Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID	:	1N2Z / pdb_00001n2z
Title	:	2.0 Angstrom structure of BtuF, the vitamin B12 binding protein of E. coli
Authors	:	Borths, E.L.; Locher, K.P.; Lee, A.T.; Rees, D.C.
Deposited on	:	2002-10-24
Resolution	:	2.00 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:

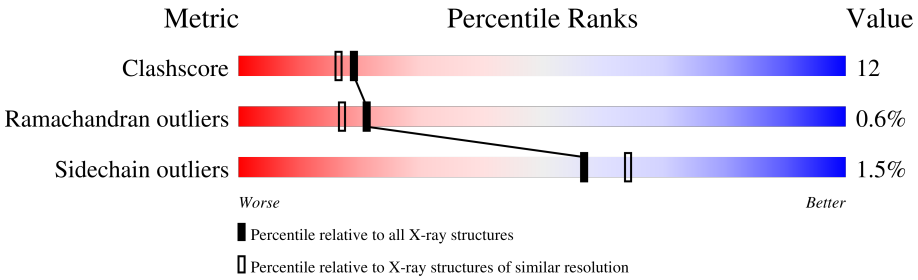
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	78% 21%
1	B	245	81% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CNC	A	400	X	-	-	-
4	CNC	B	401	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4416 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 Vitamin B12 transport protein btuF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1908	1216	332	356	4			
1	B	245	Total	C	N	O	S	0	0	0
			1908	1216	332	356	4			

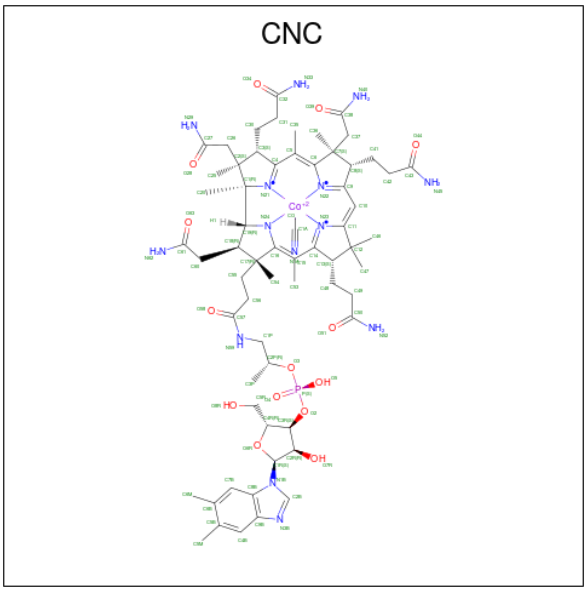
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	Cd	0	0
			13	13		
2	B	9	Total	Cd	0	0
			9	9		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

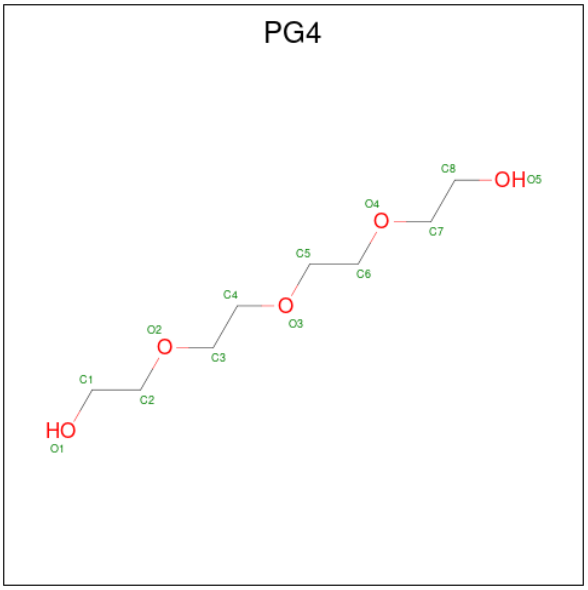
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
4	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	201	Total O 201 201	0	0
6	B	176	Total O 176 176	0	0

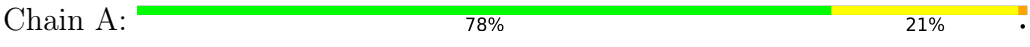
3 Residue-property plots (i)

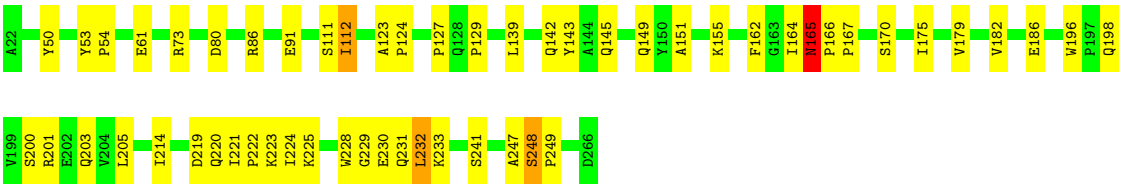
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Vitamin B12 transport protein btuF

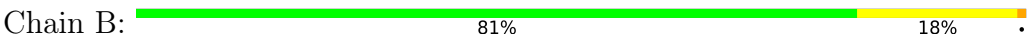
Chain A:

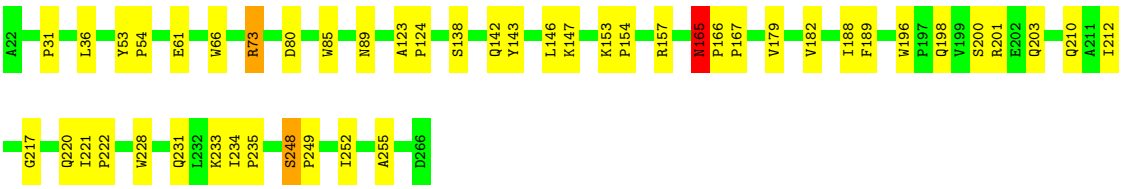




• Molecule 1: Vitamin B12 transport protein btuF

Chain B:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	133.07Å 133.07Å 67.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.189 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4416	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL, PG4, CNC

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	0.37	0/1952	0.93	8/2661 (0.3%)
1	B	0.36	0/1952	0.87	4/2661 (0.2%)
All	All	0.37	0/3904	0.90	12/5322 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	165	ASN	CA-C-N	-9.28	110.82	120.38
1	A	165	ASN	C-N-CA	-9.28	110.82	120.38
1	B	165	ASN	CA-C-N	-6.16	114.04	120.38
1	B	165	ASN	C-N-CA	-6.16	114.04	120.38
1	A	151	ALA	N-CA-C	6.15	117.98	111.28
1	A	198	GLN	N-CA-C	-6.00	99.89	109.96
1	A	80	ASP	N-CA-C	-5.68	106.18	113.23
1	A	86	ARG	N-CA-C	5.60	117.39	111.28
1	B	80	ASP	N-CA-C	-5.42	106.83	113.50
1	A	127	PRO	N-CA-C	-5.16	107.90	114.35
1	B	198	GLN	N-CA-C	-5.10	100.93	109.24
1	A	241	SER	N-CA-C	5.09	117.23	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1908	0	1923	50	0
1	B	1908	0	1923	36	0
2	A	13	0	0	0	0
2	B	9	0	0	0	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
4	A	91	0	87	6	0
4	B	91	0	86	7	0
5	A	13	0	18	0	0
6	A	201	0	0	3	0
6	B	176	0	0	1	0
All	All	4416	0	4037	95	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 12.

All (95) 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)
4:A:400:CNC:H353	4:A:400:CNC:H312	1.54	0.88
1:A:233:LYS:HD3	1:A:233:LYS:H	1.41	0.86
1:B:85:TRP:H	1:B:89:ASN:HD22	1.23	0.83
1:B:165:ASN:HB3	1:B:166:PRO:CD	2.07	0.83
1:A:165:ASN:O	1:A:167:PRO:HD3	1.80	0.82
1:B:165:ASN:O	1:B:167:PRO:HD3	1.80	0.81
1:A:165:ASN:HB3	1:A:166:PRO:CD	2.09	0.81
1:A:200:SER:H	1:A:203:GLN:HE21	1.29	0.80
1:A:220:GLN:HB3	1:A:223:LYS:HE2	1.68	0.75
1:B:66:TRP:HB2	4:B:401:CNC:O34	1.87	0.75
4:A:400:CNC:H601	4:A:400:CNC:H252	1.71	0.73
1:A:201:ARG:HG3	1:A:228:TRP:CZ3	2.24	0.72
1:B:85:TRP:H	1:B:89:ASN:ND2	1.90	0.69
1:B:143:TYR:CZ	1:B:147:LYS:HE3	2.27	0.69
1:A:200:SER:OG	1:A:203:GLN:HG3	1.94	0.66
1:B:165:ASN:HB3	1:B:166:PRO:HD3	1.76	0.65
1:B:123:ALA:HB3	1:B:124:PRO:HD3	1.80	0.63
1:B:200:SER:OG	1:B:203:GLN:HG3	1.98	0.63
1:B:157:ARG:H	1:B:210:GLN:NE2	1.96	0.62
1:A:205:LEU:HD21	1:A:232:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:HG2	6:B:487:HOH:O	1.98	0.62
1:A:231:GLN:HG3	1:A:232:LEU:HD13	1.81	0.61
1:A:165:ASN:HB3	1:A:166:PRO:HD3	1.83	0.60
1:B:61:GLU:OE2	1:B:73:ARG:HD3	2.01	0.60
1:A:205:LEU:CD2	1:A:232:LEU:HG	2.31	0.60
1:A:231:GLN:HG3	1:A:232:LEU:HD22	1.85	0.58
1:A:142:GLN:HE22	1:A:145:GLN:HE21	1.51	0.58
1:B:157:ARG:H	1:B:210:GLN:HE21	1.51	0.58
1:B:212:ILE:HD11	1:B:234:ILE:HD11	1.85	0.58
1:A:200:SER:H	1:A:203:GLN:NE2	2.00	0.57
1:A:123:ALA:HB3	1:A:124:PRO:HD3	1.87	0.57
4:A:400:CNC:H362	4:A:400:CNC:H351	1.86	0.57
1:B:143:TYR:CE2	1:B:147:LYS:HE3	2.39	0.57
4:B:401:CNC:H601	4:B:401:CNC:H252	1.86	0.56
1:B:201:ARG:HG3	1:B:228:TRP:CZ3	2.42	0.55
1:B:146:LEU:HD21	1:B:255:ALA:HB1	1.88	0.54
4:B:401:CNC:H552	4:B:401:CNC:H531	1.90	0.54
1:B:142:GLN:HE21	1:B:252:ILE:HG13	1.72	0.54
1:B:138:SER:O	1:B:142:GLN:HG3	2.07	0.54
1:A:200:SER:N	1:A:203:GLN:HE21	2.03	0.53
4:A:400:CNC:H302	4:A:400:CNC:H203	1.90	0.53
1:B:53:TYR:HA	1:B:54:PRO:C	2.34	0.53
1:A:229:GLY:C	1:A:231:GLN:H	2.17	0.52
4:A:400:CNC:H552	4:A:400:CNC:H531	1.91	0.52
1:A:112:ILE:HD12	1:A:175:ILE:HD11	1.91	0.52
1:B:179:VAL:O	1:B:182:VAL:HG12	2.10	0.52
4:B:401:CNC:H351	4:B:401:CNC:H362	1.93	0.51
1:B:221:ILE:HB	1:B:222:PRO:HD3	1.93	0.51
1:A:112:ILE:HD13	1:A:143:TYR:CE1	2.46	0.50
1:B:217:GLY:O	1:B:220:GLN:HG2	2.12	0.50
1:A:155:LYS:HB3	1:A:186:GLU:HG2	1.93	0.50
1:A:231:GLN:CG	1:A:232:LEU:HD22	2.41	0.49
1:B:200:SER:H	1:B:203:GLN:NE2	2.09	0.49
1:B:165:ASN:HB3	1:B:166:PRO:HD2	1.92	0.49
1:A:229:GLY:O	1:A:231:GLN:N	2.45	0.49
4:B:401:CNC:H353	4:B:401:CNC:H312	1.95	0.49
1:B:231:GLN:O	1:B:233:LYS:HG3	2.13	0.48
1:A:112:ILE:HG23	1:A:139:LEU:HG	1.94	0.48
1:A:232:LEU:HD22	1:A:232:LEU:H	1.79	0.48
1:B:165:ASN:CB	1:B:166:PRO:CD	2.85	0.48
1:A:112:ILE:CD1	1:A:175:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLN:O	1:A:149:GLN:HG3	2.14	0.47
1:A:162:PHE:HB3	6:A:621:HOH:O	2.14	0.47
1:A:165:ASN:HB3	1:A:166:PRO:HD2	1.91	0.47
1:B:212:ILE:HD11	1:B:234:ILE:CD1	2.45	0.47
1:A:111:SER:C	1:A:175:ILE:HD13	2.40	0.46
1:B:196:TRP:CE2	4:B:401:CNC:H491	2.50	0.46
1:A:129:PRO:HG3	6:A:548:HOH:O	2.14	0.46
1:B:142:GLN:NE2	1:B:252:ILE:HG13	2.30	0.46
1:A:221:ILE:N	1:A:222:PRO:CD	2.79	0.46
1:A:201:ARG:O	1:A:205:LEU:HG	2.16	0.45
1:B:73:ARG:HA	1:B:73:ARG:HE	1.80	0.45
1:A:165:ASN:CB	1:A:166:PRO:CD	2.88	0.45
1:A:61:GLU:OE2	1:A:73:ARG:HG2	2.17	0.44
1:A:219:ASP:O	1:A:222:PRO:HD2	2.18	0.44
1:A:164:ILE:HD11	1:A:223:LYS:HD2	2.00	0.43
1:A:233:LYS:H	1:A:233:LYS:CD	2.18	0.43
1:A:247:ALA:HB3	6:A:627:HOH:O	2.18	0.43
1:A:50:TYR:CE1	4:A:400:CNC:O34	2.72	0.42
1:B:31:PRO:HD2	4:B:401:CNC:O44	2.20	0.42
1:A:228:TRP:HB3	1:A:232:LEU:HD23	2.02	0.42
1:A:231:GLN:HG3	1:A:232:LEU:CD1	2.46	0.42
1:A:53:TYR:HA	1:A:54:PRO:C	2.45	0.42
1:A:170:SER:HB2	1:A:196:TRP:CH2	2.55	0.41
1:A:231:GLN:HG3	1:A:232:LEU:CD2	2.49	0.41
1:A:164:ILE:O	1:A:165:ASN:C	2.64	0.41
1:B:146:LEU:HD21	1:B:255:ALA:CB	2.50	0.41
1:A:179:VAL:O	1:A:182:VAL:HG12	2.20	0.40
1:B:153:LYS:HA	1:B:154:PRO:HD3	1.91	0.40
1:B:210:GLN:O	1:B:235:PRO:HD2	2.21	0.40
1:A:248:SER:HB2	1:A:249:PRO:HD2	2.03	0.40
1:A:214:ILE:HD13	1:A:224:ILE:HG13	2.02	0.40
1:A:221:ILE:CG2	1:A:225:LYS:HE3	2.52	0.40
1:B:188:ILE:HG13	1:B:189:PHE:CD1	2.57	0.40
1:B:248:SER:HB2	1:B:249:PRO:CD	2.52	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	243/245 (99%)	236 (97%)	5 (2%)	2 (1%)	16 11
1	B	243/245 (99%)	237 (98%)	5 (2%)	1 (0%)	30 27
All	All	486/490 (99%)	473 (97%)	10 (2%)	3 (1%)	21 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	230	GLU
1	B	165	ASN

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	205/205 (100%)	202 (98%)	3 (2%)	57 64
1	B	205/205 (100%)	202 (98%)	3 (2%)	57 64
All	All	410/410 (100%)	404 (98%)	6 (2%)	57 64

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

Mol	Chain	Res	Type
1	A	112	ILE
1	A	232	LEU
1	A	248	SER

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Mol	Chain	Res	Type
1	B	36	LEU
1	B	73	ARG
1	B	248	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	96	GLN
1	A	137	GLN
1	A	145	GLN
1	A	203	GLN
1	A	220	GLN
1	A	231	GLN
1	A	256	GLN
1	B	58	GLN
1	B	62	GLN
1	B	67	GLN
1	B	89	ASN
1	B	134	GLN
1	B	142	GLN
1	B	149	GLN
1	B	203	GLN
1	B	210	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 28 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PG4	A	430	-	12,12,12	0.47	0	11,11,11	0.29	0
4	CNC	B	401	3	94,101,103	1.19	9 (9%)	150,166,171	1.66	19 (12%)
4	CNC	A	400	3	94,101,103	1.21	11 (11%)	150,166,171	1.70	20 (13%)

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	PG4	A	430	-	-	9/10/10/10	-
4	CNC	B	401	3	1/1/36/38	8/56/223/235	0/3/11/11
4	CNC	A	400	3	1/1/36/38	9/56/223/235	0/3/11/11

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	CNC	C14-N23	4.08	1.40	1.30
4	B	401	CNC	C14-N23	3.91	1.40	1.30
4	A	400	CNC	C7B-C8B	3.03	1.44	1.39
4	B	401	CNC	C7B-C8B	2.97	1.44	1.39
4	A	400	CNC	C20-C1	2.80	1.59	1.53
4	B	401	CNC	C3-C4	2.78	1.58	1.51
4	B	401	CNC	C6B-C5B	2.44	1.46	1.40
4	A	400	CNC	C41-C8	2.38	1.59	1.54
4	A	400	CNC	C6B-C5B	2.36	1.46	1.40
4	B	401	CNC	C20-C1	2.23	1.57	1.53
4	A	400	CNC	C4B-C9B	2.14	1.43	1.40
4	B	401	CNC	P-O5	-2.13	1.45	1.55
4	B	401	CNC	C35-C5	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	CNC	C17-C18	2.06	1.58	1.54
4	B	401	CNC	C36-C7	2.05	1.57	1.54
4	A	400	CNC	C36-C7	2.05	1.57	1.54
4	B	401	CNC	C17-C18	2.04	1.58	1.54
4	A	400	CNC	P-O5	-2.02	1.46	1.55
4	A	400	CNC	O7R-C2R	-2.01	1.38	1.43
4	A	400	CNC	C3-C4	2.00	1.56	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	CNC	C11-N23-C14	10.92	110.44	106.31
4	B	401	CNC	C11-N23-C14	10.16	110.15	106.31
4	B	401	CNC	C30-C3-C4	7.00	126.07	109.66
4	A	400	CNC	C30-C3-C4	5.15	121.74	109.66
4	A	400	CNC	C30-C3-C2	-4.63	108.79	119.00
4	B	401	CNC	C9-N22-C6	4.54	110.74	105.28
4	A	400	CNC	C9-N22-C6	4.51	110.71	105.28
4	B	401	CNC	O3-C2P-C1P	4.21	115.28	106.94
4	A	400	CNC	O3-C2P-C1P	4.16	115.19	106.94
4	A	400	CNC	C48-C13-C12	-3.69	105.97	116.52
4	A	400	CNC	O34-C32-C31	-3.52	110.42	121.04
4	B	401	CNC	C48-C13-C12	-3.22	107.30	116.52
4	A	400	CNC	C3R-C2R-C1R	3.20	106.92	99.89
4	B	401	CNC	C3R-C2R-C1R	3.18	106.89	99.89
4	B	401	CNC	C20-C1-N21	-3.18	105.01	110.26
4	B	401	CNC	O34-C32-C31	-3.17	111.46	121.04
4	B	401	CNC	P-O3-C2P	2.91	131.02	121.10
4	B	401	CNC	C47-C12-C46	-2.85	104.69	109.41
4	A	400	CNC	C20-C1-N21	-2.82	105.59	110.26
4	A	400	CNC	P-O3-C2P	2.70	130.34	121.10
4	A	400	CNC	C47-C12-C46	-2.61	105.08	109.41
4	A	400	CNC	O7R-C2R-C3R	2.61	118.48	111.19
4	A	400	CNC	C31-C32-N33	2.55	124.65	116.49
4	A	400	CNC	C2R-C1R-N1B	2.42	119.31	113.30
4	B	401	CNC	C8B-N1B-C1R	2.42	129.50	125.41
4	A	400	CNC	O63-C61-C60	2.35	125.78	120.87
4	A	400	CNC	C9B-C8B-N1B	2.28	106.31	105.30
4	A	400	CNC	C8B-N1B-C1R	2.26	129.23	125.41
4	B	401	CNC	C31-C32-N33	2.25	123.71	116.49
4	B	401	CNC	C47-C12-C13	2.13	121.38	112.74
4	B	401	CNC	C36-C7-C6	2.13	123.44	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	CNC	C2R-C1R-N1B	2.11	118.55	113.30
4	A	400	CNC	C36-C7-C37	-2.10	107.17	110.74
4	A	400	CNC	C47-C12-C13	2.09	121.21	112.74
4	B	401	CNC	C1-C2-C3	2.09	104.23	101.60
4	B	401	CNC	C2R-C3R-C4R	2.08	106.88	103.24
4	B	401	CNC	O7R-C2R-C3R	2.06	116.95	111.19
4	B	401	CNC	C36-C7-C37	-2.05	107.25	110.74
4	A	400	CNC	C2R-C3R-C4R	2.05	106.83	103.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	400	CNC	N24
4	B	401	CNC	N24

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	CNC	C1P-C2P-O3-P
4	B	401	CNC	C4-C3-C30-C31
4	B	401	CNC	C1P-C2P-O3-P
4	B	401	CNC	C3P-C2P-O3-P
5	A	430	PG4	O3-C5-C6-O4
4	B	401	CNC	C30-C31-C32-N33
4	A	400	CNC	C30-C31-C32-O34
4	A	400	CNC	C30-C31-C32-N33
4	B	401	CNC	C30-C31-C32-O34
4	A	400	CNC	C3P-C2P-O3-P
4	B	401	CNC	C2-C3-C30-C31
5	A	430	PG4	O1-C1-C2-O2
4	A	400	CNC	C3-C30-C31-C32
4	A	400	CNC	C2P-C1P-N59-C57
5	A	430	PG4	C4-C3-O2-C2
4	B	401	CNC	C2P-C1P-N59-C57
5	A	430	PG4	C8-C7-O4-C6
5	A	430	PG4	C6-C5-O3-C4
4	A	400	CNC	C18-C60-C61-O63
4	A	400	CNC	C18-C60-C61-N62
5	A	430	PG4	O4-C7-C8-O5
5	A	430	PG4	O2-C3-C4-O3
4	B	401	CNC	C2R-C1R-N1B-C8B
5	A	430	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
4	A	400	CNC	C2P-O3-P-O5
5	A	430	PG4	C5-C6-O4-C7

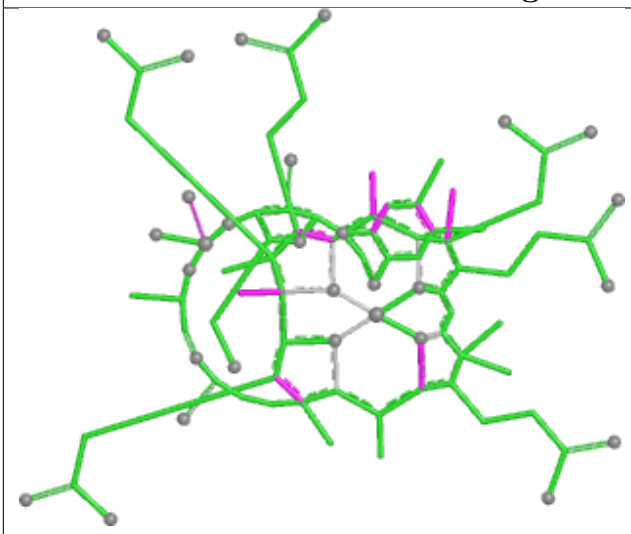
There are no ring outliers.

2 monomers are involved in 13 short contacts:

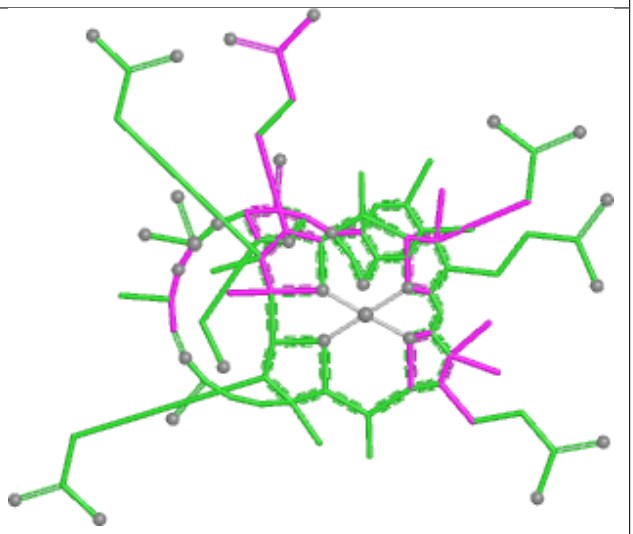
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	CNC	7	0
4	A	400	CNC	6	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

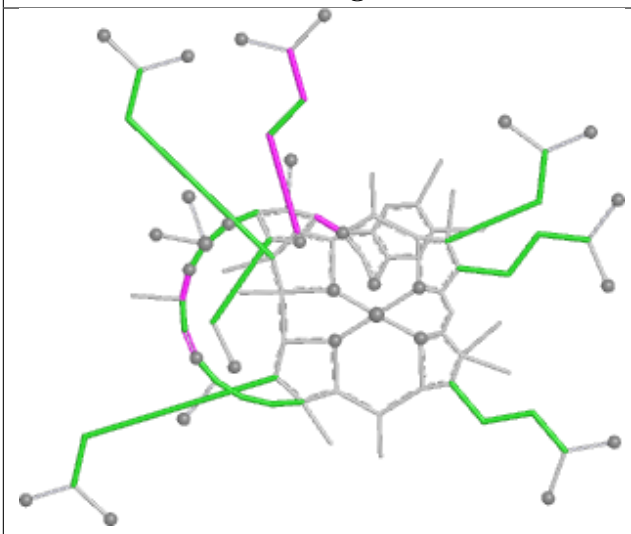
Ligand CNC B 401



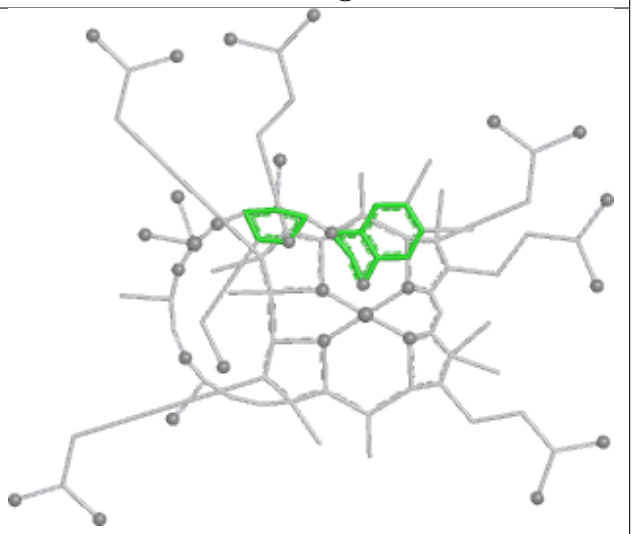
Bond lengths



Bond angles

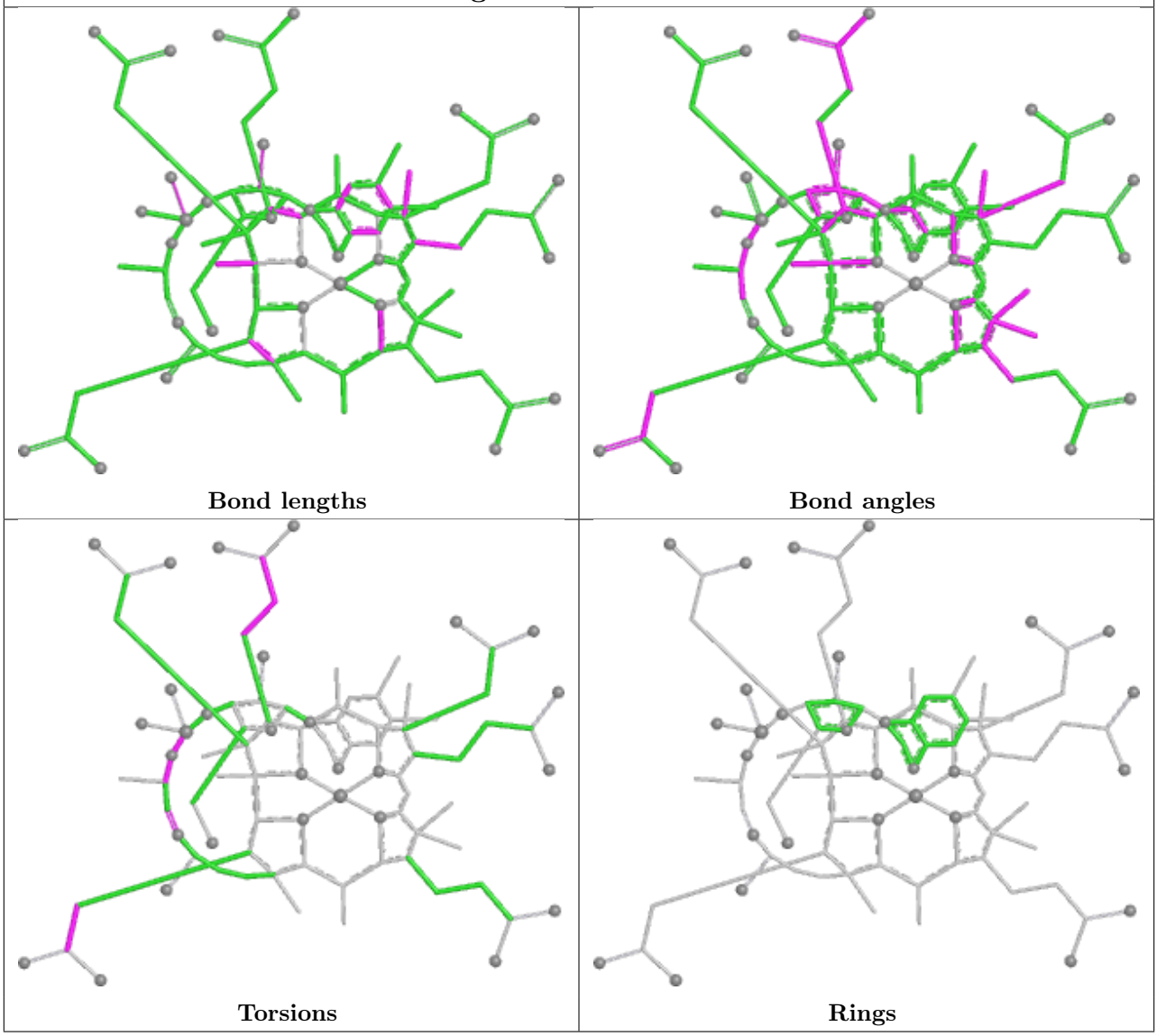


Torsions



Rings

Ligand CNC A 400



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.