



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2022 – 03:33 am GMT

PDB ID : 7QBE  
Title : TC:CD320 in complex with nanobody TC-Nb11  
Authors : Bloch, J.S.; Locher, K.P.  
Deposited on : 2021-11-19  
Resolution : 3.00 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

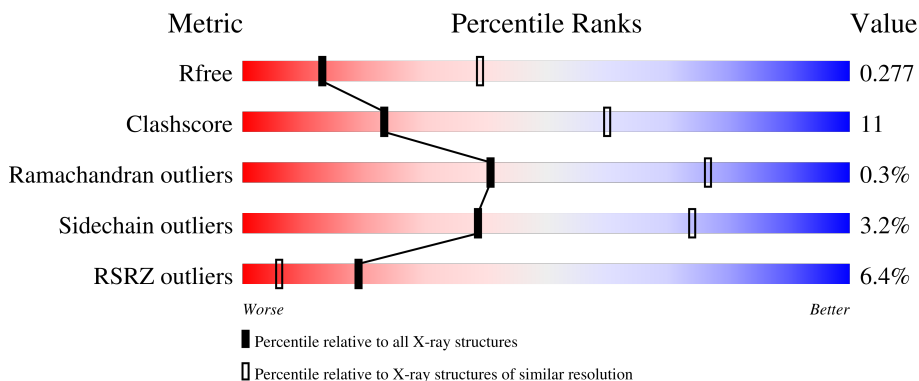
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



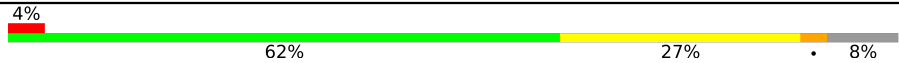
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	
1	C	409	
2	B	147	
2	D	147	
3	E	133	

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Mol	Chain	Length	Quality of chain
3	F	133	

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	C	501	X	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9439 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
			Total	C	N	O	S			
1	A	394	3064	1956	536	553	19	0	0	0
1	C	395	3069	1959	537	554	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
C	209	GLN	ARG	conflict	UNP P20062

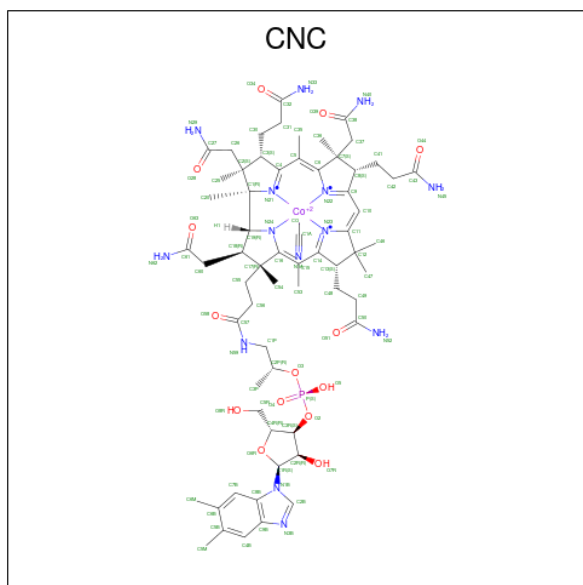
- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	80	596	353	104	127	12	0	0	0
2	D	86	642	381	113	135	13	0	0	0

- Molecule 3 is a protein called Anti-transcobalamin-2 nanobody TC-Nb11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	936	584	167	181	4	0	0	0
3	F	123	936	584	167	181	4	0	0	0

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



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

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

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

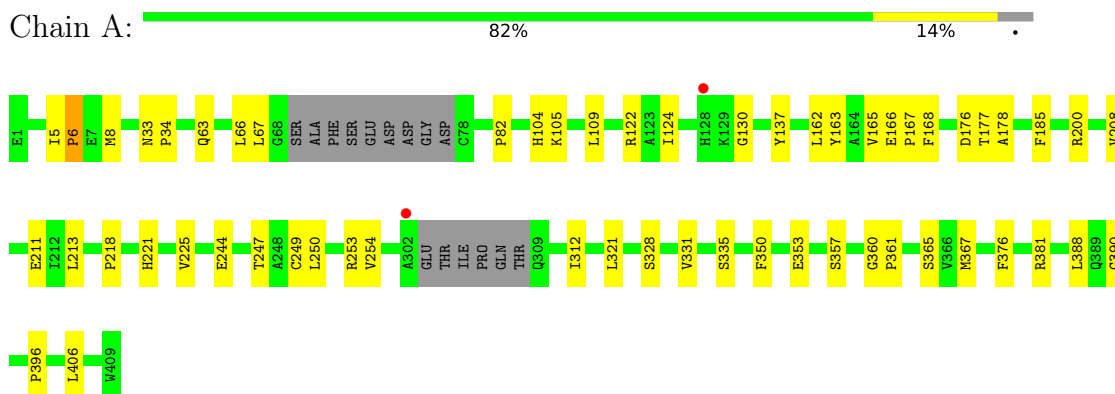
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	D	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		

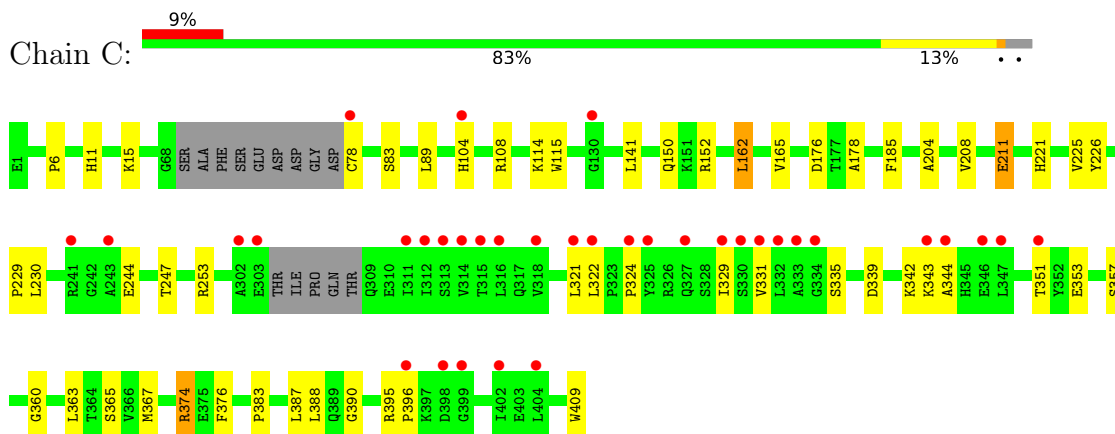
### 3 Residue-property plots [i](#)

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.

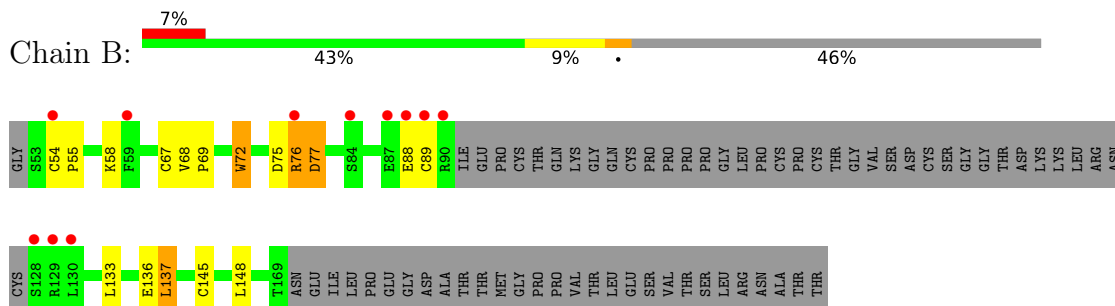
- Molecule 1: Transcobalamin-2



- Molecule 1: Transcobalamin-2



- Molecule 2: CD320 antigen





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.72Å 195.83Å 198.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 3.00 48.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.96-3.00) 99.9 (48.96-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.252 , 0.284 0.246 , 0.277	Depositor DCC
$R_{free}$ test set	2039 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.1	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.51	2/3130 (0.1%)	0.69	1/4240 (0.0%)
1	C	0.50	0/3135	0.69	0/4247
2	B	0.71	0/606	1.05	1/822 (0.1%)
2	D	0.61	0/653	0.89	0/886
3	E	0.75	0/955	1.00	1/1287 (0.1%)
3	F	0.71	2/955 (0.2%)	0.88	0/1287
All	All	0.58	4/9434 (0.0%)	0.79	3/12769 (0.0%)

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	C	0	1
2	B	0	2
3	E	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	115	CYS	CB-SG	-6.47	1.71	1.82
1	A	166	GLU	CG-CD	6.47	1.61	1.51
1	A	166	GLU	CD-OE2	5.67	1.31	1.25
3	F	76	SER	CA-CB	-5.23	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	PRO	N-CD-CG	-6.58	93.33	103.20
3	E	81	ASP	CB-CG-OD2	5.21	122.98	118.30
2	B	137	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	67	CYS	Mainchain
2	B	89	CYS	Peptide
1	C	162	LEU	Mainchain
3	E	100	LEU	Mainchain
3	E	37	GLY	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	3064	0	3078	52	0
1	C	3069	0	3080	53	0
2	B	596	0	528	11	0
2	D	642	0	572	15	0
3	E	936	0	906	44	3
3	F	936	0	906	32	0
4	A	93	0	83	14	0
4	C	93	0	81	21	0
5	B	2	0	0	0	0
5	D	2	0	0	1	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
All	All	9439	0	9234	210	3

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 11.

All (210) 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:E:100:LEU:CD2	3:E:102:MET:HE3	1.16	1.56
3:E:100:LEU:HD23	3:E:102:MET:CE	1.16	1.54
4:C:501:CNC:C49	4:C:501:CNC:C50	1.97	1.41
4:A:501:CNC:C50	4:A:501:CNC:C49	1.97	1.40
1:C:388:LEU:HD21	3:F:120:GLN:NE2	1.55	1.20
3:E:63:GLU:HG2	3:E:64:ARG:H	1.21	1.01
1:C:388:LEU:HD21	3:F:120:GLN:HE22	1.23	0.94
1:A:250:LEU:HB3	1:C:150:GLN:OE1	1.69	0.91
2:D:55:PRO:HD2	2:D:58:LYS:HD2	1.54	0.90
1:C:165:VAL:HG13	1:C:208:VAL:HG22	1.51	0.89
1:C:165:VAL:HG21	1:C:185:PHE:HE2	1.35	0.89
3:F:88:THR:HG23	3:F:101:GLN:HB3	1.55	0.88
1:A:211:GLU:HB3	3:E:123:TYR:CE1	2.10	0.86
3:E:110:THR:HG22	3:E:143:VAL:H	1.39	0.85
1:A:218:PRO:HG3	3:E:72:TRP:CD2	2.12	0.85
3:F:34:VAL:HG21	3:F:40:LEU:HD22	1.58	0.84
1:C:6:PRO:HD2	1:C:253:ARG:HD2	1.58	0.84
3:E:24:LEU:HD13	3:E:50:THR:HG22	1.59	0.84
3:E:100:LEU:CD2	3:E:102:MET:CE	2.02	0.83
3:F:34:VAL:CG2	3:F:40:LEU:HD22	2.09	0.83
1:C:104:HIS:ND1	1:C:108:ARG:NH1	2.27	0.82
3:E:63:GLU:HG2	3:E:64:ARG:N	1.96	0.80
1:A:122:ARG:NH2	2:B:136:GLU:OE2	2.17	0.77
1:C:221:HIS:CE1	1:C:225:VAL:HG23	2.19	0.77
1:C:388:LEU:CD2	3:F:120:GLN:HE22	1.97	0.77
1:C:357:SER:OG	1:C:360:GLY:O	2.03	0.76
2:D:58:LYS:HD3	2:D:67:CYS:CB	2.17	0.75
3:F:25:GLN:H	3:F:47:SER:HB3	1.53	0.74
4:C:501:CNC:C14	4:C:501:CNC:H2B	2.17	0.74
3:E:24:LEU:HD13	3:E:50:THR:CG2	2.19	0.73
2:D:92:GLU:HG3	2:D:95:THR:HG23	1.71	0.72
4:A:501:CNC:H2B	4:A:501:CNC:C14	2.19	0.72
1:C:165:VAL:HG21	1:C:185:PHE:CE2	2.24	0.71
3:F:24:LEU:CD1	3:F:48:GLY:H	2.05	0.70
3:F:30:GLY:HA3	3:F:42:LEU:HD22	1.75	0.69
1:C:388:LEU:CD2	3:F:120:GLN:NE2	2.46	0.68
3:E:33:LEU:HG	3:E:33:LEU:O	1.92	0.68
2:D:57:THR:O	2:D:70:LEU:HB2	1.93	0.68
2:D:75:ASP:OD1	5:D:201:CA:CA	1.71	0.68
3:E:64:ARG:HB3	3:E:129:ILE:HD11	1.76	0.68
1:A:218:PRO:HG3	3:E:72:TRP:CG	2.30	0.67
1:C:388:LEU:HD21	3:F:120:GLN:HE21	1.55	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:501:CNC:C2B	4:A:501:CNC:N23	2.59	0.66
4:C:501:CNC:H4B	4:C:501:CNC:C4	2.25	0.66
1:A:388:LEU:O	4:A:501:CNC:H311	1.97	0.65
1:C:329:ILE:CD1	1:C:344:ALA:HB2	2.27	0.63
1:C:165:VAL:CG1	1:C:208:VAL:HG22	2.26	0.63
3:E:72:TRP:CH2	3:E:93:ASN:HB3	2.33	0.63
1:A:357:SER:OG	1:A:360:GLY:O	2.12	0.63
1:C:329:ILE:HD11	1:C:344:ALA:HB2	1.80	0.63
4:C:501:CNC:H472	4:C:501:CNC:C15	2.29	0.63
3:E:24:LEU:CD1	3:E:50:THR:CG2	2.76	0.63
1:A:167:PRO:HB3	1:A:211:GLU:OE1	1.98	0.62
2:D:58:LYS:HD3	2:D:67:CYS:HB3	1.78	0.62
1:A:353:GLU:HB2	1:A:365:SER:HB3	1.81	0.62
3:E:29:SER:HB3	3:E:43:SER:OG	1.99	0.62
1:A:104:HIS:CE1	2:B:76:ARG:HB2	2.34	0.61
1:C:390:GLY:HA3	4:C:501:CNC:C5M	2.30	0.61
1:A:250:LEU:CB	1:C:150:GLN:OE1	2.45	0.61
2:B:68:VAL:CG1	2:B:69:PRO:HD2	2.30	0.61
3:E:24:LEU:HD21	3:E:46:ALA:HB1	1.82	0.60
1:C:104:HIS:CE1	1:C:108:ARG:HH12	2.19	0.60
1:A:218:PRO:HG3	3:E:72:TRP:CE2	2.36	0.60
1:A:312:ILE:HD11	1:A:331:VAL:HG23	1.84	0.60
1:C:390:GLY:HA3	4:C:501:CNC:HM51	1.83	0.60
4:C:501:CNC:N23	4:C:501:CNC:C2B	2.64	0.59
1:A:167:PRO:HB3	1:A:211:GLU:CD	2.23	0.58
1:A:221:HIS:NE2	1:A:225:VAL:HG22	2.18	0.58
1:A:350:PHE:HA	1:A:367:MET:SD	2.43	0.57
2:B:137:LEU:HD13	2:B:148:LEU:HA	1.86	0.57
1:A:165:VAL:HG11	1:A:208:VAL:HG23	1.86	0.57
3:E:100:LEU:CD2	3:E:102:MET:HE2	2.27	0.57
3:E:102:MET:HE1	3:E:113:TYR:CD2	2.40	0.57
1:C:351:THR:OG1	1:C:367:MET:HA	2.04	0.57
2:B:68:VAL:HG13	2:B:69:PRO:HD2	1.86	0.56
1:A:361:PRO:O	4:A:501:CNC:HM62	2.06	0.56
4:A:501:CNC:H561	4:A:501:CNC:H533	1.88	0.56
2:D:58:LYS:HB3	2:D:67:CYS:HB3	1.87	0.56
1:C:89:LEU:HG	1:C:141:LEU:HD21	1.88	0.56
1:C:244:GLU:OE1	1:C:247:THR:OG1	2.15	0.55
1:C:322:LEU:HD23	1:C:324:PRO:HD3	1.89	0.55
3:F:30:GLY:CA	3:F:42:LEU:HD22	2.36	0.55
1:A:5:ILE:HD11	1:A:249:CYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:40:LEU:HB2	3:F:105:LEU:HD11	1.88	0.55
1:A:165:VAL:CG1	1:A:208:VAL:HG23	2.37	0.54
2:B:55:PRO:HG2	2:B:58:LYS:HB2	1.89	0.54
3:F:34:VAL:HG23	3:F:40:LEU:HD22	1.89	0.54
4:C:501:CNC:H353	4:C:501:CNC:H362	1.90	0.54
4:A:501:CNC:H531	4:A:501:CNC:H543	1.90	0.54
1:A:165:VAL:HG13	1:A:208:VAL:HG22	1.88	0.54
1:A:312:ILE:CG1	1:A:331:VAL:HG23	2.38	0.53
1:C:11:HIS:O	1:C:15:LYS:HG3	2.07	0.53
1:C:390:GLY:CA	4:C:501:CNC:HM52	2.38	0.53
3:E:129:ILE:HG23	3:E:135:TRP:CZ2	2.43	0.53
3:E:24:LEU:CD1	3:E:50:THR:HG22	2.34	0.53
1:C:353:GLU:HB2	1:C:365:SER:HB3	1.90	0.53
4:C:501:CNC:N23	4:C:501:CNC:N3B	2.57	0.53
2:D:163:ASP:OD1	2:D:164:GLU:HG2	2.08	0.53
1:A:165:VAL:HG13	1:A:208:VAL:CG2	2.38	0.53
3:E:100:LEU:HD21	3:E:102:MET:CE	2.27	0.52
3:F:95:LYS:O	3:F:97:THR:HG23	2.10	0.52
1:C:331:VAL:HG12	1:C:343:LYS:HG3	1.91	0.52
1:A:244:GLU:OE1	1:A:247:THR:OG1	2.15	0.51
4:C:501:CNC:H2B	4:C:501:CNC:N23	2.25	0.51
1:A:67:LEU:HD13	1:A:105:LYS:HD3	1.93	0.51
1:A:165:VAL:CG1	1:A:208:VAL:CG2	2.88	0.51
3:E:44:CYS:HB3	3:E:98:LEU:CD1	2.41	0.51
1:C:162:LEU:HD23	1:C:185:PHE:CZ	2.47	0.50
1:C:165:VAL:CG1	1:C:208:VAL:CG2	2.89	0.50
1:A:162:LEU:HD23	1:A:185:PHE:CZ	2.47	0.49
1:A:376:PHE:CG	4:A:501:CNC:H462	2.46	0.49
3:E:79:TYR:CE1	3:E:87:PHE:HB2	2.46	0.49
3:E:100:LEU:CG	3:E:102:MET:HE3	2.23	0.49
2:B:75:ASP:C	2:B:77:ASP:H	2.15	0.49
3:E:44:CYS:HB3	3:E:98:LEU:HD12	1.94	0.49
3:F:24:LEU:HD12	3:F:47:SER:CB	2.42	0.49
3:F:59:GLY:O	3:F:65:GLU:OE1	2.30	0.49
1:C:115:TRP:CH2	2:D:147:PRO:HD3	2.47	0.49
3:E:63:GLU:CG	3:E:64:ARG:N	2.67	0.49
1:A:124:ILE:HA	1:A:130:GLY:O	2.13	0.49
2:D:160:ASP:CG	2:D:162:SER:HB3	2.33	0.49
4:C:501:CNC:N3B	4:C:501:CNC:N21	2.61	0.49
1:C:390:GLY:CA	4:C:501:CNC:C5M	2.92	0.48
3:F:42:LEU:HG	3:F:102:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:HIS:CD2	1:A:225:VAL:HG22	2.48	0.48
1:C:226:TYR:O	1:C:229:PRO:HD2	2.13	0.48
1:A:312:ILE:CD1	1:A:331:VAL:HG23	2.43	0.48
3:F:31:GLY:O	3:F:40:LEU:HD21	2.13	0.48
1:A:5:ILE:HG23	1:A:253:ARG:HG3	1.95	0.47
4:A:501:CNC:H353	4:A:501:CNC:H362	1.96	0.47
1:A:254:VAL:HG21	1:C:150:GLN:NE2	2.30	0.47
3:E:129:ILE:HG22	3:E:130:LYS:H	1.79	0.47
3:F:24:LEU:HD12	3:F:47:SER:OG	2.14	0.47
1:A:312:ILE:HG13	1:A:331:VAL:HG23	1.97	0.47
2:D:62:ARG:HG3	2:D:62:ARG:HH11	1.79	0.47
3:E:88:THR:HG22	3:E:88:THR:O	2.14	0.47
1:A:168:PHE:HA	3:E:125:ALA:CB	2.45	0.47
3:E:100:LEU:HG	3:E:102:MET:HG3	1.97	0.46
3:E:34:VAL:HB	3:E:40:LEU:HD11	1.96	0.46
3:E:102:MET:HE2	3:E:113:TYR:CE2	2.51	0.46
1:A:390:GLY:HA3	4:A:501:CNC:HM51	1.98	0.46
1:C:178:ALA:HB1	1:C:208:VAL:HG13	1.98	0.46
1:C:374:ARG:HD2	1:C:374:ARG:HA	1.58	0.46
1:C:376:PHE:CG	4:C:501:CNC:H462	2.51	0.46
3:F:110:THR:HG23	3:F:142:THR:HA	1.98	0.46
1:C:114:LYS:HB3	2:D:150:TRP:CZ2	2.51	0.45
1:A:137:TYR:HA	1:A:177:THR:HG23	1.97	0.45
1:C:211:GLU:HB3	3:F:123:TYR:CE1	2.52	0.45
4:C:501:CNC:H362	4:C:501:CNC:C35	2.47	0.45
3:E:40:LEU:HD13	3:E:141:VAL:HG13	1.99	0.45
3:F:42:LEU:HG	3:F:102:MET:HE2	1.99	0.45
1:A:178:ALA:CB	3:E:123:TYR:CE1	3.00	0.45
3:E:63:GLU:CG	3:E:64:ARG:H	2.02	0.45
3:F:92:ASP:OD1	3:F:94:ALA:HB3	2.17	0.45
2:D:58:LYS:HD3	2:D:67:CYS:HB2	1.97	0.44
4:A:501:CNC:C50	4:A:501:CNC:C48	2.83	0.44
1:A:335:SER:O	1:A:396:PRO:HD2	2.17	0.44
1:C:335:SER:O	1:C:396:PRO:HD2	2.18	0.44
3:E:102:MET:CE	3:E:113:TYR:CE2	3.01	0.44
1:C:329:ILE:HG21	1:C:343:LYS:HB2	1.99	0.44
1:A:6:PRO:HG2	1:C:152:ARG:HH22	1.82	0.44
3:F:83:VAL:HB	3:F:87:PHE:CG	2.53	0.44
3:F:72:TRP:CZ3	3:F:93:ASN:HB3	2.52	0.44
1:A:312:ILE:HG13	1:A:331:VAL:CG2	2.48	0.43
4:A:501:CNC:H362	4:A:501:CNC:C35	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ALA:O	1:C:208:VAL:HG23	2.18	0.43
1:C:363:LEU:H	4:C:501:CNC:H452	1.67	0.43
2:D:62:ARG:HG3	2:D:62:ARG:NH1	2.32	0.43
1:A:5:ILE:CD1	1:A:249:CYS:HB3	2.49	0.43
3:F:87:PHE:CD1	3:F:87:PHE:N	2.87	0.43
1:C:339:ASP:HA	1:C:342:LYS:HD2	2.01	0.43
3:F:28:GLU:HB2	3:F:139:THR:HG23	2.01	0.43
1:A:33:ASN:HA	1:A:34:PRO:HD2	1.93	0.43
3:E:129:ILE:C	3:E:131:ASP:H	2.23	0.43
1:A:104:HIS:H	2:B:77:ASP:CG	2.22	0.42
2:B:137:LEU:O	2:B:145:CYS:HA	2.19	0.42
2:D:55:PRO:CD	2:D:58:LYS:HD2	2.36	0.42
3:F:28:GLU:CB	3:F:139:THR:HG23	2.49	0.42
2:B:133:LEU:N	2:B:133:LEU:HD12	2.34	0.42
1:C:162:LEU:HD23	1:C:185:PHE:CE1	2.55	0.42
3:E:40:LEU:CD1	3:E:141:VAL:HG13	2.49	0.42
1:C:360:GLY:C	4:C:501:CNC:HM61	2.40	0.42
3:E:24:LEU:HD11	3:E:50:THR:HG23	2.02	0.42
2:B:72:TRP:HA	2:B:75:ASP:CG	2.40	0.42
1:A:162:LEU:HD23	1:A:185:PHE:CE1	2.55	0.42
4:A:501:CNC:H541	4:A:501:CNC:H602	2.00	0.42
3:E:24:LEU:HD11	3:E:50:THR:CG2	2.50	0.42
1:A:167:PRO:HB3	1:A:211:GLU:OE2	2.19	0.42
3:E:86:ARG:HB3	3:E:103:ASN:O	2.20	0.42
4:A:501:CNC:H2B	4:A:501:CNC:N23	2.28	0.42
1:A:406:LEU:HD12	1:A:406:LEU:HA	1.89	0.41
4:C:501:CNC:H363	4:C:501:CNC:H411	1.72	0.41
1:A:66:LEU:HG	1:A:82:PRO:HG2	2.01	0.41
1:C:395:ARG:HA	1:C:396:PRO:HD2	1.88	0.41
3:E:71:LYS:HD2	3:E:78:TYR:HE1	1.85	0.41
1:C:376:PHE:HE1	1:C:409:TRP:HB3	1.85	0.41
4:C:501:CNC:H422	4:C:501:CNC:H361	2.03	0.41
3:F:90:SER:O	3:F:98:LEU:HD12	2.21	0.41
1:A:163:TYR:CE1	1:A:200:ARG:NH2	2.88	0.41
3:F:38:GLY:H	3:F:105:LEU:H	1.68	0.41
1:A:63:GLN:HG2	1:A:109:LEU:HD11	2.03	0.41
1:C:321:LEU:HG	1:C:322:LEU:N	2.36	0.41
1:C:387:LEU:HD23	1:C:387:LEU:HA	1.84	0.41
4:C:501:CNC:H541	4:C:501:CNC:H602	1.86	0.40
1:C:329:ILE:HG22	1:C:331:VAL:HG13	2.03	0.40
1:A:312:ILE:HD11	1:A:331:VAL:CG2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:501:CNC:H461	4:C:501:CNC:H491	1.91	0.40
3:F:70:HIS:HA	3:F:76:SER:O	2.21	0.40
1:A:167:PRO:CB	1:A:211:GLU:OE1	2.68	0.40
1:C:230:LEU:HD12	1:C:230:LEU:HA	1.92	0.40

All (3) 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)
3:E:61:GLY:O	3:E:61:GLY:O[3_554]	1.58	0.62
3:E:61:GLY:O	3:E:62:LYS:CA[3_554]	1.73	0.47
3:E:61:GLY:C	3:E:61:GLY:O[3_554]	2.11	0.09

## 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	388/409 (95%)	384 (99%)	4 (1%)	0	100	100
1	C	389/409 (95%)	384 (99%)	4 (1%)	1 (0%)	41	76
2	B	76/147 (52%)	69 (91%)	6 (8%)	1 (1%)	12	45
2	D	82/147 (56%)	77 (94%)	5 (6%)	0	100	100
3	E	121/133 (91%)	107 (88%)	13 (11%)	1 (1%)	19	57
3	F	121/133 (91%)	113 (93%)	8 (7%)	0	100	100
All	All	1177/1378 (85%)	1134 (96%)	40 (3%)	3 (0%)	41	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	72	TRP
3	E	129	ILE

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Mol	Chain	Res	Type
1	C	383	PRO

### 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	328/348 (94%)	322 (98%)	6 (2%)	59	85
1	C	328/348 (94%)	323 (98%)	5 (2%)	65	87
2	B	71/129 (55%)	67 (94%)	4 (6%)	21	56
2	D	76/129 (59%)	73 (96%)	3 (4%)	32	69
3	E	98/107 (92%)	92 (94%)	6 (6%)	18	53
3	F	98/107 (92%)	90 (92%)	8 (8%)	11	39
All	All	999/1168 (86%)	967 (97%)	32 (3%)	39	74

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	176	ASP
1	A	213	LEU
1	A	321	LEU
1	A	328	SER
1	A	381	ARG
2	B	54	CYS
2	B	76	ARG
2	B	77	ASP
2	B	88	GLU
1	C	78	CYS
1	C	83	SER
1	C	176	ASP
1	C	211	GLU
1	C	374	ARG
2	D	92	GLU
2	D	95	THR

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Mol	Chain	Res	Type
2	D	146	ILE
3	E	34	VAL
3	E	76	SER
3	E	86	ARG
3	E	87	PHE
3	E	98	LEU
3	E	121	ILE
3	F	25	GLN
3	F	35	GLN
3	F	39	SER
3	F	40	LEU
3	F	43	SER
3	F	47	SER
3	F	49	ARG
3	F	58	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	128	HIS
2	B	60	GLN
3	F	35	GLN
3	F	58	GLN
3	F	96	ASN
3	F	120	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 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	-	90,103,103	7.86	53 (58%)	139,171,171	4.55	72 (51%)
4	CNC	C	501	-	90,103,103	7.93	56 (62%)	139,171,171	4.41	58 (41%)

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	4/52/235/235	0/3/11/11
4	CNC	C	501	-	2/2/36/38	5/52/235/235	0/3/11/11

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	CNC	C48-C13	-62.33	0.09	1.54
4	A	501	CNC	C48-C13	-62.10	0.10	1.54
4	A	501	CNC	C2R-C1R	-15.13	1.30	1.53
4	C	501	CNC	C2R-C1R	-12.00	1.35	1.53
4	A	501	CNC	C49-C50	11.84	1.97	1.51
4	C	501	CNC	C56-C57	11.70	1.73	1.51
4	C	501	CNC	C49-C50	11.64	1.97	1.51
4	A	501	CNC	C56-C57	10.63	1.71	1.51
4	C	501	CNC	C50-N52	10.20	1.66	1.32
4	A	501	CNC	C50-N52	9.68	1.64	1.32
4	C	501	CNC	O6R-C1R	9.46	1.54	1.41
4	A	501	CNC	O6R-C1R	9.42	1.54	1.41
4	C	501	CNC	C19-N24	-8.86	1.30	1.49
4	A	501	CNC	C19-N24	-8.58	1.31	1.49
4	A	501	CNC	C10-C9	8.49	1.63	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	CNC	C3R-C4R	-7.97	1.31	1.52
4	C	501	CNC	C10-C9	7.86	1.61	1.39
4	A	501	CNC	C10-C11	7.80	1.60	1.37
4	A	501	CNC	C3-C4	-7.73	1.32	1.51
4	A	501	CNC	C1-C2	-7.67	1.40	1.58
4	C	501	CNC	C3R-C4R	-7.67	1.32	1.52
4	C	501	CNC	C1-C2	-7.43	1.41	1.58
4	C	501	CNC	C10-C11	7.04	1.58	1.37
4	C	501	CNC	C3-C4	-6.97	1.34	1.51
4	C	501	CNC	C35-C5	-6.54	1.36	1.50
4	A	501	CNC	C41-C42	6.28	1.72	1.52
4	C	501	CNC	C41-C42	6.25	1.72	1.52
4	C	501	CNC	C26-C2	6.15	1.70	1.55
4	A	501	CNC	C26-C2	6.13	1.70	1.55
4	C	501	CNC	C1-C19	6.06	1.71	1.54
4	A	501	CNC	C1-C19	6.06	1.71	1.54
4	C	501	CNC	C53-C15	5.89	1.63	1.50
4	A	501	CNC	C7-C6	5.72	1.68	1.54
4	C	501	CNC	C5M-C5B	5.71	1.62	1.51
4	C	501	CNC	O6R-C4R	5.55	1.57	1.45
4	C	501	CNC	C6-C5	5.51	1.51	1.36
4	C	501	CNC	P-O2	5.48	1.74	1.60
4	A	501	CNC	C35-C5	-5.44	1.39	1.50
4	C	501	CNC	C13-C14	5.38	1.65	1.51
4	C	501	CNC	C7-C6	5.34	1.67	1.54
4	C	501	CNC	C12-C11	5.22	1.68	1.51
4	C	501	CNC	C60-C18	-5.21	1.42	1.54
4	C	501	CNC	C4-C5	5.10	1.64	1.43
4	A	501	CNC	C53-C15	5.04	1.61	1.50
4	A	501	CNC	C4-C5	4.89	1.63	1.43
4	A	501	CNC	C6-C5	4.85	1.50	1.36
4	C	501	CNC	C2R-C3R	4.76	1.63	1.52
4	A	501	CNC	C12-C11	4.67	1.66	1.51
4	C	501	CNC	C43-N45	4.53	1.47	1.32
4	A	501	CNC	C13-C14	4.44	1.63	1.51
4	A	501	CNC	C48-C49	-4.30	1.39	1.52
4	C	501	CNC	C8-C9	4.28	1.60	1.51
4	A	501	CNC	C60-C18	-4.26	1.44	1.54
4	C	501	CNC	C36-C7	-4.26	1.47	1.54
4	A	501	CNC	C17-C18	4.24	1.62	1.54
4	A	501	CNC	C5M-C5B	4.16	1.59	1.51
4	C	501	CNC	C48-C49	-4.09	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	CNC	C36-C7	-4.08	1.47	1.54
4	C	501	CNC	C6M-C6B	4.03	1.59	1.51
4	A	501	CNC	C41-C8	-3.96	1.45	1.54
4	C	501	CNC	C32-N33	3.86	1.45	1.32
4	A	501	CNC	O6R-C4R	3.80	1.53	1.45
4	C	501	CNC	C14-C15	3.78	1.58	1.43
4	A	501	CNC	C14-C15	3.76	1.58	1.43
4	C	501	CNC	C7B-C6B	3.67	1.47	1.37
4	A	501	CNC	C2R-C3R	3.57	1.60	1.52
4	C	501	CNC	C16-C15	3.57	1.58	1.42
4	A	501	CNC	C43-N45	3.54	1.44	1.32
4	A	501	CNC	C6M-C6B	3.49	1.58	1.51
4	A	501	CNC	C46-C12	3.48	1.61	1.54
4	C	501	CNC	O34-C32	-3.45	1.13	1.24
4	C	501	CNC	C42-C43	3.41	1.64	1.51
4	A	501	CNC	C55-C17	-3.38	1.46	1.54
4	C	501	CNC	C14-N23	3.34	1.40	1.30
4	C	501	CNC	C4B-C9B	3.31	1.47	1.41
4	C	501	CNC	C17-C18	3.26	1.61	1.54
4	C	501	CNC	C46-C12	3.26	1.61	1.54
4	A	501	CNC	C16-C15	3.23	1.57	1.42
4	A	501	CNC	C42-C43	3.19	1.63	1.51
4	C	501	CNC	O39-C38	-3.10	1.14	1.24
4	A	501	CNC	C32-N33	3.08	1.42	1.32
4	C	501	CNC	C41-C8	-3.08	1.47	1.54
4	A	501	CNC	C7B-C6B	3.06	1.45	1.37
4	A	501	CNC	P-O2	2.98	1.68	1.60
4	A	501	CNC	C12-C13	2.98	1.64	1.55
4	A	501	CNC	C14-N23	2.97	1.39	1.30
4	C	501	CNC	C12-C13	2.93	1.64	1.55
4	A	501	CNC	C7-C8	-2.91	1.47	1.55
4	A	501	CNC	C8-C9	2.90	1.57	1.51
4	A	501	CNC	O34-C32	-2.83	1.15	1.24
4	C	501	CNC	C7-C8	-2.81	1.47	1.55
4	C	501	CNC	C57-N59	2.68	1.39	1.33
4	C	501	CNC	C55-C17	-2.66	1.48	1.54
4	C	501	CNC	O44-C43	2.59	1.31	1.24
4	A	501	CNC	C30-C31	-2.58	1.44	1.52
4	C	501	CNC	C47-C12	-2.54	1.48	1.54
4	C	501	CNC	C37-C38	-2.46	1.43	1.51
4	A	501	CNC	O39-C38	-2.45	1.16	1.24
4	A	501	CNC	C4B-C9B	2.44	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	501	CNC	C2-C3	2.43	1.64	1.57
4	A	501	CNC	C20-C1	2.41	1.58	1.53
4	A	501	CNC	O44-C43	2.30	1.30	1.24
4	C	501	CNC	C60-C61	-2.28	1.45	1.51
4	A	501	CNC	C60-C61	-2.26	1.45	1.51
4	A	501	CNC	C47-C12	-2.24	1.49	1.54
4	A	501	CNC	C9B-N3B	-2.23	1.31	1.38
4	C	501	CNC	C30-C3	2.15	1.59	1.54
4	C	501	CNC	C20-C1	2.08	1.57	1.53
4	C	501	CNC	C30-C31	-2.01	1.46	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C3-C4-C5	-20.42	89.41	123.81
4	C	501	CNC	C3-C4-C5	-19.92	90.26	123.81
4	C	501	CNC	C12-C11-C10	-17.34	107.71	123.54
4	A	501	CNC	C6-C5-C4	-16.34	92.29	121.54
4	A	501	CNC	C8-C9-C10	-13.13	94.97	123.32
4	C	501	CNC	C8-C9-C10	-12.24	96.90	123.32
4	C	501	CNC	C12-C13-C14	-12.03	85.95	101.86
4	A	501	CNC	C26-C2-C3	-11.95	86.28	107.41
4	A	501	CNC	C18-C19-N24	11.28	119.78	101.88
4	C	501	CNC	C25-C2-C26	-11.24	86.99	109.71
4	A	501	CNC	C9-C10-C11	-10.95	109.72	125.88
4	A	501	CNC	C12-C13-C14	-10.87	87.49	101.86
4	C	501	CNC	C1-C19-C18	-10.44	106.37	121.81
4	C	501	CNC	C25-C2-C1	9.95	128.79	113.78
4	A	501	CNC	C25-C2-C26	-9.83	89.83	109.71
4	C	501	CNC	C18-C19-N24	9.81	117.46	101.88
4	A	501	CNC	C30-C3-C2	-9.77	98.42	119.09
4	A	501	CNC	C12-C11-C10	-9.42	114.94	123.54
4	A	501	CNC	C12-C11-N23	-9.30	101.42	111.48
4	C	501	CNC	C6-C5-C4	-9.11	105.23	121.54
4	C	501	CNC	C9-C10-C11	-9.10	112.44	125.88
4	A	501	CNC	C54-C17-C55	-8.95	94.49	109.25
4	C	501	CNC	C13-C14-C15	-8.76	109.06	123.81
4	C	501	CNC	C12-C11-N23	-8.69	102.08	111.48
4	C	501	CNC	C26-C2-C1	-8.36	96.99	110.01
4	A	501	CNC	C25-C2-C1	8.28	126.27	113.78
4	C	501	CNC	C26-C2-C3	-8.11	93.06	107.41
4	A	501	CNC	C13-C14-C15	-7.78	110.71	123.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	CNC	C47-C12-C46	-7.46	96.74	109.35
4	C	501	CNC	C16-C15-C14	-7.27	111.33	121.30
4	A	501	CNC	C1-C19-C18	-7.20	111.16	121.81
4	C	501	CNC	C7-C8-C9	-7.15	91.75	100.90
4	A	501	CNC	C26-C2-C1	-6.38	100.06	110.01
4	C	501	CNC	C41-C8-C9	6.10	121.94	111.19
4	A	501	CNC	C35-C5-C6	-5.95	112.95	122.43
4	A	501	CNC	C16-C15-C14	-5.82	113.33	121.30
4	A	501	CNC	C36-C7-C37	-5.68	101.44	110.80
4	C	501	CNC	C35-C5-C4	5.65	128.32	116.79
4	C	501	CNC	C47-C12-C46	-5.63	99.83	109.35
4	C	501	CNC	C30-C3-C2	-5.59	107.25	119.09
4	A	501	CNC	C25-C2-C3	5.57	127.20	112.96
4	C	501	CNC	C54-C17-C55	-5.47	100.22	109.25
4	C	501	CNC	C35-C5-C6	-5.38	113.86	122.43
4	C	501	CNC	C25-C2-C3	5.28	126.46	112.96
4	A	501	CNC	C19-N24-C16	-5.27	103.44	111.96
4	C	501	CNC	C13-C14-N23	5.20	120.56	109.39
4	A	501	CNC	C13-C14-N23	5.13	120.42	109.39
4	A	501	CNC	C55-C17-C16	5.13	127.27	116.24
4	C	501	CNC	O3-C2P-C1P	5.06	117.02	106.92
4	A	501	CNC	C56-C57-N59	4.88	124.63	116.42
4	C	501	CNC	C15-C14-N23	-4.86	117.04	126.68
4	C	501	CNC	C5-C4-N21	-4.82	116.37	124.19
4	A	501	CNC	O28-C27-N29	-4.74	109.56	122.50
4	A	501	CNC	C7-C8-C9	-4.68	94.92	100.90
4	A	501	CNC	C41-C8-C9	4.65	119.40	111.19
4	C	501	CNC	C19-N24-C16	-4.44	104.78	111.96
4	C	501	CNC	C3R-C2R-C1R	4.27	109.35	99.89
4	A	501	CNC	C17-C18-C19	-4.12	97.70	102.66
4	C	501	CNC	C53-C15-C14	4.08	125.11	116.79
4	A	501	CNC	C42-C41-C8	-4.06	103.01	114.73
4	C	501	CNC	C2-C1-N21	4.05	107.41	101.77
4	C	501	CNC	C48-C13-C12	-3.97	105.50	116.63
4	A	501	CNC	C7-C6-C5	-3.87	121.99	128.07
4	C	501	CNC	C17-C18-C19	-3.81	98.07	102.66
4	A	501	CNC	C6M-C6B-C5B	3.81	128.54	120.74
4	C	501	CNC	C56-C57-N59	3.76	122.75	116.42
4	A	501	CNC	C3R-C2R-C1R	3.75	108.20	99.89
4	A	501	CNC	C1-N21-C4	-3.75	103.45	109.37
4	A	501	CNC	C19-C1-N21	-3.74	96.91	101.67
4	A	501	CNC	C3P-C2P-C1P	-3.70	104.21	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	CNC	C17-C16-C15	-3.68	121.13	126.73
4	A	501	CNC	C26-C27-N29	3.67	128.17	116.52
4	A	501	CNC	C56-C55-C17	-3.66	108.46	115.52
4	A	501	CNC	C5M-C5B-C4B	-3.65	111.61	120.34
4	A	501	CNC	C3-C4-N21	3.61	116.50	111.97
4	A	501	CNC	C1-C2-C3	3.60	106.20	101.60
4	C	501	CNC	O7R-C2R-C3R	-3.60	100.95	111.17
4	A	501	CNC	C55-C56-C57	-3.57	103.44	111.23
4	A	501	CNC	O58-C57-N59	-3.56	116.29	123.01
4	A	501	CNC	C2-C26-C27	3.55	125.22	115.22
4	C	501	CNC	O28-C27-N29	-3.47	113.02	122.50
4	C	501	CNC	C19-C1-N21	-3.42	97.33	101.67
4	A	501	CNC	C54-C17-C18	3.38	117.98	112.98
4	C	501	CNC	C55-C17-C16	3.30	123.34	116.24
4	A	501	CNC	O8R-C5R-C4R	-3.23	100.22	111.29
4	A	501	CNC	C53-C15-C16	-3.22	113.44	120.37
4	A	501	CNC	C6M-C6B-C7B	-3.15	112.81	120.34
4	C	501	CNC	O63-C61-N62	-3.07	114.12	122.50
4	A	501	CNC	C37-C7-C6	3.04	116.69	107.12
4	C	501	CNC	C3-C4-N21	3.04	115.78	111.97
4	C	501	CNC	O6R-C1R-C2R	-2.98	102.58	106.93
4	C	501	CNC	C2-C26-C27	2.94	123.48	115.22
4	A	501	CNC	O44-C43-N45	-2.92	114.52	122.50
4	A	501	CNC	C2-C1-N21	2.89	105.80	101.77
4	C	501	CNC	C1-N21-C4	-2.84	104.88	109.37
4	A	501	CNC	C5M-C5B-C6B	2.83	126.54	120.74
4	A	501	CNC	C30-C31-C32	-2.81	103.05	112.59
4	C	501	CNC	C5M-C5B-C6B	2.76	126.39	120.74
4	A	501	CNC	C35-C5-C4	2.69	122.28	116.79
4	A	501	CNC	C5-C6-N22	-2.69	119.77	123.88
4	A	501	CNC	O3-C2P-C1P	2.68	112.26	106.92
4	C	501	CNC	C5M-C5B-C4B	-2.65	114.00	120.34
4	A	501	CNC	C20-C1-C19	2.65	115.55	110.23
4	A	501	CNC	O7R-C2R-C3R	-2.64	103.67	111.17
4	C	501	CNC	C20-C1-C19	2.62	115.48	110.23
4	C	501	CNC	C18-C17-C16	2.62	104.53	100.33
4	A	501	CNC	C60-C18-C19	2.61	120.31	114.09
4	C	501	CNC	C20-C1-C2	-2.61	108.93	113.28
4	A	501	CNC	C15-C14-N23	-2.58	121.56	126.68
4	A	501	CNC	C13-C12-C11	2.56	104.39	100.90
4	C	501	CNC	C20-C1-N21	-2.55	106.08	110.27
4	A	501	CNC	O6R-C1R-C2R	-2.54	103.22	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	CNC	C18-C60-C61	2.44	120.07	113.97
4	C	501	CNC	O58-C57-N59	-2.44	118.40	123.01
4	C	501	CNC	C8-C9-N22	2.44	115.63	110.77
4	C	501	CNC	O63-C61-C60	2.42	125.96	120.87
4	A	501	CNC	C17-C16-C15	-2.42	123.05	126.73
4	A	501	CNC	C10-C11-N23	2.35	128.78	124.93
4	A	501	CNC	C8-C9-N22	2.30	115.35	110.77
4	C	501	CNC	C2P-C1P-N59	2.25	116.26	112.93
4	A	501	CNC	C18-C17-C16	2.19	103.84	100.33
4	C	501	CNC	C1-C2-C3	2.18	104.38	101.60
4	A	501	CNC	O51-C50-N52	-2.18	116.56	122.50
4	C	501	CNC	C42-C41-C8	-2.14	108.56	114.73
4	A	501	CNC	C48-C13-C14	-2.11	104.72	109.63
4	A	501	CNC	O63-C61-C60	2.10	125.29	120.87
4	C	501	CNC	C10-C9-N22	-2.09	123.33	125.73
4	A	501	CNC	C48-C13-C12	-2.08	110.81	116.63
4	A	501	CNC	C20-C1-C2	-2.03	109.89	113.28
4	A	501	CNC	O44-C43-C42	2.00	126.95	121.07

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	501	CNC	N24
4	A	501	CNC	C13
4	C	501	CNC	N24
4	C	501	CNC	C13

All (9) torsion outliers are listed below:

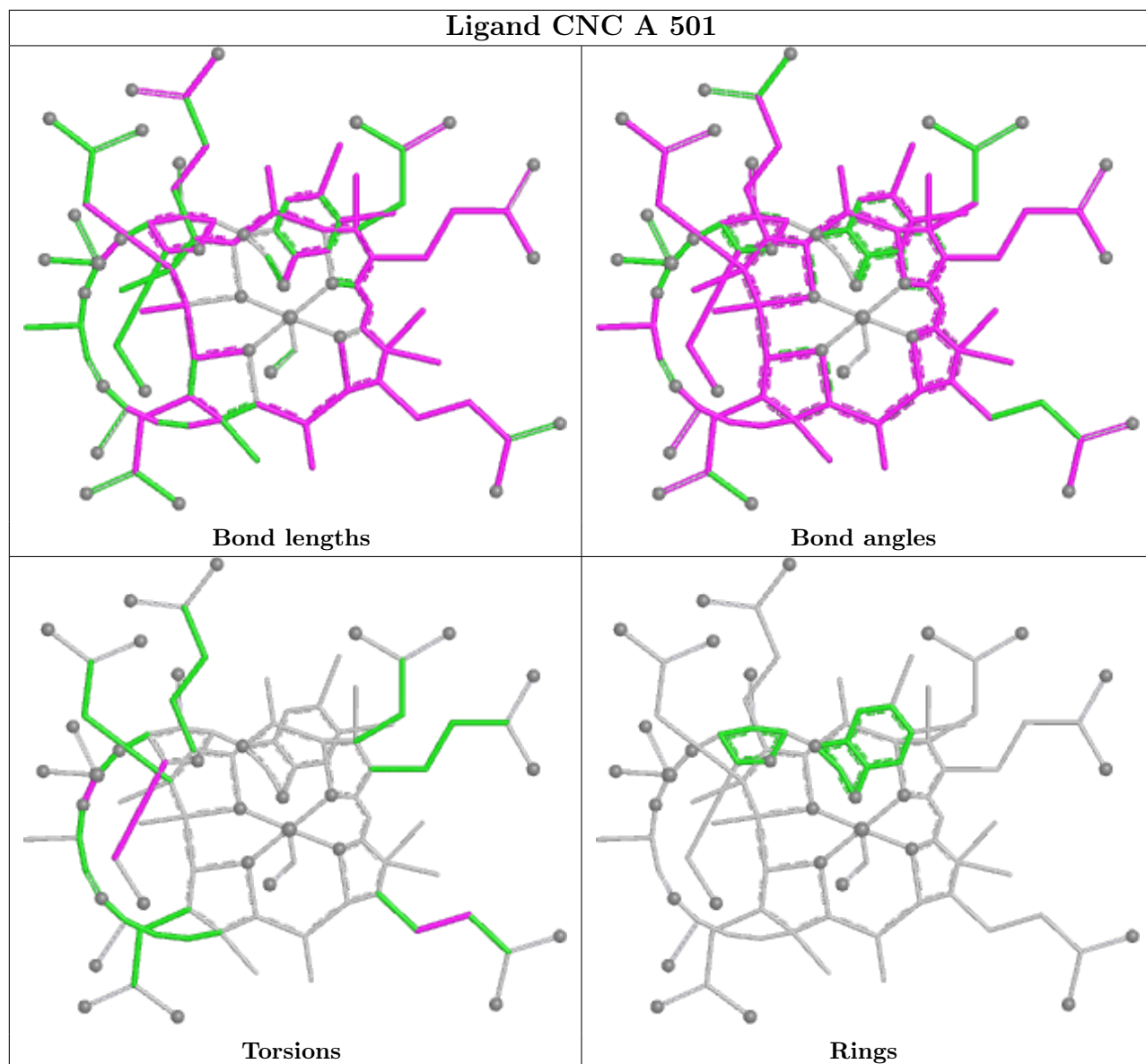
Mol	Chain	Res	Type	Atoms
4	C	501	CNC	C2P-O3-P-O2
4	A	501	CNC	O6R-C4R-C5R-O8R
4	C	501	CNC	O6R-C4R-C5R-O8R
4	A	501	CNC	C3R-C4R-C5R-O8R
4	C	501	CNC	C3R-C4R-C5R-O8R
4	A	501	CNC	C13-C48-C49-C50
4	C	501	CNC	C13-C48-C49-C50
4	A	501	CNC	C2P-O3-P-O2
4	C	501	CNC	C19-C18-C60-C61

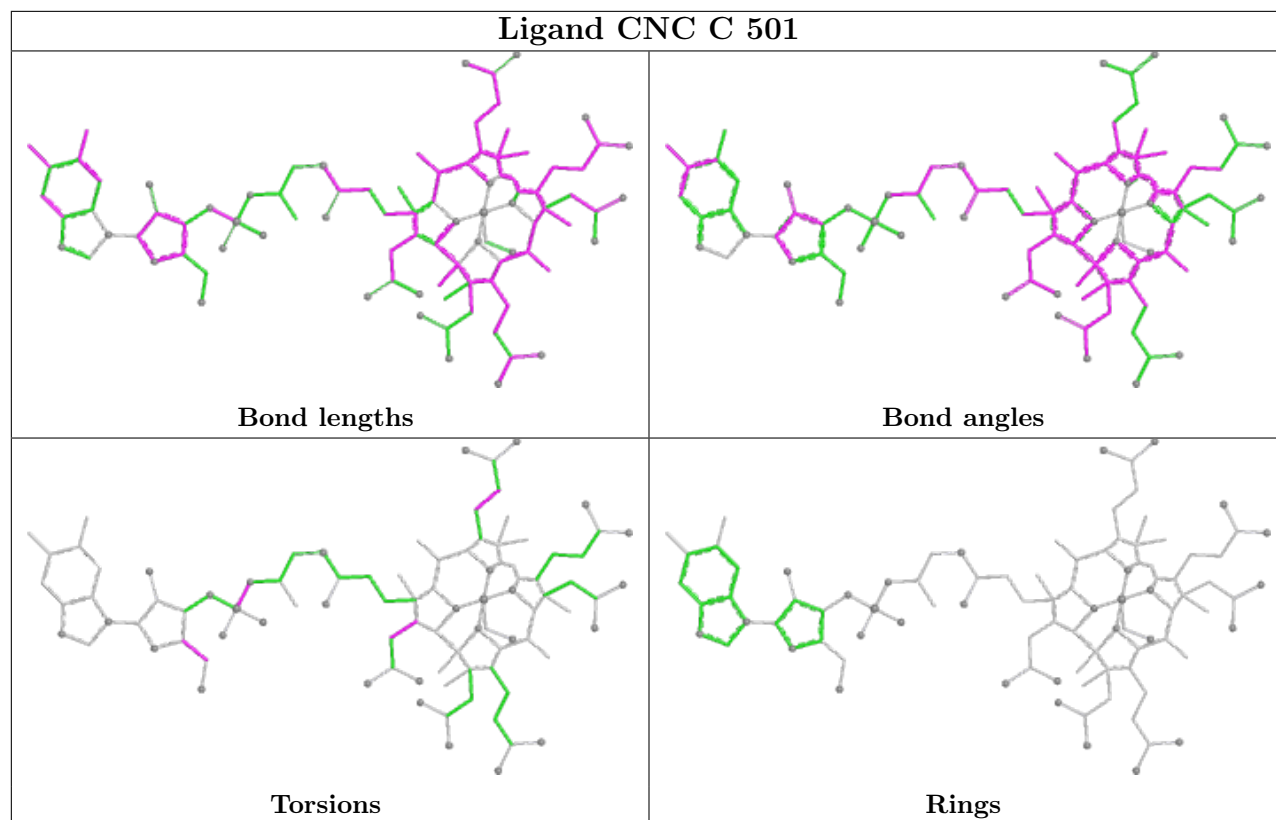
There are no ring outliers.

2 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	CNC	14	0
4	C	501	CNC	21	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	394/409 (96%)	0.18	2 (0%) 91 75	36, 55, 83, 110	0
1	C	395/409 (96%)	0.56	35 (8%) 9 3	43, 73, 103, 120	0
2	B	80/147 (54%)	0.76	11 (13%) 2 1	42, 87, 126, 138	0
2	D	86/147 (58%)	0.86	14 (16%) 1 0	57, 89, 117, 137	0
3	E	123/133 (92%)	0.53	10 (8%) 12 3	47, 67, 110, 127	0
3	F	123/133 (92%)	0.26	5 (4%) 37 14	49, 66, 90, 125	0
All	All	1201/1378 (87%)	0.44	77 (6%) 19 6	36, 66, 104, 138	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	ALA	7.0
2	D	128	SER	6.8
2	B	128	SER	6.6
3	F	59	GLY	6.0
3	F	60	PRO	5.3
2	B	129	ARG	5.2
1	C	322	LEU	4.4
2	B	88	GLU	4.2
3	F	61	GLY	4.1
2	B	89	CYS	4.1
2	D	129	ARG	4.0
2	B	87	GLU	3.9
1	C	312	ILE	3.8
2	D	168	GLY	3.8
3	E	35	GLN	3.6
2	B	130	LEU	3.6
3	E	146	HIS	3.5
1	C	330	SER	3.4
1	A	302	ALA	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	347	LEU	3.4
3	E	144	SER	3.3
1	C	303	GLU	3.2
3	E	145	SER	3.2
2	D	90	ARG	3.2
1	C	324	PRO	3.1
1	C	316	LEU	3.1
2	D	130	LEU	3.1
2	D	143	ASP	3.0
1	C	313	SER	3.0
1	C	314	VAL	3.0
1	C	327	GLN	3.0
2	B	90	ARG	2.9
3	F	39	SER	2.9
2	D	141	LEU	2.9
1	C	331	VAL	2.9
1	C	318	VAL	2.9
2	D	139	CYS	2.8
3	F	62	LYS	2.8
1	C	329	ILE	2.7
1	C	332	LEU	2.7
1	C	404	LEU	2.7
1	C	346	GLU	2.7
3	E	40	LEU	2.7
1	C	399	GLY	2.7
1	C	104	HIS	2.7
1	C	243	ALA	2.6
1	C	130	GLY	2.6
2	D	58	LYS	2.6
1	C	311	ILE	2.6
1	C	325	TYR	2.5
3	E	59	GLY	2.5
1	C	315	THR	2.5
2	D	133	LEU	2.4
2	B	59	PHE	2.4
1	C	402	ILE	2.3
2	D	57	THR	2.3
2	D	92	GLU	2.3
1	C	321	LEU	2.3
1	C	398	ASP	2.3
1	C	78	CYS	2.3
2	D	56	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	241	ARG	2.2
2	B	54	CYS	2.2
1	C	334	GLY	2.2
3	E	102	MET	2.2
1	A	128	HIS	2.2
1	C	333	ALA	2.1
2	D	95	THR	2.1
1	C	343	LYS	2.1
2	B	84	SER	2.1
1	C	344	ALA	2.1
3	E	107	SER	2.1
3	E	109	ASP	2.1
1	C	396	PRO	2.0
1	C	351	THR	2.0
3	E	65	GLU	2.0
2	B	76	ARG	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](#)

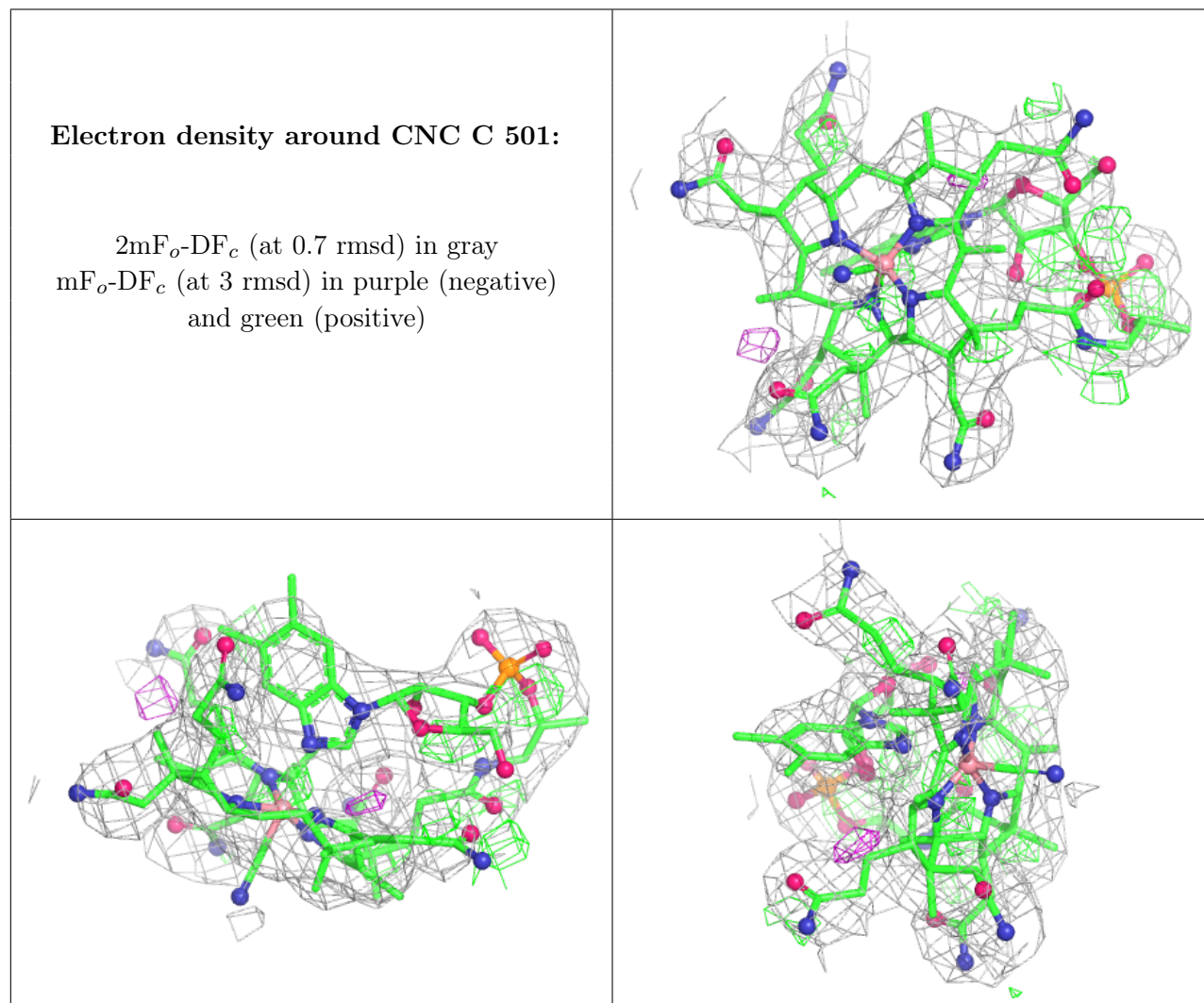
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

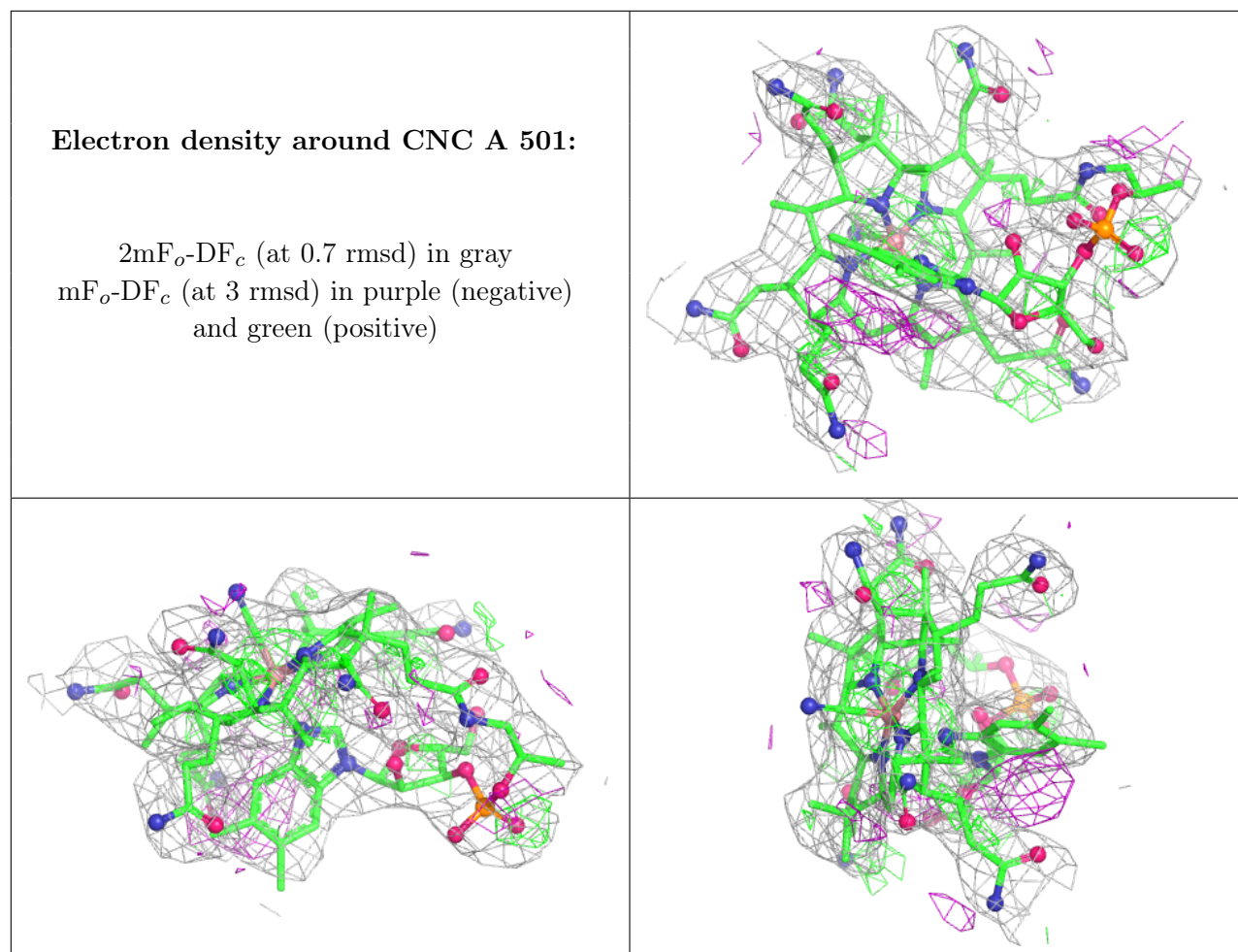
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	CA	D	202	1/1	0.72	0.10	67,67,67,67	0
5	CA	B	202	1/1	0.87	0.05	91,91,91,91	0
4	CNC	C	501	93/93	0.91	0.28	61,74,92,107	4
4	CNC	A	501	93/93	0.93	0.27	31,48,65,96	4
5	CA	D	201	1/1	0.95	0.07	66,66,66,66	0
5	CA	B	201	1/1	0.97	0.15	46,46,46,46	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.