



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:40 AM UTC

PDB ID : 6YVR / pdb_00006yvr
Title : Crystal structure of the neurotensin receptor 1 in complex with the peptide full agonist NTS8-13
Authors : Deluigi, M.; Merklinger, L.; Hilge, M.; Ernst, P.; Klipp, A.; Klenk, C.; Plueckthun, A.
Deposited on : 2020-04-28
Resolution : 2.46 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

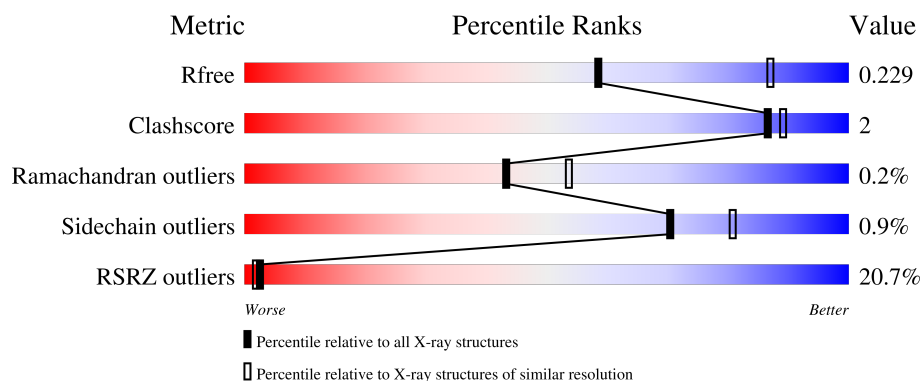
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	AAA	482	20% 91% 7%
1	BBB	482	20% 91% 6%
2	CCC	8	50% 88% 12%
2	DDD	8	12% 88% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14715 atoms, of which 7365 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 Neurotensin receptor type 1, Neurotensin receptor type 1, DARPin crystallisation chaperone.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	470	Total	C	H	N	O	S	190	0	0
			7008	2274	3502	591	627	14			
1	BBB	470	Total	C	H	N	O	S	193	0	0
			6975	2266	3479	589	627	14			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	46	GLY	-	expression tag	UNP P20789
AAA	47	PRO	-	expression tag	UNP P20789
AAA	48	GLY	-	expression tag	UNP P20789
AAA	49	SER	-	expression tag	UNP P20789
AAA	83	GLY	SER	engineered mutation	UNP P20789
AAA	86	LEU	ALA	engineered mutation	UNP P20789
AAA	101	ARG	THR	engineered mutation	UNP P20789
AAA	103	ASP	HIS	engineered mutation	UNP P20789
AAA	105	TYR	HIS	engineered mutation	UNP P20789
AAA	119	PHE	LEU	engineered mutation	UNP P20789
AAA	121	LEU	MET	engineered mutation	UNP P20789
AAA	124	ASP	GLU	engineered mutation	UNP P20789
AAA	143	LYS	ARG	engineered mutation	UNP P20789
AAA	150	GLU	ASP	engineered mutation	UNP P20789
AAA	161	VAL	ALA	engineered mutation	UNP P20789
AAA	167	LEU	ARG	engineered mutation	UNP P20789
AAA	213	LEU	ARG	engineered mutation	UNP P20789
AAA	234	LEU	VAL	engineered mutation	UNP P20789
AAA	235	ARG	LYS	engineered mutation	UNP P20789
AAA	240	LEU	VAL	engineered mutation	UNP P20789
AAA	253	ALA	ILE	engineered mutation	UNP P20789
AAA	260	ALA	ILE	engineered mutation	UNP P20789
AAA	262	ARG	ASN	engineered mutation	UNP P20789
AAA	263	ARG	LYS	engineered mutation	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	GLU	deletion	UNP P20789
AAA	?	-	GLN	deletion	UNP P20789
AAA	?	-	GLY	deletion	UNP P20789
AAA	?	-	ARG	deletion	UNP P20789
AAA	?	-	VAL	deletion	UNP P20789
AAA	?	-	CYS	deletion	UNP P20789
AAA	?	-	THR	deletion	UNP P20789
AAA	?	-	VAL	deletion	UNP P20789
AAA	?	-	GLY	deletion	UNP P20789
AAA	?	-	THR	deletion	UNP P20789
AAA	?	-	HIS	deletion	UNP P20789
AAA	?	-	ASN	deletion	UNP P20789
AAA	?	-	GLY	deletion	UNP P20789
AAA	?	-	LEU	deletion	UNP P20789
AAA	?	-	GLU	deletion	UNP P20789
AAA	?	-	HIS	deletion	UNP P20789
AAA	?	-	SER	deletion	UNP P20789
AAA	?	-	THR	deletion	UNP P20789
AAA	305	ARG	HIS	engineered mutation	UNP P20789
AAA	332	VAL	CYS	engineered mutation	UNP P20789
AAA	342	ALA	PHE	engineered mutation	UNP P20789
AAA	354	SER	THR	engineered mutation	UNP P20789
AAA	358	VAL	PHE	engineered mutation	UNP P20789
AAA	362	ALA	SER	engineered mutation	UNP P20789
AAA	372	ALA	-	linker	UNP P20789
AAA	373	GLU	-	linker	UNP P20789
AAA	374	ASP	-	linker	UNP P20789
AAA	375	LEU	-	linker	UNP P20789
AAA	376	VAL	-	linker	UNP P20789
AAA	377	GLU	-	linker	UNP P20789
AAA	378	ASP	-	linker	UNP P20789
AAA	379	TRP	-	linker	UNP P20789
AAA	380	GLU	-	linker	UNP P20789
BBB	46	GLY	-	expression tag	UNP P20789
BBB	47	PRO	-	expression tag	UNP P20789
BBB	48	GLY	-	expression tag	UNP P20789
BBB	49	SER	-	expression tag	UNP P20789
BBB	83	GLY	SER	engineered mutation	UNP P20789
BBB	86	LEU	ALA	engineered mutation	UNP P20789
BBB	101	ARG	THR	engineered mutation	UNP P20789
BBB	103	ASP	HIS	engineered mutation	UNP P20789
BBB	105	TYR	HIS	engineered mutation	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	119	PHE	LEU	engineered mutation	UNP P20789
BBB	121	LEU	MET	engineered mutation	UNP P20789
BBB	124	ASP	GLU	engineered mutation	UNP P20789
BBB	143	LYS	ARG	engineered mutation	UNP P20789
BBB	150	GLU	ASP	engineered mutation	UNP P20789
BBB	161	VAL	ALA	engineered mutation	UNP P20789
BBB	167	LEU	ARG	engineered mutation	UNP P20789
BBB	213	LEU	ARG	engineered mutation	UNP P20789
BBB	234	LEU	VAL	engineered mutation	UNP P20789
BBB	235	ARG	LYS	engineered mutation	UNP P20789
BBB	240	LEU	VAL	engineered mutation	UNP P20789
BBB	253	ALA	ILE	engineered mutation	UNP P20789
BBB	260	ALA	ILE	engineered mutation	UNP P20789
BBB	262	ARG	ASN	engineered mutation	UNP P20789
BBB	263	ARG	LYS	engineered mutation	UNP P20789
BBB	?	-	GLU	deletion	UNP P20789
BBB	?	-	GLN	deletion	UNP P20789
BBB	?	-	GLY	deletion	UNP P20789
BBB	?	-	ARG	deletion	UNP P20789
BBB	?	-	VAL	deletion	UNP P20789
BBB	?	-	CYS	deletion	UNP P20789
BBB	?	-	THR	deletion	UNP P20789
BBB	?	-	VAL	deletion	UNP P20789
BBB	?	-	GLY	deletion	UNP P20789
BBB	?	-	THR	deletion	UNP P20789
BBB	?	-	HIS	deletion	UNP P20789
BBB	?	-	ASN	deletion	UNP P20789
BBB	?	-	GLY	deletion	UNP P20789
BBB	?	-	LEU	deletion	UNP P20789
BBB	?	-	GLU	deletion	UNP P20789
BBB	?	-	HIS	deletion	UNP P20789
BBB	?	-	SER	deletion	UNP P20789
BBB	?	-	THR	deletion	UNP P20789
BBB	305	ARG	HIS	engineered mutation	UNP P20789
BBB	332	VAL	CYS	engineered mutation	UNP P20789
BBB	342	ALA	PHE	engineered mutation	UNP P20789
BBB	354	SER	THR	engineered mutation	UNP P20789
BBB	358	VAL	PHE	engineered mutation	UNP P20789
BBB	362	ALA	SER	engineered mutation	UNP P20789
BBB	372	ALA	-	linker	UNP P20789
BBB	373	GLU	-	linker	UNP P20789
BBB	374	ASP	-	linker	UNP P20789

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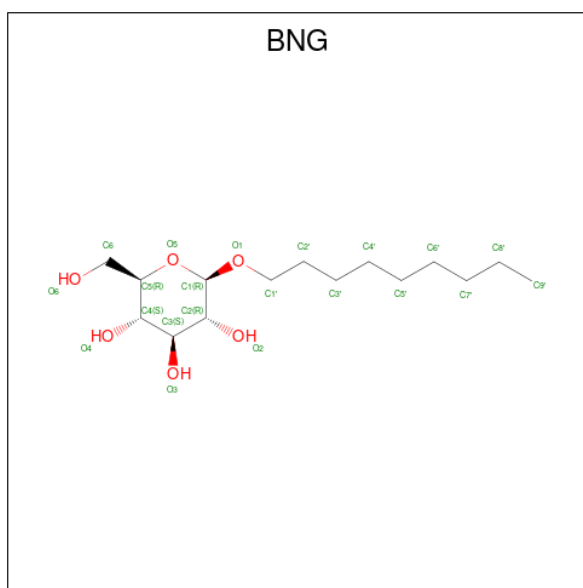
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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	375	LEU	-	linker	UNP P20789
BBB	376	VAL	-	linker	UNP P20789
BBB	377	GLU	-	linker	UNP P20789
BBB	378	ASP	-	linker	UNP P20789
BBB	379	TRP	-	linker	UNP P20789
BBB	380	GLU	-	linker	UNP P20789

- Molecule 2 is a protein called neurotensin NTS8-13 (full agonist).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	8	Total 138	C 42	H 72	N 14	O 10	1	0	0
2	DDD	8	Total 138	C 42	H 72	N 14	O 10	1	0	0

- Molecule 3 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	4	0
			51	15	30	6		
3	AAA	1	Total	C	H	O	4	0
			51	15	30	6		
3	AAA	1	Total	C	H	O	4	0
			51	15	30	6		
3	BBB	1	Total	C	H	O	4	0
			51	15	30	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	BBB	1	Total	C	H	O	4	0
			51	15	30	6		
3	BBB	1	Total	C	H	O	4	0
			51	15	30	6		
3	BBB	1	Total	C	H	O	4	0
			51	15	30	6		
3	BBB	1	Total	C	H	O	4	0
			51	15	30	6		

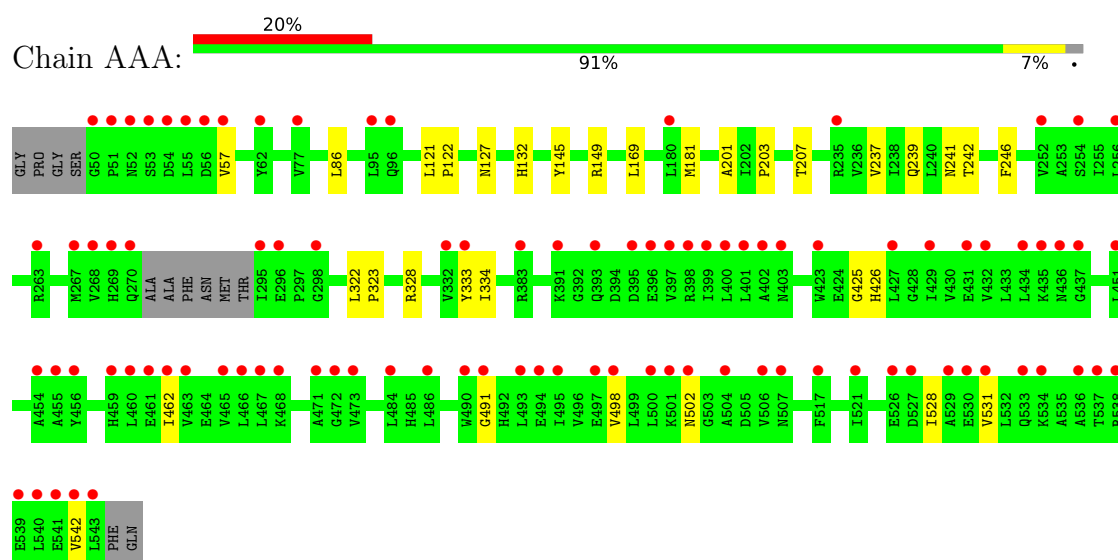
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	21	Total	O	0	0
			21	21		
4	BBB	27	Total	O	0	0
			27	27		

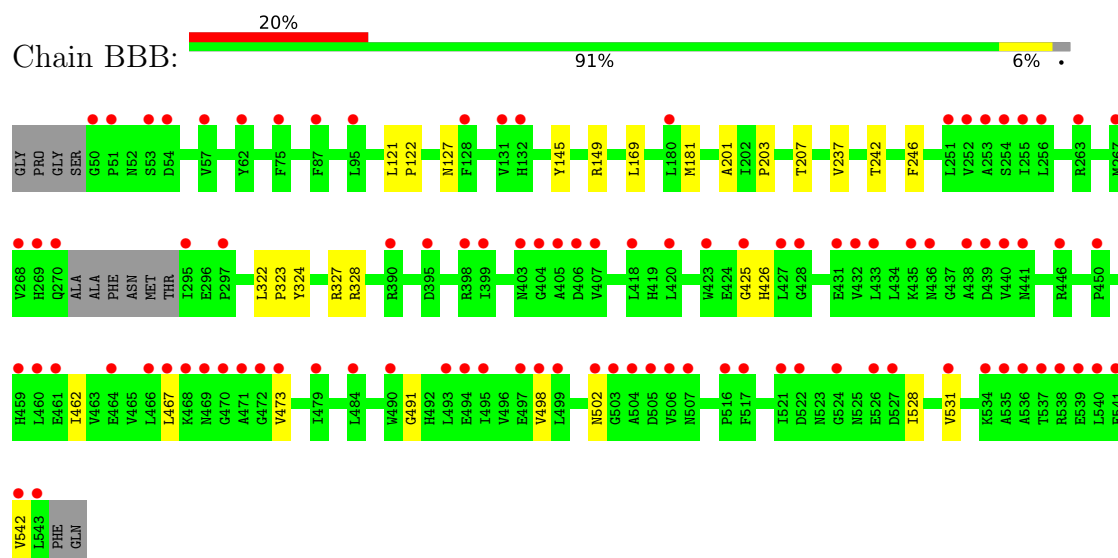
3 Residue-property plots [i](#)

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: Neurotensin receptor type 1,Neurotensin receptor type 1,DARPin crystallisation chaperone

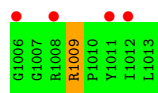


- Molecule 1: Neurotensin receptor type 1,Neurotensin receptor type 1,DARPin crystallisation chaperone



- Molecule 2: neurotensin NTS8-13 (full agonist)

Chain CCC: 



- Molecule 2: neurotensin NTS8-13 (full agonist)

Chain DDD: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.89Å 114.00Å 195.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.46 29.63 – 2.46	Depositor EDS
% Data completeness (in resolution range)	81.2 (29.63-2.46) 81.2 (29.63-2.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.237 (Not available) , 0.229	Depositor DCC
R_{free} test set	2958 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14715	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BNG

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	AAA	1.04	0/3585	1.56	2/4909 (0.0%)
1	BBB	1.04	0/3575	1.57	2/4898 (0.0%)
2	CCC	0.88	0/67	1.19	0/87
2	DDD	0.85	0/67	1.15	0/87
All	All	1.04	0/7294	1.56	4/9981 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	201	ALA	CA-C-N	5.45	123.68	120.24
1	BBB	201	ALA	C-N-CA	5.45	123.68	120.24
1	AAA	201	ALA	CA-C-N	5.15	123.48	120.24
1	AAA	201	ALA	C-N-CA	5.15	123.48	120.24

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	AAA	3506	3502	3409	16	0
1	BBB	3496	3479	3380	14	0
2	CCC	66	72	69	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DDD	66	72	69	1	0
3	AAA	63	90	90	0	0
3	BBB	105	150	150	0	0
4	AAA	21	0	0	1	0
4	BBB	27	0	0	0	0
All	All	7350	7365	7167	30	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 2.

All (30) 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:AAA:334:ILE:O	2:CCC:1009:ARG:NH2	2.07	0.88
1:AAA:207:THR:HG21	1:AAA:237:VAL:HG11	1.85	0.59
1:BBB:498:VAL:O	1:BBB:502:ASN:ND2	2.36	0.58
1:AAA:498:VAL:O	1:AAA:502:ASN:ND2	2.36	0.56
1:BBB:207:THR:HG21	1:BBB:237:VAL:HG11	1.91	0.53
1:AAA:203:PRO:O	1:AAA:207:THR:HG23	2.09	0.52
1:BBB:203:PRO:O	1:BBB:207:THR:HG23	2.08	0.52
1:BBB:425:GLY:O	1:BBB:462:ILE:HD11	2.11	0.51
1:AAA:425:GLY:O	1:AAA:462:ILE:HD11	2.13	0.48
1:BBB:467:LEU:CD2	1:BBB:473:VAL:HG22	2.43	0.47
1:AAA:121:LEU:HB3	1:AAA:122:PRO:HD3	1.97	0.47
1:BBB:491:GLY:HA2	1:BBB:528:ILE:CD1	2.46	0.46
1:BBB:322:LEU:HB3	1:BBB:323:PRO:HD3	1.98	0.45
1:AAA:169:LEU:HD12	1:AAA:181:MET:HE2	1.98	0.45
1:AAA:491:GLY:HA2	1:AAA:528:ILE:CD1	2.46	0.45
1:BBB:121:LEU:HB3	1:BBB:122:PRO:HD3	1.99	0.44
1:BBB:145:TYR:CZ	1:BBB:149:ARG:HD2	2.52	0.44
1:AAA:322:LEU:HB3	1:AAA:323:PRO:HD3	1.99	0.44
1:AAA:145:TYR:CZ	1:AAA:149:ARG:HD2	2.53	0.44
1:BBB:327:ARG:NH1	2:DDD:1013:LEU:O	2.45	0.43
1:BBB:169:LEU:HD12	1:BBB:181:MET:HE2	2.02	0.42
1:AAA:239:GLN:OE1	1:AAA:333:TYR:OH	2.34	0.42
1:BBB:324:TYR:CE1	1:BBB:328:ARG:HD2	2.55	0.42
1:AAA:86:LEU:HD23	1:AAA:86:LEU:HA	1.82	0.42
1:BBB:242:THR:O	1:BBB:246:PHE:HB3	2.20	0.42
1:AAA:57:VAL:HG21	1:AAA:132:HIS:CD2	2.56	0.41
1:AAA:242:THR:O	1:AAA:246:PHE:HB3	2.21	0.41
1:AAA:528:ILE:O	1:AAA:531:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:241:ASN:HB2	4:AAA:4106:HOH:O	2.21	0.40
1:BBB:528:ILE:O	1:BBB:531:VAL:HG22	2.21	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	AAA	466/482 (97%)	452 (97%)	13 (3%)	1 (0%)	43	54
1	BBB	466/482 (97%)	452 (97%)	13 (3%)	1 (0%)	43	54
2	CCC	6/8 (75%)	6 (100%)	0	0	100	100
2	DDD	6/8 (75%)	6 (100%)	0	0	100	100
All	All	944/980 (96%)	916 (97%)	26 (3%)	2 (0%)	43	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	542	VAL
1	BBB	542	VAL

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	AAA	347/397 (87%)	344 (99%)	3 (1%)	70	81
1	BBB	344/397 (87%)	342 (99%)	2 (1%)	78	86
2	CCC	6/6 (100%)	5 (83%)	1 (17%)	2	1
2	DDD	6/6 (100%)	6 (100%)	0	100	100
All	All	703/806 (87%)	697 (99%)	6 (1%)	70	81

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	127	ASN
1	AAA	328	ARG
1	AAA	426	HIS
1	BBB	127	ASN
1	BBB	426	HIS
2	CCC	1009	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
3	BNG	BBB	4001	-	21,21,21	0.66	1 (4%)	26,26,26	0.84	1 (3%)
3	BNG	BBB	4005	-	21,21,21	0.55	0	26,26,26	0.53	0
3	BNG	BBB	4002	-	21,21,21	0.63	1 (4%)	26,26,26	0.78	0
3	BNG	AAA	4003	-	21,21,21	0.70	1 (4%)	26,26,26	0.97	1 (3%)
3	BNG	BBB	4003	-	21,21,21	0.60	1 (4%)	26,26,26	0.81	1 (3%)
3	BNG	BBB	4004	-	21,21,21	0.56	0	26,26,26	0.58	0
3	BNG	AAA	4002	-	21,21,21	0.61	1 (4%)	26,26,26	0.47	0
3	BNG	AAA	4001	-	21,21,21	0.65	1 (4%)	26,26,26	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BNG	BBB	4001	-	-	7/12/32/32	0/1/1/1
3	BNG	BBB	4005	-	-	6/12/32/32	0/1/1/1
3	BNG	BBB	4002	-	-	3/12/32/32	0/1/1/1
3	BNG	AAA	4003	-	-	7/12/32/32	0/1/1/1
3	BNG	BBB	4003	-	-	7/12/32/32	0/1/1/1
3	BNG	BBB	4004	-	-	7/12/32/32	0/1/1/1
3	BNG	AAA	4002	-	-	4/12/32/32	0/1/1/1
3	BNG	AAA	4001	-	-	7/12/32/32	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	4003	BNG	O1-C1	2.50	1.44	1.40
3	AAA	4001	BNG	O1-C1	2.32	1.44	1.40
3	BBB	4002	BNG	O1-C1	2.31	1.44	1.40
3	BBB	4001	BNG	O1-C1	2.29	1.44	1.40
3	AAA	4002	BNG	O1-C1	2.19	1.43	1.40
3	BBB	4003	BNG	O1-C1	2.09	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	4003	BNG	C1'-O1-C1	3.32	119.34	113.68
3	BBB	4001	BNG	C3-C4-C5	2.43	114.63	110.23
3	BBB	4003	BNG	C1-C2-C3	2.13	114.50	110.01

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	4003	BNG	O5-C1-O1-C1'
3	AAA	4003	BNG	C2'-C1'-O1-C1
3	BBB	4002	BNG	C2'-C1'-O1-C1
3	BBB	4005	BNG	O5-C1-O1-C1'
3	AAA	4003	BNG	O5-C5-C6-O6
3	AAA	4003	BNG	C4-C5-C6-O6
3	BBB	4001	BNG	C4-C5-C6-O6
3	BBB	4001	BNG	O5-C5-C6-O6
3	BBB	4003	BNG	O5-C5-C6-O6
3	BBB	4004	BNG	C4-C5-C6-O6
3	BBB	4003	BNG	C2'-C1'-O1-C1
3	BBB	4005	BNG	C1'-C2'-C3'-C4'
3	BBB	4005	BNG	C3'-C4'-C5'-C6'
3	BBB	4005	BNG	C4-C5-C6-O6
3	BBB	4004	BNG	O5-C5-C6-O6
3	AAA	4001	BNG	C4-C5-C6-O6
3	BBB	4002	BNG	O5-C5-C6-O6
3	AAA	4002	BNG	C1'-C2'-C3'-C4'
3	BBB	4001	BNG	C5'-C6'-C7'-C8'
3	AAA	4001	BNG	C6'-C7'-C8'-C9'
3	BBB	4004	BNG	C2'-C1'-O1-C1
3	AAA	4001	BNG	C2-C1-O1-C1'
3	AAA	4001	BNG	C1'-C2'-C3'-C4'
3	BBB	4001	BNG	C6'-C7'-C8'-C9'
3	AAA	4002	BNG	O1-C1'-C2'-C3'
3	AAA	4001	BNG	O5-C1-O1-C1'
3	BBB	4003	BNG	C3'-C4'-C5'-C6'
3	BBB	4003	BNG	C4-C5-C6-O6
3	BBB	4003	BNG	C4'-C5'-C6'-C7'
3	AAA	4001	BNG	C2'-C3'-C4'-C5'
3	BBB	4001	BNG	C1'-C2'-C3'-C4'
3	BBB	4004	BNG	O5-C1-O1-C1'
3	BBB	4004	BNG	C4'-C5'-C6'-C7'
3	AAA	4003	BNG	C2-C1-O1-C1'
3	AAA	4002	BNG	C2'-C1'-O1-C1

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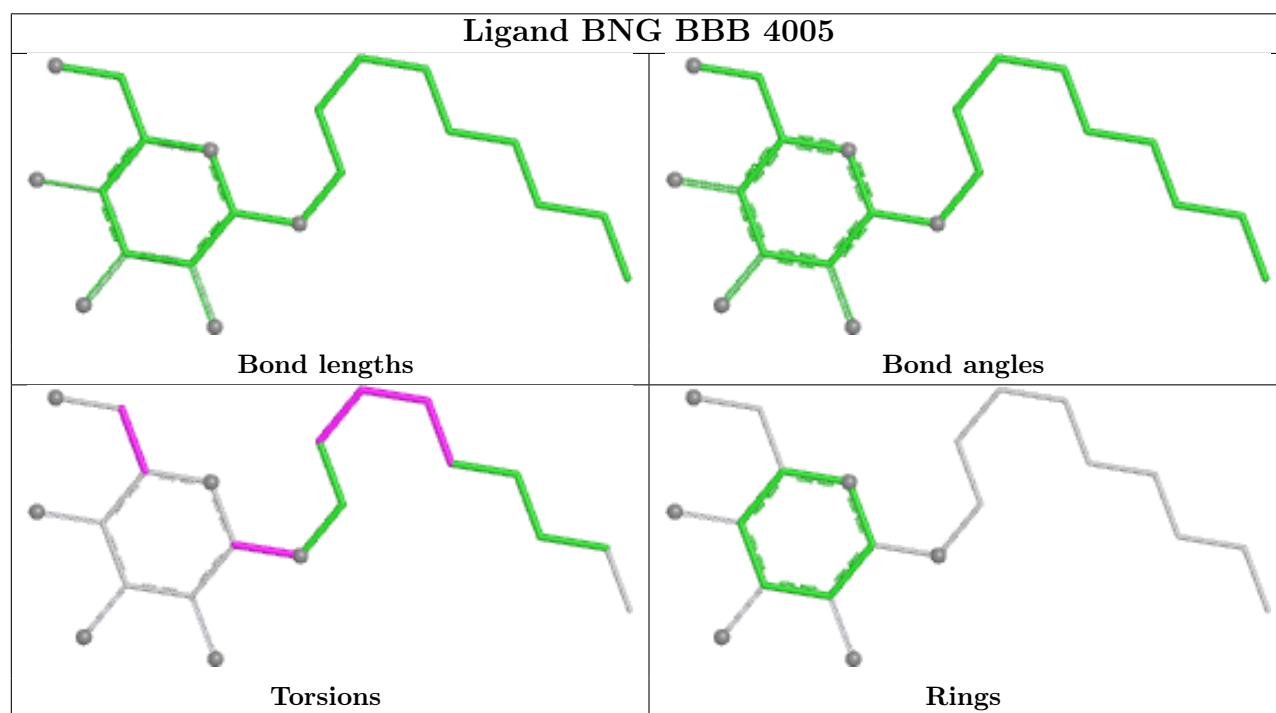
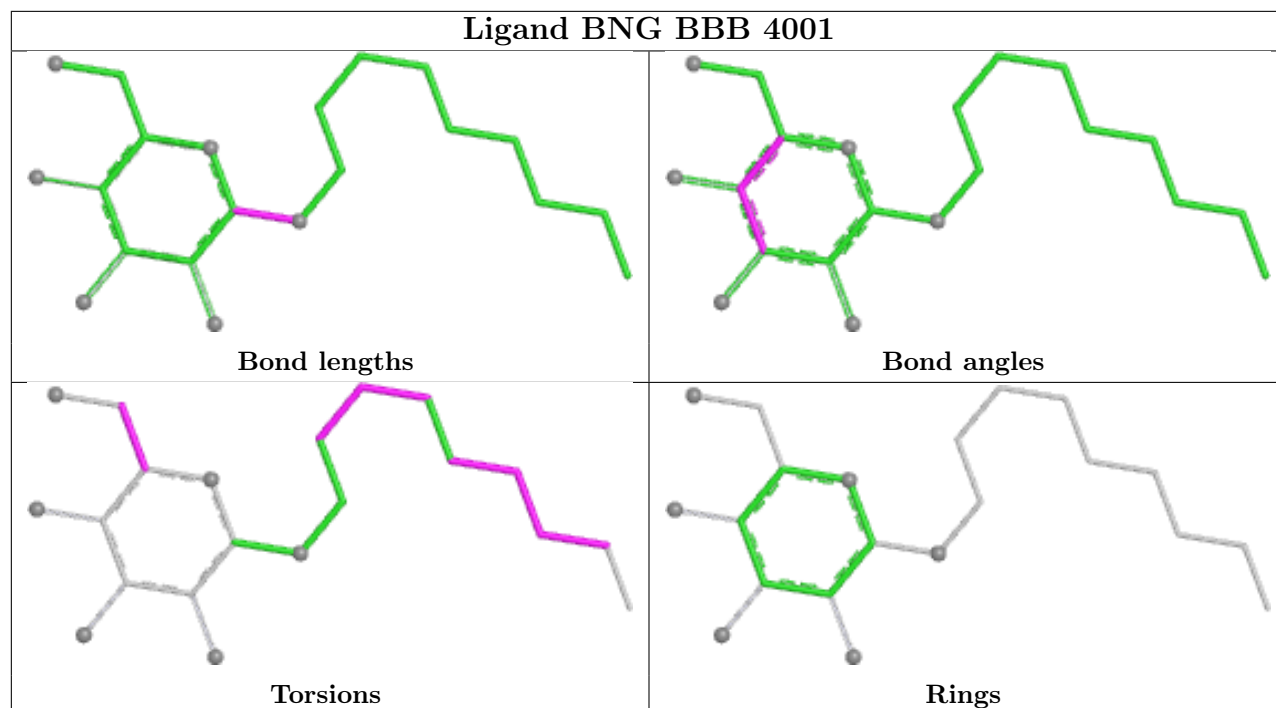
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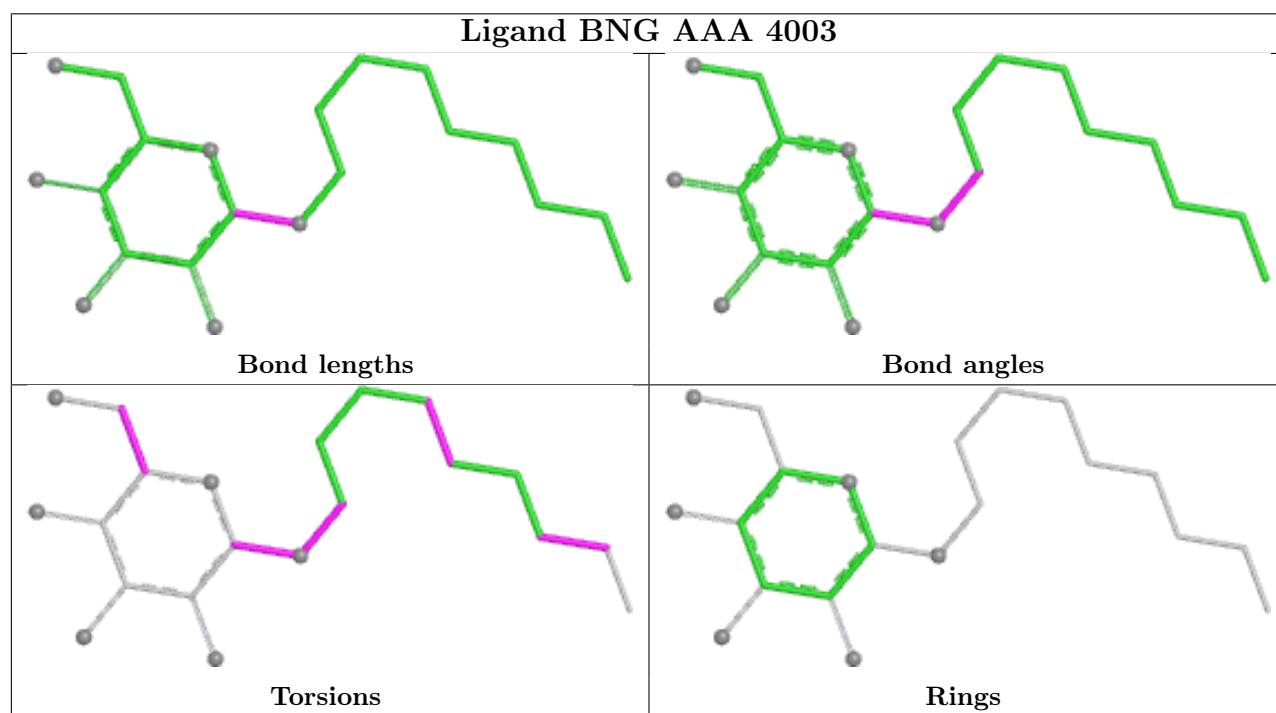
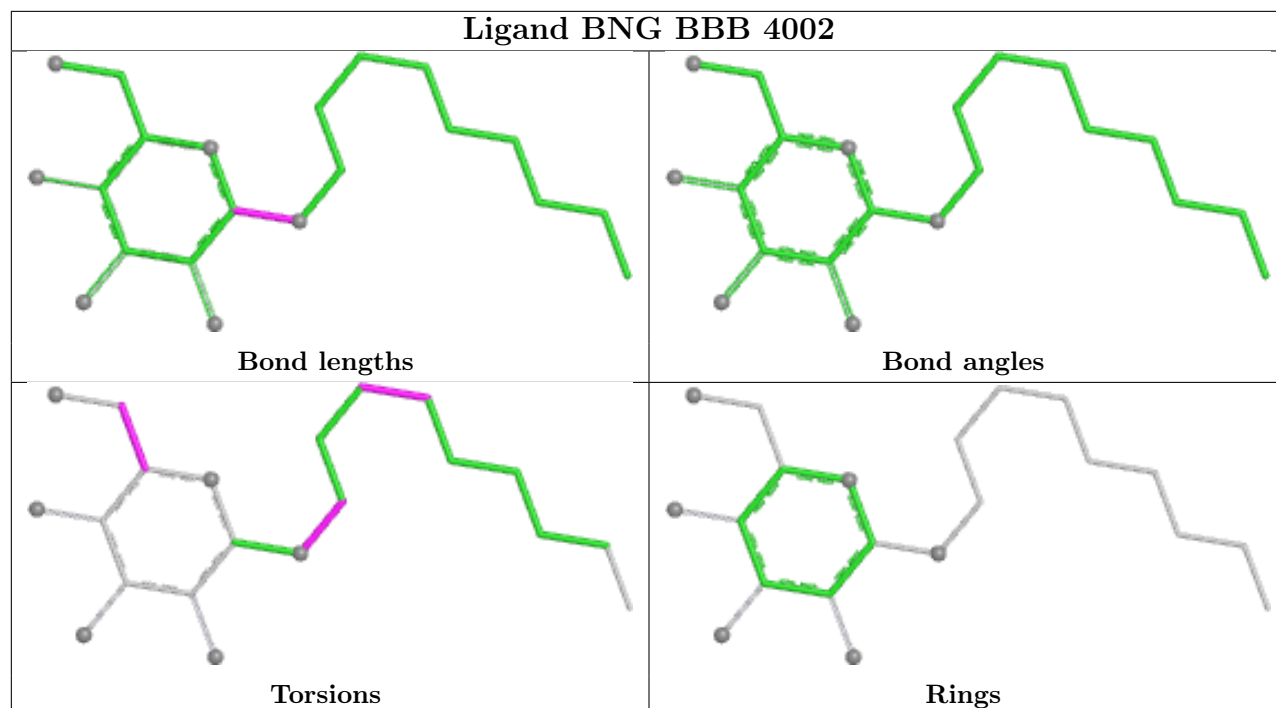
Mol	Chain	Res	Type	Atoms
3	BBB	4005	BNG	O5-C5-C6-O6
3	BBB	4003	BNG	C1'-C2'-C3'-C4'
3	BBB	4005	BNG	C2'-C3'-C4'-C5'
3	AAA	4002	BNG	C5'-C6'-C7'-C8'
3	BBB	4004	BNG	C1'-C2'-C3'-C4'
3	AAA	4003	BNG	C6'-C7'-C8'-C9'
3	BBB	4004	BNG	C3'-C4'-C5'-C6'
3	AAA	4003	BNG	C3'-C4'-C5'-C6'
3	BBB	4003	BNG	O1-C1'-C2'-C3'
3	BBB	4001	BNG	C4'-C5'-C6'-C7'
3	BBB	4002	BNG	C2'-C3'-C4'-C5'
3	AAA	4001	BNG	O5-C5-C6-O6
3	BBB	4001	BNG	C2'-C3'-C4'-C5'

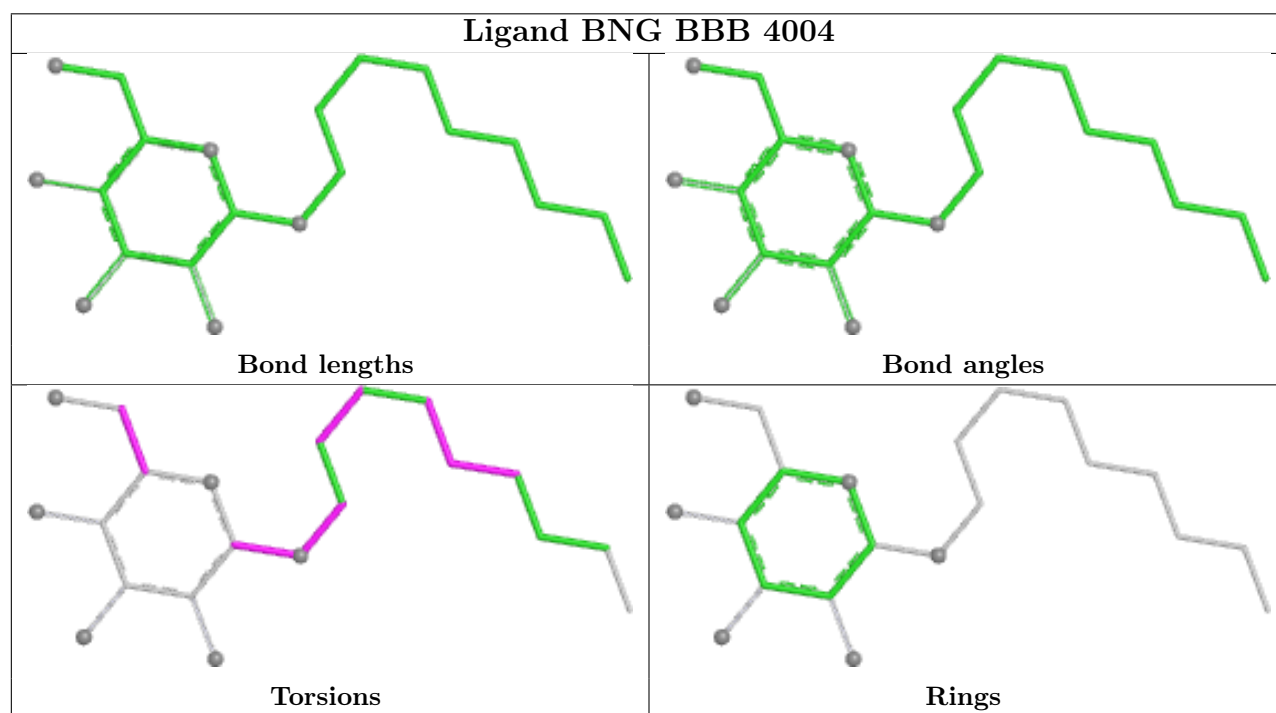
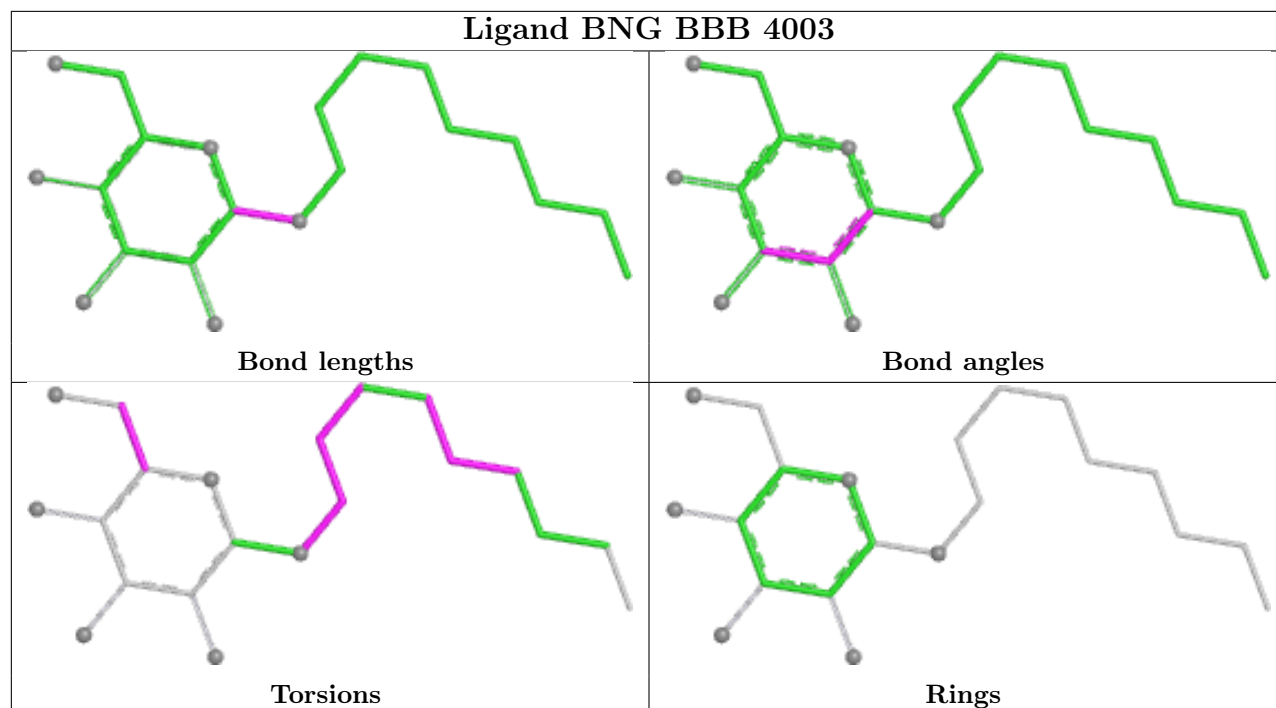
There are no ring outliers.

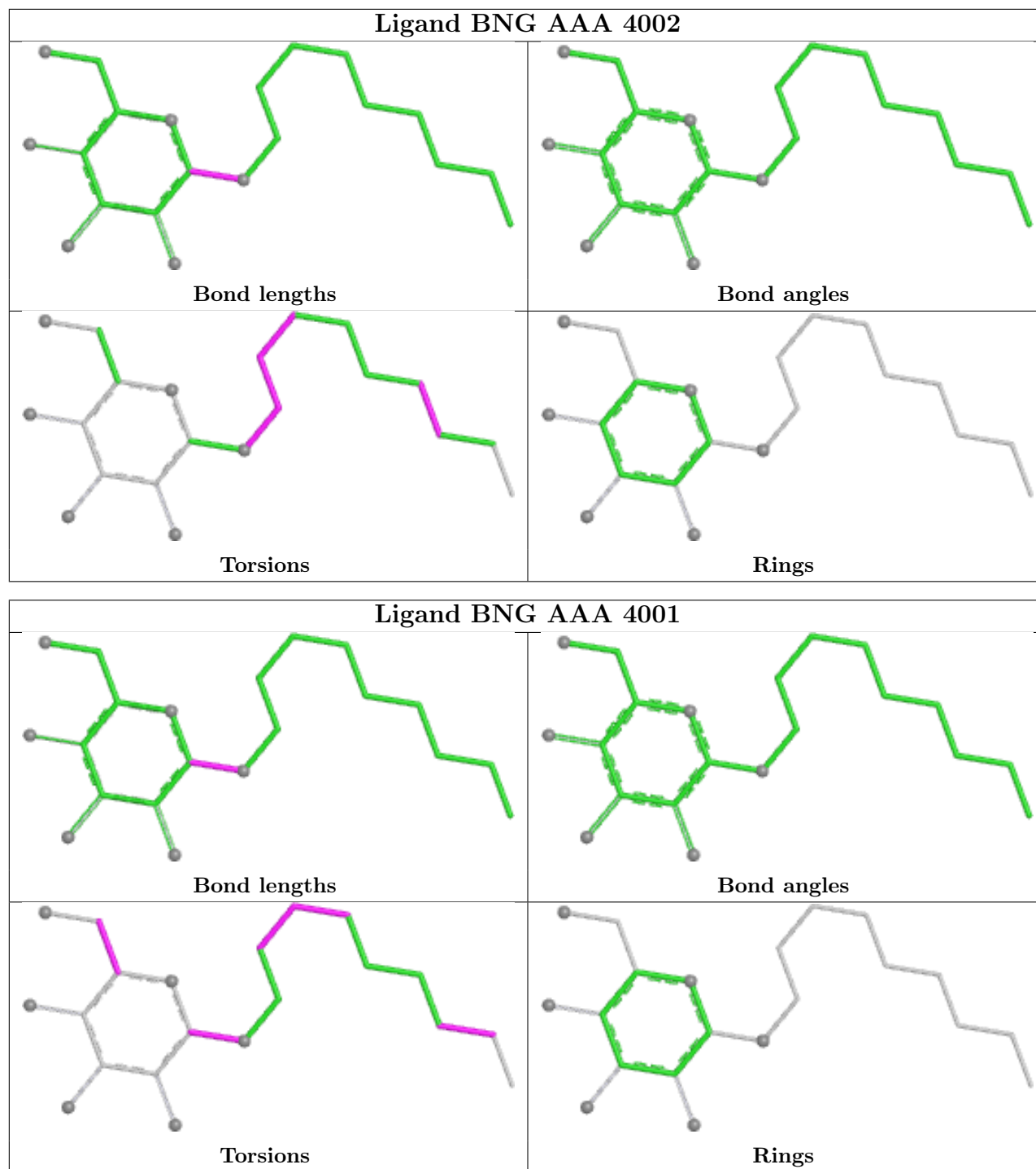
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	AAA	470/482 (97%)	1.01	96 (20%) 3 2	42, 70, 125, 149	0
1	BBB	470/482 (97%)	1.02	97 (20%) 2 2	40, 72, 125, 166	0
2	CCC	8/8 (100%)	1.80	4 (50%) 0 0	61, 71, 105, 124	0
2	DDD	8/8 (100%)	1.08	1 (12%) 8 6	56, 67, 109, 114	0
All	All	956/980 (97%)	1.02	198 (20%) 2 2	40, 71, 125, 166	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	268	VAL	8.4
1	AAA	471	ALA	7.4
1	BBB	484	LEU	7.2
1	BBB	494	GLU	6.3
1	BBB	469	ASN	6.3
1	AAA	494	GLU	6.1
1	BBB	395	ASP	6.0
1	BBB	440	VAL	5.8
1	AAA	527	ASP	5.7
1	AAA	541	GLU	5.7
1	AAA	493	LEU	5.6
1	BBB	295	ILE	5.6
1	AAA	543	LEU	5.5
1	BBB	543	LEU	5.5
1	AAA	540	LEU	5.3
1	AAA	403	ASN	5.3
1	AAA	504	ALA	5.2
1	BBB	471	ALA	5.2
1	BBB	502	ASN	5.2
1	AAA	484	LEU	5.2
1	AAA	62	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	50	GLY	5.1
1	AAA	295	ILE	5.1
1	AAA	461	GLU	5.1
1	BBB	537	THR	5.1
1	BBB	467	LEU	5.0
1	AAA	526	GLU	5.0
1	BBB	507	ASN	4.9
1	AAA	472	GLY	4.8
1	AAA	539	GLU	4.7
1	BBB	95	LEU	4.7
1	BBB	493	LEU	4.7
1	AAA	537	THR	4.7
1	BBB	438	ALA	4.6
1	AAA	95	LEU	4.6
1	AAA	270	GLN	4.6
1	BBB	541	GLU	4.5
1	BBB	253	ALA	4.5
1	AAA	542	VAL	4.5
1	AAA	395	ASP	4.5
1	AAA	536	ALA	4.5
1	AAA	50	GLY	4.4
1	AAA	456	TYR	4.4
1	AAA	432	VAL	4.3
1	BBB	427	LEU	4.3
1	BBB	270	GLN	4.3
1	BBB	504	ALA	4.2
1	AAA	473	VAL	4.2
1	AAA	460	LEU	4.2
1	AAA	256	LEU	4.1
1	BBB	527	ASP	4.1
1	BBB	499	LEU	4.0
1	AAA	490	TRP	4.0
1	AAA	451	LEU	3.9
1	BBB	53	SER	3.9
1	BBB	472	GLY	3.9
1	AAA	427	LEU	3.9
1	BBB	521	ILE	3.9
1	BBB	435	LYS	3.9
2	CCC	1006	GLY	3.8
1	BBB	466	LEU	3.8
1	BBB	526	GLU	3.8
1	AAA	269	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	462	ILE	3.8
2	DDD	1006	GLY	3.8
1	AAA	252	VAL	3.8
1	BBB	268	VAL	3.8
1	AAA	399	ILE	3.8
1	BBB	131	VAL	3.7
1	AAA	52	ASN	3.7
1	BBB	57	VAL	3.7
1	AAA	529	ALA	3.7
1	BBB	431	GLU	3.6
1	AAA	429	ILE	3.6
1	AAA	497	GLU	3.6
1	BBB	269	HIS	3.6
1	BBB	432	VAL	3.6
1	BBB	407	VAL	3.5
1	BBB	470	GLY	3.5
1	AAA	534	LYS	3.5
1	AAA	400	LEU	3.4
1	BBB	256	LEU	3.4
1	BBB	254	SER	3.4
1	AAA	498	VAL	3.4
1	AAA	517	PHE	3.4
1	AAA	298	GLY	3.4
1	BBB	461	GLU	3.4
1	BBB	517	PHE	3.3
1	AAA	468	LYS	3.3
1	BBB	251	LEU	3.3
1	BBB	497	GLU	3.3
1	AAA	57	VAL	3.2
1	AAA	506	VAL	3.2
1	AAA	54	ASP	3.2
1	AAA	466	LEU	3.2
1	AAA	463	VAL	3.2
2	CCC	1012	ILE	3.2
1	AAA	55	LEU	3.1
1	AAA	235	ARG	3.1
1	AAA	465	VAL	3.1
1	AAA	267	MET	3.1
1	BBB	506	VAL	3.1
1	BBB	62	TYR	3.0
1	AAA	431	GLU	3.0
1	AAA	401	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	460	LEU	3.0
1	AAA	56	ASP	3.0
1	AAA	530	GLU	3.0
1	BBB	51	PRO	3.0
1	BBB	446	ARG	2.9
1	BBB	531	VAL	2.9
1	AAA	398	ARG	2.9
1	BBB	468	LYS	2.9
1	BBB	406	ASP	2.9
1	AAA	533	GLN	2.9
1	AAA	296	GLU	2.9
1	BBB	403	ASN	2.9
1	BBB	252	VAL	2.9
1	BBB	473	VAL	2.9
1	BBB	398	ARG	2.8
1	BBB	459	HIS	2.8
1	BBB	87	PHE	2.8
1	BBB	441	ASN	2.8
1	AAA	397	VAL	2.8
1	BBB	399	ILE	2.8
1	BBB	436	ASN	2.8
1	BBB	495	ILE	2.7
1	AAA	435	LYS	2.7
1	AAA	53	SER	2.7
1	AAA	501	LYS	2.7
1	BBB	542	VAL	2.7
1	BBB	539	GLU	2.6
1	BBB	534	LYS	2.6
1	BBB	297	PRO	2.6
1	AAA	538	ARG	2.6
1	BBB	132	HIS	2.6
1	BBB	404	GLY	2.6
1	BBB	267	MET	2.6
1	BBB	405	ALA	2.6
1	AAA	383	ARG	2.6
1	AAA	495	ILE	2.6
1	BBB	420	LEU	2.6
1	AAA	333	TYR	2.6
1	AAA	491	GLY	2.5
1	AAA	77	VAL	2.5
1	AAA	521	ILE	2.5
1	BBB	516	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	396	GLU	2.5
2	CCC	1011	TYR	2.5
1	AAA	391	LYS	2.5
1	AAA	467	LEU	2.5
1	AAA	486	LEU	2.5
1	BBB	128	PHE	2.5
1	AAA	180	LEU	2.4
1	BBB	423	TRP	2.4
1	AAA	455	ALA	2.4
1	BBB	75	PHE	2.4
1	AAA	254	SER	2.4
1	BBB	428	GLY	2.4
1	AAA	507	ASN	2.4
1	BBB	479	ILE	2.4
1	AAA	393	GLN	2.4
1	AAA	500	LEU	2.4
1	AAA	531	VAL	2.4
1	AAA	423	TRP	2.4
1	BBB	490	TRP	2.4
1	BBB	538	ARG	2.3
1	BBB	433	LEU	2.3
1	AAA	502	ASN	2.3
1	AAA	454	ALA	2.3
1	BBB	263	ARG	2.3
1	AAA	437	GLY	2.3
1	BBB	503	GLY	2.3
1	BBB	180	LEU	2.3
1	BBB	540	LEU	2.3
1	BBB	450	PRO	2.3
1	AAA	96	GLN	2.3
1	BBB	255	ILE	2.3
2	CCC	1008	ARG	2.2
1	AAA	402	ALA	2.2
1	BBB	425	GLY	2.2
1	AAA	434	LEU	2.2
1	BBB	418	LEU	2.2
1	BBB	54	ASP	2.2
1	BBB	505	ASP	2.2
1	BBB	522	ASP	2.2
1	BBB	390	ARG	2.2
1	AAA	51	PRO	2.2
1	AAA	436	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	459	HIS	2.2
1	BBB	498	VAL	2.1
1	BBB	535	ALA	2.1
1	BBB	524	GLY	2.1
1	AAA	332	VAL	2.1
1	BBB	464	GLU	2.1
1	AAA	263	ARG	2.0
1	BBB	536	ALA	2.0
1	BBB	439	ASP	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](#)

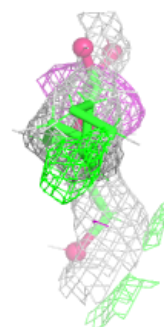
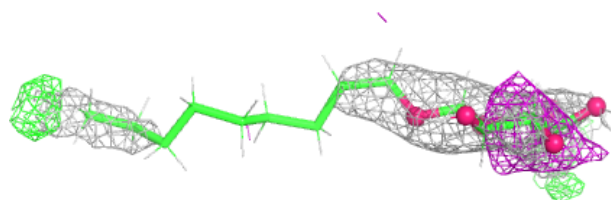
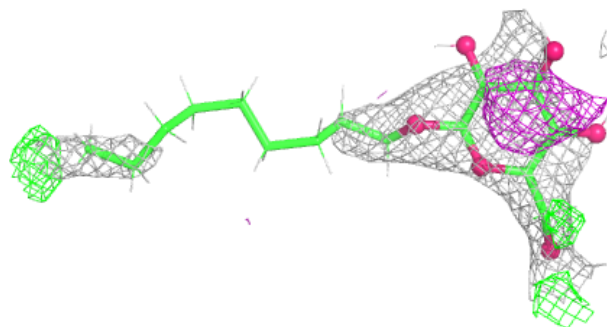
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BNG	BBB	4001	21/21	0.66	0.25	58,93,100,106	4
3	BNG	AAA	4001	21/21	0.73	0.27	58,94,120,121	4
3	BNG	AAA	4003	21/21	0.74	0.21	58,90,121,125	4
3	BNG	BBB	4005	21/21	0.74	0.21	58,78,97,100	4
3	BNG	BBB	4004	21/21	0.78	0.19	58,84,100,104	4
3	BNG	BBB	4002	21/21	0.79	0.18	58,78,118,123	4
3	BNG	BBB	4003	21/21	0.83	0.16	58,83,119,123	4
3	BNG	AAA	4002	21/21	0.84	0.17	58,75,125,137	4

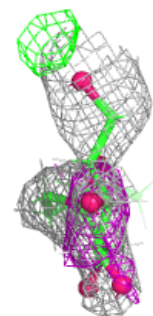
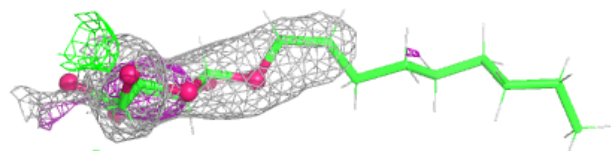
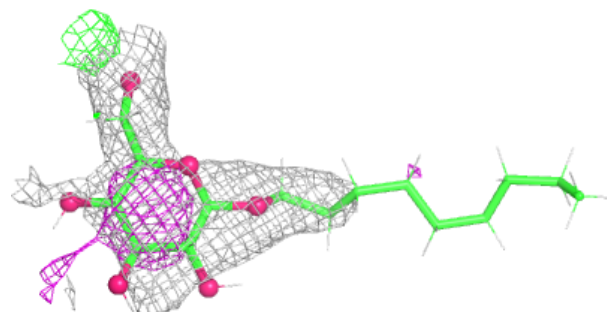
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG BBB 4001:

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

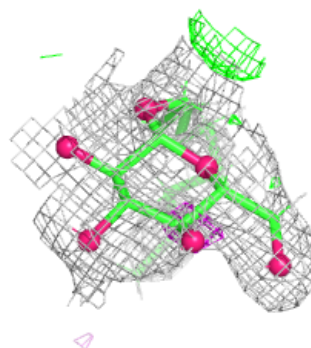
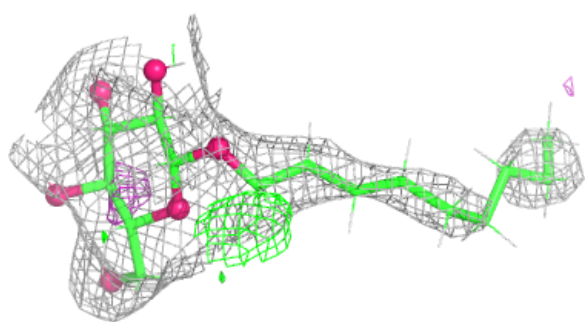
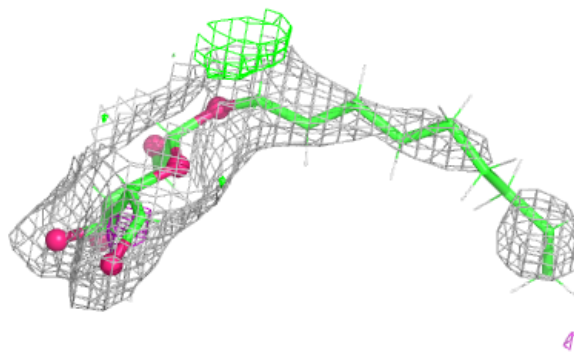
**Electron density around BNG AAA 4001:**

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

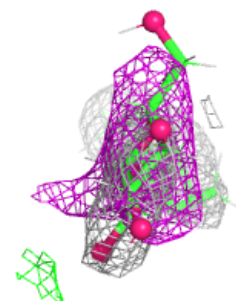
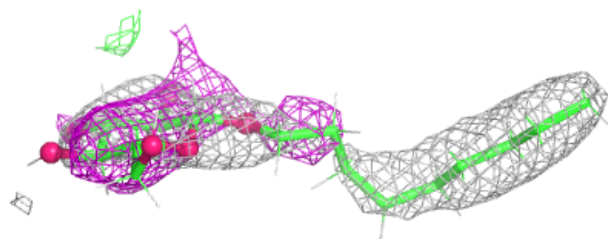
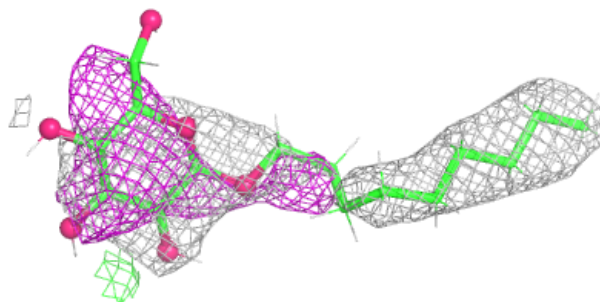


Electron density around BNG AAA 4003:

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

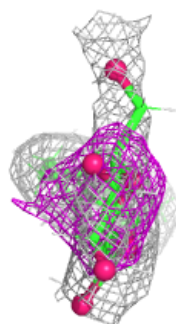
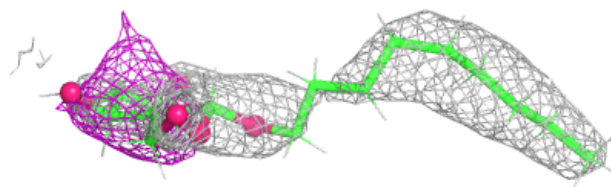
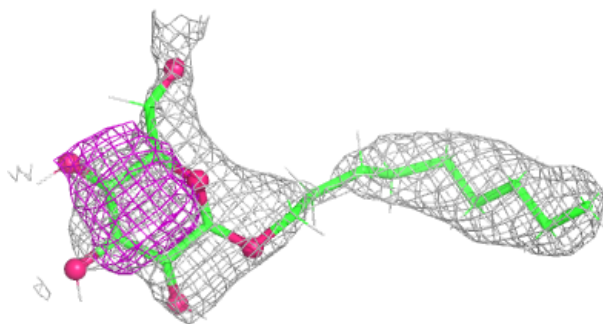
**Electron density around BNG BBB 4005:**

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

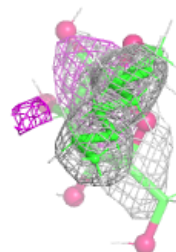
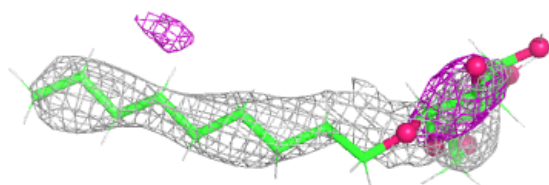
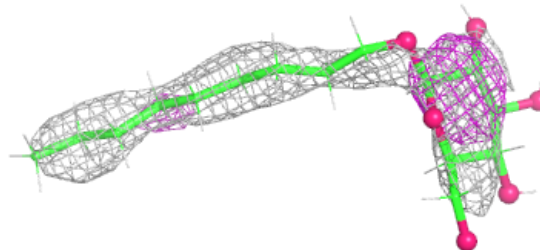


Electron density around BNG BBB 4004:

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

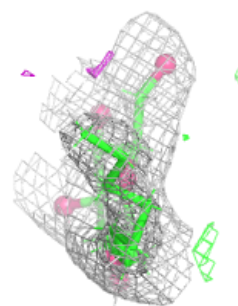
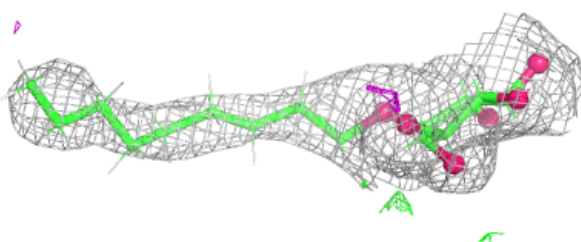
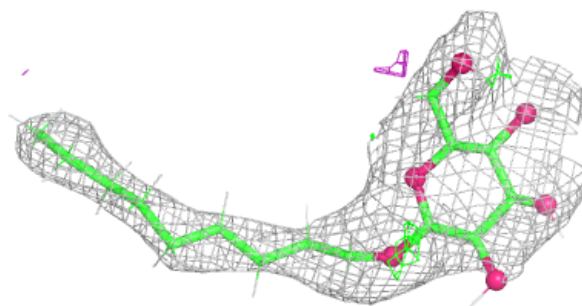
**Electron density around BNG BBB 4002:**

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

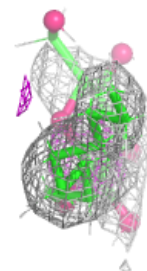
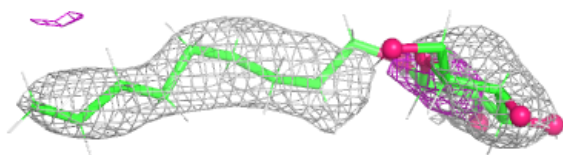
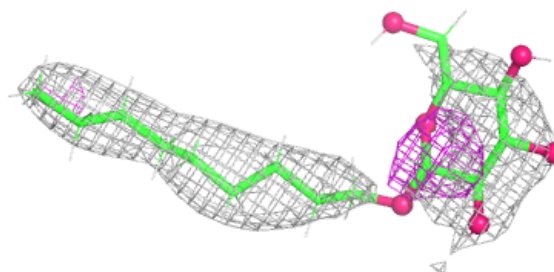


Electron density around BNG BBB 4003:

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

**Electron density around BNG AAA 4002:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.