W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 17, 2021 – 12:05 pm BST

PDB ID	:	4ZRQ
Title	:	E88 deletion mutant of CD320 in complex with TC2
Authors	:	Alam, A.; Locher, K.P.
Deposited on	:	2015-05-12
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

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

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 2.60 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.
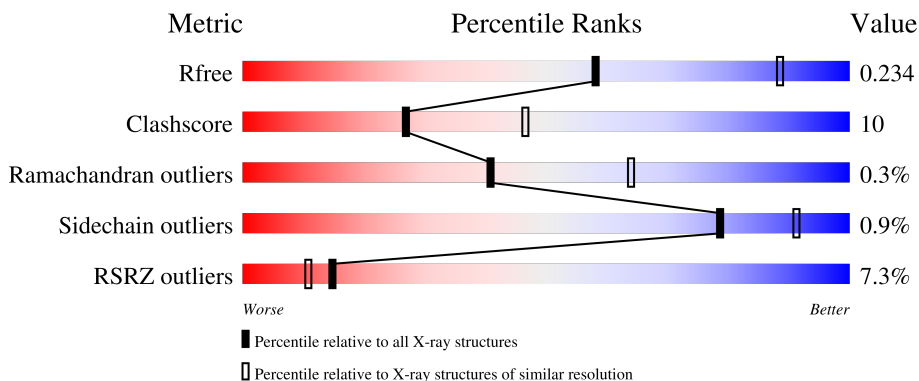
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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% 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	2% 88% 9% •
1	B	409	4% 87% 10% ••
2	C	118	19% 41% 20% •• 36%
2	D	118	17% 44% 18% • 36%

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
3	CNC	A	501	X	-	X	-
3	CNC	B	501	X	-	X	-
4	GOL	A	503	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7560 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 3119	C 1989	N 542	O 569	S 19	0	0	0
1	B	399	Total 3119	C 1989	N 543	O 568	S 19	0	0	0

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 530	C 316	N 87	O 116	S 11	0	0	0
2	D	75	Total 534	C 319	N 89	O 115	S 11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q9NPF0
D	?	-	GLU	deletion	UNP Q9NPF0

- Molecule 3 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).
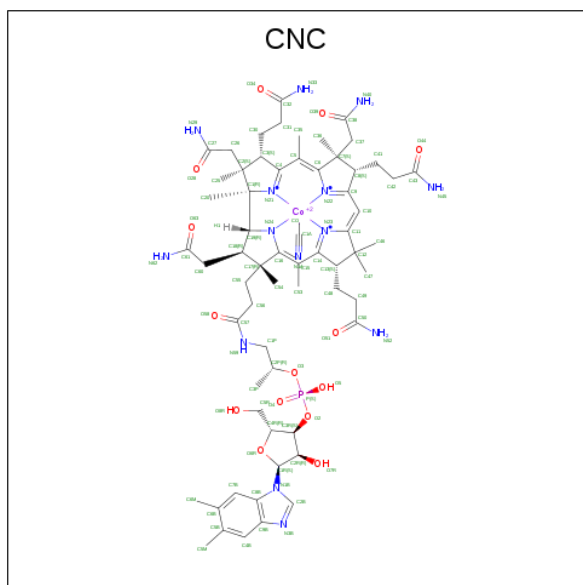
CNC

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

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
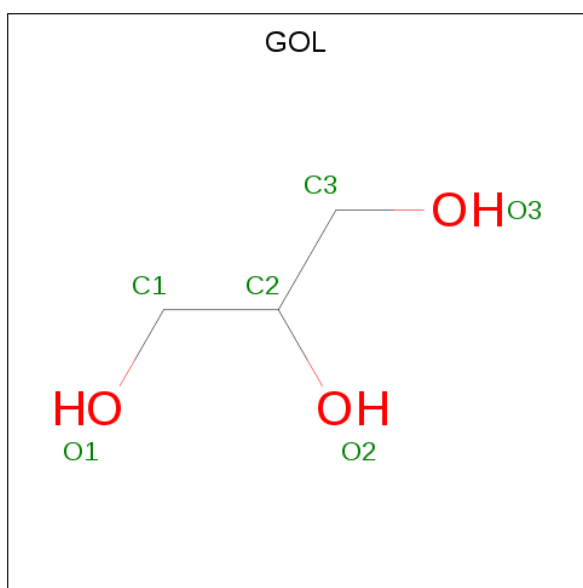
GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total 25	O 25	0	0
6	B	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

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.
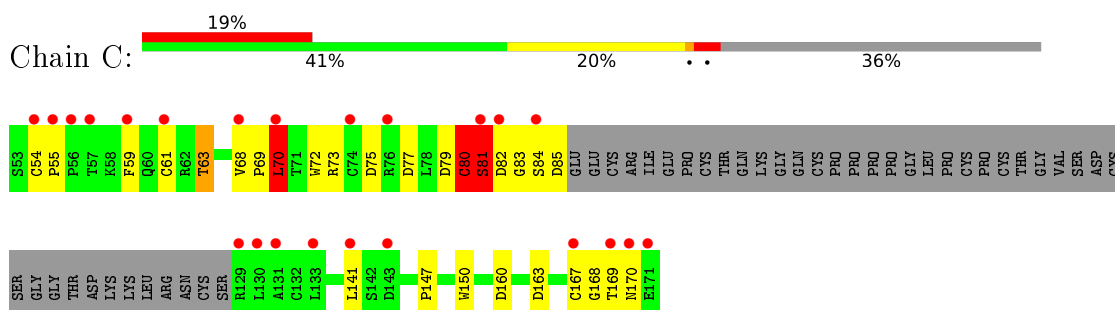
- Molecule 1: Transcobalamin-2
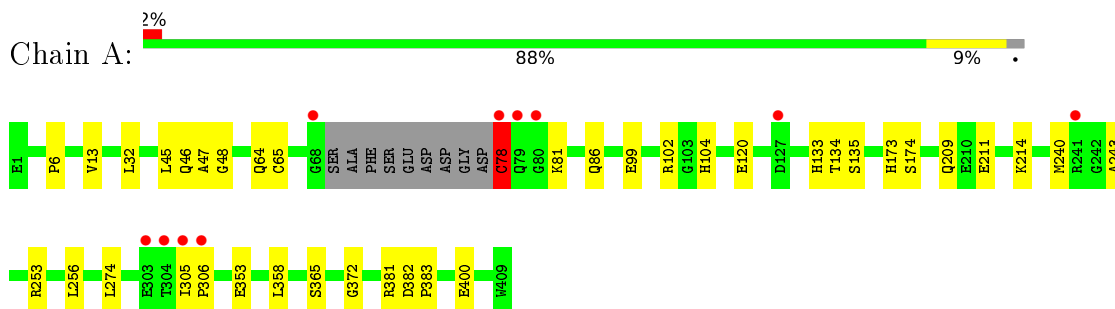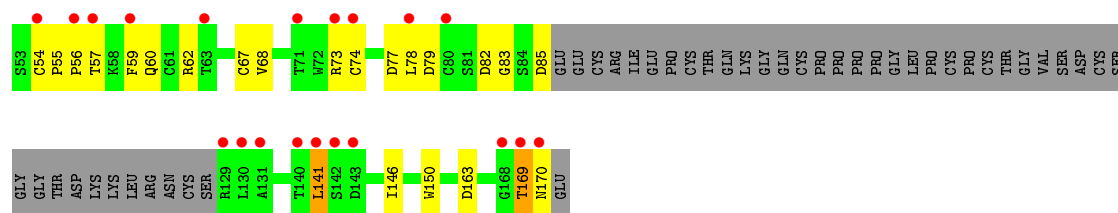

- Molecule 1: Transcobalamin-2
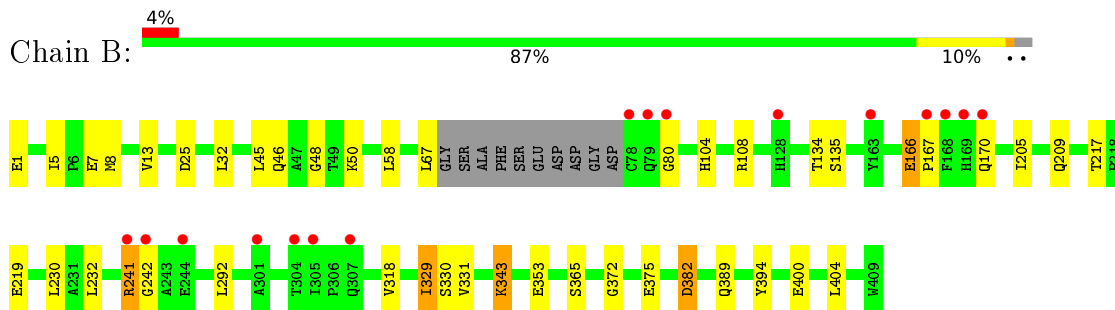
- Molecule 2: CD320 antigen

- Molecule 2: CD320 antigen

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.40Å 98.40Å 356.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.43 – 2.60 29.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.43-2.60) 93.7 (29.43-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.199 , 0.231 0.205 , 0.234	Depositor DCC
R_{free} test set	2732 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.0	EDS
L-test for twinning[2]	$<|L|> = 0.47$, $<L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7560	wwPDB-VP
Average B, all atoms (Å^2)	74.0	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: CNC, CA, GOL

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	0.32	1/3187 (0.0%)	0.44	0/4320
1	B	0.29	0/3187	0.55	3/4320 (0.1%)
2	C	0.45	0/540	1.08	3/740 (0.4%)
2	D	0.37	0/544	0.87	2/744 (0.3%)
All	All	0.33	1/7458 (0.0%)	0.59	8/10124 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
2	D	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	CYS	CB-SG	11.77	2.02	1.82

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	ILE	CG1-CB-CG2	-12.52	83.85	111.40
2	C	70	LEU	CA-CB-CG	10.03	138.36	115.30
1	B	343	LYS	CD-CE-NZ	-8.12	93.02	111.70
2	C	81	SER	N-CA-C	7.27	130.64	111.00
1	B	382	ASP	CB-CG-OD1	6.93	124.54	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	GLU	Peptide
2	C	80	CYS	Peptide
2	D	169	THR	Peptide
2	D	57	THR	Peptide

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	3119	0	3131	31	0
1	B	3119	0	3136	38	0
2	C	530	0	438	30	0
2	D	534	0	456	13	0
3	A	93	0	84	23	0
3	B	93	0	84	24	0
4	A	18	0	24	3	0
4	B	6	0	8	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	25	0	0	4	0
6	B	19	0	0	5	0
All	All	7560	0	7361	152	0

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

The worst 5 of 152 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)
3:B:501:CNC:C31	3:B:501:CNC:C30	1.79	1.59
3:A:501:CNC:C30	3:A:501:CNC:C31	1.78	1.53
3:B:501:CNC:C31	3:B:501:CNC:C3	1.84	1.52
1:A:78:CYS:SG	1:A:78:CYS:CB	2.02	1.46
3:A:501:CNC:C19	3:A:501:CNC:C1	1.77	1.43

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	396/409 (97%)	389 (98%)	7 (2%)	0	100	100
1	B	395/409 (97%)	385 (98%)	9 (2%)	1 (0%)	41	64
2	C	72/118 (61%)	65 (90%)	6 (8%)	1 (1%)	11	22
2	D	71/118 (60%)	63 (89%)	7 (10%)	1 (1%)	11	22
All	All	934/1054 (89%)	902 (97%)	29 (3%)	3 (0%)	41	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	81	SER
2	D	56	PRO
1	B	80	GLY

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	336/348 (97%)	335 (100%)	1 (0%)	92	98
1	B	337/348 (97%)	335 (99%)	2 (1%)	86	95
2	C	60/105 (57%)	57 (95%)	3 (5%)	24	47
2	D	62/105 (59%)	61 (98%)	1 (2%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	795/906 (88%)	788 (99%)	7 (1%)	78 91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	63	THR
2	C	70	LEU
2	D	141	LEU
2	C	80	CYS
1	B	382	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	209	GLN
2	D	170	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

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

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 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	#$|Z| > 2$
4	GOL	A	502	-	5,5,5	0.33	0	5,5,5	0.27	0
4	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.21	0
3	CNC	A	501	-	77,103,103	3.79	33 (42%)	100,171,171	3.70	31 (31%)
3	CNC	B	501	-	77,103,103	3.85	33 (42%)	100,171,171	3.67	32 (32%)
4	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	B	502	-	5,5,5	0.37	0	5,5,5	0.29	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
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
3	CNC	A	501	-	2/2/36/38	4/51/235/235	0/3/11/11
3	CNC	B	501	-	2/2/36/38	8/51/235/235	0/3/11/11
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	B	502	-	-	4/4/4/4	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CNC	C11-C10	12.76	1.62	1.40
3	B	501	CNC	C11-C10	12.41	1.61	1.40
3	B	501	CNC	C1-C19	10.82	1.78	1.55
3	B	501	CNC	C32-N33	10.54	1.67	1.32
3	A	501	CNC	C2R-C3R	-10.53	1.29	1.52

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	CNC	C25-C2-C26	-14.78	79.83	109.71
3	A	501	CNC	C25-C2-C26	-13.65	82.12	109.71
3	A	501	CNC	C26-C2-C1	-13.17	89.55	110.02
3	B	501	CNC	C26-C2-C1	-12.77	90.18	110.02
3	A	501	CNC	C1-C19-C18	-12.71	100.91	121.93

All (4) chirality outliers are listed below:

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

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CNC	C2P-O3-P-O2
4	A	502	GOL	C1-C2-C3-O3
4	A	503	GOL	O1-C1-C2-O2
4	A	503	GOL	O1-C1-C2-C3
4	A	504	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	GOL	1	0
4	A	503	GOL	1	0
3	A	501	CNC	23	0
3	B	501	CNC	24	0
4	A	504	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand CNC B 501

Bond lengths

Bond angles

Torsions

Rings
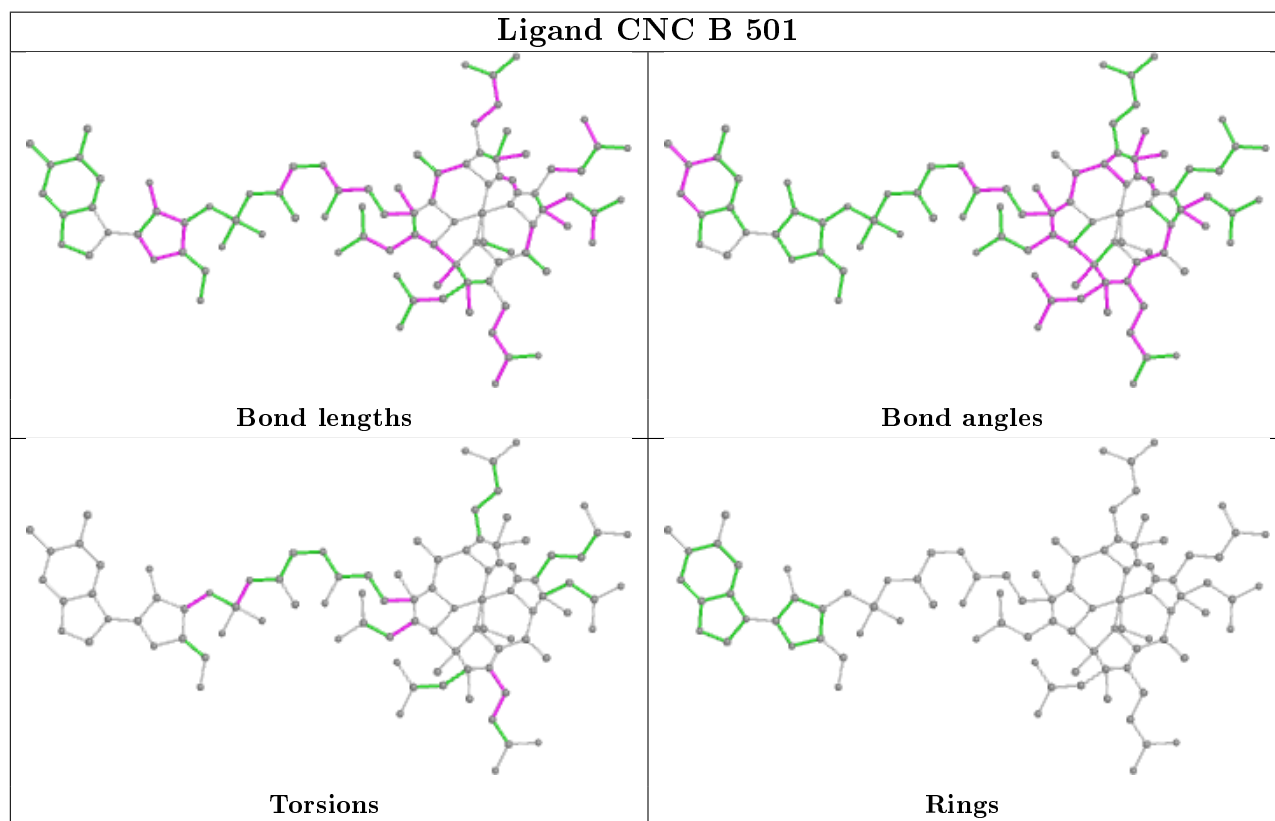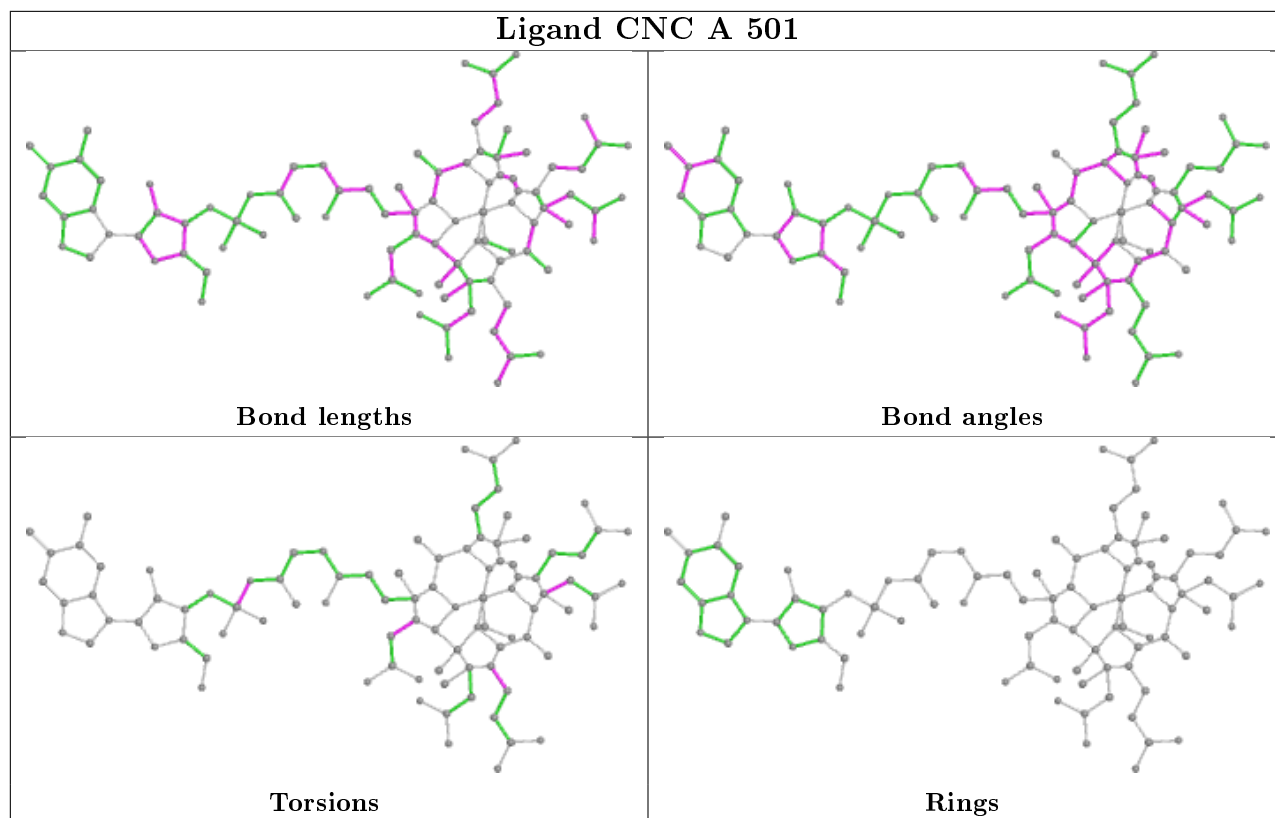
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	400/409 (97%)	-0.16	10 (2%)	57	51	41, 63, 96, 113	0
1	B	399/409 (97%)	-0.12	16 (4%)	38	31	41, 67, 102, 119	0
2	C	76/118 (64%)	1.40	23 (30%)	0	0	66, 119, 158, 166	0
2	D	75/118 (63%)	1.07	20 (26%)	0	0	59, 114, 140, 155	0
All	All	950/1054 (90%)	0.08	69 (7%)	15	11	41, 68, 128, 166	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	171	GLU	7.3
2	C	131	ALA	5.9
2	C	130	LEU	5.7
2	D	129	ARG	5.4
2	D	130	LEU	5.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	GOL	A	503	6/6	0.75	0.48	109,111,112,112	0
4	GOL	B	502	6/6	0.78	0.40	105,107,107,110	0
4	GOL	A	504	6/6	0.83	0.31	94,99,101,101	0
4	GOL	A	502	6/6	0.83	0.23	90,91,95,95	0
5	CA	D	202	1/1	0.88	0.05	110,110,110,110	0
5	CA	C	202	1/1	0.94	0.14	116,116,116,116	0
3	CNC	B	501	93/93	0.95	0.24	37,48,80,91	23
3	CNC	A	501	93/93	0.96	0.26	32,44,72,82	28
5	CA	D	201	1/1	0.99	0.08	53,53,53,53	0
5	CA	C	201	1/1	0.99	0.12	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.