



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2021 – 12:13 am BST

PDB ID : 7O82
Title : The L-arginine/agmatine antiporter from *E. coli* at 1.7 Å resolution
Authors : Jeckelmann, J.M.; Ilgue, H.; Kalbermatter, D.; Fotiadis, D.
Deposited on : 2021-04-14
Resolution : 1.69 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRS	A	502	-	X	-	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7313 atoms, of which 260 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.

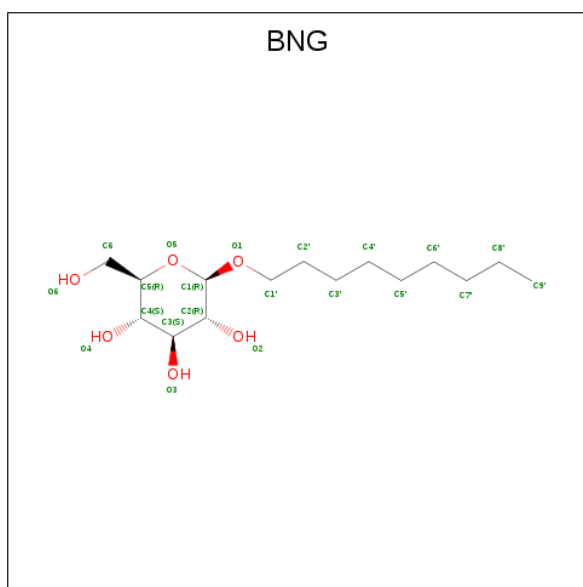
- Molecule 1 is a protein called Arginine/agmatine antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	Total 3279	C 2175	N 523	O 556	S 25	0	5	0
1	B	436	Total 3274	C 2172	N 522	O 555	S 25	0	5	0

There are 16 discrepancies between the modelled and reference sequences:

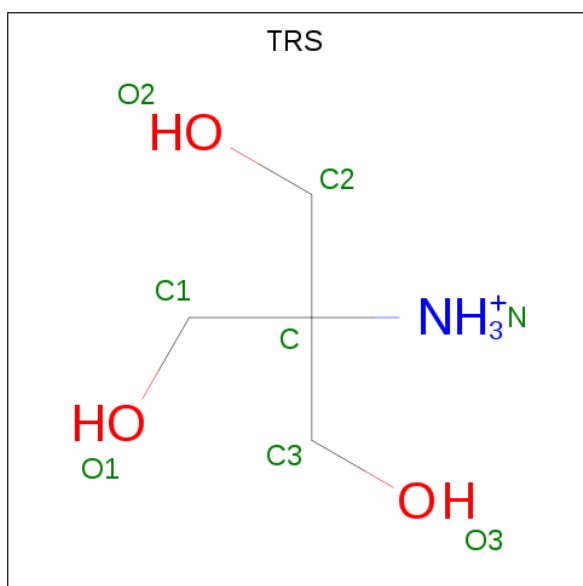
Chain	Residue	Modelled	Actual	Comment	Reference
A	446	LEU	-	expression tag	UNP P60063
A	447	GLU	-	expression tag	UNP P60063
A	448	LEU	-	expression tag	UNP P60063
A	449	GLU	-	expression tag	UNP P60063
A	450	VAL	-	expression tag	UNP P60063
A	451	LEU	-	expression tag	UNP P60063
A	452	PHE	-	expression tag	UNP P60063
A	453	GLN	-	expression tag	UNP P60063
B	446	LEU	-	expression tag	UNP P60063
B	447	GLU	-	expression tag	UNP P60063
B	448	LEU	-	expression tag	UNP P60063
B	449	GLU	-	expression tag	UNP P60063
B	450	VAL	-	expression tag	UNP P60063
B	451	LEU	-	expression tag	UNP P60063
B	452	PHE	-	expression tag	UNP P60063
B	453	GLN	-	expression tag	UNP P60063

- Molecule 2 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: C₁₅H₃₀O₆).



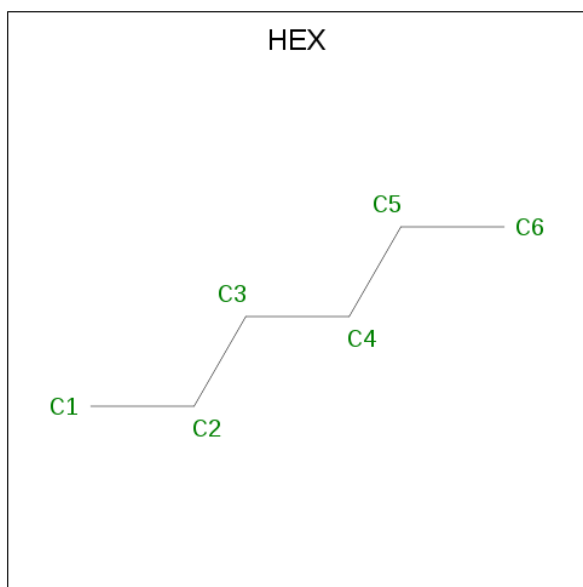
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	51	15	30	6	0	0
2	B	1	51	15	30	6	0	0
2	B	1	51	15	30	6	0	0

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



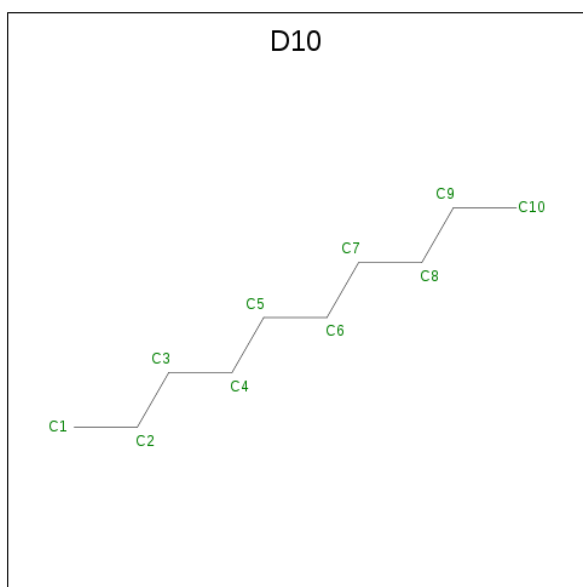
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
3	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 4 is HEXANE (three-letter code: HEX) (formula: C₆H₁₄).



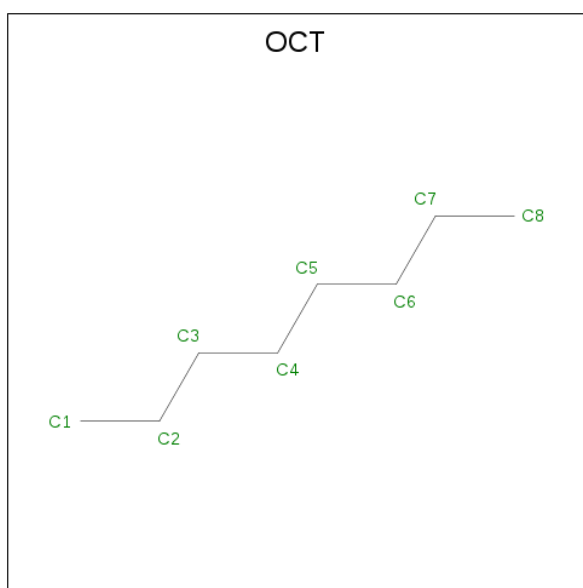
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C H	0	0
			20	6 14		
4	B	1	Total	C H	0	0
			20	6 14		
4	B	1	Total	C H	0	0
			20	6 14		
4	B	1	Total	C H	0	0
			20	6 14		
4	B	1	Total	C H	0	0
			20	6 14		

- Molecule 5 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	H	0	0
			32	10	22		
5	B	1	Total	C	H	0	0
			32	10	22		

- Molecule 6 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	H	0	0
			26	8	18		

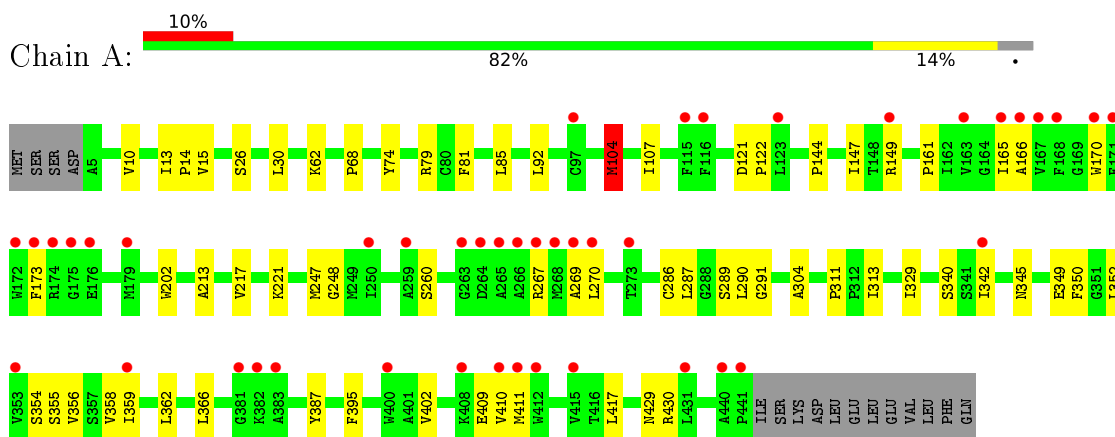
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	198	Total 198	O 198	0	0
7	B	159	Total 159	O 159	0	0

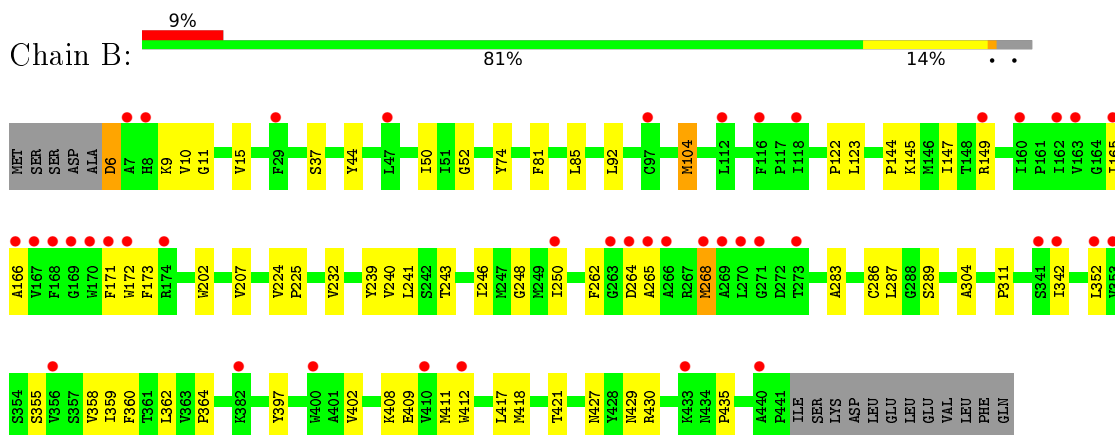
3 Residue-property plots [i](#)

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: Arginine/agmatine antiporter



- Molecule 1: Arginine/agmatine antiporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.71Å 175.59Å 73.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.58 – 1.69 56.81 – 1.69	Depositor EDS
% Data completeness (in resolution range)	78.3 (34.58-1.69) 74.7 (56.81-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 1.69Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.195 , 0.203 0.196 , 0.204	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7313	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: OCT, BNG, HEX, TRS, D10

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	0.59	0/3370	0.70	8/4612 (0.2%)
1	B	0.56	2/3365 (0.1%)	0.66	2/4605 (0.0%)
All	All	0.58	2/6735 (0.0%)	0.68	10/9217 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104[A]	MET	CA-C	5.27	1.66	1.52
1	B	104[B]	MET	CA-C	5.27	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104[A]	MET	N-CA-C	6.46	128.44	111.00
1	A	104[B]	MET	N-CA-C	6.46	128.44	111.00
1	B	104[A]	MET	CA-C-O	6.06	132.82	120.10
1	B	104[B]	MET	CA-C-O	6.06	132.82	120.10
1	A	104[A]	MET	N-CA-CB	-5.83	100.11	110.60
1	A	104[B]	MET	N-CA-CB	-5.83	100.11	110.60
1	A	104[A]	MET	CA-C-O	5.77	132.22	120.10
1	A	104[B]	MET	CA-C-O	5.77	132.22	120.10
1	A	104[A]	MET	CA-C-N	-5.38	105.36	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104[B]	MET	CA-C-N	-5.38	105.36	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104[A]	MET	Mainchain
1	A	411[B]	MET	Mainchain

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	3279	0	3389	60	0
1	B	3274	0	3384	73	0
2	A	21	30	30	1	0
2	B	42	60	60	5	0
3	A	8	12	12	2	0
3	B	8	12	12	3	0
4	A	6	14	14	0	0
4	B	30	70	70	3	0
5	A	10	22	22	4	0
5	B	10	22	22	0	0
6	A	8	18	18	0	0
7	A	198	0	0	18	0
7	B	159	0	0	8	0
All	All	7053	260	7033	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (132) 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:355:SER:HB2	7:B:605:HOH:O	1.36	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:SER:HB2	7:A:603:HOH:O	1.48	1.13
1:B:145:LYS:HD3	1:B:149:ARG:NH2	1.82	0.94
1:A:345:ASN:ND2	7:A:601:HOH:O	1.98	0.94
1:A:149:ARG:CD	5:A:504:D10:H102	1.99	0.93
1:A:355:SER:CB	7:A:603:HOH:O	2.10	0.84
1:B:352:LEU:HA	7:B:605:HOH:O	1.77	0.84
1:B:250:ILE:HD11	1:B:265:ALA:HB2	1.59	0.83
1:A:352:LEU:HA	7:A:603:HOH:O	1.76	0.83
1:B:145:LYS:HD3	1:B:149:ARG:HH21	1.45	0.81
1:A:247:MET:HE2	7:A:634:HOH:O	1.81	0.80
1:A:149:ARG:HD3	5:A:504:D10:H102	1.60	0.80
1:A:149:ARG:HD2	5:A:504:D10:H102	1.63	0.79
1:A:269:ALA:HB3	7:A:741:HOH:O	1.82	0.78
1:B:264:ASP:O	1:B:268:MET:HG2	1.85	0.76
1:A:311:PRO:HD3	3:A:502:TRS:H22	1.68	0.75
1:A:270:LEU:HD13	7:A:741:HOH:O	1.88	0.74
1:A:417:LEU:CD1	7:A:793:HOH:O	2.37	0.73
1:B:44:TYR:CE2	4:B:507:HEX:H22	2.24	0.72
1:A:202:TRP:CH2	1:A:362:LEU:HD11	2.25	0.71
1:B:250:ILE:HD11	1:B:265:ALA:CB	2.20	0.71
1:A:352:LEU:HD23	2:A:501:BNG:H1'2	1.73	0.69
1:A:260:SER:OG	7:A:602:HOH:O	2.11	0.69
1:B:429:ASN:O	1:B:430:ARG:HB2	1.94	0.67
1:A:417:LEU:HD12	7:A:793:HOH:O	1.95	0.66
1:B:145:LYS:O	1:B:149:ARG:HG3	1.97	0.65
1:A:410:VAL:HB	1:B:411[B]:MET:HG3	1.80	0.64
1:A:149:ARG:HD2	5:A:504:D10:C10	2.27	0.64
1:B:250:ILE:CD1	1:B:265:ALA:HB2	2.29	0.62
1:B:166:ALA:HB1	1:B:241:LEU:HB3	1.82	0.60
1:B:104[A]:MET:HE1	7:B:604:HOH:O	2.00	0.60
1:B:408:LYS:HD3	2:B:501:BNG:O6	2.01	0.60
1:B:122:PRO:HB2	1:B:342:ILE:O	2.02	0.60
1:A:122:PRO:HB2	1:A:342:ILE:O	2.03	0.59
1:A:355:SER:OG	7:A:603:HOH:O	2.11	0.59
1:A:13:ILE:HB	1:A:14:PRO:HD3	1.84	0.59
3:B:503:TRS:O3	3:B:503:TRS:O1	2.21	0.59
1:B:165:ILE:HD13	1:B:246:ILE:CG1	2.33	0.59
1:A:429:ASN:O	1:A:430:ARG:HB2	2.02	0.58
1:B:144:PRO:HA	1:B:147:ILE:HG22	1.84	0.58
1:B:352:LEU:HD23	2:B:501:BNG:H1'1	1.87	0.57
1:A:354:SER:O	1:A:358:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:CD1	1:B:246:ILE:CG1	2.84	0.55
1:B:37:SER:HB3	7:B:627:HOH:O	2.06	0.54
1:B:173:PHE:CE2	1:B:248:GLY:HA3	2.42	0.54
1:A:26:SER:HB2	1:A:107:ILE:HG21	1.88	0.53
1:B:165:ILE:CD1	1:B:246:ILE:HG12	2.38	0.53
1:B:246:ILE:HD11	1:B:262:PHE:CZ	2.42	0.53
1:B:355:SER:CB	7:B:605:HOH:O	2.19	0.53
1:A:121:ASP:OD1	1:A:122:PRO:HD2	2.09	0.53
4:B:508:HEX:C2	7:B:756:HOH:O	2.58	0.52
1:A:79:ARG:O	1:B:435:PRO:HD2	2.10	0.52
1:B:6:ASP:HA	1:B:9:LYS:CG	2.40	0.51
1:B:165:ILE:HD13	1:B:246:ILE:HG13	1.91	0.51
1:B:202:TRP:CH2	1:B:362:LEU:HD11	2.44	0.51
1:B:10:VAL:HG12	1:B:15:VAL:HG23	1.92	0.51
1:B:246:ILE:HD11	1:B:262:PHE:CE2	2.46	0.51
1:B:207:VAL:HG23	1:B:232:VAL:HG21	1.92	0.51
1:A:81:PHE:HB3	1:A:85:LEU:HD12	1.92	0.50
1:A:92:LEU:HD11	1:A:417:LEU:HD21	1.92	0.50
1:B:104[B]:MET:HE3	7:B:633:HOH:O	2.10	0.50
1:B:352:LEU:HD23	2:B:501:BNG:H3'2	1.93	0.50
1:B:362:LEU:HD12	1:B:402:VAL:CG2	2.42	0.50
1:B:74:TYR:CZ	1:B:304:ALA:HA	2.47	0.49
1:B:166:ALA:HB1	1:B:241:LEU:CB	2.42	0.49
1:B:173:PHE:CD2	1:B:248:GLY:HA3	2.48	0.49
1:B:81:PHE:HB3	1:B:85:LEU:HD12	1.95	0.48
1:A:313:ILE:HD13	1:A:329:ILE:HD11	1.96	0.48
1:B:52:GLY:HA3	1:B:397:TYR:HD2	1.79	0.48
1:B:11:GLY:O	1:B:15:VAL:HG23	2.14	0.48
1:B:207:VAL:HG23	1:B:232:VAL:CG2	2.43	0.47
1:A:286[B]:CYS:O	1:A:289:SER:HB3	2.15	0.47
1:B:171:PHE:HD1	1:B:172:TRP:CD2	2.33	0.47
4:B:508:HEX:H22	7:B:756:HOH:O	2.14	0.47
1:B:6:ASP:N	1:B:6:ASP:OD1	2.46	0.46
1:B:165:ILE:CD1	1:B:246:ILE:HG13	2.45	0.46
1:B:283:ALA:O	1:B:287:LEU:HG	2.15	0.46
1:A:81:PHE:CB	1:A:85:LEU:HD12	2.45	0.46
1:B:311:PRO:HG3	3:B:503:TRS:H21	1.97	0.46
1:A:340:SER:CB	1:A:350:PHE:HB2	2.45	0.46
1:A:104[A]:MET:HE1	7:A:604:HOH:O	2.16	0.46
1:A:147:ILE:HD11	1:A:291:GLY:HA3	1.97	0.45
1:B:286[A]:CYS:O	1:B:289:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD11	1:B:417:LEU:HD21	1.99	0.45
1:A:355:SER:HB3	1:A:409:GLU:HG2	1.99	0.45
1:B:355:SER:HB3	1:B:409:GLU:HG2	1.99	0.45
1:B:145:LYS:HG2	1:B:149:ARG:NE	2.32	0.44
1:A:81:PHE:CG	1:A:85:LEU:HD12	2.53	0.44
1:B:224:VAL:HB	1:B:225:PRO:HD3	1.99	0.44
1:B:6:ASP:HA	1:B:9:LYS:HG3	1.99	0.44
7:A:793:HOH:O	1:B:417:LEU:CD1	2.66	0.44
3:A:502:TRS:H32	7:A:703:HOH:O	2.18	0.44
1:A:402:VAL:HG21	1:B:418:MET:SD	2.58	0.44
1:A:417:LEU:HD13	7:A:793:HOH:O	2.08	0.44
1:B:239:TYR:O	1:B:243:THR:HG23	2.18	0.44
1:B:360:PHE:O	1:B:364:PRO:HD2	2.18	0.44
7:A:793:HOH:O	1:B:417:LEU:HD13	2.17	0.43
1:A:62:LYS:HE2	1:A:387:TYR:OH	2.17	0.43
1:A:30:LEU:HD23	7:A:619:HOH:O	2.19	0.43
1:B:352:LEU:HD23	2:B:501:BNG:C3'	2.48	0.43
1:B:202:TRP:CZ3	1:B:358:VAL:HG12	2.53	0.43
1:A:144:PRO:HA	1:A:147:ILE:HG22	1.99	0.43
1:A:74:TYR:CZ	1:A:304:ALA:HA	2.54	0.43
1:B:411[B]:MET:HE1	1:B:412:TRP:CE2	2.53	0.43
1:A:213:ALA:O	1:A:217:VAL:HG23	2.18	0.42
1:A:366:LEU:HD12	1:A:395:PHE:CE1	2.54	0.42
1:A:173:PHE:CD2	1:A:248:GLY:HA3	2.54	0.42
1:B:50:ILE:HD11	1:B:240:VAL:CG2	2.49	0.42
1:A:161:PRO:O	1:A:165:ILE:HG12	2.19	0.42
1:A:287:LEU:O	1:A:290:LEU:HB2	2.18	0.42
1:B:352:LEU:CD2	2:B:501:BNG:HI'1	2.49	0.42
1:A:62:LYS:HE2	1:A:387:TYR:CE1	2.54	0.42
1:A:173:PHE:CE2	1:A:248:GLY:HA3	2.54	0.42
1:A:366:LEU:HD21	1:B:421:THR:HB	2.02	0.42
1:A:166:ALA:O	1:A:170:TRP:NE1	2.50	0.42
1:A:68:PRO:HG3	1:A:221:LYS:HG2	2.02	0.41
1:B:362:LEU:CD1	1:B:402:VAL:HG23	2.50	0.41
1:A:352:LEU:O	1:A:356:VAL:HG23	2.20	0.41
1:B:246:ILE:CD1	1:B:262:PHE:CZ	3.04	0.41
1:A:68:PRO:HG3	1:A:221:LYS:CG	2.51	0.41
1:B:427:ASN:OD1	3:B:503:TRS:H31	2.19	0.41
1:A:92:LEU:HD11	1:A:417:LEU:CD2	2.51	0.41
1:B:52:GLY:HA3	1:B:397:TYR:CD2	2.56	0.41
1:A:10:VAL:HG12	1:A:15:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASN:O	1:A:349:GLU:HG2	2.21	0.41
1:A:410:VAL:HG11	1:B:411[A]:MET:HG2	2.03	0.41
1:A:267:ARG:NH1	7:A:605:HOH:O	2.36	0.41
1:B:123:LEU:HA	1:B:342:ILE:CD1	2.51	0.40
1:A:359:ILE:CD1	1:A:409:GLU:HB3	2.51	0.40
1:B:202:TRP:CH2	1:B:359:ILE:HD13	2.56	0.40
1:B:362:LEU:HD12	1:B:402:VAL:HG23	2.04	0.40
1:B:429:ASN:O	1:B:430:ARG:CB	2.67	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	440/453 (97%)	436 (99%)	4 (1%)	0	100	100
1	B	439/453 (97%)	436 (99%)	3 (1%)	0	100	100
All	All	879/906 (97%)	872 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	340/351 (97%)	340 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/351 (97%)	338 (99%)	2 (1%)	86	80
All	All	680/702 (97%)	678 (100%)	2 (0%)	92	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	ASP
1	B	268	MET

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
5	D10	B	509	-	9,9,9	0.20	0	8,8,8	0.30	0
6	OCT	A	505	-	7,7,7	0.18	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	D10	A	504	-	9,9,9	0.24	0	8,8,8	0.50	0
4	HEX	B	505	-	5,5,5	0.12	0	4,4,4	0.22	0
4	HEX	B	504	-	5,5,5	0.30	0	4,4,4	0.24	0
4	HEX	B	506	-	5,5,5	0.31	0	4,4,4	0.21	0
4	HEX	B	508	-	5,5,5	0.28	0	4,4,4	0.19	0
3	TRS	A	502	-	7,7,7	0.76	0	9,9,9	1.12	1 (11%)
2	BNG	A	501	-	21,21,21	0.58	0	26,26,26	0.86	0
2	BNG	B	502	-	21,21,21	1.20	1 (4%)	26,26,26	1.61	5 (19%)
3	TRS	B	503	-	7,7,7	0.58	0	9,9,9	0.99	0
2	BNG	B	501	-	21,21,21	0.59	0	26,26,26	1.29	4 (15%)
4	HEX	A	503	-	5,5,5	0.24	0	4,4,4	0.20	0
4	HEX	B	507	-	5,5,5	0.16	0	4,4,4	0.24	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
5	D10	B	509	-	-	1/7/7/7	-
6	OCT	A	505	-	-	4/5/5/5	-
5	D10	A	504	-	-	4/7/7/7	-
4	HEX	B	505	-	-	0/3/3/3	-
4	HEX	B	504	-	-	0/3/3/3	-
4	HEX	B	506	-	-	0/3/3/3	-
4	HEX	B	508	-	-	0/3/3/3	-
3	TRS	A	502	-	-	9/9/9/9	-
2	BNG	A	501	-	-	4/12/32/32	0/1/1/1
2	BNG	B	502	-	-	6/12/32/32	0/1/1/1
3	TRS	B	503	-	-	7/9/9/9	-
2	BNG	B	501	-	-	6/12/32/32	0/1/1/1
4	HEX	A	503	-	-	0/3/3/3	-
4	HEX	B	507	-	-	0/3/3/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	BNG	O5-C5	-3.23	1.36	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	BNG	C4-C3-C2	-3.99	103.85	110.82
2	B	501	BNG	O5-C5-C4	3.04	115.21	109.69
2	B	502	BNG	C1-C2-C3	-2.94	103.87	110.00
2	B	502	BNG	C6-C5-C4	-2.92	106.16	113.00
2	B	501	BNG	C3-C4-C5	-2.60	105.61	110.24
2	B	501	BNG	O1-C1-C2	2.53	112.26	108.30
3	A	502	TRS	C2-C-N	-2.53	100.43	107.98
2	B	502	BNG	C1'-O1-C1	2.41	117.83	113.84
2	B	501	BNG	C6-C5-C4	-2.32	107.57	113.00
2	B	502	BNG	O5-C1-C2	-2.14	105.82	110.35

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	BNG	C2-C1-O1-C1'
2	A	501	BNG	O5-C1-O1-C1'
2	A	501	BNG	C2'-C1'-O1-C1
2	B	501	BNG	C2'-C1'-O1-C1
2	B	502	BNG	O5-C1-O1-C1'
3	A	502	TRS	C3-C-C1-O1
3	A	502	TRS	N-C-C1-O1
3	A	502	TRS	N-C-C2-O2
3	A	502	TRS	C1-C-C3-O3
3	A	502	TRS	C2-C-C3-O3
3	A	502	TRS	N-C-C3-O3
3	B	503	TRS	C2-C-C1-O1
3	B	503	TRS	C3-C-C1-O1
3	B	503	TRS	N-C-C1-O1
3	B	503	TRS	N-C-C3-O3
2	B	502	BNG	C2'-C3'-C4'-C5'
2	B	501	BNG	O5-C1-O1-C1'
2	A	501	BNG	O1-C1'-C2'-C3'
5	A	504	D10	C4-C5-C6-C7
2	B	502	BNG	C6'-C7'-C8'-C9'
6	A	505	OCT	C2-C3-C4-C5
2	B	501	BNG	C5'-C6'-C7'-C8'
3	A	502	TRS	C3-C-C2-O2
2	B	501	BNG	C6'-C7'-C8'-C9'
6	A	505	OCT	C4-C5-C6-C7
5	A	504	D10	C6-C7-C8-C9
3	A	502	TRS	C2-C-C1-O1
2	B	501	BNG	C4'-C5'-C6'-C7'

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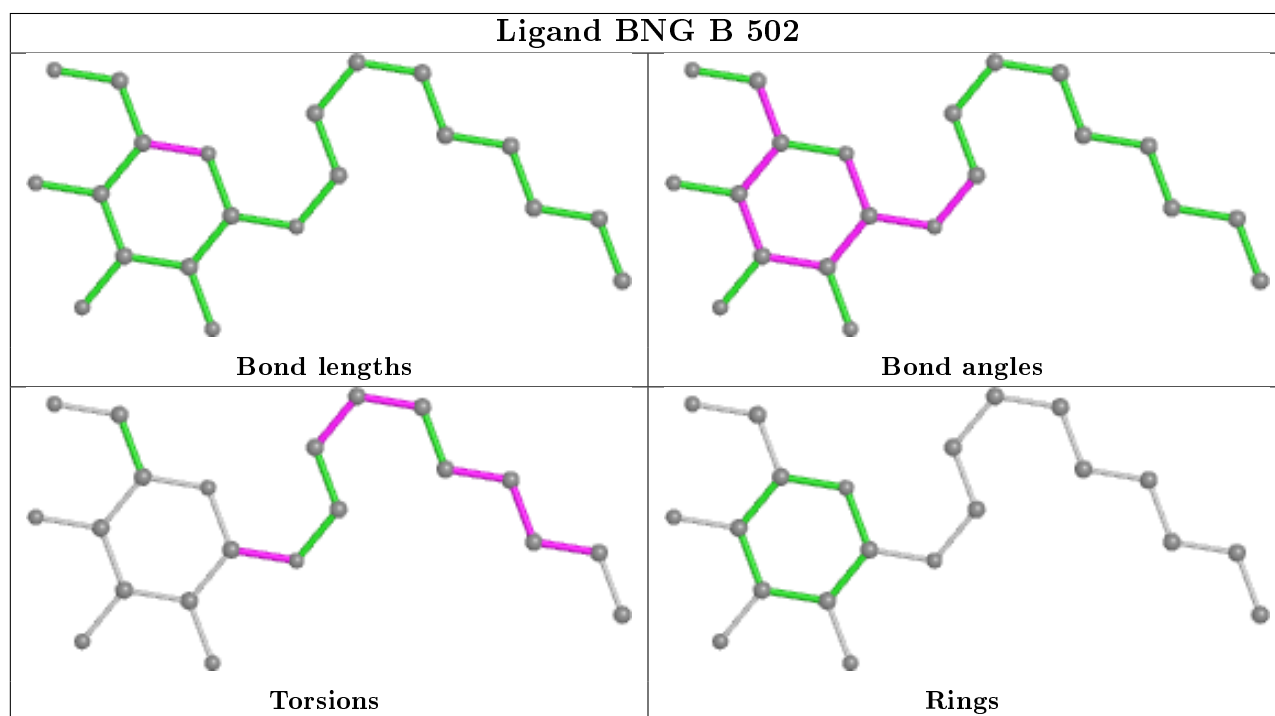
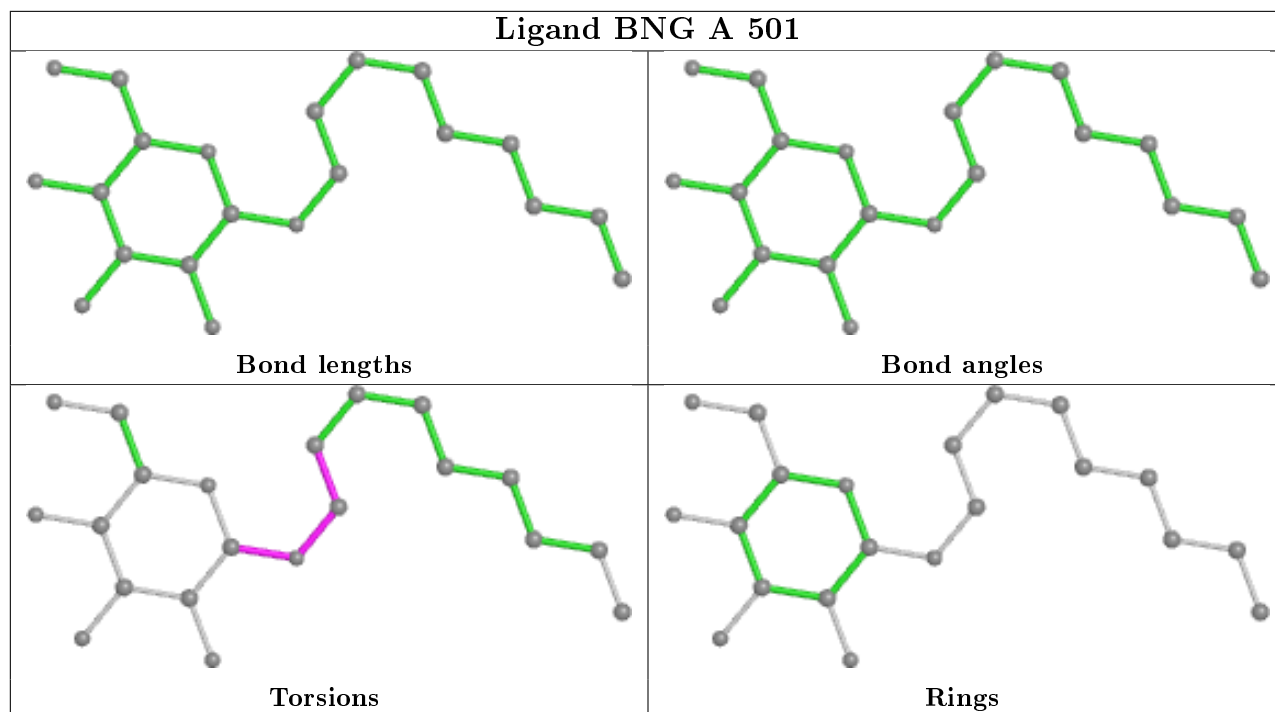
Mol	Chain	Res	Type	Atoms
2	B	501	BNG	O1-C1'-C2'-C3'
6	A	505	OCT	C3-C4-C5-C6
5	A	504	D10	C7-C8-C9-C10
2	B	502	BNG	C4'-C5'-C6'-C7'
2	B	502	BNG	C1'-C2'-C3'-C4'
3	B	503	TRS	C1-C-C3-O3
2	B	502	BNG	C5'-C6'-C7'-C8'
5	B	509	D10	C7-C8-C9-C10
3	A	502	TRS	C1-C-C2-O2
3	B	503	TRS	C3-C-C2-O2
3	B	503	TRS	C2-C-C3-O3
6	A	505	OCT	C1-C2-C3-C4
5	A	504	D10	C5-C6-C7-C8

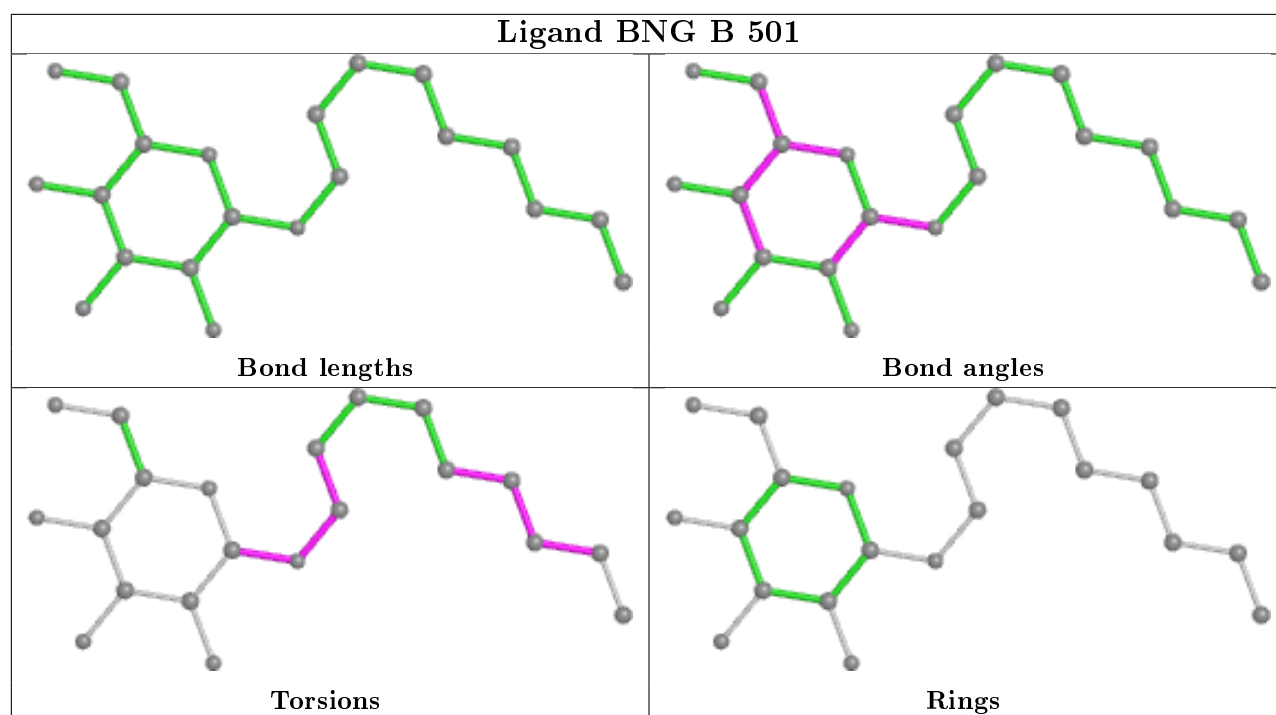
There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	D10	4	0
4	B	508	HEX	2	0
3	A	502	TRS	2	0
2	A	501	BNG	1	0
3	B	503	TRS	3	0
2	B	501	BNG	5	0
4	B	507	HEX	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	437/453 (96%)	0.50	44 (10%) 7 8	29, 43, 80, 137	0
1	B	436/453 (96%)	0.53	42 (9%) 8 9	32, 46, 83, 135	0
All	All	873/906 (96%)	0.51	86 (9%) 7 8	29, 45, 82, 137	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	VAL	7.9
1	B	170	TRP	7.8
1	B	168	PHE	7.7
1	B	171	PHE	7.5
1	A	266	ALA	7.4
1	B	269	ALA	7.3
1	A	268	MET	7.3
1	A	171	PHE	7.1
1	B	270	LEU	6.9
1	B	268	MET	6.8
1	B	97	CYS	6.8
1	A	263	GLY	6.6
1	A	172	TRP	5.9
1	A	170	TRP	5.4
1	A	264	ASP	5.4
1	A	441	PRO	5.4
1	B	266	ALA	5.0
1	A	168	PHE	4.6
1	B	172	TRP	4.5
1	B	264	ASP	4.4
1	A	440	ALA	4.4
1	A	166	ALA	4.4
1	A	269	ALA	4.1
1	B	166	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	4.1
1	B	400[A]	TRP	4.0
1	A	123	LEU	3.9
1	B	263	GLY	3.9
1	B	265	ALA	3.9
1	B	163	VAL	3.9
1	B	273	THR	3.7
1	A	259	ALA	3.6
1	B	440	ALA	3.5
1	B	118	ILE	3.4
1	B	149	ARG	3.2
1	B	116	PHE	3.2
1	A	382	LYS	3.1
1	A	167	VAL	3.1
1	A	116	PHE	3.1
1	A	250	ILE	3.0
1	B	356	VAL	3.0
1	A	267	ARG	3.0
1	B	8	HIS	2.9
1	B	412	TRP	2.9
1	B	162	ILE	2.9
1	A	415	VAL	2.8
1	B	29	PHE	2.8
1	B	271	GLY	2.8
1	A	174	ARG	2.8
1	A	412	TRP	2.7
1	A	273	THR	2.6
1	B	7	ALA	2.6
1	A	353	VAL	2.6
1	A	408	LYS	2.5
1	A	176	GLU	2.5
1	A	400[A]	TRP	2.5
1	A	173	PHE	2.5
1	B	352	LEU	2.5
1	B	353	VAL	2.5
1	A	431	LEU	2.5
1	B	112	LEU	2.5
1	A	265	ALA	2.5
1	A	163	VAL	2.4
1	A	410	VAL	2.4
1	B	47	LEU	2.4
1	B	382	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	165	ILE	2.4
1	A	359	ILE	2.3
1	B	342	ILE	2.3
1	B	174	ARG	2.3
1	B	341	SER	2.3
1	A	97	CYS	2.2
1	A	175	GLY	2.2
1	B	250	ILE	2.2
1	A	383	ALA	2.1
1	A	381	GLY	2.1
1	A	165	ILE	2.1
1	B	160	ILE	2.1
1	A	179	MET	2.1
1	B	169	GLY	2.1
1	A	342	ILE	2.1
1	B	433	LYS	2.0
1	A	411[A]	MET	2.0
1	A	115	PHE	2.0
1	A	149	ARG	2.0
1	B	410	VAL	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 monosaccharides 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	HEX	B	508	6/6	0.34	0.17	74,92,96,96	0
4	HEX	B	505	6/6	0.49	0.23	70,87,92,92	0
4	HEX	B	504	6/6	0.63	0.12	69,87,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	HEX	B	506	6/6	0.64	0.34	65,81,89,89	0
3	TRS	A	502	8/8	0.65	0.17	80,106,116,116	0
5	D10	B	509	10/10	0.68	0.36	67,85,101,101	0
4	HEX	B	507	6/6	0.71	0.31	71,87,91,91	0
3	TRS	B	503	8/8	0.74	0.18	68,92,109,110	0
2	BNG	B	501	21/21	0.75	0.21	63,107,173,180	0
5	D10	A	504	10/10	0.76	0.20	62,83,100,101	0
2	BNG	A	501	21/21	0.79	0.19	62,100,158,161	0
4	HEX	A	503	6/6	0.83	0.42	76,92,96,96	0
6	OCT	A	505	8/8	0.83	0.20	62,78,91,92	0
2	BNG	B	502	21/21	0.86	0.37	83,105,151,158	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.