



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 06:22 PM UTC

PDB ID : 7BIZ / pdb_00007biz
Title : Structure of a B12 binding lipoprotein from Bacteroides thetaiotaomicron
Authors : Abellon-Ruiz, J.; van den Berg, B.
Deposited on : 2021-01-13
Resolution : 1.53 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

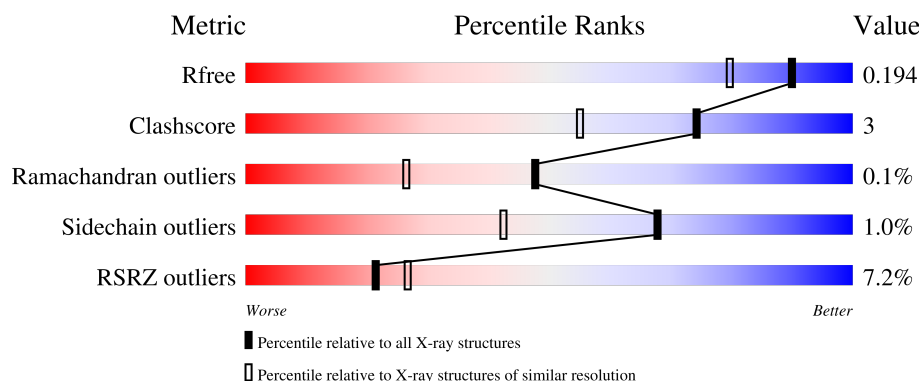
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

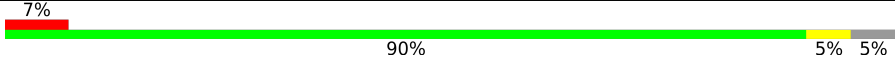
The reported resolution of this entry is 1.53 Å.

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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	501	
1	B	501	

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	701	X	-	-	-
2	CNC	B	701	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9101 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.

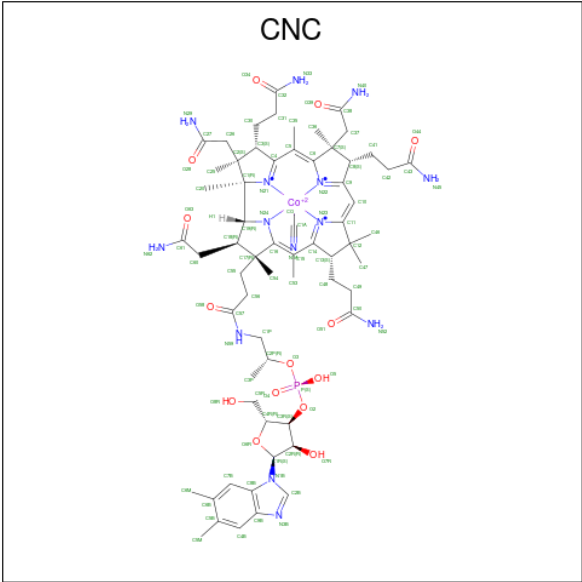
- Molecule 1 is a protein called Cell surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3764	2378	611	764	11			
1	B	467	Total	C	N	O	S	0	0	0
			3685	2332	597	745	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MET	-	initiating methionine	UNP A0A0N7IAT3
A	102	GLY	-	cloning artifact	UNP A0A0N7IAT3
A	594	LEU	-	cloning artifact	UNP A0A0N7IAT3
A	595	GLU	-	expression tag	UNP A0A0N7IAT3
A	596	HIS	-	expression tag	UNP A0A0N7IAT3
A	597	HIS	-	expression tag	UNP A0A0N7IAT3
A	598	HIS	-	expression tag	UNP A0A0N7IAT3
A	599	HIS	-	expression tag	UNP A0A0N7IAT3
A	600	HIS	-	expression tag	UNP A0A0N7IAT3
A	601	HIS	-	expression tag	UNP A0A0N7IAT3
B	101	MET	-	initiating methionine	UNP A0A0N7IAT3
B	102	GLY	-	cloning artifact	UNP A0A0N7IAT3
B	594	LEU	-	cloning artifact	UNP A0A0N7IAT3
B	595	GLU	-	expression tag	UNP A0A0N7IAT3
B	596	HIS	-	expression tag	UNP A0A0N7IAT3
B	597	HIS	-	expression tag	UNP A0A0N7IAT3
B	598	HIS	-	expression tag	UNP A0A0N7IAT3
B	599	HIS	-	expression tag	UNP A0A0N7IAT3
B	600	HIS	-	expression tag	UNP A0A0N7IAT3
B	601	HIS	-	expression tag	UNP A0A0N7IAT3

- Molecule 2 is CYANOCOBALAMIN (CCD ID: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$) (labeled as "Ligand of Interest" by depositor).

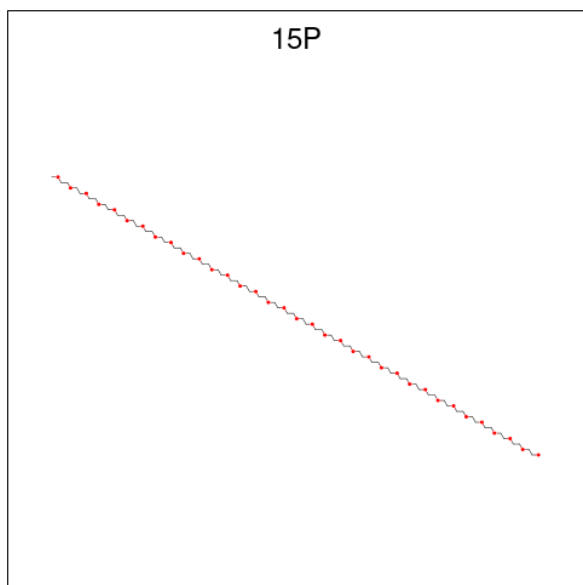


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: C₆₉H₁₄₀O₃₅).

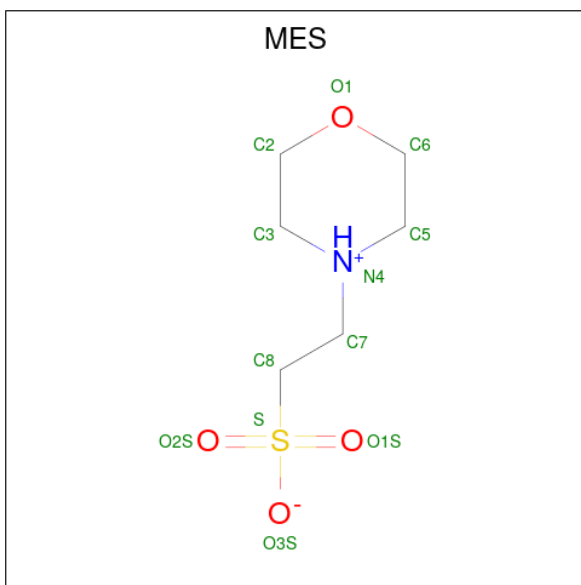


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	9	5		
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

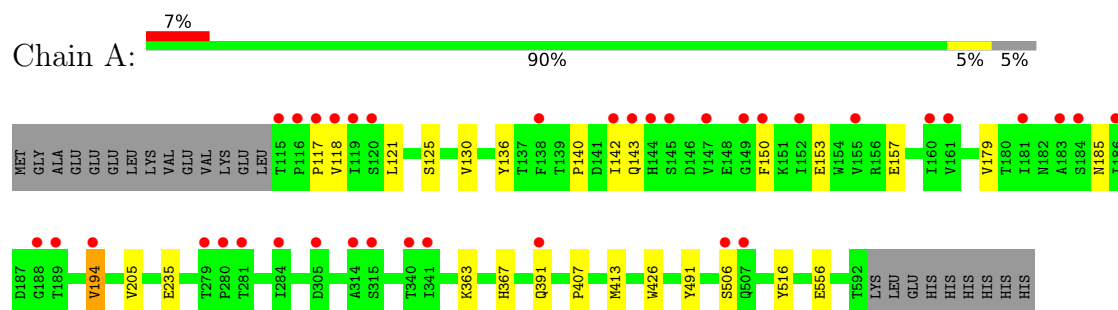
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	718	Total	O	0	0
			718	718		
7	B	687	Total	O	0	0
			687	687		

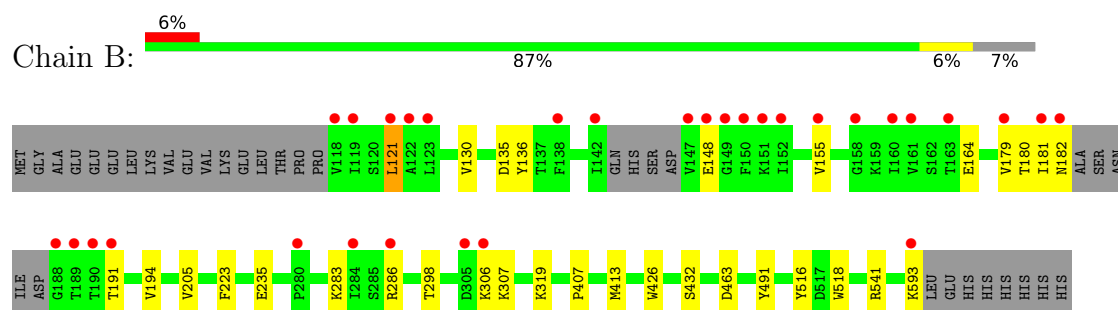
3 Residue-property plots [i](#)

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: Cell surface protein



• Molecule 1: Cell surface protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.05Å 128.05Å 135.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.70 – 1.53 85.70 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.70-1.53) 100.0 (85.70-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.53Å)	Xtriage
Refinement program	PHENIX v1.18_3855	Depositor
R, R_{free}	0.165 , 0.192 0.166 , 0.194	Depositor DCC
R_{free} test set	9277 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9101	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, CA, 15P, NA, 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	0.39	0/3860	0.58	0/5256
1	B	0.38	0/3776	0.56	0/5135
All	All	0.38	0/7636	0.57	0/10391

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3764	0	3533	18	0
1	B	3685	0	3468	19	0
2	A	93	0	87	5	0
2	B	93	0	87	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	27	0	34	3	0
4	B	16	0	21	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	718	0	0	3	0
7	B	687	0	0	3	0
All	All	9101	0	7242	46	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 3.

All (46) 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:541:ARG:HD3	7:B:1055:HOH:O	1.93	0.68
1:B:155:VAL:HG13	1:B:180:THR:HB	1.75	0.67
1:B:463:ASP:OD2	7:B:801:HOH:O	2.12	0.66
1:A:363:LYS:HZ3	4:A:704:15P:H26	1.60	0.65
1:A:118:VAL:HG12	1:A:143:GLN:HB2	1.78	0.65
1:B:223:PHE:HE1	1:B:306:LYS:HE2	1.61	0.65
2:A:701:CNC:H552	2:A:701:CNC:H531	1.79	0.65
2:A:701:CNC:H362	2:A:701:CNC:H351	1.80	0.63
2:B:701:CNC:H552	2:B:701:CNC:H531	1.78	0.63
2:B:701:CNC:H362	2:B:701:CNC:H351	1.81	0.61
1:A:363:LYS:HG2	4:A:704:15P:H16	1.86	0.56
1:B:182:ASN:ND2	1:B:191:THR:OG1	2.39	0.55
1:A:367:HIS:HD2	7:A:1381:HOH:O	1.88	0.55
1:A:391:GLN:NE2	7:A:814:HOH:O	2.39	0.54
1:B:182:ASN:HB3	1:B:191:THR:HA	1.91	0.53
1:A:506:SER:OG	1:B:135:ASP:OD2	2.21	0.52
2:B:701:CNC:N3B	2:B:701:CNC:N23	2.58	0.52
1:A:121:LEU:HD12	1:A:140:PRO:HB3	1.92	0.52
1:A:142:ILE:HG21	1:A:150:PHE:CZ	2.44	0.52
1:B:121:LEU:HD12	1:B:181:ILE:HD11	1.91	0.51
1:A:556:GLU:OE2	7:A:801:HOH:O	2.19	0.51
2:B:701:CNC:H531	2:B:701:CNC:C55	2.42	0.50
2:A:701:CNC:N3B	2:A:701:CNC:N23	2.59	0.49
1:A:179:VAL:HB	1:A:194:VAL:HG23	1.92	0.49
1:B:413:MET:HE3	1:B:426:TRP:CE2	2.46	0.49
2:B:701:CNC:C6	2:B:701:CNC:H4B	2.43	0.49
1:A:117:PRO:HD3	1:A:185:ASN:ND2	2.28	0.49
1:A:130:VAL:HB	1:A:136:TYR:CE1	2.48	0.48
1:B:130:VAL:HB	1:B:136:TYR:CZ	2.49	0.47
1:A:363:LYS:HZ3	4:A:704:15P:H18	1.79	0.47
1:B:306:LYS:HG2	1:B:307:LYS:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:701:CNC:H531	2:A:701:CNC:C55	2.42	0.47
1:A:130:VAL:HB	1:A:136:TYR:CZ	2.49	0.46
1:B:130:VAL:HB	1:B:136:TYR:CE1	2.52	0.45
1:A:413:MET:HE3	1:A:426:TRP:CE2	2.52	0.44
1:A:205:VAL:HB	1:A:235:GLU:HB2	1.99	0.44
1:B:179:VAL:HG22	1:B:194:VAL:HB	2.00	0.44
1:B:205:VAL:HB	1:B:235:GLU:HB2	2.01	0.42
1:B:407:PRO:HG3	1:B:516:TYR:CE1	2.54	0.42
1:A:117:PRO:HD3	1:A:185:ASN:CG	2.45	0.42
1:A:407:PRO:HG3	1:A:516:TYR:CE1	2.55	0.41
1:B:298:THR:HG22	7:B:1349:HOH:O	2.20	0.41
2:A:701:CNC:HM61	2:A:701:CNC:HM53	1.86	0.40
1:B:319:LYS:HE3	1:B:593:LYS:HD2	2.02	0.40
1:B:283:LYS:HE2	1:B:286:ARG:HA	2.02	0.40
1:B:432:SER:HB3	1:B:518:TRP:CD1	2.57	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	476/501 (95%)	464 (98%)	12 (2%)	0	100	100
1	B	461/501 (92%)	446 (97%)	14 (3%)	1 (0%)	43	25
All	All	937/1002 (94%)	910 (97%)	26 (3%)	1 (0%)	48	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	GLU

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	413/434 (95%)	408 (99%)	5 (1%)	63	34
1	B	403/434 (93%)	400 (99%)	3 (1%)	76	55
All	All	816/868 (94%)	808 (99%)	8 (1%)	68	42

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	SER
1	A	153	GLU
1	A	157	GLU
1	A	194	VAL
1	A	491	TYR
1	B	121	LEU
1	B	164	GLU
1	B	491	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	249	GLN
1	A	367	HIS
1	A	390	ASN
1	A	458	GLN
1	A	514	GLN
1	B	441	GLN
1	B	558	ASN

5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
6	MES	B	704	-	12,12,12	2.05	1 (8%)	15,16,16	2.09	6 (40%)
4	15P	B	705	-	15,15,103	0.62	0	14,14,102	0.64	0
2	CNC	A	701	3,5	93,103,103	1.29	11 (11%)	149,171,171	2.85	37 (24%)
4	15P	A	705	-	12,12,103	0.56	0	11,11,102	0.51	0
2	CNC	B	701	3,5	93,103,103	1.21	11 (11%)	149,171,171	3.05	35 (23%)
4	15P	A	704	-	13,13,103	0.63	0	12,12,102	0.53	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
6	MES	B	704	-	-	0/6/14/14	0/1/1/1
4	15P	B	705	-	-	5/13/13/101	-
2	CNC	A	701	3,5	1/1/36/38	2/56/235/235	0/3/11/11
4	15P	A	705	-	-	1/10/10/101	-
2	CNC	B	701	3,5	1/1/36/38	2/56/235/235	0/3/11/11
4	15P	A	704	-	-	5/11/11/101	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	704	MES	C8-S	-6.80	1.68	1.77
2	A	701	CNC	C1-N21	-4.03	1.44	1.50
2	A	701	CNC	C35-C5	3.83	1.58	1.50
2	B	701	CNC	C35-C5	3.20	1.57	1.50
2	A	701	CNC	C2B-N1B	-3.06	1.32	1.37
2	B	701	CNC	C1-N21	-3.01	1.45	1.50
2	B	701	CNC	C2B-N1B	-2.81	1.32	1.37
2	A	701	CNC	C36-C7	2.51	1.58	1.54
2	A	701	CNC	C30-C3	2.49	1.60	1.54
2	A	701	CNC	C46-C12	2.41	1.58	1.54
2	B	701	CNC	C54-C17	2.34	1.58	1.54
2	B	701	CNC	C19-N24	-2.33	1.44	1.49
2	B	701	CNC	C1-C2	-2.31	1.53	1.58
2	A	701	CNC	C48-C13	2.28	1.59	1.54
2	A	701	CNC	P-O2	2.26	1.66	1.59
2	A	701	CNC	C1-C2	-2.26	1.53	1.58
2	B	701	CNC	C48-C13	2.21	1.59	1.54
2	A	701	CNC	C54-C17	2.21	1.58	1.54
2	B	701	CNC	C55-C56	2.16	1.57	1.53
2	B	701	CNC	C46-C12	2.09	1.58	1.54
2	B	701	CNC	C53-C15	2.08	1.55	1.50
2	A	701	CNC	C53-C15	2.07	1.55	1.50
2	B	701	CNC	C36-C7	2.06	1.58	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	CNC	C1-C19-C18	14.94	144.20	121.75
2	B	701	CNC	C20-C1-N21	-14.49	86.32	110.26
2	A	701	CNC	C1-C19-C18	13.32	141.76	121.75
2	A	701	CNC	C20-C1-N21	-12.28	89.97	110.26
2	B	701	CNC	C19-C1-N21	11.31	115.94	101.69
2	B	701	CNC	C20-C1-C19	-10.75	88.90	110.23
2	A	701	CNC	C19-C1-N21	10.75	115.24	101.69
2	A	701	CNC	C20-C1-C19	-10.65	89.11	110.23
2	B	701	CNC	C2-C1-N21	9.02	114.30	101.78
2	B	701	CNC	C20-C1-C2	-8.42	99.39	113.28
2	A	701	CNC	C2-C1-N21	8.14	113.08	101.78
2	A	701	CNC	C20-C1-C2	-7.91	100.23	113.28
2	A	701	CNC	C2-C1-C19	6.91	130.69	118.77
2	B	701	CNC	C1-N21-C4	-6.42	99.04	109.48
2	A	701	CNC	C26-C2-C1	-6.42	100.09	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CNC	C12-C11-C10	-6.23	117.94	123.54
2	B	701	CNC	C2-C1-C19	6.20	129.47	118.77
2	B	701	CNC	C12-C11-C10	-5.55	118.56	123.54
2	B	701	CNC	C12-C11-N23	5.43	117.30	111.49
2	B	701	CNC	C9-C10-C11	-5.38	117.92	125.84
2	B	701	CNC	C8-C9-C10	-5.27	112.11	123.33
2	B	701	CNC	C17-C16-C15	-4.98	119.21	126.70
6	B	704	MES	C5-N4-C3	4.98	119.57	108.84
2	B	701	CNC	C26-C2-C1	-4.93	102.39	110.00
2	A	701	CNC	C17-C16-C15	-4.77	119.53	126.70
2	A	701	CNC	C9B-N3B-C2B	4.68	110.14	104.40
2	A	701	CNC	C8B-N1B-C2B	4.60	110.44	106.26
2	A	701	CNC	C12-C11-N23	4.47	116.27	111.49
2	A	701	CNC	N1B-C2B-N3B	-4.30	107.84	113.94
2	A	701	CNC	C1-N21-C4	-4.15	102.72	109.48
2	A	701	CNC	C13-C14-C15	-4.15	116.88	123.82
2	B	701	CNC	C5-C6-N22	-4.09	117.69	123.88
2	B	701	CNC	C15-C16-N24	4.01	126.41	122.38
2	A	701	CNC	C8B-C9B-N3B	-3.76	105.94	110.00
2	A	701	CNC	C9-C10-C11	-3.75	120.32	125.84
2	A	701	CNC	C60-C18-C19	-3.73	105.28	114.08
2	B	701	CNC	C7-C6-C5	-3.65	122.37	128.07
2	B	701	CNC	C13-C14-C15	-3.62	117.77	123.82
2	B	701	CNC	C9B-N3B-C2B	3.53	108.73	104.40
2	A	701	CNC	C2R-C3R-C4R	-3.52	97.08	103.24
2	B	701	CNC	C60-C18-C19	-3.50	105.84	114.08
2	B	701	CNC	C8B-C9B-N3B	-3.29	106.44	110.00
2	A	701	CNC	C25-C2-C1	3.26	118.63	113.75
2	A	701	CNC	C15-C16-N24	3.22	125.61	122.38
2	B	701	CNC	C8-C7-C6	-3.13	95.61	100.92
2	B	701	CNC	C8B-N1B-C2B	3.09	109.07	106.26
2	B	701	CNC	C25-C2-C1	3.03	118.28	113.75
2	A	701	CNC	C8-C9-C10	-2.96	117.03	123.33
6	B	704	MES	O2S-S-C8	2.95	111.19	106.73
2	B	701	CNC	C10-C9-N22	-2.95	122.38	125.74
2	B	701	CNC	N1B-C2B-N3B	-2.94	109.76	113.94
2	B	701	CNC	C55-C17-C18	-2.90	105.58	111.12
2	B	701	CNC	C54-C17-C18	-2.85	108.90	112.99
2	B	701	CNC	C13-C14-N23	2.80	115.36	109.39
2	A	701	CNC	C2R-C1R-N1B	-2.80	106.34	113.30
2	A	701	CNC	C16-C15-C14	-2.70	117.62	121.29
2	A	701	CNC	C5-C6-N22	-2.68	119.82	123.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	CNC	C55-C17-C18	-2.68	106.00	111.12
2	A	701	CNC	C3-C4-C5	-2.67	119.36	123.82
2	B	701	CNC	C41-C8-C7	-2.59	107.06	114.19
6	B	704	MES	C7-N4-C3	2.57	118.10	111.24
2	A	701	CNC	C8-C9-N22	2.49	115.69	110.77
2	B	701	CNC	C12-C13-C14	-2.49	98.62	101.86
2	A	701	CNC	C7-C6-N22	2.43	112.36	107.94
2	A	701	CNC	C54-C17-C18	-2.42	109.52	112.99
2	A	701	CNC	C13-C14-N23	2.27	114.22	109.39
6	B	704	MES	C2-C3-N4	-2.24	106.71	110.12
6	B	704	MES	C8-C7-N4	-2.23	103.92	112.36
2	A	701	CNC	C12-C13-C14	-2.18	99.02	101.86
2	A	701	CNC	C1P-N59-C57	-2.16	118.06	122.69
2	B	701	CNC	C2R-C1R-N1B	-2.13	108.00	113.30
2	A	701	CNC	C18-C17-C16	-2.11	96.99	100.34
2	B	701	CNC	C8-C9-N22	2.09	114.89	110.77
2	B	701	CNC	C30-C3-C2	-2.08	114.40	119.00
2	B	701	CNC	C7-C8-C9	-2.08	98.25	100.89
2	A	701	CNC	C41-C8-C7	-2.08	108.47	114.19
6	B	704	MES	O1S-S-C8	2.05	109.83	106.73
2	A	701	CNC	C4B-C9B-N3B	2.04	133.95	130.51

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	CNC	N24
2	B	701	CNC	N24

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	705	15P	C4-C3-O1-C2
4	A	705	15P	O3-C7-C8-O4
4	B	705	15P	O1-C3-C4-O2
4	A	704	15P	O1-C3-C4-O2
4	B	705	15P	OXT-C1-C2-O1
4	A	704	15P	C8-C7-O3-C6
4	A	704	15P	C7-C8-O4-C9
4	A	704	15P	C1-C2-O1-C3
4	B	705	15P	C10-C9-O4-C8
4	B	705	15P	C3-C4-O2-C5
2	A	701	CNC	C18-C60-C61-O63

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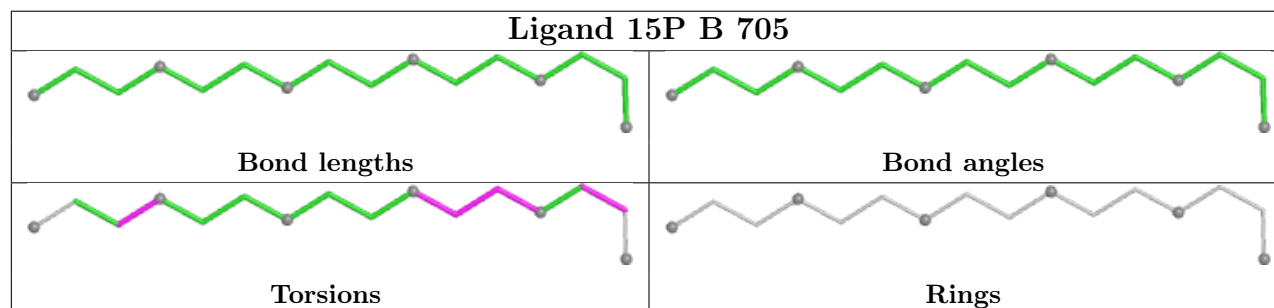
Mol	Chain	Res	Type	Atoms
2	B	701	CNC	C18-C60-C61-O63
2	B	701	CNC	C18-C60-C61-N62
4	A	704	15P	O3-C7-C8-O4
2	A	701	CNC	C18-C60-C61-N62

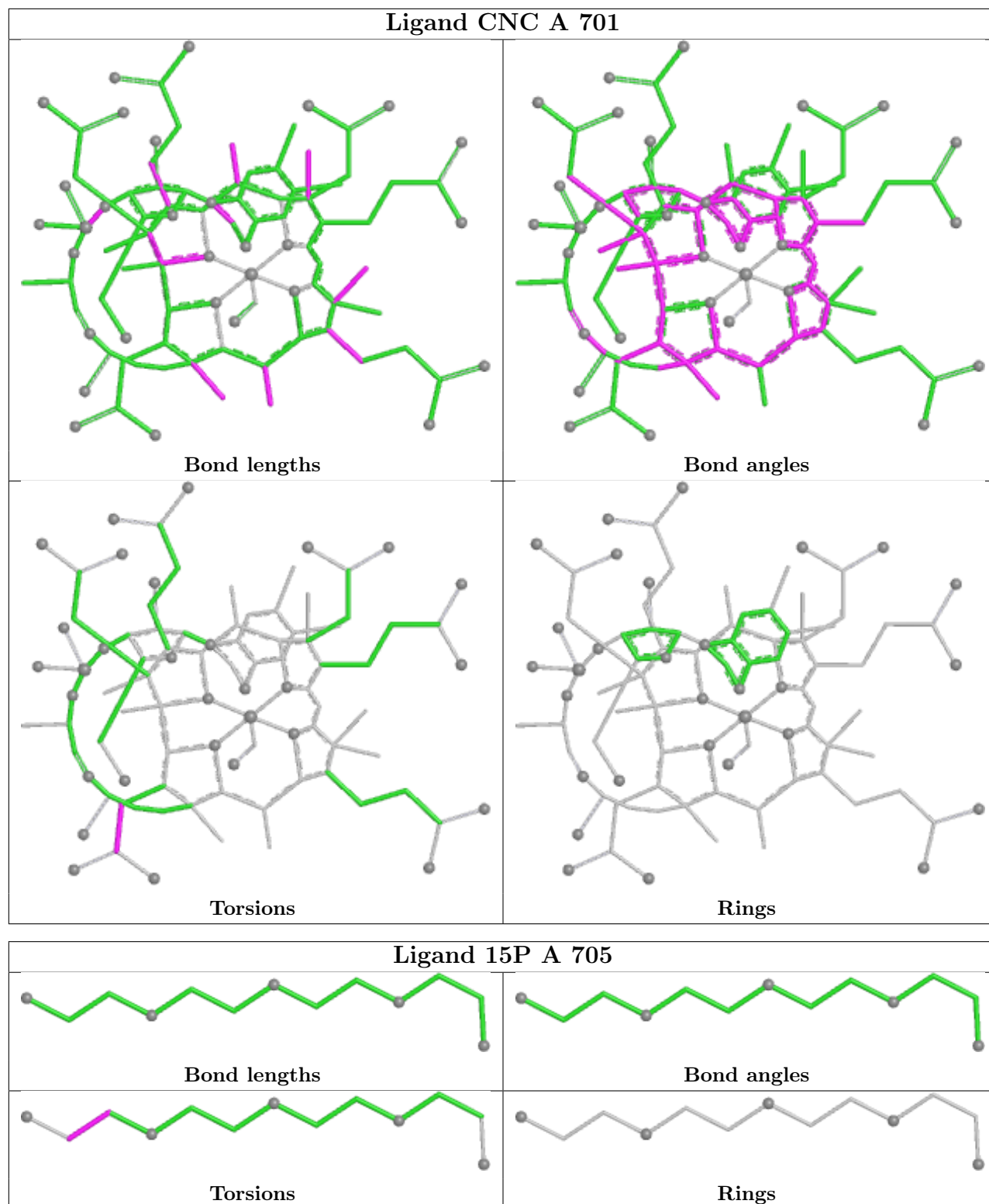
There are no ring outliers.

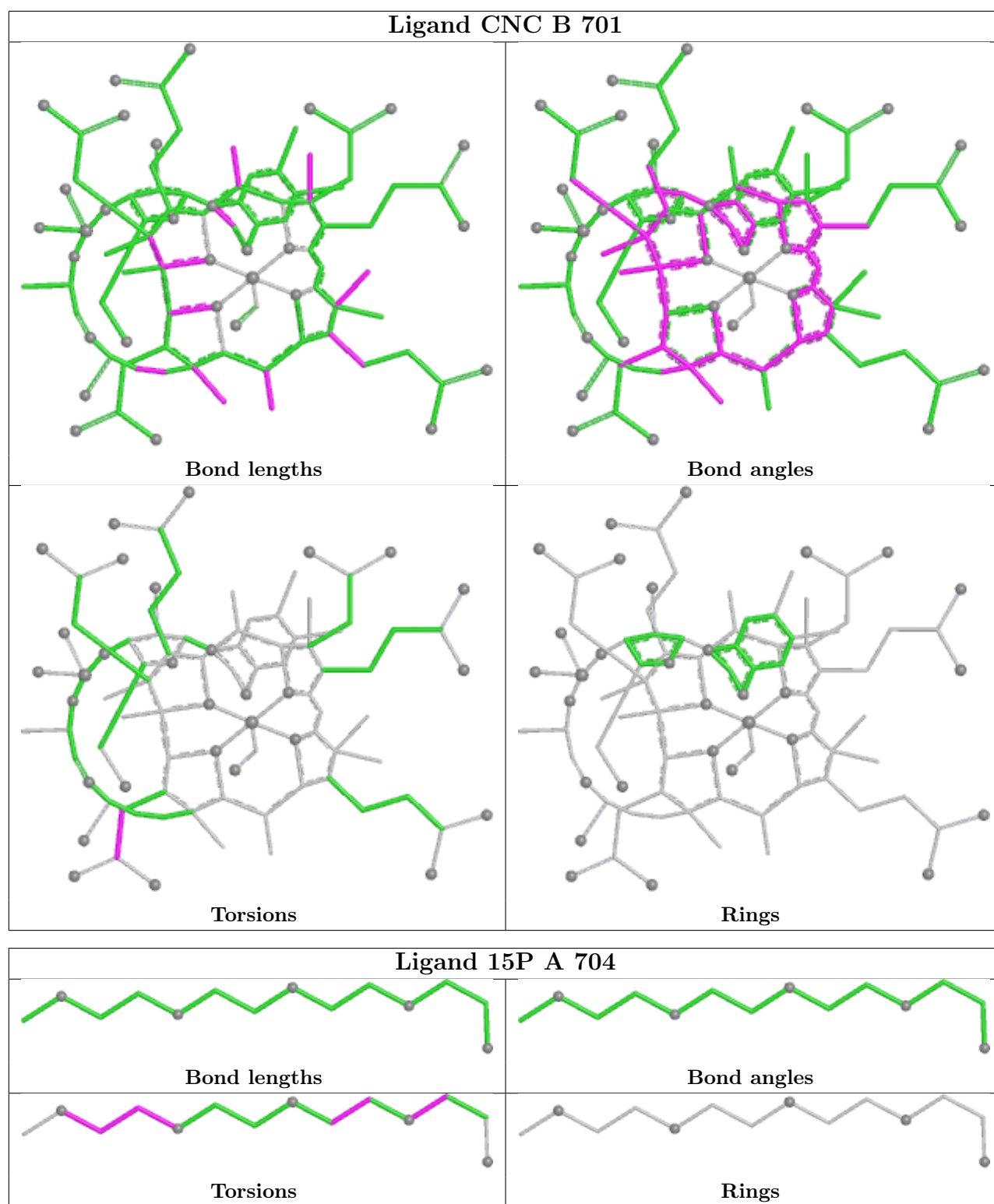
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CNC	5	0
2	B	701	CNC	5	0
4	A	704	15P	3	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 ⓘ

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	478/501 (95%)	0.08	37 (7%)	19 24	14, 22, 74, 124	0
1	B	467/501 (93%)	0.10	31 (6%)	24 30	16, 24, 70, 123	0
All	All	945/1002 (94%)	0.09	68 (7%)	21 27	14, 23, 72, 124	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ILE	7.0
1	B	147	VAL	6.7
1	B	160	ILE	6.0
1	B	118	VAL	5.8
1	A	315	SER	5.0
1	B	150	PHE	4.8
1	B	189	THR	4.8
1	B	188	GLY	4.6
1	A	280	PRO	4.4
1	B	181	ILE	4.2
1	A	186	ILE	4.1
1	A	118	VAL	4.1
1	B	152	ILE	4.0
1	A	160	ILE	3.9
1	A	142	ILE	3.8
1	B	119	ILE	3.7
1	B	593	LYS	3.6
1	A	183	ALA	3.4
1	A	188	GLY	3.4
1	A	115	THR	3.4
1	B	149	GLY	3.4
1	B	155	VAL	3.3
1	A	506	SER	3.3
1	A	305	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	189	THR	3.2
1	B	280	PRO	3.2
1	A	507	GLN	3.1
1	A	341	ILE	3.1
1	A	161	VAL	3.0
1	A	281	THR	3.0
1	B	161	VAL	2.9
1	A	119	ILE	2.9
1	B	148	GLU	2.9
1	B	182	ASN	2.9
1	B	138	PHE	2.8
1	A	181	ILE	2.8
1	B	191	THR	2.8
1	A	147	VAL	2.7
1	A	194	VAL	2.7
1	B	179	VAL	2.7
1	A	150	PHE	2.7
1	B	123	LEU	2.6
1	A	149	GLY	2.6
1	A	155	VAL	2.6
1	A	143	GLN	2.6
1	A	117	PRO	2.5
1	B	305	ASP	2.4
1	B	163	THR	2.4
1	B	190	THR	2.4
1	A	314	ALA	2.4
1	B	286	ARG	2.3
1	A	340	THR	2.3
1	B	121	LEU	2.3
1	B	158	GLY	2.3
1	B	122	ALA	2.3
1	A	116	PRO	2.2
1	A	144	HIS	2.2
1	B	306	LYS	2.2
1	A	152	ILE	2.2
1	A	284	ILE	2.2
1	B	151	LYS	2.2
1	B	284	ILE	2.1
1	A	391	GLN	2.1
1	A	120	SER	2.0
1	A	279	THR	2.0
1	A	138	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	145	SER	2.0
1	A	184	SER	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](#)

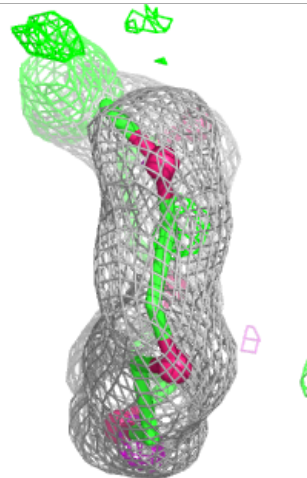
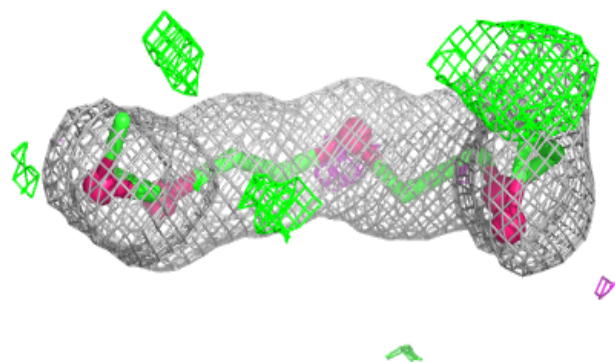
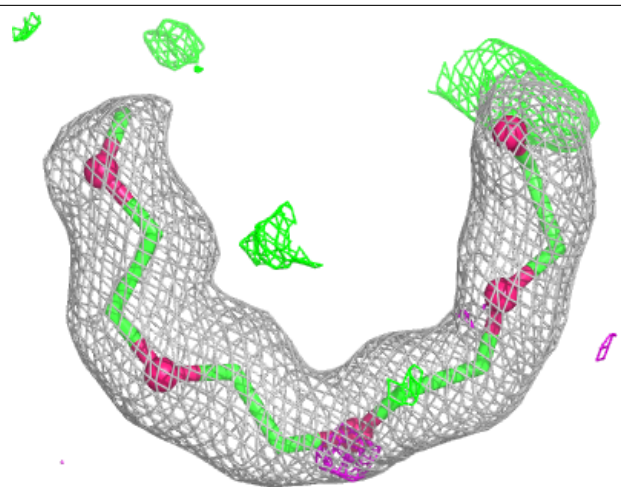
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	15P	A	704	14/104	0.83	0.15	27,38,50,54	0
4	15P	A	705	13/104	0.85	0.15	31,36,44,47	0
4	15P	B	705	16/104	0.85	0.14	32,38,45,45	0
6	MES	B	704	12/12	0.95	0.10	27,35,40,40	0
2	CNC	A	701	93/93	0.97	0.07	17,21,28,34	0
2	CNC	B	701	93/93	0.97	0.07	20,25,34,39	0
5	NA	B	706	1/1	0.98	0.04	21,21,21,21	0
3	CA	B	703	1/1	0.98	0.04	21,21,21,21	0
3	CA	A	702	1/1	0.99	0.03	17,17,17,17	0
5	NA	A	706	1/1	0.99	0.02	17,17,17,17	0
3	CA	A	703	1/1	0.99	0.03	17,17,17,17	0
3	CA	B	702	1/1	0.99	0.03	20,20,20,20	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.

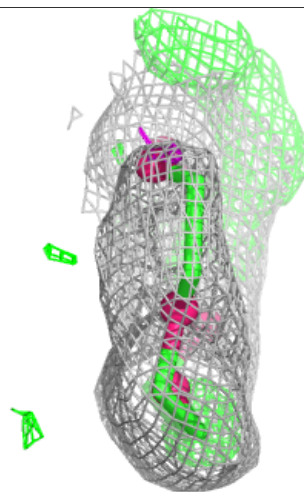
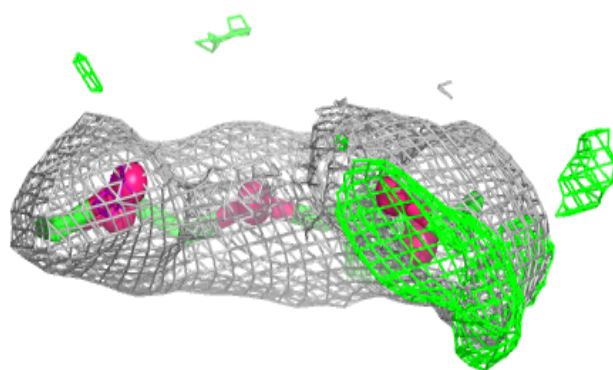
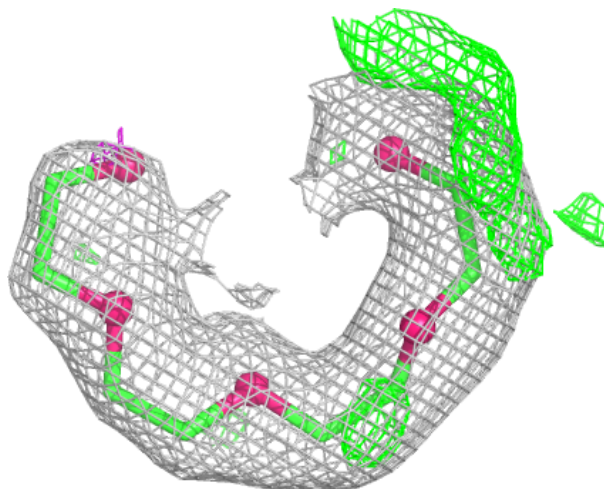
Electron density around 15P A 704:

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



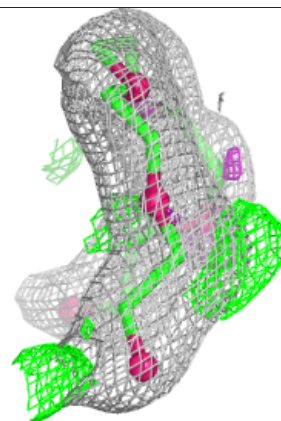
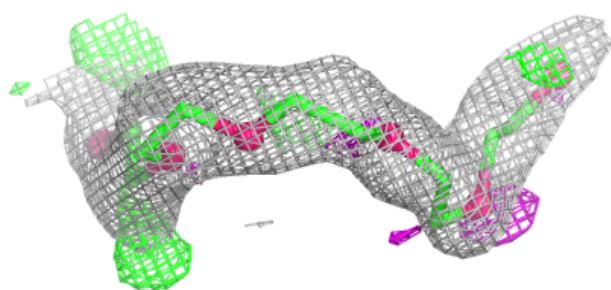
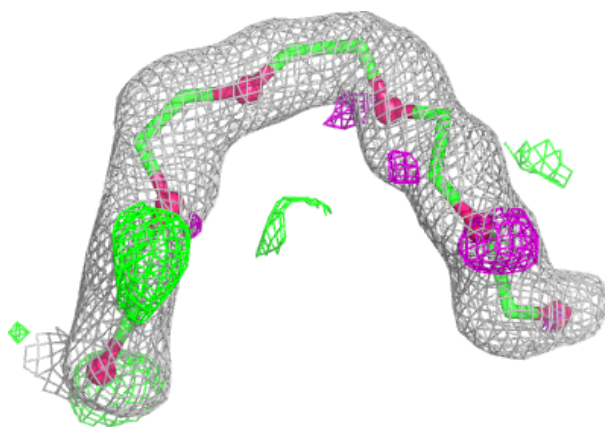
Electron density around 15P A 705:

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



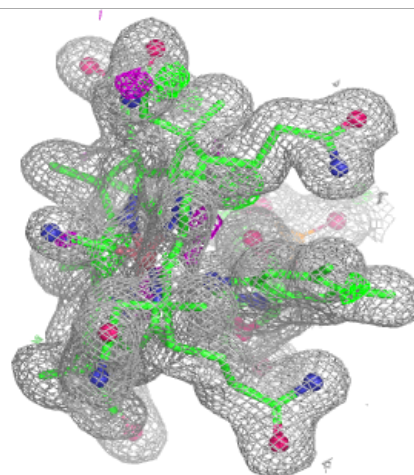
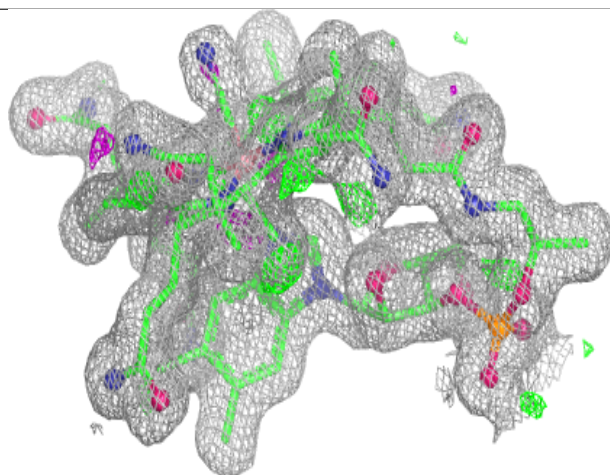
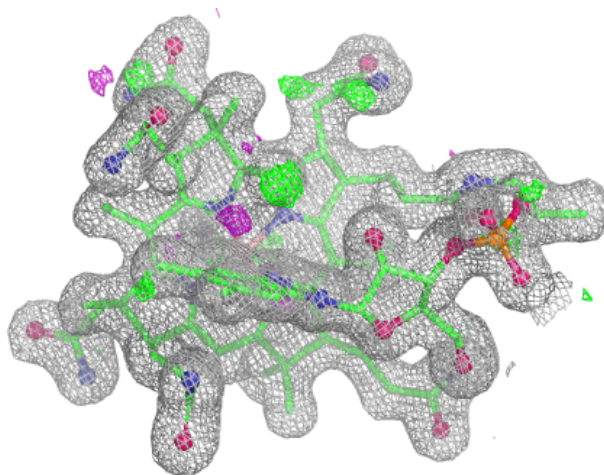
Electron density around 15P B 705:

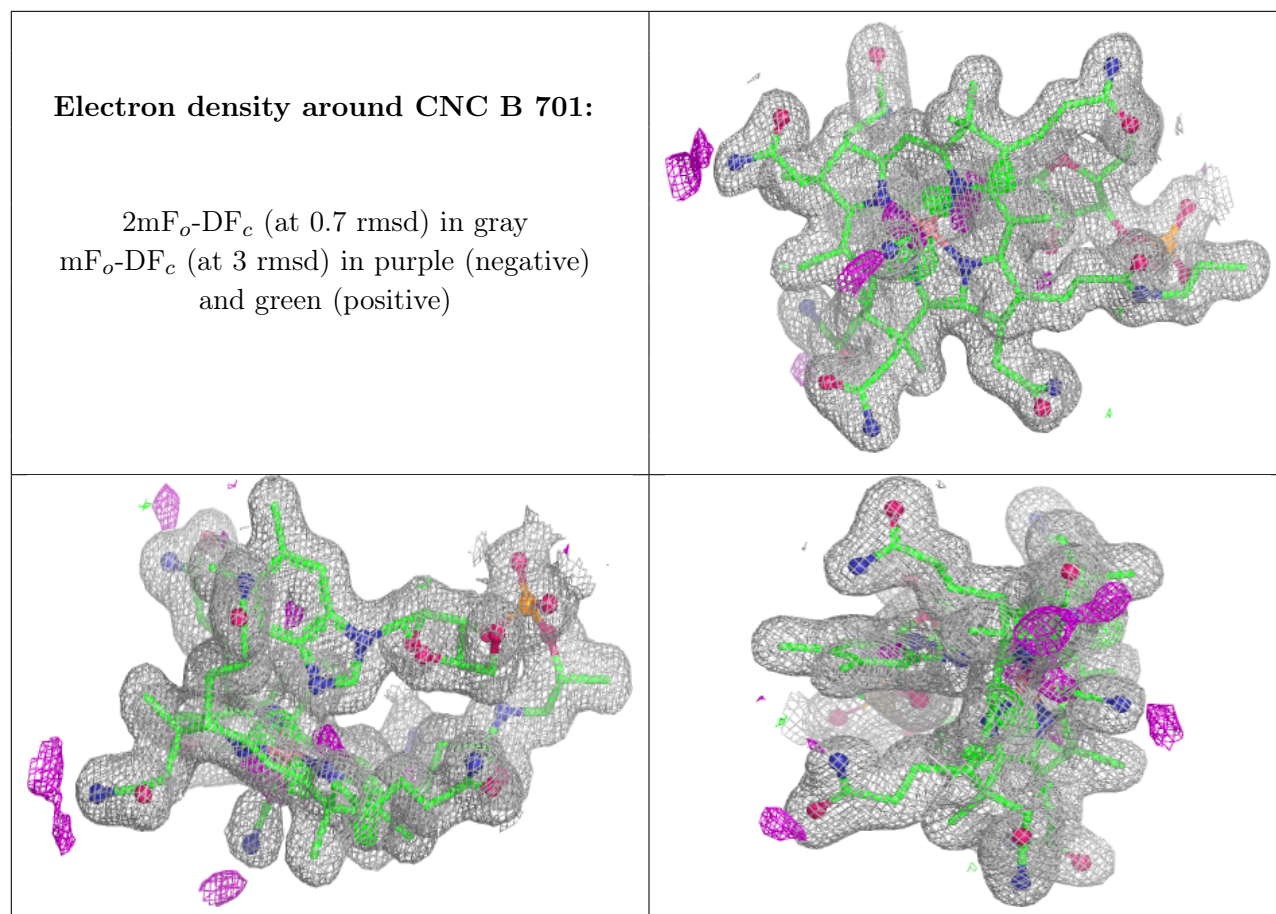
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CNC A 701:

$2mF_o-DF_c$ (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.