3358
1	D	0.24	0/2472	0.42	2/3374 (0.1%)
2	E	0.21	0/8476	0.43	5/11747 (0.0%)
2	G	0.41	0/1290	0.76	8/1784 (0.4%)
All	All	0.25	0/19669	0.46	19/27059 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	203	LYS	CA-C-N	10.43	131.12	120.38
2	G	203	LYS	C-N-CA	10.43	131.12	120.38
2	E	902	LEU	N-CA-C	8.76	120.91	111.36
2	G	19	VAL	N-CA-C	7.88	118.67	110.72
2	G	189	ARG	N-CA-C	7.71	119.32	111.07
2	G	198	ASN	CA-C-N	7.58	127.56	119.76
2	G	198	ASN	C-N-CA	7.58	127.56	119.76
2	E	241	LYS	CA-C-N	6.89	127.06	120.31
2	E	241	LYS	C-N-CA	6.89	127.06	120.31
1	A	24	LYS	CA-C-N	6.64	126.58	119.28
1	A	24	LYS	C-N-CA	6.64	126.58	119.28
1	A	30	ARG	N-CA-C	6.61	118.48	111.28
1	B	34	ALA	N-CA-C	6.51	119.42	110.24
2	E	238	ALA	N-CA-C	6.40	117.92	111.07
1	D	31	LEU	CA-C-N	6.03	126.48	120.52
1	D	31	LEU	C-N-CA	6.03	126.48	120.52
2	E	225	LYS	N-CA-C	-5.70	101.21	109.59
2	G	194	VAL	N-CA-C	5.45	120.68	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	17	HIS	N-CA-C	5.32	116.76	111.07

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	2448	0	2219	61	0
1	B	2426	0	2213	64	0
1	C	2407	0	2238	59	0
1	D	2423	0	2234	50	0
2	E	8338	0	5692	94	0
2	G	1261	0	895	10	0
3	F	28	0	25	1	0
3	N	28	0	25	0	0
4	A	2	0	0	0	0
5	A	31	0	12	1	0
5	B	62	0	24	6	0
5	C	31	0	12	2	0
5	E	31	0	12	0	0
6	A	128	0	148	2	0
6	C	64	0	74	6	0
6	D	32	0	37	0	0
6	E	96	0	111	1	0
7	B	36	0	45	0	0
7	C	36	0	45	1	0
7	D	36	0	45	1	0
8	E	33	0	28	5	0
All	All	19977	0	16134	308	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 9.

All (308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ALA:HB2	1:C:333:GLY:O	1.37	1.25
1:B:35:ARG:NH1	1:B:39:LYS:HG2	1.61	1.12
2:E:230:TRP:CH2	2:E:1210:ALA:CB	2.35	1.09
1:C:31:LEU:CB	1:C:32:PRO:HD2	1.82	1.08
1:C:31:LEU:CB	1:C:32:PRO:CD	2.34	1.06
1:D:196:HIS:NE2	1:D:319:GLN:OE1	1.86	1.06
1:B:34:ALA:CB	1:C:333:GLY:O	2.05	1.05
1:B:35:ARG:HH12	1:B:39:LYS:CG	1.74	1.00
1:D:196:HIS:CD2	1:D:319:GLN:OE1	2.13	1.00
2:E:230:TRP:CZ2	2:E:1210:ALA:CB	2.50	0.94
1:B:35:ARG:HH12	1:B:39:LYS:HG2	0.79	0.93
1:A:248:ILE:CB	1:A:269:HIS:HE1	1.89	0.86
1:B:208:PHE:HB3	1:B:269:HIS:HB3	1.57	0.86
1:B:34:ALA:HB2	1:C:333:GLY:C	2.01	0.84
2:E:230:TRP:CH2	2:E:1210:ALA:HB2	2.11	0.84
1:D:196:HIS:CD2	1:D:319:GLN:CD	2.57	0.82
1:D:196:HIS:HD2	1:D:319:GLN:HG3	1.44	0.81
1:B:148:MET:HE1	1:B:159:LEU:HD22	1.62	0.81
2:E:230:TRP:CZ2	2:E:1210:ALA:HB1	2.15	0.81
2:E:552:PHE:O	2:E:555:HIS:HB3	1.80	0.80
2:E:230:TRP:CZ2	2:E:1210:ALA:HB2	2.16	0.77
1:A:139:VAL:HG12	1:A:139:VAL:O	1.84	0.77
1:A:248:ILE:CB	1:A:269:HIS:CE1	2.68	0.77
1:C:241:VAL:HG12	1:C:243:ILE:O	1.87	0.75
2:E:377:GLY:HA2	2:E:425:LEU:HD23	1.67	0.75
2:E:230:TRP:CH2	2:E:1210:ALA:HB3	2.22	0.73
2:E:1213:ARG:NH1	8:E:1602:GBM:O5	2.22	0.70
1:D:196:HIS:CD2	1:D:319:GLN:HG3	2.27	0.69
2:G:4:SER:OG	2:G:8:ASN:N	2.26	0.69
1:A:328:VAL:HG22	1:A:337:VAL:HG22	1.75	0.68
2:E:230:TRP:HH2	2:E:1210:ALA:CB	2.04	0.67
1:C:84:TRP:HE1	1:C:138:GLN:HG2	1.60	0.67
1:C:174:LEU:HD23	1:D:174:LEU:HD11	1.76	0.66
1:B:57:LEU:O	1:B:60:ILE:HG22	1.96	0.66
1:D:163:ASN:HD22	1:D:163:ASN:C	2.03	0.65
1:D:230:VAL:HB	1:D:291:GLU:HB3	1.78	0.65
1:C:226:ARG:NH1	1:C:297:GLU:OE2	2.30	0.65
1:D:196:HIS:NE2	1:D:319:GLN:CD	2.56	0.64
1:C:69:TRP:NE1	1:C:180:LYS:HG2	2.13	0.64
2:E:707:LYS:NZ	2:E:833:ASP:OD2	2.27	0.64
2:E:464:ALA:HB2	2:E:582:LEU:HD23	1.80	0.64
1:D:196:HIS:HD2	1:D:319:GLN:CG	2.10	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:515:VAL:O	2:E:518:THR:HB	1.98	0.63
1:B:239:GLU:OE2	1:C:323:ARG:NE	2.32	0.63
1:D:36:PHE:HD1	1:D:37:ILE:HG13	1.64	0.63
2:E:1145:ILE:HA	2:E:1148:TYR:CD2	2.34	0.63
1:B:359:ASP:HA	1:B:362:PRO:HB3	1.82	0.62
1:A:24:LYS:CB	1:A:25:PRO:CD	2.78	0.62
1:B:57:LEU:HD12	6:C:502:PTY:HC11	1.81	0.62
1:D:299:VAL:HG12	1:D:306:THR:HA	1.81	0.62
1:B:202:ARG:NE	1:B:209:MET:SD	2.73	0.62
1:D:196:HIS:CD2	1:D:319:GLN:CG	2.83	0.62
1:C:328:VAL:HG22	1:C:337:VAL:HG22	1.81	0.62
2:E:1209:SER:HB2	8:E:1602:GBM:H8	1.82	0.61
3:F:2:NAG:N2	3:F:2:NAG:O4	2.34	0.61
1:A:51:ARG:NH2	5:B:501:ATP:N7	2.43	0.61
1:C:196:HIS:ND1	1:C:319:GLN:OE1	2.34	0.61
1:D:226:ARG:NH2	1:D:297:GLU:OE2	2.33	0.61
1:A:175:GLY:HA2	1:B:178:PHE:HD1	1.65	0.60
1:A:228:GLN:NE2	1:A:247:ASP:OD1	2.34	0.60
1:D:293:ILE:HG22	1:D:312:SER:HB2	1.84	0.59
1:A:174:LEU:HD23	1:B:174:LEU:HD11	1.84	0.59
2:G:155:TYR:O	2:G:159:GLY:N	2.35	0.59
1:B:98:HIS:O	1:B:98:HIS:ND1	2.29	0.59
2:E:1389:LEU:HD23	2:E:1393:ILE:H	1.66	0.58
1:C:216:ARG:H	1:C:216:ARG:HD3	1.69	0.58
1:B:354:SER:OG	1:B:355:ALA:N	2.37	0.58
2:E:1540:PHE:HA	2:E:1543:ALA:HB3	1.86	0.58
1:B:51:ARG:H	5:B:502:ATP:HN62	1.52	0.58
1:C:163:ASN:HD21	1:D:139:VAL:HG21	1.69	0.57
1:C:231:LYS:NZ	1:C:232:LYS:O	2.38	0.56
1:B:272:ASP:OD1	1:B:273:LYS:N	2.38	0.56
2:E:1536:VAL:O	2:E:1540:PHE:N	2.29	0.56
2:E:1104:PRO:HG2	2:E:1105:PRO:HD3	1.87	0.56
1:A:148:MET:O	1:B:146:ARG:NH2	2.30	0.56
2:G:185:ILE:O	2:G:188:ILE:CB	2.53	0.56
1:A:202:ARG:HH21	1:A:209:MET:HE2	1.71	0.55
6:C:502:PTY:N1	6:C:502:PTY:O12	2.38	0.55
2:E:1131:PHE:HA	2:E:1134:ALA:HB3	1.88	0.55
2:E:387:MET:HE3	2:E:606:LEU:HD23	1.88	0.55
1:C:178:PHE:HD2	1:D:178:PHE:CE1	2.24	0.55
1:B:152:CYS:SG	1:B:155:ALA:CB	2.95	0.55
2:E:293:PHE:HZ	2:E:380:LEU:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1603:PTY:H311	6:E:1603:PTY:H141	1.90	0.54
1:C:84:TRP:NE1	1:C:138:GLN:HG2	2.22	0.54
1:A:31:LEU:N	1:A:32:PRO:HD2	2.22	0.54
1:B:207:CYS:SG	1:B:208:PHE:N	2.81	0.54
1:C:320:TRP:O	1:C:322:HIS:ND1	2.37	0.54
1:A:224:SER:OG	1:A:257:ASN:ND2	2.41	0.54
2:E:78:ALA:O	2:E:82:VAL:HG13	2.07	0.54
2:E:749:ALA:HB3	2:E:829:VAL:HA	1.90	0.54
1:D:221:ILE:HB	1:D:299:VAL:HG23	1.91	0.53
2:E:293:PHE:CZ	2:E:380:LEU:HA	2.43	0.53
1:A:225:VAL:HG12	1:A:296:LEU:HB2	1.90	0.53
1:A:362:PRO:HD2	1:A:365:LEU:HA	1.90	0.53
2:E:230:TRP:CH2	2:E:1210:ALA:HB1	2.36	0.53
2:E:545:ILE:O	2:E:548:VAL:HG12	2.08	0.53
1:A:338:ASP:OD1	1:A:341:LYS:N	2.35	0.53
2:E:228:TYR:HB2	2:E:1214:TRP:HD1	1.73	0.53
1:C:69:TRP:HE3	6:C:502:PTY:HC51	1.73	0.53
1:D:86:LEU:O	1:D:89:ILE:HG22	2.08	0.53
2:E:187:VAL:O	2:E:190:VAL:HG12	2.08	0.53
1:B:195:ARG:HH21	5:B:501:ATP:PG	2.31	0.53
1:C:46:ALA:HB3	1:D:336:SER:HA	1.91	0.53
1:B:237:GLU:OE1	1:C:323:ARG:NH2	2.42	0.53
1:C:58:GLN:OE1	6:C:503:PTY:N1	2.39	0.53
1:A:139:VAL:O	1:A:139:VAL:CG1	2.53	0.53
1:B:195:ARG:NE	5:B:501:ATP:O1B	2.42	0.52
2:E:858:ASP:OD1	2:E:859:LYS:N	2.35	0.52
2:E:1157:GLN:O	2:E:1161:ASP:N	2.39	0.52
1:B:147:MET:SD	1:C:145:GLY:HA3	2.49	0.52
2:E:230:TRP:HH2	2:E:1210:ALA:HB2	1.68	0.52
1:C:324:PHE:HA	1:C:345:THR:HG22	1.91	0.52
1:B:214:ASP:OD1	1:B:215:LEU:N	2.43	0.51
1:A:197:ALA:HB3	1:A:318:ILE:HG23	1.91	0.51
1:D:214:ASP:OD1	1:D:215:LEU:N	2.43	0.51
1:B:185:HIS:O	1:B:185:HIS:ND1	2.43	0.51
1:C:179:MET:HE3	1:D:182:ALA:HA	1.92	0.51
2:G:198:ASN:N	2:G:199:PRO:CD	2.73	0.51
2:E:1163:THR:O	2:E:1201:ASN:ND2	2.44	0.51
1:D:98:HIS:ND1	1:D:120:CYS:HB2	2.25	0.51
2:E:148:LYS:HZ3	2:E:173:MET:HG2	1.76	0.51
2:E:1516:LYS:N	2:E:1519:ASN:O	2.38	0.51
1:B:175:GLY:HA2	1:C:178:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:THR:HG22	1:C:240:VAL:HG12	1.93	0.51
1:B:34:ALA:CB	1:C:333:GLY:C	2.72	0.50
2:E:818:VAL:O	2:E:822:LEU:HG	2.11	0.50
1:A:175:GLY:HA2	1:B:178:PHE:CD1	2.45	0.50
2:E:1490:ALA:O	2:E:1494:ARG:N	2.44	0.50
1:A:51:ARG:HB2	5:B:501:ATP:C6	2.46	0.50
2:E:1227:VAL:HG22	2:E:1251:ALA:HB1	1.92	0.50
1:A:138:GLN:HB2	1:A:162:GLN:HE21	1.77	0.50
1:B:144:GLY:HA3	1:C:143:PHE:O	2.11	0.50
1:B:178:PHE:CD2	1:C:178:PHE:CZ	2.99	0.50
2:E:148:LYS:NZ	2:E:173:MET:HG2	2.27	0.50
2:E:462:LEU:C	2:E:465:PRO:HD2	2.37	0.50
1:C:31:LEU:CB	1:C:32:PRO:HD3	2.37	0.49
1:D:228:GLN:NE2	1:D:247:ASP:OD1	2.45	0.49
1:A:178:PHE:CD2	1:B:178:PHE:CZ	2.99	0.49
1:A:24:LYS:CB	1:A:25:PRO:HD3	2.43	0.49
1:A:219:MET:SD	1:A:220:ILE:N	2.80	0.49
1:D:76:PHE:CZ	1:D:173:MET:HB3	2.48	0.49
1:B:152:CYS:SG	1:B:155:ALA:HB3	2.52	0.49
1:C:51:ARG:HB2	5:C:501:ATP:N1	2.28	0.49
1:D:272:ASP:H	1:D:275:SER:HB3	1.78	0.49
2:E:1145:ILE:HA	2:E:1148:TYR:HD2	1.77	0.49
2:E:1515:MET:HA	2:E:1520:ILE:HA	1.95	0.49
2:E:38:LEU:HD11	2:E:42:PHE:CE2	2.48	0.49
2:E:786:LEU:O	2:E:790:ILE:N	2.42	0.49
1:C:241:VAL:CG1	1:C:243:ILE:O	2.59	0.48
2:E:1490:ALA:HA	2:E:1494:ARG:H	1.77	0.48
1:B:152:CYS:SG	1:B:155:ALA:HB2	2.53	0.48
2:E:423:TRP:HZ3	8:E:1602:GBM:H19	1.78	0.48
2:E:762:VAL:O	2:E:766:ILE:HG13	2.13	0.48
1:A:24:LYS:N	1:A:25:PRO:HD2	2.28	0.48
1:B:132:LEU:HA	1:B:135:ILE:HG22	1.96	0.48
2:E:83:HIS:HE1	2:E:111:GLY:HA3	1.78	0.48
2:E:318:ILE:O	2:E:322:VAL:HG23	2.12	0.48
2:G:22:ASN:OD1	2:G:25:PHE:N	2.29	0.48
1:A:98:HIS:O	1:A:98:HIS:ND1	2.47	0.48
1:B:178:PHE:HD2	1:C:178:PHE:CZ	2.32	0.48
6:A:507:PTY:HC52	2:E:5:PHE:HB2	1.96	0.48
2:E:771:SER:O	2:E:823:TYR:OH	2.23	0.48
2:E:677:TRP:CG	2:E:677:TRP:O	2.67	0.47
1:A:330:GLU:OE1	1:A:330:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:HD2	1:B:178:PHE:CZ	2.33	0.47
1:D:229:VAL:HG11	1:D:276:PRO:HG3	1.96	0.47
2:E:543:ILE:N	2:E:544:PRO:HD2	2.30	0.47
2:E:710:LEU:O	2:E:714:ILE:HG12	2.15	0.47
1:B:121:VAL:O	1:B:124:VAL:HG12	2.15	0.47
1:A:190:THR:OG1	1:A:216:ARG:NH1	2.48	0.47
1:C:178:PHE:HD2	1:D:178:PHE:CZ	2.33	0.47
1:A:138:GLN:HB2	1:A:162:GLN:NE2	2.28	0.47
1:B:155:ALA:HA	1:B:158:VAL:HG22	1.96	0.47
1:B:223:ALA:O	1:B:258:ASN:HA	2.14	0.47
1:A:45:LEU:HG	1:A:46:ALA:H	1.80	0.46
1:B:290:LEU:HG	1:B:291:GLU:H	1.79	0.46
1:B:127:PHE:O	1:B:130:ALA:N	2.48	0.46
1:B:136:GLU:OE2	1:B:146:ARG:NH1	2.49	0.46
1:B:149:THR:HA	1:C:146:ARG:NH2	2.30	0.46
2:E:580:THR:HB	2:E:581:PRO:HD3	1.98	0.46
2:E:751:ALA:HB2	2:E:821:ALA:HB2	1.97	0.46
2:E:1389:LEU:HB3	2:E:1392:PRO:HA	1.97	0.46
2:E:347:ASN:HB3	2:E:350:VAL:HG22	1.97	0.46
1:D:211:ARG:CZ	1:D:324:PHE:HD2	2.29	0.46
1:D:121:VAL:O	1:D:124:VAL:HG12	2.16	0.46
1:C:104:TYR:HE2	1:C:123:ASN:HA	1.81	0.45
2:E:397:THR:HA	2:E:1178:LEU:O	2.16	0.45
2:E:974:PRO:HB2	2:E:978:CYS:HG	1.81	0.45
1:A:338:ASP:OD1	1:A:340:SER:N	2.49	0.45
1:D:62:THR:O	1:D:65:VAL:HG12	2.17	0.45
1:A:195:ARG:NH2	5:A:503:ATP:O2G	2.50	0.45
8:E:1602:GBM:H20	8:E:1602:GBM:O7	2.17	0.45
1:A:242:PRO:HG2	1:B:328:VAL:HB	1.98	0.45
1:B:328:VAL:HG22	1:B:337:VAL:HG12	1.98	0.45
1:B:331:GLU:HB2	1:B:334:VAL:O	2.16	0.45
2:E:116:THR:O	2:E:119:ILE:HG22	2.16	0.45
2:E:1102:HIS:O	2:E:1105:PRO:HD2	2.16	0.45
1:D:91:TRP:CH2	1:D:148:MET:HE1	2.52	0.45
1:B:34:ALA:HB1	1:C:333:GLY:O	2.06	0.45
1:A:280:ILE:O	1:A:355:ALA:HB3	2.17	0.45
1:D:163:ASN:C	1:D:163:ASN:ND2	2.74	0.45
2:E:83:HIS:CE1	2:E:111:GLY:HA3	2.52	0.45
2:E:979:TRP:O	2:E:983:THR:OG1	2.25	0.45
1:A:31:LEU:N	1:A:32:PRO:CD	2.79	0.45
1:B:57:LEU:HB2	6:C:502:PTY:HC6	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:MET:HE3	1:D:159:LEU:HD22	1.98	0.45
2:E:71:LEU:HD12	2:E:71:LEU:HA	1.80	0.45
2:E:1271:GLN:O	2:E:1275:VAL:HG23	2.17	0.45
1:A:44:ASN:O	1:A:44:ASN:ND2	2.51	0.44
2:G:203:LYS:HA	2:G:204:PRO:HD3	1.56	0.44
1:A:93:LEU:HD11	2:E:32:VAL:HG21	1.99	0.44
1:C:163:ASN:HD21	1:D:139:VAL:HG11	1.82	0.44
2:E:38:LEU:HD11	2:E:42:PHE:HE2	1.80	0.44
2:E:119:ILE:HD12	2:E:119:ILE:HA	1.85	0.44
1:B:323:ARG:HG2	1:B:324:PHE:N	2.32	0.44
2:E:106:MET:N	2:E:107:PRO:HD2	2.33	0.44
1:B:194:SER:OG	1:B:196:HIS:O	2.30	0.44
1:C:212:VAL:O	1:C:264:PRO:HA	2.17	0.44
1:A:214:ASP:OD1	1:A:215:LEU:N	2.50	0.43
6:A:507:PTY:HC12	2:E:5:PHE:HB2	1.99	0.43
2:G:30:ASN:O	2:G:33:PRO:HD2	2.18	0.43
1:C:267:ILE:H	1:C:267:ILE:HG12	1.64	0.43
1:A:216:ARG:HD3	1:A:218:SER:HB3	1.99	0.43
1:A:319:GLN:HB2	1:A:322:HIS:CE1	2.53	0.43
1:C:148:MET:HE3	1:C:159:LEU:HD22	2.00	0.43
1:C:180:LYS:HB2	1:C:180:LYS:HE2	1.79	0.43
1:C:280:ILE:HD12	1:C:280:ILE:HA	1.89	0.43
2:G:5:PHE:HE2	2:G:28:ALA:HB2	1.83	0.43
1:C:311:THR:OG1	1:C:312:SER:N	2.51	0.43
2:E:132:LYS:HE3	2:E:132:LYS:HB3	1.91	0.43
1:D:87:PHE:CZ	1:D:162:GLN:HA	2.54	0.43
2:E:445:LEU:O	2:E:449:LEU:CB	2.67	0.43
1:C:69:TRP:CZ3	6:C:502:PTY:H122	2.53	0.43
1:D:200:ALA:HB3	1:D:209:MET:HE3	2.00	0.43
2:E:228:TYR:HB2	2:E:1214:TRP:CD1	2.53	0.43
1:B:53:GLN:OE1	1:B:53:GLN:N	2.52	0.42
2:E:669:LYS:O	2:E:726:TYR:N	2.32	0.42
2:E:1317:TYR:C	2:E:1323:PRO:HB3	2.44	0.42
2:E:1514:VAL:HG12	2:E:1530:LEU:HA	2.01	0.42
1:C:178:PHE:CD2	1:D:178:PHE:CZ	3.07	0.42
1:C:328:VAL:HA	1:C:336:SER:O	2.19	0.42
1:D:76:PHE:CE2	1:D:173:MET:HB3	2.54	0.42
2:E:1104:PRO:CG	2:E:1105:PRO:HD3	2.49	0.42
1:D:278:TYR:O	1:D:355:ALA:HB3	2.20	0.42
1:A:260:PHE:HD1	1:A:261:LEU:H	1.67	0.42
2:E:1310:ILE:HA	2:E:1366:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:PHE:O	1:B:79:SER:OG	2.29	0.42
1:B:148:MET:HE2	1:B:148:MET:HB3	1.85	0.42
1:C:48:LYS:HE2	1:C:48:LYS:HB2	1.71	0.42
1:D:69:TRP:CD1	1:D:180:LYS:HZ1	2.37	0.42
1:D:72:THR:HA	1:D:75:ILE:HG22	2.00	0.42
2:G:22:ASN:OD1	2:G:24:CYS:N	2.53	0.42
1:A:57:LEU:O	1:A:60:ILE:HG22	2.19	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.87	0.42
1:C:211:ARG:HH21	1:C:324:PHE:HD2	1.67	0.42
1:A:33:LYS:HD3	1:A:33:LYS:HA	1.89	0.42
1:B:34:ALA:HB2	1:C:333:GLY:CA	2.49	0.42
1:D:252:ASN:HA	1:D:253:PRO:HD3	1.89	0.42
1:B:87:PHE:CZ	1:B:162:GLN:HA	2.55	0.42
1:A:242:PRO:HG3	1:B:328:VAL:O	2.20	0.41
1:C:323:ARG:NH1	1:C:348:VAL:HG21	2.35	0.41
2:G:106:MET:N	2:G:107:PRO:HD2	2.35	0.41
2:E:148:LYS:HA	2:E:148:LYS:HD3	1.86	0.41
2:E:1395:PHE:O	2:E:1441:GLY:N	2.49	0.41
1:A:178:PHE:CZ	1:D:178:PHE:HD2	2.37	0.41
1:A:233:THR:OG1	1:A:234:THR:N	2.53	0.41
2:E:152:LEU:HD13	2:E:170:THR:HG22	2.03	0.41
2:E:1490:ALA:CA	2:E:1494:ARG:H	2.33	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.90	0.41
1:A:138:GLN:OE1	1:A:162:GLN:NE2	2.53	0.41
1:A:235:THR:OG1	1:A:239:GLU:O	2.25	0.41
2:E:125:ILE:HD13	2:E:125:ILE:HA	1.88	0.41
2:E:1116:LEU:HD23	2:E:1116:LEU:HA	1.87	0.41
1:A:155:ALA:O	1:A:158:VAL:HG12	2.20	0.41
1:C:51:ARG:NH1	5:C:501:ATP:N7	2.68	0.41
1:C:197:ALA:HB3	1:C:318:ILE:HG23	2.02	0.41
1:D:164:ILE:HD13	1:D:164:ILE:HA	1.95	0.41
2:E:974:PRO:HB2	2:E:978:CYS:SG	2.60	0.41
1:A:90:MET:HE3	1:A:90:MET:HB2	2.00	0.41
2:E:1465:ILE:HD13	2:E:1465:ILE:HA	1.97	0.41
1:A:96:PHE:HE1	2:E:13:TYR:HB2	1.85	0.41
1:B:132:LEU:O	1:B:135:ILE:HG22	2.20	0.41
1:A:87:PHE:CE2	1:A:165:VAL:HG11	2.55	0.41
1:B:51:ARG:N	5:B:502:ATP:HN62	2.17	0.41
1:D:208:PHE:CE2	1:D:292:VAL:HG11	2.56	0.41
1:A:139:VAL:O	1:A:140:THR:OG1	2.38	0.41
1:B:52:GLU:HG3	1:B:54:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:900:VAL:C	2:E:902:LEU:N	2.79	0.41
1:A:35:ARG:NH2	1:A:39:LYS:HB2	2.36	0.40
1:A:211:ARG:HG2	1:A:342:PHE:CZ	2.55	0.40
1:B:124:VAL:HA	1:B:129:SER:OG	2.21	0.40
1:C:37:ILE:HG22	1:C:43:CYS:HA	2.03	0.40
1:C:139:VAL:O	1:C:140:THR:OG1	2.39	0.40
2:E:1397:GLY:HA3	2:E:1437:THR:HG22	2.03	0.40
1:A:181:THR:OG1	1:D:61:PHE:HZ	2.04	0.40
2:E:1103:ILE:N	2:E:1104:PRO:HD2	2.37	0.40
1:A:178:PHE:CE1	1:D:178:PHE:HD2	2.40	0.40
1:B:36:PHE:HD2	1:B:293:ILE:HD11	1.87	0.40
1:C:320:TRP:C	1:C:322:HIS:H	2.29	0.40
7:C:504:POV:H11	7:C:504:POV:H15B	1.88	0.40
1:D:252:ASN:ND2	1:D:256:SER:O	2.55	0.40
2:E:483:ASP:O	2:E:486:THR:OG1	2.30	0.40
1:A:339:TYR:HB2	1:D:49:ASN:O	2.21	0.40
1:C:245:GLN:N	1:C:245:GLN:OE1	2.55	0.40
7:D:801:POV:H13B	7:D:801:POV:H11	1.85	0.40
2:E:453:ALA:O	2:E:457:ALA:N	2.55	0.40
2:E:1205:TYR:CZ	8:E:1602:GBM:H13	2.56	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	343/424 (81%)	317 (92%)	26 (8%)	0	100	100
1	B	335/424 (79%)	300 (90%)	35 (10%)	0	100	100
1	C	335/424 (79%)	305 (91%)	30 (9%)	0	100	100
1	D	335/424 (79%)	304 (91%)	31 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	1408/1545 (91%)	1276 (91%)	132 (9%)	0	100	100
2	G	203/1545 (13%)	191 (94%)	12 (6%)	0	100	100
All	All	2959/4786 (62%)	2693 (91%)	266 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/376 (57%)	213 (100%)	0	100	100
1	B	216/376 (57%)	216 (100%)	0	100	100
1	C	218/376 (58%)	218 (100%)	0	100	100
1	D	218/376 (58%)	218 (100%)	0	100	100
2	E	374/1348 (28%)	374 (100%)	0	100	100
2	G	71/1348 (5%)	71 (100%)	0	100	100
All	All	1310/4200 (31%)	1310 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	163	ASN
1	A	269	HIS
1	C	44	ASN
1	C	163	ASN
1	C	258	ASN
1	D	203	ASN
1	D	288	GLN
2	E	17	HIS

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Mol	Chain	Res	Type
2	E	1501	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 ⓘ

4 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$
3	NAG	F	1	2,3	14,14,15	2.69	8 (57%)	17,19,21	2.01	4 (23%)
3	NAG	F	2	3	14,14,15	2.82	7 (50%)	17,19,21	1.21	1 (5%)
3	NAG	N	1	2,3	14,14,15	2.71	8 (57%)	17,19,21	2.11	3 (17%)
3	NAG	N	2	3	14,14,15	2.77	7 (50%)	17,19,21	1.45	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C5	5.65	1.54	1.43
3	N	2	NAG	O5-C5	5.35	1.53	1.43
3	F	1	NAG	O5-C5	5.30	1.53	1.43
3	N	1	NAG	O5-C5	5.16	1.53	1.43
3	N	2	NAG	C2-N2	4.71	1.54	1.46
3	N	1	NAG	C2-N2	4.17	1.53	1.46
3	F	1	NAG	C2-N2	4.16	1.53	1.46
3	F	2	NAG	C2-N2	4.12	1.53	1.46
3	N	2	NAG	C7-N2	3.89	1.46	1.34
3	F	1	NAG	C7-N2	3.83	1.46	1.34
3	N	1	NAG	C7-N2	3.82	1.46	1.34
3	F	2	NAG	C7-N2	3.71	1.46	1.34
3	F	2	NAG	C6-C5	-3.27	1.40	1.51
3	F	1	NAG	C6-C5	-3.27	1.40	1.51
3	N	1	NAG	C6-C5	-3.24	1.41	1.51
3	N	2	NAG	C6-C5	-3.22	1.41	1.51
3	F	2	NAG	C3-C2	-3.20	1.45	1.52
3	F	2	NAG	O5-C1	3.08	1.48	1.43
3	N	1	NAG	C3-C2	-2.89	1.46	1.52
3	F	1	NAG	C3-C2	-2.62	1.47	1.52
3	N	2	NAG	O5-C1	2.61	1.48	1.43
3	N	2	NAG	C3-C2	-2.52	1.47	1.52
3	F	1	NAG	O5-C1	2.42	1.47	1.43
3	N	1	NAG	C1-C2	-2.14	1.49	1.52
3	N	1	NAG	O5-C1	2.09	1.47	1.43
3	N	1	NAG	O3-C3	2.09	1.48	1.43
3	N	2	NAG	O3-C3	2.08	1.48	1.43
3	F	2	NAG	C8-C7	2.07	1.54	1.50
3	F	1	NAG	O3-C3	2.06	1.48	1.43
3	F	1	NAG	C8-C7	2.02	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C4-C3-C2	5.53	119.13	111.02
3	F	1	NAG	C4-C3-C2	4.54	117.67	111.02
3	N	1	NAG	C3-C4-C5	4.26	117.96	110.23
3	N	2	NAG	C4-C3-C2	3.74	116.49	111.02
3	F	1	NAG	C1-O5-C5	-3.68	107.26	112.19
3	F	2	NAG	C8-C7-N2	2.65	120.51	116.12
3	F	1	NAG	O3-C3-C2	-2.56	104.09	109.40
3	N	2	NAG	C3-C4-C5	2.38	114.55	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C8-C7-N2	2.34	120.00	116.12
3	F	1	NAG	C8-C7-N2	2.12	119.64	116.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

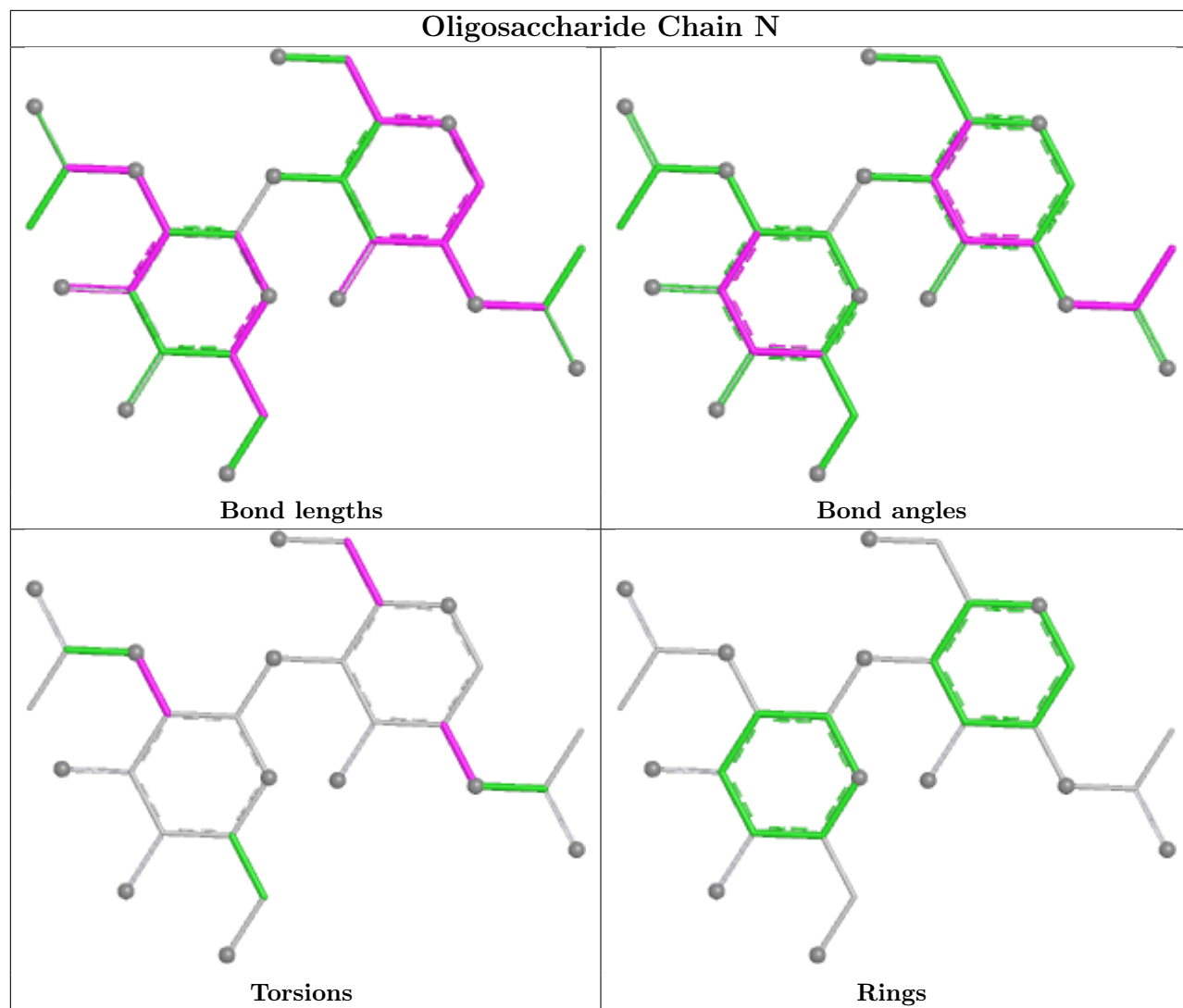
Mol	Chain	Res	Type	Atoms
3	N	2	NAG	C1-C2-N2-C7
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7

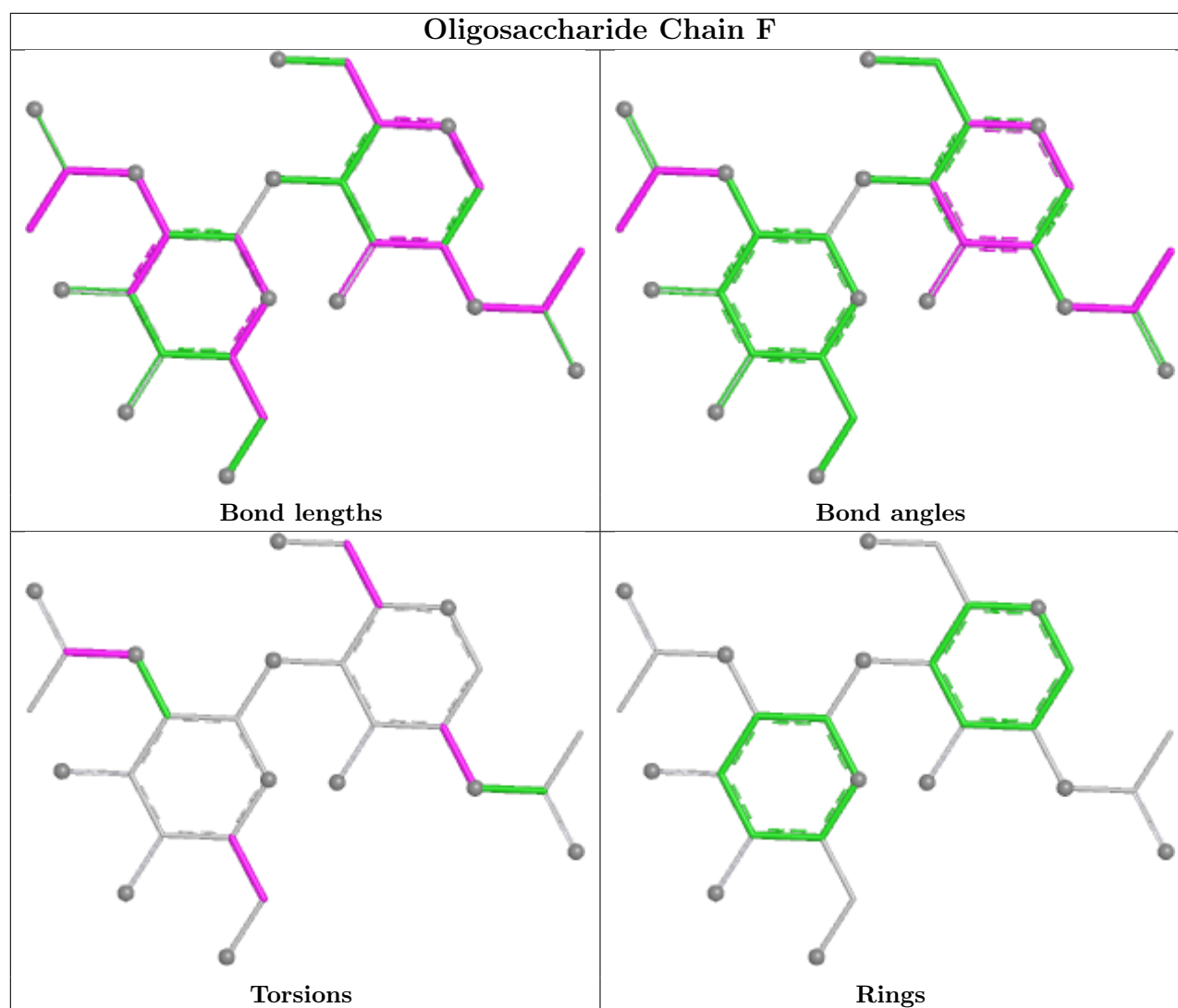
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	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 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z > 2$
8	GBM	E	1602	-	35,35,35	4.82	8 (22%)	48,48,48	1.95	8 (16%)
6	PTY	C	502	-	31,31,49	1.09	4 (12%)	34,36,54	1.08	2 (5%)
5	ATP	B	501	-	32,33,33	1.34	5 (15%)	48,52,52	1.79	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PTY	E	1605	-	31,31,49	1.10	4 (12%)	34,36,54	1.06	2 (5%)
5	ATP	E	1601	-	32,33,33	1.39	4 (12%)	48,52,52	1.76	9 (18%)
7	POV	D	801	-	35,35,51	1.46	4 (11%)	41,43,59	1.15	3 (7%)
6	PTY	C	503	-	31,31,49	1.09	4 (12%)	34,36,54	1.06	2 (5%)
6	PTY	A	505	-	31,31,49	1.10	4 (12%)	34,36,54	1.01	2 (5%)
5	ATP	B	502	-	32,33,33	1.35	5 (15%)	48,52,52	1.75	8 (16%)
6	PTY	A	504	-	31,31,49	1.11	4 (12%)	34,36,54	1.06	2 (5%)
6	PTY	E	1603	-	31,31,49	1.10	4 (12%)	34,36,54	1.07	2 (5%)
7	POV	B	503	-	35,35,51	1.46	4 (11%)	41,43,59	1.19	4 (9%)
5	ATP	C	501	-	32,33,33	1.33	5 (15%)	48,52,52	1.75	10 (20%)
6	PTY	A	506	-	31,31,49	1.11	4 (12%)	34,36,54	1.02	2 (5%)
7	POV	C	504	-	35,35,51	1.46	4 (11%)	41,43,59	1.16	4 (9%)
6	PTY	A	507	-	31,31,49	1.12	3 (9%)	34,36,54	1.11	3 (8%)
6	PTY	E	1604	-	31,31,49	1.09	4 (12%)	34,36,54	1.08	2 (5%)
5	ATP	A	503	-	32,33,33	1.36	5 (15%)	48,52,52	1.72	9 (18%)
6	PTY	D	802	-	31,31,49	1.11	4 (12%)	34,36,54	1.04	2 (5%)

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
8	GBM	E	1602	-	-	13/27/35/35	0/3/3/3
6	PTY	C	502	-	-	18/35/35/53	-
5	ATP	B	501	-	-	5/22/38/38	0/3/3/3
6	PTY	E	1605	-	-	16/35/35/53	-
5	ATP	E	1601	-	-	1/22/38/38	0/3/3/3
7	POV	D	801	-	-	13/39/39/55	-
6	PTY	C	503	-	-	14/35/35/53	-
6	PTY	A	505	-	-	21/35/35/53	-
5	ATP	B	502	-	-	6/22/38/38	0/3/3/3
6	PTY	A	504	-	-	13/35/35/53	-
6	PTY	E	1603	-	-	16/35/35/53	-
7	POV	B	503	-	-	18/39/39/55	-
5	ATP	C	501	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PTY	A	506	-	-	14/35/35/53	-
7	POV	C	504	-	-	17/39/39/55	-
6	PTY	A	507	-	-	15/35/35/53	-
6	PTY	E	1604	-	-	13/35/35/53	-
5	ATP	A	503	-	-	6/22/38/38	0/3/3/3
6	PTY	D	802	-	-	13/35/35/53	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1602	GBM	O4-S2	19.04	1.65	1.43
8	E	1602	GBM	O5-S2	18.91	1.65	1.43
8	E	1602	GBM	C26-N10	5.66	1.46	1.33
5	E	1601	ATP	C5-C4	4.65	1.47	1.39
5	B	501	ATP	C5-C4	4.48	1.47	1.39
5	A	503	ATP	C5-C4	4.44	1.47	1.39
5	C	501	ATP	C5-C4	4.41	1.46	1.39
5	B	502	ATP	C5-C4	4.39	1.46	1.39
7	B	503	POV	C210-C29	3.99	1.54	1.29
7	D	801	POV	C210-C29	3.98	1.54	1.29
7	C	504	POV	C210-C29	3.98	1.54	1.29
8	E	1602	GBM	C18-S2	3.60	1.82	1.76
8	E	1602	GBM	C17-N8	3.44	1.45	1.35
7	B	503	POV	O31-C31	3.12	1.42	1.33
7	C	504	POV	O31-C31	3.05	1.42	1.33
6	A	507	PTY	O7-C6	-3.04	1.39	1.46
7	D	801	POV	O31-C31	3.03	1.42	1.33
7	C	504	POV	O21-C21	2.90	1.42	1.34
6	D	802	PTY	O7-C6	-2.85	1.39	1.46
7	D	801	POV	O21-C2	-2.85	1.39	1.46
7	B	503	POV	O21-C2	-2.84	1.39	1.46
6	A	504	PTY	O7-C6	-2.81	1.40	1.46
7	B	503	POV	O21-C21	2.80	1.42	1.34
7	D	801	POV	O21-C21	2.79	1.42	1.34
6	C	503	PTY	O7-C6	-2.79	1.40	1.46
6	A	505	PTY	O7-C6	-2.78	1.40	1.46
6	A	506	PTY	O7-C6	-2.77	1.40	1.46
6	E	1605	PTY	O7-C6	-2.75	1.40	1.46
8	E	1602	GBM	S2-N9	2.72	1.70	1.64
6	C	502	PTY	O7-C6	-2.71	1.40	1.46
6	E	1603	PTY	O7-C6	-2.70	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1601	ATP	C5-C6	2.66	1.48	1.41
7	C	504	POV	O21-C2	-2.65	1.40	1.46
6	E	1604	PTY	O7-C6	-2.62	1.40	1.46
8	E	1602	GBM	C17-N9	2.58	1.45	1.39
5	A	503	ATP	C5-N7	-2.58	1.34	1.39
5	C	501	ATP	C5-C6	2.56	1.48	1.41
5	B	502	ATP	C5-N7	-2.51	1.34	1.39
5	B	501	ATP	C5-N7	-2.49	1.34	1.39
5	B	502	ATP	C5-C6	2.48	1.47	1.41
5	C	501	ATP	C5-N7	-2.45	1.34	1.39
5	A	503	ATP	C5-C6	2.44	1.47	1.41
6	A	507	PTY	O4-C30	2.43	1.40	1.33
6	E	1605	PTY	O4-C30	2.42	1.40	1.33
6	E	1603	PTY	O4-C30	2.40	1.40	1.33
6	A	505	PTY	O4-C30	2.40	1.40	1.33
6	C	503	PTY	O4-C30	2.39	1.40	1.33
6	C	502	PTY	O4-C30	2.38	1.40	1.33
6	A	506	PTY	O4-C30	2.38	1.40	1.33
6	A	504	PTY	O4-C30	2.37	1.40	1.33
6	E	1604	PTY	O4-C30	2.35	1.40	1.33
6	D	802	PTY	O4-C1	-2.33	1.40	1.45
5	B	501	ATP	C5-C6	2.32	1.47	1.41
6	D	802	PTY	O4-C30	2.31	1.40	1.33
5	E	1601	ATP	C5-N7	-2.29	1.34	1.39
5	C	501	ATP	C8-N7	2.28	1.36	1.31
6	A	504	PTY	O4-C1	-2.28	1.40	1.45
6	A	507	PTY	O4-C1	-2.27	1.40	1.45
6	E	1604	PTY	O4-C1	-2.26	1.40	1.45
6	E	1603	PTY	O4-C1	-2.26	1.40	1.45
5	E	1601	ATP	C8-N7	2.25	1.36	1.31
6	A	506	PTY	O4-C1	-2.24	1.40	1.45
6	A	505	PTY	O4-C1	-2.23	1.40	1.45
6	C	502	PTY	O4-C1	-2.22	1.40	1.45
5	B	501	ATP	C8-N7	2.22	1.35	1.31
6	C	503	PTY	O4-C1	-2.20	1.40	1.45
6	E	1603	PTY	O7-C8	2.19	1.40	1.34
8	E	1602	GBM	O3-C17	-2.19	1.18	1.23
6	E	1604	PTY	O7-C8	2.19	1.40	1.34
6	E	1605	PTY	O4-C1	-2.19	1.40	1.45
5	B	502	ATP	C4-N9	-2.18	1.33	1.37
5	A	503	ATP	C8-N7	2.18	1.35	1.31
6	D	802	PTY	O7-C8	2.17	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	504	PTY	O7-C8	2.16	1.40	1.34
5	A	503	ATP	C4-N9	-2.15	1.33	1.37
5	B	501	ATP	C4-N9	-2.14	1.33	1.37
5	B	502	ATP	C8-N7	2.14	1.35	1.31
6	E	1605	PTY	O7-C8	2.14	1.40	1.34
6	C	502	PTY	O7-C8	2.12	1.40	1.34
5	C	501	ATP	C4-N9	-2.12	1.33	1.37
6	A	506	PTY	O7-C8	2.11	1.40	1.34
6	C	503	PTY	O7-C8	2.09	1.40	1.34
6	A	505	PTY	O7-C8	2.09	1.40	1.34

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	1602	GBM	O5-S2-O4	-8.02	109.79	119.52
5	B	501	ATP	C5-C4-N3	-5.78	118.76	126.72
5	E	1601	ATP	C5-C4-N3	-5.76	118.79	126.72
5	B	502	ATP	C5-C4-N3	-5.73	118.82	126.72
5	C	501	ATP	C5-C4-N3	-5.66	118.93	126.72
5	A	503	ATP	C5-C4-N3	-5.59	119.02	126.72
8	E	1602	GBM	C27-C26-N10	5.01	127.06	117.32
5	B	501	ATP	N3-C4-N9	4.71	135.18	127.17
5	B	502	ATP	N3-C4-N9	4.70	135.16	127.17
5	E	1601	ATP	N3-C4-N9	4.63	135.03	127.17
5	A	503	ATP	N3-C4-N9	4.59	134.98	127.17
5	C	501	ATP	N3-C4-N9	4.43	134.69	127.17
6	E	1604	PTY	O7-C8-C11	4.25	120.67	111.48
7	D	801	POV	O21-C21-C22	4.16	120.49	111.48
6	C	502	PTY	O7-C8-C11	4.13	120.41	111.48
6	E	1605	PTY	O7-C8-C11	4.12	120.39	111.48
7	B	503	POV	O21-C21-C22	4.05	120.25	111.48
6	E	1603	PTY	O7-C8-C11	4.02	120.18	111.48
7	C	504	POV	O21-C21-C22	4.01	120.16	111.48
6	A	506	PTY	O7-C8-C11	4.00	120.13	111.48
6	A	504	PTY	O7-C8-C11	3.99	120.11	111.48
6	D	802	PTY	O7-C8-C11	3.99	120.10	111.48
6	A	507	PTY	O7-C8-C11	3.91	119.94	111.48
6	C	503	PTY	O7-C8-C11	3.85	119.81	111.48
8	E	1602	GBM	O7-C28-C27	3.81	122.10	116.55
6	A	505	PTY	O7-C8-C11	3.80	119.71	111.48
5	E	1601	ATP	C2-N3-C4	3.68	120.83	111.83
5	C	501	ATP	C2-N3-C4	3.68	120.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	1602	GBM	O7-C28-C30	-3.65	118.15	124.30
5	B	502	ATP	C2-N3-C4	3.61	120.66	111.83
5	B	501	ATP	C2-N3-C4	3.57	120.55	111.83
5	A	503	ATP	C2-N3-C4	3.56	120.53	111.83
5	C	501	ATP	C4-C5-N7	-3.42	106.68	110.58
5	E	1601	ATP	C4-C5-N7	-3.38	106.72	110.58
5	C	501	ATP	N3-C2-N1	-3.32	123.56	128.58
5	E	1601	ATP	N3-C2-N1	-3.27	123.63	128.58
5	B	502	ATP	C4-C5-N7	-3.24	106.88	110.58
5	B	501	ATP	C4-C5-N7	-3.24	106.88	110.58
8	E	1602	GBM	O6-C26-N10	-3.21	116.33	122.59
5	B	501	ATP	N3-C2-N1	-3.20	123.74	128.58
5	B	502	ATP	N3-C2-N1	-3.19	123.75	128.58
5	A	503	ATP	N3-C2-N1	-3.18	123.77	128.58
5	A	503	ATP	C4-C5-N7	-3.18	106.95	110.58
6	A	507	PTY	O4-C30-C31	3.01	121.00	111.83
5	B	502	ATP	C4-N9-C8	2.98	108.87	105.74
6	A	504	PTY	O4-C30-C31	2.91	120.70	111.83
5	A	503	ATP	C4-N9-C8	2.90	108.79	105.74
5	B	501	ATP	C4-N9-C8	2.90	108.78	105.74
6	E	1603	PTY	O4-C30-C31	2.79	120.33	111.83
6	C	503	PTY	O4-C30-C31	2.78	120.30	111.83
6	E	1605	PTY	O4-C30-C31	2.75	120.21	111.83
7	C	504	POV	O31-C31-C32	2.72	120.14	111.83
6	C	502	PTY	O4-C30-C31	2.72	120.13	111.83
5	E	1601	ATP	C4-N9-C8	2.71	108.59	105.74
7	B	503	POV	O31-C31-C32	2.71	120.08	111.83
5	C	501	ATP	C4-N9-C8	2.70	108.57	105.74
6	A	505	PTY	O4-C30-C31	2.64	119.90	111.83
7	D	801	POV	O31-C31-C32	2.63	119.84	111.83
6	D	802	PTY	O4-C30-C31	2.62	119.82	111.83
6	E	1604	PTY	O4-C30-C31	2.57	119.67	111.83
6	A	506	PTY	O4-C30-C31	2.57	119.66	111.83
5	E	1601	ATP	C5-N7-C8	2.50	107.38	103.45
5	C	501	ATP	C5-N7-C8	2.46	107.32	103.45
8	E	1602	GBM	O6-C26-C27	-2.45	116.54	121.03
5	B	502	ATP	C5-N7-C8	2.41	107.24	103.45
5	A	503	ATP	C5-N7-C8	2.40	107.22	103.45
5	B	501	ATP	C5-N7-C8	2.39	107.21	103.45
5	B	501	ATP	C3'-C2'-C1'	2.39	105.98	101.46
7	B	503	POV	C14-N-C12	2.37	119.33	109.91
7	C	504	POV	C14-N-C12	2.36	119.31	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	1602	GBM	C25-N10-C26	2.36	127.45	122.11
5	B	501	ATP	C2'-C1'-N9	-2.33	107.53	113.30
5	E	1601	ATP	C3'-C2'-C1'	2.30	105.82	101.46
7	D	801	POV	C14-N-C12	2.29	119.02	109.91
6	A	507	PTY	C6-O7-C8	-2.12	112.73	117.80
8	E	1602	GBM	C11-N8-C17	-2.11	118.38	122.92
5	C	501	ATP	C6-C5-N7	2.09	136.11	132.09
5	B	502	ATP	N9-C8-N7	-2.07	111.00	113.94
5	C	501	ATP	O4'-C1'-N9	2.05	112.03	108.09
5	E	1601	ATP	C6-C5-N7	2.04	136.03	132.09
5	A	503	ATP	N9-C8-N7	-2.04	111.04	113.94
5	A	503	ATP	C3'-C2'-C1'	2.04	105.32	101.46
5	C	501	ATP	N9-C8-N7	-2.03	111.05	113.94
7	C	504	POV	C11-C12-N	-2.03	109.31	115.82
5	B	501	ATP	N9-C8-N7	-2.02	111.06	113.94
7	B	503	POV	C11-C12-N	-2.01	109.38	115.82

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	ATP	C5'-O5'-PA-O3A
5	B	501	ATP	C5'-O5'-PA-O3A
5	B	502	ATP	C5'-O5'-PA-O2A
5	B	502	ATP	O4'-C4'-C5'-O5'
5	C	501	ATP	C5'-O5'-PA-O2A
5	C	501	ATP	C5'-O5'-PA-O3A
6	A	504	PTY	O4-C1-C6-O7
6	A	504	PTY	N1-C2-C3-O11
6	A	504	PTY	C3-O11-P1-O14
6	A	505	PTY	N1-C2-C3-O11
6	A	505	PTY	C3-O11-P1-O12
6	A	505	PTY	C3-O11-P1-O14
6	A	505	PTY	C5-O14-P1-O11
6	A	505	PTY	C5-O14-P1-O12
6	A	506	PTY	N1-C2-C3-O11
6	A	506	PTY	C11-C8-O7-C6
6	A	506	PTY	C3-O11-P1-O12
6	A	506	PTY	C3-O11-P1-O13
6	A	506	PTY	C3-O11-P1-O14
6	A	506	PTY	C5-O14-P1-O11
6	A	506	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
6	A	506	PTY	C5-O14-P1-O13
6	A	507	PTY	N1-C2-C3-O11
6	A	507	PTY	O10-C8-O7-C6
6	A	507	PTY	C11-C8-O7-C6
6	A	507	PTY	C3-O11-P1-O12
6	A	507	PTY	C3-O11-P1-O14
6	C	502	PTY	O30-C30-O4-C1
6	C	502	PTY	C3-O11-P1-O13
6	C	502	PTY	C5-O14-P1-O11
6	C	502	PTY	C5-O14-P1-O12
6	C	502	PTY	C5-O14-P1-O13
6	C	503	PTY	C3-O11-P1-O12
6	C	503	PTY	C3-O11-P1-O13
6	C	503	PTY	C3-O11-P1-O14
6	D	802	PTY	N1-C2-C3-O11
6	D	802	PTY	C11-C8-O7-C6
6	D	802	PTY	C5-O14-P1-O11
6	D	802	PTY	C5-O14-P1-O12
6	E	1603	PTY	N1-C2-C3-O11
6	E	1603	PTY	C3-O11-P1-O12
6	E	1603	PTY	C3-O11-P1-O14
6	E	1603	PTY	C5-O14-P1-O13
6	E	1604	PTY	N1-C2-C3-O11
6	E	1604	PTY	C11-C8-O7-C6
6	E	1605	PTY	N1-C2-C3-O11
6	E	1605	PTY	O10-C8-O7-C6
6	E	1605	PTY	C11-C8-O7-C6
6	E	1605	PTY	C3-O11-P1-O14
6	E	1605	PTY	C5-O14-P1-O11
6	E	1605	PTY	C5-O14-P1-O13
7	B	503	POV	C1-O11-P-O12
7	B	503	POV	C1-O11-P-O13
7	B	503	POV	C11-O12-P-O11
7	B	503	POV	C11-O12-P-O13
7	B	503	POV	O11-C1-C2-O21
7	B	503	POV	C22-C21-O21-C2
7	B	503	POV	O22-C21-O21-C2
7	C	504	POV	C1-O11-P-O12
7	C	504	POV	C1-O11-P-O13
7	C	504	POV	C1-O11-P-O14
7	C	504	POV	O22-C21-O21-C2
8	E	1602	GBM	N9-C17-N8-C11

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Mol	Chain	Res	Type	Atoms
8	E	1602	GBM	C19-C20-C25-N10
6	C	502	PTY	C31-C30-O4-C1
8	E	1602	GBM	O3-C17-N8-C11
6	A	506	PTY	O10-C8-O7-C6
6	D	802	PTY	O10-C8-O7-C6
7	C	504	POV	C22-C21-O21-C2
6	A	507	PTY	O30-C30-O4-C1
6	E	1604	PTY	O10-C8-O7-C6
6	A	504	PTY	C11-C8-O7-C6
6	C	503	PTY	C11-C8-O7-C6
7	D	801	POV	C22-C21-O21-C2
8	E	1602	GBM	O6-C26-N10-C25
5	B	502	ATP	C3'-C4'-C5'-O5'
6	A	507	PTY	C31-C30-O4-C1
6	C	503	PTY	O10-C8-O7-C6
8	E	1602	GBM	C27-C26-N10-C25
7	D	801	POV	O22-C21-O21-C2
6	C	503	PTY	C8-C11-C12-C13
6	A	504	PTY	O10-C8-O7-C6
6	C	503	PTY	O4-C1-C6-O7
5	C	501	ATP	O4'-C4'-C5'-O5'
6	E	1604	PTY	C8-C11-C12-C13
6	E	1604	PTY	C30-C31-C32-C33
7	D	801	POV	C31-C32-C33-C34
6	A	505	PTY	C11-C8-O7-C6
6	E	1603	PTY	C11-C8-O7-C6
6	C	502	PTY	C30-C31-C32-C33
6	A	504	PTY	C31-C32-C33-C34
6	A	505	PTY	O10-C8-O7-C6
6	E	1603	PTY	O10-C8-O7-C6
5	A	503	ATP	O4'-C4'-C5'-O5'
7	B	503	POV	C22-C23-C24-C25
6	E	1603	PTY	O4-C1-C6-O7
6	E	1605	PTY	C15-C16-C17-C18
6	A	507	PTY	C13-C14-C15-C16
6	A	504	PTY	C11-C12-C13-C14
8	E	1602	GBM	C22-C18-S2-O4
8	E	1602	GBM	C21-C18-S2-O4
6	C	502	PTY	C11-C12-C13-C14
7	D	801	POV	C33-C34-C35-C36
6	E	1605	PTY	C13-C14-C15-C16
6	E	1605	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	B	503	POV	C24-C25-C26-C27
6	A	507	PTY	C12-C13-C14-C15
6	D	802	PTY	C15-C16-C17-C18
7	D	801	POV	C24-C25-C26-C27
6	A	505	PTY	C11-C12-C13-C14
6	E	1603	PTY	C16-C17-C18-C19
6	C	502	PTY	C31-C32-C33-C34
7	C	504	POV	C32-C33-C34-C35
6	E	1604	PTY	C11-C12-C13-C14
7	C	504	POV	C24-C25-C26-C27
6	D	802	PTY	C30-C31-C32-C33
7	B	503	POV	C34-C35-C36-C37
6	D	802	PTY	C11-C12-C13-C14
7	D	801	POV	C27-C28-C29-C210
6	E	1603	PTY	C12-C13-C14-C15
7	B	503	POV	C32-C33-C34-C35
6	E	1603	PTY	C13-C14-C15-C16
6	C	502	PTY	O14-C5-C6-C1
6	E	1603	PTY	O14-C5-C6-C1
7	B	503	POV	O11-C1-C2-C3
7	C	504	POV	C23-C24-C25-C26
7	D	801	POV	C21-C22-C23-C24
6	C	503	PTY	O4-C1-C6-C5
6	E	1603	PTY	O4-C1-C6-C5
6	E	1603	PTY	C15-C16-C17-C18
7	D	801	POV	C25-C26-C27-C28
7	C	504	POV	C32-C31-O31-C3
6	A	504	PTY	C12-C13-C14-C15
6	E	1604	PTY	O14-C5-C6-O7
6	E	1604	PTY	C16-C17-C18-C19
6	A	507	PTY	C17-C18-C19-C20
6	C	502	PTY	C17-C18-C19-C20
6	A	505	PTY	C31-C30-O4-C1
6	A	507	PTY	C32-C33-C34-C35
6	A	506	PTY	C30-C31-C32-C33
7	B	503	POV	C21-C22-C23-C24
6	D	802	PTY	C17-C18-C19-C20
8	E	1602	GBM	C21-C18-S2-N9
8	E	1602	GBM	C22-C18-S2-N9
6	C	503	PTY	O14-C5-C6-C1
6	A	504	PTY	O4-C1-C6-C5
6	A	506	PTY	O4-C1-C6-C5

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Mol	Chain	Res	Type	Atoms
7	B	503	POV	C1-C2-C3-O31
7	C	504	POV	O32-C31-O31-C3
6	C	502	PTY	O14-C5-C6-O7
5	C	501	ATP	C3'-C4'-C5'-O5'
6	C	503	PTY	C30-C31-C32-C33
6	A	505	PTY	O14-C5-C6-C1
6	D	802	PTY	C14-C15-C16-C17
6	A	505	PTY	C8-C11-C12-C13
6	A	505	PTY	O30-C30-O4-C1
6	A	505	PTY	O14-C5-C6-O7
6	A	506	PTY	O14-C5-C6-O7
6	C	503	PTY	O14-C5-C6-O7
7	C	504	POV	C1-C2-C3-O31
6	E	1605	PTY	C11-C12-C13-C14
6	A	505	PTY	C2-C3-O11-P1
6	A	507	PTY	C2-C3-O11-P1
6	E	1603	PTY	C2-C3-O11-P1
7	D	801	POV	O12-C11-C12-N
6	D	802	PTY	C32-C33-C34-C35
6	E	1604	PTY	O14-C5-C6-C1
6	E	1605	PTY	O14-C5-C6-C1
7	C	504	POV	O11-C1-C2-C3
7	D	801	POV	O11-C1-C2-C3
6	C	503	PTY	C11-C12-C13-C14
6	E	1604	PTY	C12-C13-C14-C15
6	A	505	PTY	C31-C32-C33-C34
6	E	1605	PTY	O14-C5-C6-O7
7	C	504	POV	O11-C1-C2-O21
7	D	801	POV	O11-C1-C2-O21
6	A	505	PTY	C13-C14-C15-C16
6	A	506	PTY	O4-C1-C6-O7
7	B	503	POV	O21-C2-C3-O31
7	C	504	POV	O21-C2-C3-O31
6	C	502	PTY	C8-C11-C12-C13
5	A	503	ATP	C5'-O5'-PA-O1A
5	B	501	ATP	C5'-O5'-PA-O1A
5	B	502	ATP	C5'-O5'-PA-O1A
5	B	502	ATP	C5'-O5'-PA-O3A
5	E	1601	ATP	C5'-O5'-PA-O1A
6	A	504	PTY	C3-O11-P1-O13
6	A	505	PTY	C5-O14-P1-O13
6	C	503	PTY	N1-C2-C3-O11

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Mol	Chain	Res	Type	Atoms
6	D	802	PTY	C3-O11-P1-O12
6	D	802	PTY	C3-O11-P1-O14
6	E	1604	PTY	C3-O11-P1-O14
6	E	1605	PTY	C5-O14-P1-O12
7	B	503	POV	C1-O11-P-O14
7	B	503	POV	C11-O12-P-O14
7	D	801	POV	C11-O12-P-O14
6	C	503	PTY	C6-C5-O14-P1
6	E	1604	PTY	C13-C14-C15-C16
6	E	1603	PTY	O14-C5-C6-O7
7	C	504	POV	C35-C36-C37-C38
6	A	505	PTY	C12-C11-C8-O7
5	A	503	ATP	C3'-C4'-C5'-O5'
8	E	1602	GBM	O6-C26-C27-C28
6	E	1605	PTY	C14-C15-C16-C17
8	E	1602	GBM	N10-C26-C27-C28
6	A	507	PTY	C14-C15-C16-C17
6	A	507	PTY	O4-C1-C6-O7
6	A	505	PTY	C1-C6-O7-C8
6	A	505	PTY	C5-C6-O7-C8
6	C	502	PTY	C13-C14-C15-C16
7	B	503	POV	C27-C28-C29-C210
6	C	502	PTY	O4-C1-C6-O7
5	A	503	ATP	PB-O3A-PA-O1A
5	B	501	ATP	PB-O3A-PA-O1A
5	B	501	ATP	PB-O3A-PA-O2A
6	A	506	PTY	O14-C5-C6-C1
8	E	1602	GBM	C17-N9-S2-O5
6	A	507	PTY	C11-C12-C13-C14
6	E	1603	PTY	C11-C12-C13-C14
6	A	504	PTY	C13-C14-C15-C16
6	E	1604	PTY	C2-C3-O11-P1
7	D	801	POV	C12-C11-O12-P
6	E	1605	PTY	O4-C30-C31-C32
6	C	502	PTY	O4-C30-C31-C32
5	A	503	ATP	PB-O3A-PA-O2A
7	C	504	POV	O12-C11-C12-N
6	A	504	PTY	C12-C11-C8-O7
6	C	502	PTY	C12-C13-C14-C15
7	C	504	POV	C27-C28-C29-C210
8	E	1602	GBM	C30-C28-O7-C33
6	A	505	PTY	C6-C5-O14-P1

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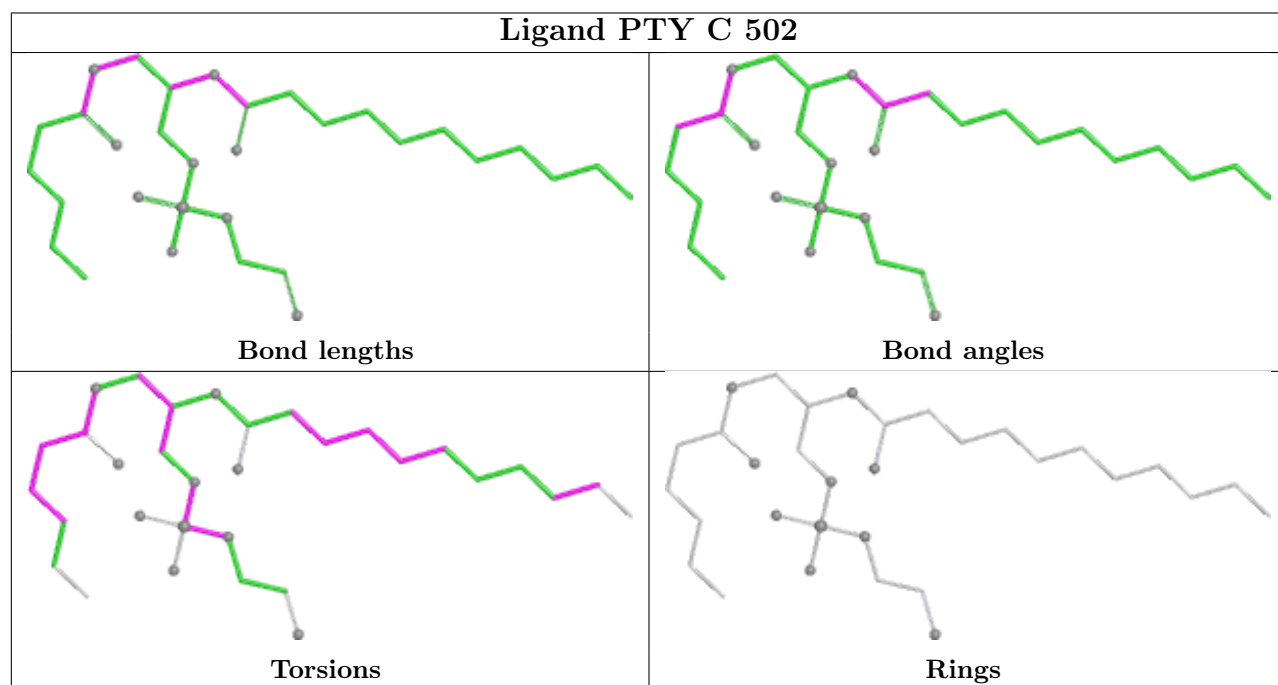
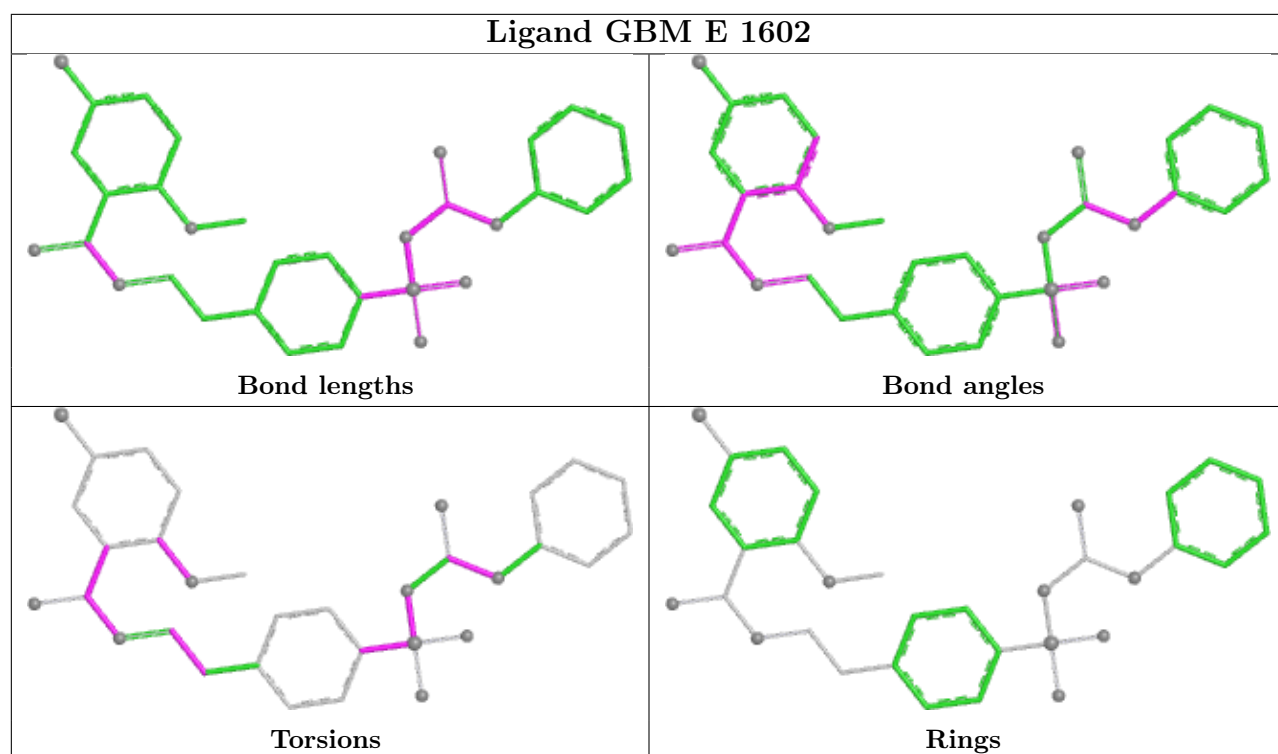
Mol	Chain	Res	Type	Atoms
6	A	504	PTY	C12-C11-C8-O10
6	E	1605	PTY	O30-C30-C31-C32
6	C	502	PTY	O30-C30-C31-C32
5	B	501	ATP	PG-O3B-PB-O2B
5	B	502	ATP	PA-O3A-PB-O2B

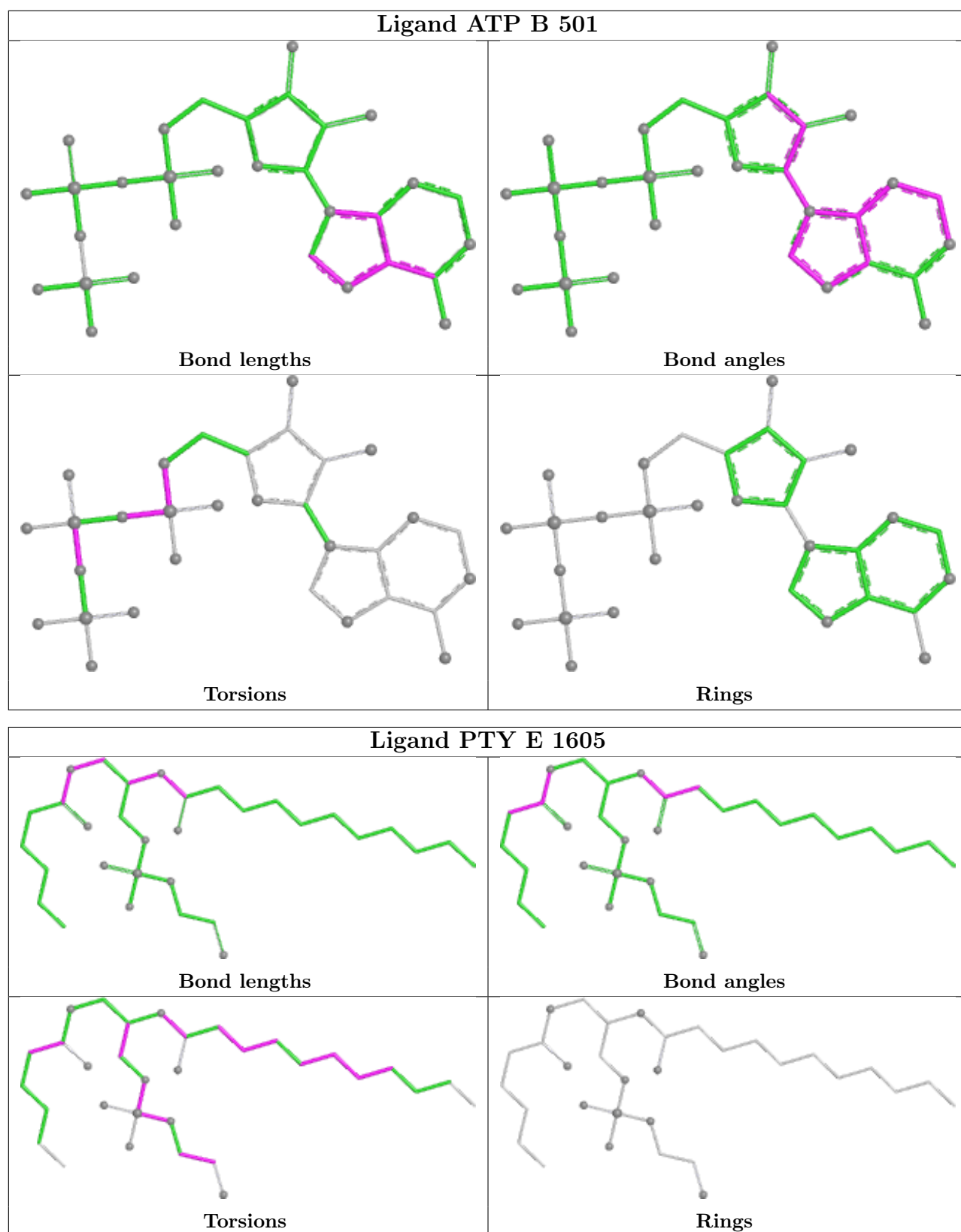
There are no ring outliers.

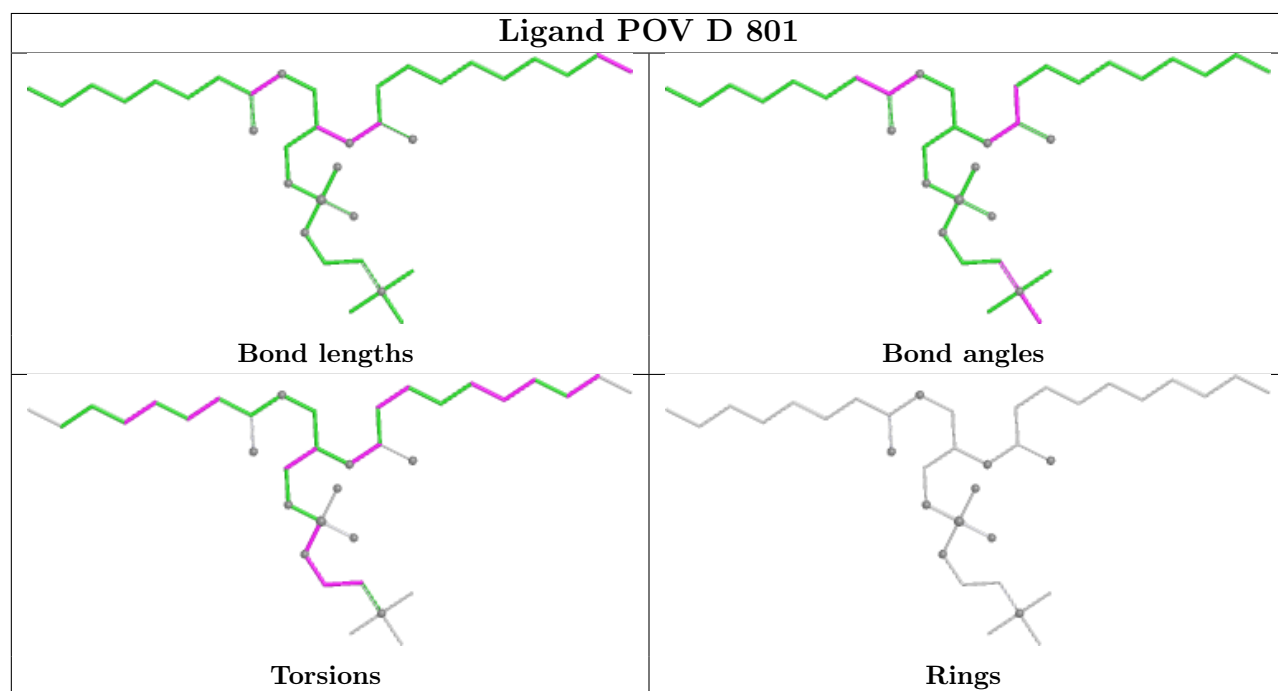
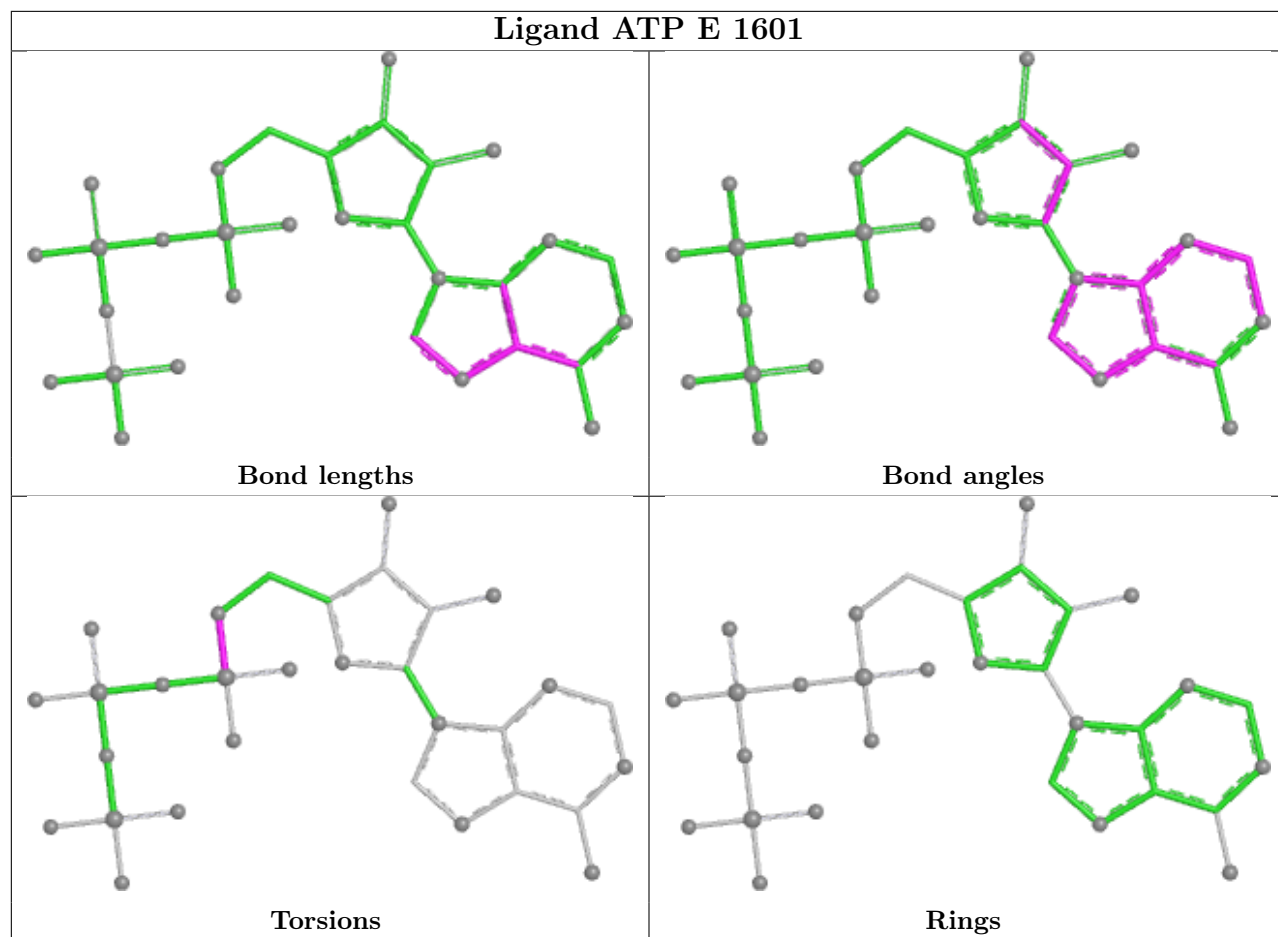
11 monomers are involved in 25 short contacts:

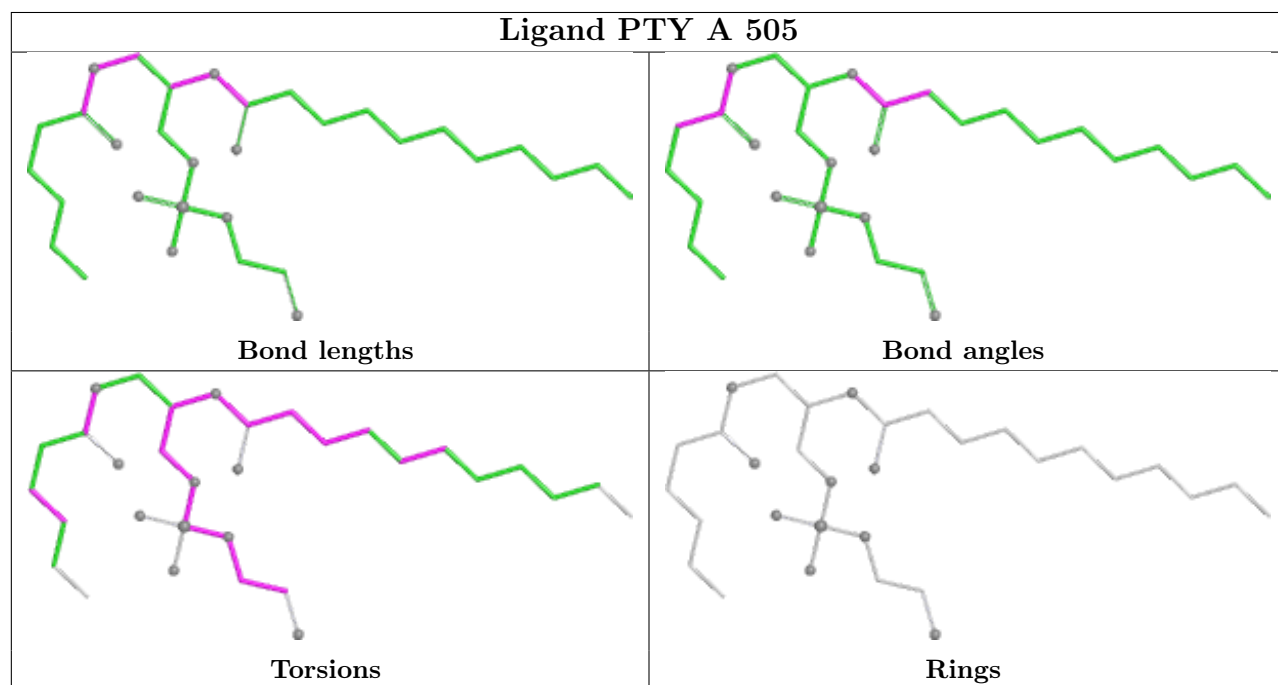
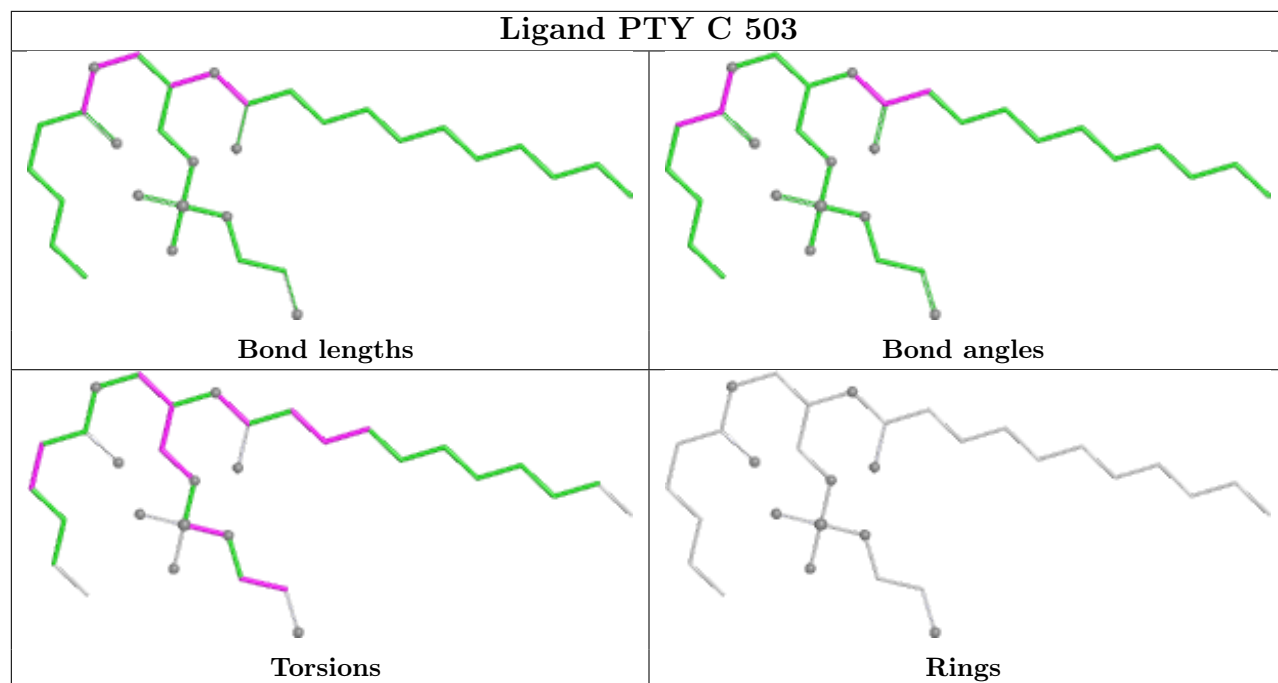
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1602	GBM	5	0
6	C	502	PTY	5	0
5	B	501	ATP	4	0
7	D	801	POV	1	0
6	C	503	PTY	1	0
5	B	502	ATP	2	0
6	E	1603	PTY	1	0
5	C	501	ATP	2	0
7	C	504	POV	1	0
6	A	507	PTY	2	0
5	A	503	ATP	1	0

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

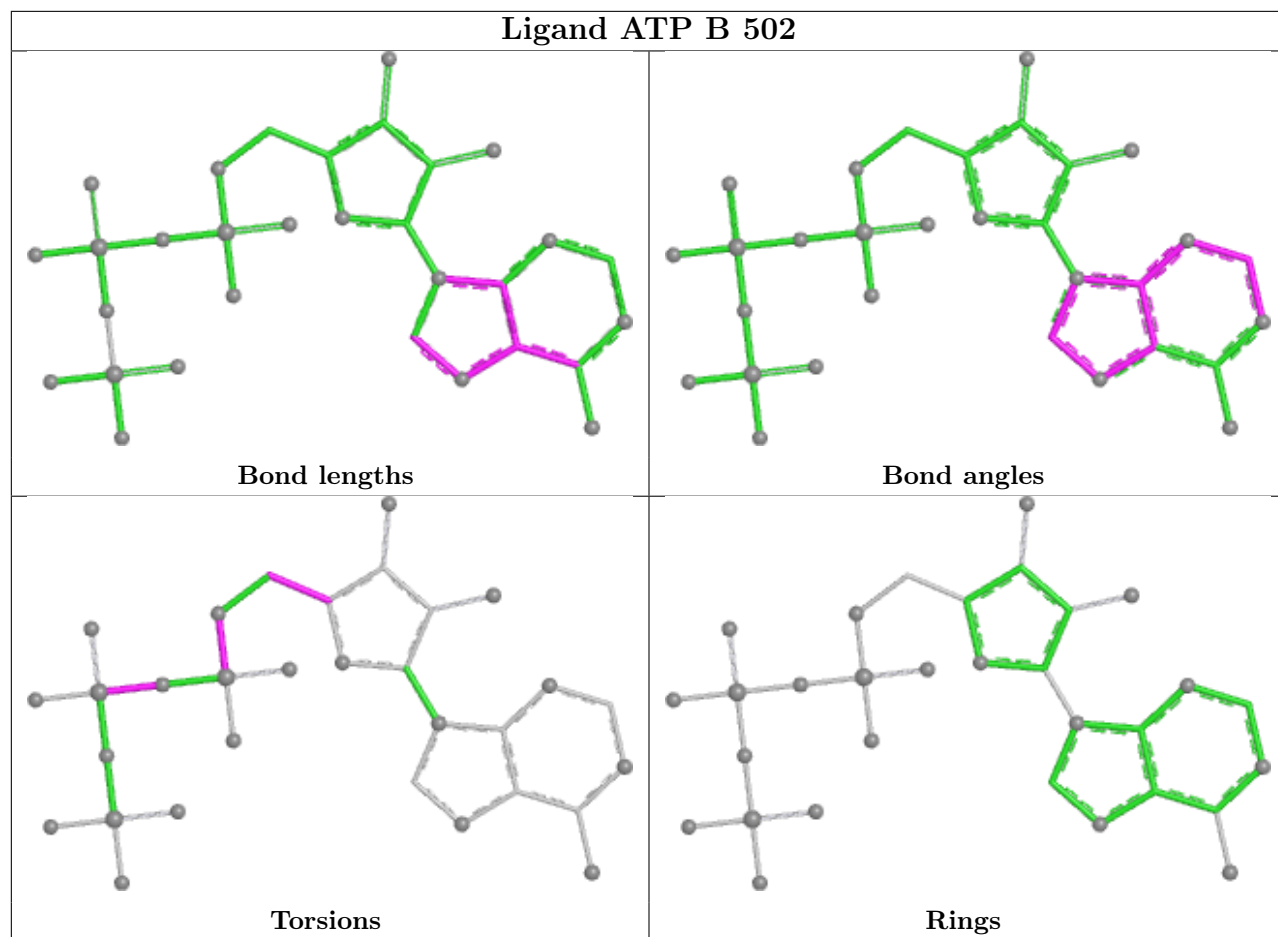




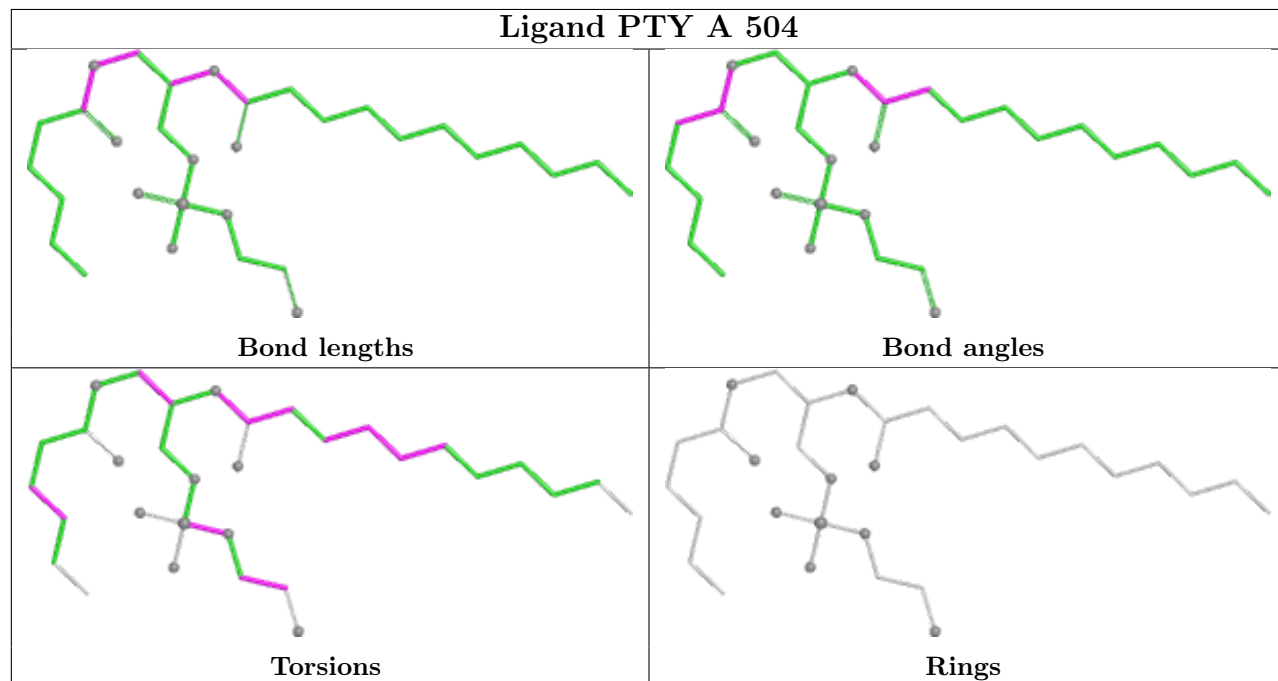


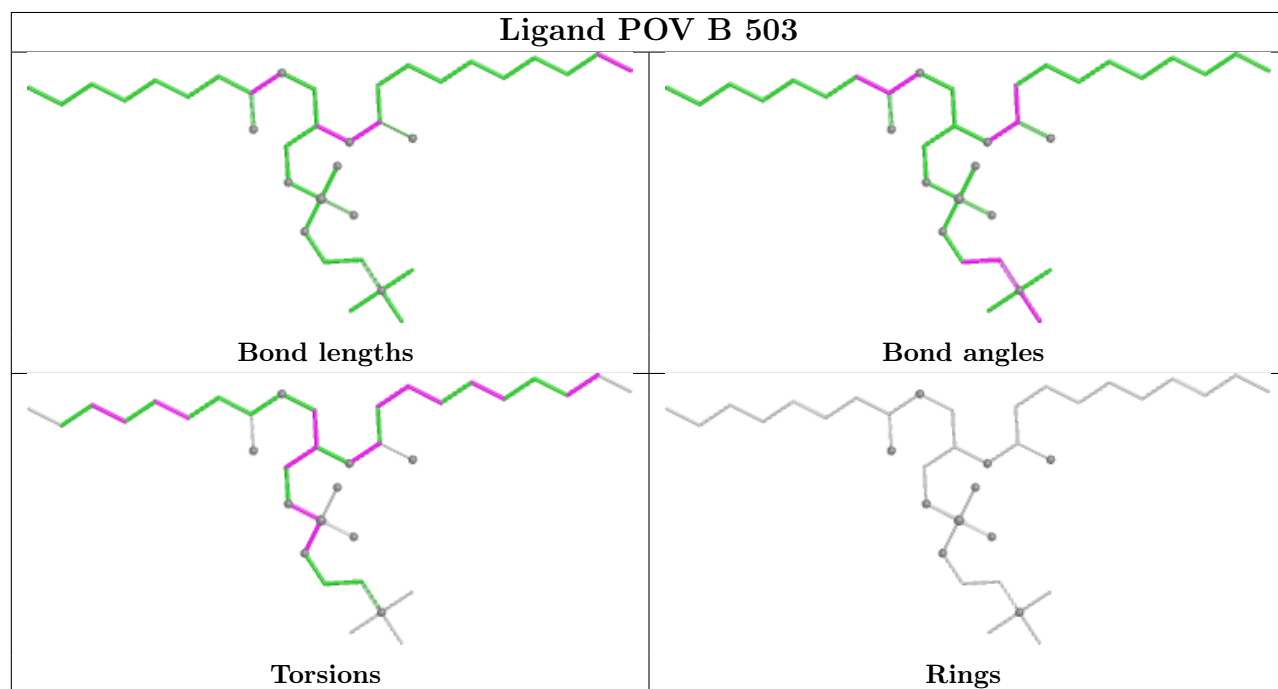
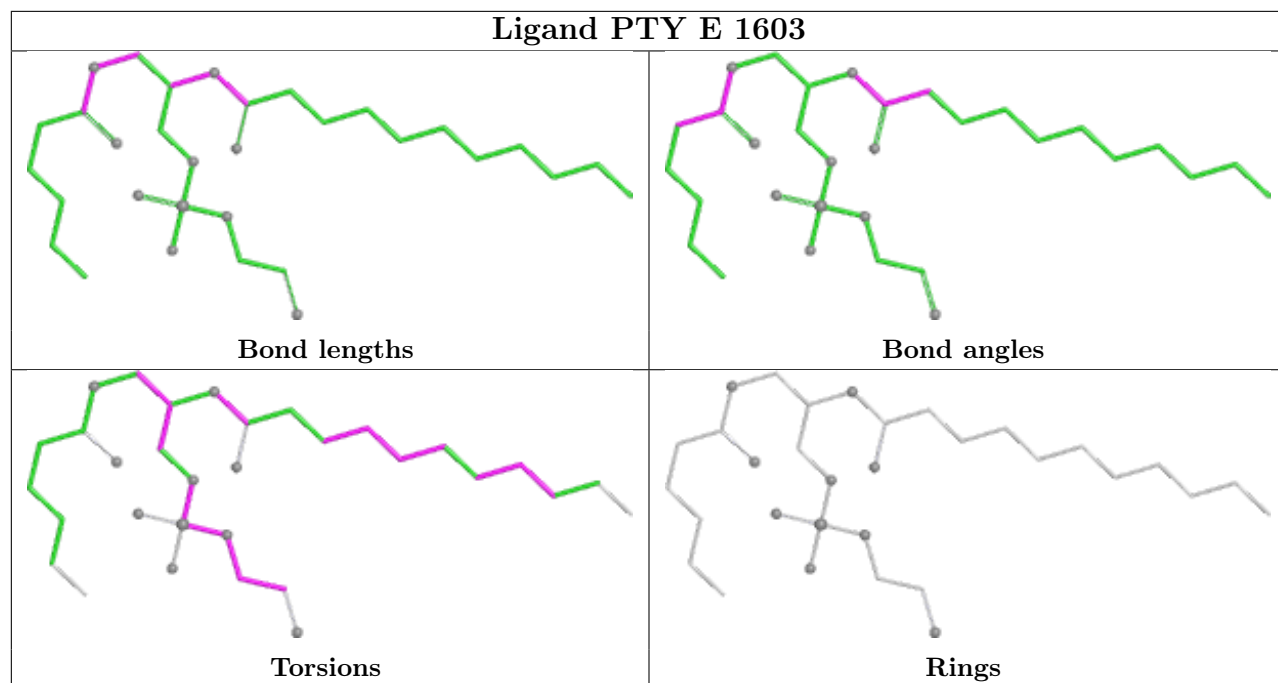


Ligand ATP B 502

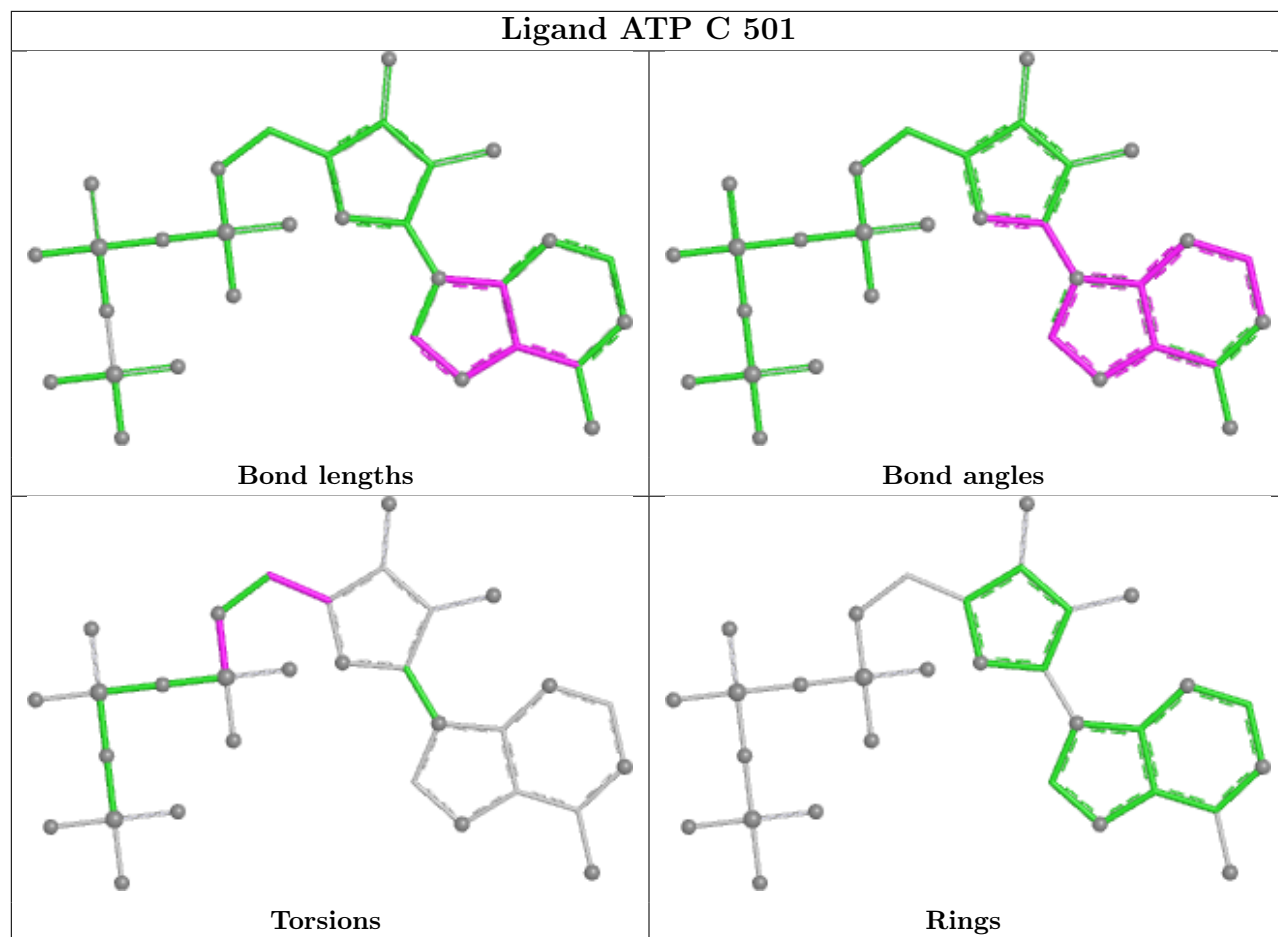


Ligand PTY A 504

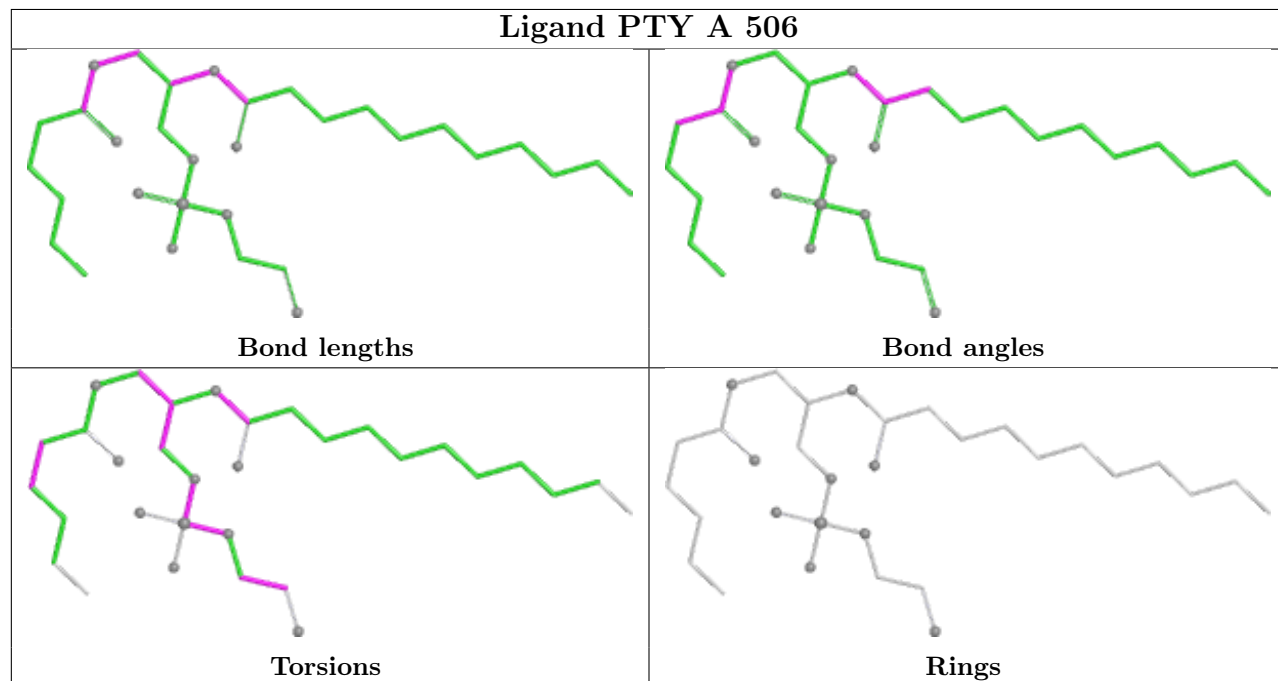


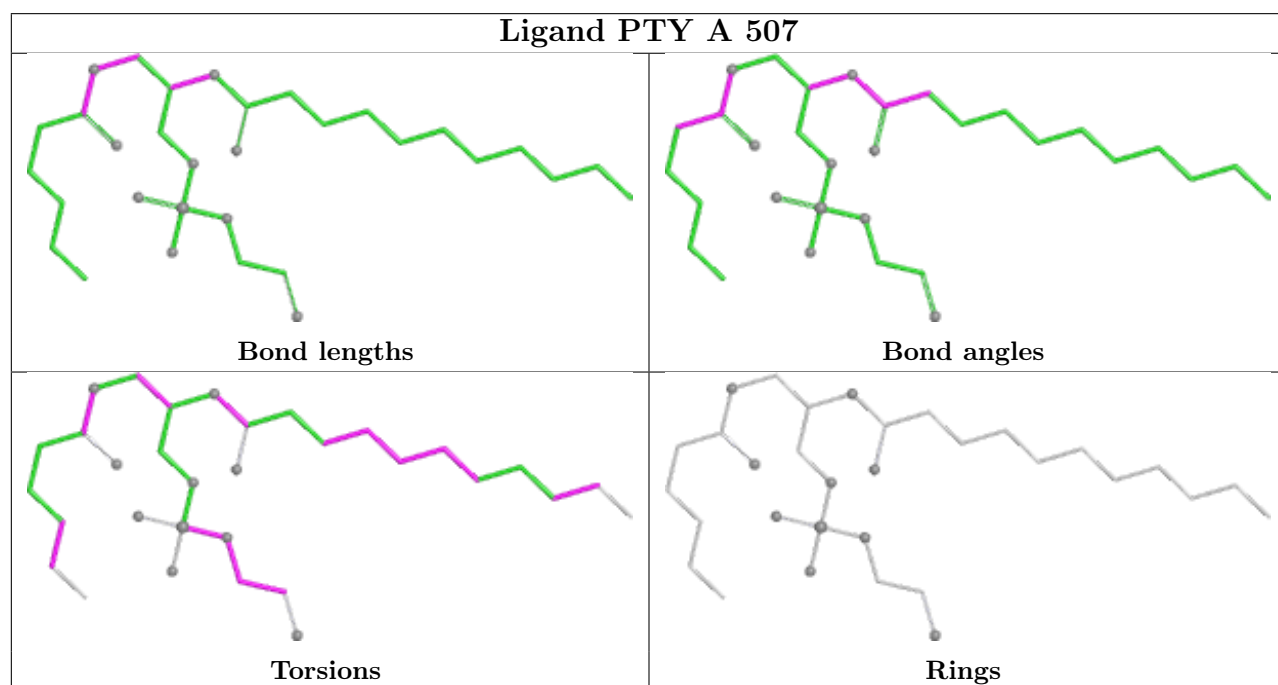
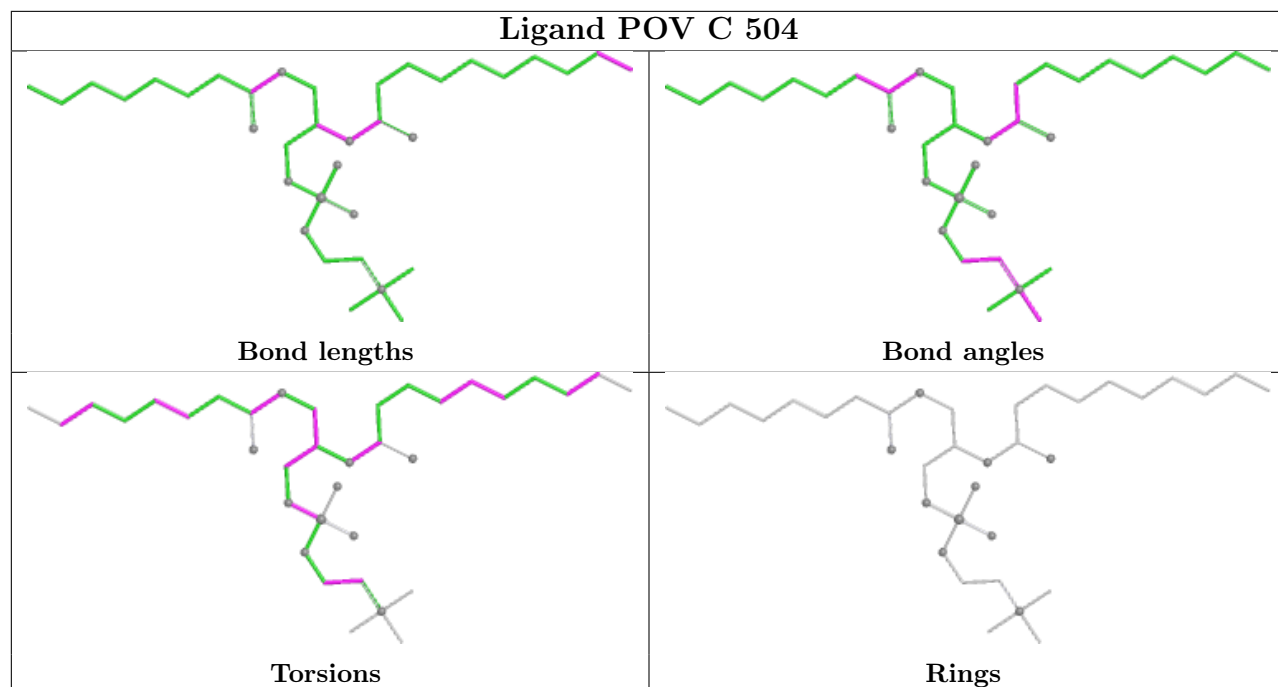


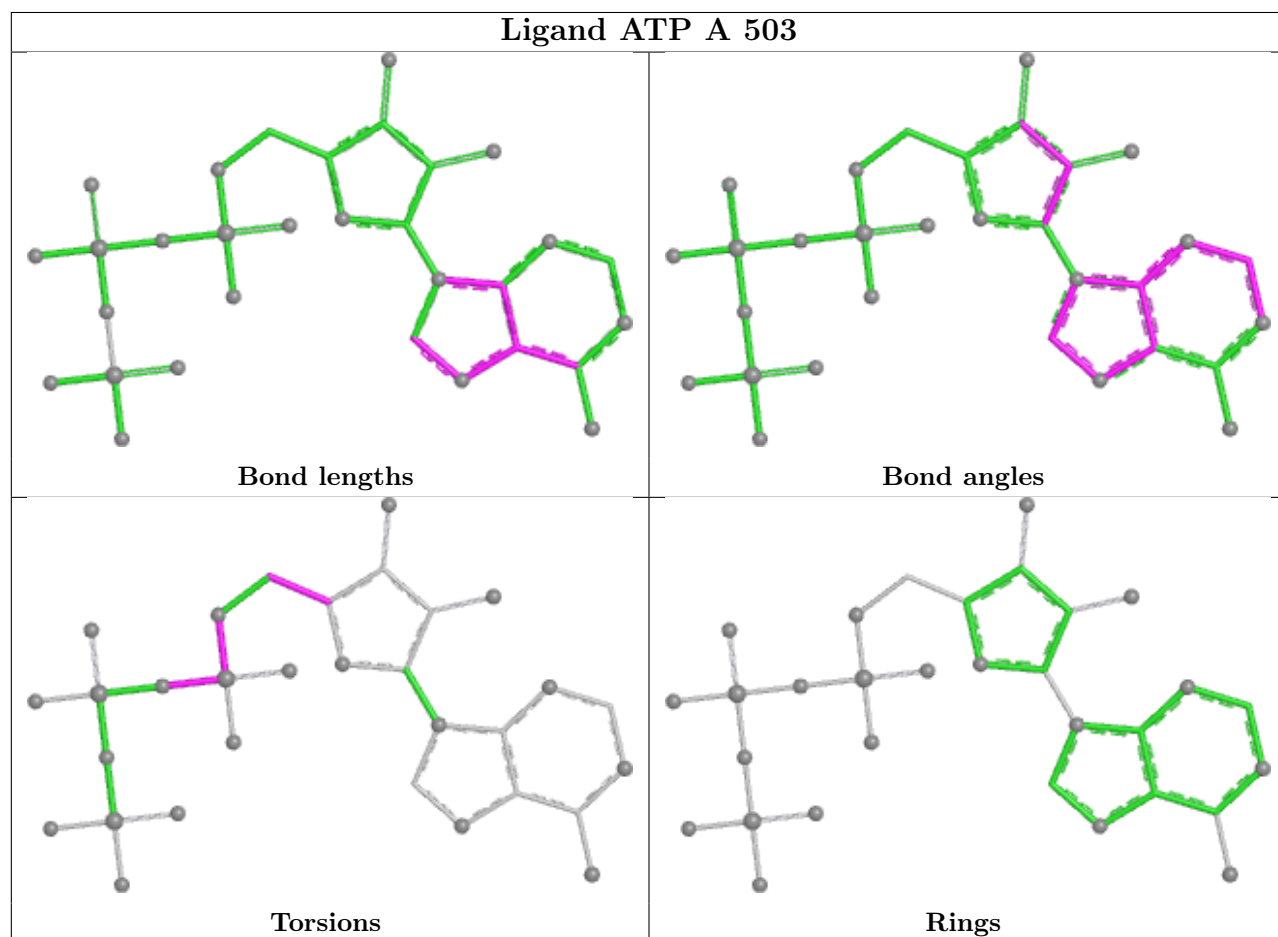
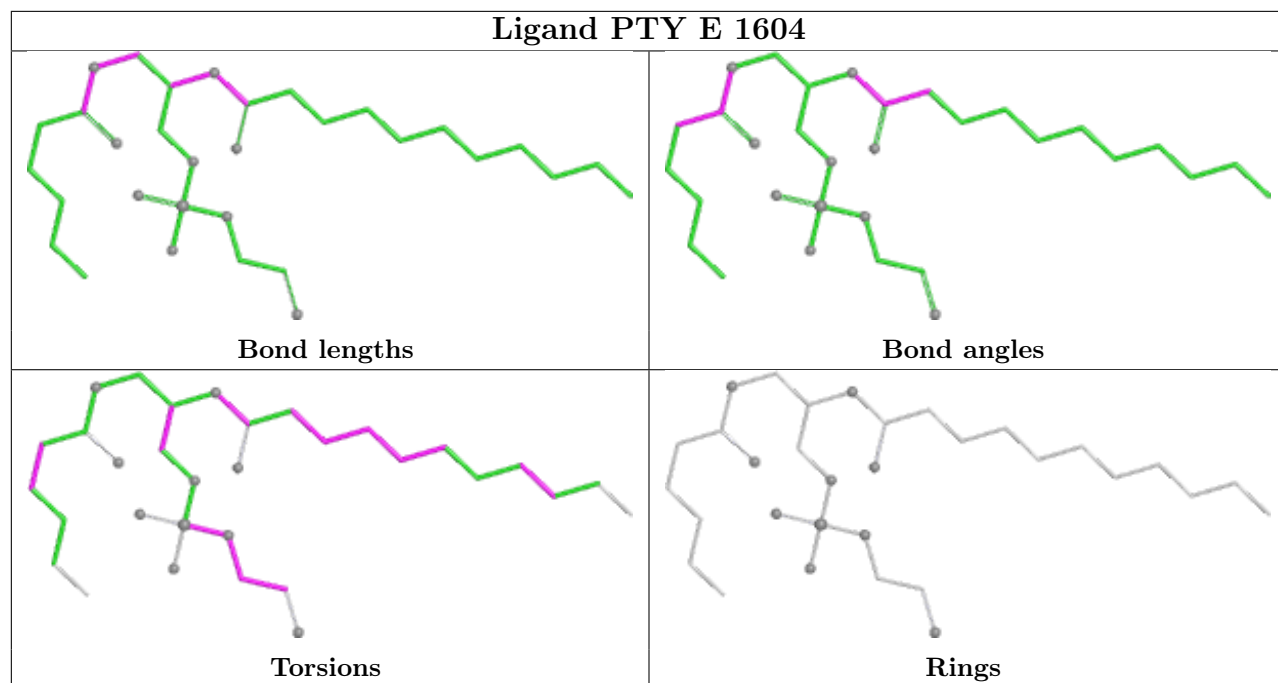
Ligand ATP C 501

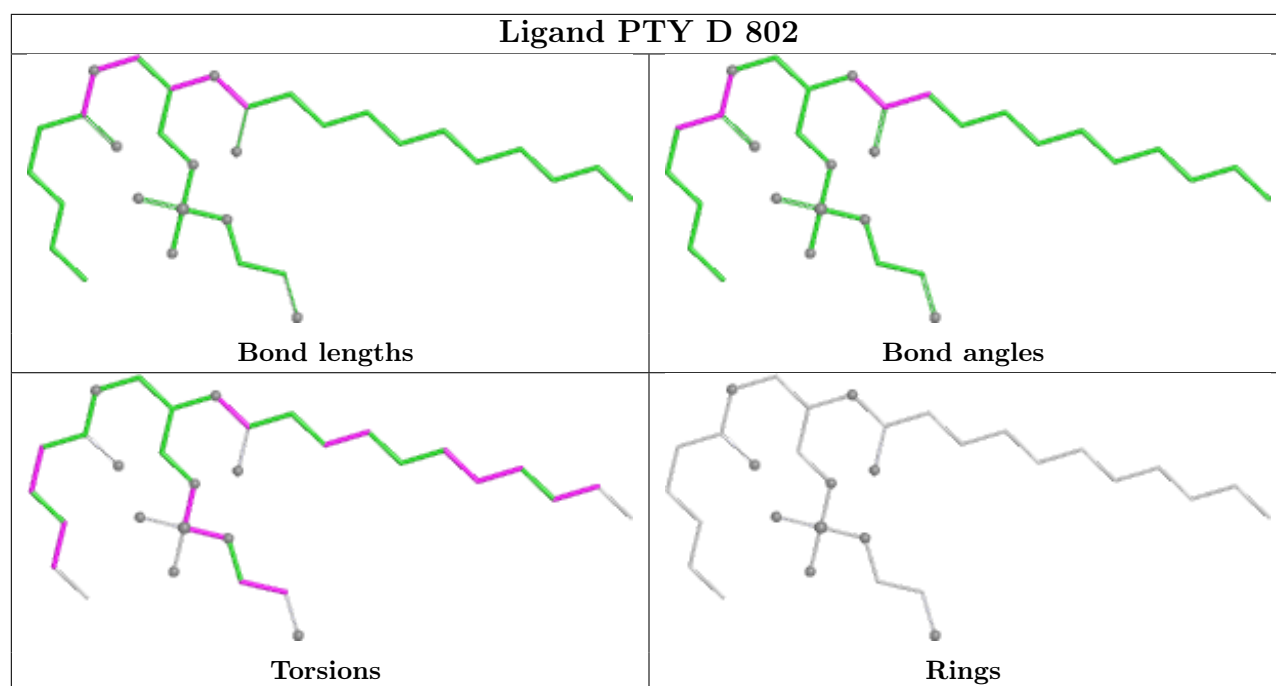


Ligand PTY A 506









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.

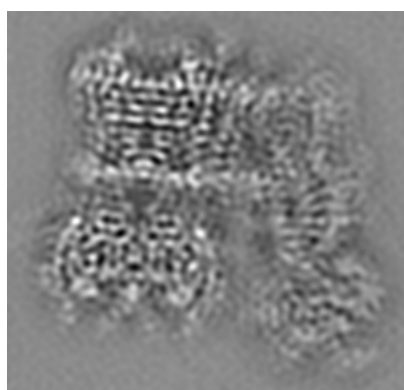
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23880. These allow visual inspection of the internal detail of the map and identification of artifacts.

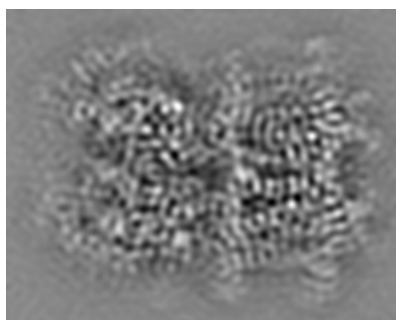
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

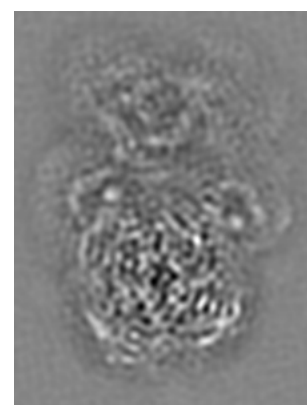
6.1.1 Primary map



X



Y

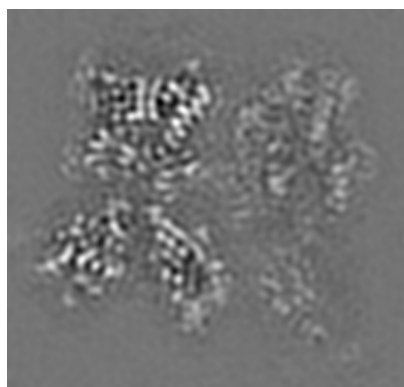


Z

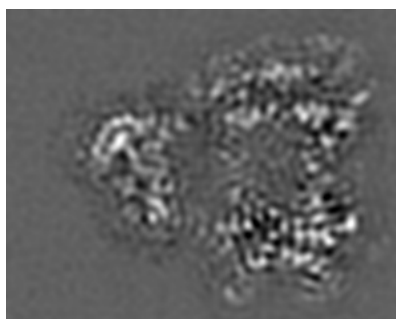
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

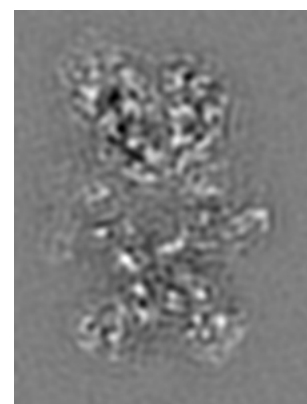
6.2.1 Primary map



X Index: 37



Y Index: 49

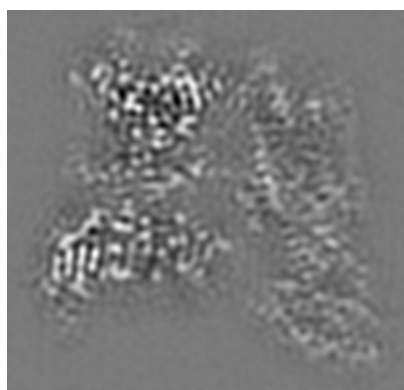


Z Index: 47

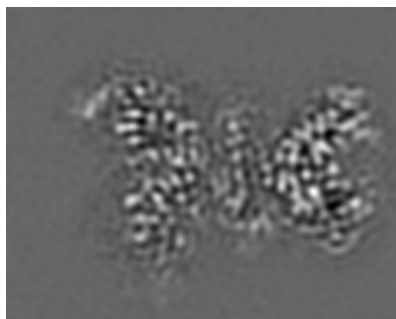
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

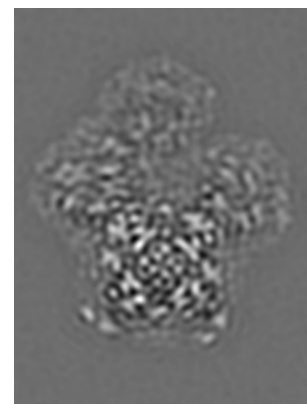
6.3.1 Primary map



X Index: 29



Y Index: 26

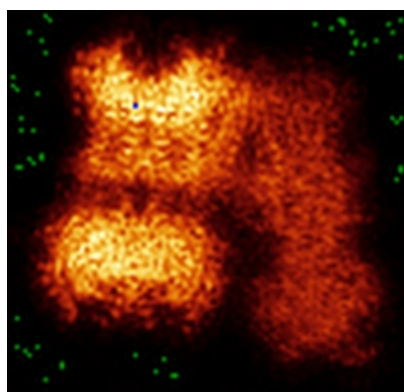


Z Index: 72

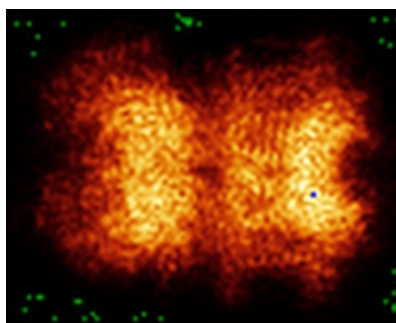
The images above show the largest variance slices of the map in three orthogonal directions.

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

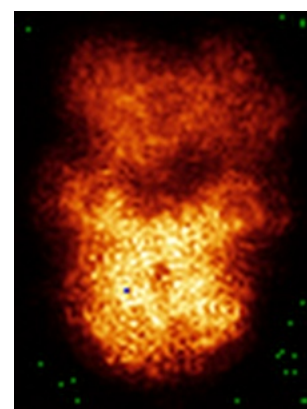
6.4.1 Primary map



X



Y

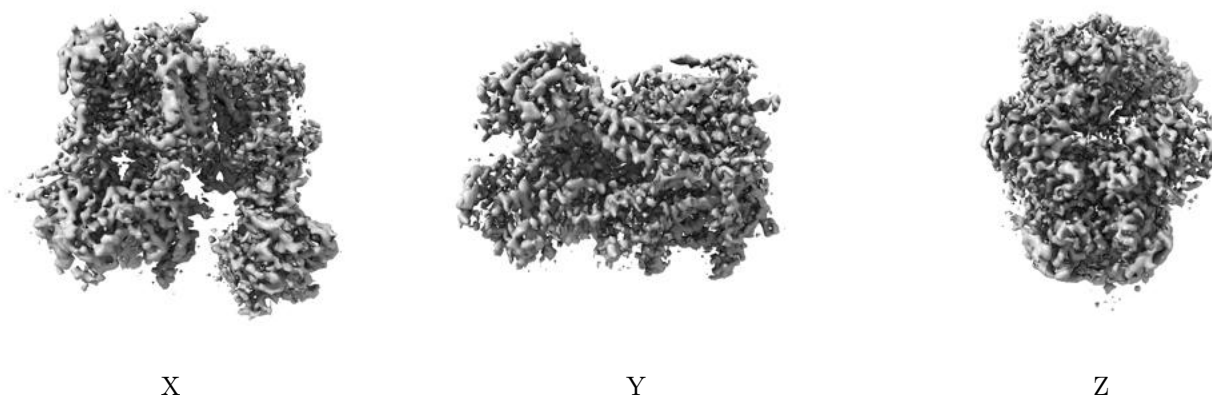


Z

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

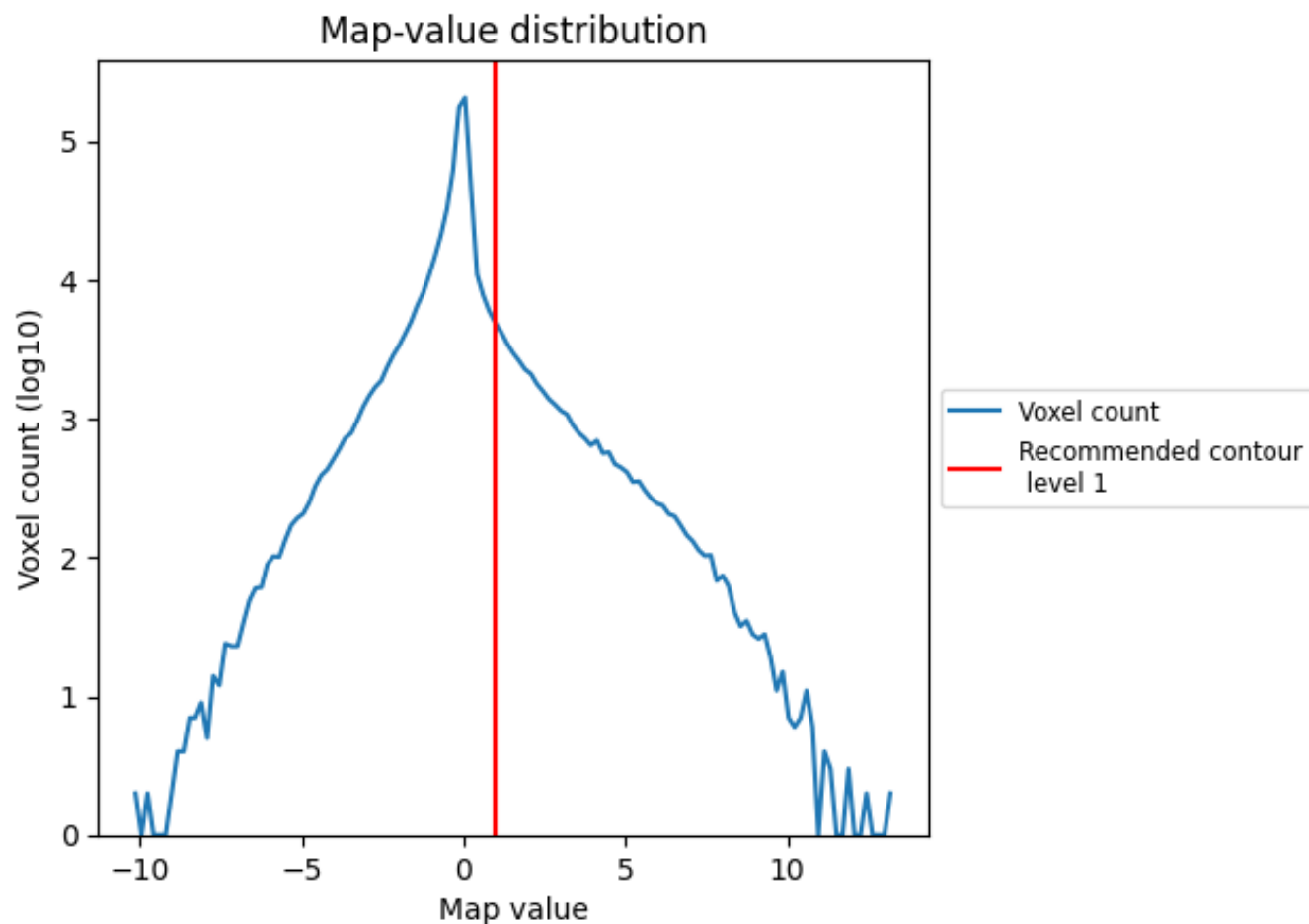
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

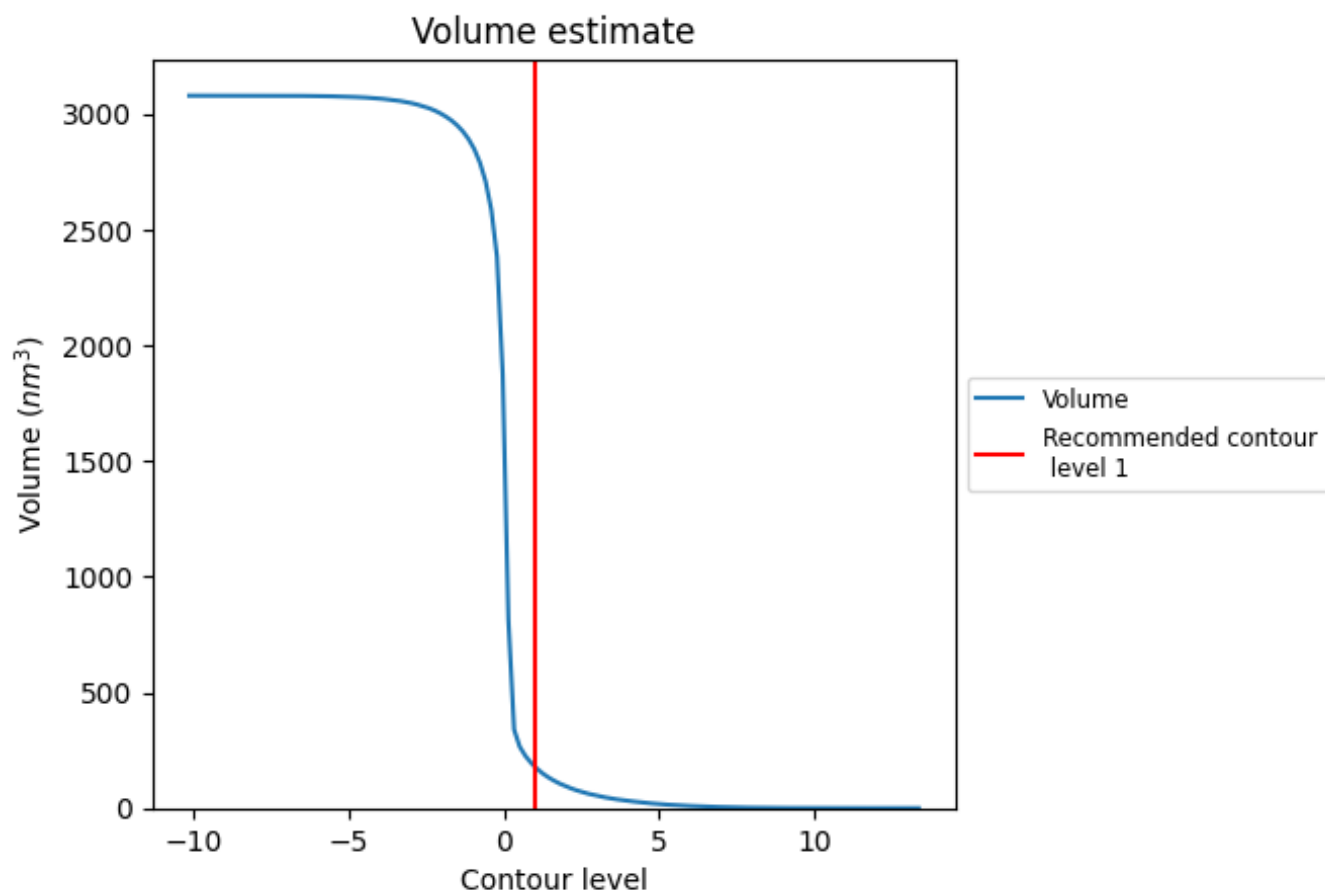
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 162 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

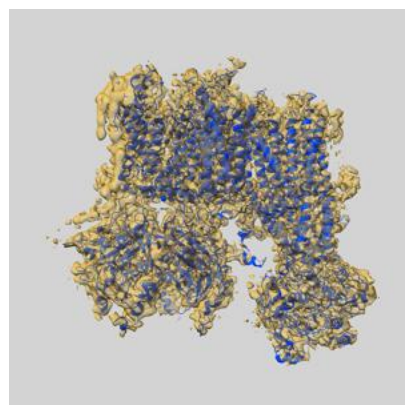
8 Fourier-Shell correlation

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

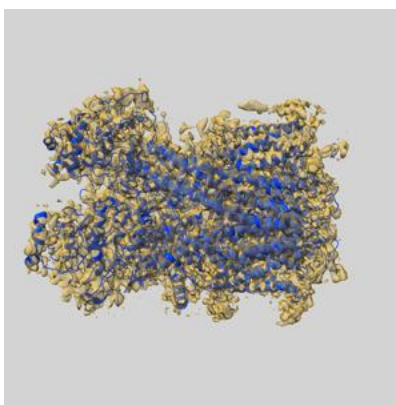
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23880 and PDB model 7MJO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

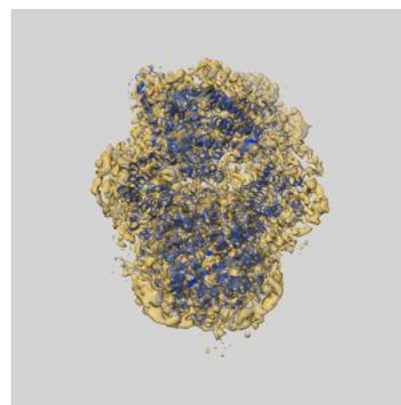
9.1 Map-model overlay [i](#)



X



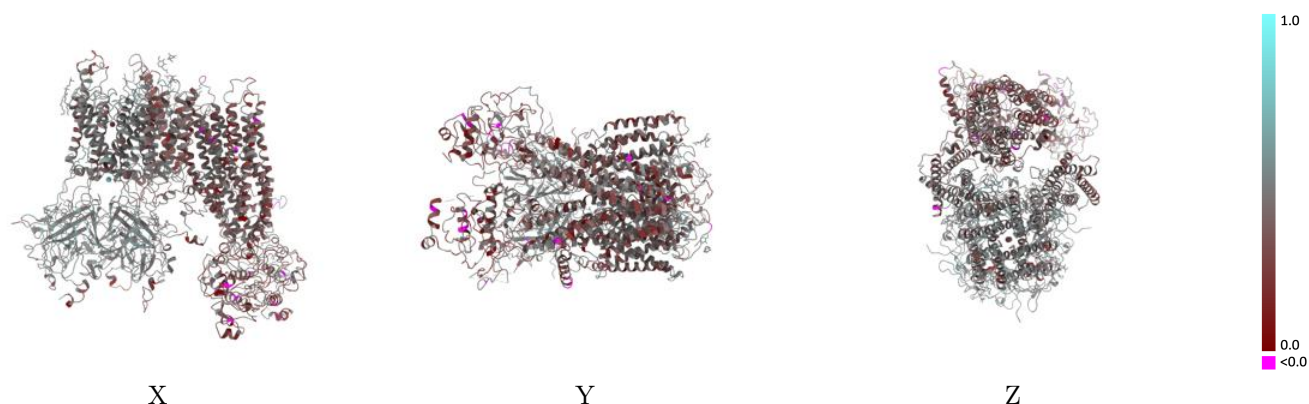
Y



Z

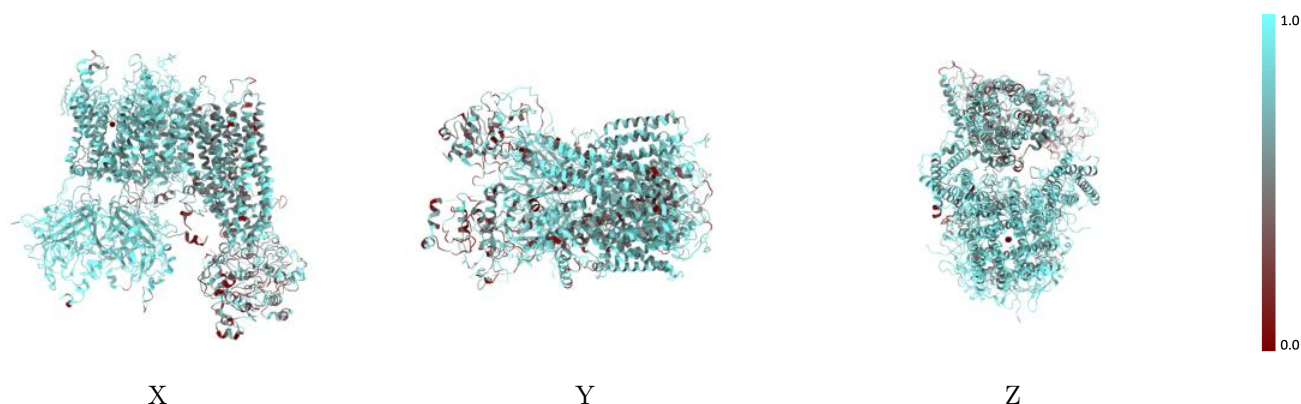
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



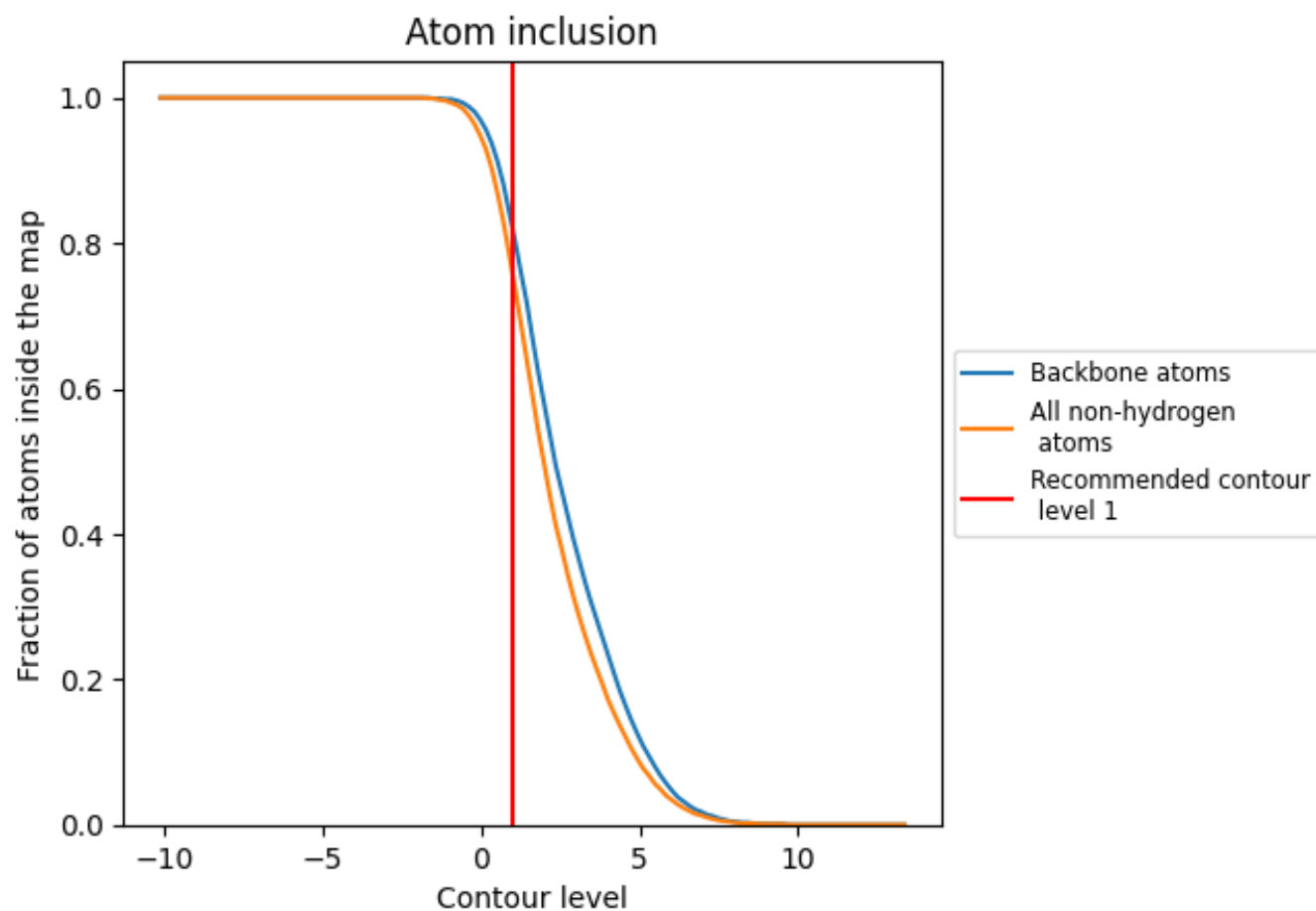
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 75% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7540	0.4290
A	0.8150	0.4730
B	0.8540	0.4770
C	0.8430	0.4800
D	0.8400	0.4800
E	0.6520	0.3720
F	0.7860	0.4890
G	0.7740	0.4210
N	0.8210	0.4570

1.0

0.0

<0.0