



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:45 AM UTC

PDB ID : 8OMZ / pdb_00008omz
Title : Wide inward-open unliganded UraA in complex with a conformation-selective synthetic nanobody
Authors : Kuhn, B.T.; Geertsma, E.R.
Deposited on : 2023-03-31
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

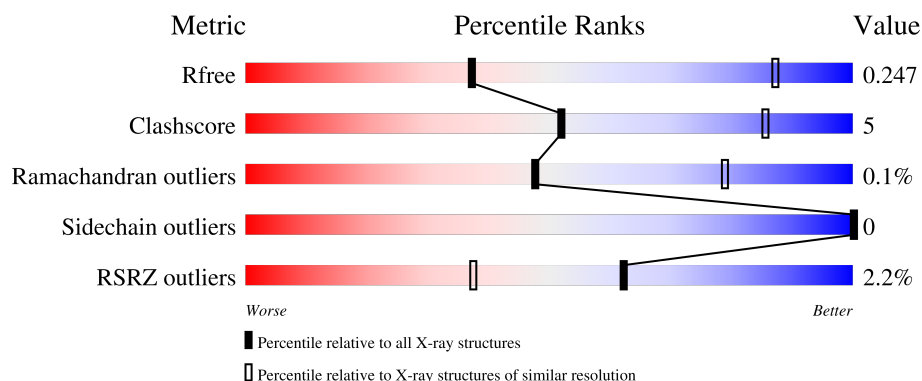
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	437	2% 81% 13% 6%
1	C	437	3% 83% 11% 6%
2	B	154	3% 72% 10% 18%
2	D	154	% 73% 9% 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8347 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Uracil permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3030	2024	481	511	14			
1	C	409	Total	C	N	O	S	0	0	0
			3019	2018	477	510	14			

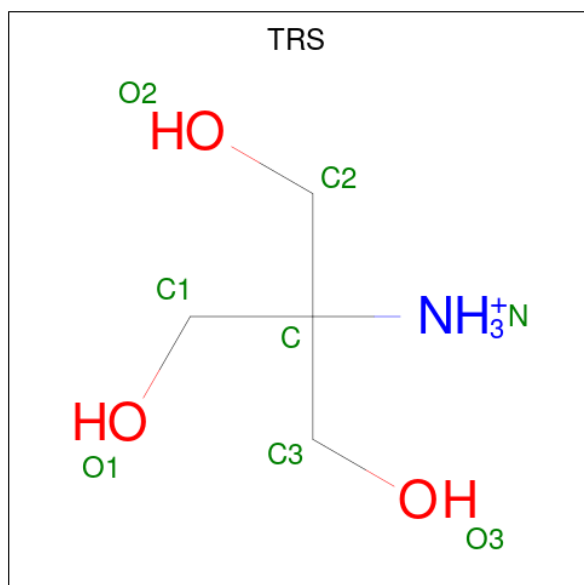
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AGM7
A	1	SER	-	expression tag	UNP P0AGM7
A	320	PRO	GLY	engineered mutation	UNP P0AGM7
A	430	ALA	-	expression tag	UNP P0AGM7
A	431	LEU	-	expression tag	UNP P0AGM7
A	432	GLU	-	expression tag	UNP P0AGM7
A	433	VAL	-	expression tag	UNP P0AGM7
A	434	LEU	-	expression tag	UNP P0AGM7
A	435	PHE	-	expression tag	UNP P0AGM7
A	436	GLN	-	expression tag	UNP P0AGM7
C	0	MET	-	initiating methionine	UNP P0AGM7
C	1	SER	-	expression tag	UNP P0AGM7
C	320	PRO	GLY	engineered mutation	UNP P0AGM7
C	430	ALA	-	expression tag	UNP P0AGM7
C	431	LEU	-	expression tag	UNP P0AGM7
C	432	GLU	-	expression tag	UNP P0AGM7
C	433	VAL	-	expression tag	UNP P0AGM7
C	434	LEU	-	expression tag	UNP P0AGM7
C	435	PHE	-	expression tag	UNP P0AGM7
C	436	GLN	-	expression tag	UNP P0AGM7

- Molecule 2 is a protein called Sy45.

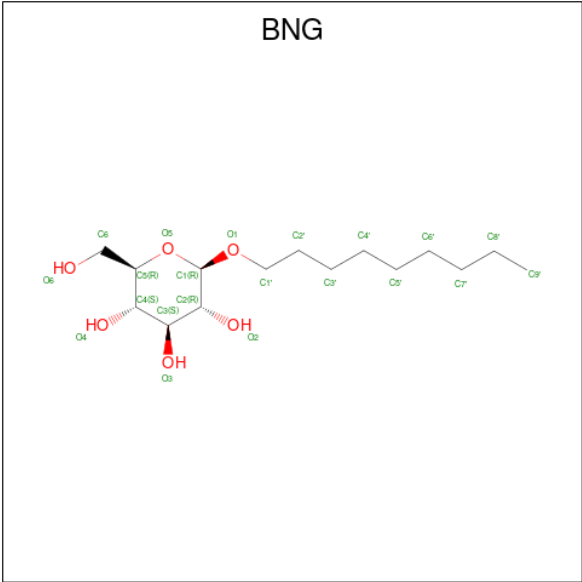
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	0
			963	607	164	188	4			
2	D	126	Total	C	N	O	S	0	0	0
			957	604	163	186	4			

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	A	1	Total	C	O	0	0
			21	15	6		
4	C	1	Total	C	O	0	0
			21	15	6		
4	C	1	Total	C	O	0	0
			21	15	6		
4	C	1	Total	C	O	0	0
			21	15	6		
4	C	1	Total	C	O	0	0
			21	15	6		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).

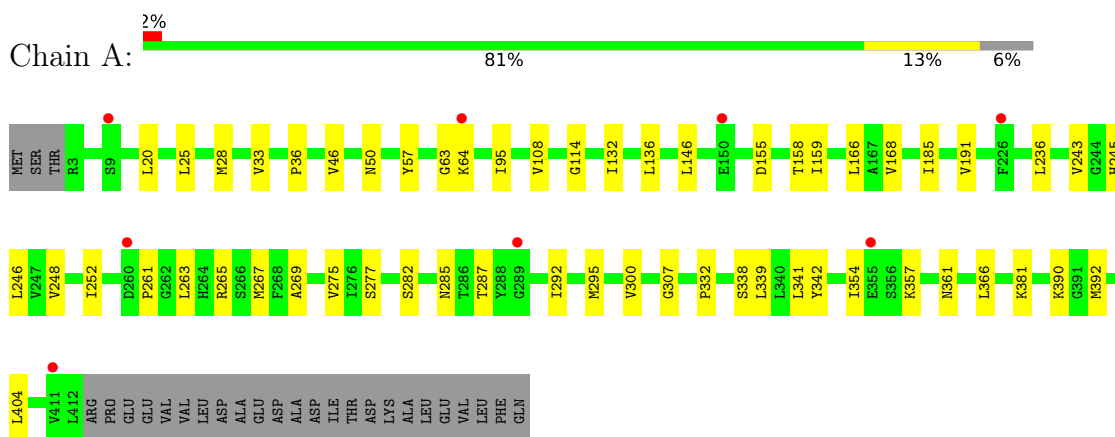
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			33	22	11		
6	D	1	Total	C	O	0	0
			33	22	11		

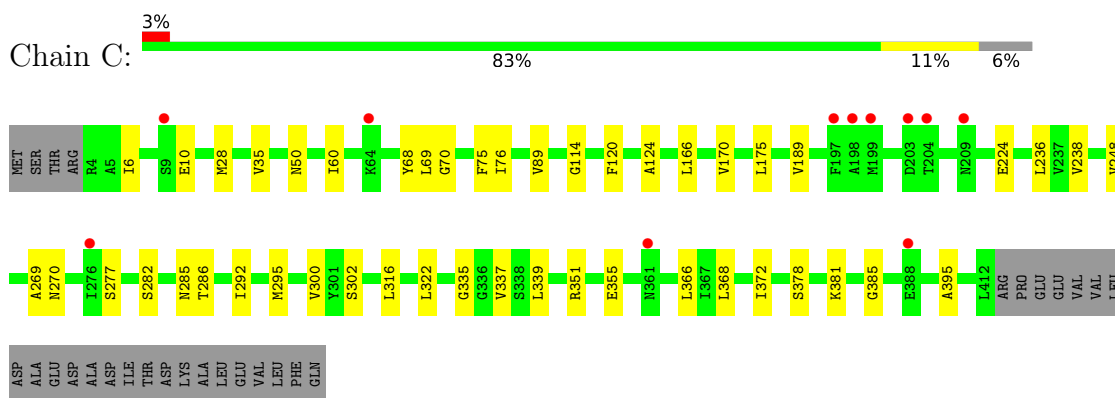
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

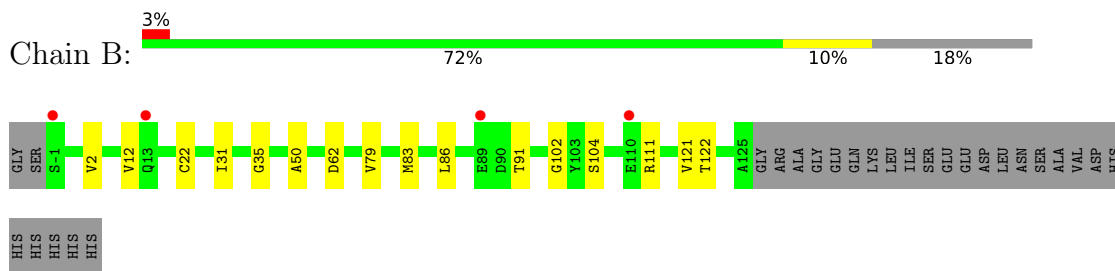
• Molecule 1: Uracil permease



• Molecule 1: Uracil permease



• Molecule 2: Sy45



• Molecule 2: Sy45



GLY	SER	SER	SO	A23	G35	Q39	A40	K43	E44	R45	Y48	A49	A50	V64	N74	T78	T91	S104	R111	T122	A125	GLY	ARG	ALA	GLY	GLU	GLN	LYS	LEU	TLE	SER	GLU	GLU	ASP	LEU	ASN	SER	ALA	VAL	ASP	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.14Å 118.11Å 94.93Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	29.53 – 3.50 29.53 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.53-3.50) 98.2 (29.53-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.05 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.17.1-3660-000	Depositor
R, R_{free}	0.241 , 0.260 0.245 , 0.247	Depositor DCC
R_{free} test set	1142 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 16.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8347	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMU, TRS, BNG, 1PE

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	0.07	0/3096	0.21	0/4229
1	C	0.08	0/3085	0.21	0/4215
2	B	0.06	0/985	0.20	0/1337
2	D	0.07	0/979	0.20	0/1329
All	All	0.07	0/8145	0.21	0/11110

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3030	0	3261	39	0
1	C	3019	0	3248	30	0
2	B	963	0	921	9	0
2	D	957	0	916	7	0
3	A	8	0	12	0	0
3	C	8	0	12	0	0
4	A	147	0	210	6	0
4	C	84	0	120	6	0
5	A	16	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	16	0	22	2	0
6	A	33	0	42	3	0
6	B	33	0	42	3	0
6	D	33	0	42	0	0
All	All	8347	0	8870	88	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 5.

All (88) 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:C:277:SER:HB3	1:C:282:SER:HB3	1.71	0.73
1:C:60:ILE:HG21	1:C:269:ALA:HB2	1.80	0.63
1:A:277:SER:HB3	1:A:282:SER:HB2	1.81	0.62
1:C:316:LEU:HD12	1:C:322:LEU:HD22	1.82	0.61
1:A:158:THR:HG23	1:A:332:PRO:HG3	1.82	0.61
1:C:248:VAL:HG11	5:C:505:1PE:H121	1.82	0.61
1:A:381:LYS:HB3	1:A:390:LYS:HB2	1.83	0.60
1:A:354:ILE:HG12	6:B:201:DMU:H7	1.82	0.59
1:A:307:GLY:HA3	6:A:510:DMU:H25	1.85	0.59
2:D:48:VAL:HG23	2:D:64:VAL:HG21	1.86	0.58
1:A:57:TYR:HA	1:A:269:ALA:HB1	1.85	0.57
1:A:248:VAL:HG21	5:A:508:1PE:H152	1.87	0.57
2:B:104:SER:HB3	2:B:111:ARG:HD2	1.87	0.56
1:A:166:LEU:HD22	1:A:339:LEU:HD23	1.88	0.55
1:C:114:GLY:HA3	4:C:506:BNG:H3	1.88	0.55
1:A:168:VAL:HG21	1:A:191:VAL:HG11	1.88	0.54
1:A:108:VAL:HG21	1:A:267:MET:HE1	1.91	0.53
2:D:39:GLN:HB2	2:D:45:ARG:HG2	1.90	0.53
2:D:104:SER:HB2	2:D:111:ARG:HD2	1.91	0.53
1:A:46:VAL:O	1:A:50:ASN:ND2	2.32	0.53
1:C:372:ILE:HG23	1:C:395:ALA:HB1	1.90	0.52
1:C:69:LEU:HB3	1:C:285:ASN:HB3	1.91	0.52
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.91	0.52
1:A:252:ILE:HD11	5:A:508:1PE:H222	1.90	0.52
5:C:505:1PE:H222	5:C:505:1PE:H252	1.91	0.51
1:C:166:LEU:HD22	1:C:339:LEU:HD23	1.92	0.51
1:A:146:LEU:HD13	4:C:503:BNG:H6'2	1.93	0.50
2:B:83:MET:HE1	2:B:121:VAL:HG11	1.93	0.49
1:C:35:VAL:HG22	1:C:76:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ILE:HA	1:C:295:MET:HE2	1.94	0.49
1:A:243:VAL:HG22	1:A:263:LEU:HD21	1.95	0.49
1:C:70:GLY:O	1:C:285:ASN:HA	2.13	0.49
1:C:6:ILE:HD13	1:C:300:VAL:HG22	1.94	0.48
1:A:261:PRO:HB2	1:A:265:ARG:HD2	1.95	0.48
1:C:270:ASN:HD21	1:C:286:THR:HA	1.78	0.48
1:C:351:ARG:NH1	1:C:355:GLU:OE2	2.47	0.48
1:A:25:LEU:HD12	1:A:28:MET:HE1	1.95	0.48
2:D:91:THR:HG23	2:D:122:THR:HA	1.93	0.48
1:A:64:LYS:HB2	1:A:261:PRO:HD3	1.95	0.48
2:B:91:THR:HG23	2:B:122:THR:HA	1.96	0.48
1:C:170:VAL:HG21	4:C:503:BNG:H7'1	1.96	0.48
1:A:20:LEU:HD13	1:A:300:VAL:HG11	1.95	0.47
2:D:40:ALA:HB3	2:D:43:LYS:HD3	1.96	0.47
1:A:361:ASN:HA	4:A:502:BNG:H5'1	1.96	0.47
1:A:114:GLY:HA3	4:A:505:BNG:H3	1.97	0.47
1:A:185:ILE:HD12	1:A:341:LEU:HD11	1.97	0.46
1:C:189:VAL:HG23	1:C:337:VAL:HG21	1.97	0.46
1:A:245:HIS:ND1	1:A:287:THR:O	2.48	0.46
1:C:50:ASN:CG	1:C:70:GLY:HA2	2.41	0.46
1:A:155:ASP:HB3	1:A:158:THR:HB	1.98	0.45
1:A:146:LEU:HD22	4:C:503:BNG:H4'1	1.97	0.45
2:B:35:GLY:HA2	2:B:50:ALA:HA	1.98	0.45
6:A:510:DMU:H12	6:A:510:DMU:H7	1.55	0.45
1:A:28:MET:HE3	1:A:28:MET:HB3	1.85	0.45
1:A:246:LEU:HD23	1:A:263:LEU:HD13	1.98	0.45
1:A:404:LEU:HD21	4:A:505:BNG:H8'2	1.98	0.45
2:D:35:GLY:HA2	2:D:50:ALA:HA	1.99	0.44
1:C:120:PHE:HZ	1:C:236:LEU:HB3	1.82	0.44
1:A:132:ILE:HD11	1:A:392:MET:HE3	2.00	0.44
2:D:23:ALA:HA	2:D:78:THR:HG22	1.99	0.44
1:A:285:ASN:OD1	1:A:285:ASN:N	2.49	0.44
1:C:28:MET:HE3	1:C:28:MET:HB3	1.89	0.43
1:A:357:LYS:HZ3	6:B:201:DMU:H36	1.83	0.43
1:C:335:GLY:O	1:C:339:LEU:HB2	2.18	0.43
1:A:63:GLY:HA3	6:A:510:DMU:H13	2.00	0.43
1:A:136:LEU:HB3	1:A:342:TYR:CG	2.54	0.43
1:C:124:ALA:HB2	1:C:368:LEU:HD23	2.00	0.43
2:B:2:VAL:HG11	2:B:31:ILE:HD11	2.01	0.42
1:C:10:GLU:O	1:C:302:SER:OG	2.33	0.42
1:C:28:MET:HE2	1:C:68:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ILE:HA	1:A:295:MET:HE2	2.02	0.42
1:A:95:ILE:HG23	1:A:275:VAL:HG13	2.02	0.42
1:A:366:LEU:HD22	4:A:502:BNG:H6'2	2.01	0.42
1:C:381:LYS:HB2	1:C:381:LYS:HE2	1.82	0.42
4:A:502:BNG:H1	1:C:378:SER:HB2	2.00	0.41
2:B:62:ASP:OD2	6:B:201:DMU:O2	2.32	0.41
1:A:159:ILE:HB	1:C:175:LEU:HD21	2.00	0.41
4:A:505:BNG:O6	4:A:505:BNG:O4	2.32	0.41
1:C:75:PHE:CE2	1:C:238:VAL:HG21	2.56	0.41
1:C:89:VAL:HG13	1:C:224:GLU:HG3	2.02	0.41
1:A:33:VAL:C	1:A:36:PRO:HD2	2.46	0.41
1:A:338:SER:HB3	1:A:342:TYR:CE2	2.56	0.41
1:C:368:LEU:O	1:C:372:ILE:HG12	2.21	0.41
4:C:503:BNG:H5'1	4:C:503:BNG:H2'2	1.92	0.41
1:C:366:LEU:HD22	4:C:502:BNG:H7'2	2.01	0.41
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.93	0.40
2:B:22:CYS:HB3	2:B:79:VAL:HG12	2.03	0.40
2:B:102:GLY:O	2:B:111:ARG:NH1	2.54	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 X-ray entries followed by that with respect to entries of similar resolution.

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	408/437 (93%)	395 (97%)	13 (3%)	0	100	100
1	C	407/437 (93%)	391 (96%)	15 (4%)	1 (0%)	43	74
2	B	125/154 (81%)	120 (96%)	5 (4%)	0	100	100
2	D	124/154 (80%)	120 (97%)	4 (3%)	0	100	100
All	All	1064/1182 (90%)	1026 (96%)	37 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	385	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	324/348 (93%)	324 (100%)	0	100	100
1	C	323/348 (93%)	323 (100%)	0	100	100
2	B	98/120 (82%)	98 (100%)	0	100	100
2	D	97/120 (81%)	97 (100%)	0	100	100
All	All	842/936 (90%)	842 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	242	HIS
1	A	270	ASN
1	A	365	ASN
2	B	82	GLN
1	C	24	HIS
1	C	285	ASN
1	C	291	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 ligands 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
4	BNG	A	507	-	21,21,21	0.55	0	26,26,26	1.16	2 (7%)
4	BNG	A	503	-	21,21,21	0.54	0	26,26,26	1.17	2 (7%)
4	BNG	C	504	-	21,21,21	0.54	0	26,26,26	1.14	2 (7%)
5	1PE	A	508	-	15,15,15	0.55	0	14,14,14	0.21	0
5	1PE	C	505	-	15,15,15	0.54	0	14,14,14	0.20	0
6	DMU	D	201	-	34,34,34	0.49	0	45,45,45	0.75	0
6	DMU	B	201	-	34,34,34	0.50	0	45,45,45	0.70	0
4	BNG	C	506	-	21,21,21	0.56	0	26,26,26	1.14	2 (7%)
4	BNG	A	509	-	21,21,21	0.56	0	26,26,26	1.20	2 (7%)
4	BNG	A	502	-	21,21,21	0.54	0	26,26,26	1.19	2 (7%)
3	TRS	A	501	-	7,7,7	0.34	0	9,9,9	0.30	0
4	BNG	C	503	-	21,21,21	0.55	0	26,26,26	1.19	2 (7%)
4	BNG	A	506	-	21,21,21	0.55	0	26,26,26	1.16	2 (7%)
4	BNG	A	505	-	21,21,21	0.54	0	26,26,26	1.16	2 (7%)
6	DMU	A	510	-	34,34,34	0.51	0	45,45,45	0.71	0
3	TRS	C	501	-	7,7,7	0.35	0	9,9,9	0.35	0
4	BNG	A	504	-	21,21,21	0.55	0	26,26,26	1.07	2 (7%)
4	BNG	C	502	-	21,21,21	0.54	0	26,26,26	1.15	2 (7%)

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
4	BNG	A	507	-	-	1/12/32/32	0/1/1/1
4	BNG	A	503	-	-	5/12/32/32	0/1/1/1
4	BNG	C	504	-	-	5/12/32/32	0/1/1/1
5	1PE	A	508	-	-	9/13/13/13	-
5	1PE	C	505	-	-	8/13/13/13	-
6	DMU	D	201	-	-	6/19/59/59	0/2/2/2
6	DMU	B	201	-	-	11/19/59/59	0/2/2/2
4	BNG	C	506	-	-	2/12/32/32	0/1/1/1
4	BNG	A	509	-	-	6/12/32/32	0/1/1/1
4	BNG	A	502	-	-	2/12/32/32	0/1/1/1
3	TRS	A	501	-	-	0/9/9/9	-
4	BNG	C	503	-	-	0/12/32/32	0/1/1/1
4	BNG	A	506	-	-	3/12/32/32	0/1/1/1
4	BNG	A	505	-	-	3/12/32/32	0/1/1/1
6	DMU	A	510	-	-	11/19/59/59	0/2/2/2
3	TRS	C	501	-	-	0/9/9/9	-
4	BNG	A	504	-	-	4/12/32/32	0/1/1/1
4	BNG	C	502	-	-	0/12/32/32	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	BNG	C1'-O1-C1	-4.18	106.53	113.68
4	A	509	BNG	C1'-O1-C1	-4.12	106.65	113.68
4	A	502	BNG	C1'-O1-C1	-4.06	106.74	113.68
4	A	505	BNG	C1'-O1-C1	-3.97	106.89	113.68
4	A	506	BNG	C1'-O1-C1	-3.94	106.95	113.68
4	A	503	BNG	C1'-O1-C1	-3.93	106.97	113.68
4	C	506	BNG	C1'-O1-C1	-3.90	107.02	113.68
4	A	507	BNG	C1'-O1-C1	-3.87	107.08	113.68
4	C	502	BNG	C1'-O1-C1	-3.83	107.13	113.68
4	C	504	BNG	C1'-O1-C1	-3.81	107.17	113.68
4	A	504	BNG	C1'-O1-C1	-3.48	107.73	113.68
4	A	509	BNG	C1-O5-C5	-3.03	107.80	113.72
4	A	507	BNG	C1-O5-C5	-2.96	107.95	113.72
4	A	502	BNG	C1-O5-C5	-2.92	108.02	113.72
4	A	503	BNG	C1-O5-C5	-2.84	108.17	113.72
4	A	506	BNG	C1-O5-C5	-2.78	108.29	113.72
4	C	502	BNG	C1-O5-C5	-2.77	108.31	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	BNG	C1-O5-C5	-2.75	108.36	113.72
4	C	503	BNG	C1-O5-C5	-2.70	108.45	113.72
4	C	504	BNG	C1-O5-C5	-2.67	108.51	113.72
4	C	506	BNG	C1-O5-C5	-2.64	108.57	113.72
4	A	504	BNG	C1-O5-C5	-2.50	108.83	113.72

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	BNG	C2-C1-O1-C1'
4	A	509	BNG	C2'-C1'-O1-C1
6	A	510	DMU	O5-C6-O16-C18
6	B	201	DMU	O1-C10-O7-C3
6	D	201	DMU	C1-C6-O16-C18
6	D	201	DMU	O5-C6-O16-C18
4	A	509	BNG	C4-C5-C6-O6
4	A	502	BNG	O5-C5-C6-O6
6	B	201	DMU	O5-C4-C57-O61
6	A	510	DMU	C2-C3-O7-C10
4	A	509	BNG	O5-C5-C6-O6
4	A	503	BNG	O5-C5-C6-O6
6	A	510	DMU	O5-C4-C57-O61
4	A	502	BNG	C4-C5-C6-O6
6	B	201	DMU	O6-C11-C9-O1
6	A	510	DMU	C3-C4-C57-O61
6	B	201	DMU	C3-C4-C57-O61
6	B	201	DMU	O6-C11-C9-C8
4	A	503	BNG	O5-C1-O1-C1'
4	C	504	BNG	O5-C1-O1-C1'
4	A	504	BNG	C4-C5-C6-O6
4	A	506	BNG	C4-C5-C6-O6
5	C	505	1PE	OH4-C13-C23-OH3
4	C	504	BNG	C2-C1-O1-C1'
4	A	506	BNG	O5-C5-C6-O6
4	A	503	BNG	C4-C5-C6-O6
6	A	510	DMU	O6-C11-C9-O1
4	A	505	BNG	O5-C1-O1-C1'
4	A	509	BNG	O5-C1-O1-C1'
4	A	504	BNG	O5-C5-C6-O6
5	C	505	1PE	OH5-C14-C24-OH4
4	A	505	BNG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	505	BNG	C2-C1-O1-C1'
4	A	509	BNG	C2-C1-O1-C1'
5	A	508	1PE	OH6-C15-C25-OH5
4	C	506	BNG	C3'-C4'-C5'-C6'
4	A	509	BNG	O1-C1'-C2'-C3'
6	A	510	DMU	C28-C31-C34-C37
6	A	510	DMU	C19-C22-C25-C28
6	A	510	DMU	C18-C19-C22-C25
5	C	505	1PE	OH6-C15-C25-OH5
4	A	507	BNG	O5-C5-C6-O6
4	C	506	BNG	O5-C5-C6-O6
6	A	510	DMU	C4-C3-O7-C10
6	A	510	DMU	C22-C25-C28-C31
5	A	508	1PE	OH4-C13-C23-OH3
6	D	201	DMU	C22-C25-C28-C31
5	A	508	1PE	OH5-C14-C24-OH4
4	A	504	BNG	C1'-C2'-C3'-C4'
5	C	505	1PE	C24-C14-OH5-C25
6	A	510	DMU	O6-C11-C9-C8
5	C	505	1PE	C14-C24-OH4-C13
6	B	201	DMU	C25-C28-C31-C34
6	D	201	DMU	C28-C31-C34-C37
5	A	508	1PE	C14-C24-OH4-C13
4	C	504	BNG	C4-C5-C6-O6
5	A	508	1PE	C12-C22-OH3-C23
5	A	508	1PE	C15-C25-OH5-C14
6	B	201	DMU	C19-C22-C25-C28
5	A	508	1PE	C16-C26-OH6-C15
6	D	201	DMU	C31-C34-C37-C40
5	C	505	1PE	C12-C22-OH3-C23
4	C	504	BNG	C2'-C1'-O1-C1
6	D	201	DMU	C19-C18-O16-C6
5	A	508	1PE	C23-C13-OH4-C24
5	A	508	1PE	C24-C14-OH5-C25
4	A	504	BNG	C2'-C3'-C4'-C5'
4	A	506	BNG	O5-C1-O1-C1'
4	A	503	BNG	C1'-C2'-C3'-C4'
5	C	505	1PE	C23-C13-OH4-C24
6	B	201	DMU	C28-C31-C34-C37
6	B	201	DMU	O5-C6-O16-C18
6	B	201	DMU	C19-C18-O16-C6
6	B	201	DMU	C1-C6-O16-C18

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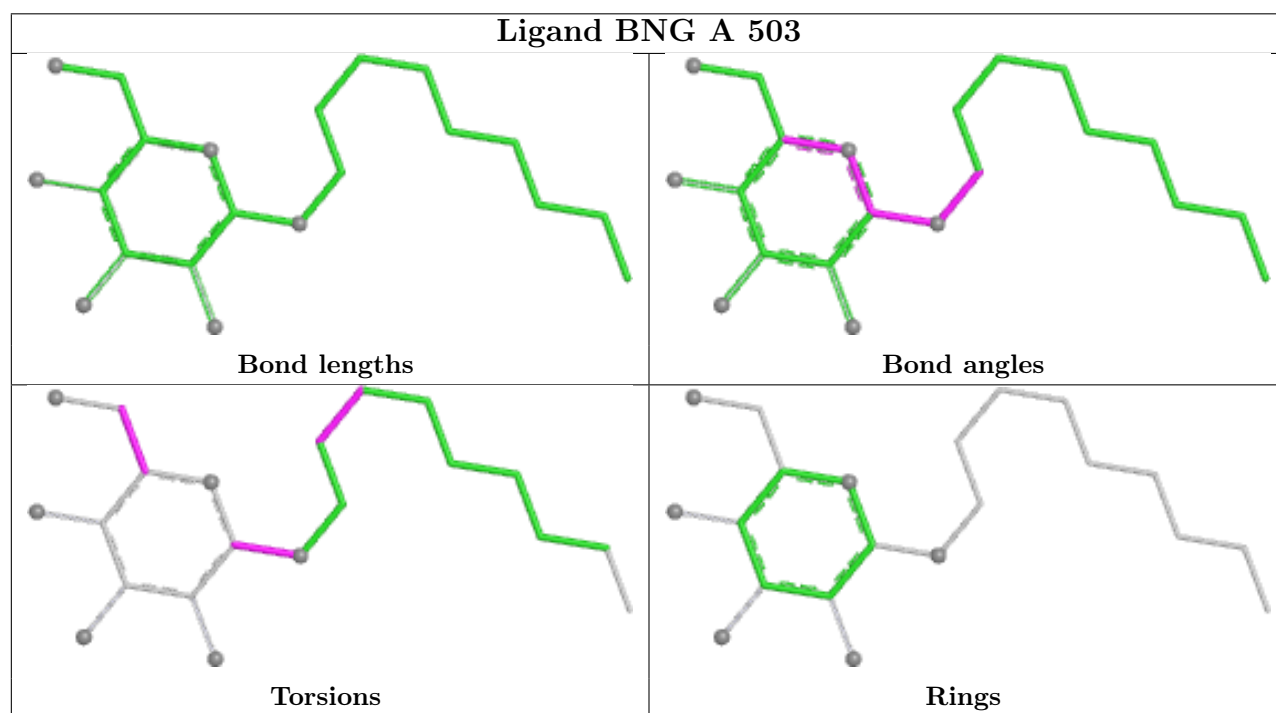
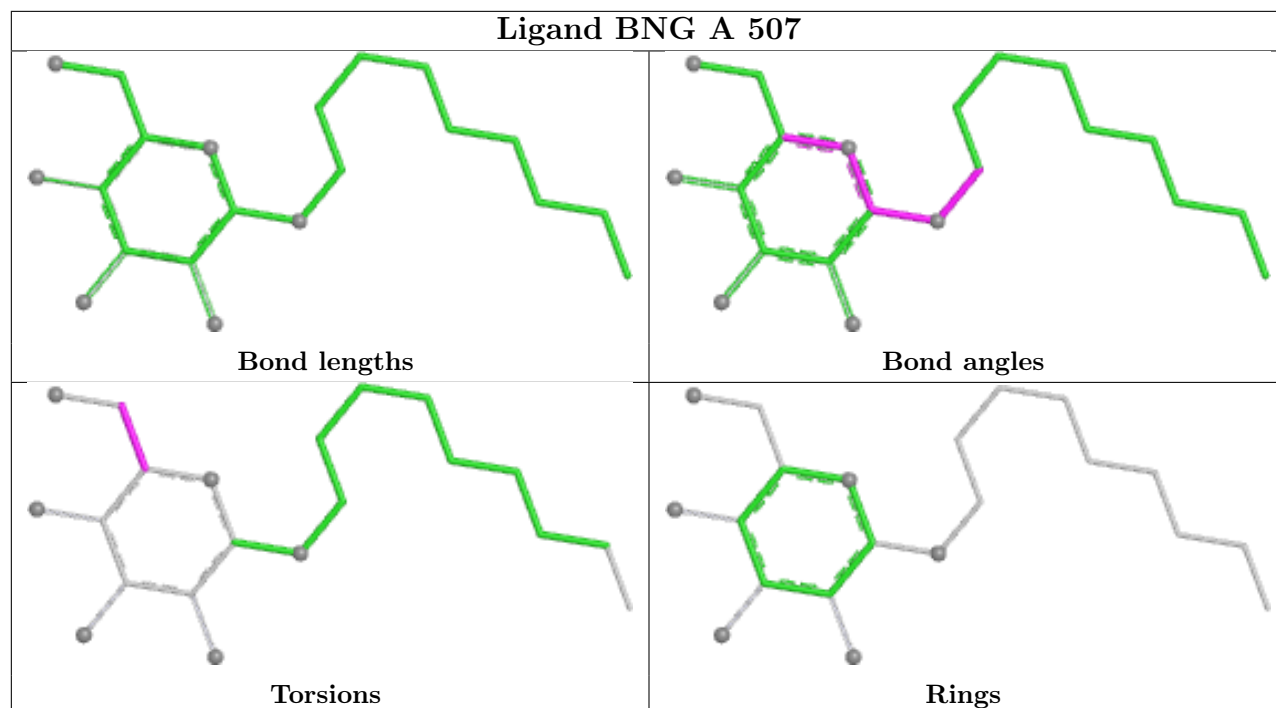
Mol	Chain	Res	Type	Atoms
5	C	505	1PE	OH7-C16-C26-OH6
4	C	504	BNG	O5-C5-C6-O6

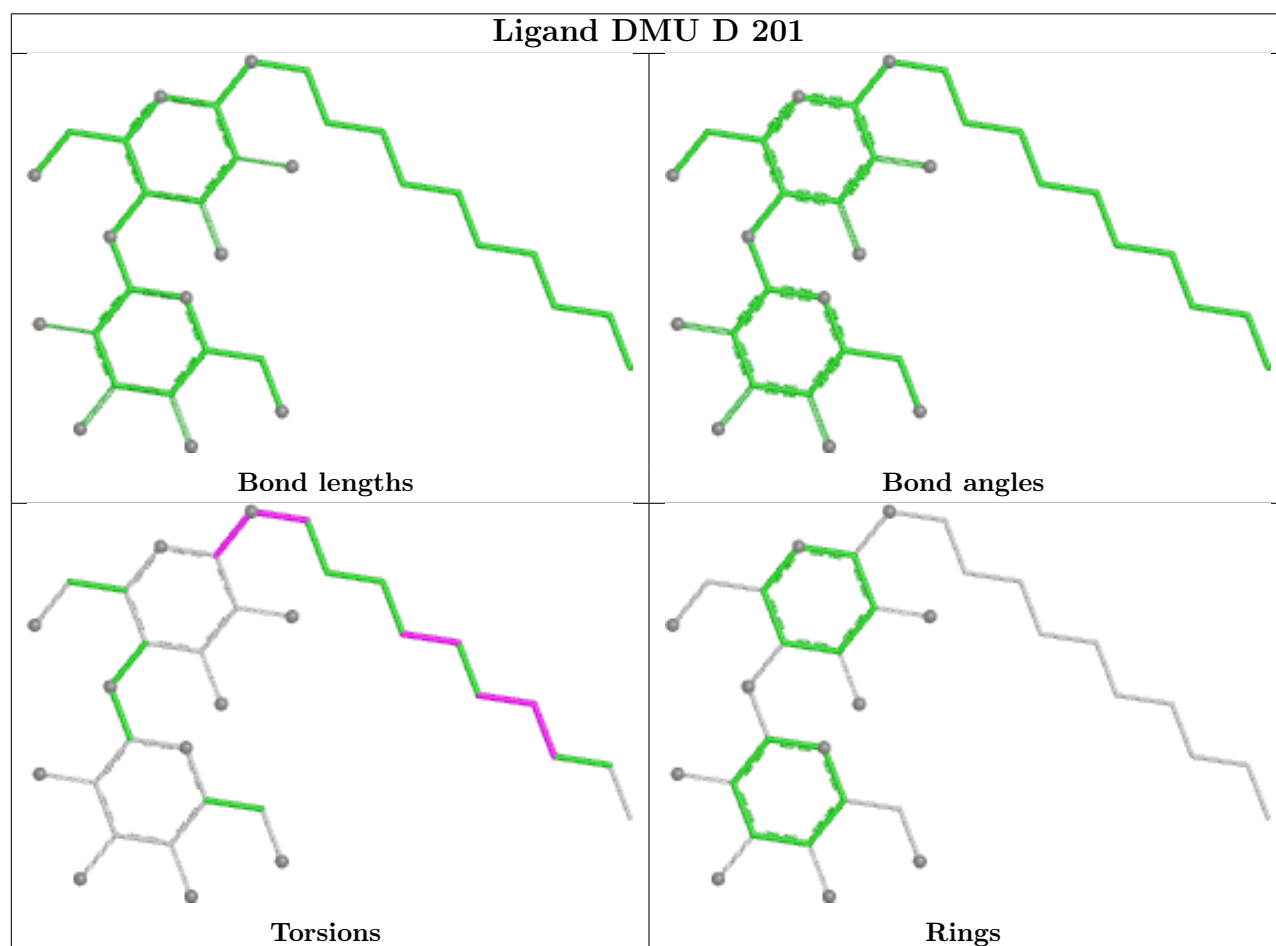
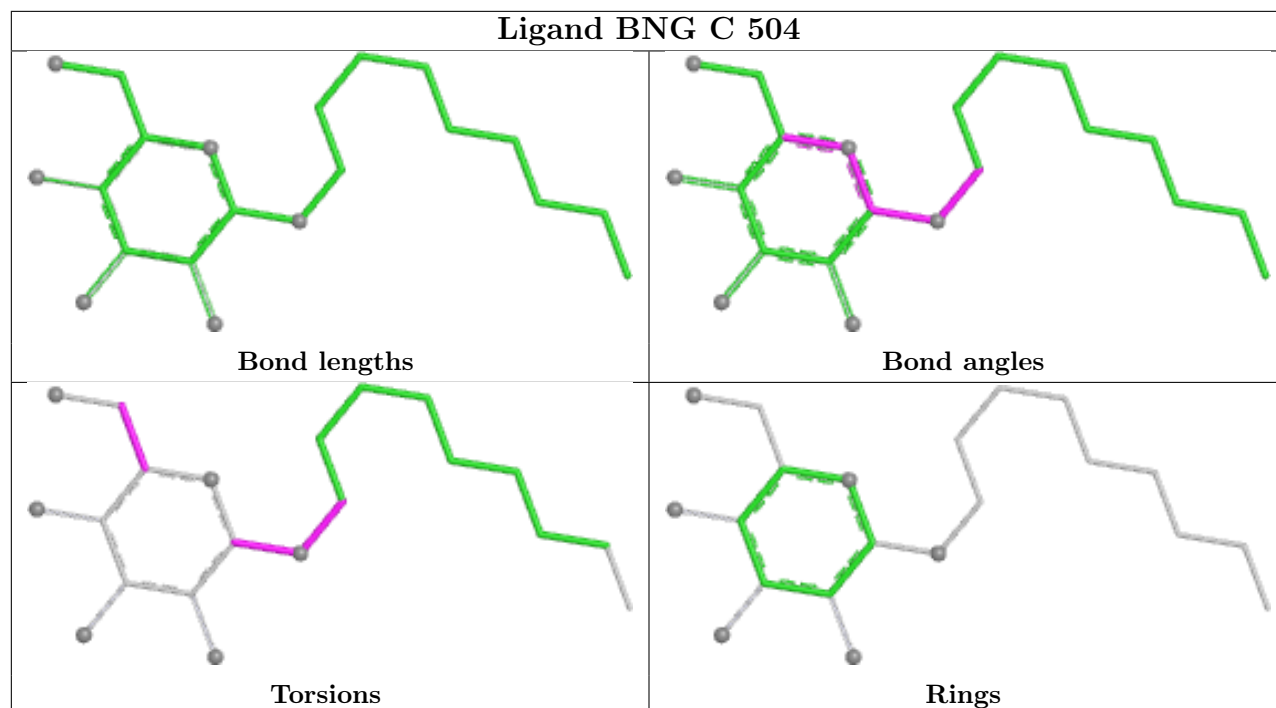
There are no ring outliers.

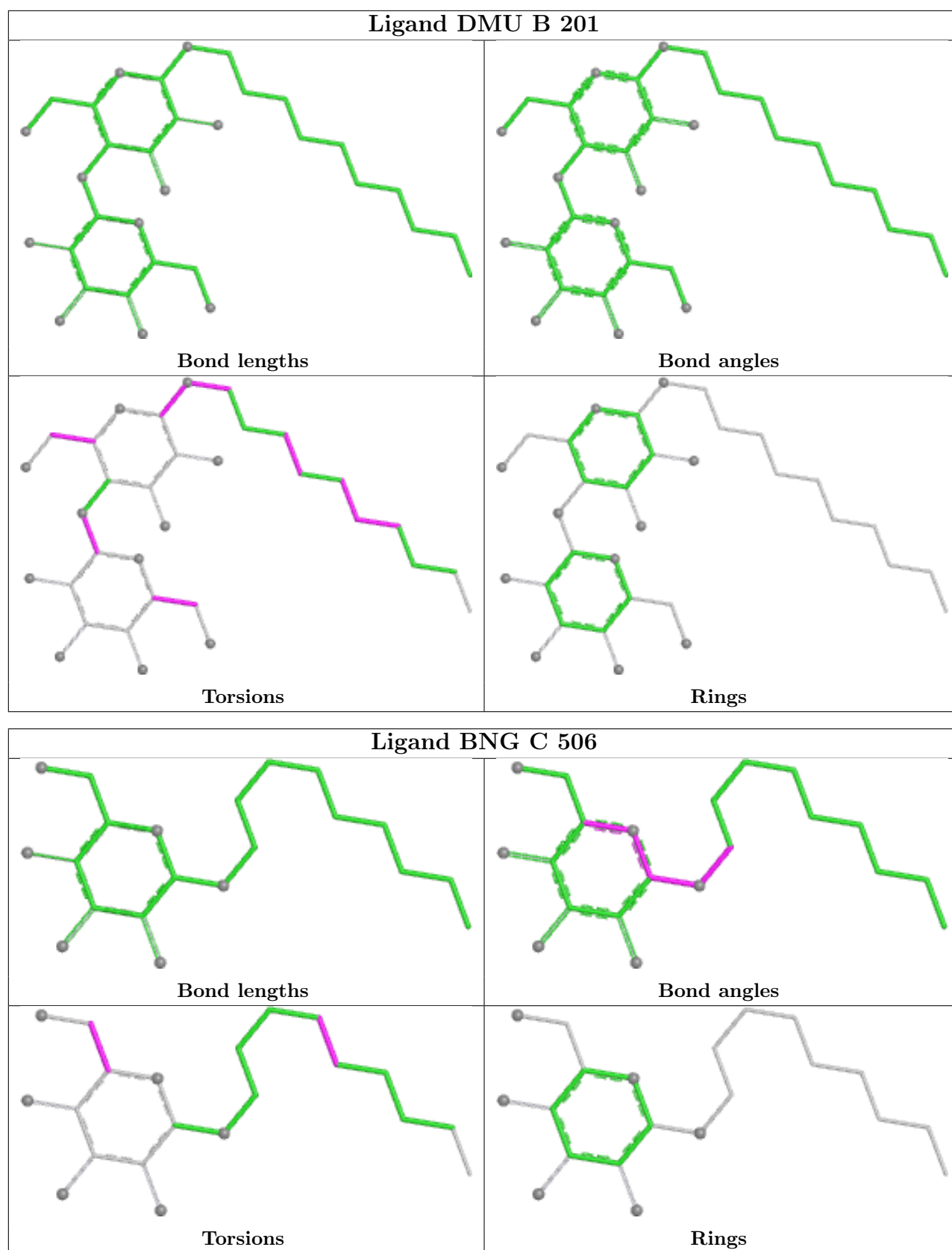
9 monomers are involved in 22 short contacts:

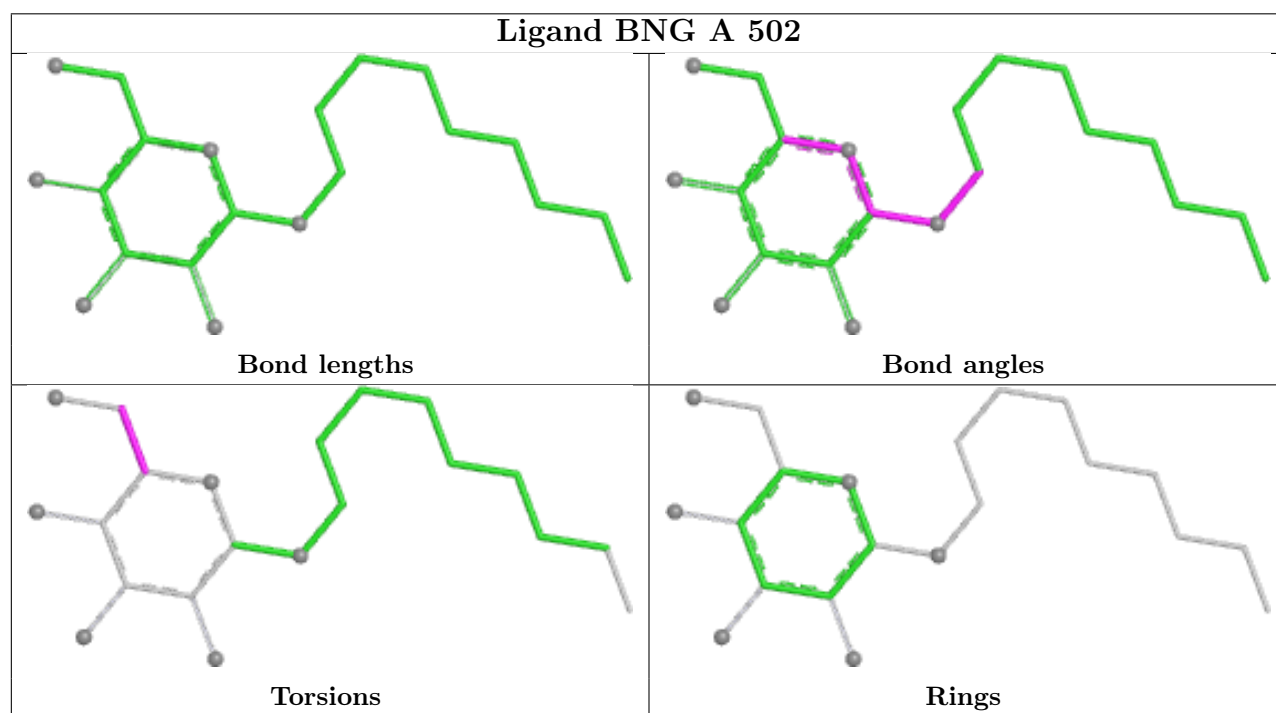
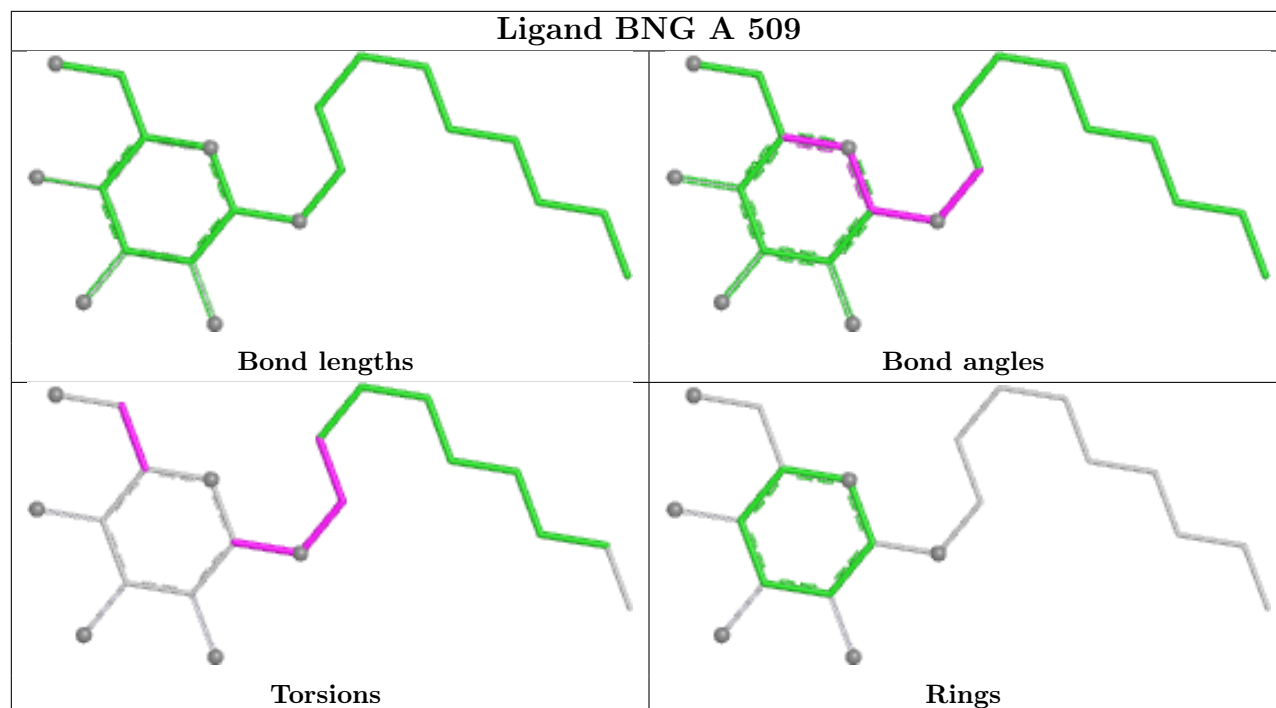
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	1PE	2	0
5	C	505	1PE	2	0
6	B	201	DMU	3	0
4	C	506	BNG	1	0
4	A	502	BNG	3	0
4	C	503	BNG	4	0
4	A	505	BNG	3	0
6	A	510	DMU	3	0
4	C	502	BNG	1	0

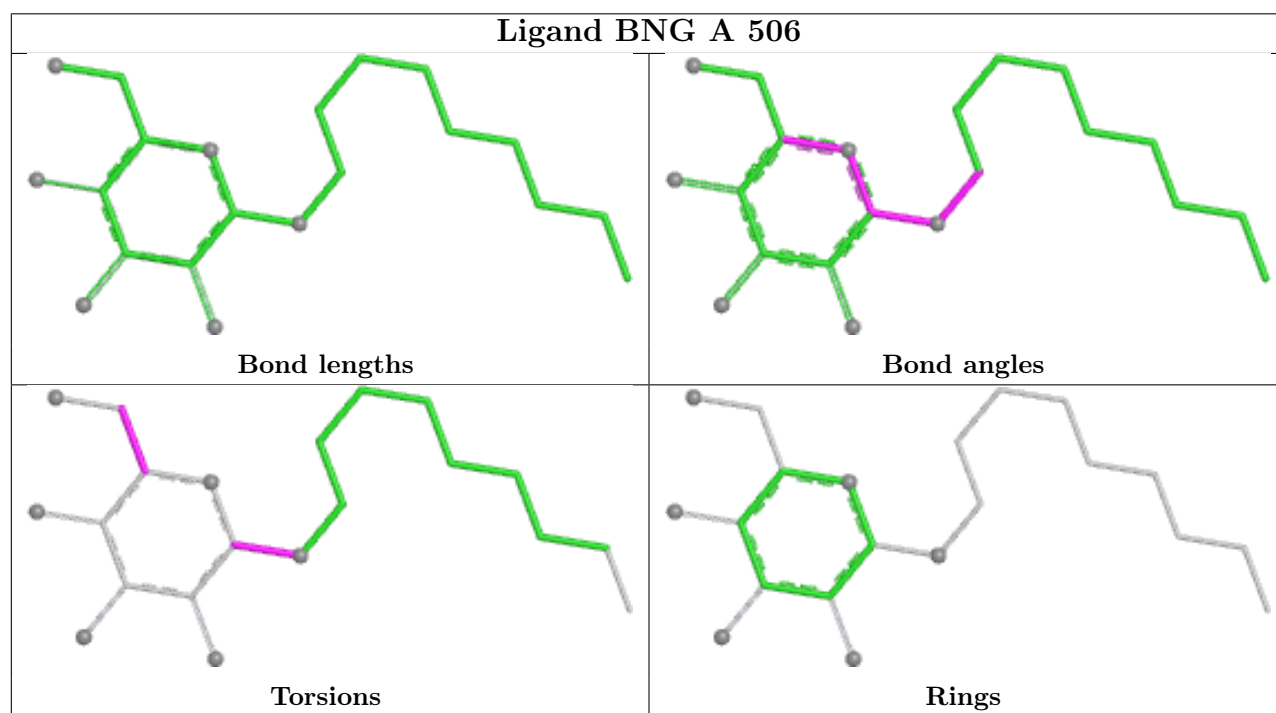
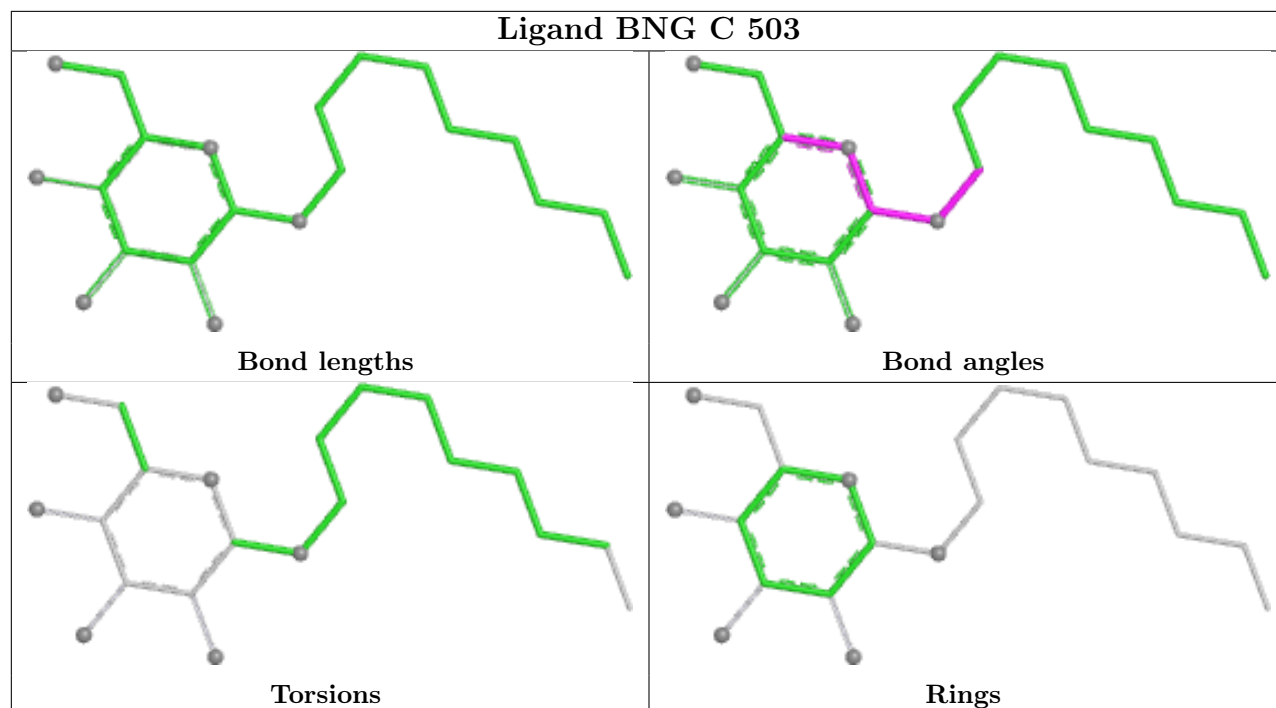
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

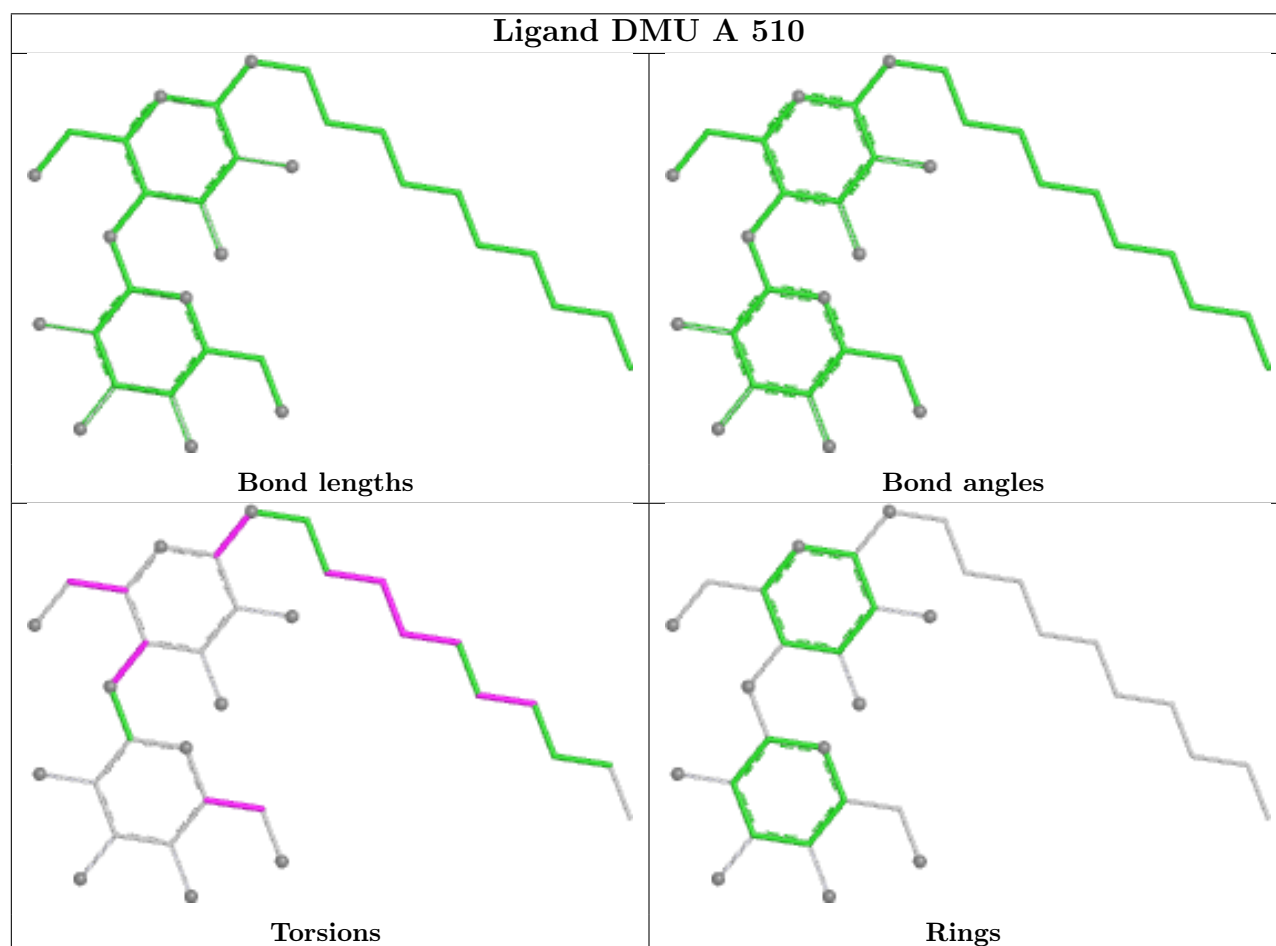
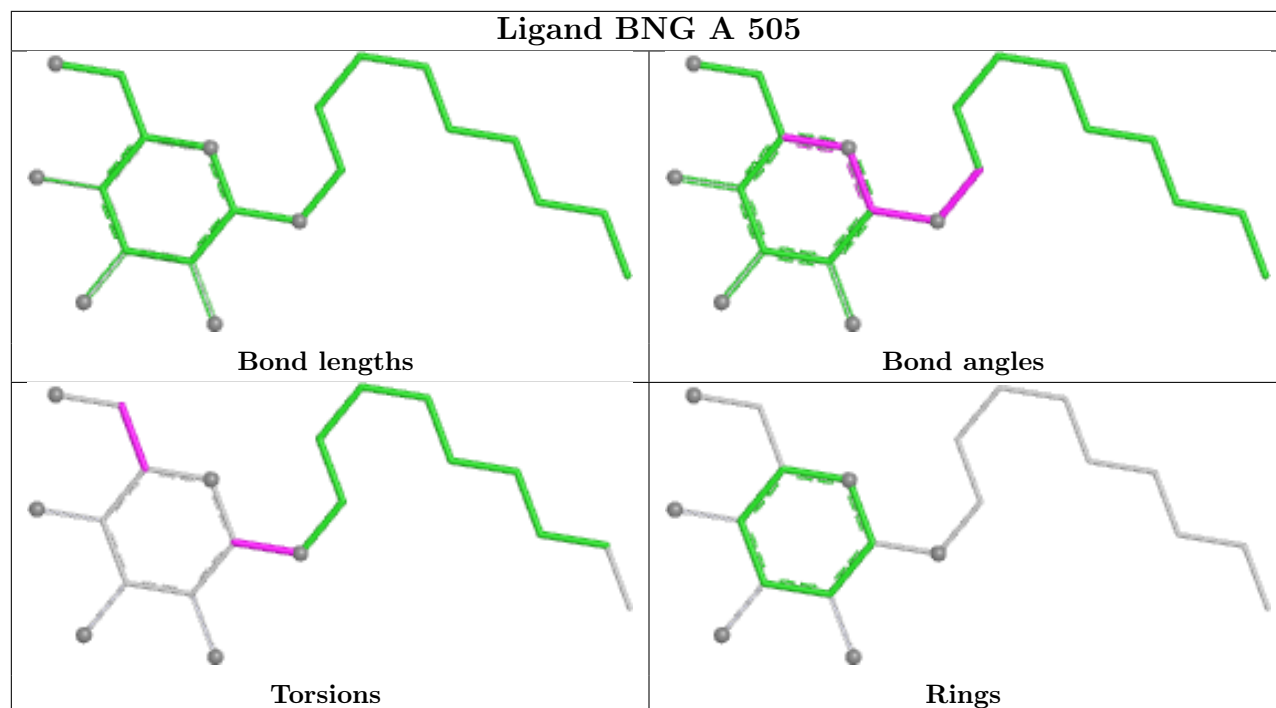


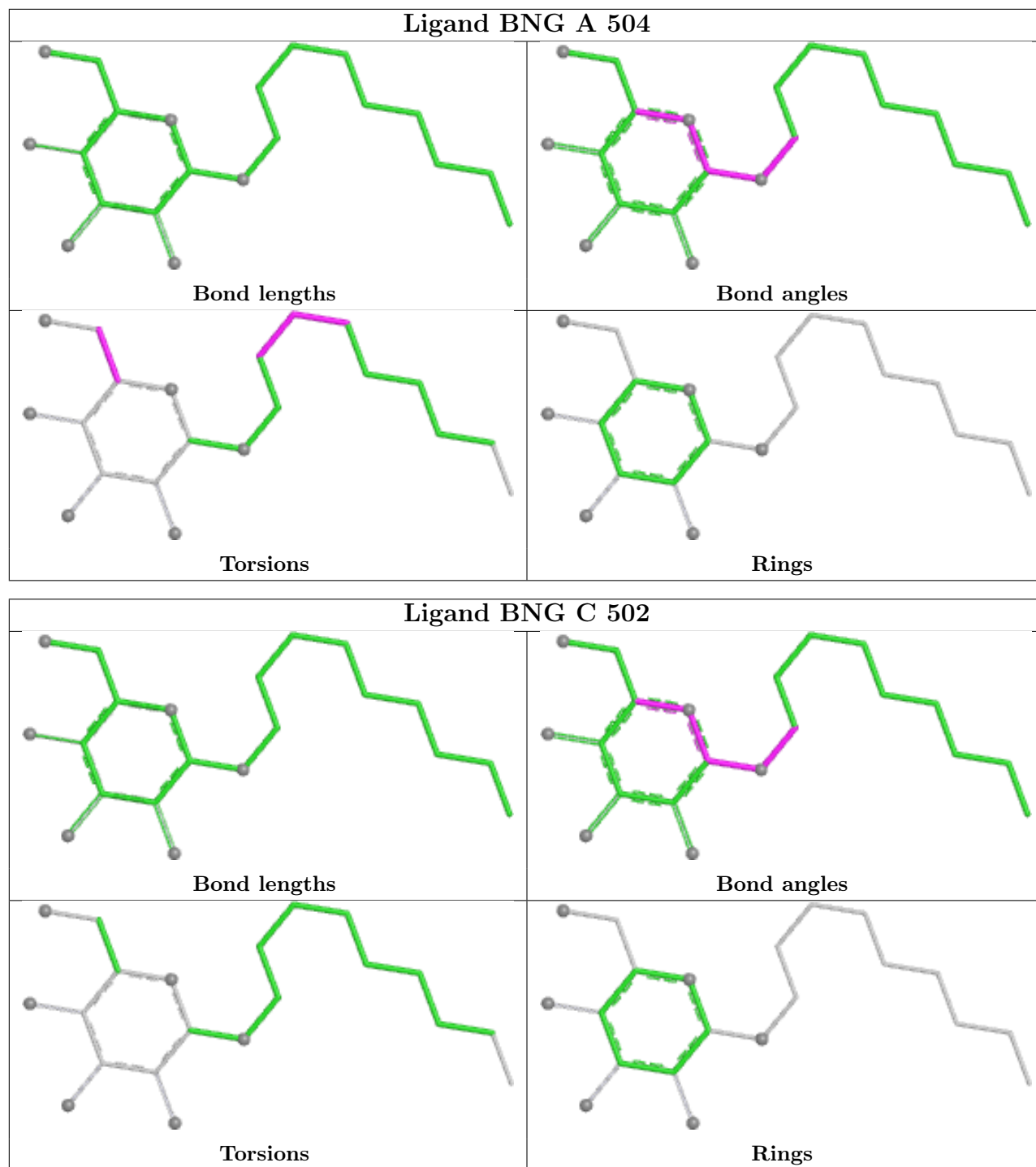












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	410/437 (93%)	0.24	8 (1%) 65 39	37, 61, 98, 129	0
1	C	409/437 (93%)	0.30	11 (2%) 56 33	38, 65, 102, 143	0
2	B	127/154 (82%)	0.41	4 (3%) 51 29	46, 66, 94, 109	0
2	D	126/154 (81%)	0.43	1 (0%) 82 60	50, 65, 92, 120	0
All	All	1072/1182 (90%)	0.31	24 (2%) 62 37	37, 64, 101, 143	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	MET	4.5
2	D	74	ASN	4.5
1	C	64	LYS	4.3
1	C	388	GLU	4.1
1	C	9	SER	3.9
2	B	89	GLU	3.6
1	A	260	ASP	3.4
1	C	198	ALA	3.4
1	C	276	ILE	3.4
1	C	203	ASP	3.3
1	A	9	SER	3.1
1	C	209	ASN	3.0
1	C	204	THR	2.8
1	A	64	LYS	2.6
2	B	13	GLN	2.5
1	A	226	PHE	2.3
1	A	150	GLU	2.3
2	B	110	GLU	2.3
1	A	411	VAL	2.3
2	B	-1	SER	2.3
1	A	355	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	197	PHE	2.1
1	C	361	ASN	2.0
1	A	289	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

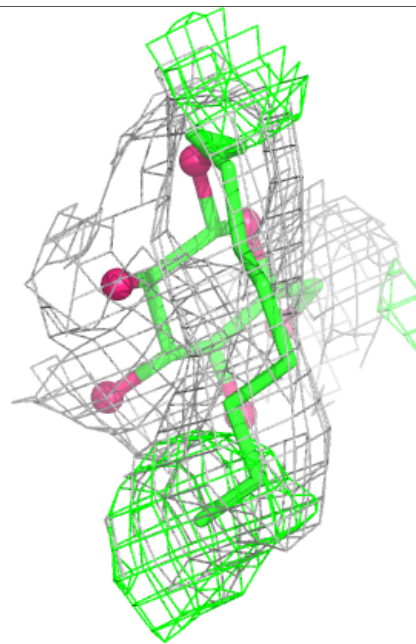
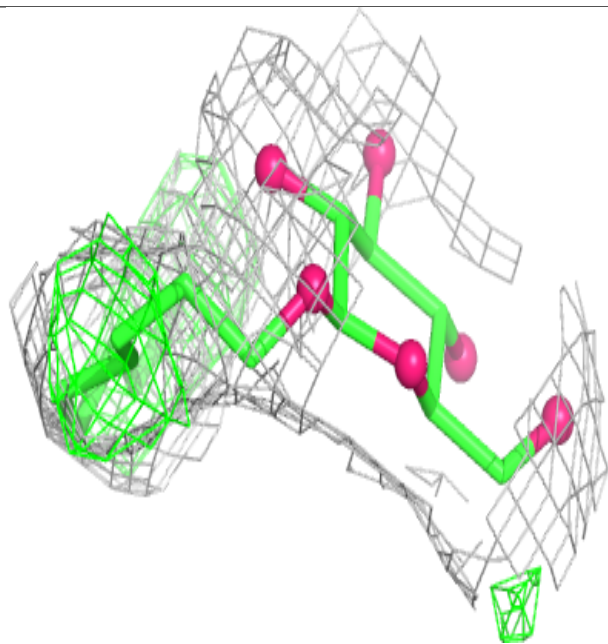
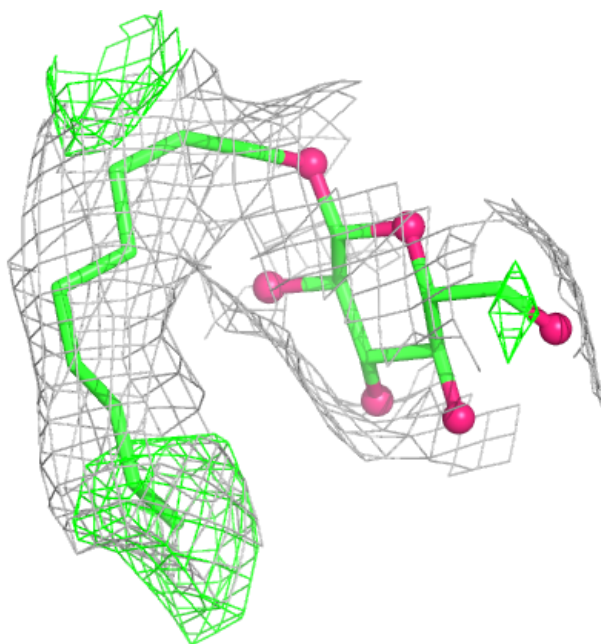
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BNG	A	509	21/21	0.66	0.19	94,101,102,104	0
6	DMU	A	510	33/33	0.71	0.20	93,97,98,99	0
4	BNG	C	506	21/21	0.72	0.20	82,84,84,85	0
4	BNG	A	505	21/21	0.75	0.18	52,79,89,91	0
5	1PE	C	505	16/16	0.78	0.23	61,62,69,69	0
4	BNG	A	507	21/21	0.80	0.16	41,59,95,101	0
5	1PE	A	508	16/16	0.82	0.20	69,71,77,78	0
4	BNG	A	506	21/21	0.83	0.16	63,95,118,124	0
6	DMU	D	201	33/33	0.86	0.12	32,52,76,102	0
4	BNG	C	504	21/21	0.87	0.19	36,60,81,93	0
4	BNG	A	503	21/21	0.87	0.17	34,61,86,98	0
6	DMU	B	201	33/33	0.87	0.13	34,53,78,86	0
4	BNG	C	503	21/21	0.87	0.13	37,66,83,87	0
4	BNG	A	504	21/21	0.90	0.11	40,59,74,77	0
4	BNG	A	502	21/21	0.92	0.11	39,47,85,97	0
3	TRS	A	501	8/8	0.92	0.18	37,46,50,71	0
3	TRS	C	501	8/8	0.92	0.14	41,41,42,46	0
4	BNG	C	502	21/21	0.95	0.11	42,58,81,93	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

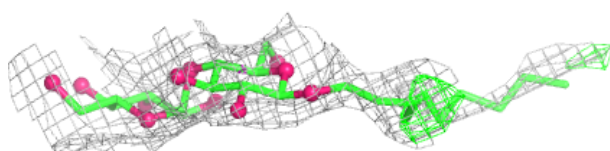
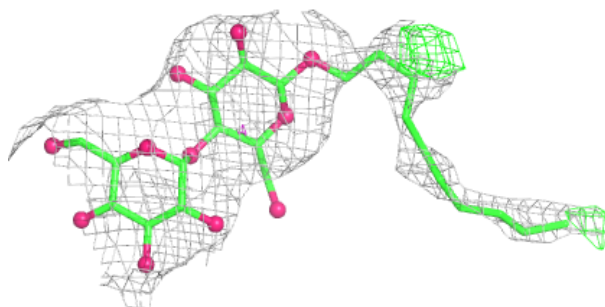
Electron density around BNG A 509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

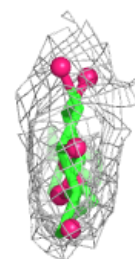
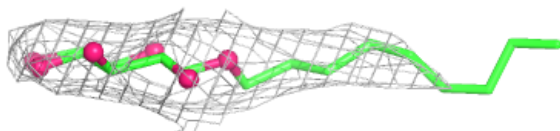
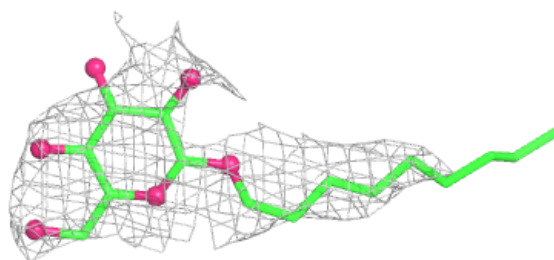


Electron density around DMU A 510:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

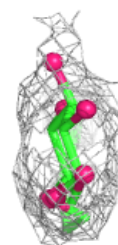
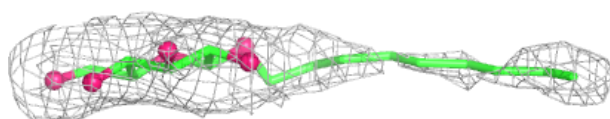
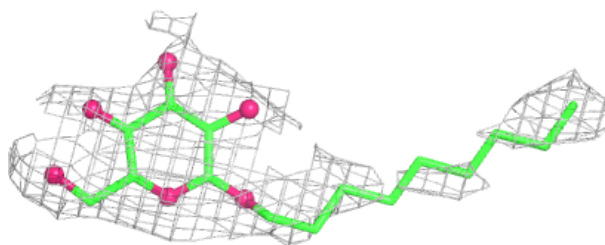
**Electron density around BNG C 506:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

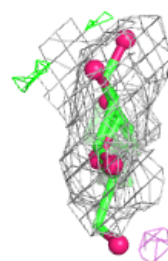
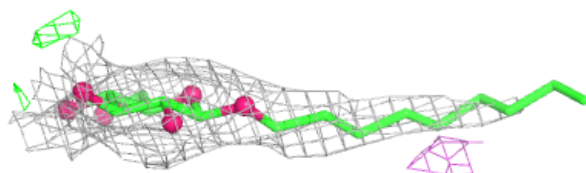
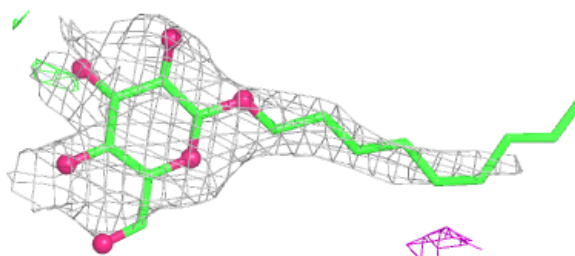


Electron density around BNG A 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

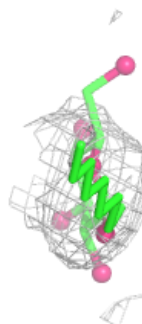
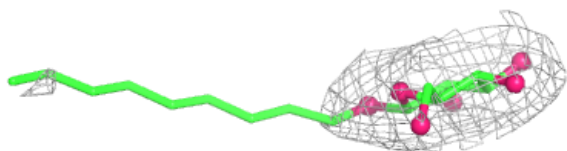
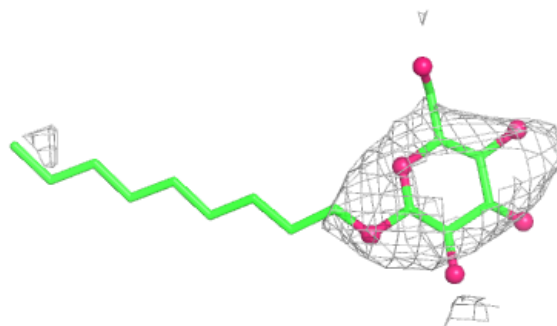
**Electron density around BNG A 507:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

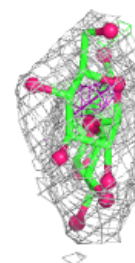
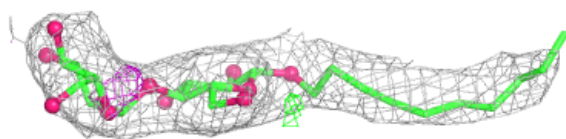
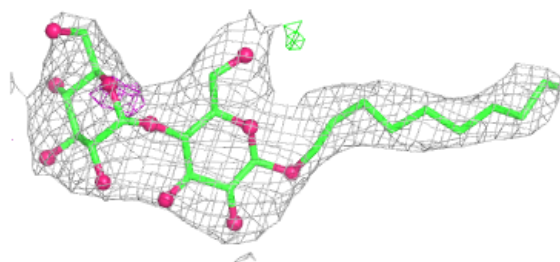


Electron density around BNG A 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

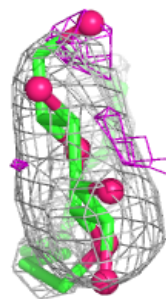
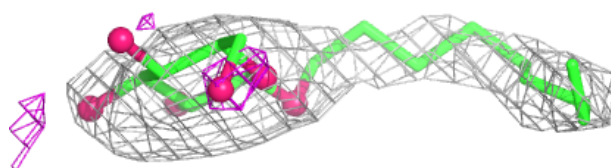
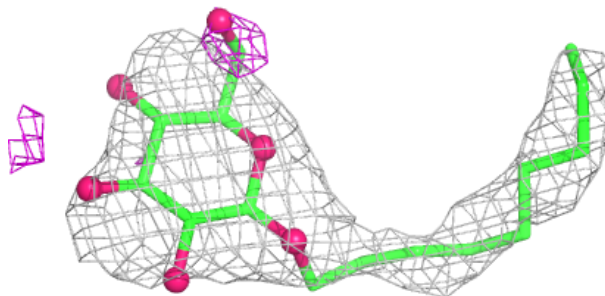
**Electron density around DMU D 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

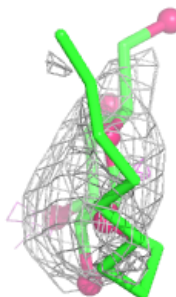
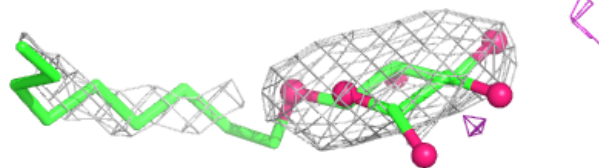
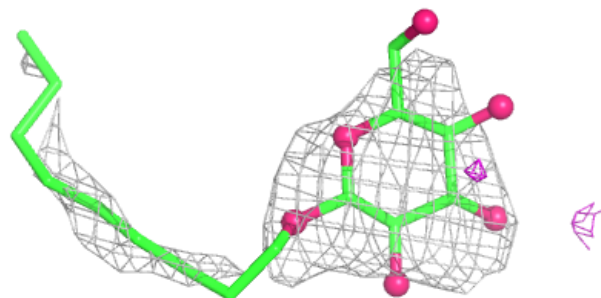


Electron density around BNG C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

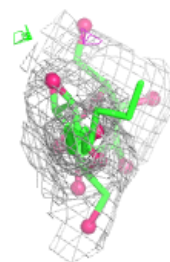
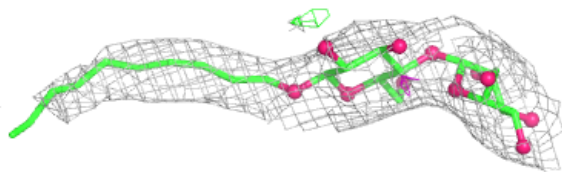
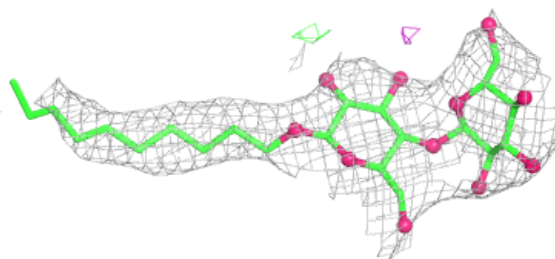
**Electron density around BNG A 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

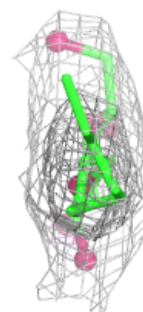
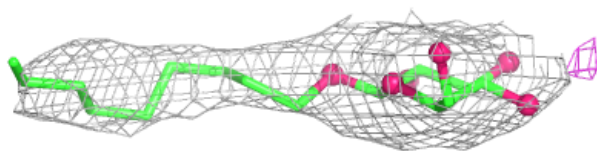
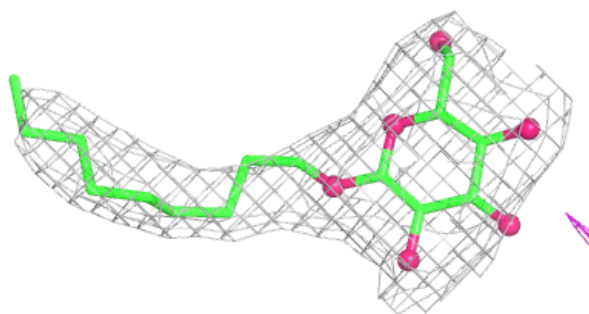


Electron density around DMU B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

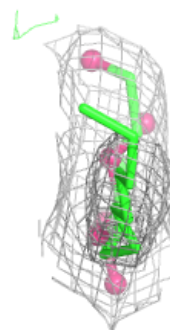
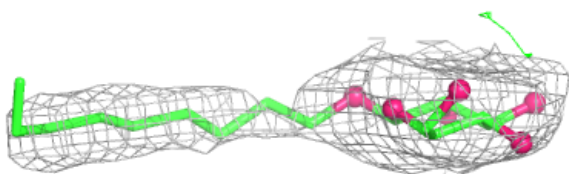
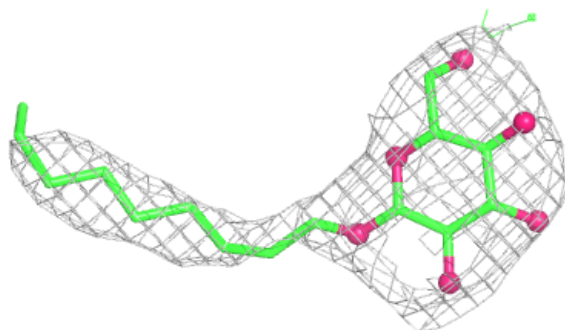
**Electron density around BNG C 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

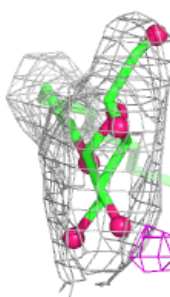
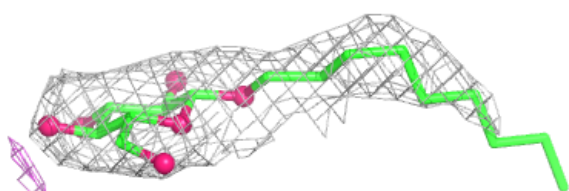
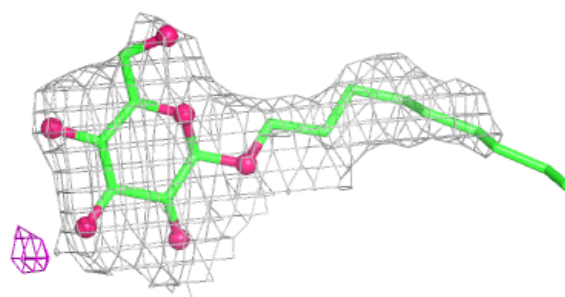


Electron density around BNG A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

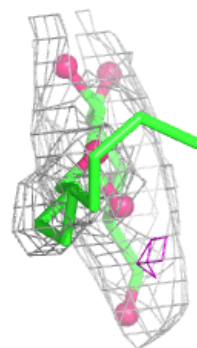
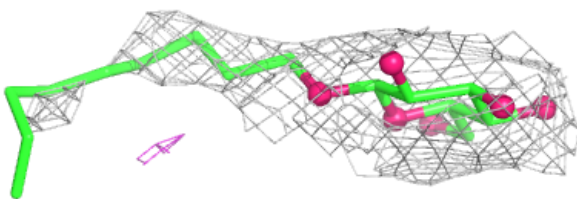
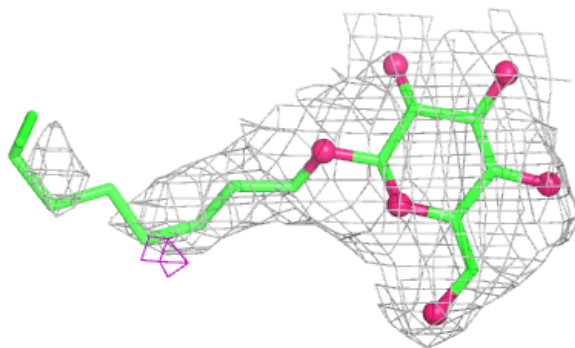
**Electron density around BNG A 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BNG C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.