



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2021 – 05:22 pm BST

PDB ID : 6ZTI  
Title : Phospholipase PlaB from Legionella pneumophila in complex with thio-NAD  
Authors : Diwo, M.G.; Flieger, A.; Blankenfeldt, W.  
Deposited on : 2020-07-20  
Resolution : 1.81 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

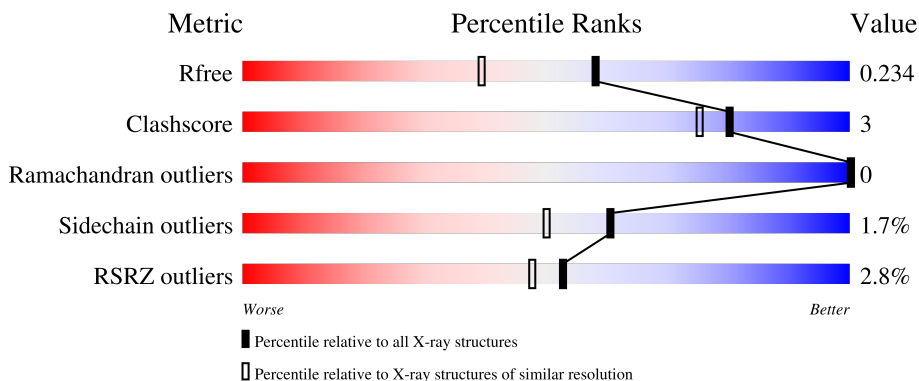
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	489	 3% 88% 7% 5%
1	B	489	 2% 87% 8% 5%
1	C	489	 2% 89% 6% 5%
1	D	489	 4% 90% 6% 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32173 atoms, of which 15156 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 PlaB phospholipase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	465	7464	2369	3729	656	692	18	0	5	0
1	B	466	7507	2384	3751	662	692	18	0	9	0
1	C	464	7437	2360	3718	655	686	18	0	5	0
1	D	466	7444	2365	3715	652	694	18	0	4	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP A0A378K488
A	-13	ALA	-	expression tag	UNP A0A378K488
A	-12	SER	-	expression tag	UNP A0A378K488
A	-11	TRP	-	expression tag	UNP A0A378K488
A	-10	SER	-	expression tag	UNP A0A378K488
A	-9	HIS	-	expression tag	UNP A0A378K488
A	-8	PRO	-	expression tag	UNP A0A378K488
A	-7	GLN	-	expression tag	UNP A0A378K488
A	-6	PHE	-	expression tag	UNP A0A378K488
A	-5	GLU	-	expression tag	UNP A0A378K488
A	-4	LYS	-	expression tag	UNP A0A378K488
A	-3	GLY	-	expression tag	UNP A0A378K488
A	-2	ALA	-	expression tag	UNP A0A378K488
A	-1	GLY	-	expression tag	UNP A0A378K488
A	0	THR	-	expression tag	UNP A0A378K488
A	203	ASN	ASP	conflict	UNP A0A378K488
B	-14	MET	-	initiating methionine	UNP A0A378K488
B	-13	ALA	-	expression tag	UNP A0A378K488
B	-12	SER	-	expression tag	UNP A0A378K488
B	-11	TRP	-	expression tag	UNP A0A378K488
B	-10	SER	-	expression tag	UNP A0A378K488

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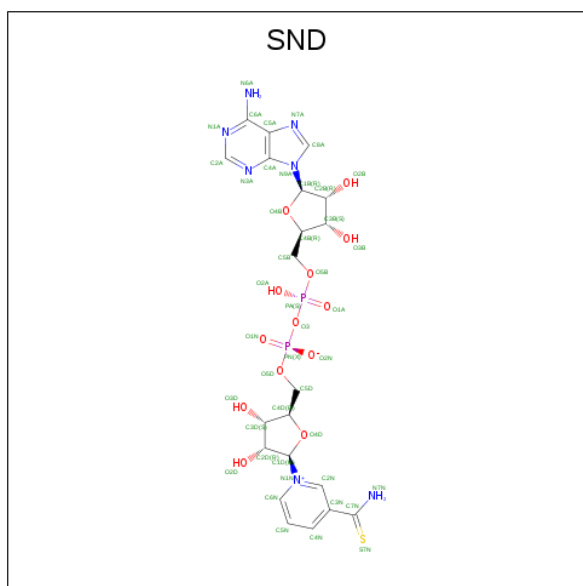
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A378K488
B	-8	PRO	-	expression tag	UNP A0A378K488
B	-7	GLN	-	expression tag	UNP A0A378K488
B	-6	PHE	-	expression tag	UNP A0A378K488
B	-5	GLU	-	expression tag	UNP A0A378K488
B	-4	LYS	-	expression tag	UNP A0A378K488
B	-3	GLY	-	expression tag	UNP A0A378K488
B	-2	ALA	-	expression tag	UNP A0A378K488
B	-1	GLY	-	expression tag	UNP A0A378K488
B	0	THR	-	expression tag	UNP A0A378K488
B	203	ASN	ASP	conflict	UNP A0A378K488
C	-14	MET	-	initiating methionine	UNP A0A378K488
C	-13	ALA	-	expression tag	UNP A0A378K488
C	-12	SER	-	expression tag	UNP A0A378K488
C	-11	TRP	-	expression tag	UNP A0A378K488
C	-10	SER	-	expression tag	UNP A0A378K488
C	-9	HIS	-	expression tag	UNP A0A378K488
C	-8	PRO	-	expression tag	UNP A0A378K488
C	-7	GLN	-	expression tag	UNP A0A378K488
C	-6	PHE	-	expression tag	UNP A0A378K488
C	-5	GLU	-	expression tag	UNP A0A378K488
C	-4	LYS	-	expression tag	UNP A0A378K488
C	-3	GLY	-	expression tag	UNP A0A378K488
C	-2	ALA	-	expression tag	UNP A0A378K488
C	-1	GLY	-	expression tag	UNP A0A378K488
C	0	THR	-	expression tag	UNP A0A378K488
C	203	ASN	ASP	conflict	UNP A0A378K488
D	-14	MET	-	initiating methionine	UNP A0A378K488
D	-13	ALA	-	expression tag	UNP A0A378K488
D	-12	SER	-	expression tag	UNP A0A378K488
D	-11	TRP	-	expression tag	UNP A0A378K488
D	-10	SER	-	expression tag	UNP A0A378K488
D	-9	HIS	-	expression tag	UNP A0A378K488
D	-8	PRO	-	expression tag	UNP A0A378K488
D	-7	GLN	-	expression tag	UNP A0A378K488
D	-6	PHE	-	expression tag	UNP A0A378K488
D	-5	GLU	-	expression tag	UNP A0A378K488
D	-4	LYS	-	expression tag	UNP A0A378K488
D	-3	GLY	-	expression tag	UNP A0A378K488
D	-2	ALA	-	expression tag	UNP A0A378K488
D	-1	GLY	-	expression tag	UNP A0A378K488
D	0	THR	-	expression tag	UNP A0A378K488

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Chain	Residue	Modelled	Actual	Comment	Reference
D	203	ASN	ASP	conflict	UNP A0A378K488

- Molecule 2 is THIONICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: SND) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>13</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
2	A	1	Total	C	H	N	O	P	S	0	0
			70	21	26	7	13	2	1		
2	A	1	Total	C	H	N	O	P	S	0	0
			70	21	26	7	13	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			70	21	26	7	13	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			71	21	27	7	13	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			70	21	26	7	13	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			71	21	27	7	13	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			70	21	26	7	13	2	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			71	21	27	7	13	2	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	14	3	8	3	0	0
3	B	1	14	3	8	3	0	0
3	C	1	14	3	8	3	0	0
3	D	1	14	3	8	3	0	0

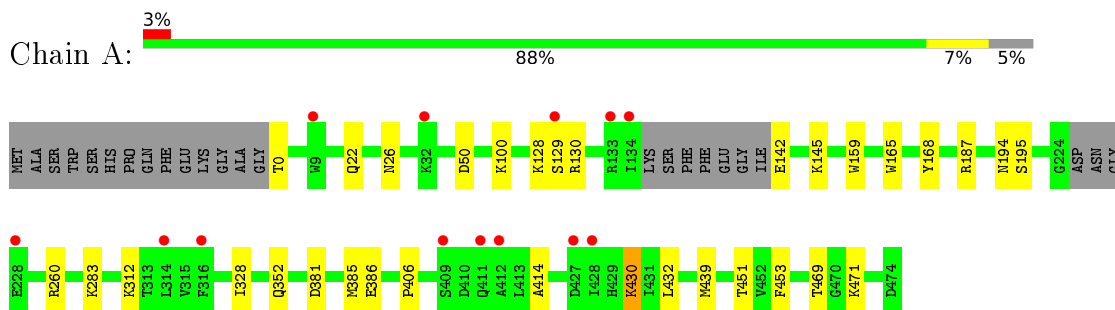
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	450	450	450	0	0
4	B	402	402	402	0	0
4	C	416	416	416	0	0
4	D	434	434	434	0	0

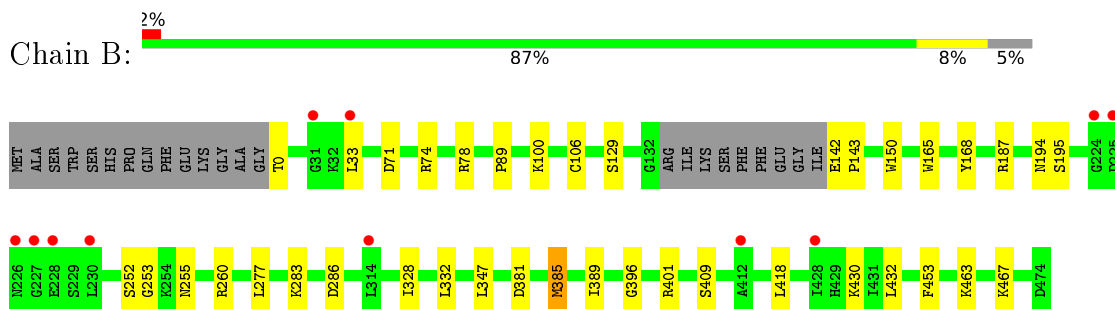
### 3 Residue-property plots [i](#)

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.

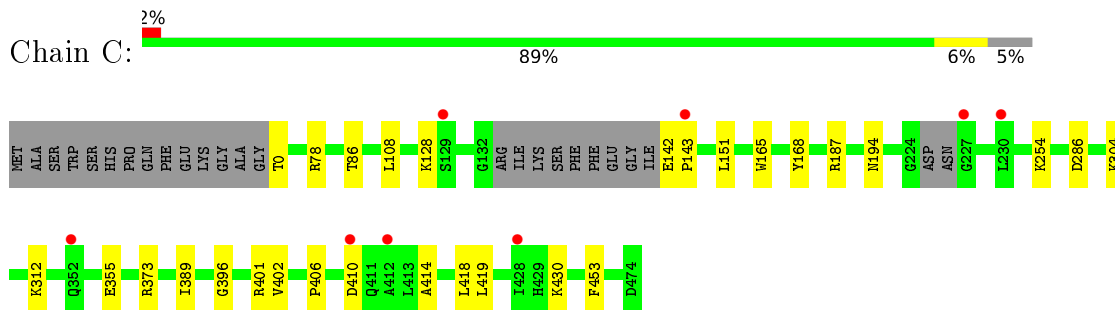
- Molecule 1: PlaB phospholipase



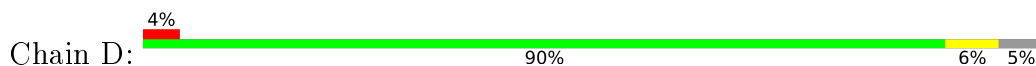
- Molecule 1: PlaB phospholipase

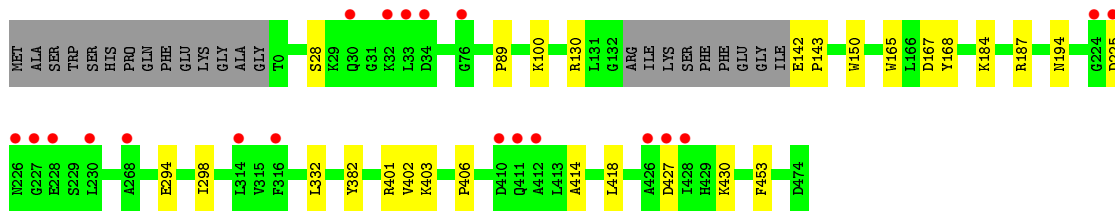


- Molecule 1: PlaB phospholipase



- Molecule 1: PlaB phospholipase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.83Å 90.72Å 92.79Å 78.44° 90.26° 75.41°	Depositor
Resolution (Å)	46.91 – 1.81 46.91 – 1.81	Depositor EDS
% Data completeness (in resolution range)	75.9 (46.91-1.81) 75.9 (46.91-1.81)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.81Å)	Xtrriage
Refinement program	PHENIX dev_3922	Depositor
R, $R_{free}$	0.186 , 0.234 0.186 , 0.234	Depositor DCC
$R_{free}$ test set	8002 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32173	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.24% 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: GOL, SND

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	0.38	0/3826	0.54	0/5171
1	B	0.36	0/3860	0.54	0/5217
1	C	0.37	0/3810	0.53	0/5148
1	D	0.37	0/3818	0.53	0/5164
All	All	0.37	0/15314	0.53	0/20700

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	3735	3729	3734	20	0
1	B	3756	3751	3768	22	0
1	C	3719	3718	3723	20	0
1	D	3729	3715	3719	16	0
2	A	88	52	52	7	0
2	B	132	79	78	6	0
2	C	88	53	52	6	0
2	D	44	27	26	2	0
3	A	6	8	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	8	8	3	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
4	A	450	0	0	6	0
4	B	402	0	0	5	1
4	C	416	0	0	6	0
4	D	434	0	0	6	1
All	All	17017	15156	15184	82	1

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 (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386[A]:GLU:OE1	4:A:601:HOH:O	1.98	0.80
1:C:142:GLU:OE1	4:C:601:HOH:O	1.98	0.80
1:A:26:ASN:OD1	4:A:602:HOH:O	2.04	0.76
1:C:286:ASP:OD1	4:C:602:HOH:O	2.04	0.76
1:C:254:LYS:NZ	4:C:604:HOH:O	2.19	0.76
1:D:427:ASP:OD1	4:D:601:HOH:O	2.04	0.73
1:D:167:ASP:OD2	4:D:602:HOH:O	2.08	0.72
1:C:86:THR:HG22	1:C:151:LEU:HD21	1.72	0.71
1:D:403[A]:LYS:NZ	4:D:606:HOH:O	2.24	0.70
1:A:430:LYS:NZ	4:A:605:HOH:O	2.25	0.69
1:A:100:LYS:O	4:A:603:HOH:O	2.11	0.68
1:D:28:SER:O	4:D:603:HOH:O	2.11	0.68
1:B:71[B]:ASP:OD1	1:B:74:ARG:NH2	2.33	0.61
1:D:100:LYS:O	4:D:604:HOH:O	2.16	0.61
1:B:142:GLU:HB3	1:B:143:PRO:HD3	1.83	0.60
1:C:128:LYS:NZ	1:C:143:PRO:O	2.35	0.57
1:A:130:ARG:HD3	4:A:700:HOH:O	2.09	0.52
2:B:503:SND:S7N	1:D:187:ARG:NH1	2.76	0.52
1:A:194:ASN:C	2:A:501:SND:S7N	2.89	0.51
1:C:312:LYS:NZ	4:C:615:HOH:O	2.35	0.50
2:B:501:SND:H2N	2:B:501:SND:O5D	2.12	0.50
1:B:78[A]:ARG:NH1	1:B:106:CYS:O	2.42	0.49
1:B:165:TRP:HA	1:B:168:TYR:CD1	2.47	0.49
1:D:406:PRO:HG2	1:D:414:ALA:O	2.13	0.49
1:C:194:ASN:C	2:C:501:SND:S7N	2.91	0.49
1:D:130:ARG:HD3	4:D:861:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:TYR:OH	1:D:430:LYS:NZ	2.46	0.48
1:A:195:SER:N	2:A:501:SND:S7N	2.87	0.48
1:B:194:ASN:C	2:B:501:SND:S7N	2.92	0.47
1:B:187:ARG:NH1	2:B:502:SND:S7N	2.81	0.46
1:C:128:LYS:NZ	4:C:616:HOH:O	2.37	0.46
1:B:401:ARG:CZ	1:B:418:LEU:HD11	2.46	0.46
2:D:501:SND:O5D	2:D:501:SND:H2N	2.15	0.46
1:D:142:GLU:HB3	1:D:143:PRO:HD3	1.97	0.46
1:D:165:TRP:HA	1:D:168:TYR:CD1	2.51	0.46
1:C:187:ARG:NH1	2:C:502:SND:S7N	2.73	0.46
1:C:389:ILE:HG22	1:C:396:GLY:HA2	1.96	0.46
1:A:194:ASN:CA	2:A:501:SND:S7N	3.05	0.45
1:A:328:ILE:HD11	1:A:432:LEU:HD21	1.98	0.45
1:A:381:ASP:O	1:A:385:MET:HG3	2.16	0.45
2:A:501:SND:H2N	2:A:501:SND:O5D	2.16	0.45
1:B:195:SER:N	2:B:501:SND:S7N	2.90	0.45
1:C:165:TRP:HA	1:C:168:TYR:CD1	2.52	0.45
2:C:501:SND:O5D	2:C:501:SND:H2N	2.17	0.45
1:B:33:LEU:HD21	1:B:277:LEU:HD12	1.99	0.44
1:B:255[B]:ASN:OD1	4:B:603:HOH:O	2.21	0.44
1:B:286:ASP:OD2	4:B:602:HOH:O	2.21	0.44
1:C:355:GLU:OE2	4:C:605:HOH:O	2.21	0.44
1:B:194:ASN:CA	2:B:501:SND:S7N	3.06	0.44
1:C:406:PRO:HG2	1:C:414:ALA:O	2.18	0.44
1:B:253:GLY:H	3:B:504:GOL:H31	1.83	0.43
1:C:401:ARG:CZ	1:C:418:LEU:HD11	2.48	0.43
1:A:165:TRP:HA	1:A:168:TYR:CD1	2.54	0.43
1:B:430:LYS:NZ	4:B:634:HOH:O	2.50	0.43
1:C:402[B]:VAL:CG2	1:C:419:LEU:HB3	2.48	0.43
1:A:145:LYS:NZ	4:A:636:HOH:O	2.51	0.43
1:D:89:PRO:HB3	1:D:150:TRP:CH2	2.54	0.43
1:A:260:ARG:HE	3:A:503:GOL:H11	1.84	0.43
1:D:194:ASN:C	2:D:501:SND:S7N	2.97	0.43
1:B:328:ILE:HD11	1:B:432:LEU:HD21	2.01	0.42
1:B:252:SER:HB3	3:B:504:GOL:H31	2.00	0.42
1:A:159:TRP:CH2	1:A:439:MET:HB3	2.54	0.42
1:B:100:LYS:O	4:B:604:HOH:O	2.21	0.42
1:B:89:PRO:HB3	1:B:150:TRP:CH2	2.54	0.42
1:C:78:ARG:NH2	1:C:108:LEU:O	2.51	0.42
1:D:332:LEU:HD11	1:D:402:VAL:HG11	2.02	0.42
1:C:187:ARG:CG	2:C:502:SND:S7N	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:GLU:HB3	1:C:143:PRO:HD3	2.01	0.42
1:A:50:ASP:OD2	1:A:128:LYS:NZ	2.46	0.42
1:A:406:PRO:HG2	1:A:414:ALA:O	2.20	0.41
1:A:187:ARG:NH1	2:A:502:SND:S7N	2.80	0.41
1:B:381:ASP:O	1:B:385:MET:HG3	2.20	0.41
1:B:389:ILE:HG22	1:B:396:GLY:HA2	2.02	0.41
1:D:401:ARG:CZ	1:D:418:LEU:HD11	2.50	0.41
1:A:187:ARG:HD3	2:A:502:SND:S7N	2.60	0.41
1:A:194:ASN:HA	2:A:501:SND:S7N	2.61	0.41
1:C:194:ASN:CA	2:C:501:SND:S7N	3.09	0.41
1:D:294:GLU:O	1:D:298:ILE:HG12	2.20	0.41
1:B:260:ARG:HE	3:B:504:GOL:H11	1.86	0.41
1:B:409:SER:O	4:B:605:HOH:O	2.22	0.41
1:C:187:ARG:HD3	2:C:502:SND:S7N	2.61	0.41
1:A:451:THR:OG1	1:A:469:THR:HG23	2.20	0.40

All (1) 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)
4:B:904:HOH:O	4:D:807:HOH:O 1_655	2.14	0.06

## 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	464/489 (95%)	449 (97%)	15 (3%)	0	100 100
1	B	471/489 (96%)	454 (96%)	17 (4%)	0	100 100
1	C	463/489 (95%)	451 (97%)	12 (3%)	0	100 100
1	D	466/489 (95%)	452 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1864/1956 (95%)	1806 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	408/422 (97%)	397 (97%)	11 (3%)	44	30
1	B	410/422 (97%)	400 (98%)	10 (2%)	49	35
1	C	405/422 (96%)	399 (98%)	6 (2%)	65	55
1	D	407/422 (96%)	404 (99%)	3 (1%)	84	80
All	All	1630/1688 (97%)	1600 (98%)	30 (2%)	60	48

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	THR
1	A	22	GLN
1	A	129	SER
1	A	142	GLU
1	A	283	LYS
1	A	312[A]	LYS
1	A	312[B]	LYS
1	A	352	GLN
1	A	430	LYS
1	A	453	PHE
1	A	471	LYS
1	B	0	THR
1	B	129	SER
1	B	283[A]	LYS
1	B	283[B]	LYS
1	B	332	LEU
1	B	347	LEU

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Mol	Chain	Res	Type
1	B	385	MET
1	B	453	PHE
1	B	463	LYS
1	B	467	LYS
1	C	0	THR
1	C	304	LYS
1	C	373	ARG
1	C	410	ASP
1	C	430	LYS
1	C	453	PHE
1	D	184	LYS
1	D	225	ASP
1	D	453	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	D	221	HIS

### 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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	502	-	5,5,5	1.13	0	5,5,5	0.70	0
2	SND	B	503	-	42,48,48	0.58	0	49,73,73	0.63	1 (2%)
3	GOL	A	503	-	5,5,5	1.12	0	5,5,5	1.06	0
2	SND	A	501	-	42,48,48	0.56	0	49,73,73	0.68	2 (4%)
2	SND	C	501	-	42,48,48	0.61	0	49,73,73	0.67	1 (2%)
3	GOL	C	503	-	5,5,5	0.86	0	5,5,5	0.71	0
2	SND	A	502	-	42,48,48	0.57	0	49,73,73	0.62	1 (2%)
2	SND	D	501	-	42,48,48	0.56	0	49,73,73	0.63	1 (2%)
2	SND	C	502	-	42,48,48	0.56	0	49,73,73	0.67	1 (2%)
2	SND	B	502	-	42,48,48	0.57	0	49,73,73	0.67	1 (2%)
3	GOL	B	504	-	5,5,5	0.96	0	5,5,5	1.19	1 (20%)
2	SND	B	501	-	42,48,48	0.56	0	49,73,73	0.68	1 (2%)

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
3	GOL	D	502	-	-	2/4/4/4	-
2	SND	B	503	-	-	2/26/62/62	0/5/5/5
3	GOL	A	503	-	-	0/4/4/4	-
2	SND	A	501	-	-	2/26/62/62	0/5/5/5
2	SND	C	501	-	-	2/26/62/62	0/5/5/5
3	GOL	C	503	-	-	2/4/4/4	-
2	SND	A	502	-	-	3/26/62/62	0/5/5/5
2	SND	D	501	-	-	1/26/62/62	0/5/5/5
2	SND	C	502	-	-	3/26/62/62	0/5/5/5
2	SND	B	502	-	-	2/26/62/62	0/5/5/5
3	GOL	B	504	-	-	0/4/4/4	-
2	SND	B	501	-	-	1/26/62/62	0/5/5/5

There are no bond length outliers.



All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SND	C5A-C6A-N6A	2.33	123.90	120.35
2	B	502	SND	C5A-C6A-N6A	2.25	123.78	120.35
2	B	503	SND	C5A-C6A-N6A	2.24	123.75	120.35
2	C	502	SND	C5A-C6A-N6A	2.22	123.73	120.35
2	C	501	SND	C5A-C6A-N6A	2.17	123.65	120.35
2	B	501	SND	C5A-C6A-N6A	2.17	123.64	120.35
2	D	501	SND	C5A-C6A-N6A	2.09	123.52	120.35
2	A	502	SND	C5A-C6A-N6A	2.09	123.52	120.35
3	B	504	GOL	C3-C2-C1	-2.07	103.64	111.70
2	A	501	SND	O5B-PA-O1A	2.03	116.99	109.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	SND	PN-O3-PA-O5B
2	A	502	SND	O4D-C1D-N1N-C6N
2	B	502	SND	C5D-O5D-PN-O3
2	B	502	SND	C5D-O5D-PN-O1N
2	B	503	SND	C5D-O5D-PN-O1N
2	C	502	SND	O4D-C1D-N1N-C6N
2	D	501	SND	PN-O3-PA-O5B
3	C	503	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-O2
3	D	502	GOL	O1-C1-C2-O2
2	B	501	SND	PN-O3-PA-O5B
2	C	501	SND	PN-O3-PA-O5B
2	A	502	SND	C5D-O5D-PN-O2N
2	A	501	SND	C5B-O5B-PA-O3
2	A	502	SND	C5D-O5D-PN-O3
2	B	503	SND	C5D-O5D-PN-O3
2	C	501	SND	C5B-O5B-PA-O3
2	C	502	SND	C5D-O5D-PN-O3
2	C	502	SND	C5D-O5D-PN-O2N

There are no ring outliers.

10 monomers are involved in 25 short contacts:

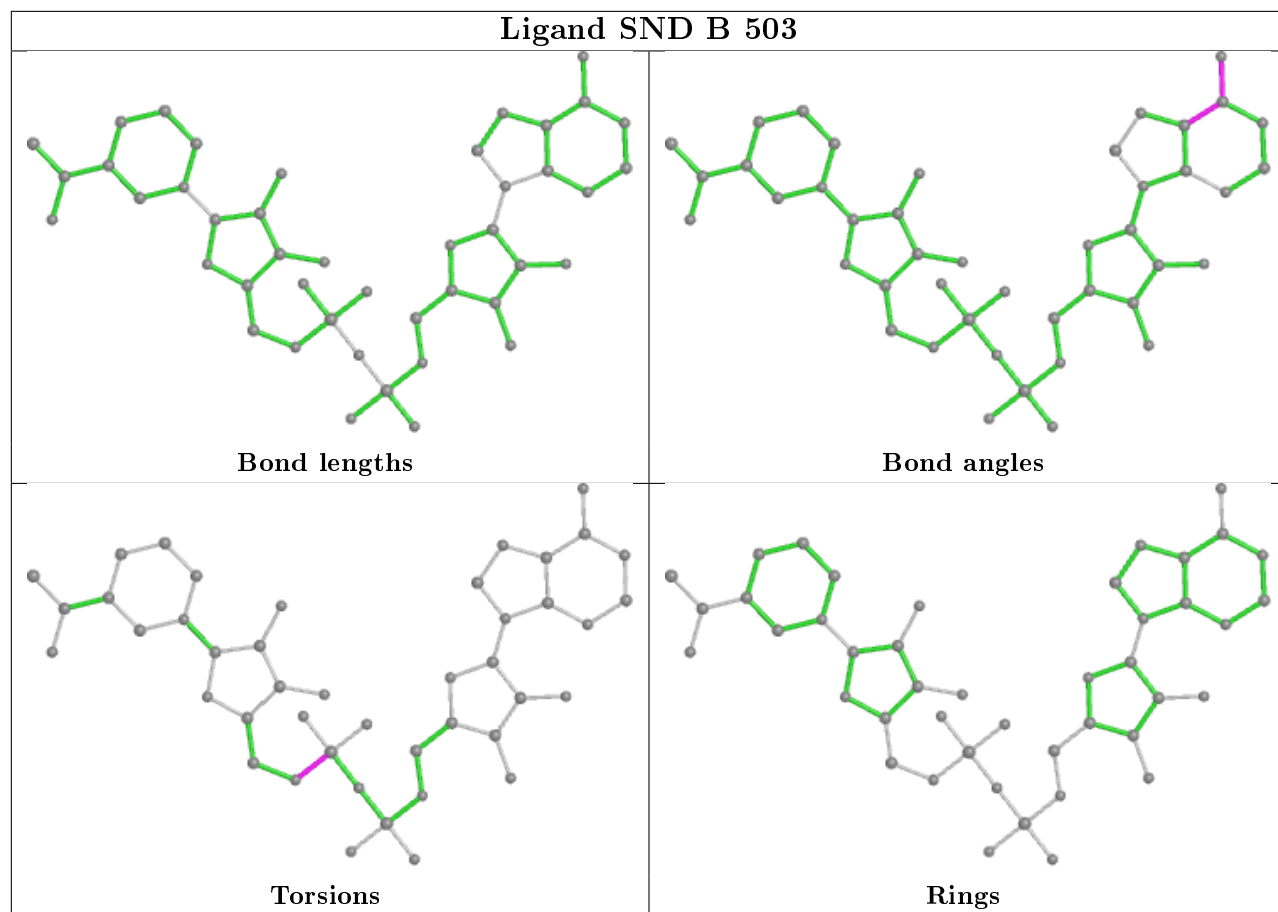
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	SND	1	0

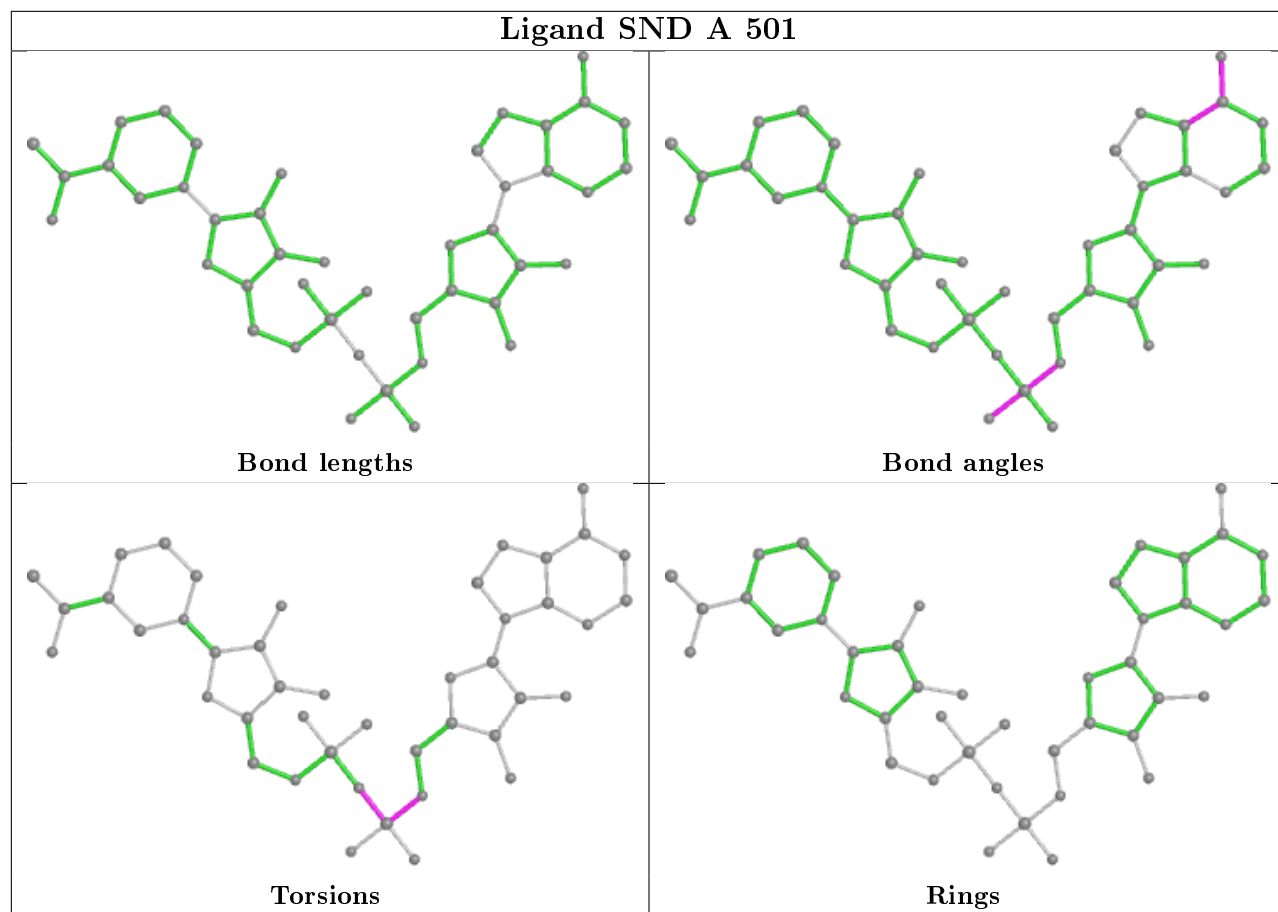
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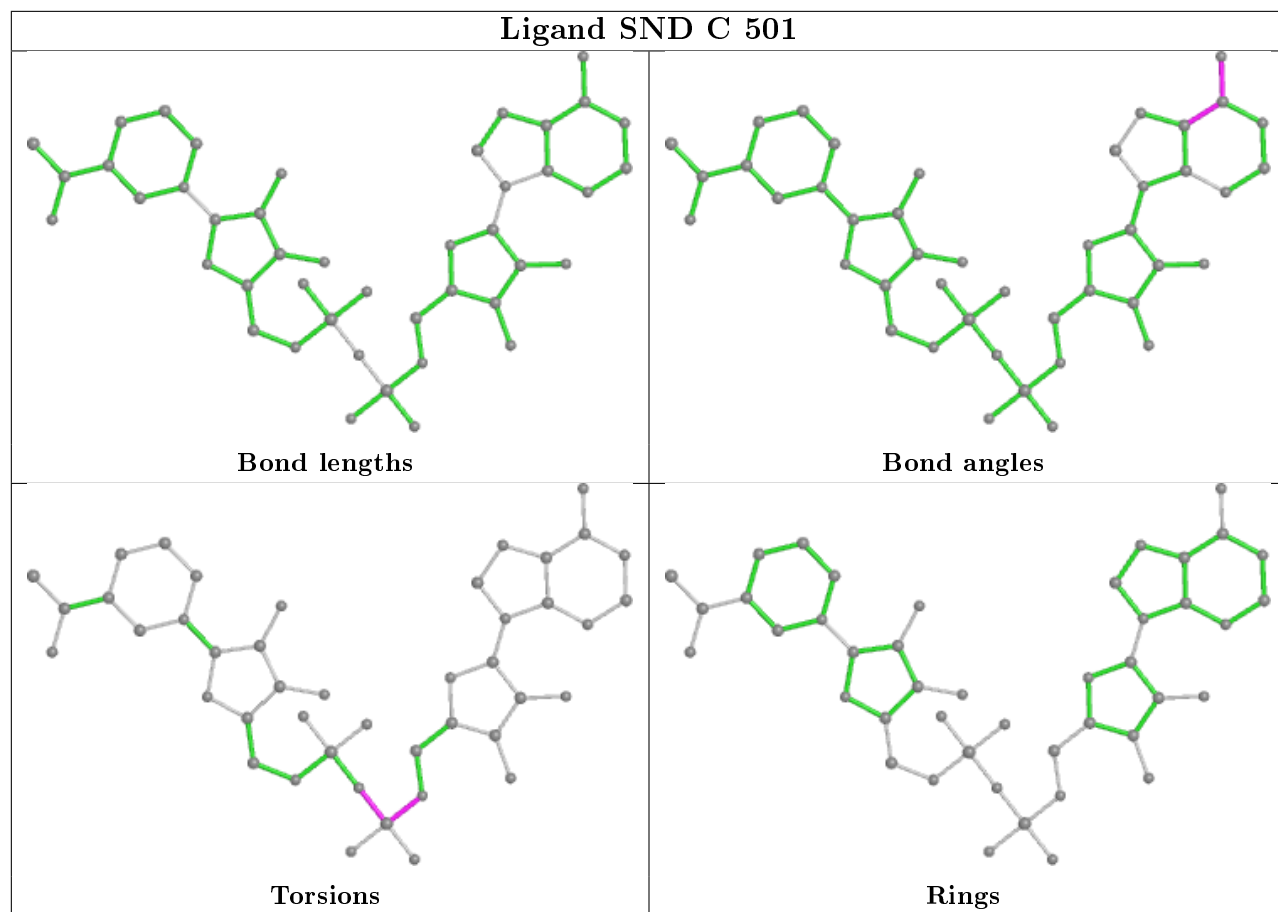
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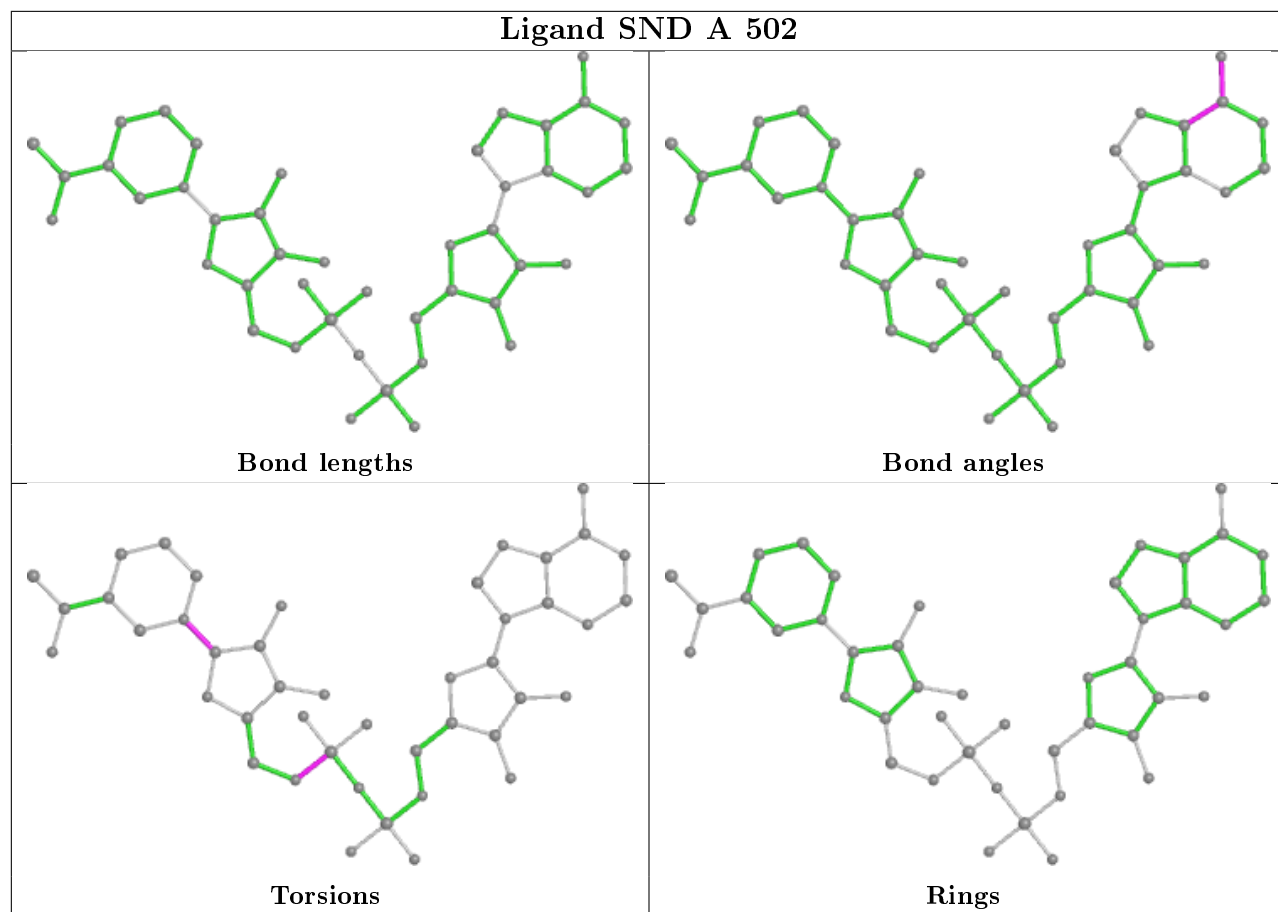
<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Clashes</b>	<b>Symm-Clashes</b>
3	A	503	GOL	1	0
2	A	501	SND	5	0
2	C	501	SND	3	0
2	A	502	SND	2	0
2	D	501	SND	2	0
2	C	502	SND	3	0
2	B	502	SND	1	0
3	B	504	GOL	3	0
2	B	501	SND	4	0

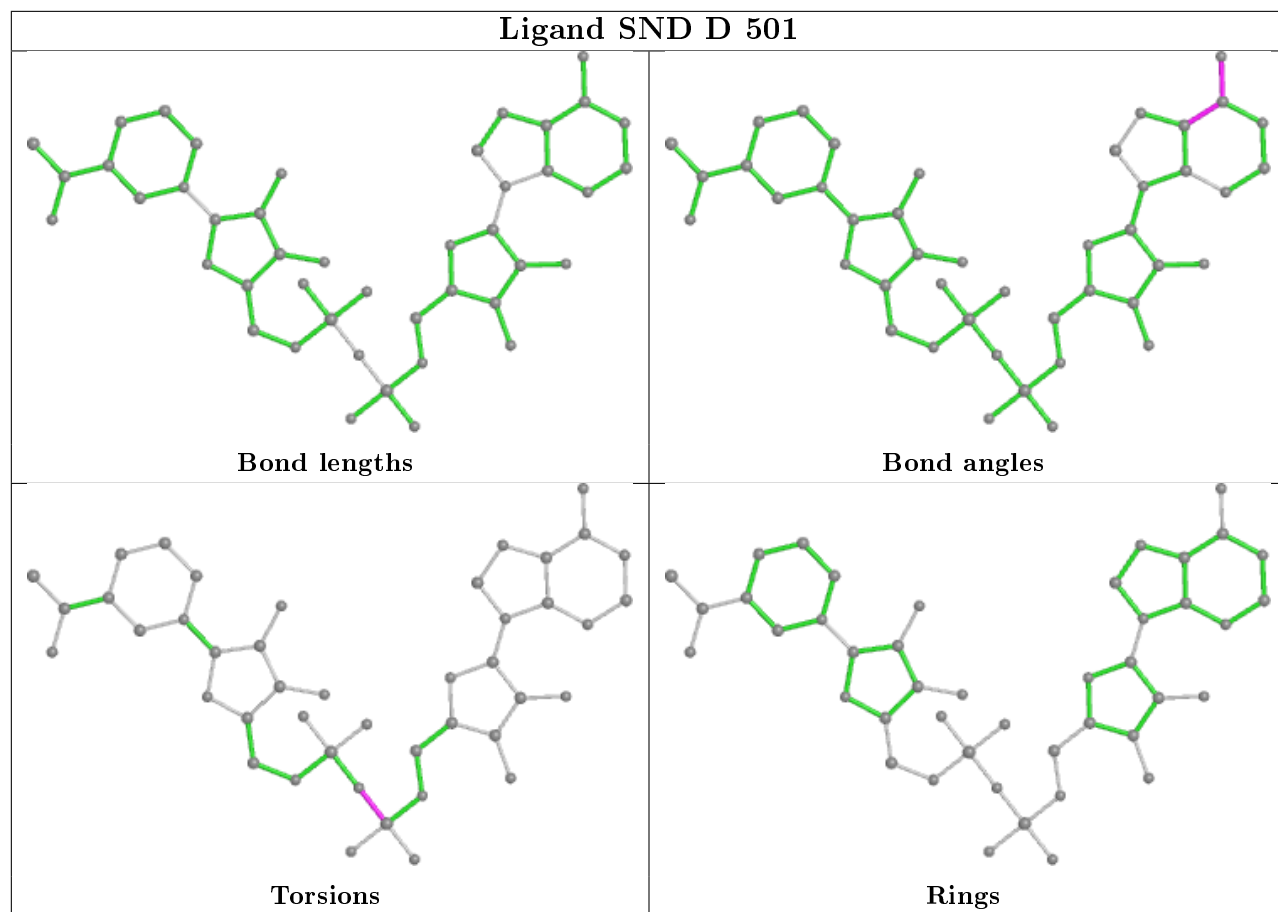
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

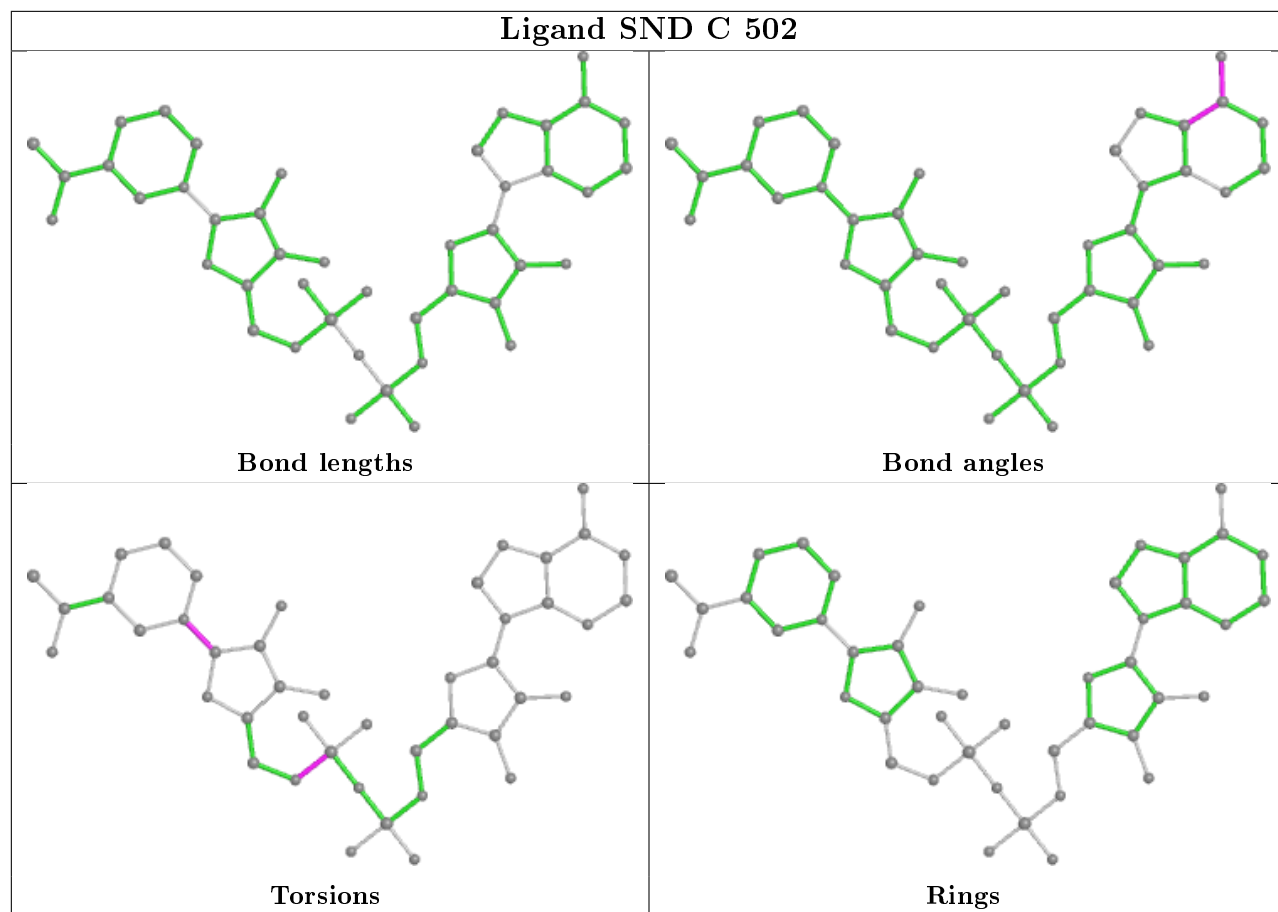




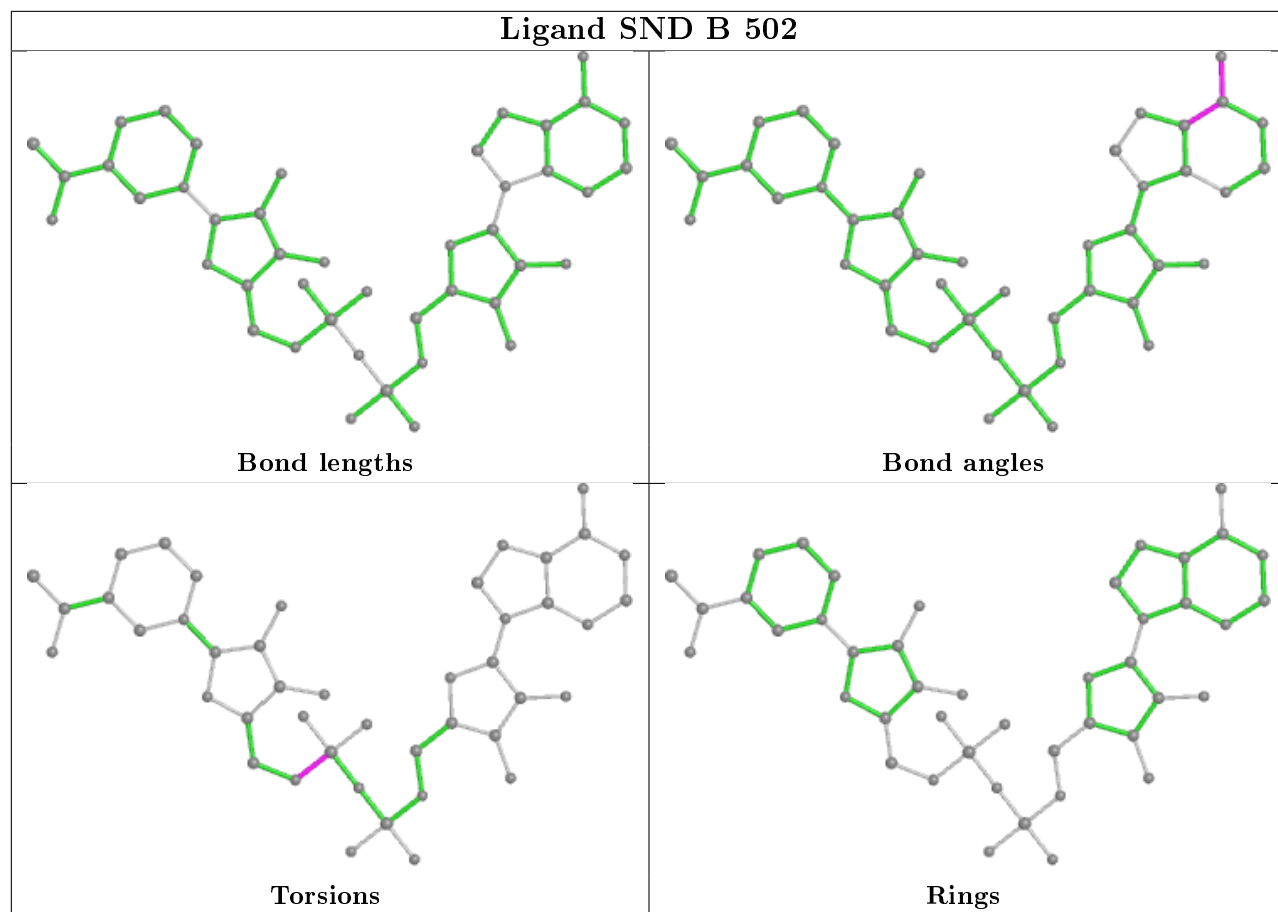


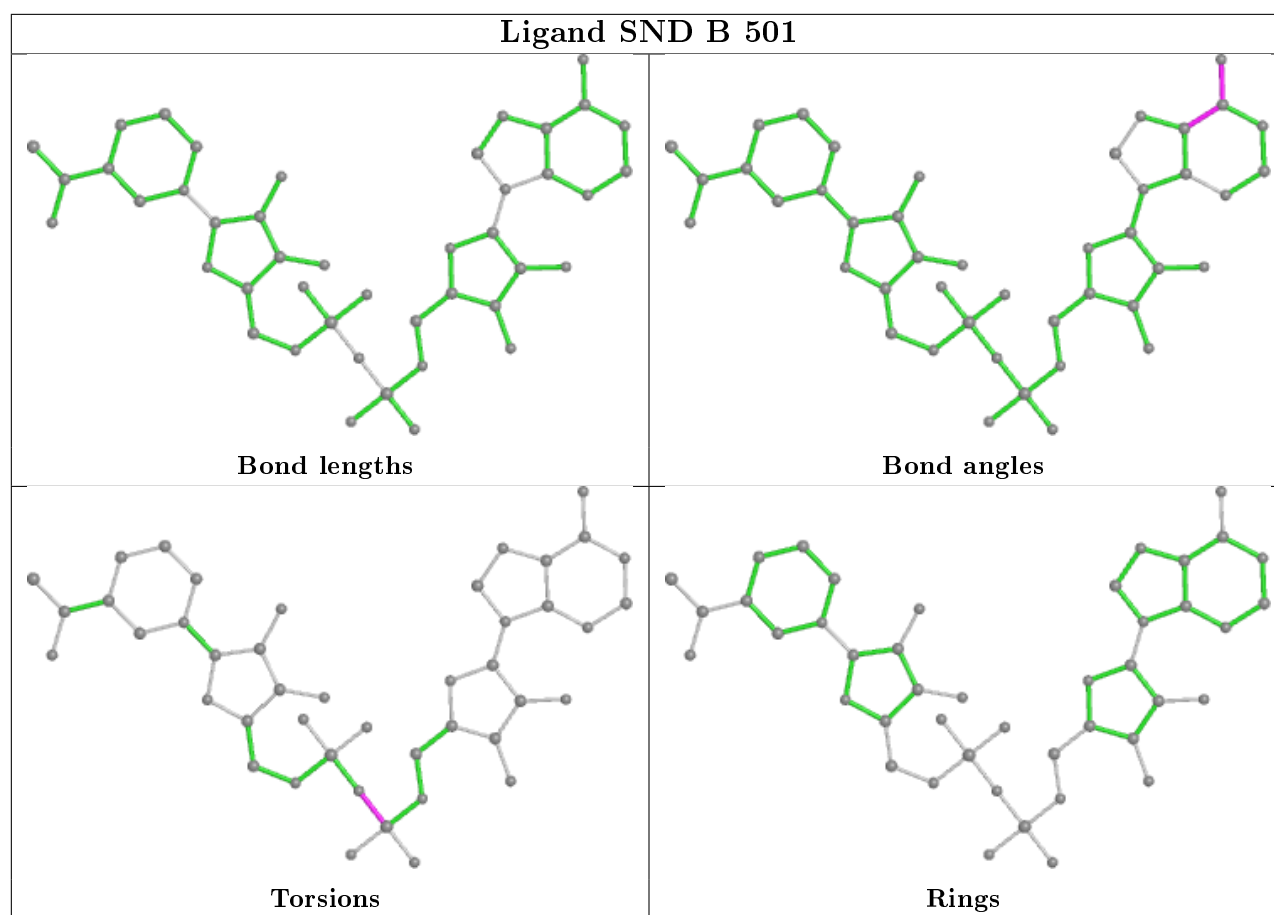












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	465/489 (95%)	-0.18	13 (2%) 53 48	7, 17, 42, 78	0
1	B	466/489 (95%)	-0.16	11 (2%) 59 54	6, 17, 43, 79	0
1	C	464/489 (94%)	-0.22	8 (1%) 70 66	7, 17, 39, 75	0
1	D	466/489 (95%)	-0.08	20 (4%) 35 29	6, 18, 41, 79	0
All	All	1861/1956 (95%)	-0.16	52 (2%) 53 48	6, 17, 42, 79	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ASN	8.8
1	D	227	GLY	5.4
1	D	428	ILE	5.4
1	B	428	ILE	5.2
1	B	227	GLY	4.8
1	A	228	GLU	4.7
1	B	226	ASN	4.6
1	A	32	LYS	4.3
1	D	228	GLU	4.1
1	D	225	ASP	4.0
1	A	134	ILE	4.0
1	C	227	GLY	3.9
1	B	314	LEU	3.6
1	B	31	GLY	3.6
1	A	133	ARG	3.5
1	B	230	LEU	3.3
1	D	412	ALA	3.2
1	D	30	GLN	3.0
1	B	225	ASP	3.0
1	D	230	LEU	3.0
1	B	228	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	34	ASP	2.8
1	D	32	LYS	2.8
1	C	428	ILE	2.8
1	D	427	ASP	2.8
1	C	412	ALA	2.7
1	A	427	ASP	2.7
1	A	428	ILE	2.7
1	D	411	GLN	2.6
1	A	314	LEU	2.6
1	A	412	ALA	2.5
1	D	224	GLY	2.5
1	D	314	LEU	2.5
1	A	316	PHE	2.4
1	A	9	TRP	2.4
1	B	33	LEU	2.4
1	C	230	LEU	2.4
1	A	409	SER	2.4
1	C	129	SER	2.3
1	B	412	ALA	2.3
1	C	143	PRO	2.3
1	D	268	ALA	2.3
1	D	76	GLY	2.2
1	D	316	PHE	2.2
1	D	426	ALA	2.2
1	C	410	ASP	2.2
1	A	129	SER	2.1
1	A	411	GLN	2.1
1	D	33	LEU	2.1
1	D	410	ASP	2.0
1	B	224	GLY	2.0
1	C	352	GLN	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](#)

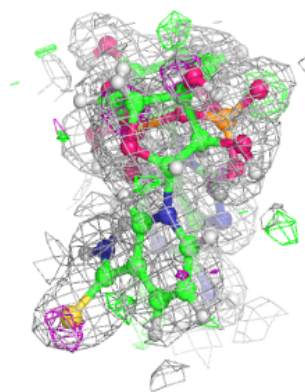
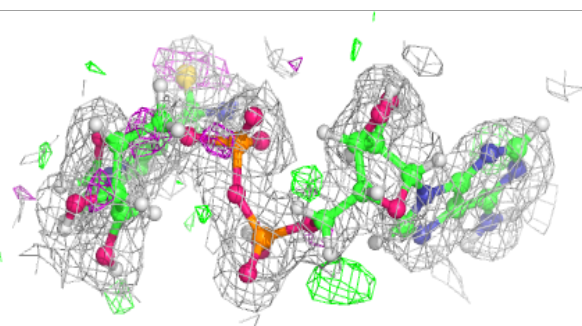
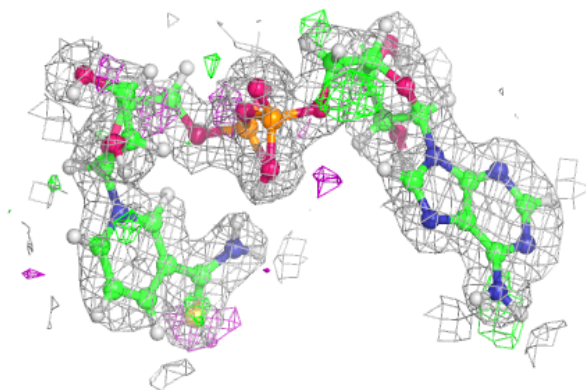
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
3	GOL	A	503	6/6	0.87	0.17	17,37,45,48	0
3	GOL	C	503	6/6	0.88	0.22	7,40,48,48	0
3	GOL	B	504	6/6	0.90	0.14	15,35,52,62	0
3	GOL	D	502	6/6	0.93	0.12	9,28,40,48	0
2	SND	D	501	44/44	0.96	0.09	8,15,25,29	0
2	SND	C	501	44/44	0.97	0.09	6,16,25,30	0
2	SND	A	501	44/44	0.97	0.09	6,18,26,31	0
2	SND	B	501	44/44	0.97	0.09	8,16,23,27	0
2	SND	B	503	44/44	0.98	0.09	5,9,17,39	0
2	SND	A	502	44/44	0.98	0.09	6,10,15,33	0
2	SND	C	502	44/44	0.98	0.10	5,10,15,31	0
2	SND	B	502	44/44	0.98	0.08	4,9,15,32	0

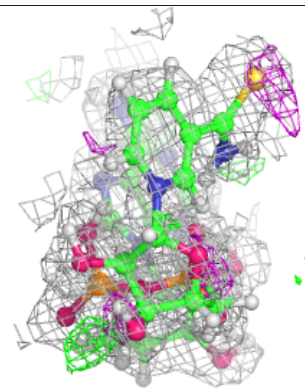
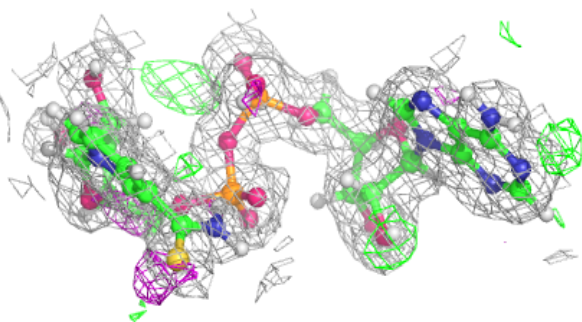
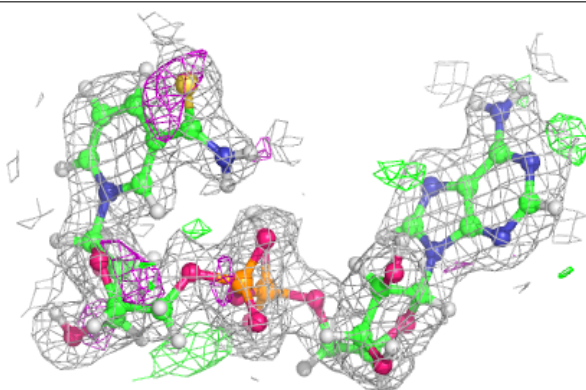
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around SND D 501:**

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

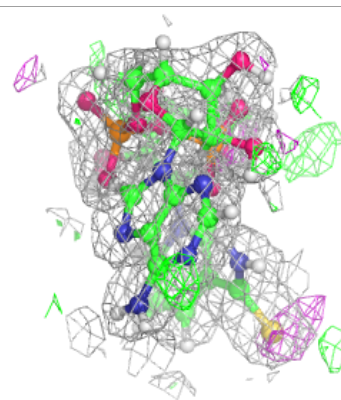
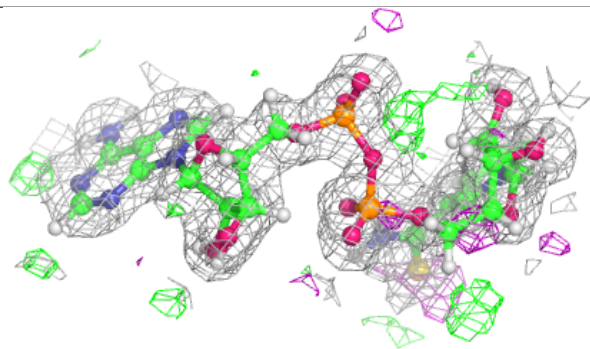
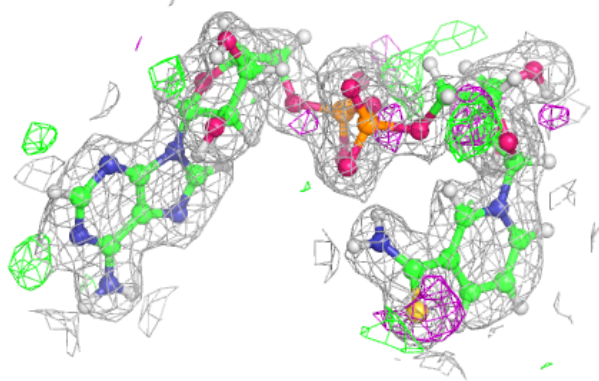
**Electron density around SND C 501:**

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

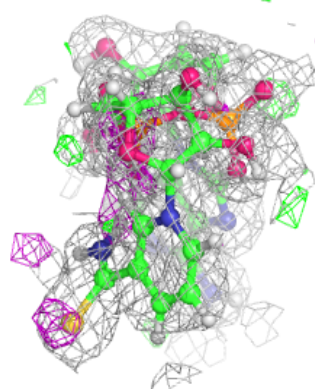
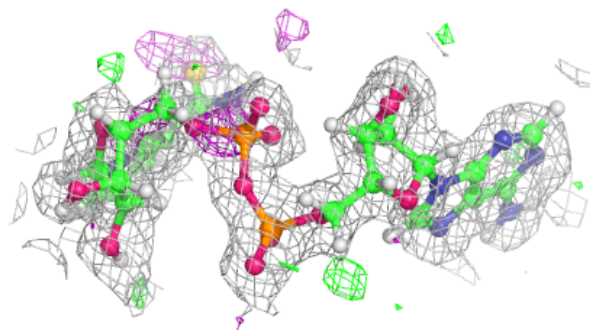
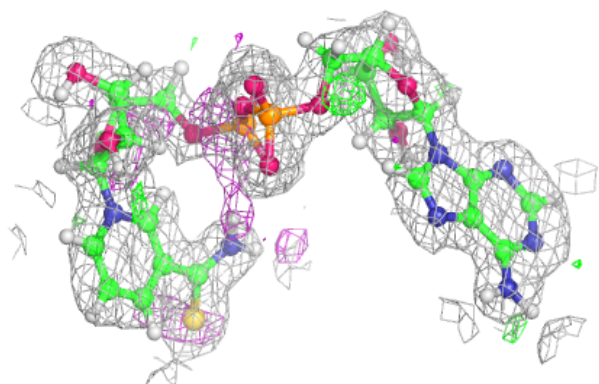


**Electron density around SND A 501:**

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

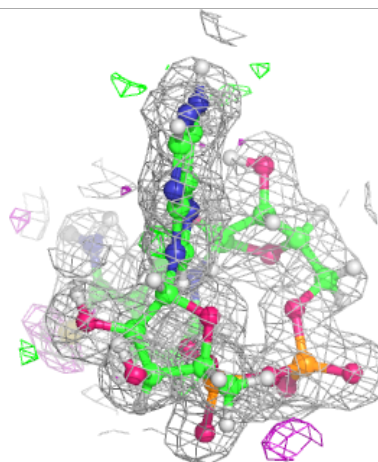
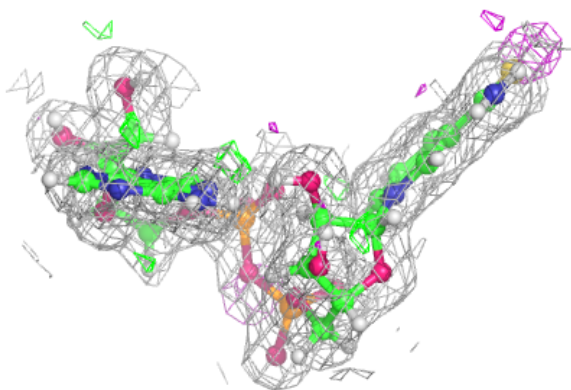
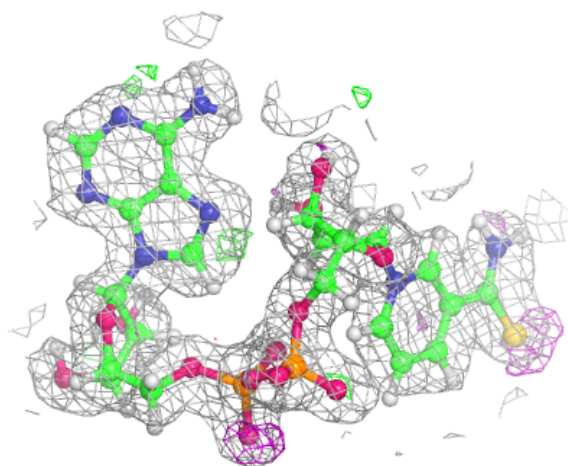
**Electron density around SND B 501:**

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



**Electron density around SND B 503:**

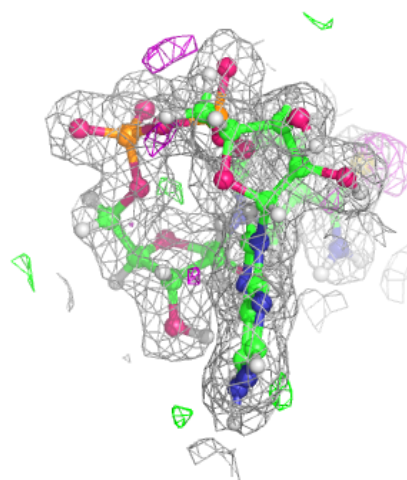
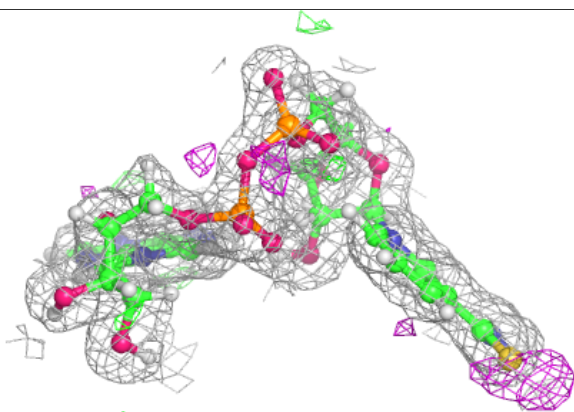
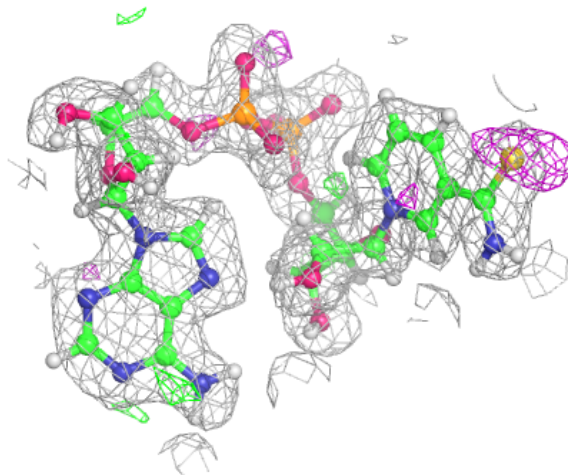
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

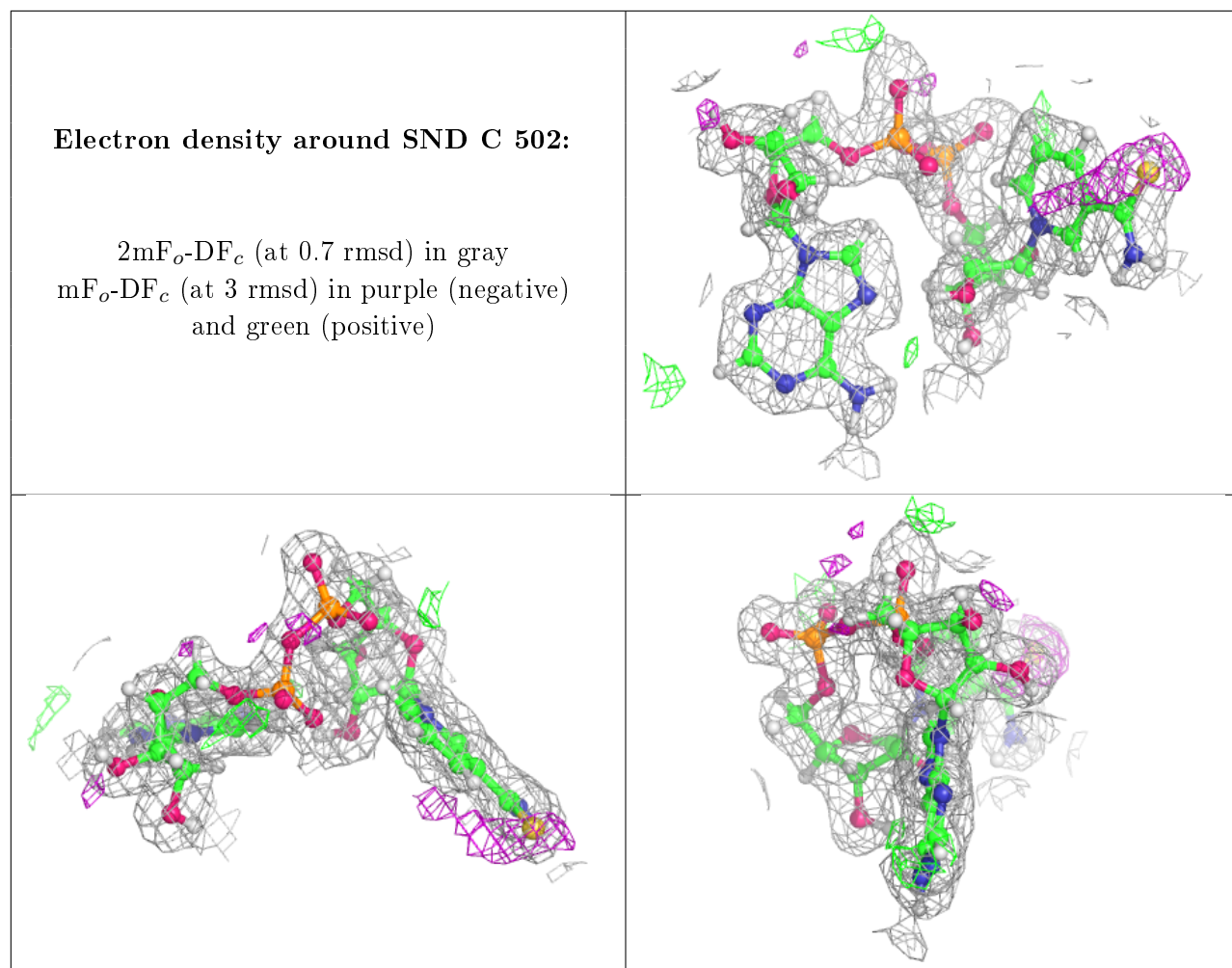


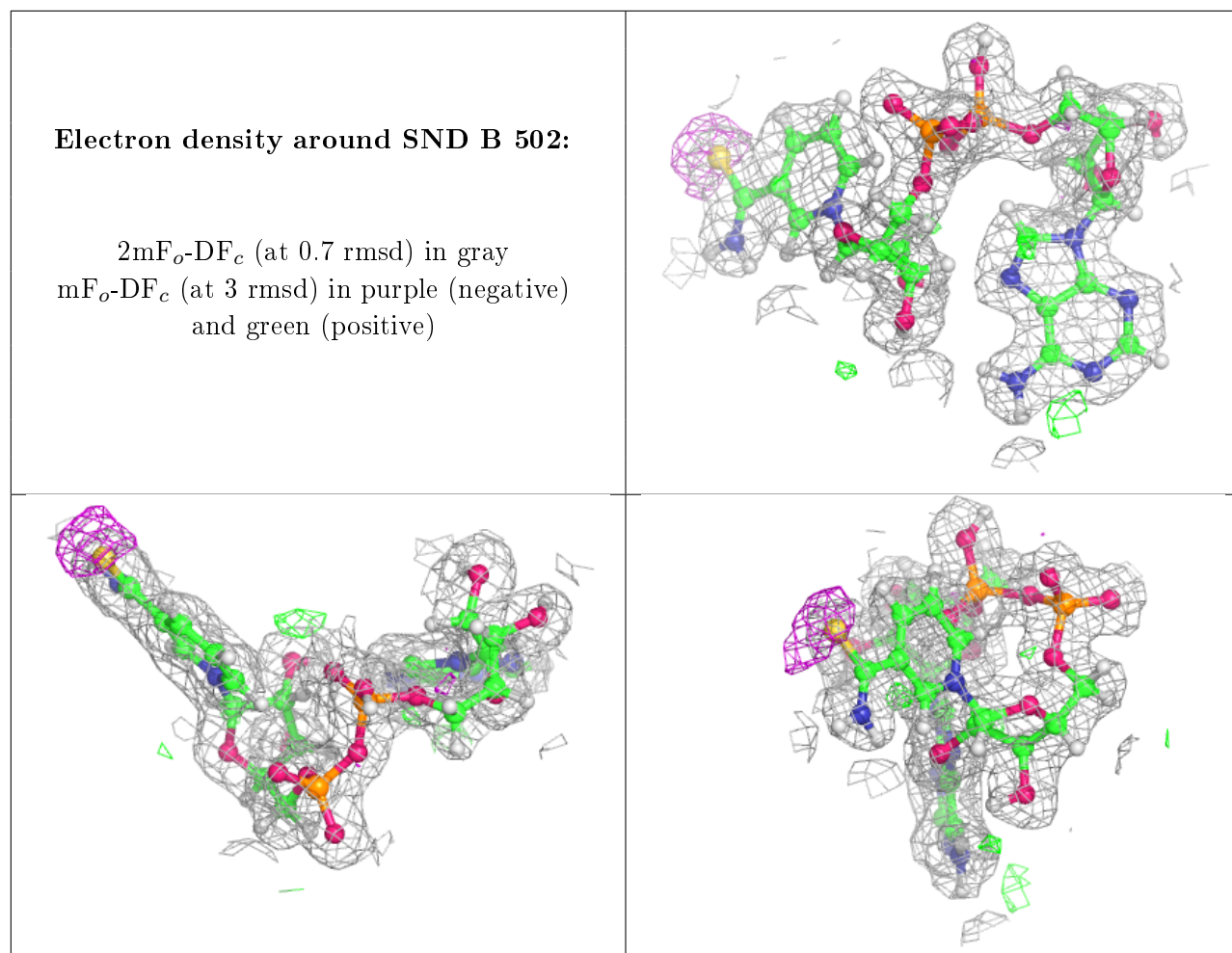


**Electron density around SND A 502:**

$2mF_o-DF_c$  (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.