



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 02:44 pm BST

PDB ID : 6ZTI / pdb_00006zti
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

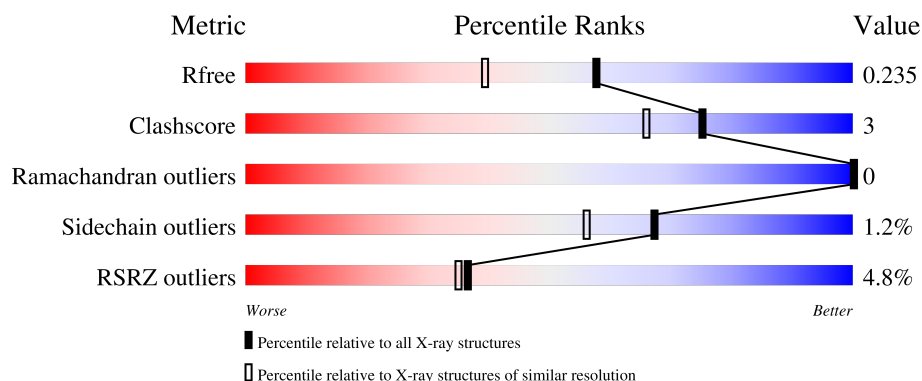
1 Overall quality at a glance

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}	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (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 ≥ 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	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	489	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	489	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	D	489	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>

2 Entry composition

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

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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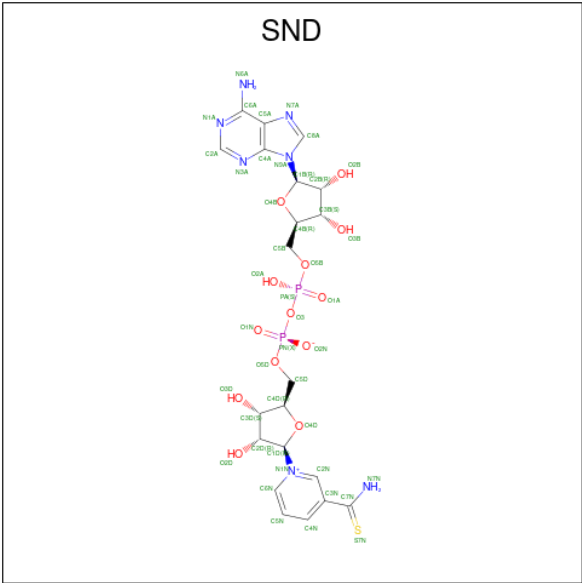
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A378K488
B	-8	PRO	-	expression tag	UNP A0A378K488
B	-7	GLN	-	expression tag	UNP A0A378K488
B	-6	PHE	-	expression tag	UNP A0A378K488
B	-5	GLU	-	expression tag	UNP A0A378K488
B	-4	LYS	-	expression tag	UNP A0A378K488
B	-3	GLY	-	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 (CCD ID: SND) (formula: C₂₁H₂₇N₇O₁₃P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
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 (CCD ID: GOL) (formula: C₃H₈O₃).



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

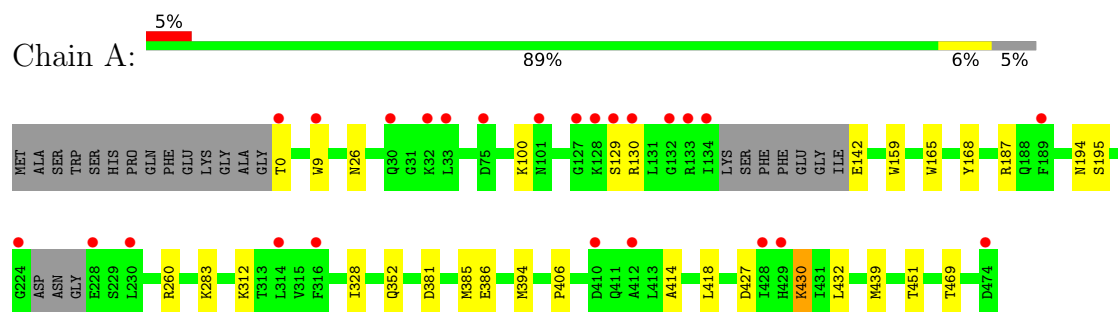
- Molecule 4 is water.

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

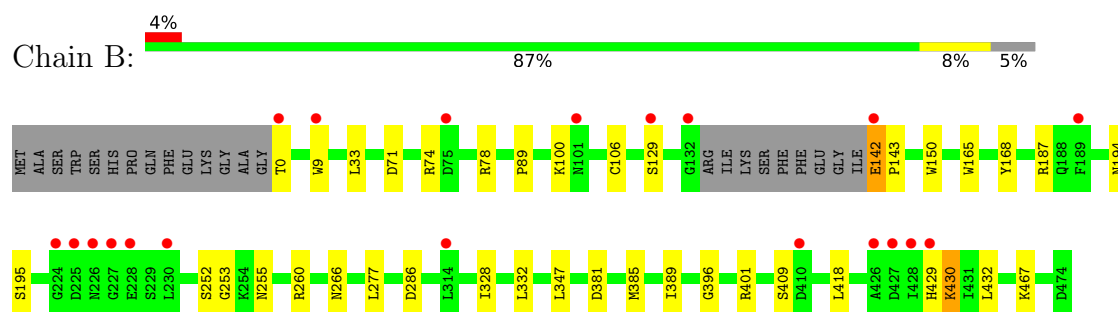
3 Residue-property plots [i](#)

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.

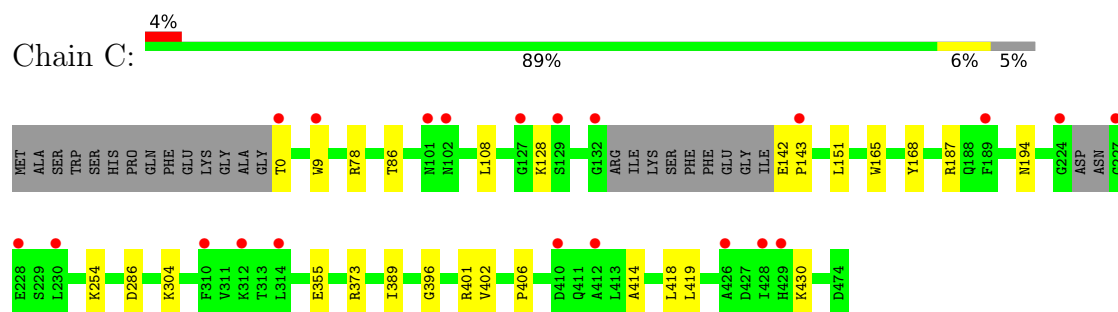
• Molecule 1: PlaB phospholipase



• Molecule 1: PlaB phospholipase

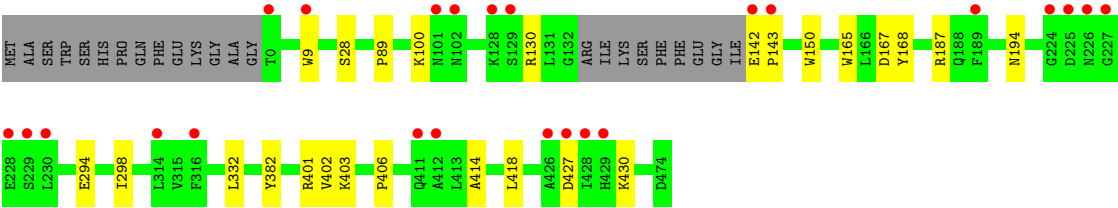


• Molecule 1: PlaB phospholipase



• Molecule 1: PlaB phospholipase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.81Å)	Xtriage
Refinement program	PHENIX dev_3922	Depositor
R, R_{free}	0.186 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	55218 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32173	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.28	0/3826	0.44	0/5171
1	B	0.28	0/3860	0.44	0/5217
1	C	0.28	0/3810	0.44	0/5148
1	D	0.28	0/3818	0.43	0/5164
All	All	0.28	0/15314	0.44	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	22	0
1	B	3756	3751	3768	25	0
1	C	3719	3718	3723	19	0
1	D	3729	3715	3719	17	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	4	0
4	D	434	0	0	6	1
All	All	17017	15156	15184	87	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 (87) 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	0.58
1:A:194:ASN:C	2:A:501:SND:S7N	2.89	0.55
1:C:194:ASN:C	2:C:501:SND:S7N	2.91	0.54
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:B:194:ASN:C	2:B:501:SND:S7N	2.92	0.52
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: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:D:194:ASN:C	2:D:501:SND:S7N	2.97	0.47
1:B:187:ARG:NH1	2:B:502:SND:S7N	2.81	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:A:9:TRP:H	1:A:9:TRP:CD1	2.33	0.46
1:B:9:TRP:CD1	1:B:9:TRP:H	2.34	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
1:A:451:THR:HG1	1:A:469:THR:HG23	1.81	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:9:TRP:CD1	1:C:9:TRP:H	2.35	0.43
1:C:402[B]:VAL:CG2	1:C:419:LEU:HB3	2.48	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:B:418:LEU:C	1:B:418:LEU:HD23	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:142:GLU:HB3	1:C:143:PRO:HD3	2.01	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:A:394:MET:HE3	4:A:696:HOH:O	2.19	0.41
1:B:266:ASN:OD1	1:B:266:ASN:C	2.63	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:A:418:LEU:C	1:A:418:LEU:HD23	2.45	0.41
1:C:194:ASN:CA	2:C:501:SND:S7N	3.09	0.41
1:D:9:TRP:H	1:D:9:TRP:CD1	2.37	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

5.3.1 Protein backbone

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/422 (97%)	399 (98%)	9 (2%)	47	31
1	B	410/422 (97%)	402 (98%)	8 (2%)	50	35
1	C	405/422 (96%)	401 (99%)	4 (1%)	73	62
1	D	407/422 (96%)	407 (100%)	0	100	100
All	All	1630/1688 (97%)	1609 (99%)	21 (1%)	67	52

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	THR
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	427	ASP
1	A	430	LYS
1	B	0	THR
1	B	129	SER
1	B	142	GLU
1	B	332	LEU

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Mol	Chain	Res	Type
1	B	347	LEU
1	B	429	HIS
1	B	430	LYS
1	B	467	LYS
1	C	0	THR
1	C	304	LYS
1	C	373	ARG
1	C	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	183	GLN
1	A	303	GLN
1	A	307	HIS
1	A	367	GLN
1	A	433	HIS
1	A	435	ASN
1	B	125	GLN
1	B	183	GLN
1	B	239	GLN
1	B	303	GLN
1	B	339	HIS
1	B	367	GLN
1	B	435	ASN
1	C	26	ASN
1	C	183	GLN
1	C	255	ASN
1	C	303	GLN
1	C	338	ASN
1	C	339	HIS
1	C	422	HIS
1	C	433	HIS
1	C	435	ASN
1	D	26	ASN
1	D	101	ASN
1	D	160	GLN
1	D	183	GLN
1	D	255	ASN
1	D	303	GLN
1	D	338	ASN

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Mol	Chain	Res	Type
1	D	435	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 oligosaccharides 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	$\# Z > 2$
2	SND	A	501	-	42,48,48	0.56	0	49,73,73	0.68	2 (4%)
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	C	502	-	42,48,48	0.56	0	49,73,73	0.67	1 (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%)
2	SND	D	501	-	42,48,48	0.56	0	49,73,73	0.63	1 (2%)
2	SND	B	501	-	42,48,48	0.56	0	49,73,73	0.68	1 (2%)
2	SND	B	502	-	42,48,48	0.57	0	49,73,73	0.67	1 (2%)
3	GOL	A	503	-	5,5,5	1.12	0	5,5,5	1.06	0
3	GOL	B	504	-	5,5,5	0.96	0	5,5,5	1.19	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SND	C	501	-	42,48,48	0.61	0	49,73,73	0.67	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
2	SND	A	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	C	502	-	-	3/26/62/62	0/5/5/5
3	GOL	D	502	-	-	2/4/4/4	-
2	SND	B	503	-	-	2/26/62/62	0/5/5/5
2	SND	D	501	-	-	1/26/62/62	0/5/5/5
2	SND	B	501	-	-	1/26/62/62	0/5/5/5
2	SND	B	502	-	-	2/26/62/62	0/5/5/5
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
2	SND	C	501	-	-	2/26/62/62	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

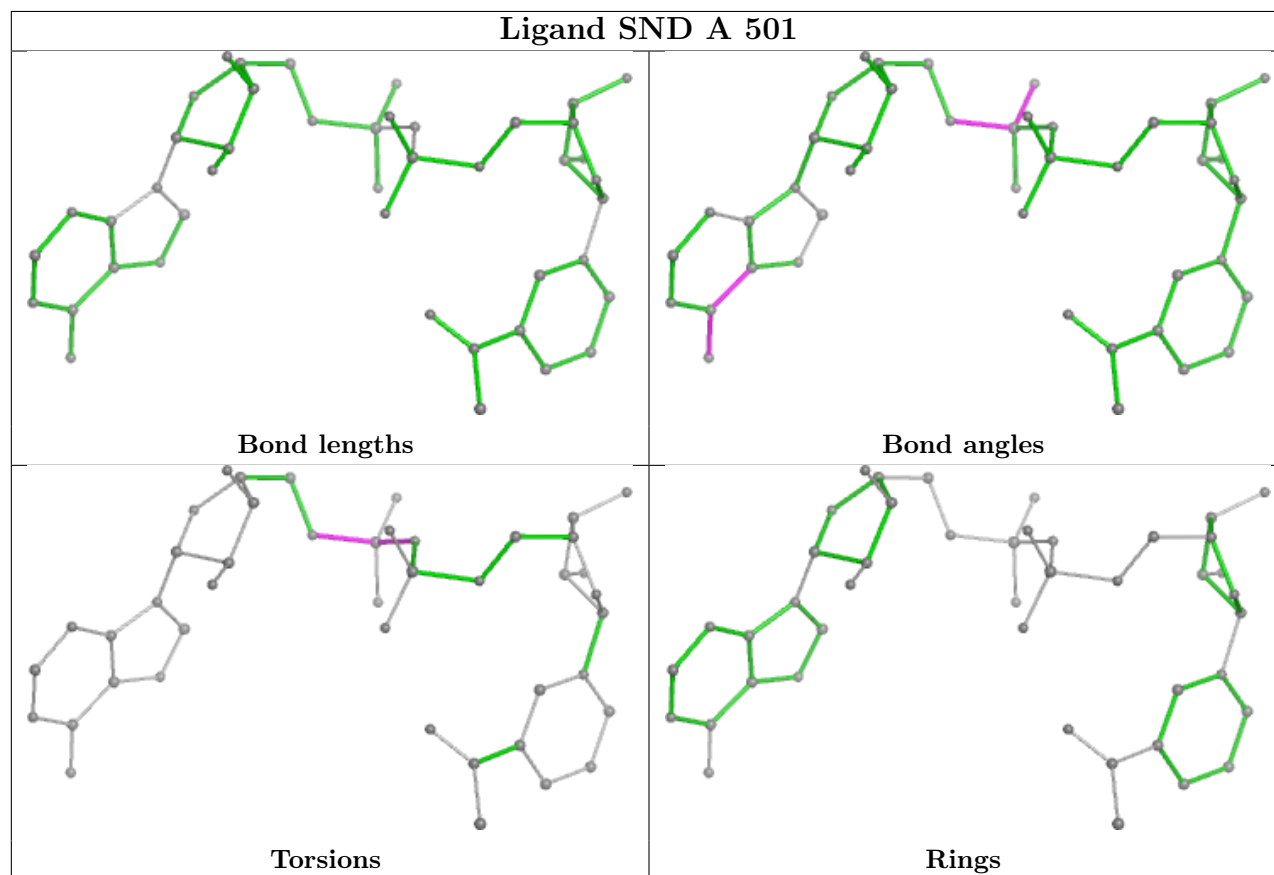
There are no ring outliers.

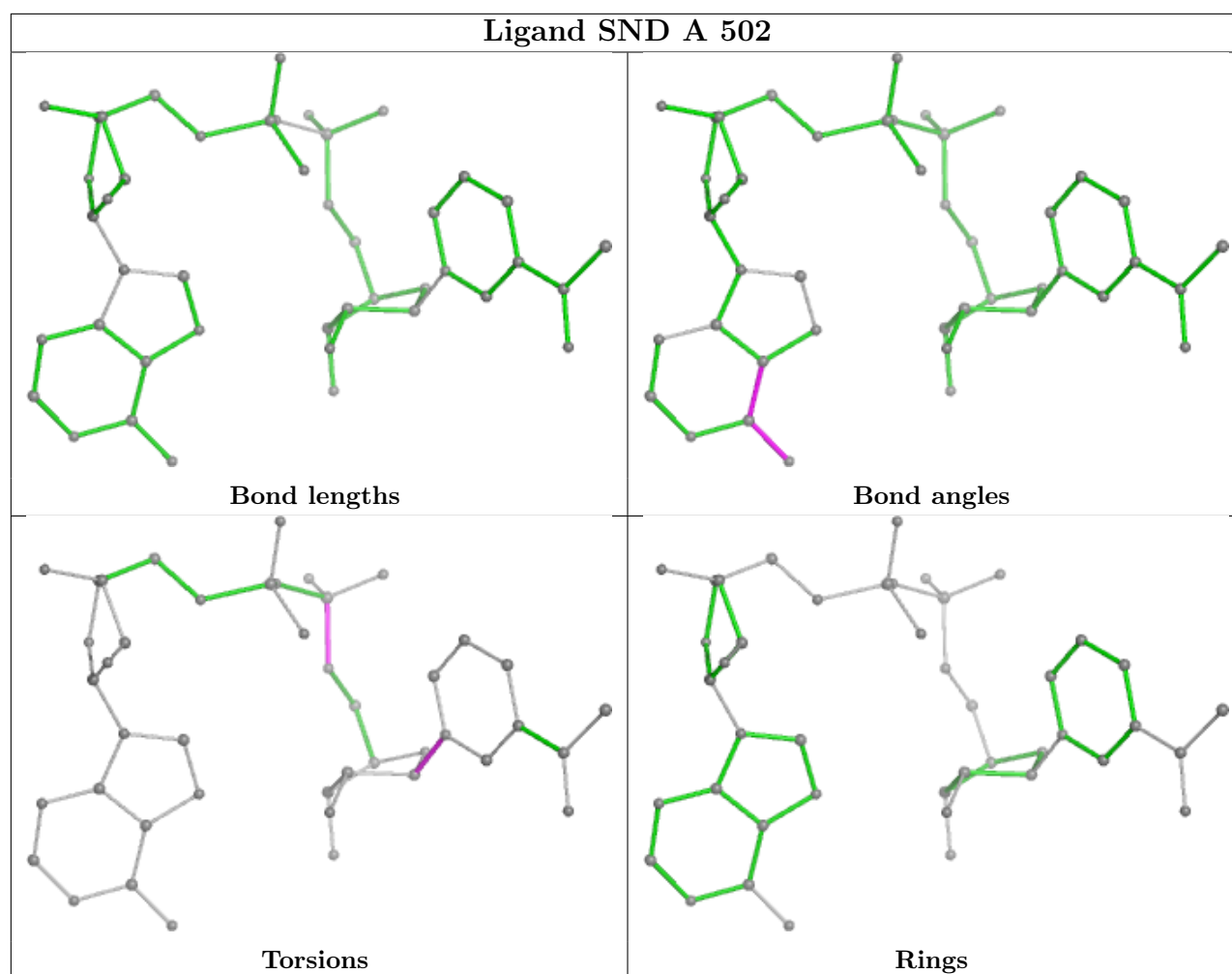
10 monomers are involved in 25 short contacts:

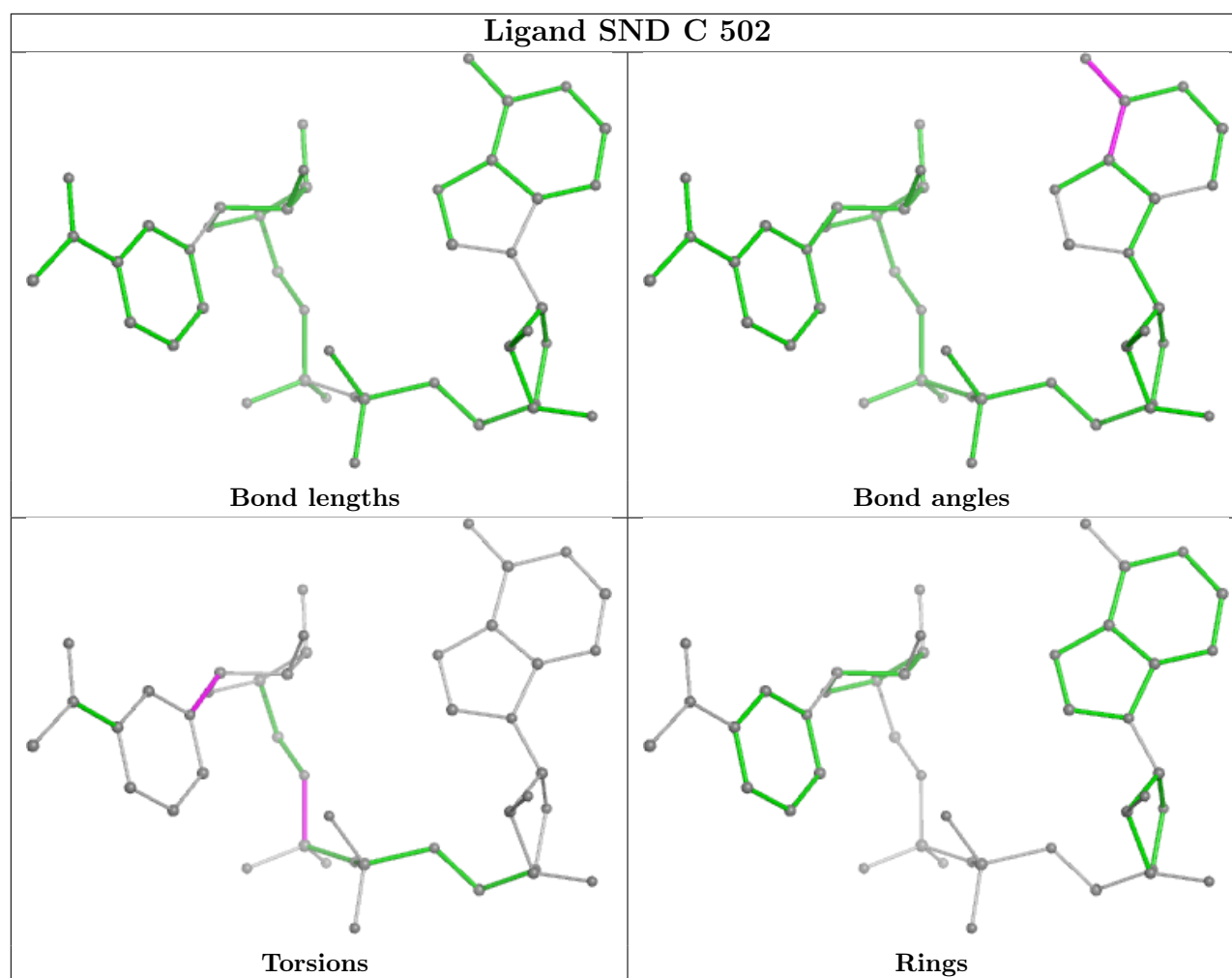
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SND	5	0
2	A	502	SND	2	0
2	C	502	SND	3	0
2	B	503	SND	1	0
2	D	501	SND	2	0
2	B	501	SND	4	0
2	B	502	SND	1	0
3	A	503	GOL	1	0
3	B	504	GOL	3	0
2	C	501	SND	3	0

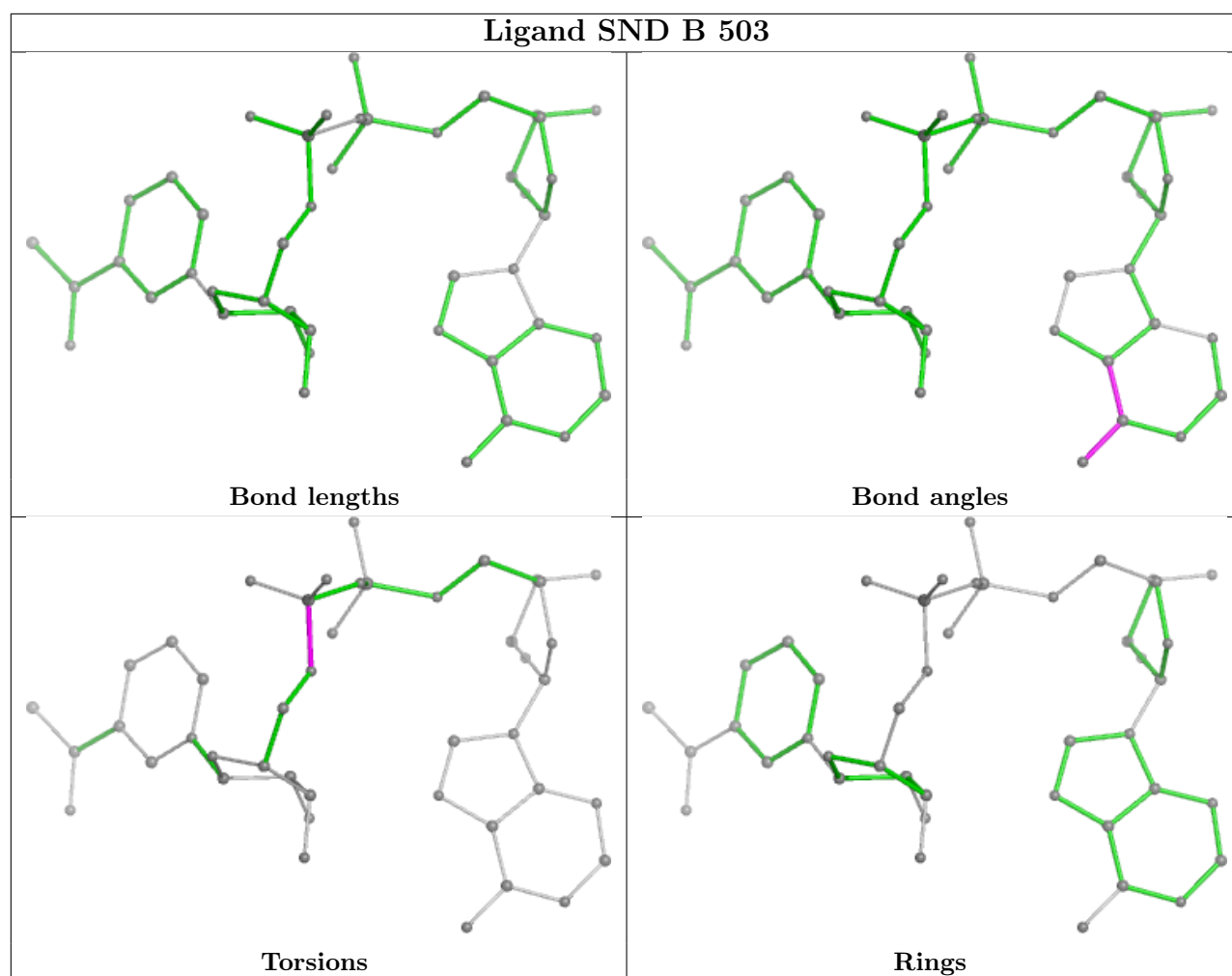
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

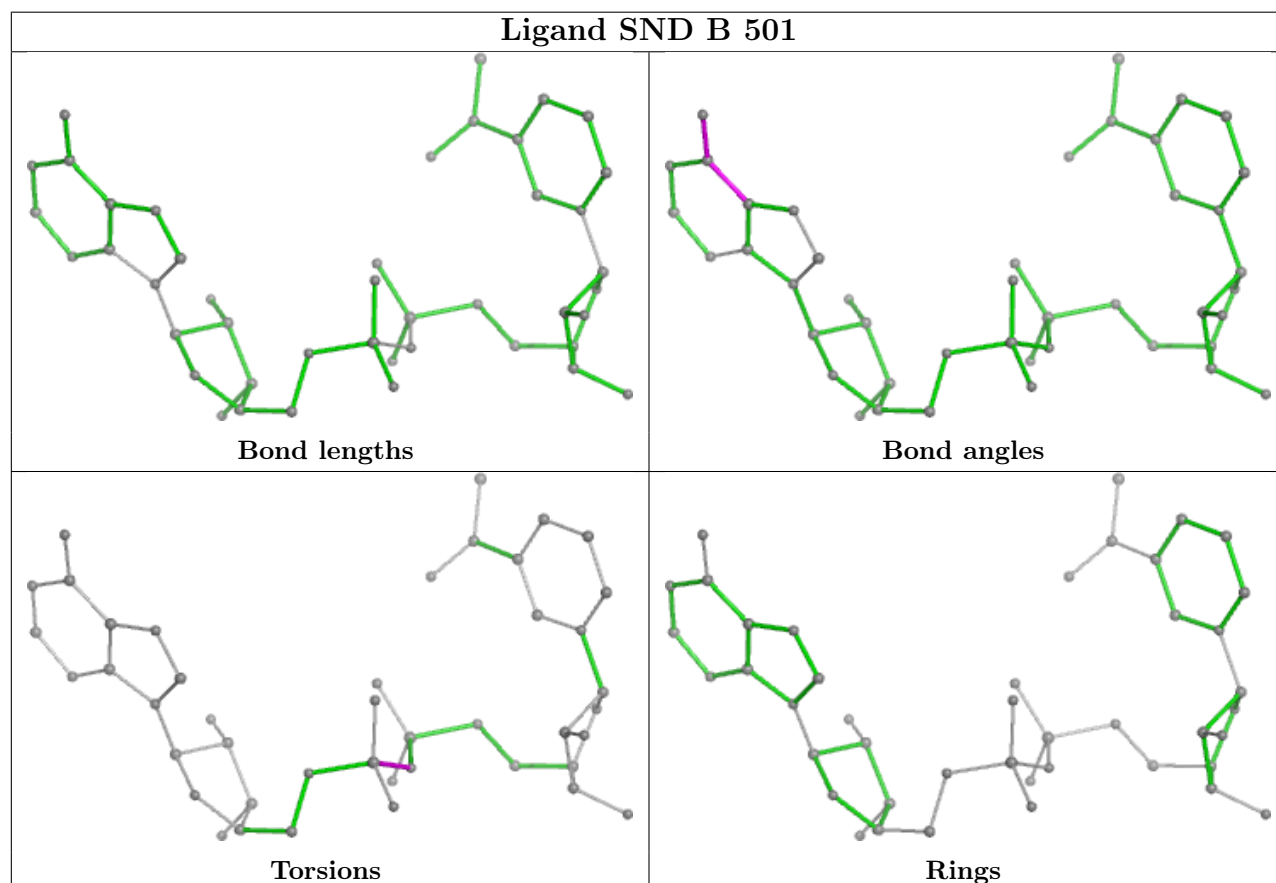
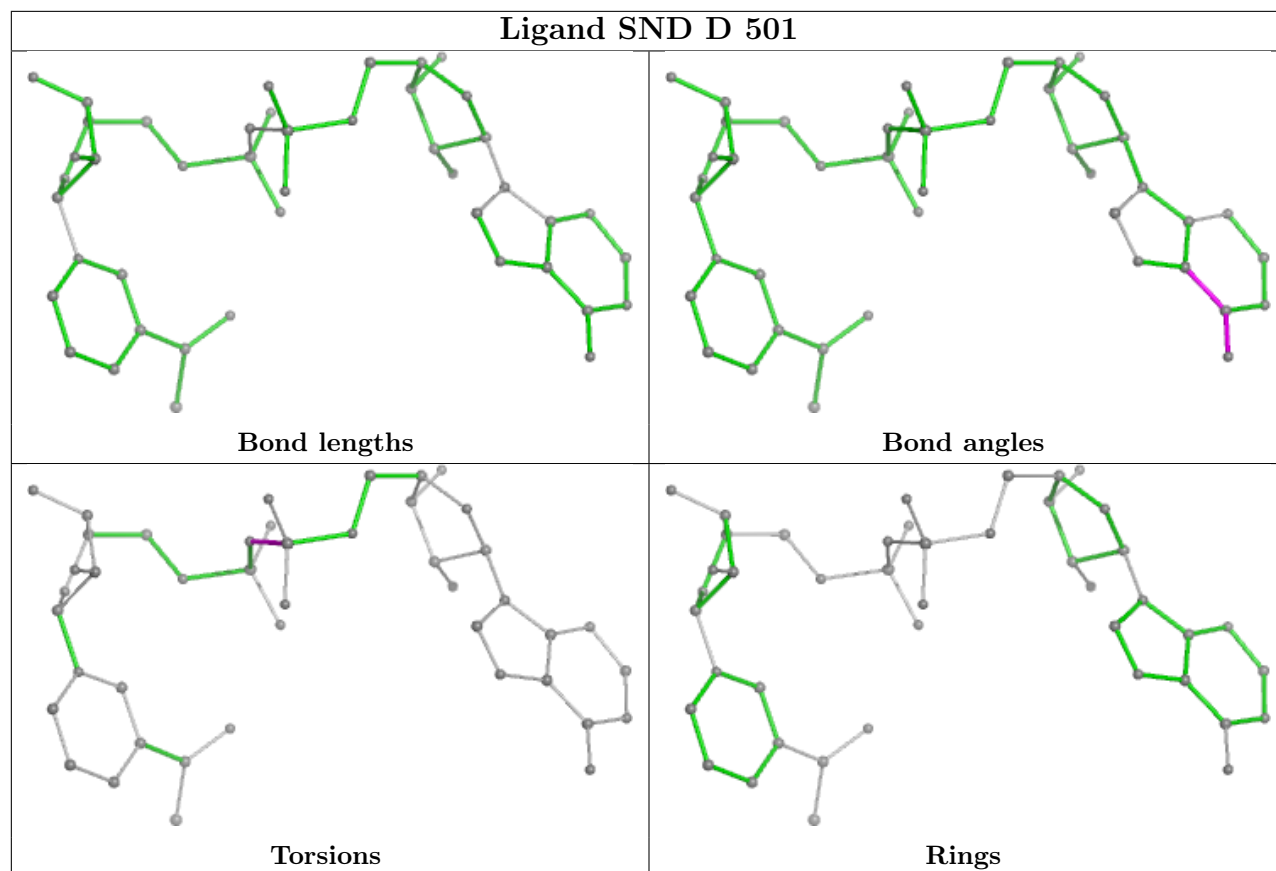
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

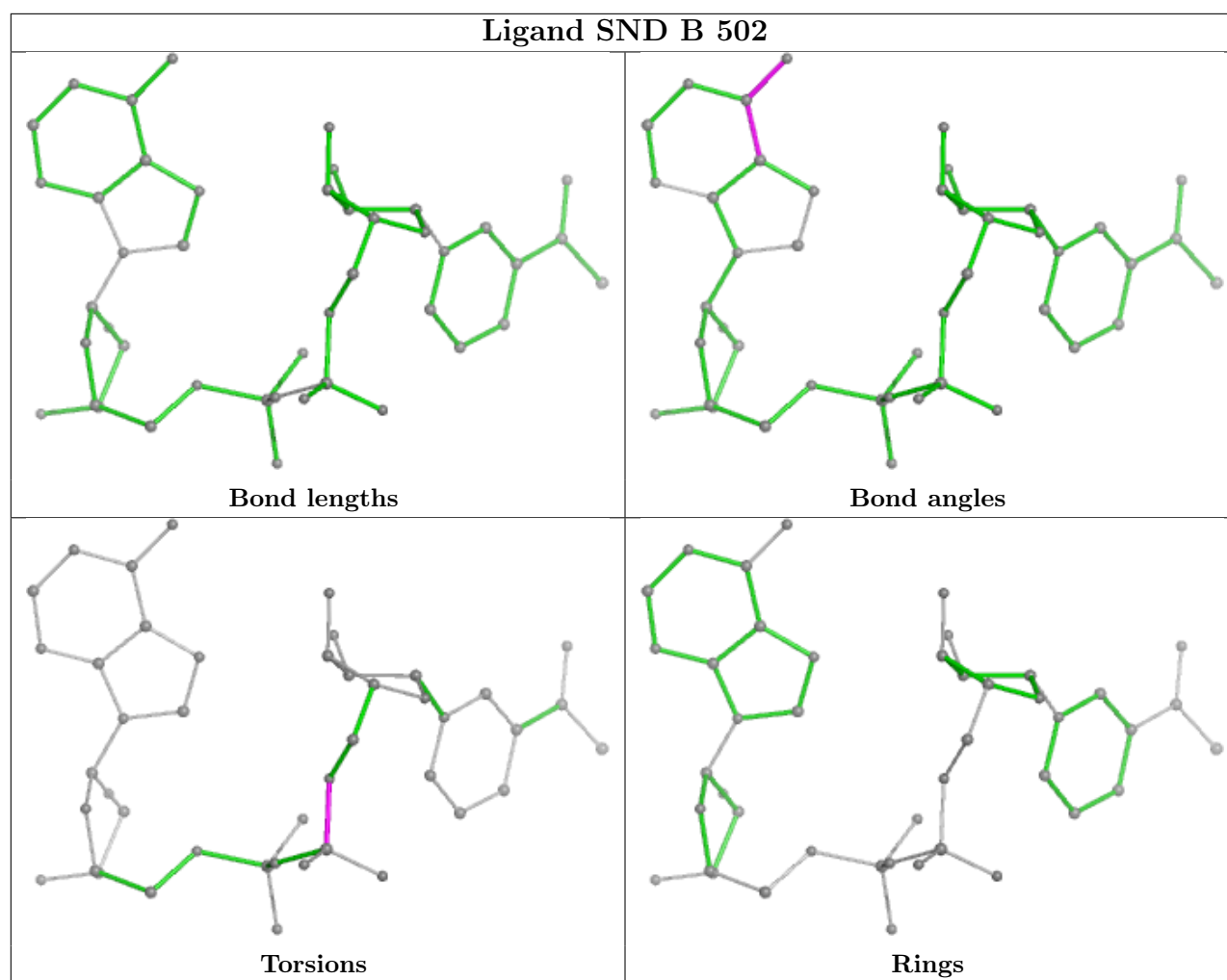


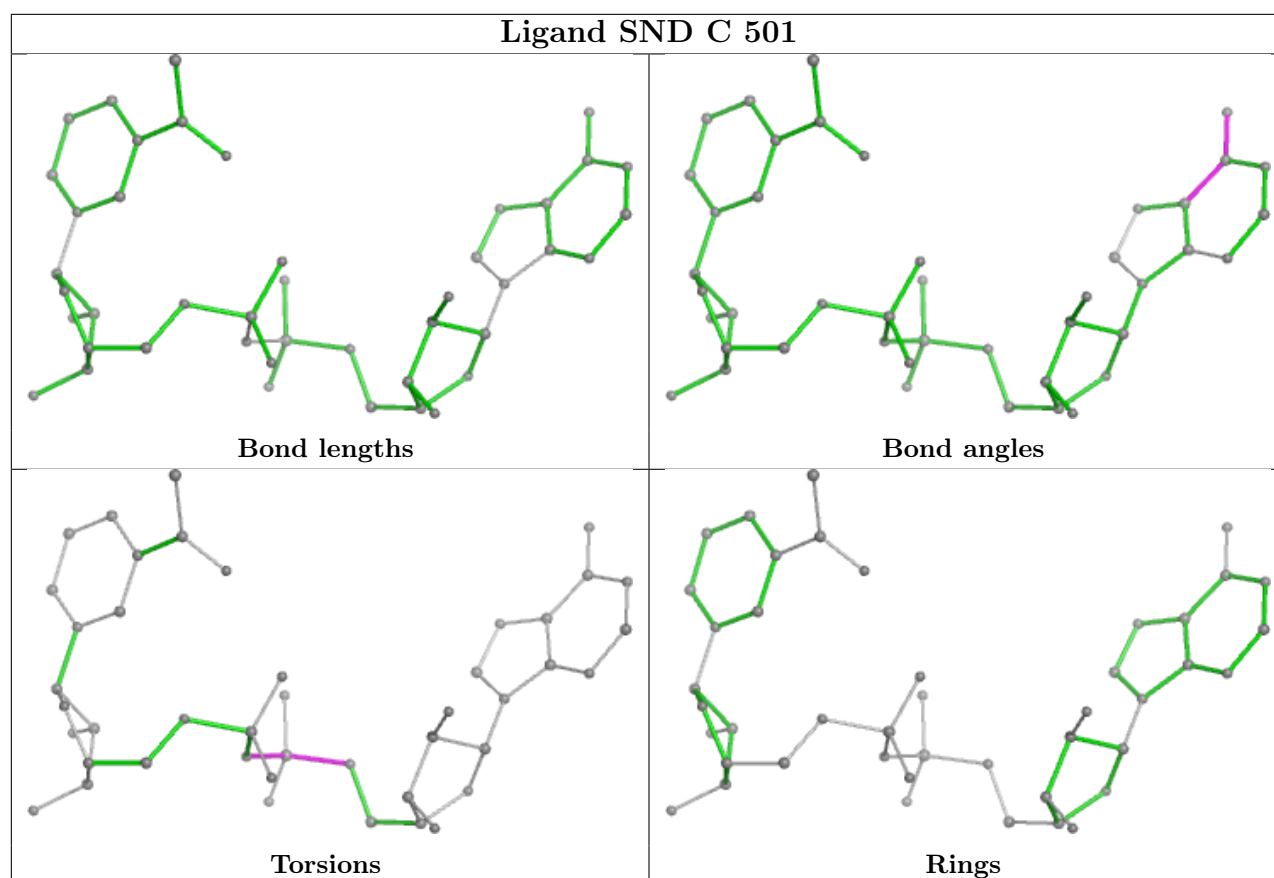












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/489 (95%)	-0.05	25 (5%) 32 31	6, 19, 47, 85	5 (1%)
1	B	466/489 (95%)	-0.08	20 (4%) 40 39	7, 19, 47, 84	9 (1%)
1	C	464/489 (94%)	-0.08	21 (4%) 39 37	7, 19, 48, 76	5 (1%)
1	D	466/489 (95%)	-0.07	24 (5%) 34 32	6, 20, 48, 86	4 (0%)
All	All	1861/1956 (95%)	-0.07	90 (4%) 36 35	6, 19, 48, 86	23 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ASN	6.0
1	C	227	GLY	5.2
1	B	428	ILE	5.0
1	D	428	ILE	5.0
1	B	225	ASP	4.9
1	A	32	LYS	4.7
1	C	428	ILE	4.5
1	A	9	TRP	4.5
1	D	224	GLY	4.4
1	B	427	ASP	4.3
1	A	134	ILE	4.2
1	B	226	ASN	4.2
1	A	133	ARG	4.0
1	A	128	LYS	4.0
1	A	129	SER	3.9
1	C	429	HIS	3.9
1	C	412	ALA	3.9
1	A	224	GLY	3.9
1	A	428	ILE	3.9
1	B	227	GLY	3.8
1	D	129	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	230	LEU	3.6
1	A	30	GLN	3.6
1	D	227	GLY	3.6
1	C	9	TRP	3.6
1	D	128	LYS	3.5
1	B	9	TRP	3.5
1	C	224	GLY	3.5
1	C	102	ASN	3.4
1	D	427	ASP	3.4
1	C	129	SER	3.4
1	A	228	GLU	3.4
1	D	429	HIS	3.4
1	C	230	LEU	3.3
1	D	225	ASP	3.3
1	B	228	GLU	3.3
1	D	228	GLU	3.3
1	D	189	PHE	3.3
1	B	129	SER	3.3
1	B	429	HIS	3.3
1	C	0	THR	3.2
1	B	0	THR	3.1
1	D	143	PRO	3.1
1	A	230	LEU	3.0
1	D	9	TRP	3.0
1	B	314	LEU	2.9
1	C	312	LYS	2.9
1	A	33	LEU	2.9
1	B	189	PHE	2.9
1	D	314	LEU	2.8
1	C	410	ASP	2.8
1	A	189	PHE	2.7
1	C	228	GLU	2.7
1	D	411	GLN	2.7
1	D	230	LEU	2.7
1	B	142	GLU	2.6
1	C	143	PRO	2.6
1	A	101	ASN	2.6
1	C	314	LEU	2.6
1	A	316	PHE	2.5
1	B	132	GLY	2.5
1	D	0	THR	2.5
1	A	429	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	142	GLU	2.5
1	D	316	PHE	2.5
1	A	412	ALA	2.4
1	C	310	PHE	2.4
1	B	426	ALA	2.4
1	A	474	ASP	2.4
1	C	127	GLY	2.3
1	B	101	ASN	2.3
1	A	314	LEU	2.2
1	C	189	PHE	2.2
1	D	229	SER	2.2
1	C	101	ASN	2.2
1	D	102	ASN	2.2
1	D	426	ALA	2.2
1	A	130	ARG	2.1
1	A	410	ASP	2.1
1	B	75	ASP	2.1
1	A	0	THR	2.1
1	A	75	ASP	2.1
1	A	127	GLY	2.1
1	D	412	ALA	2.1
1	A	132	GLY	2.1
1	B	410	ASP	2.0
1	D	101	ASN	2.0
1	B	224	GLY	2.0
1	C	132	GLY	2.0
1	C	426	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

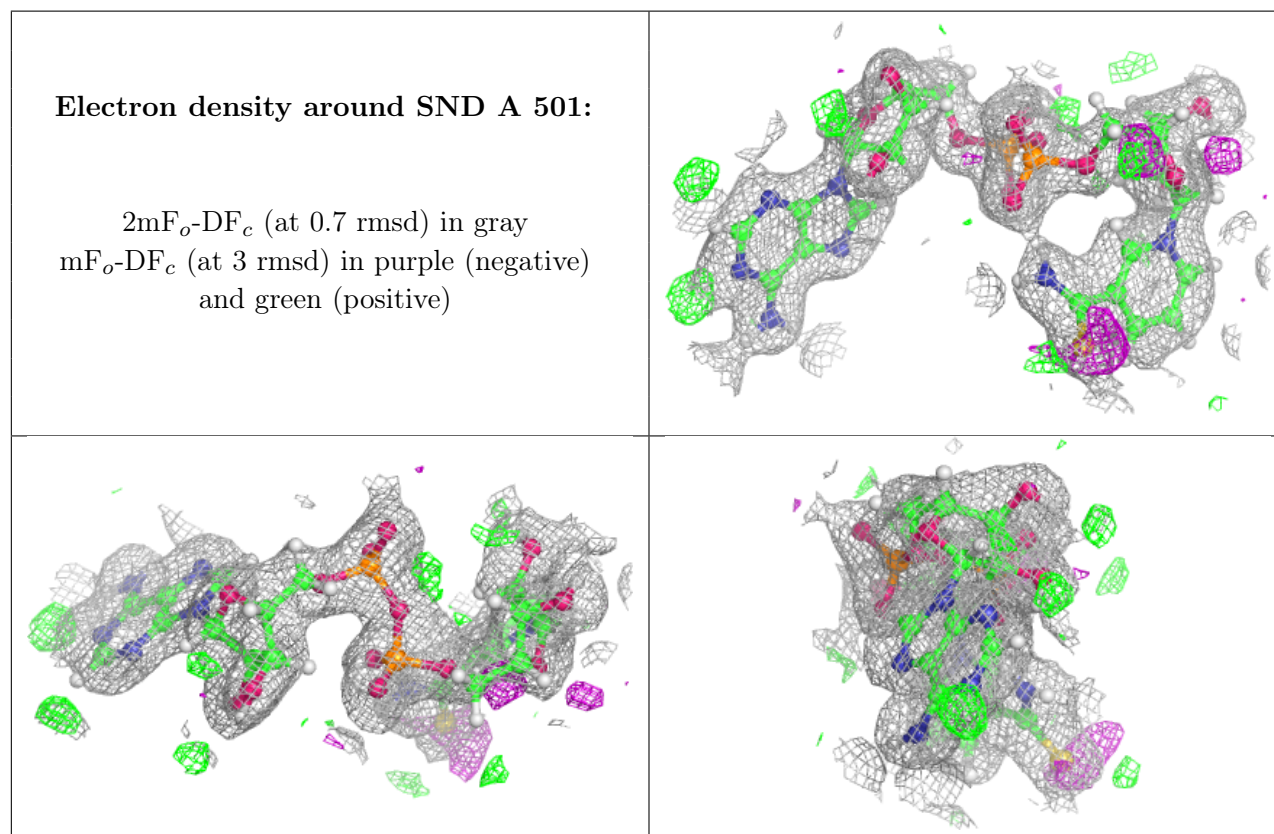
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

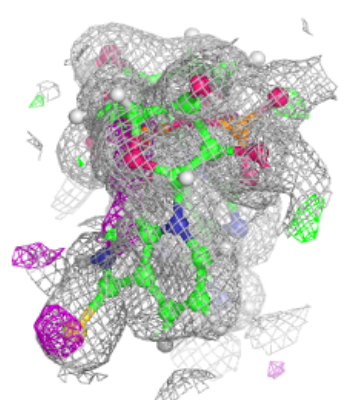
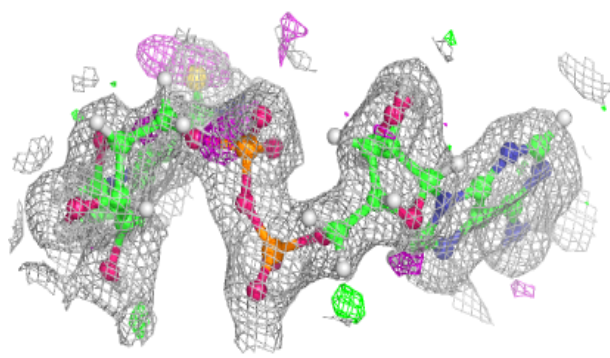
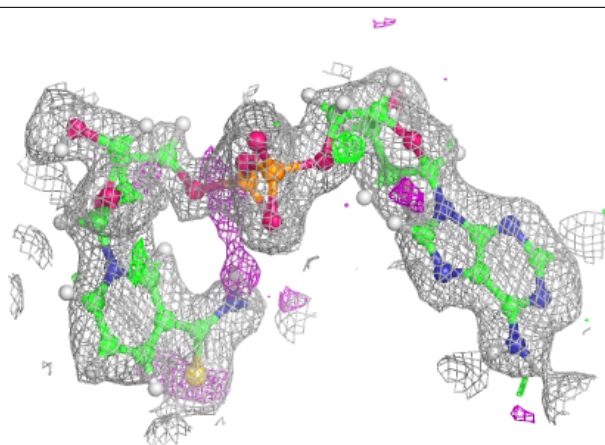
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	504	6/6	0.86	0.15	15,35,52,62	0
3	GOL	A	503	6/6	0.87	0.16	17,37,45,48	0
3	GOL	C	503	6/6	0.88	0.21	7,40,48,48	0
3	GOL	D	502	6/6	0.90	0.12	9,28,40,48	0
2	SND	A	501	44/44	0.96	0.07	6,18,26,31	0
2	SND	B	501	44/44	0.96	0.07	8,16,23,27	0
2	SND	C	501	44/44	0.96	0.07	6,16,25,30	0
2	SND	D	501	44/44	0.96	0.07	8,15,25,29	0
2	SND	B	503	44/44	0.97	0.05	5,9,17,39	0
2	SND	A	502	44/44	0.97	0.06	6,10,15,33	0
2	SND	C	502	44/44	0.97	0.05	5,10,15,31	0
2	SND	B	502	44/44	0.97	0.05	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.

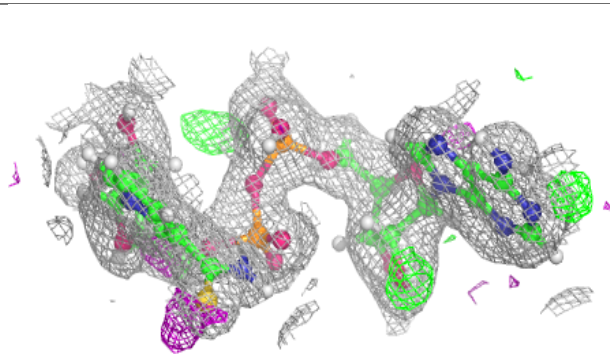
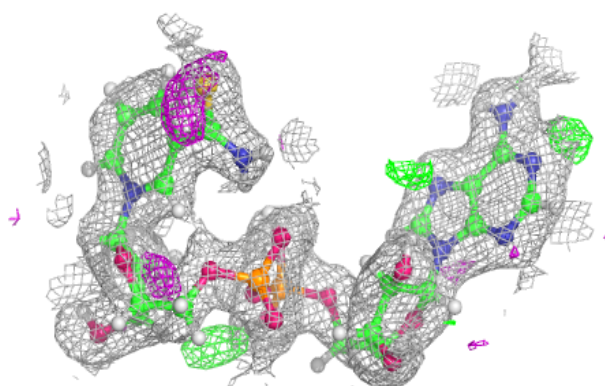


Electron density around SND B 501:

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

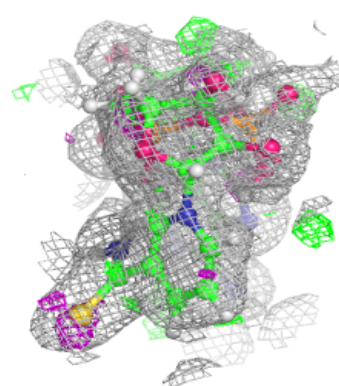
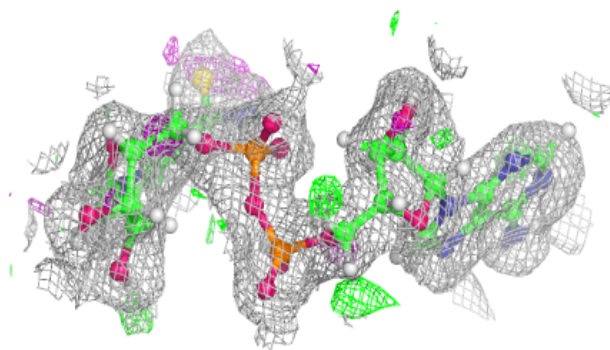
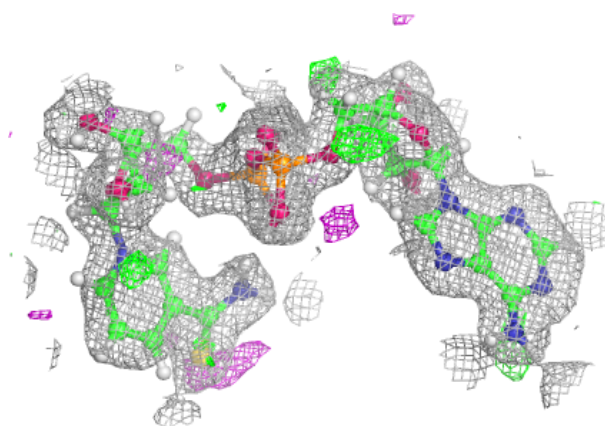
**Electron density around SND C 501:**

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



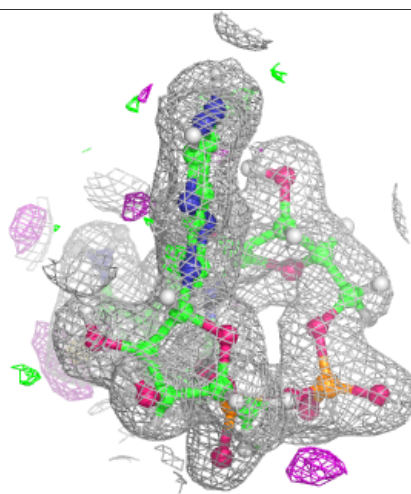
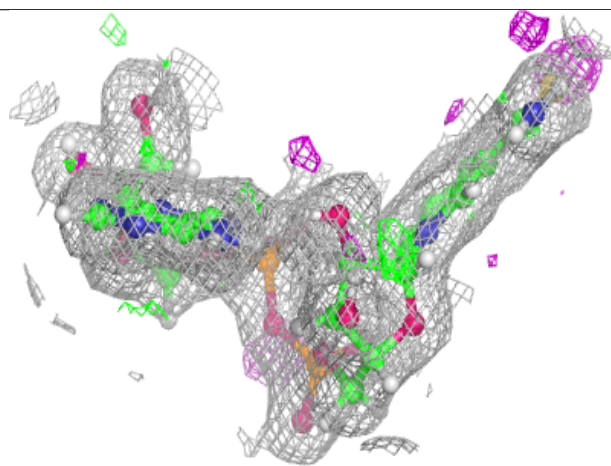
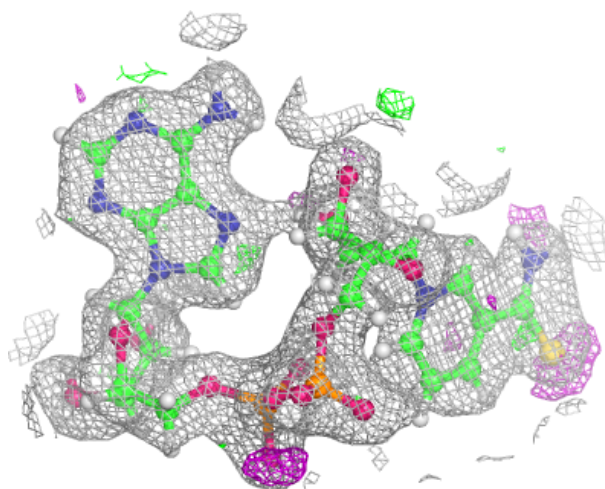
Electron density around SND D 501:

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



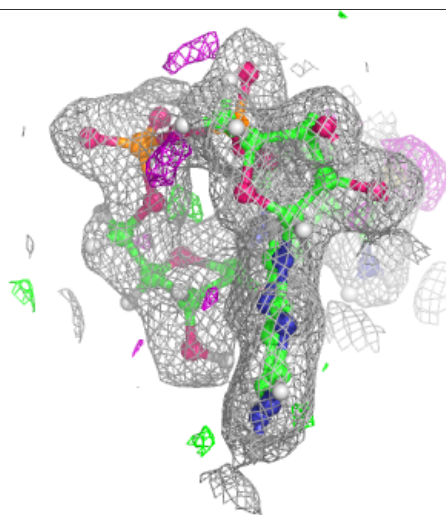
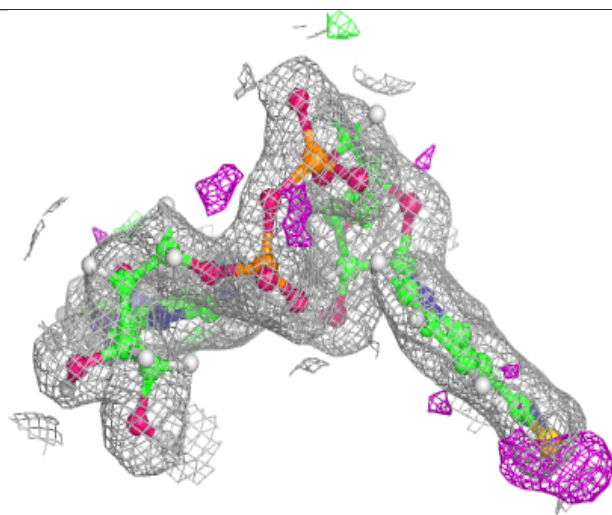
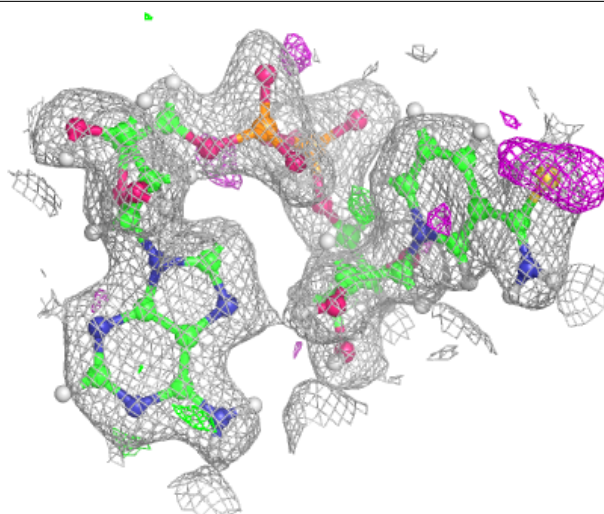
Electron density around SND B 503:

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



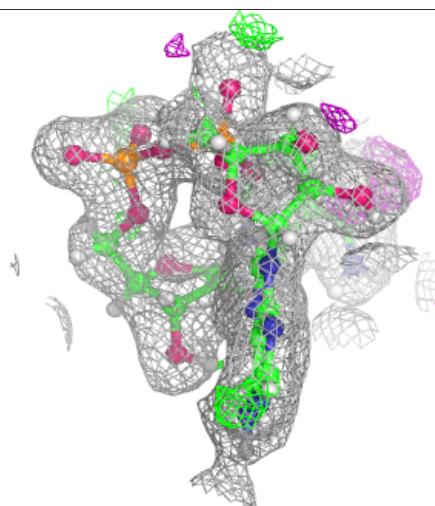
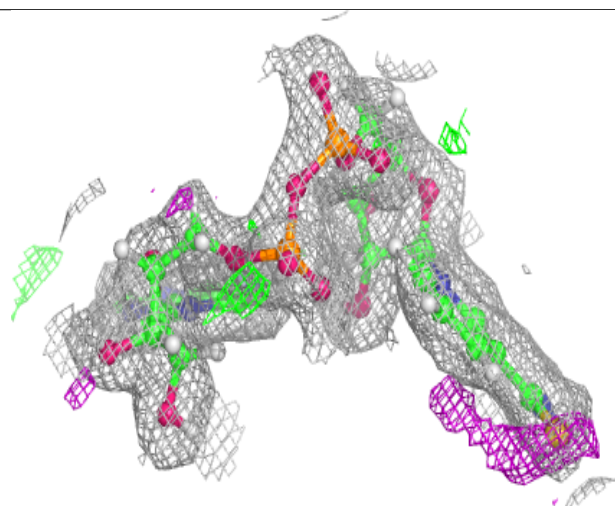
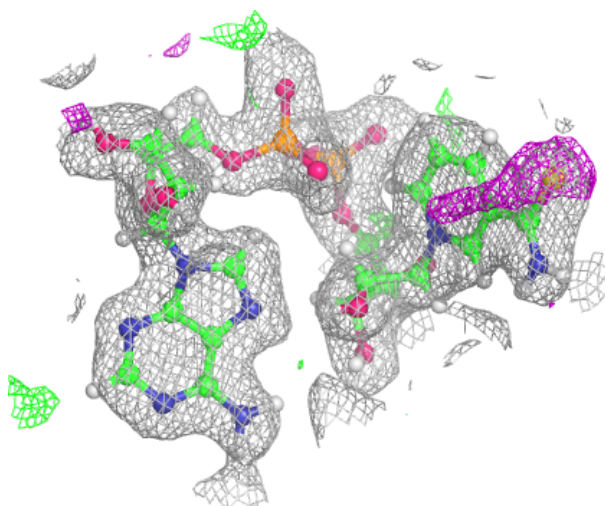
Electron density around SND A 502:

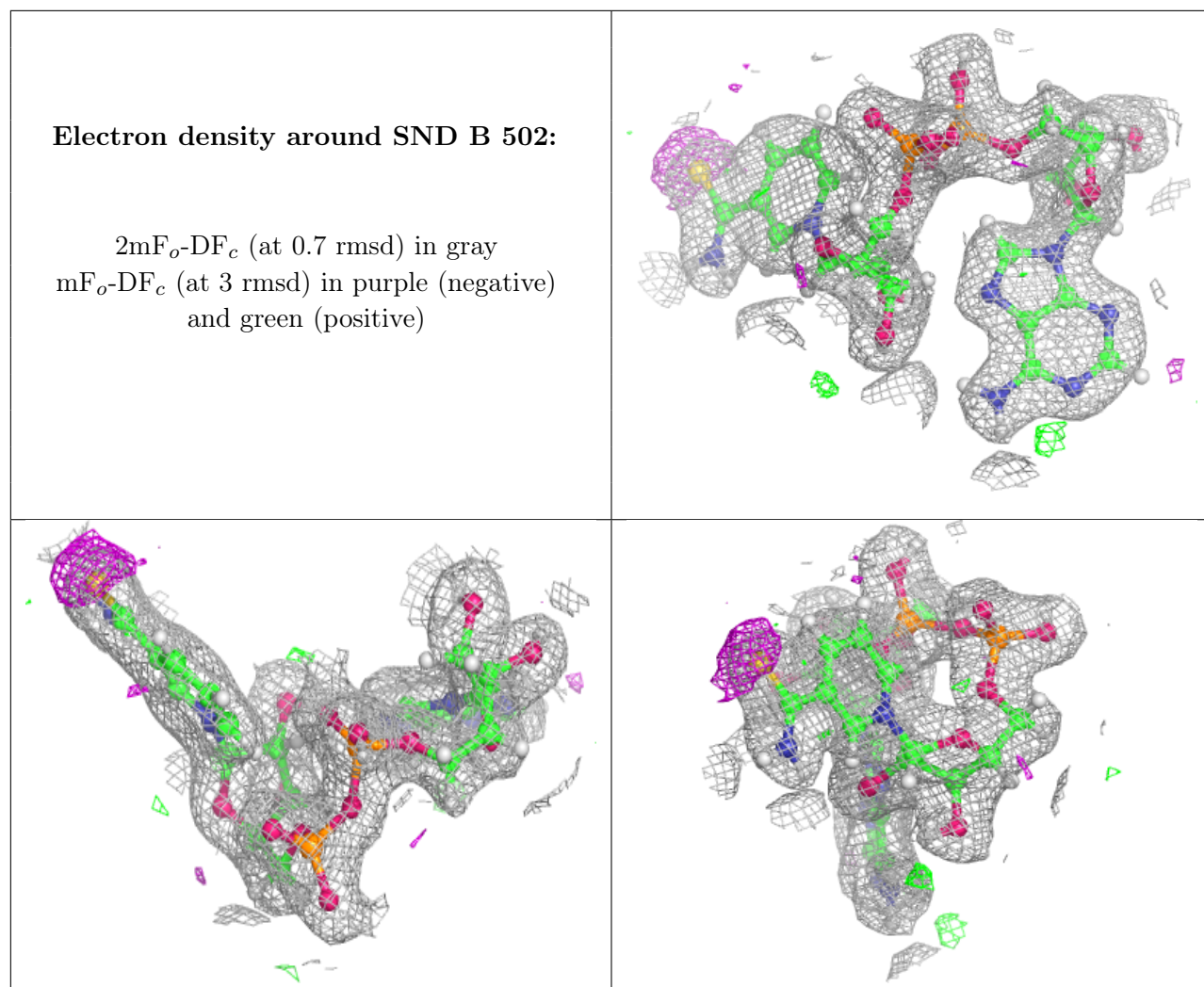
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SND C 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 ⓘ

There are no such residues in this entry.