



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:32 PM UTC

PDB ID : 1N4A / pdb_00001n4a
Title : The Ligand Bound Structure of E.coli BtuF, the Periplasmic Binding Protein for Vitamin B12
Authors : Karpowich, N.K.; Smith, P.C.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2002-10-30
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)	:	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

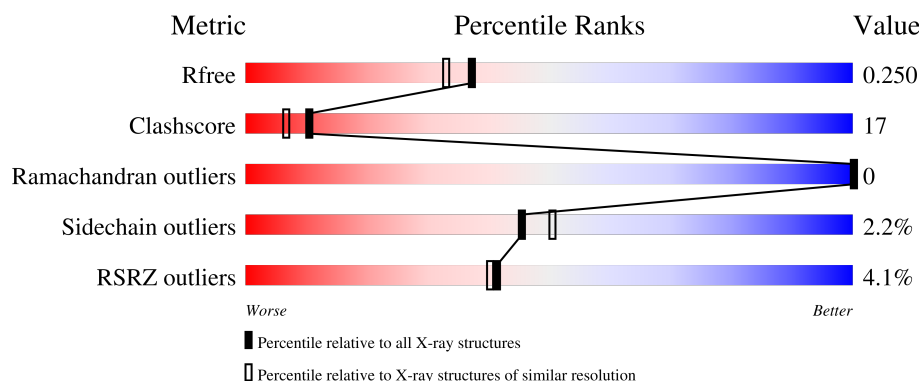
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	252	3% 70% 25% ..
1	B	252	5% 69% 27% ..

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
2	CNC	A	501	X	-	-	-
2	CNC	B	5501	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4539 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.

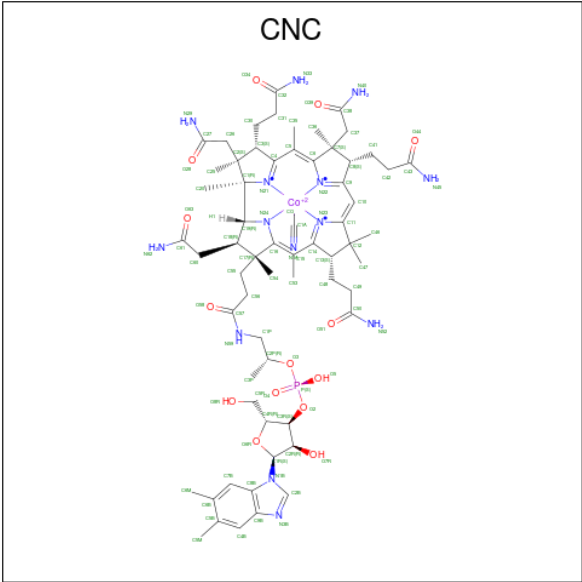
- Molecule 1 is a protein called Vitamin B12 transport protein btuF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	Se	0	0	0
			1902	1213	331	354	2	2			
1	B	244	Total	C	N	O	S	Se	0	0	0
			1902	1213	331	354	2	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MSE	MET	modified residue	UNP P37028
A	83	MSE	MET	modified residue	UNP P37028
A	245	LEU	-	expression tag	UNP P37028
A	246	GLU	-	expression tag	UNP P37028
A	247	HIS	-	expression tag	UNP P37028
A	248	HIS	-	expression tag	UNP P37028
A	249	HIS	-	expression tag	UNP P37028
A	250	HIS	-	expression tag	UNP P37028
A	251	HIS	-	expression tag	UNP P37028
A	252	HIS	-	expression tag	UNP P37028
B	5047	MSE	MET	modified residue	UNP P37028
B	5083	MSE	MET	modified residue	UNP P37028
B	5245	LEU	-	expression tag	UNP P37028
B	5246	GLU	-	expression tag	UNP P37028
B	5247	HIS	-	expression tag	UNP P37028
B	5248	HIS	-	expression tag	UNP P37028
B	5249	HIS	-	expression tag	UNP P37028
B	5250	HIS	-	expression tag	UNP P37028
B	5251	HIS	-	expression tag	UNP P37028
B	5252	HIS	-	expression tag	UNP P37028

- Molecule 2 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

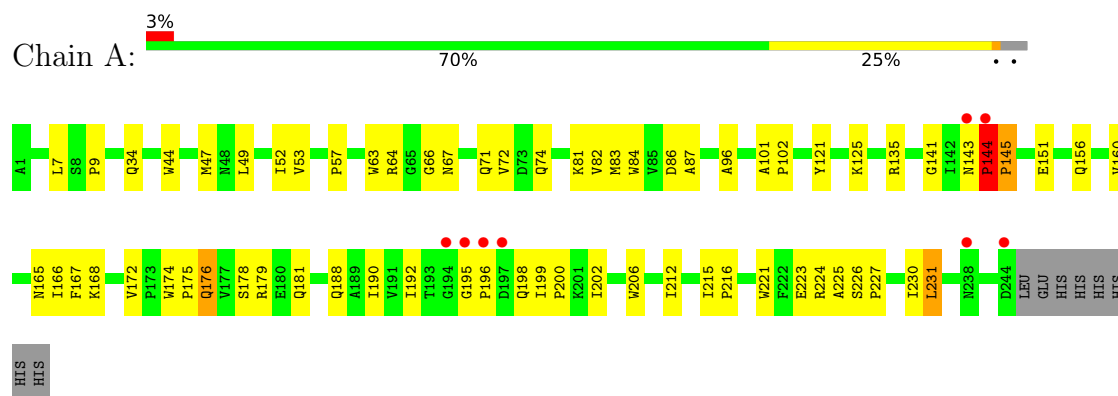
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	296	Total	O	0	0
			296	296		
3	B	253	Total	O	0	0
			253	253		

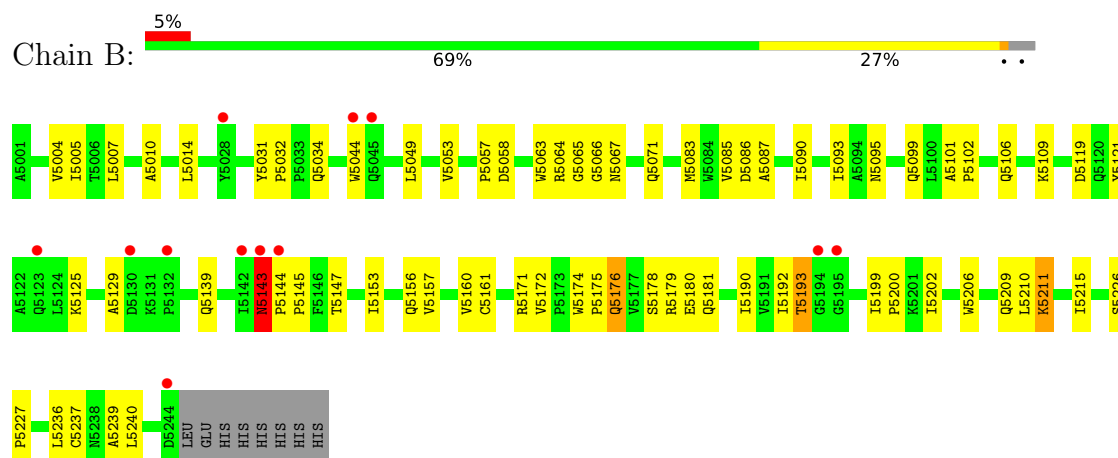
3 Residue-property plots [i](#)

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: Vitamin B12 transport protein btuF



- Molecule 1: Vitamin B12 transport protein btuF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.73Å 92.02Å 44.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	24.4 (20.00-2.00) 91.9 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	33.49 (at 1.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.261 0.206 , 0.250	Depositor DCC
R_{free} test set	1751 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.4	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	0.95	EDS
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: 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	0.42	0/1944	0.94	8/2648 (0.3%)
1	B	0.42	0/1944	0.92	6/2648 (0.2%)
All	All	0.42	0/3888	0.93	14/5296 (0.3%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5143	ASN	C-N-CD	-9.21	100.34	120.60
1	A	143	ASN	C-N-CD	-6.97	105.27	120.60
1	A	144	PRO	N-CA-C	6.66	129.41	112.10
1	A	144	PRO	CA-C-N	6.62	142.89	127.00
1	A	144	PRO	C-N-CA	6.62	142.89	127.00
1	B	5227	PRO	N-CA-C	5.78	122.19	113.81
1	B	5058	ASP	N-CA-C	-5.59	106.30	113.23
1	A	144	PRO	C-N-CD	-5.43	108.65	120.60
1	B	5176	GLN	N-CA-C	-5.41	100.87	109.96
1	B	5193	THR	N-CA-C	5.30	121.15	114.31
1	A	215	ILE	N-CA-C	5.21	112.71	107.55
1	A	151	GLU	N-CA-C	5.17	117.38	109.62
1	A	176	GLN	N-CA-C	-5.04	101.10	109.46
1	B	5004	VAL	N-CA-C	5.04	115.73	108.48

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	1902	0	1922	54	0
1	B	1902	0	1921	63	0
2	A	93	0	87	20	0
2	B	93	0	87	14	0
3	A	296	0	0	12	0
3	B	253	0	0	18	0
All	All	4539	0	4017	134	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 17.

All (134) 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:A:135:ARG:H	1:A:188:GLN:HE21	1.18	0.92
1:A:145:PRO:HA	3:A:7442:HOH:O	1.72	0.88
1:B:5063:TRP:H	1:B:5067:ASN:HD22	1.23	0.86
1:B:5139:GLN:HE22	1:B:5206:TRP:HE1	1.21	0.85
1:A:82:VAL:H	1:B:5095:ASN:HD21	1.24	0.85
1:A:224:ARG:HE	2:A:501:CNC:H402	1.30	0.79
1:B:5063:TRP:H	1:B:5067:ASN:ND2	1.81	0.78
1:A:83:MSE:SE	3:A:7478:HOH:O	2.53	0.77
2:B:5501:CNC:H552	2:B:5501:CNC:H531	1.67	0.76
2:B:5501:CNC:H492	2:B:5501:CNC:H471	1.67	0.75
2:B:5501:CNC:H492	2:B:5501:CNC:C47	2.19	0.72
1:B:5190:ILE:HD11	1:B:5210:LEU:HD23	1.74	0.70
1:B:5083:MSE:HE2	1:B:5085:VAL:HG22	1.73	0.69
1:A:63:TRP:H	1:A:67:ASN:ND2	1.90	0.68
2:A:501:CNC:H531	2:A:501:CNC:H552	1.76	0.67
1:B:5179:ARG:HH21	1:B:5209:GLN:HE21	1.42	0.67
1:A:63:TRP:H	1:A:67:ASN:HD22	1.43	0.67
2:A:501:CNC:H492	2:A:501:CNC:H471	1.77	0.66
1:B:5178:SER:H	1:B:5181:GLN:HE21	1.43	0.66
1:A:135:ARG:H	1:A:188:GLN:NE2	1.91	0.66
2:A:501:CNC:H492	2:A:501:CNC:C47	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:CNC:H601	2:A:501:CNC:H252	1.77	0.65
1:A:81:LYS:HB3	1:B:5099:GLN:HE22	1.62	0.65
1:A:81:LYS:HB3	1:B:5099:GLN:NE2	2.13	0.64
1:A:87:ALA:HB2	3:A:7084:HOH:O	1.97	0.64
2:A:501:CNC:H362	2:A:501:CNC:H351	1.78	0.64
1:B:5174:TRP:CE2	2:B:5501:CNC:H491	2.33	0.63
1:B:5067:ASN:HA	3:B:7414:HOH:O	1.98	0.62
1:B:5192:ILE:HG21	1:B:5202:ILE:HG12	1.82	0.61
1:B:5215:ILE:HG21	3:B:7058:HOH:O	1.99	0.61
1:B:5066:GLY:O	2:B:5501:CNC:H2R	2.00	0.61
1:B:5034:GLN:HG3	3:B:7090:HOH:O	2.00	0.60
2:B:5501:CNC:H362	2:B:5501:CNC:H351	1.82	0.60
1:A:165:ASN:ND2	1:A:167:PHE:H	1.99	0.60
1:B:5236:LEU:HD12	3:B:7058:HOH:O	2.00	0.60
1:A:179:ARG:HD2	3:A:7415:HOH:O	2.01	0.60
1:B:5139:GLN:NE2	1:B:5206:TRP:HE1	1.97	0.59
1:A:141:GLY:O	1:A:145:PRO:HB3	2.03	0.58
1:A:66:GLY:HA2	2:A:501:CNC:H1R	1.85	0.57
1:B:5193:THR:HG23	3:B:7125:HOH:O	2.04	0.57
1:A:34:GLN:HG3	3:A:7199:HOH:O	2.04	0.57
1:A:9:PRO:HD2	2:A:501:CNC:N45	2.20	0.56
1:A:121:TYR:CE1	1:A:160:VAL:HG21	2.40	0.56
1:B:5178:SER:H	1:B:5181:GLN:NE2	2.03	0.56
1:A:71:GLN:HA	1:A:74:GLN:HE21	1.70	0.56
1:A:174:TRP:CE2	2:A:501:CNC:H491	2.41	0.56
1:A:64:ARG:HB2	1:A:86:ASP:HB2	1.87	0.55
1:B:5180:GLU:HB3	3:B:7441:HOH:O	2.07	0.55
2:B:5501:CNC:H601	2:B:5501:CNC:H252	1.89	0.54
2:A:501:CNC:N40	2:A:501:CNC:H361	2.23	0.54
1:A:156:GLN:O	1:A:160:VAL:HG23	2.08	0.54
1:B:5090:ILE:HD13	1:B:5153:ILE:HD11	1.91	0.53
1:A:121:TYR:HE1	1:A:160:VAL:HG21	1.74	0.53
1:A:192:ILE:HG21	1:A:202:ILE:HG12	1.91	0.53
1:A:47:MSE:HE1	1:A:72:VAL:HG22	1.90	0.53
1:B:5144:PRO:N	1:B:5145:PRO:HA	2.24	0.53
1:A:47:MSE:HE1	1:A:72:VAL:CG2	2.39	0.52
1:B:5063:TRP:CD2	1:B:5066:GLY:HA3	2.44	0.52
1:A:96:ALA:HB2	3:A:7084:HOH:O	2.10	0.52
2:B:5501:CNC:H482	2:B:5501:CNC:H533	1.91	0.52
1:A:178:SER:H	1:A:181:GLN:HE21	1.58	0.51
1:B:5174:TRP:CD2	2:B:5501:CNC:H491	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:7136:HOH:O	1:B:5083:MSE:HE3	2.11	0.51
1:B:5099:GLN:HG3	3:B:7443:HOH:O	2.11	0.51
2:A:501:CNC:H1P1	2:A:501:CNC:O4	2.11	0.51
1:A:198:GLN:HG2	3:A:7509:HOH:O	2.10	0.50
1:B:5064:ARG:HB3	1:B:5086:ASP:HB2	1.94	0.50
1:B:5087:ALA:HB2	3:B:7007:HOH:O	2.11	0.50
1:A:223:GLU:OE2	2:A:501:CNC:H371	2.12	0.49
1:B:5156:GLN:O	1:B:5160:VAL:HG23	2.11	0.49
1:B:5172:VAL:O	1:B:5175:PRO:HD3	2.11	0.49
1:A:196:PRO:HA	1:A:199:ILE:HG13	1.95	0.49
1:A:125:LYS:HA	1:A:160:VAL:HG13	1.95	0.48
1:B:5005:ILE:HG12	1:B:5057:PRO:HB3	1.95	0.48
1:B:5010:ALA:H	2:B:5501:CNC:H452	1.61	0.47
1:B:5200:PRO:HG2	3:B:7404:HOH:O	2.13	0.47
1:B:5044:TRP:HB2	2:B:5501:CNC:H331	1.79	0.47
1:B:5147:THR:O	1:B:5174:TRP:HA	2.15	0.47
1:B:5119:ASP:HB3	3:B:7255:HOH:O	2.14	0.47
1:B:5236:LEU:HD11	3:B:7096:HOH:O	2.15	0.47
1:B:5014:LEU:HD11	3:B:7004:HOH:O	2.15	0.46
1:B:5215:ILE:HD13	3:B:7058:HOH:O	2.14	0.46
1:A:190:ILE:HG13	1:A:212:ILE:HD11	1.98	0.46
1:B:5144:PRO:HD2	1:B:5176:GLN:HG3	1.98	0.46
1:A:200:PRO:HG2	3:A:7536:HOH:O	2.16	0.46
2:A:501:CNC:O4	2:A:501:CNC:C1P	2.64	0.46
1:A:101:ALA:HB3	1:A:102:PRO:HD3	1.98	0.46
1:B:5121:TYR:HE1	1:B:5160:VAL:HG21	1.81	0.46
1:A:195:GLY:HA2	1:A:216:PRO:HB2	1.98	0.45
2:A:501:CNC:H531	2:A:501:CNC:C55	2.45	0.45
1:A:144:PRO:HB2	1:A:176:GLN:HG3	1.97	0.45
2:B:5501:CNC:C5	2:B:5501:CNC:H4B	2.47	0.45
1:B:5239:ALA:HB3	3:B:7058:HOH:O	2.16	0.45
1:A:52:ILE:O	1:A:57:PRO:HD3	2.17	0.44
1:A:44:TRP:HB2	2:A:501:CNC:H331	1.81	0.44
2:A:501:CNC:H401	2:A:501:CNC:H8	1.83	0.44
1:A:64:ARG:HG2	1:A:84:TRP:CE3	2.53	0.44
1:A:44:TRP:HB2	2:A:501:CNC:N33	2.32	0.44
1:A:165:ASN:HD22	1:A:165:ASN:C	2.25	0.44
1:B:5101:ALA:HB3	1:B:5102:PRO:HD3	1.99	0.44
1:B:5093:ILE:HD11	1:B:5153:ILE:CD1	2.48	0.43
1:A:44:TRP:HA	2:A:501:CNC:HM62	2.01	0.43
1:B:5106:GLN:NE2	1:B:5109:LYS:HE3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5143:ASN:HD22	1:B:5143:ASN:N	2.16	0.43
1:A:63:TRP:CE3	1:A:66:GLY:HA3	2.53	0.43
1:A:168:LYS:HG3	3:A:7106:HOH:O	2.18	0.43
1:A:225:ALA:HB3	3:A:7376:HOH:O	2.17	0.43
1:B:5190:ILE:HD11	1:B:5210:LEU:CD2	2.47	0.43
1:A:221:TRP:CE3	1:A:231:LEU:HB3	2.53	0.43
1:B:5143:ASN:HA	1:B:5144:PRO:HA	1.55	0.43
2:A:501:CNC:H2P	3:A:7069:HOH:O	2.18	0.43
1:B:5071:GLN:HG2	3:B:7107:HOH:O	2.19	0.43
2:B:5501:CNC:P	2:B:5501:CNC:N59	2.92	0.43
1:A:227:PRO:O	1:A:230:ILE:HG22	2.18	0.42
1:A:165:ASN:HD22	1:A:166:ILE:N	2.17	0.42
2:A:501:CNC:H401	2:A:501:CNC:C8	2.32	0.42
1:B:5121:TYR:CE1	1:B:5160:VAL:HG21	2.54	0.42
1:B:5143:ASN:C	1:B:5145:PRO:HA	2.45	0.42
1:B:5031:TYR:HA	1:B:5032:PRO:C	2.45	0.42
1:A:172:VAL:O	1:A:175:PRO:HD3	2.20	0.42
1:A:165:ASN:HD22	1:A:167:PHE:H	1.65	0.42
1:B:5125:LYS:O	1:B:5129:ALA:HB2	2.20	0.42
1:A:49:LEU:O	1:A:53:VAL:HG23	2.20	0.41
1:B:5157:VAL:HG12	1:B:5236:LEU:HD23	2.02	0.41
1:B:5171:ARG:HD2	3:B:7398:HOH:O	2.19	0.41
1:A:179:ARG:NH1	1:A:206:TRP:HA	2.34	0.41
1:B:5199:ILE:N	1:B:5200:PRO:HD2	2.35	0.41
1:B:5044:TRP:HB2	2:B:5501:CNC:N33	2.36	0.41
1:B:5065:GLY:HA3	3:B:7138:HOH:O	2.19	0.41
1:B:5049:LEU:O	1:B:5053:VAL:HG23	2.21	0.40
1:B:5161:CYS:HB3	1:B:5237:CYS:HA	2.04	0.40
1:B:5240:LEU:HD22	3:B:7096:HOH:O	2.20	0.40
1:A:196:PRO:HA	1:A:199:ILE:CD1	2.51	0.40
1:B:5211:LYS:HB3	1:B:5211:LYS:NZ	2.36	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	242/252 (96%)	238 (98%)	4 (2%)	0	100	100
1	B	242/252 (96%)	237 (98%)	5 (2%)	0	100	100
All	All	484/504 (96%)	475 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	205/211 (97%)	200 (98%)	5 (2%)	43	47
1	B	205/211 (97%)	201 (98%)	4 (2%)	48	54
All	All	410/422 (97%)	401 (98%)	9 (2%)	45	50

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	144	PRO
1	A	145	PRO
1	A	226	SER
1	A	231	LEU
1	B	5007	LEU
1	B	5143	ASN
1	B	5211	LYS
1	B	5226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN

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Mol	Chain	Res	Type
1	A	40	GLN
1	A	67	ASN
1	A	74	GLN
1	A	106	GLN
1	A	112	GLN
1	A	120	GLN
1	A	123	GLN
1	A	165	ASN
1	A	181	GLN
1	A	188	GLN
1	A	198	GLN
1	B	5045	GLN
1	B	5067	ASN
1	B	5095	ASN
1	B	5099	GLN
1	B	5139	GLN
1	B	5143	ASN
1	B	5181	GLN
1	B	5204	GLN
1	B	5209	GLN
1	B	5234	GLN

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](#)

2 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
2	CNC	A	501	-	93,103,103	0.79	1 (1%)	149,171,171	1.22	15 (10%)
2	CNC	B	5501	-	93,103,103	0.72	0	149,171,171	1.16	14 (9%)

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
2	CNC	A	501	-	1/1/36/38	10/56/235/235	0/3/11/11
2	CNC	B	5501	-	1/1/36/38	14/56/235/235	0/3/11/11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CNC	P-O5	-2.09	1.45	1.55

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5501	CNC	C9B-C8B-N1B	3.76	106.97	105.30
2	A	501	CNC	O3-C2P-C1P	3.48	113.83	106.94
2	A	501	CNC	C48-C13-C12	-3.34	106.96	116.52
2	A	501	CNC	C9B-C8B-N1B	3.25	106.75	105.30
2	B	5501	CNC	O34-C32-C31	-3.09	111.72	121.04
2	A	501	CNC	C3R-C2R-C1R	2.96	106.40	99.89
2	A	501	CNC	O7R-C2R-C3R	2.92	119.37	111.19
2	B	5501	CNC	C30-C3-C4	2.88	116.42	109.66
2	A	501	CNC	O34-C32-C31	-2.87	112.36	121.04
2	B	5501	CNC	O7R-C2R-C3R	2.69	118.73	111.19
2	B	5501	CNC	C3R-C2R-C1R	2.65	105.71	99.89
2	B	5501	CNC	O3-C2P-C1P	2.62	112.14	106.94
2	A	501	CNC	C2R-C1R-N1B	2.61	119.80	113.30
2	B	5501	CNC	C36-C7-C37	-2.58	106.35	110.74
2	A	501	CNC	P-O3-C2P	2.58	129.91	121.10
2	B	5501	CNC	C2R-C3R-C4R	2.52	107.66	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5501	CNC	C48-C13-C12	-2.38	109.71	116.52
2	A	501	CNC	C30-C3-C4	2.33	115.11	109.66
2	A	501	CNC	C36-C7-C37	-2.28	106.87	110.74
2	B	5501	CNC	C31-C32-N33	2.21	123.57	116.49
2	A	501	CNC	C20-C1-N21	-2.20	106.62	110.26
2	A	501	CNC	C2R-C3R-C4R	2.19	107.07	103.24
2	A	501	CNC	C36-C7-C6	2.18	123.72	112.41
2	B	5501	CNC	C31-C30-C3	-2.18	108.48	114.65
2	B	5501	CNC	C36-C7-C6	2.17	123.68	112.41
2	B	5501	CNC	P-O3-C2P	2.13	128.39	121.10
2	B	5501	CNC	C20-C1-N21	-2.13	106.74	110.26
2	A	501	CNC	C1-C19-C18	-2.07	118.64	121.75
2	A	501	CNC	C8B-N1B-C1R	2.03	128.84	125.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	CNC	N24
2	B	5501	CNC	N24

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CNC	C7-C37-C38-O39
2	A	501	CNC	C2P-C1P-N59-C57
2	A	501	CNC	C1P-C2P-O3-P
2	B	5501	CNC	C4-C3-C30-C31
2	B	5501	CNC	C1P-C2P-O3-P
2	B	5501	CNC	C3P-C2P-O3-P
2	B	5501	CNC	O6R-C4R-C5R-O8R
2	B	5501	CNC	C3R-C4R-C5R-O8R
2	A	501	CNC	C7-C37-C38-N40
2	B	5501	CNC	C2-C3-C30-C31
2	B	5501	CNC	C16-C17-C55-C56
2	A	501	CNC	C30-C31-C32-N33
2	B	5501	CNC	C30-C31-C32-N33
2	A	501	CNC	C30-C31-C32-O34
2	B	5501	CNC	C30-C31-C32-O34
2	B	5501	CNC	C2R-C1R-N1B-C8B
2	B	5501	CNC	O6R-C1R-N1B-C8B
2	B	5501	CNC	C18-C17-C55-C56
2	A	501	CNC	C2P-O3-P-O4

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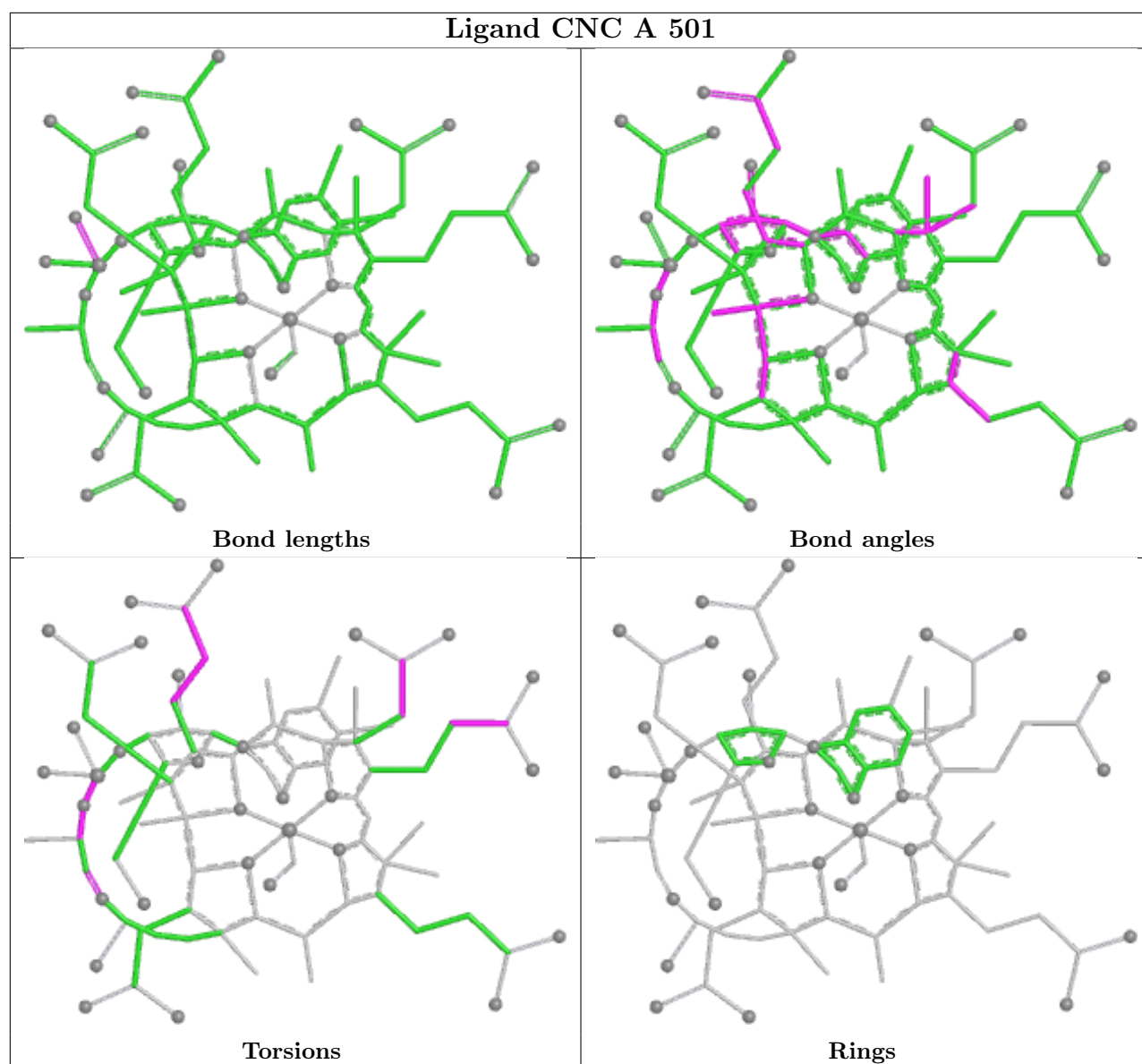
Mol	Chain	Res	Type	Atoms
2	A	501	CNC	C3-C30-C31-C32
2	A	501	CNC	C41-C42-C43-N45
2	A	501	CNC	C41-C42-C43-O44
2	B	5501	CNC	C41-C42-C43-O44
2	B	5501	CNC	C41-C42-C43-N45

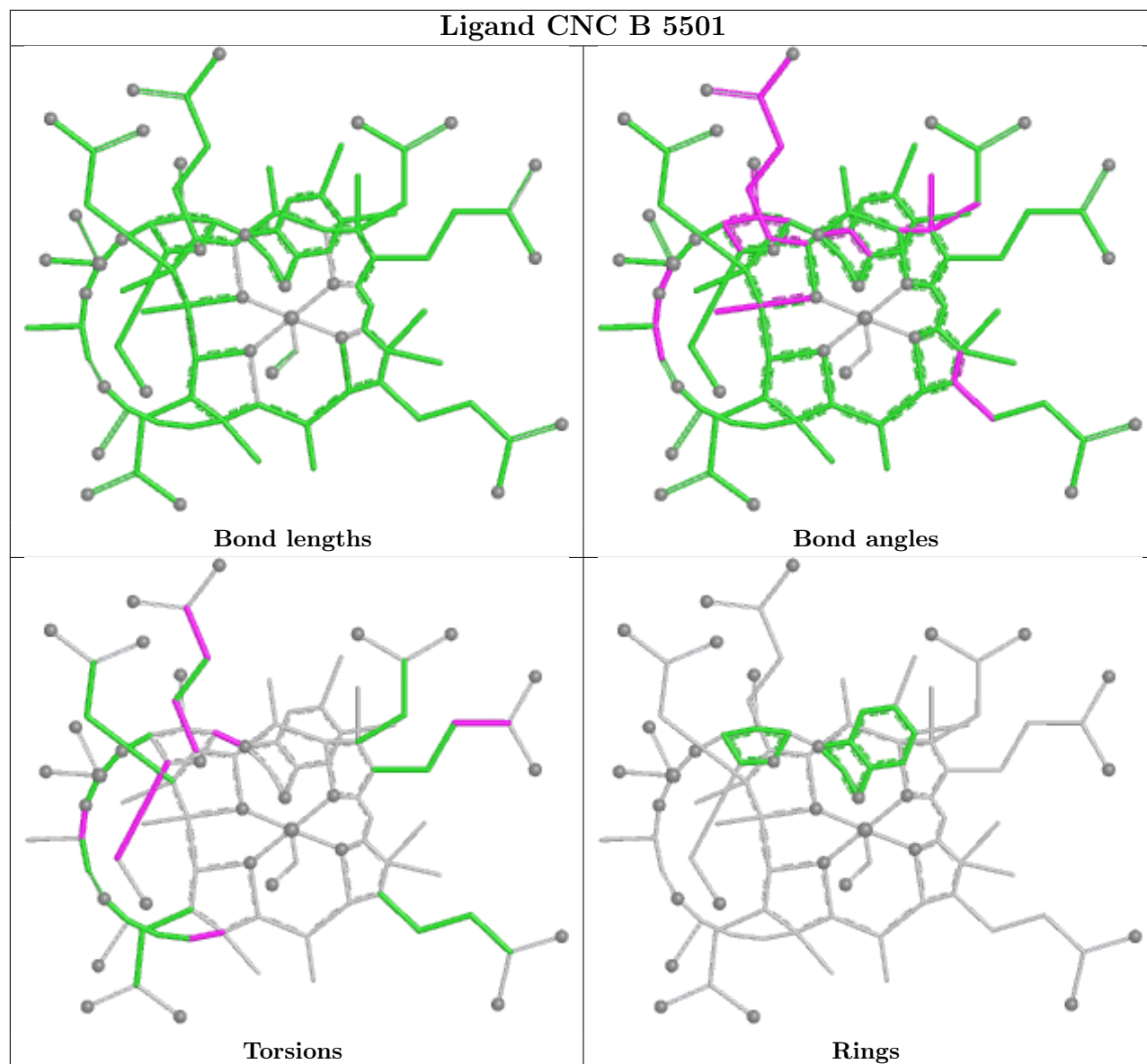
There are no ring outliers.

2 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CNC	20	0
2	B	5501	CNC	14	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	242/252 (96%)	-0.11	8 (3%) 49 48	11, 23, 57, 111	0
1	B	242/252 (96%)	0.06	12 (4%) 34 33	11, 24, 68, 139	0
All	All	484/504 (96%)	-0.03	20 (4%) 41 40	11, 24, 65, 139	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	7.7
1	B	5144	PRO	5.0
1	B	5143	ASN	4.3
1	A	194	GLY	4.2
1	B	5044	TRP	3.7
1	B	5195	GLY	3.7
1	A	144	PRO	3.4
1	A	196	PRO	3.4
1	B	5130	ASP	2.9
1	B	5142	ILE	2.8
1	B	5244	ASP	2.6
1	B	5194	GLY	2.4
1	B	5132	PRO	2.4
1	A	143	ASN	2.3
1	A	197	ASP	2.3
1	A	238	ASN	2.2
1	B	5123	GLN	2.2
1	A	244	ASP	2.0
1	B	5045	GLN	2.0
1	B	5028	TYR	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](#)

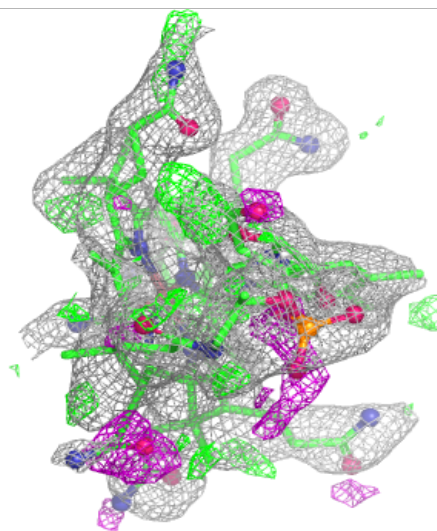
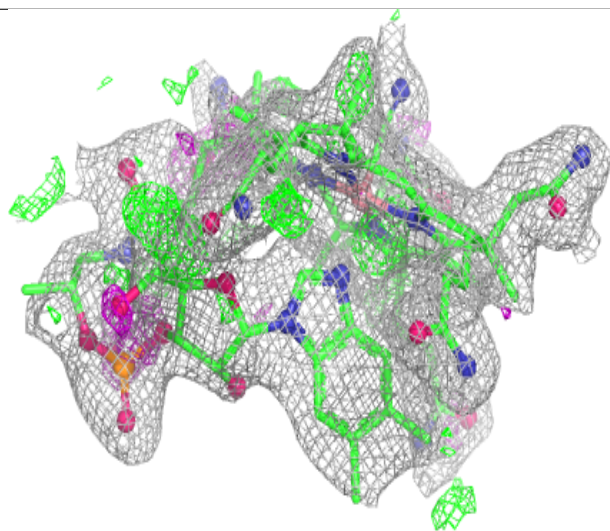
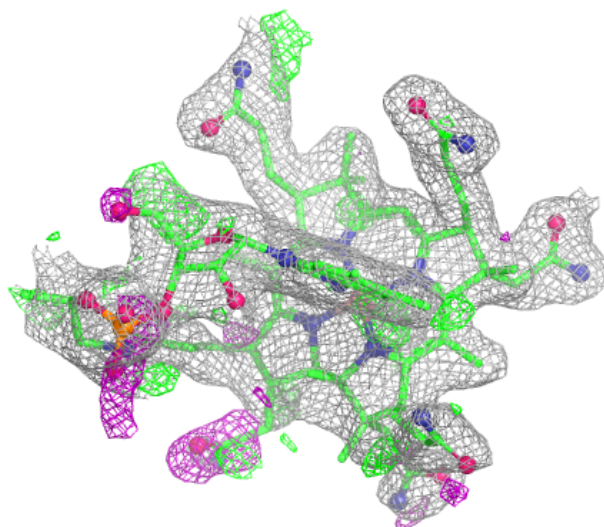
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	CNC	B	5501	93/93	0.90	0.12	13,36,52,55	0
2	CNC	A	501	93/93	0.94	0.08	11,18,29,35	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.

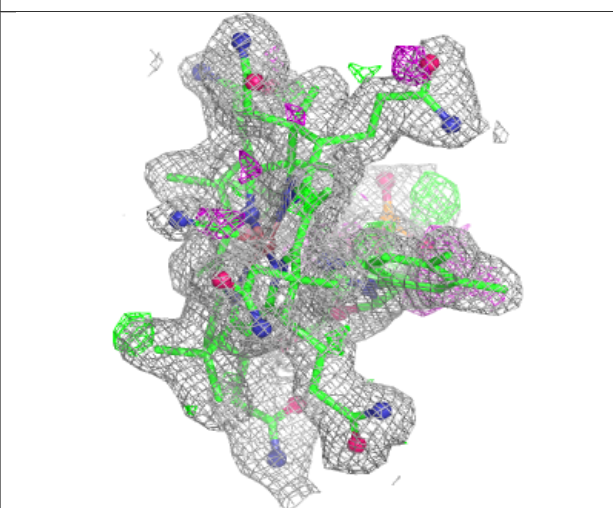
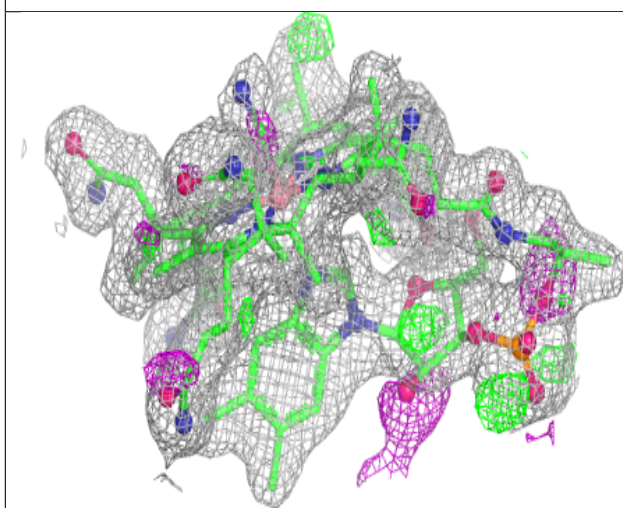
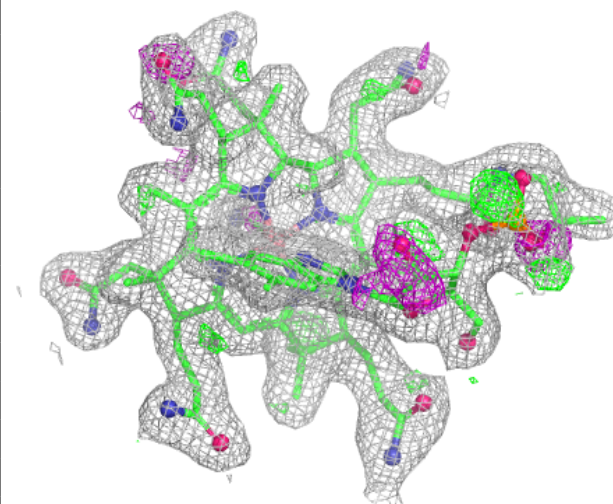
Electron density around CNC B 5501:

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



Electron density around CNC A 501:

$2mF_o-DF_c$ (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.