



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 4QTN / pdb_00004qtn
Title : Crystal structure of the Vitamin B3 transporter PnuC
Authors : Guskov, A.; Jaehme, M.; Slotboom, D.J.
Deposited on : 2014-07-08
Resolution : 2.80 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

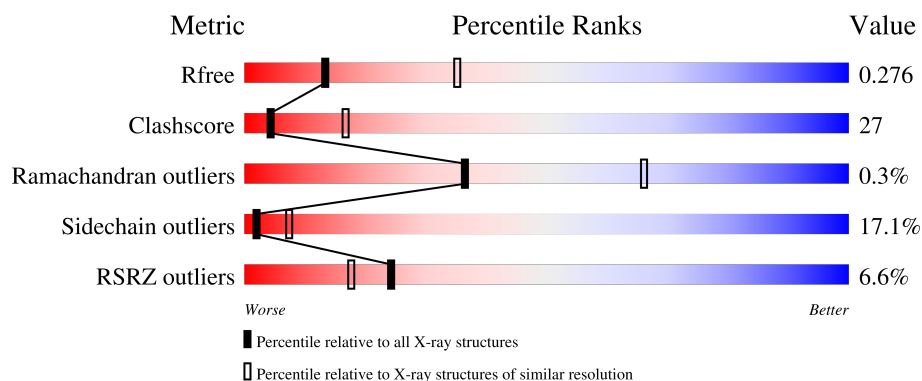
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	244	5% 56% 34% 7% .
1	B	244	11% 45% 40% 10% .
1	C	244	3% 57% 34% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5808 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 Nicotinamide riboside transporter PnuC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	Se	0	0	0
			1887	1269	298	310	2	8			
1	B	235	Total	C	N	O	S	Se	0	0	0
			1887	1269	298	310	2	8			
1	C	237	Total	C	N	O	S	Se	0	0	0
			1900	1276	301	313	2	8			

There are 24 discrepancies between the modelled and reference sequences:

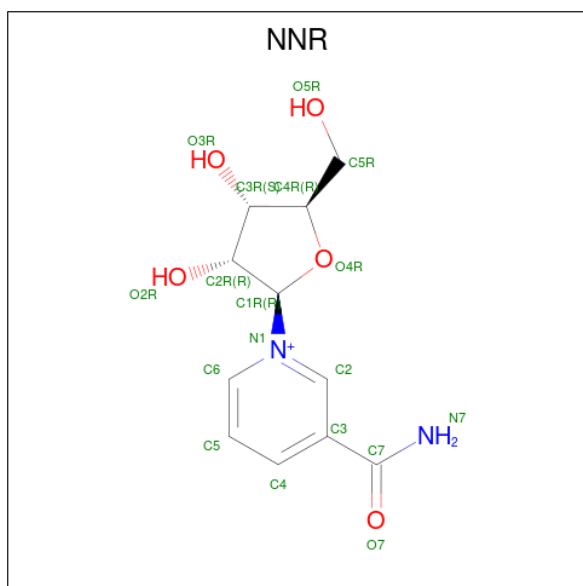
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP D2ZZC1
A	2	GLY	-	expression tag	UNP D2ZZC1
A	239	HIS	-	expression tag	UNP D2ZZC1
A	240	HIS	-	expression tag	UNP D2ZZC1
A	241	HIS	-	expression tag	UNP D2ZZC1
A	242	HIS	-	expression tag	UNP D2ZZC1
A	243	HIS	-	expression tag	UNP D2ZZC1
A	244	HIS	-	expression tag	UNP D2ZZC1
B	1	MSE	-	expression tag	UNP D2ZZC1
B	2	GLY	-	expression tag	UNP D2ZZC1
B	239	HIS	-	expression tag	UNP D2ZZC1
B	240	HIS	-	expression tag	UNP D2ZZC1
B	241	HIS	-	expression tag	UNP D2ZZC1
B	242	HIS	-	expression tag	UNP D2ZZC1
B	243	HIS	-	expression tag	UNP D2ZZC1
B	244	HIS	-	expression tag	UNP D2ZZC1
C	1	MSE	-	expression tag	UNP D2ZZC1
C	2	GLY	-	expression tag	UNP D2ZZC1
C	239	HIS	-	expression tag	UNP D2ZZC1
C	240	HIS	-	expression tag	UNP D2ZZC1
C	241	HIS	-	expression tag	UNP D2ZZC1
C	242	HIS	-	expression tag	UNP D2ZZC1
C	243	HIS	-	expression tag	UNP D2ZZC1

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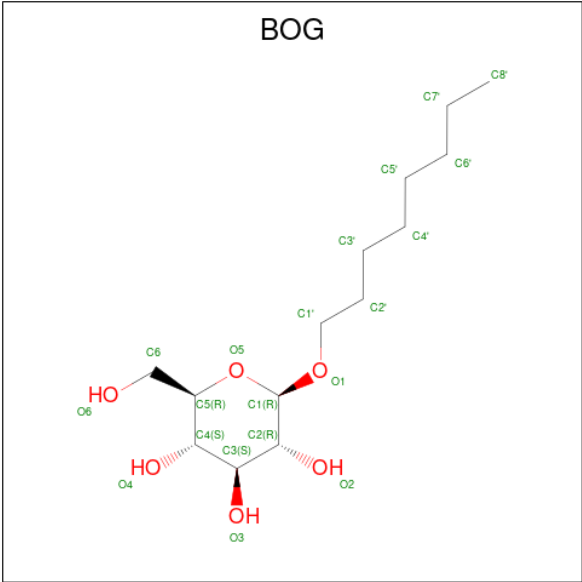
Chain	Residue	Modelled	Actual	Comment	Reference
C	244	HIS	-	expression tag	UNP D2ZZC1

- Molecule 2 is Nicotinamide riboside (CCD ID: NNR) (formula: $C_{11}H_{15}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	11	2	5		
2	B	1	Total	C	N	O	0	0
			18	11	2	5		
2	C	1	Total	C	N	O	0	0
			18	11	2	5		

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).

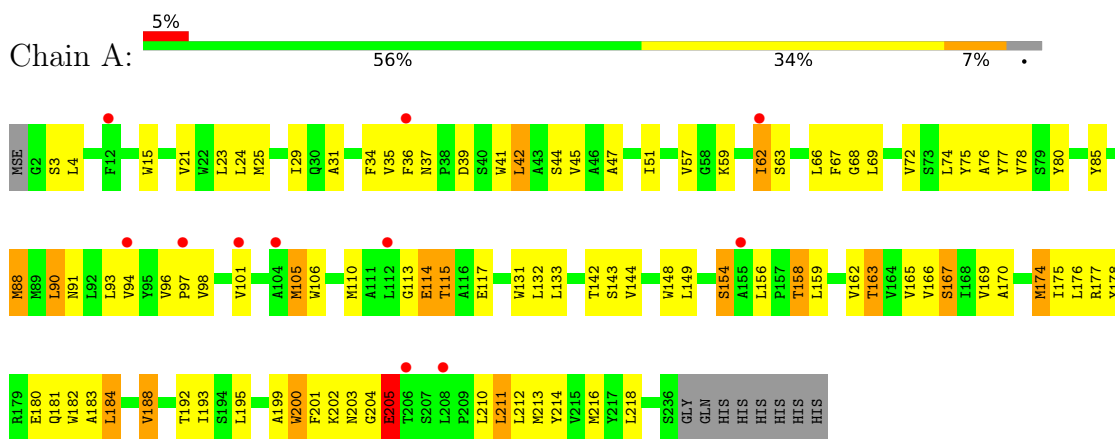


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		
3	C	1	Total	C	O	0	0
			20	14	6		

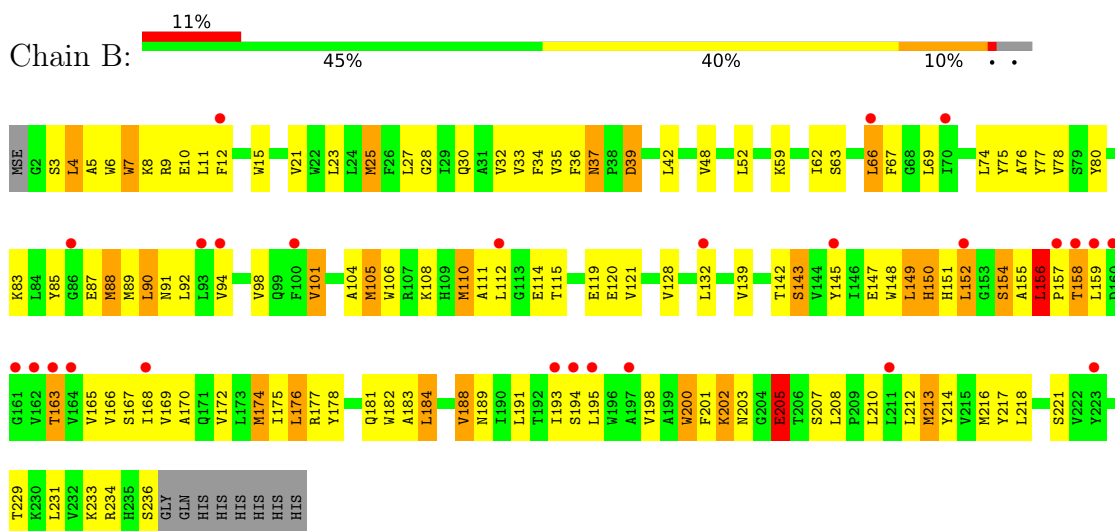
3 Residue-property plots [i](#)

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.

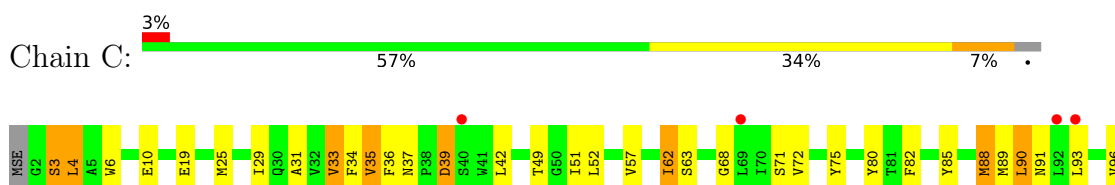
• Molecule 1: Nicotinamide riboside transporter PnuC

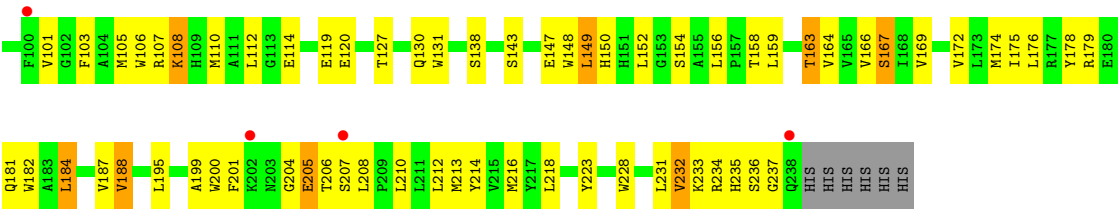


• Molecule 1: Nicotinamide riboside transporter PnuC



• Molecule 1: Nicotinamide riboside transporter PnuC





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.32Å 112.93Å 120.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.80 48.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.31-2.80) 99.8 (48.31-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.244 , 0.276 0.245 , 0.276	Depositor DCC
R_{free} test set	1597 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.7	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.9	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	0.91	EDS
Total number of atoms	5808	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: NNR, BOG

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	0.83	0/1936	0.88	2/2633 (0.1%)
1	B	0.84	0/1936	0.94	6/2633 (0.2%)
1	C	0.73	0/1949	0.88	3/2650 (0.1%)
All	All	0.80	0/5821	0.90	11/7916 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLU	N-CA-C	6.51	119.09	108.55
1	B	150	HIS	N-CA-C	-6.46	104.28	111.71
1	A	114	GLU	N-CA-C	5.50	117.27	111.28
1	C	205	GLU	N-CA-C	5.48	117.42	108.76
1	B	110	MSE	CA-CB-CG	-5.45	103.20	114.10
1	C	114	GLU	N-CA-C	5.23	117.73	111.71
1	C	237	GLY	N-CA-C	5.17	118.89	112.64
1	B	114	GLU	N-CA-C	5.09	116.91	111.36
1	B	156	LEU	CA-C-N	-5.09	114.54	119.78
1	B	156	LEU	C-N-CA	-5.09	114.54	119.78
1	B	205	GLU	N-CA-C	5.01	116.56	108.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	GLY	Peptide

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	1887	0	1931	111	0
1	B	1887	0	1931	127	0
1	C	1900	0	1942	112	0
2	A	18	0	14	1	0
2	B	18	0	14	0	0
2	C	18	0	14	1	0
3	A	20	0	28	1	0
3	B	40	0	56	3	0
3	C	20	0	28	0	0
All	All	5808	0	5958	316	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 27.

All (316) 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:25:MSE:HE1	1:C:184:LEU:CD1	1.67	1.22
1:A:154:SER:HB2	1:A:156:LEU:CD2	1.74	1.15
1:C:62:ILE:HD12	1:C:110:MSE:HE3	1.33	1.10
1:C:200:TRP:CD1	1:C:201:PHE:HE1	1.70	1.08
1:B:154:SER:HB2	1:B:156:LEU:HD22	1.31	1.08
1:A:154:SER:CB	1:A:156:LEU:HD22	1.86	1.04
1:C:200:TRP:CD1	1:C:201:PHE:CE1	2.45	1.04
1:A:25:MSE:HE1	1:B:183:ALA:HB1	1.39	1.03
1:C:200:TRP:HB2	1:C:206:THR:HG22	1.39	1.02
1:B:166:VAL:HG12	1:B:188:VAL:HG12	1.36	1.02
1:C:200:TRP:HD1	1:C:201:PHE:CE1	1.78	1.01
1:A:200:TRP:HD1	1:A:201:PHE:CD1	1.79	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:MSE:HE1	1:C:184:LEU:HD13	1.00	0.99
1:B:25:MSE:CE	1:C:184:LEU:HD13	1.93	0.99
1:A:159:LEU:HD23	1:A:195:LEU:CD2	1.96	0.95
1:C:234:ARG:C	1:C:235:HIS:CD2	2.45	0.95
1:C:234:ARG:O	1:C:235:HIS:HD2	1.50	0.94
1:A:154:SER:CB	1:A:156:LEU:CD2	2.46	0.93
1:A:184:LEU:HD13	1:C:25:MSE:HE2	1.48	0.93
1:C:200:TRP:HB2	1:C:206:THR:CG2	1.98	0.92
1:B:62:ILE:HD12	1:B:110:MSE:HE3	1.48	0.91
1:B:156:LEU:HD23	1:B:156:LEU:H	1.37	0.88
1:A:106:TRP:HB3	1:A:110:MSE:CE	2.04	0.88
1:A:159:LEU:HD23	1:A:195:LEU:HD23	1.56	0.87
1:A:154:SER:HB2	1:A:156:LEU:HD22	1.49	0.87
1:C:166:VAL:HG12	1:C:188:VAL:HG12	1.56	0.87
1:B:120:GLU:OE2	1:B:234:ARG:NH1	2.08	0.87
1:A:200:TRP:CD1	1:A:201:PHE:CD1	2.63	0.86
1:C:149:LEU:O	1:C:154:SER:OG	1.91	0.86
1:A:156:LEU:HG	1:A:156:LEU:O	1.75	0.84
1:A:154:SER:HB2	1:A:156:LEU:HD23	1.58	0.84
1:A:94:VAL:O	1:A:98:VAL:HG23	1.79	0.83
1:C:234:ARG:C	1:C:235:HIS:HD2	1.83	0.83
1:A:154:SER:HB3	1:A:156:LEU:HD22	1.58	0.82
1:A:25:MSE:CE	1:B:183:ALA:HB1	2.09	0.81
1:B:166:VAL:CG1	1:B:188:VAL:HG12	2.10	0.81
1:B:166:VAL:HG12	1:B:188:VAL:CG1	2.11	0.81
1:A:36:PHE:C	1:A:37:ASN:HD22	1.89	0.80
1:B:106:TRP:HB3	1:B:110:MSE:HE3	1.63	0.78
1:B:149:LEU:O	1:B:154:SER:OG	2.00	0.78
1:B:106:TRP:HB3	1:B:110:MSE:CE	2.13	0.78
1:C:131:TRP:HH2	1:C:184:LEU:CD2	1.95	0.78
1:C:159:LEU:CD2	1:C:195:LEU:HD21	2.12	0.78
1:A:25:MSE:HE1	1:B:183:ALA:CB	2.15	0.76
1:A:159:LEU:HD23	1:A:195:LEU:HD21	1.67	0.75
1:A:205:GLU:OE1	1:A:205:GLU:HA	1.84	0.75
1:A:159:LEU:CD2	1:A:195:LEU:HD23	2.17	0.74
1:B:155:ALA:O	1:B:157:PRO:HD3	1.87	0.73
1:C:205:GLU:OE1	1:C:206:THR:N	2.22	0.72
1:A:68:GLY:O	1:A:72:VAL:HG22	1.91	0.70
1:B:101:VAL:O	1:B:105:MSE:HE2	1.91	0.70
1:A:183:ALA:CB	1:C:25:MSE:HE1	2.21	0.70
1:C:10:GLU:HG2	1:C:63:SER:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TRP:CD1	1:A:201:PHE:CE1	2.80	0.69
1:B:143:SER:O	1:B:147:GLU:HG3	1.93	0.69
1:B:4:LEU:HD22	1:B:4:LEU:O	1.93	0.68
1:A:149:LEU:HG	1:A:154:SER:OG	1.93	0.68
1:B:145:TYR:O	1:B:149:LEU:HD22	1.93	0.68
1:A:162:VAL:HG21	1:C:33:VAL:HG23	1.76	0.68
1:B:156:LEU:H	1:B:156:LEU:CD2	2.07	0.68
1:B:75:TYR:CD1	1:B:210:LEU:HD13	2.29	0.68
1:A:183:ALA:HB3	1:C:25:MSE:HE1	1.77	0.67
1:A:193:ILE:HG23	1:A:211:LEU:HD11	1.77	0.67
1:B:36:PHE:C	1:B:37:ASN:HD22	2.03	0.67
1:C:62:ILE:CD1	1:C:110:MSE:HE3	2.20	0.67
1:A:159:LEU:O	1:A:163:THR:HG22	1.95	0.66
1:C:166:VAL:HG13	1:C:184:LEU:HD12	1.77	0.66
1:A:178:TYR:O	1:A:181:GLN:HG2	1.97	0.65
1:B:10:GLU:HG2	1:B:63:SER:HB3	1.77	0.65
1:C:159:LEU:C	1:C:159:LEU:HD23	2.22	0.65
1:B:25:MSE:HE1	1:C:184:LEU:HD11	1.73	0.64
1:B:106:TRP:CZ2	1:B:174:MSE:HE2	2.32	0.64
1:A:93:LEU:O	1:A:97:PRO:HG2	1.99	0.63
1:C:57:VAL:HG11	2:C:301:NNR:H5	1.80	0.63
1:B:105:MSE:HE1	1:B:175:ILE:HD12	1.80	0.63
1:C:234:ARG:O	1:C:235:HIS:CD2	2.40	0.62
1:B:7:TRP:HH2	1:B:66:LEU:CD1	2.11	0.62
1:B:148:TRP:HE3	1:B:149:LEU:HB3	1.65	0.62
1:B:37:ASN:HD21	1:C:158:THR:CG2	2.11	0.62
1:C:10:GLU:HG2	1:C:63:SER:CB	2.30	0.62
1:A:201:PHE:HZ	1:B:201:PHE:CZ	2.17	0.62
1:B:212:LEU:HD22	1:B:216:MSE:HE3	1.81	0.62
1:B:3:SER:O	1:B:6:TRP:HB3	2.00	0.62
1:B:6:TRP:O	1:B:8:LYS:N	2.32	0.62
1:B:4:LEU:HD13	1:B:4:LEU:C	2.26	0.61
1:B:7:TRP:CH2	1:B:66:LEU:HD11	2.36	0.61
1:B:90:LEU:O	1:B:94:VAL:HB	2.00	0.61
1:C:159:LEU:CD2	1:C:195:LEU:CD2	2.79	0.61
1:A:77:TYR:O	1:A:80:TYR:HB3	2.01	0.61
1:B:52:LEU:HD13	1:B:67:PHE:CE1	2.36	0.61
1:B:85:TYR:HA	1:B:88:MSE:HG2	1.84	0.60
1:B:7:TRP:CH2	1:B:66:LEU:CD1	2.85	0.60
1:C:75:TYR:CD1	1:C:210:LEU:HD13	2.36	0.60
1:B:205:GLU:OE1	1:B:205:GLU:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLY:O	1:C:72:VAL:HG22	2.03	0.59
1:C:105:MSE:HE1	1:C:175:ILE:HD12	1.85	0.59
1:A:36:PHE:HE1	1:B:142:THR:CG2	2.16	0.58
1:B:156:LEU:O	1:B:156:LEU:HG	2.02	0.58
1:A:166:VAL:HG12	1:A:188:VAL:HG12	1.84	0.58
1:A:36:PHE:HB3	1:B:158:THR:CG2	2.33	0.58
1:C:131:TRP:HH2	1:C:184:LEU:HD21	1.68	0.58
1:B:147:GLU:O	1:B:150:HIS:HB2	2.04	0.58
1:C:106:TRP:HB3	1:C:110:MSE:CE	2.34	0.58
1:B:37:ASN:HD22	1:B:37:ASN:N	2.02	0.57
1:C:105:MSE:HE1	1:C:175:ILE:HB	1.86	0.57
1:C:3:SER:O	1:C:6:TRP:HB3	2.04	0.57
1:B:159:LEU:O	1:B:163:THR:CG2	2.52	0.57
1:C:101:VAL:HG12	1:C:105:MSE:HE2	1.85	0.57
1:C:232:VAL:O	1:C:236:SER:OG	2.20	0.57
1:B:74:LEU:O	1:B:78:VAL:HG23	2.04	0.56
1:A:51:ILE:HD11	1:A:216:MSE:SE	2.55	0.56
1:A:159:LEU:CD2	1:A:195:LEU:CD2	2.78	0.56
1:C:31:ALA:O	1:C:35:VAL:HG23	2.05	0.56
1:C:159:LEU:O	1:C:163:THR:HG22	2.06	0.55
1:B:15:TRP:CZ3	1:B:59:LYS:HG3	2.42	0.55
1:C:159:LEU:HD23	1:C:195:LEU:HD21	1.87	0.55
1:A:158:THR:HG23	1:C:36:PHE:HB3	1.88	0.55
1:C:34:PHE:C	1:C:36:PHE:H	2.14	0.55
1:B:76:ALA:HB2	1:B:91:ASN:HB2	1.89	0.55
1:B:154:SER:CB	1:B:156:LEU:HD22	2.22	0.55
1:B:28:GLY:O	1:B:32:VAL:HG23	2.08	0.54
1:B:210:LEU:HD22	1:B:213:MSE:HE2	1.89	0.54
1:B:37:ASN:HD21	1:C:158:THR:HG21	1.70	0.54
1:A:184:LEU:N	1:C:25:MSE:HE1	2.21	0.54
1:B:172:VAL:O	1:B:176:LEU:HD12	2.08	0.54
1:C:75:TYR:HD1	1:C:210:LEU:HD13	1.70	0.54
1:A:184:LEU:HD13	1:C:25:MSE:CE	2.31	0.54
1:C:138:SER:OG	1:C:169:VAL:HG21	2.08	0.54
1:A:199:ALA:O	1:A:205:GLU:O	2.25	0.54
1:C:143:SER:O	1:C:147:GLU:HG2	2.08	0.54
1:C:103:PHE:O	1:C:107:ARG:HB2	2.08	0.53
1:B:5:ALA:O	1:B:8:LYS:HB3	2.08	0.53
1:B:182:TRP:CZ3	1:B:221:SER:HA	2.43	0.53
1:C:29:ILE:HB	1:C:216:MSE:HE1	1.90	0.53
1:A:75:TYR:CD1	1:A:210:LEU:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HG	1:A:154:SER:HG	1.74	0.53
1:B:202:LYS:HE3	1:B:203:ASN:HB2	1.90	0.53
1:C:105:MSE:CE	1:C:175:ILE:HB	2.38	0.53
1:A:106:TRP:C	1:A:110:MSE:HE2	2.34	0.53
1:B:106:TRP:CE3	1:B:110:MSE:HE1	2.44	0.53
1:C:4:LEU:O	1:C:4:LEU:HD13	2.08	0.53
1:C:178:TYR:O	1:C:181:GLN:HG2	2.09	0.53
1:B:85:TYR:O	1:B:89:MSE:HE3	2.09	0.53
1:A:66:LEU:HD23	1:A:67:PHE:H	1.73	0.53
1:C:131:TRP:CH2	1:C:184:LEU:HD21	2.44	0.53
1:A:106:TRP:HB3	1:A:110:MSE:HE1	1.87	0.52
1:B:189:ASN:O	1:B:193:ILE:HG13	2.09	0.52
1:A:37:ASN:C	1:A:39:ASP:H	2.17	0.52
1:A:63:SER:O	1:A:66:LEU:HD23	2.08	0.52
1:B:11:LEU:HD22	3:B:303:BOG:H8'1	1.92	0.52
1:B:202:LYS:HE3	1:B:202:LYS:HA	1.92	0.52
1:A:62:ILE:O	1:A:62:ILE:HG13	2.10	0.52
1:B:181:GLN:HG3	1:B:182:TRP:N	2.24	0.52
1:B:7:TRP:CZ2	1:B:66:LEU:HD11	2.45	0.51
1:B:148:TRP:CE3	1:B:149:LEU:CB	2.93	0.51
1:C:106:TRP:CE3	1:C:110:MSE:HE1	2.45	0.51
1:C:199:ALA:O	1:C:205:GLU:O	2.28	0.51
1:B:6:TRP:O	1:B:9:ARG:N	2.43	0.51
1:A:25:MSE:CE	1:B:183:ALA:CB	2.80	0.51
1:A:106:TRP:HB3	1:A:110:MSE:HE2	1.92	0.51
1:C:25:MSE:O	1:C:25:MSE:HG2	2.11	0.51
1:C:200:TRP:HA	1:C:205:GLU:C	2.36	0.51
1:A:85:TYR:HA	1:A:88:MSE:HG2	1.92	0.51
1:B:6:TRP:C	1:B:8:LYS:N	2.68	0.51
1:C:181:GLN:HG3	1:C:182:TRP:N	2.26	0.51
1:B:25:MSE:CE	1:C:184:LEU:CD1	2.63	0.51
1:C:127:THR:OG1	1:C:130:GLN:HG3	2.10	0.51
1:B:178:TYR:O	1:B:181:GLN:HG2	2.11	0.50
1:C:201:PHE:C	1:C:204:GLY:H	2.19	0.50
1:B:159:LEU:O	1:B:163:THR:HG22	2.11	0.50
1:B:35:VAL:HG12	1:B:35:VAL:O	2.11	0.50
1:B:101:VAL:O	1:B:104:ALA:HB3	2.12	0.50
1:A:47:ALA:HA	1:A:213:MSE:SE	2.61	0.50
1:B:148:TRP:CE3	1:B:149:LEU:HB3	2.46	0.50
1:A:37:ASN:C	1:A:39:ASP:N	2.67	0.50
1:C:148:TRP:O	1:C:149:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:VAL:CG1	1:C:188:VAL:HG12	2.34	0.50
1:C:200:TRP:HB2	1:C:206:THR:HG21	1.92	0.50
1:A:90:LEU:HD11	1:A:167:SER:HB3	1.94	0.50
1:B:195:LEU:O	1:B:198:VAL:HG22	2.12	0.50
1:C:39:ASP:OD1	1:C:39:ASP:N	2.38	0.49
1:A:74:LEU:O	1:A:78:VAL:HG23	2.11	0.49
1:A:170:ALA:HB2	1:A:184:LEU:HB3	1.93	0.49
1:A:183:ALA:C	1:C:25:MSE:HE1	2.36	0.49
1:C:89:MSE:O	1:C:93:LEU:HG	2.12	0.49
1:B:149:LEU:O	1:B:149:LEU:HG	2.12	0.49
1:B:149:LEU:HD21	1:B:156:LEU:HD13	1.95	0.49
1:C:51:ILE:HD11	1:C:216:MSE:SE	2.63	0.49
1:A:101:VAL:HG12	1:A:105:MSE:HE1	1.94	0.48
1:C:91:ASN:O	1:C:96:VAL:HG23	2.13	0.48
1:C:200:TRP:O	1:C:204:GLY:HA2	2.13	0.48
1:A:203:ASN:O	1:A:204:GLY:C	2.56	0.48
1:A:29:ILE:HB	1:A:216:MSE:HE1	1.95	0.48
1:C:85:TYR:HA	1:C:88:MSE:HG2	1.95	0.48
1:C:235:HIS:CD2	1:C:235:HIS:N	2.79	0.48
1:B:85:TYR:O	1:B:89:MSE:HG2	2.14	0.48
1:C:200:TRP:CD1	1:C:201:PHE:CD1	3.00	0.48
1:A:15:TRP:CZ3	1:A:59:LYS:HG3	2.49	0.48
1:B:27:LEU:HD22	1:B:48:VAL:HG13	1.94	0.48
1:A:36:PHE:HB3	1:B:158:THR:HG22	1.94	0.48
1:B:159:LEU:HD23	1:B:195:LEU:HD23	1.96	0.48
1:C:88:MSE:HG3	1:C:89:MSE:N	2.29	0.48
1:B:6:TRP:O	1:B:7:TRP:C	2.56	0.47
1:B:111:ALA:O	1:B:119:GLU:HB3	2.14	0.47
1:B:170:ALA:HB2	1:B:184:LEU:HB3	1.95	0.47
1:B:87:GLU:O	1:B:91:ASN:ND2	2.41	0.47
1:B:191:LEU:O	1:B:194:SER:HB2	2.14	0.47
1:A:106:TRP:CE3	1:A:110:MSE:HE1	2.49	0.47
1:A:75:TYR:HD1	1:A:210:LEU:HD13	1.79	0.47
1:A:163:THR:O	1:A:167:SER:HB2	2.13	0.47
1:A:201:PHE:CZ	1:B:201:PHE:CZ	3.02	0.47
1:B:165:VAL:O	1:B:169:VAL:HG23	2.14	0.47
1:A:148:TRP:CE3	1:A:149:LEU:HA	2.50	0.47
1:C:25:MSE:O	1:C:29:ILE:HG12	2.15	0.47
1:C:106:TRP:HE3	1:C:110:MSE:HE1	1.80	0.47
1:A:106:TRP:O	1:A:110:MSE:HE2	2.14	0.46
1:C:179:ARG:O	1:C:179:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:TYR:C	1:C:82:PHE:H	2.24	0.46
1:A:193:ILE:HG23	1:A:211:LEU:CD1	2.43	0.46
1:A:142:THR:CG2	1:C:36:PHE:CE1	2.98	0.46
1:A:180:GLU:N	1:A:180:GLU:OE1	2.48	0.46
1:B:151:HIS:O	1:B:152:LEU:HB2	2.15	0.46
1:C:49:THR:O	1:C:71:SER:HB2	2.16	0.46
1:A:57:VAL:HG11	2:A:301:NNR:H5	1.97	0.46
1:A:158:THR:CG2	1:C:36:PHE:HB3	2.45	0.46
1:B:11:LEU:CD2	3:B:303:BOG:H8'1	2.45	0.46
1:C:19:GLU:OE1	1:C:223:TYR:OH	2.32	0.46
1:C:101:VAL:O	1:C:105:MSE:HE2	2.16	0.46
1:B:75:TYR:HD1	1:B:210:LEU:HD13	1.76	0.46
1:A:106:TRP:HE3	1:A:110:MSE:HE1	1.80	0.46
1:B:11:LEU:HD21	1:B:67:PHE:HZ	1.80	0.45
1:C:90:LEU:HD11	1:C:167:SER:HB3	1.98	0.45
1:A:106:TRP:CZ2	1:A:174:MSE:HE2	2.52	0.45
1:B:39:ASP:OD1	1:B:39:ASP:N	2.46	0.45
1:C:4:LEU:CD1	1:C:4:LEU:C	2.89	0.45
1:C:34:PHE:C	1:C:36:PHE:N	2.75	0.45
1:A:176:LEU:O	1:A:177:ARG:HB2	2.16	0.45
1:B:75:TYR:CE1	1:B:210:LEU:HD13	2.51	0.45
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.83	0.45
1:B:37:ASN:C	1:B:39:ASP:H	2.24	0.45
1:C:200:TRP:C	1:C:201:PHE:CD1	2.95	0.45
1:A:192:THR:HG21	1:A:214:TYR:CZ	2.52	0.45
1:A:200:TRP:O	1:A:204:GLY:HA2	2.17	0.45
1:B:83:LYS:HA	1:B:85:TYR:CZ	2.52	0.44
1:A:200:TRP:O	1:A:205:GLU:N	2.51	0.44
1:A:202:LYS:HA	1:A:203:ASN:HA	1.59	0.44
1:A:203:ASN:O	1:A:205:GLU:N	2.50	0.44
1:A:166:VAL:CG1	1:A:188:VAL:HG12	2.46	0.44
1:B:77:TYR:O	1:B:80:TYR:HB3	2.17	0.44
1:C:57:VAL:HG12	1:C:182:TRP:CZ2	2.53	0.44
1:A:76:ALA:HB2	1:A:91:ASN:HB3	1.99	0.44
1:A:181:GLN:HG3	1:A:182:TRP:N	2.32	0.44
1:B:105:MSE:CE	1:B:175:ILE:HB	2.46	0.44
1:A:165:VAL:O	1:A:169:VAL:HG23	2.17	0.44
1:B:4:LEU:HD13	1:B:5:ALA:N	2.32	0.44
1:B:202:LYS:HE3	1:B:202:LYS:CA	2.47	0.44
1:B:105:MSE:HE1	1:B:175:ILE:HB	1.98	0.44
1:B:201:PHE:HZ	1:C:201:PHE:HE2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:ND2	1:B:158:THR:HG21	2.32	0.44
1:A:36:PHE:C	1:A:37:ASN:ND2	2.66	0.43
1:B:105:MSE:HE3	1:B:105:MSE:HB2	1.78	0.43
1:C:82:PHE:CZ	1:C:207:SER:HB3	2.53	0.43
1:C:201:PHE:CD1	1:C:201:PHE:N	2.85	0.43
1:B:4:LEU:HD22	1:B:4:LEU:C	2.43	0.43
1:A:63:SER:O	1:A:66:LEU:CD2	2.66	0.43
1:B:201:PHE:CZ	1:C:201:PHE:HE2	2.36	0.43
1:A:200:TRP:O	1:A:204:GLY:CA	2.67	0.43
1:B:194:SER:O	1:B:198:VAL:HG13	2.18	0.43
1:B:34:PHE:C	1:B:36:PHE:H	2.27	0.43
1:A:24:LEU:CD1	1:B:132:LEU:HB2	2.49	0.43
1:C:3:SER:HB2	1:C:6:TRP:H	1.84	0.43
1:A:115:THR:HB	1:A:117:GLU:HG3	2.00	0.42
1:A:142:THR:HG23	1:C:36:PHE:HE1	1.84	0.42
1:C:131:TRP:CH2	1:C:184:LEU:CD2	2.86	0.42
1:A:59:LYS:HA	1:A:59:LYS:HD2	1.88	0.42
1:B:121:VAL:HG21	1:B:177:ARG:HG2	2.01	0.42
1:B:159:LEU:O	1:B:163:THR:HG23	2.19	0.42
1:B:23:LEU:HD11	1:B:52:LEU:HD23	2.01	0.42
1:C:206:THR:OG1	1:C:207:SER:N	2.52	0.42
1:A:35:VAL:O	1:A:35:VAL:HG12	2.19	0.42
1:A:101:VAL:O	1:A:105:MSE:HE2	2.18	0.42
1:C:149:LEU:O	1:C:149:LEU:HG	2.19	0.42
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.76	0.42
1:C:200:TRP:C	1:C:201:PHE:HD1	2.27	0.42
1:A:105:MSE:CE	1:A:175:ILE:HB	2.50	0.42
1:A:142:THR:CG2	1:C:36:PHE:HE1	2.33	0.42
1:B:6:TRP:C	1:B:8:LYS:H	2.28	0.42
1:A:101:VAL:HG12	1:A:105:MSE:CE	2.50	0.42
1:A:131:TRP:HH2	1:A:184:LEU:HD22	1.84	0.42
1:A:37:ASN:HD22	1:A:37:ASN:N	2.10	0.41
1:A:76:ALA:HB2	1:A:91:ASN:CB	2.51	0.41
1:B:203:ASN:O	1:B:205:GLU:N	2.53	0.41
1:C:80:TYR:C	1:C:82:PHE:N	2.77	0.41
1:C:90:LEU:HG	1:C:164:VAL:HG13	2.03	0.41
1:C:101:VAL:C	1:C:105:MSE:HE2	2.45	0.41
1:C:108:LYS:HE2	1:C:108:LYS:HB2	1.77	0.41
1:A:37:ASN:HD21	1:B:158:THR:CG2	2.33	0.41
1:B:201:PHE:CZ	1:C:201:PHE:CE2	3.09	0.41
1:B:214:TYR:HA	1:B:217:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CE3	1:A:42:LEU:HA	2.55	0.41
1:A:105:MSE:HE2	1:A:105:MSE:HB2	1.70	0.41
1:B:12:PHE:O	3:B:303:BOG:O2	2.27	0.41
1:A:23:LEU:HD23	3:A:302:BOG:C5'	2.52	0.40
1:A:105:MSE:HE3	1:A:175:ILE:HB	2.03	0.40
1:B:37:ASN:C	1:B:39:ASP:N	2.77	0.40
1:B:101:VAL:C	1:B:105:MSE:HE2	2.46	0.40
1:B:168:ILE:O	1:B:172:VAL:HG23	2.22	0.40
1:A:45:VAL:HG12	1:A:74:LEU:CD1	2.51	0.40
1:B:198:VAL:O	1:B:200:TRP:N	2.54	0.40
1:B:202:LYS:O	1:B:202:LYS:HG3	2.20	0.40
1:A:149:LEU:HD23	1:A:156:LEU:HD13	2.02	0.40
1:B:34:PHE:C	1:B:34:PHE:CD1	3.00	0.40
1:B:148:TRP:O	1:B:149:LEU:HB3	2.22	0.40
1:C:213:MSE:HE3	1:C:214:TYR:CE2	2.56	0.40
1:A:31:ALA:O	1:A:34:PHE:HB3	2.22	0.40
1:C:182:TRP:HE1	1:C:228:TRP:CG	2.40	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 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	233/244 (96%)	220 (94%)	13 (6%)	0	100	100
1	B	233/244 (96%)	214 (92%)	18 (8%)	1 (0%)	30	60
1	C	235/244 (96%)	217 (92%)	17 (7%)	1 (0%)	30	60
All	All	701/732 (96%)	651 (93%)	48 (7%)	2 (0%)	36	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	TRP
1	C	35	VAL

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 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	200/199 (100%)	171 (86%)	29 (14%)	3	11
1	B	200/199 (100%)	156 (78%)	44 (22%)	1	3
1	C	201/199 (101%)	171 (85%)	30 (15%)	3	10
All	All	601/597 (101%)	498 (83%)	103 (17%)	2	7

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	LEU
1	A	21	VAL
1	A	42	LEU
1	A	44	SER
1	A	62	ILE
1	A	69	LEU
1	A	88	MSE
1	A	90	LEU
1	A	96	VAL
1	A	105	MSE
1	A	114	GLU
1	A	115	THR
1	A	132	LEU
1	A	133	LEU
1	A	143	SER
1	A	144	VAL
1	A	154	SER
1	A	158	THR
1	A	163	THR
1	A	167	SER

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Mol	Chain	Res	Type
1	A	174	MSE
1	A	184	LEU
1	A	188	VAL
1	A	200	TRP
1	A	205	GLU
1	A	211	LEU
1	A	212	LEU
1	A	218	LEU
1	B	4	LEU
1	B	21	VAL
1	B	25	MSE
1	B	30	GLN
1	B	33	VAL
1	B	37	ASN
1	B	39	ASP
1	B	42	LEU
1	B	66	LEU
1	B	69	LEU
1	B	88	MSE
1	B	90	LEU
1	B	92	LEU
1	B	98	VAL
1	B	101	VAL
1	B	105	MSE
1	B	108	LYS
1	B	112	LEU
1	B	115	THR
1	B	128	VAL
1	B	139	VAL
1	B	143	SER
1	B	149	LEU
1	B	152	LEU
1	B	154	SER
1	B	156	LEU
1	B	158	THR
1	B	163	THR
1	B	167	SER
1	B	174	MSE
1	B	176	LEU
1	B	184	LEU
1	B	188	VAL
1	B	200	TRP

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Mol	Chain	Res	Type
1	B	202	LYS
1	B	205	GLU
1	B	207	SER
1	B	208	LEU
1	B	213	MSE
1	B	218	LEU
1	B	229	THR
1	B	231	LEU
1	B	233	LYS
1	B	236	SER
1	C	3	SER
1	C	4	LEU
1	C	33	VAL
1	C	37	ASN
1	C	39	ASP
1	C	42	LEU
1	C	52	LEU
1	C	62	ILE
1	C	88	MSE
1	C	90	LEU
1	C	108	LYS
1	C	112	LEU
1	C	119	GLU
1	C	120	GLU
1	C	149	LEU
1	C	150	HIS
1	C	152	LEU
1	C	163	THR
1	C	167	SER
1	C	172	VAL
1	C	174	MSE
1	C	176	LEU
1	C	184	LEU
1	C	187	VAL
1	C	188	VAL
1	C	208	LEU
1	C	218	LEU
1	C	231	LEU
1	C	232	VAL
1	C	233	LYS

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	37	ASN
1	A	91	ASN
1	A	109	HIS
1	A	171	GLN
1	B	37	ASN
1	B	109	HIS
1	B	189	ASN
1	B	235	HIS
1	C	37	ASN
1	C	235	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	BOG	C	302	-	20,20,20	1.34	3 (15%)	25,25,25	1.18	3 (12%)
2	NNR	C	301	-	17,19,19	4.82	8 (47%)	21,27,27	1.20	1 (4%)
2	NNR	A	301	-	17,19,19	4.87	8 (47%)	21,27,27	1.55	3 (14%)
3	BOG	B	303	-	20,20,20	1.42	2 (10%)	25,25,25	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BOG	B	302	-	20,20,20	1.53	2 (10%)	25,25,25	1.25	3 (12%)
3	BOG	A	302	-	20,20,20	1.23	2 (10%)	25,25,25	1.11	3 (12%)
2	NNR	B	301	-	17,19,19	5.12	8 (47%)	21,27,27	1.51	3 (14%)

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	BOG	C	302	-	-	5/11/31/31	0/1/1/1
2	NNR	C	301	-	-	0/10/26/26	0/2/2/2
2	NNR	A	301	-	-	6/10/26/26	0/2/2/2
3	BOG	B	303	-	-	6/11/31/31	0/1/1/1
3	BOG	B	302	-	-	7/11/31/31	0/1/1/1
3	BOG	A	302	-	-	6/11/31/31	0/1/1/1
2	NNR	B	301	-	-	4/10/26/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NNR	O4R-C1R	16.86	1.63	1.40
2	A	301	NNR	O4R-C1R	16.29	1.62	1.40
2	C	301	NNR	O4R-C1R	15.48	1.61	1.40
2	B	301	NNR	C7-N7	6.98	1.45	1.33
2	C	301	NNR	O4R-C4R	-6.39	1.30	1.45
2	B	301	NNR	O4R-C4R	-6.29	1.31	1.45
2	C	301	NNR	C7-N7	6.13	1.44	1.33
2	A	301	NNR	C7-N7	6.10	1.44	1.33
2	A	301	NNR	O4R-C4R	-5.88	1.31	1.45
2	C	301	NNR	C2-N1	5.23	1.40	1.35
2	A	301	NNR	O2R-C2R	4.65	1.54	1.43
2	B	301	NNR	C2-N1	4.55	1.40	1.35
2	B	301	NNR	O2R-C2R	4.37	1.53	1.43
2	C	301	NNR	O2R-C2R	4.34	1.53	1.43
3	B	303	BOG	O5-C1	3.98	1.52	1.41
3	B	302	BOG	O5-C1	3.67	1.51	1.41
3	B	302	BOG	O2-C2	3.65	1.52	1.43
3	C	302	BOG	O5-C1	3.38	1.50	1.41
2	A	301	NNR	C2-N1	3.10	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NNR	O3R-C3R	-2.89	1.35	1.43
2	A	301	NNR	O3R-C3R	-2.81	1.36	1.43
3	A	302	BOG	O5-C1	2.74	1.48	1.41
2	C	301	NNR	O3R-C3R	-2.74	1.36	1.43
2	A	301	NNR	O7-C7	-2.64	1.19	1.24
3	B	303	BOG	O5-C5	2.59	1.50	1.44
3	C	302	BOG	O5-C5	2.51	1.50	1.44
3	A	302	BOG	O2-C2	2.49	1.49	1.43
2	B	301	NNR	C2-C3	2.44	1.42	1.39
2	A	301	NNR	C5R-C4R	2.24	1.59	1.51
2	C	301	NNR	O7-C7	-2.23	1.20	1.24
2	B	301	NNR	O7-C7	-2.19	1.20	1.24
2	C	301	NNR	C5R-C4R	2.14	1.59	1.51
3	C	302	BOG	O2-C2	2.12	1.48	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NNR	C6-N1-C2	-3.96	118.51	121.88
2	B	301	NNR	C4R-O4R-C1R	-3.58	106.65	109.92
3	C	302	BOG	O5-C5-C4	3.44	115.89	109.70
3	B	302	BOG	O1-C1-C2	3.36	113.38	108.27
2	A	301	NNR	C4R-O4R-C1R	-3.29	106.92	109.92
2	C	301	NNR	C6-N1-C2	-3.17	119.18	121.88
3	A	302	BOG	O5-C5-C4	2.66	114.49	109.70
2	B	301	NNR	C6-N1-C2	-2.59	119.67	121.88
3	A	302	BOG	O1-C1-C2	2.53	112.11	108.27
2	B	301	NNR	C5R-C4R-C3R	-2.46	109.29	115.10
2	A	301	NNR	C5R-C4R-C3R	-2.46	109.29	115.10
3	C	302	BOG	C3-C4-C5	2.43	114.64	110.23
3	C	302	BOG	C6-C5-C4	-2.33	107.30	113.02
3	A	302	BOG	C6-C5-C4	-2.24	107.51	113.02
3	B	302	BOG	C4-C3-C2	2.17	114.64	110.83
3	B	302	BOG	C3-C4-C5	2.06	113.96	110.23

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	BOG	C2'-C1'-O1-C1
3	B	303	BOG	O5-C1-O1-C1'
2	A	301	NNR	O4R-C4R-C5R-O5R

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Mol	Chain	Res	Type	Atoms
2	A	301	NNR	C3R-C4R-C5R-O5R
3	A	302	BOG	O5-C5-C6-O6
3	B	302	BOG	O5-C1-O1-C1'
3	C	302	BOG	O5-C1-O1-C1'
3	A	302	BOG	C4-C5-C6-O6
3	B	302	BOG	C2-C1-O1-C1'
3	C	302	BOG	C2-C1-O1-C1'
3	B	303	BOG	O5-C5-C6-O6
3	A	302	BOG	C1'-C2'-C3'-C4'
3	A	302	BOG	C5'-C6'-C7'-C8'
3	A	302	BOG	C4'-C5'-C6'-C7'
3	B	302	BOG	C2'-C3'-C4'-C5'
3	C	302	BOG	C4'-C5'-C6'-C7'
3	B	303	BOG	C1'-C2'-C3'-C4'
3	B	303	BOG	O1-C1'-C2'-C3'
3	B	302	BOG	C3'-C4'-C5'-C6'
3	C	302	BOG	C5'-C6'-C7'-C8'
3	B	302	BOG	C1'-C2'-C3'-C4'
3	C	302	BOG	C4-C5-C6-O6
3	B	303	BOG	C4'-C5'-C6'-C7'
3	A	302	BOG	O1-C1'-C2'-C3'
2	B	301	NNR	O4R-C4R-C5R-O5R
2	A	301	NNR	C2-C3-C7-O7
3	B	303	BOG	C2'-C1'-O1-C1
2	A	301	NNR	C2-C3-C7-N7
2	B	301	NNR	C2R-C1R-N1-C2
2	B	301	NNR	C2R-C1R-N1-C6
3	B	302	BOG	O1-C1'-C2'-C3'
2	A	301	NNR	C4-C3-C7-N7
2	A	301	NNR	C4-C3-C7-O7
2	B	301	NNR	C3R-C4R-C5R-O5R

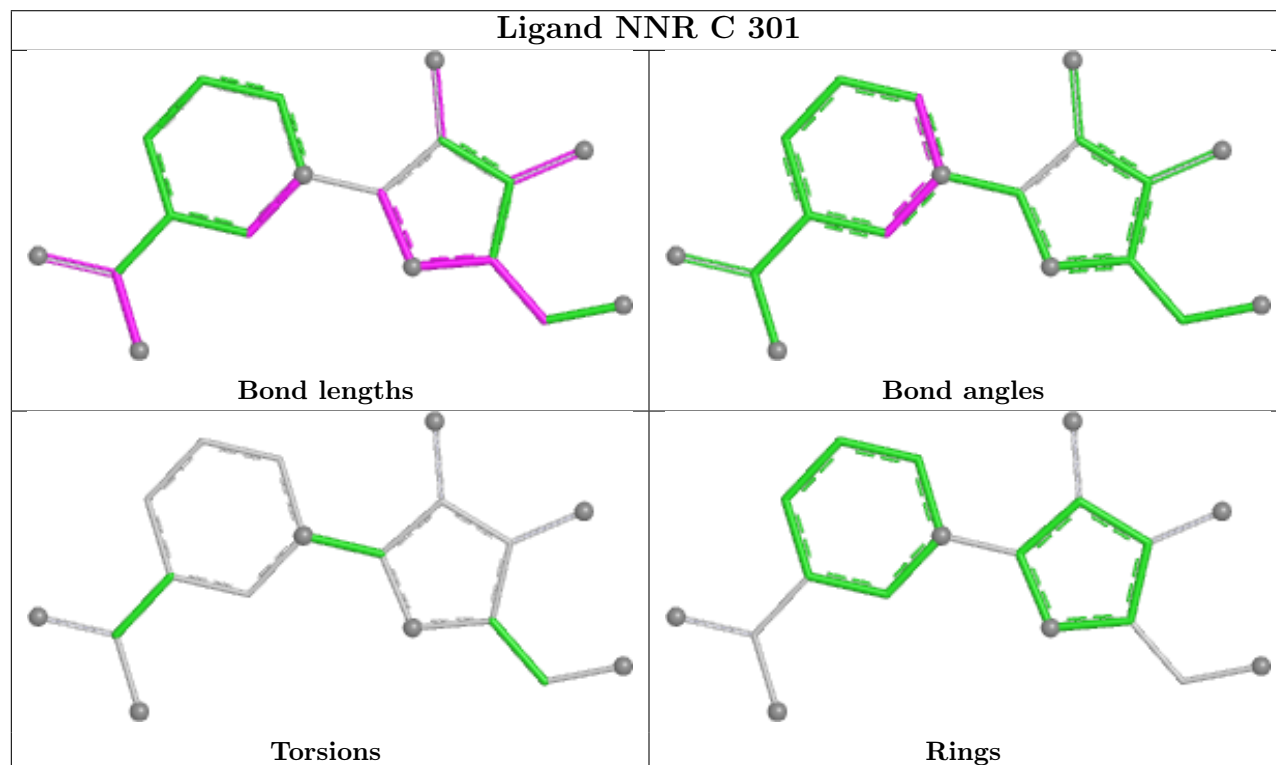
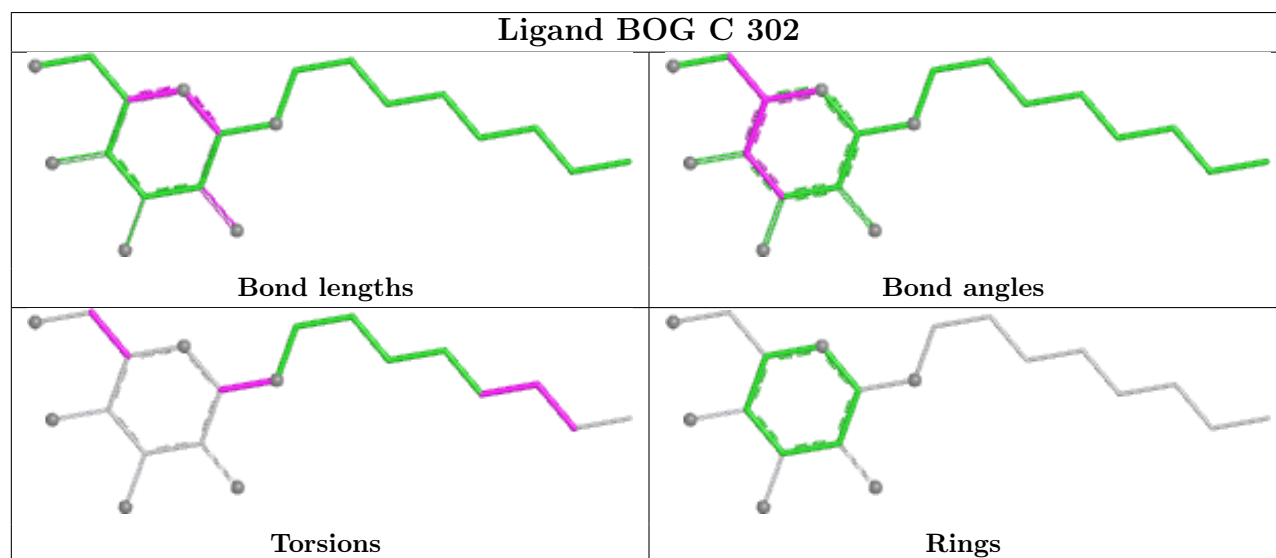
There are no ring outliers.

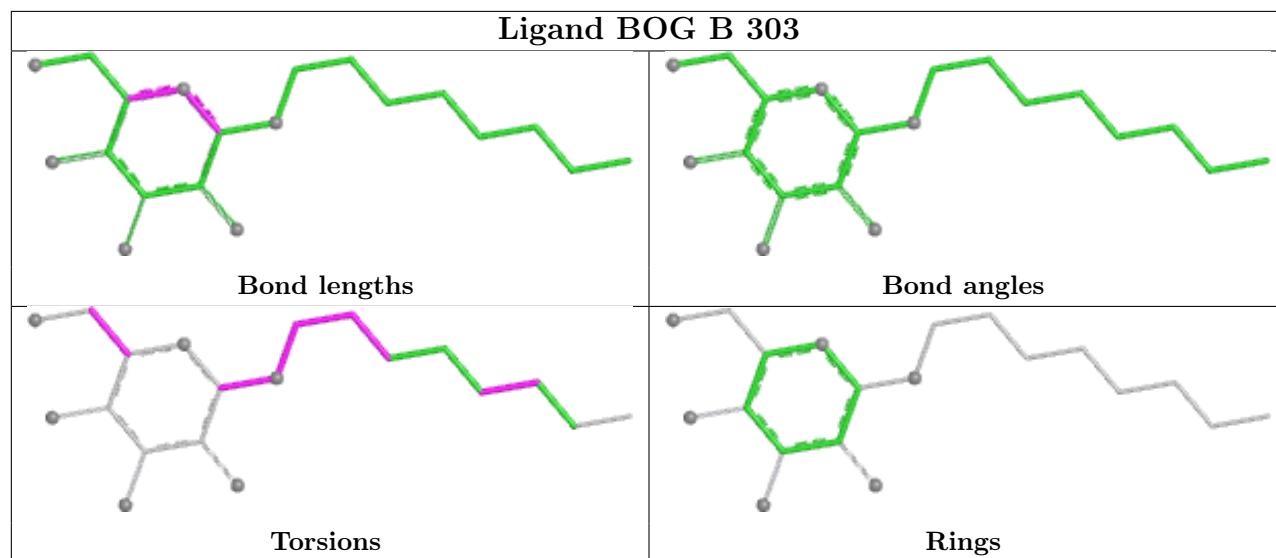
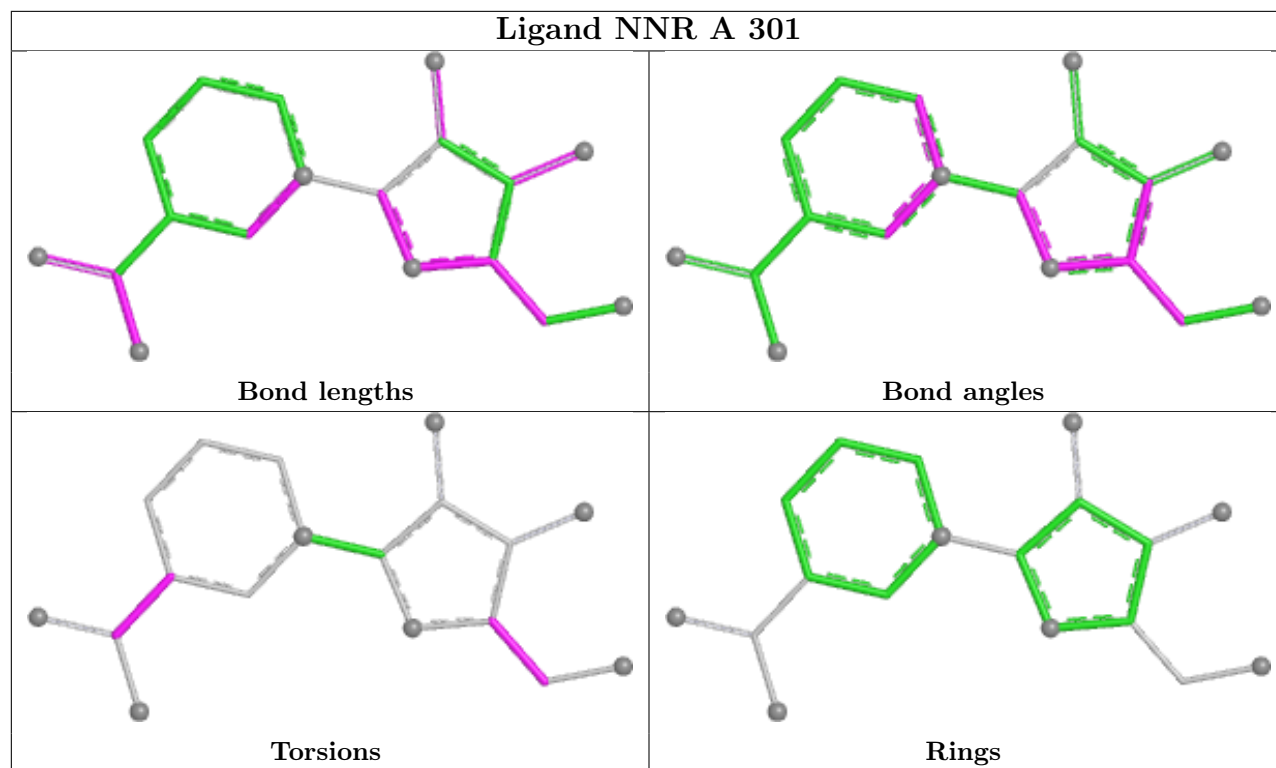
4 monomers are involved in 6 short contacts:

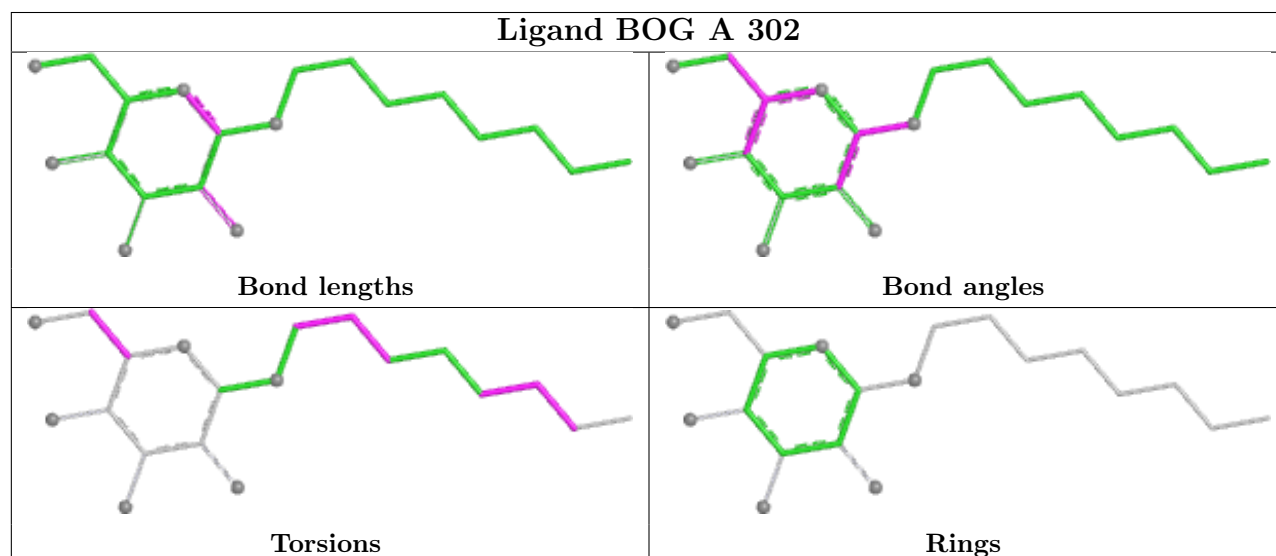
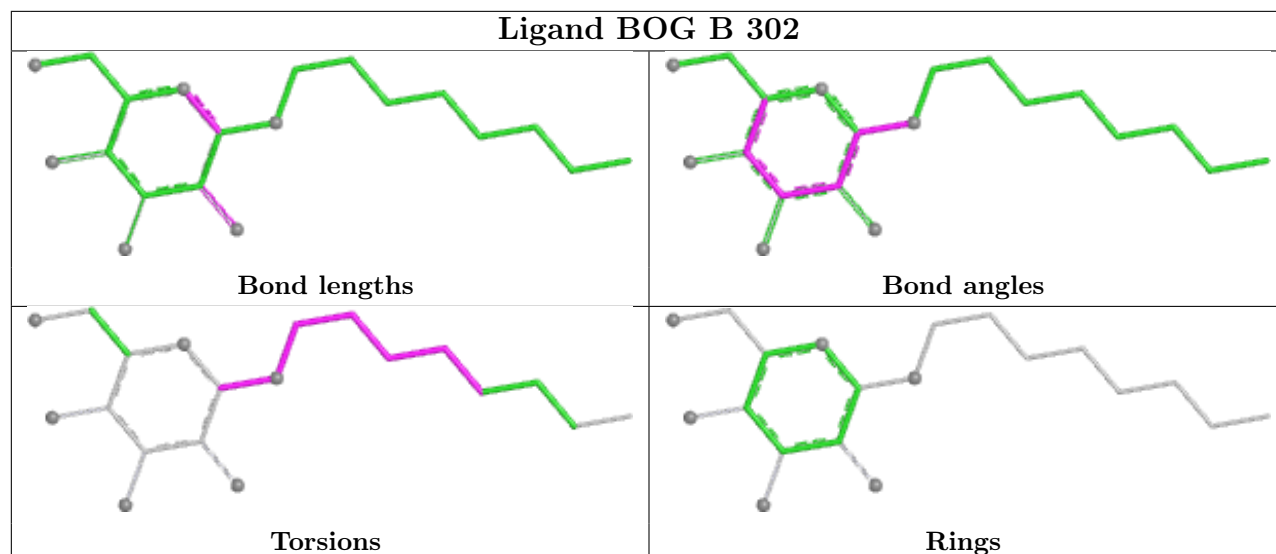
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NNR	1	0
2	A	301	NNR	1	0
3	B	303	BOG	3	0
3	A	302	BOG	1	0

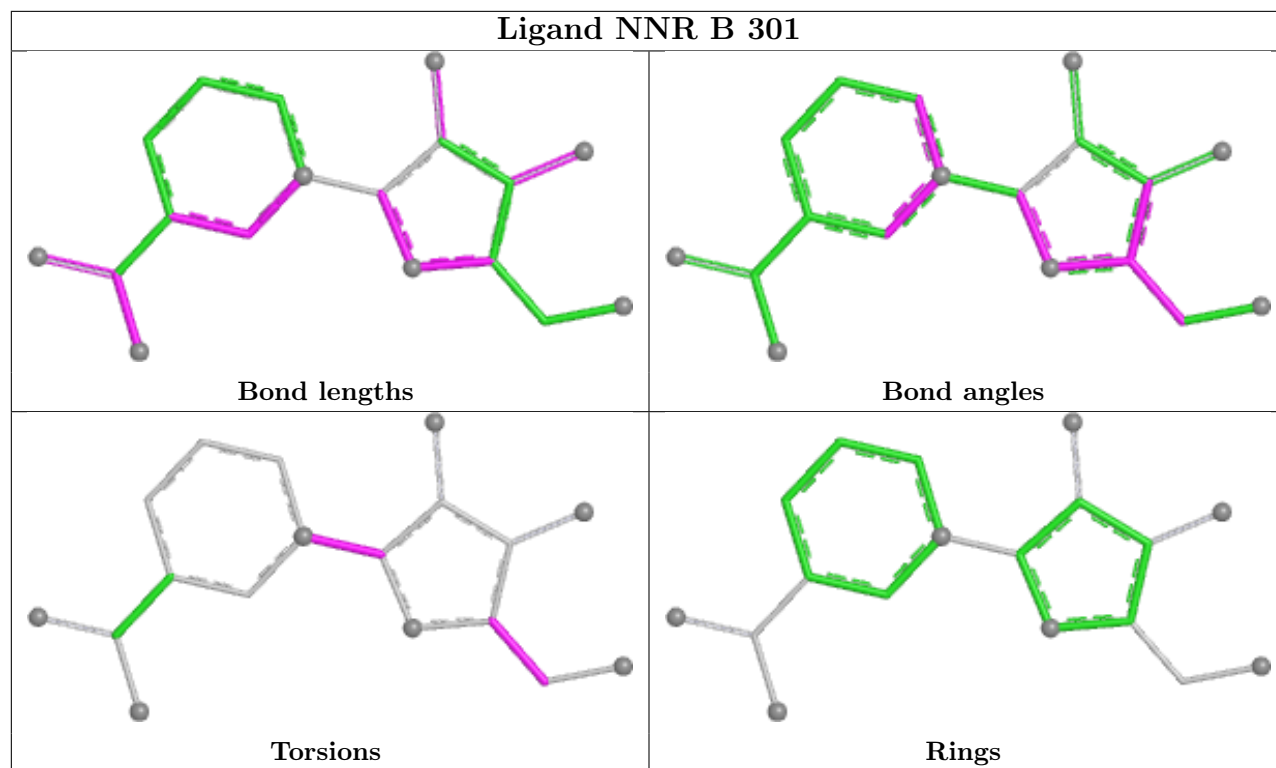
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	227/244 (93%)	0.29	11 (4%) 35 28	70, 112, 168, 196	0
1	B	227/244 (93%)	0.50	26 (11%) 9 7	72, 108, 174, 211	0
1	C	229/244 (93%)	0.18	8 (3%) 47 38	72, 115, 179, 210	0
All	All	683/732 (93%)	0.32	45 (6%) 24 18	70, 112, 175, 211	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ASP	9.8
1	B	159	LEU	8.0
1	A	101	VAL	5.1
1	B	158	THR	4.9
1	A	12	PHE	4.8
1	B	193	ILE	4.4
1	B	163	THR	4.2
1	B	93	LEU	4.0
1	C	238	GLN	4.0
1	B	112	LEU	3.8
1	B	145	TYR	3.8
1	B	100	PHE	3.8
1	B	194	SER	3.6
1	B	94	VAL	3.5
1	A	104	ALA	3.3
1	C	93	LEU	3.3
1	B	162	VAL	3.2
1	B	157	PRO	3.2
1	A	206	THR	3.1
1	B	70	ILE	3.1
1	C	202	LYS	3.0
1	A	112	LEU	3.0
1	B	152	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	2.9
1	B	164	VAL	2.9
1	C	40	SER	2.8
1	B	12	PHE	2.7
1	B	66	LEU	2.7
1	A	36	PHE	2.6
1	B	223	TYR	2.6
1	A	155	ALA	2.6
1	B	197	ALA	2.6
1	A	62	ILE	2.6
1	B	168	ILE	2.5
1	B	195	LEU	2.5
1	A	97	PRO	2.4
1	B	86	GLY	2.4
1	C	100	PHE	2.3
1	C	92	LEU	2.3
1	B	161	GLY	2.3
1	C	207	SER	2.2
1	B	132	LEU	2.1
1	B	211	LEU	2.1
1	A	94	VAL	2.0
1	C	69	LEU	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.

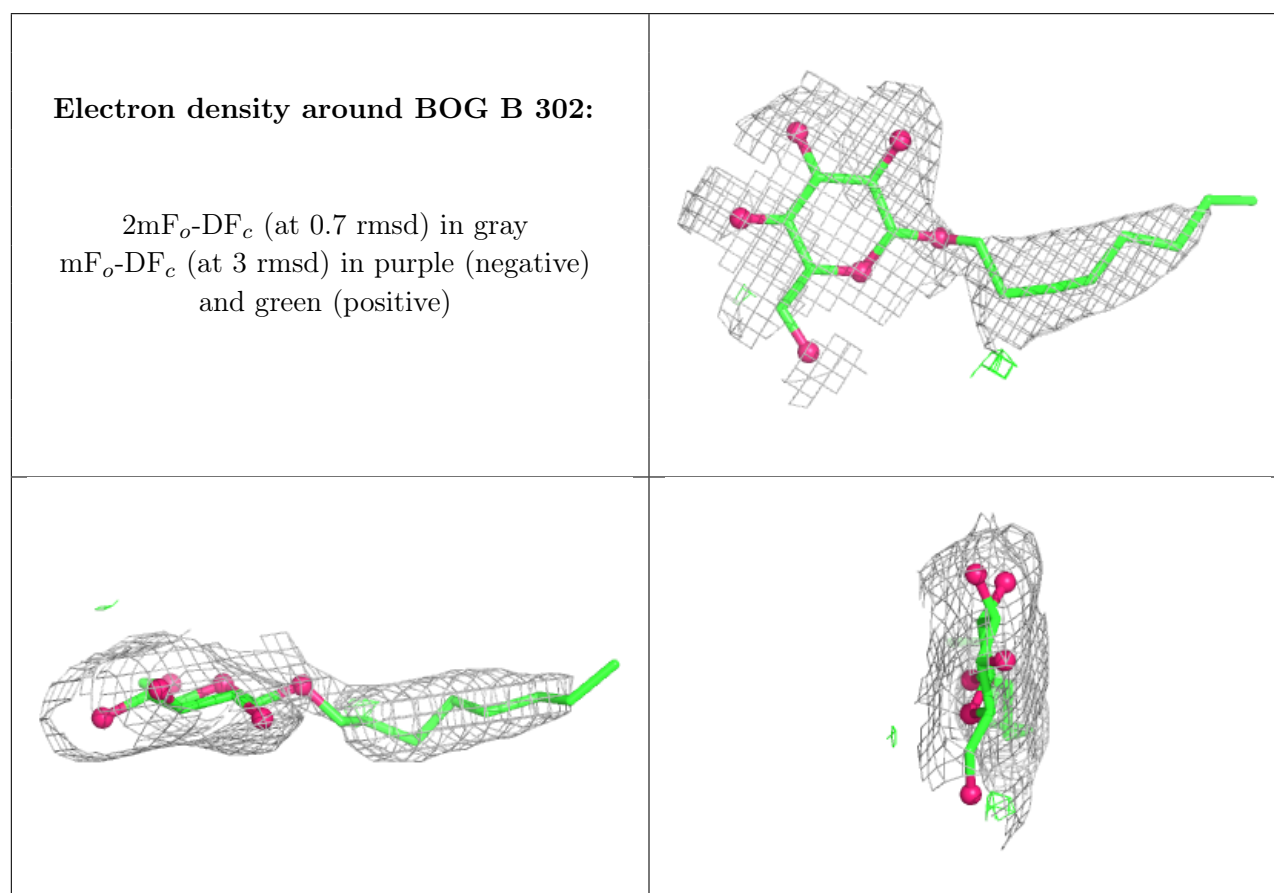
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BOG	B	302	20/20	0.90	0.14	76,100,122,135	0

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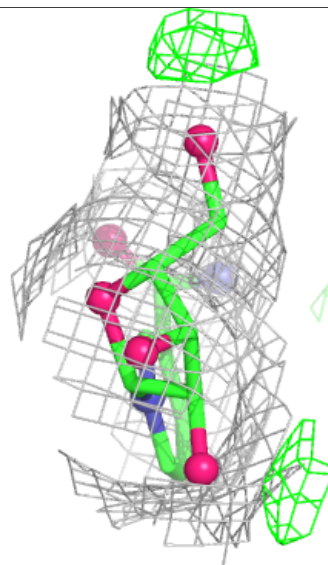
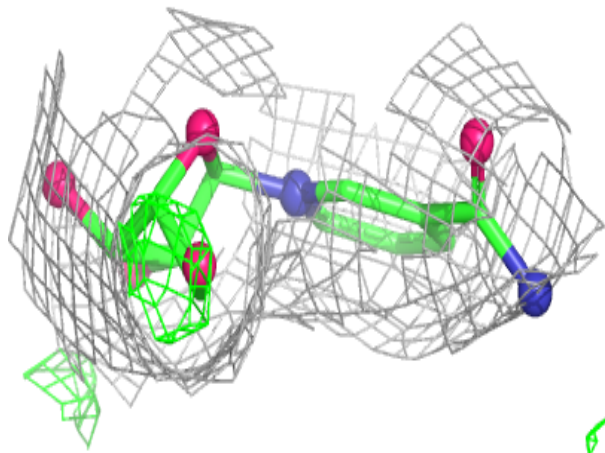
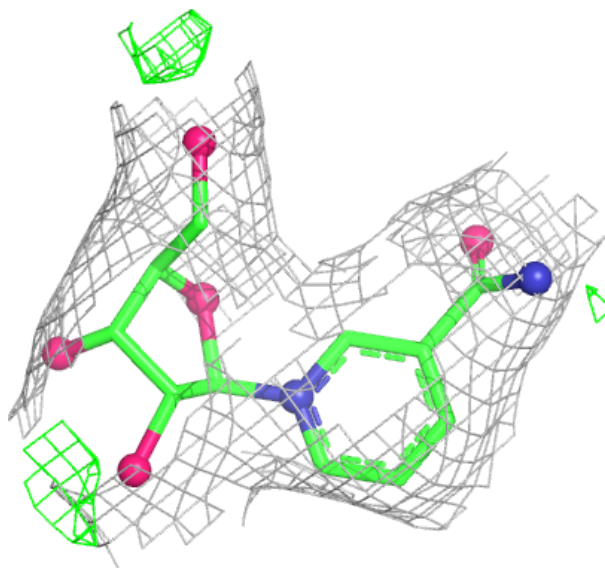
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NNR	A	301	18/18	0.93	0.10	97,105,122,129	0
3	BOG	A	302	20/20	0.94	0.10	72,102,127,142	0
2	NNR	B	301	18/18	0.94	0.08	80,95,109,111	0
3	BOG	B	303	20/20	0.94	0.10	92,99,116,126	0
3	BOG	C	302	20/20	0.94	0.12	81,124,153,158	0
2	NNR	C	301	18/18	0.95	0.09	77,99,117,125	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.



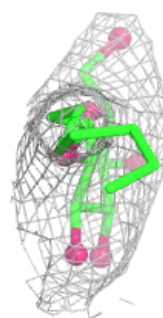
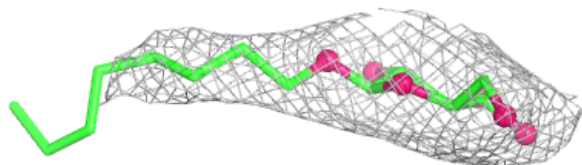
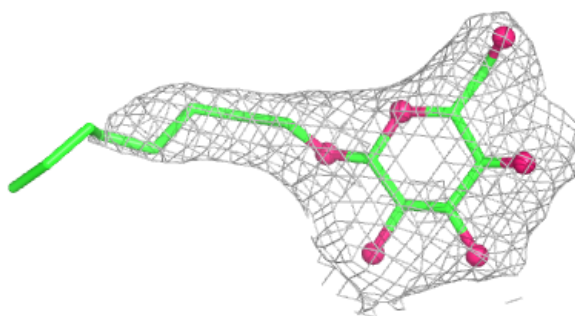
Electron density around NNR A 301:

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



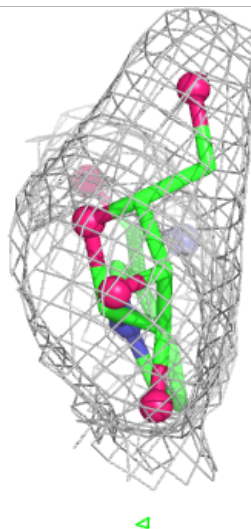
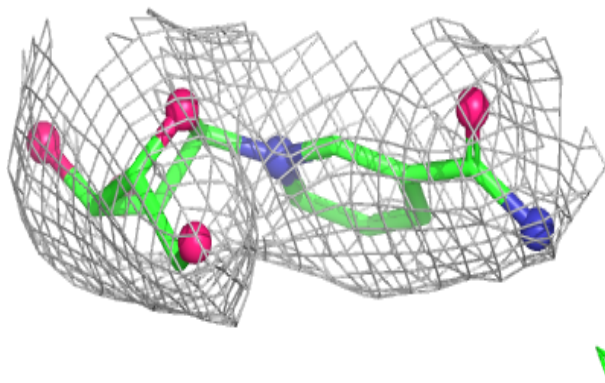
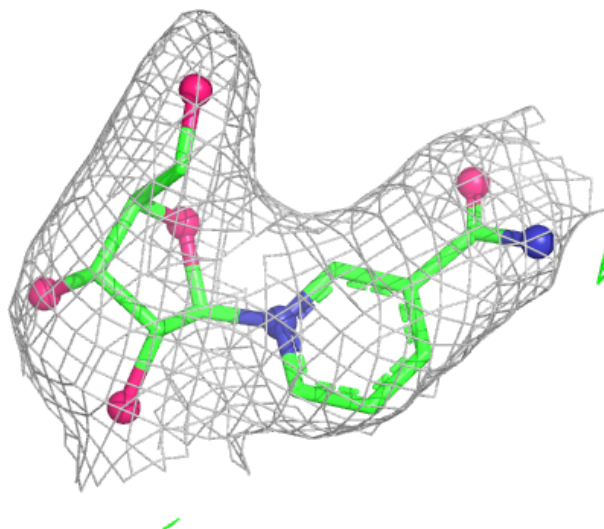
Electron density around BOG A 302:

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



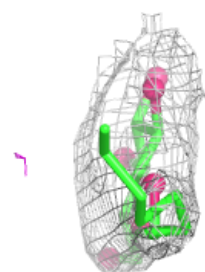
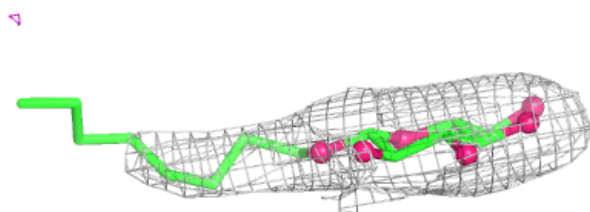
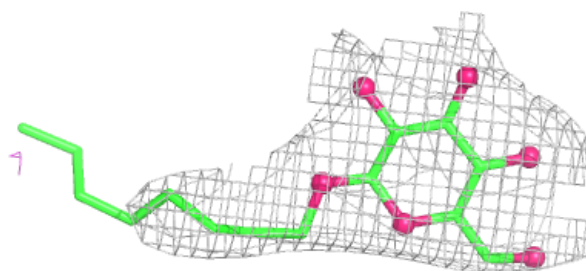
Electron density around NNR B 301:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

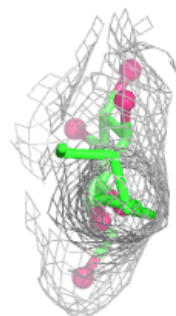
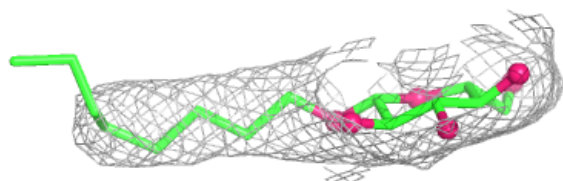
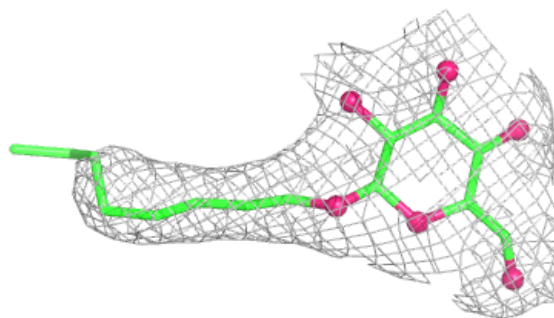


Electron density around BOG B 303:

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

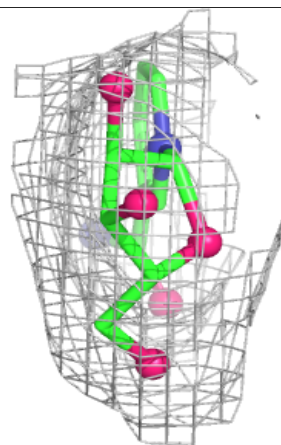
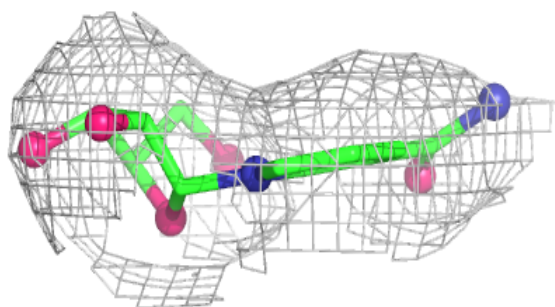
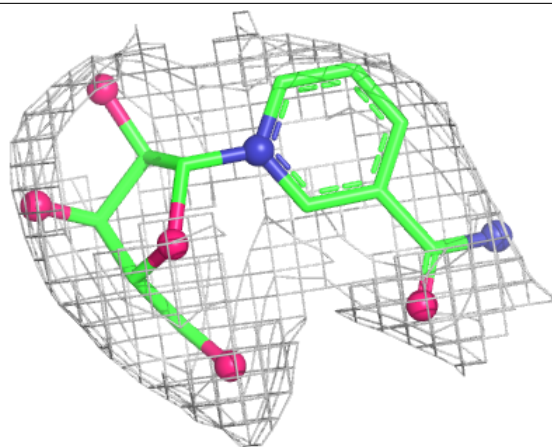
**Electron density around BOG C 302:**

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



Electron density around NNR C 301:

$2mF_o-DF_c$ (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.