



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:04 AM UTC

PDB ID : 7QBD / pdb_00007qbd
Title : TC:CD320 in complex with nanobody TC-Nb26
Authors : Bloch, J.S.; Locher, K.P.
Deposited on : 2021-11-19
Resolution : 4.18 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

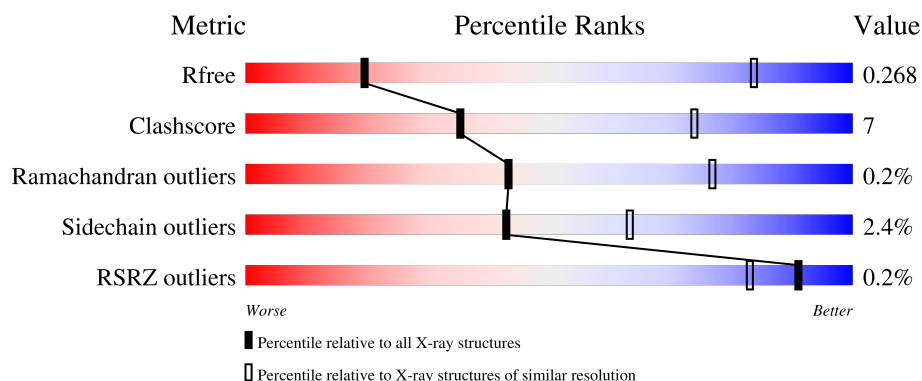
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.18 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	1026 (4.50-3.86)
Clashscore	190562	1071 (4.50-3.86)
Ramachandran outliers	187476	1014 (4.52-3.84)
Sidechain outliers	187428	1000 (4.52-3.84)
RSRZ outliers	180081	1023 (4.50-3.86)

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	409	94%
1	B	409	91% 6%
2	C	147	37% 14% 48%
2	D	147	41% 10% 47%
3	E	132	46% 36% 14%

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	501	X	-	-	-
4	CNC	B	501	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8393 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 Transcobalamin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3103	1981	542	561	19			
1	B	400	Total	C	N	O	S	0	0	0
			3103	1981	542	561	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLN	ARG	conflict	UNP P20062
B	209	GLN	ARG	conflict	UNP P20062

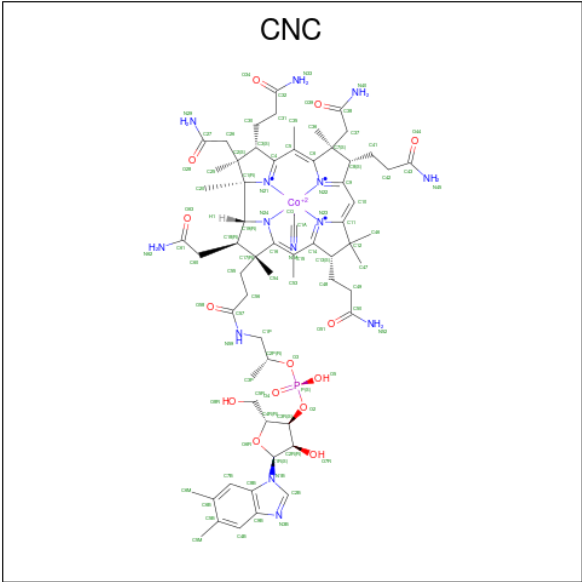
- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	76	Total	C	N	O	S	0	0	0
			545	326	88	119	12			
2	D	78	Total	C	N	O	S	0	0	0
			560	334	91	123	12			

- Molecule 3 is a protein called Antitranscobalamin-nanobody TC-Nb26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	114	Total	C	N	O	S	0	0	0
			890	556	161	169	4			

- Molecule 4 is CYANOCOBALAMIN (CCD ID: CNC) (formula: C₆₃H₈₉CoN₁₄O₁₄P).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	2	Total	Ca	0	0
			2	2		
5	D	2	Total	Ca	0	0
			2	2		

- Molecule 1: Transcobalamin-2

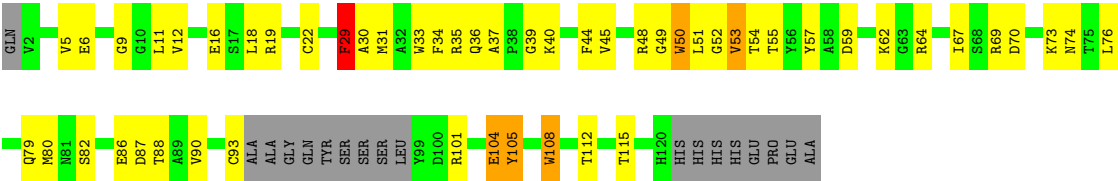
E1	P6	C65	G68	SER	ALA	PHE	SER	GLU	ASP	ASP	GLY	ASP	C78	K81	P92	L230	R241	E244	T247	R253	M270	Q307	S320	L321	E353	S365	V366	M367	E400	F406
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Sequence logo visualization showing the conservation of amino acids across positions. The y-axis represents information content in bits (0 to 4.00). The x-axis lists positions from E1 to P383. A red dot is placed above position L213. The bars are color-coded: green for positions E1, P6, E7, S10, N33, P34, C65, G68, Y163, F168, L213, R241, E244, T247, R253, N270, Q307, T308, S320, L321, S328, E353, S365, Y366, K367, D382, and P383. The bars for G68, L213, and C78 are grey and contain text labels for the amino acids: SER, ALA, PHE, SER, GLU, ASP, ASP, GLY, and ASP respectively.

CYS	ARG	ARG	L130	L137	P147	L148	T149	W150	R151	G166	C167	G168	THR	ASN	GLU	ILE	LEU	PRO	PRO	GLY	GLY	ASP	ALA	THR	THR	THR	MET	GLY	PRO	PRO	VAL	THR	THR	LEU	GLU	GLU	SER	VAL	THR	THR	SER	LEU	ARG	ASN	ALA	THR	THR					
GLY	S53	C54	P55	P56	T57	K58	F59	Q60	C61	R62	G65	L66	C67	D68	D65	E66	E67	E68	C69	ARG	ILE	GLU	PRO	CYS	CYS	THR	GLN	LYS	GLY	GLN	CYS	CYS	PRO	PRO	PRO	GLY	GLY	LEU	PRO	CYS	ASP	SER	CYS	SER	GLY	GLY	THR	ASP	LYS	LYS	LEU	ASN

[illegible]

● Molecule 3: Antitranscobalamin-nanobody TC-Nb26



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.13Å 102.13Å 361.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 4.18 49.14 – 4.18	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.14-4.18) 94.7 (49.14-4.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.262 , 0.272 0.258 , 0.268	Depositor DCC
R_{free} test set	714 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	161.3	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 156.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8393	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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: CA, 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	0.44	0/3171	0.69	0/4300
1	B	0.45	0/3171	0.74	1/4300 (0.0%)
2	C	0.67	0/555	1.25	5/757 (0.7%)
2	D	0.67	0/570	1.23	3/778 (0.4%)
3	E	0.64	0/908	1.24	7/1227 (0.6%)
All	All	0.50	0/8375	0.87	16/11362 (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
2	C	0	1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	51	LEU	N-CA-C	-12.81	97.31	111.28
2	D	169	THR	N-CA-C	8.12	120.71	109.18
3	E	29	PHE	CB-CA-C	-7.82	98.30	110.81
3	E	29	PHE	CA-CB-CG	6.71	120.51	113.80
3	E	53	VAL	CA-C-N	-6.35	113.96	122.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	53	SER	Mainchain

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	3103	0	3115	24	0
1	B	3103	0	3115	27	4
2	C	545	0	464	10	0
2	D	560	0	477	9	0
3	E	890	0	847	47	3
4	A	93	0	84	10	0
4	B	93	0	84	13	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	8393	0	8186	123	4

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 7.

The worst 5 of 123 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:501:CNC:C30	4:A:501:CNC:C31	1.88	1.52
4:B:501:CNC:C31	4:B:501:CNC:C30	1.88	1.51
1:A:241:ARG:HH21	1:B:241:ARG:NH2	1.04	1.41
1:A:241:ARG:NH2	1:B:241:ARG:HH21	0.93	1.39
4:A:501:CNC:C31	4:A:501:CNC:C3	1.91	1.39

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:CE2	3:E:90:VAL:CG2[6_555]	1.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:CB	1:B:328:SER:OG[8_555]	1.85	0.35
1:B:163:TYR:CE1	3:E:39:GLY:CA[6_555]	1.99	0.21
1:B:163:TYR:OH	3:E:39:GLY:CA[6_555]	2.09	0.11

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	396/409 (97%)	391 (99%)	5 (1%)	0	100	100
1	B	396/409 (97%)	391 (99%)	5 (1%)	0	100	100
2	C	72/147 (49%)	66 (92%)	6 (8%)	0	100	100
2	D	74/147 (50%)	66 (89%)	8 (11%)	0	100	100
3	E	110/132 (83%)	98 (89%)	10 (9%)	2 (2%)	6	34
All	All	1048/1244 (84%)	1012 (97%)	34 (3%)	2 (0%)	43	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	53	VAL
3	E	105	TYR

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	332/348 (95%)	330 (99%)	2 (1%)	78	80
1	B	332/348 (95%)	328 (99%)	4 (1%)	63	72
2	C	64/129 (50%)	59 (92%)	5 (8%)	11	33
2	D	66/129 (51%)	61 (92%)	5 (8%)	12	34
3	E	91/107 (85%)	86 (94%)	5 (6%)	19	43
All	All	885/1061 (83%)	864 (98%)	21 (2%)	43	63

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	87	GLU
3	E	50	TRP
3	E	108	TRP
3	E	74	ASN
3	E	29	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	378	GLN
1	B	389	GLN
2	C	60	GLN
1	A	378	GLN
1	A	389	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

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
4	CNC	A	501	-	93,103,103	7.65	40 (43%)	149,171,171	3.77	67 (44%)
4	CNC	B	501	-	93,103,103	7.66	40 (43%)	149,171,171	3.77	66 (44%)

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
4	CNC	A	501	-	2/2/36/38	4/56/235/235	0/3/11/11
4	CNC	B	501	-	2/2/36/38	4/56/235/235	0/3/11/11

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	CNC	C30-C3	-64.75	0.06	1.54
4	A	501	CNC	C30-C3	-64.73	0.06	1.54
4	A	501	CNC	C30-C31	11.79	1.88	1.52
4	B	501	CNC	C30-C31	11.78	1.88	1.52
4	A	501	CNC	C19-N24	-10.15	1.28	1.49

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C25-C2-C26	-13.18	83.56	109.74
4	A	501	CNC	C3-C4-C5	-13.17	101.78	123.82
4	B	501	CNC	C25-C2-C26	-13.16	83.59	109.74
4	B	501	CNC	C3-C4-C5	-13.15	101.81	123.82
4	A	501	CNC	C8-C9-C10	-12.91	95.84	123.33

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	CNC	C3
4	A	501	CNC	N24
4	B	501	CNC	C3
4	B	501	CNC	N24

5 of 8 torsion outliers are listed below:

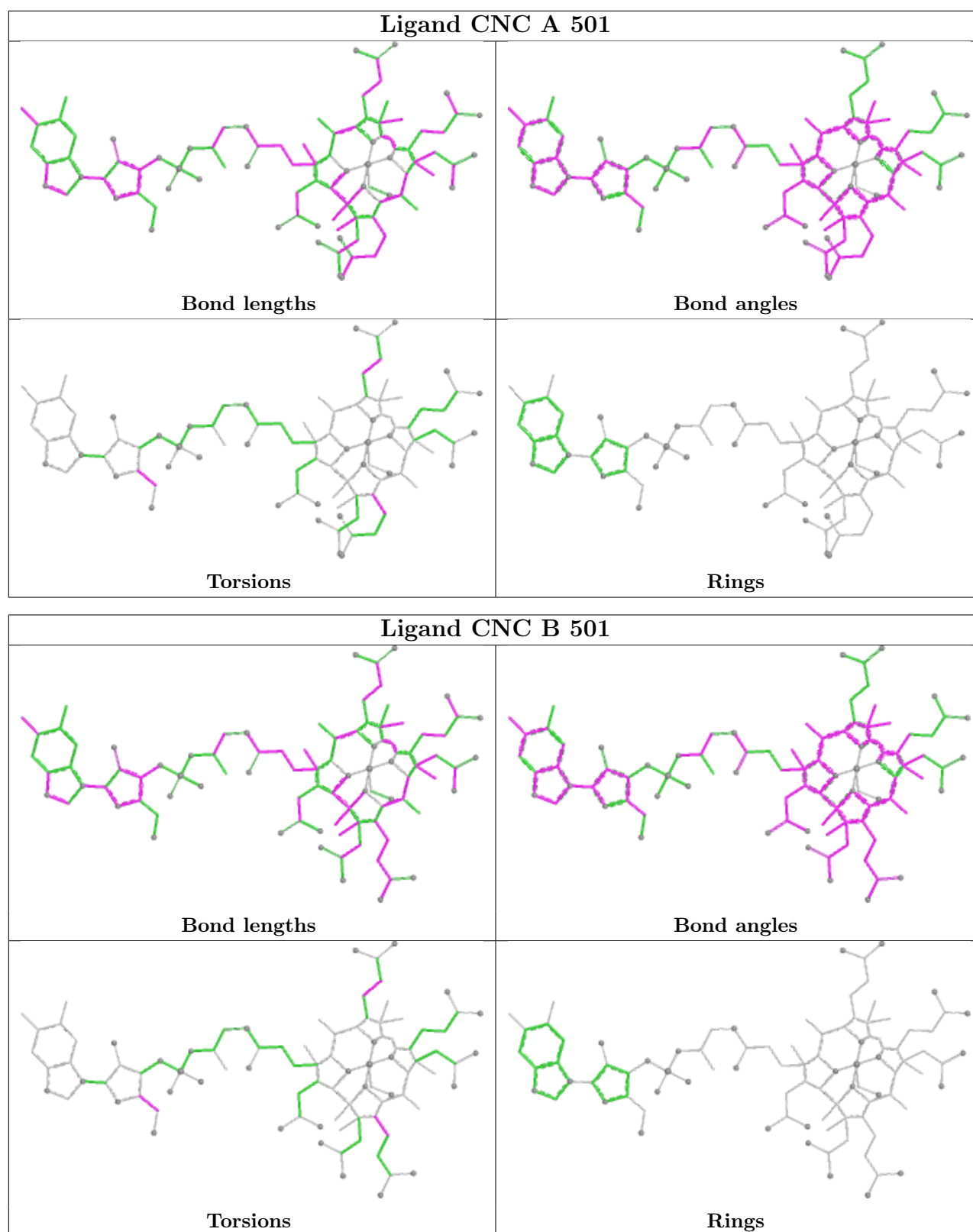
Mol	Chain	Res	Type	Atoms
4	A	501	CNC	C3R-C4R-C5R-O8R
4	B	501	CNC	C3R-C4R-C5R-O8R
4	A	501	CNC	O6R-C4R-C5R-O8R
4	B	501	CNC	O6R-C4R-C5R-O8R
4	A	501	CNC	C2-C3-C30-C31

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	CNC	10	0
4	B	501	CNC	13	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 ⓘ

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 [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	400/409 (97%)	-0.42	0 100 100	143, 184, 223, 298	0
1	B	400/409 (97%)	-0.35	1 (0%) 90 80	146, 179, 219, 270	0
2	C	76/147 (51%)	-0.48	1 (1%) 75 59	200, 250, 270, 289	0
2	D	78/147 (53%)	-0.47	0 100 100	204, 237, 269, 292	0
3	E	114/132 (86%)	-0.31	0 100 100	127, 189, 220, 249	0
All	All	1068/1244 (85%)	-0.39	2 (0%) 91 83	127, 187, 256, 298	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	LEU	3.1
2	C	168	GLY	2.6

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](#)

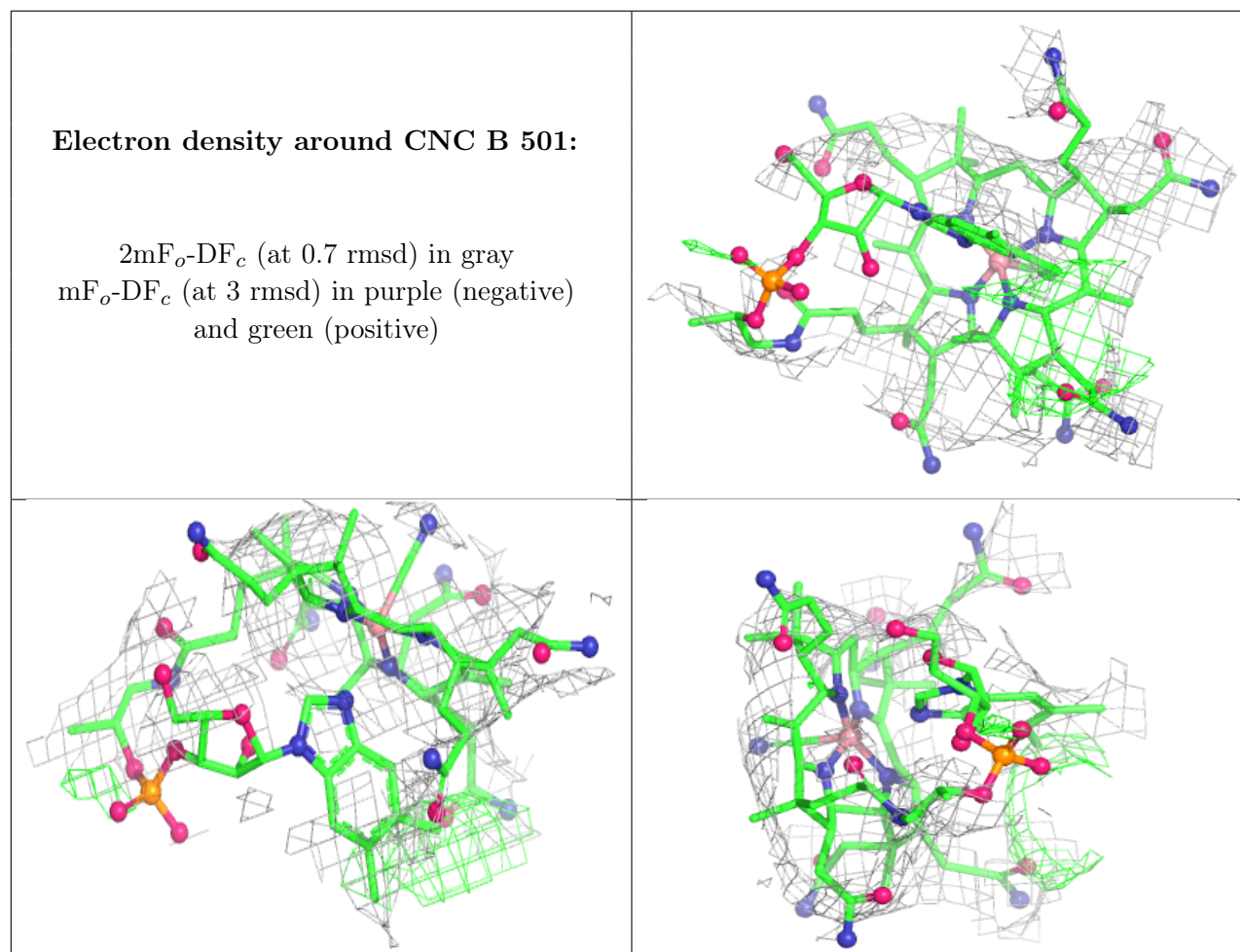
There are no oligosaccharides in this entry.

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.

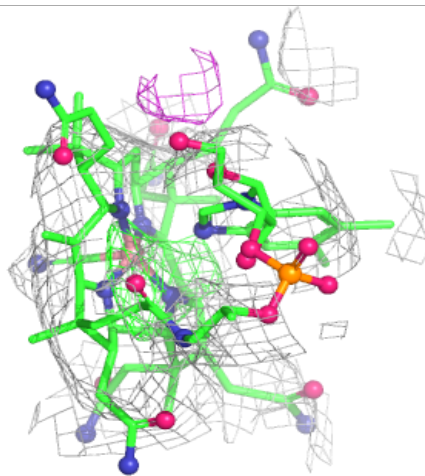
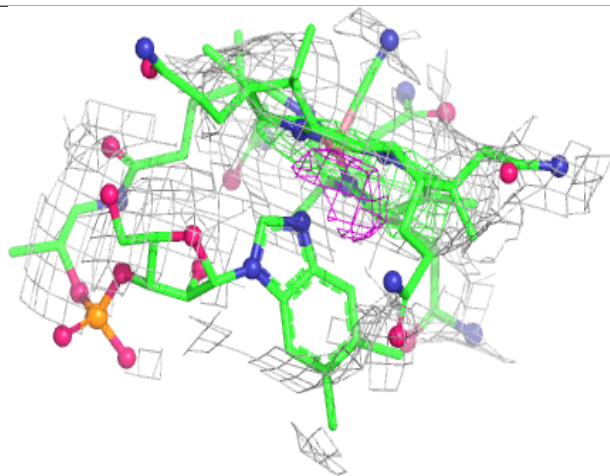
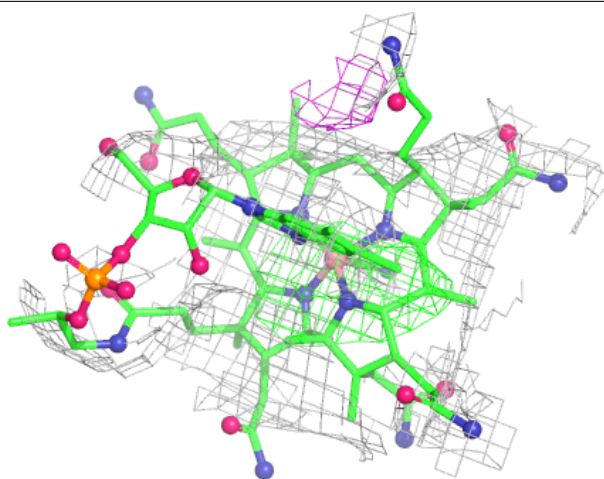
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	502	1/1	0.54	0.19	214,214,214,214	0
5	CA	B	502	1/1	0.66	0.09	179,179,179,179	0
4	CNC	B	501	93/93	0.94	0.08	131,150,162,168	8
4	CNC	A	501	93/93	0.96	0.09	148,159,173,178	8
5	CA	C	202	1/1	0.96	0.05	251,251,251,251	0
5	CA	D	202	1/1	0.97	0.04	249,249,249,249	0
5	CA	D	201	1/1	0.98	0.04	218,218,218,218	0
5	CA	C	201	1/1	0.98	0.03	224,224,224,224	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 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.