



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 06:33 AM EDT

PDB ID : 3PKJ  
Title : Human SIRT6 crystal structure in complex with 2'-N-Acetyl ADP ribose  
Authors : Pan, P.W.; Dong, A.; Qiu, W.; Loppnau, P.; Wang, J.; Ravichandran, M.; Walker, J.R.; Bountra, C.; Weigelt, J.; Arrowsmith, C.H.; Min, J.; Edwards, A.M.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-11-11  
Resolution : 2.12 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.

The types of validation reports are described at

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

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

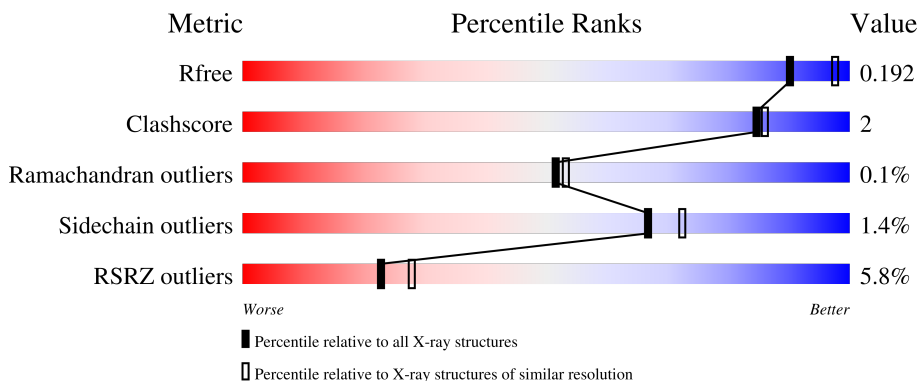
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	355	
1	B	355	
1	C	355	
1	D	355	

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Mol	Chain	Length	Quality of chain
1	E	355	
1	F	355	

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	SO4	F	1001	-	-	-	X
5	UNX	A	355	-	-	-	X
5	UNX	B	358	-	-	-	X
5	UNX	B	359	-	-	-	X
5	UNX	C	359	-	-	-	X
5	UNX	C	363	-	-	-	X
5	UNX	C	365	-	-	-	X
5	UNX	D	356	-	-	-	X
5	UNX	D	357	-	-	-	X
5	UNX	E	358	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13208 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.

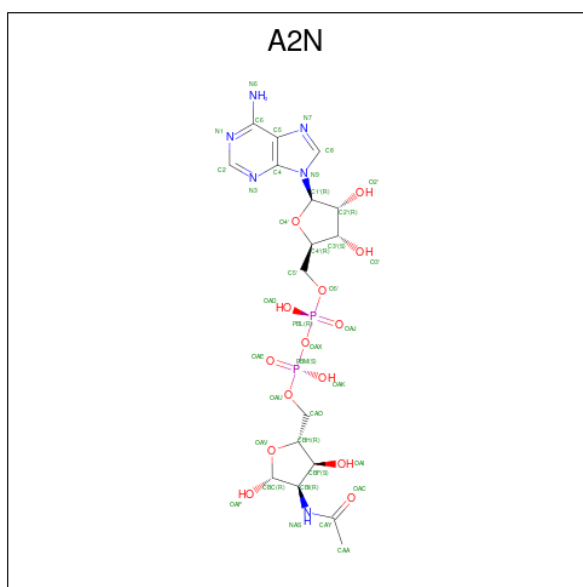
- Molecule 1 is a protein called NAD-dependent deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	Total 2050	C 1293	N 364	O 382	S 11	0	0	0
1	B	280	Total 2091	C 1314	N 371	O 395	S 11	0	0	0
1	C	276	Total 2083	C 1307	N 377	O 388	S 11	0	0	0
1	D	276	Total 2067	C 1307	N 371	O 379	S 10	0	0	0
1	E	278	Total 2049	C 1295	N 358	O 385	S 11	0	0	0
1	F	277	Total 2038	C 1281	N 367	O 379	S 11	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8N6T7
A	265	GLU	LYS	engineered mutation	UNP Q8N6T7
B	-1	GLY	-	expression tag	UNP Q8N6T7
B	265	GLU	LYS	engineered mutation	UNP Q8N6T7
C	-1	GLY	-	expression tag	UNP Q8N6T7
C	265	GLU	LYS	engineered mutation	UNP Q8N6T7
D	-1	GLY	-	expression tag	UNP Q8N6T7
D	265	GLU	LYS	engineered mutation	UNP Q8N6T7
E	-1	GLY	-	expression tag	UNP Q8N6T7
E	265	GLU	LYS	engineered mutation	UNP Q8N6T7
F	-1	GLY	-	expression tag	UNP Q8N6T7
F	265	GLU	LYS	engineered mutation	UNP Q8N6T7

- Molecule 2 is [(2R,3S,4R,5R)-4-(acetylamino)-3,5-dihydroxytetrahydrofuran-2-yl]methyl [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: A2N) (formula: C<sub>17</sub>H<sub>26</sub>N<sub>6</sub>O<sub>14</sub>P<sub>2</sub>).

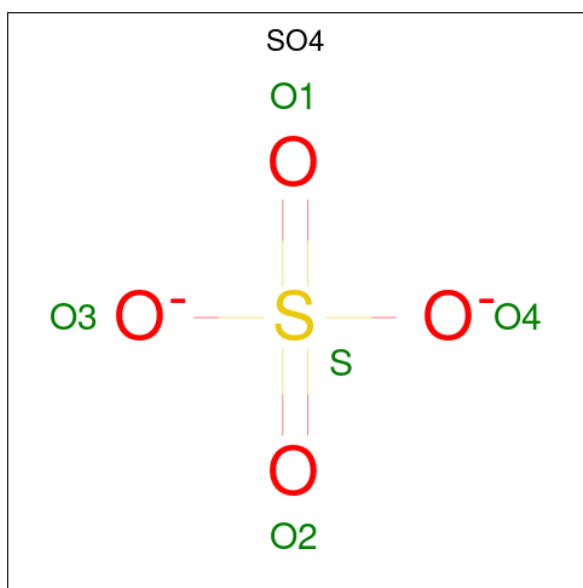


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	39	17	6	14	2	0	0
2	B	1	39	17	6	14	2	0	0
2	C	1	39	17	6	14	2	0	0
2	D	1	39	17	6	14	2	0	0
2	E	1	39	17	6	14	2	0	0
2	F	1	39	17	6	14	2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0
3	F	1	1	1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

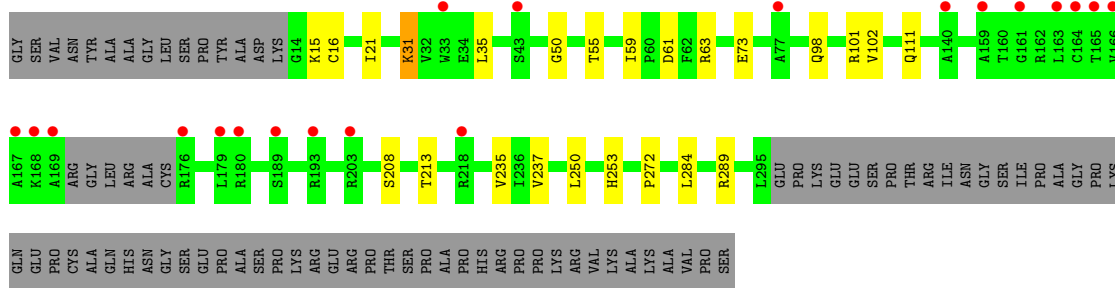
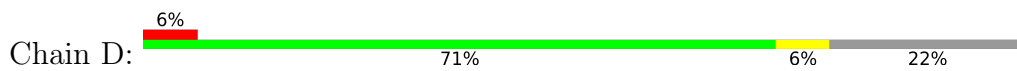
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total X 3 3	0	0
5	B	5	Total X 5 5	0	0
5	C	12	Total X 12 12	0	0
5	D	3	Total X 3 3	0	0
5	E	4	Total X 4 4	0	0
5	F	8	Total X 8 8	0	0

- Molecule 6 is water.

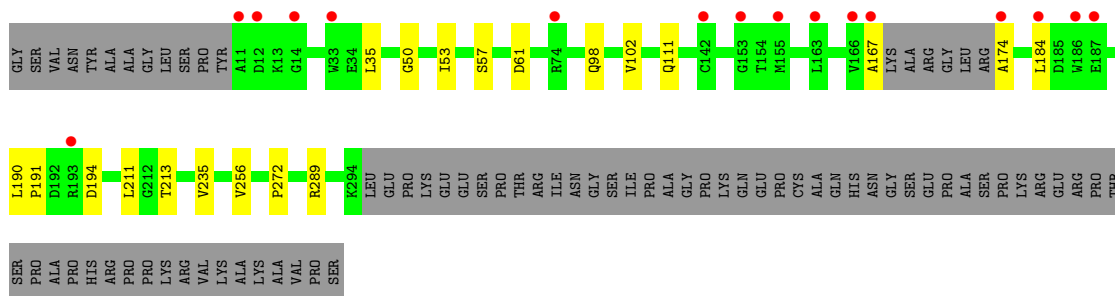
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	90	Total O 91 91	0	1
6	B	86	Total O 88 88	0	2
6	C	70	Total O 71 71	0	1
6	D	93	Total O 93 93	0	0
6	E	78	Total O 80 80	0	2
6	F	69	Total O 72 72	0	3



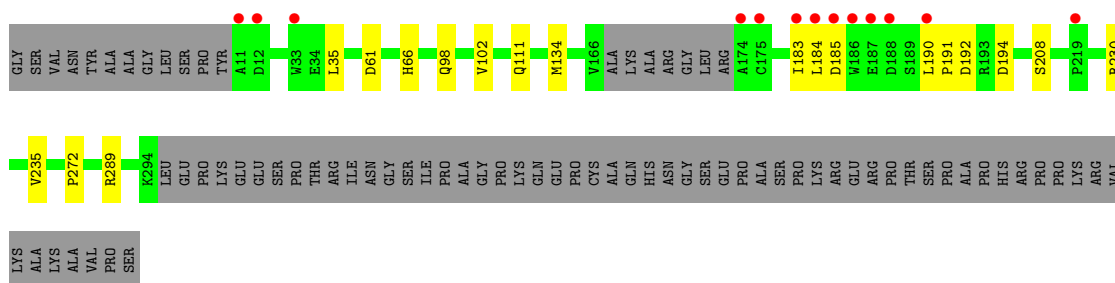




• Molecule 1: NAD-dependent deacetylase sirtuin-6



• Molecule 1: NAD-dependent deacetylase sirtuin-6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.04Å 135.78Å 89.11Å 90.00° 120.02° 90.00°	Depositor
Resolution (Å)	20.50 – 2.12 20.50 – 2.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.50-2.12) 96.1 (20.50-2.12)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.11Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.234 , 0.265 0.187 , 0.192	Depositor DCC
$R_{free}$ test set	4924 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 21.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.247 for l,k,-h-l 0.247 for -h-l,k,h 0.166 for h,-k,-h-l 0.164 for l,-k,h 0.145 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: UNX, ZN, A2N, SO4

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	0.50	0/2097	0.55	0/2865
1	B	0.49	0/2138	0.56	0/2917
1	C	0.50	0/2130	0.55	0/2902
1	D	0.51	0/2114	0.57	0/2884
1	E	0.49	0/2096	0.56	0/2863
1	F	0.50	0/2085	0.56	0/2843
All	All	0.50	0/12660	0.56	0/17274

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	2050	0	1952	3	0
1	B	2091	0	1989	9	0
1	C	2083	0	2002	9	0
1	D	2067	0	2002	13	0
1	E	2049	0	1941	11	0
1	F	2038	0	1895	9	0
2	A	39	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	24	2	0
2	C	39	0	24	1	0
2	D	39	0	24	2	0
2	E	39	0	24	3	0
2	F	39	0	24	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	15	0	0	0	0
4	F	15	0	0	0	0
5	A	3	0	0	0	0
5	B	5	0	0	0	0
5	C	12	0	0	0	0
5	D	3	0	0	0	0
5	E	4	0	0	0	0
5	F	8	0	0	0	0
6	A	91	0	0	0	0
6	B	88	0	0	0	0
6	C	71	0	0	0	0
6	D	93	0	0	1	0
6	E	80	0	0	0	0
6	F	72	0	0	0	0
All	All	13208	0	11925	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (57) 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:F:134:MET:HA	1:F:183:ILE:HD11	1.83	0.60
1:F:184:LEU:HD21	1:F:190:LEU:HA	1.85	0.59
1:F:184:LEU:HD11	1:F:191:PRO:HD3	1.86	0.56
1:F:35:LEU:HD13	1:F:235:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD13	1:D:235:VAL:HG11	1.89	0.54
1:E:35:LEU:HD13	1:E:235:VAL:HG11	1.89	0.54
1:C:245:ASP:HB3	1:D:73:GLU:HG3	1.90	0.53
1:A:35:LEU:HD13	1:A:235:VAL:HG11	1.91	0.53
1:E:102:VAL:HB	1:E:289:ARG:HB3	1.94	0.50
1:E:191:PRO:HG2	1:E:194:ASP:HB2	1.93	0.49
1:C:35:LEU:HD13	1:C:235:VAL:HG11	1.94	0.49
1:F:102:VAL:HB	1:F:289:ARG:HB3	1.94	0.49
1:E:50:GLY:HA3	1:E:213:THR:HB	1.95	0.48
1:B:102:VAL:HB	1:B:289:ARG:HB3	1.94	0.48
2:B:1000:A2N:HAA	2:B:1000:A2N:HBI	1.66	0.48
1:C:102:VAL:HB	1:C:289:ARG:HB3	1.95	0.47
1:A:53:ILE:HG22	1:A:256:VAL:HG21	1.95	0.47
1:B:51:ALA:HB1	1:B:61:ASP:HA	1.97	0.47
2:E:1000:A2N:HBI	2:E:1000:A2N:HAA	1.66	0.47
1:D:102:VAL:HB	1:D:289:ARG:HB3	1.95	0.46
1:E:167:ALA:HA	1:E:174:ALA:HA	1.97	0.46
1:B:27:GLU:HG2	1:B:31:LYS:HE3	1.98	0.46
1:D:31:LYS:HG3	1:D:250:LEU:HD11	1.98	0.45
1:D:101:ARG:HH12	1:D:284:LEU:HD12	1.82	0.45
1:B:167:ALA:HA	1:B:174:ALA:HA	1.98	0.45
1:B:98:GLN:HB2	1:B:272:PRO:HD3	1.99	0.44
2:A:1000:A2N:HBI	2:A:1000:A2N:HAA	1.67	0.44
1:B:50:GLY:HA3	1:B:213:THR:HB	2.00	0.44
1:D:16:CYS:SG	1:D:63:ARG:HG2	2.57	0.44
1:E:184:LEU:HD11	1:E:190:LEU:HA	1.99	0.44
1:E:98:GLN:HB2	1:E:272:PRO:HD3	2.00	0.43
1:F:98:GLN:HB2	1:F:272:PRO:HD3	2.00	0.43
1:B:136:VAL:HG22	1:B:147:VAL:HG22	2.01	0.43
1:E:211:LEU:HB3	1:E:256:VAL:HG21	2.01	0.43
1:D:237:VAL:CG1	6:D:417:HOH:O	2.66	0.42
1:C:50:GLY:HA3	1:C:213:THR:HB	2.02	0.42
2:F:1000:A2N:HAA	2:F:1000:A2N:HBI	1.66	0.42
1:C:111:GLN:OE1	2:C:1000:A2N:HAO	2.20	0.42
1:D:21:ILE:HB	1:D:253:HIS:CD2	2.55	0.42
1:D:55:THR:HA	1:D:59:ILE:O	2.20	0.42
1:D:61:ASP:OD1	2:D:1000:A2N:H8	2.20	0.42
1:F:191:PRO:HG2	1:F:194:ASP:HB2	2.01	0.42
1:E:61:ASP:OD1	2:E:1000:A2N:H8	2.20	0.41
1:F:111:GLN:OE1	2:F:1000:A2N:HAO	2.20	0.41
1:C:53:ILE:HA	1:C:256:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLN:HB2	1:C:272:PRO:HD3	2.01	0.41
1:E:53:ILE:HG22	1:E:256:VAL:HG11	2.02	0.41
1:B:35:LEU:HD13	1:B:235:VAL:HG11	2.02	0.41
1:A:111:GLN:OE1	2:A:1000:A2N:HAO	2.21	0.41
1:C:21:ILE:HB	1:C:253:HIS:CD2	2.56	0.41
1:D:111:GLN:OE1	2:D:1000:A2N:HAO	2.21	0.41
1:D:98:GLN:HB2	1:D:272:PRO:HD3	2.02	0.41
1:B:111:GLN:OE1	2:B:1000:A2N:HAO	2.21	0.40
1:C:191:PRO:HG2	1:C:194:ASP:HB2	2.04	0.40
1:F:61:ASP:OD1	2:F:1000:A2N:H8	2.21	0.40
1:E:111:GLN:OE1	2:E:1000:A2N:HAO	2.21	0.40
1:D:50:GLY:HA3	1:D:213:THR:HB	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/355 (77%)	271 (99%)	2 (1%)	0	100	100
1	B	276/355 (78%)	274 (99%)	2 (1%)	0	100	100
1	C	272/355 (77%)	270 (99%)	2 (1%)	0	100	100
1	D	272/355 (77%)	270 (99%)	2 (1%)	0	100	100
1	E	274/355 (77%)	270 (98%)	4 (2%)	0	100	100
1	F	274/355 (77%)	270 (98%)	3 (1%)	1 (0%)	34	32
All	All	1641/2130 (77%)	1625 (99%)	15 (1%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	192	ASP

### 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	208/297 (70%)	205 (99%)	3 (1%)	67	72
1	B	213/297 (72%)	210 (99%)	3 (1%)	67	72
1	C	215/297 (72%)	212 (99%)	3 (1%)	67	72
1	D	212/297 (71%)	209 (99%)	3 (1%)	67	72
1	E	205/297 (69%)	204 (100%)	1 (0%)	88	92
1	F	196/297 (66%)	192 (98%)	4 (2%)	55	59
All	All	1249/1782 (70%)	1232 (99%)	17 (1%)	67	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	187	GLU
1	A	229	ARG
1	B	57	SER
1	B	208	SER
1	B	265	GLU
1	C	38	LEU
1	C	208	SER
1	C	228	LYS
1	D	15	LYS
1	D	31	LYS
1	D	208	SER
1	E	57	SER
1	F	66	HIS
1	F	185	ASP
1	F	208	SER
1	F	230	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 59 ligands modelled in this entry, 6 are monoatomic and 35 are unknown - leaving 18 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
2	A2N	E	1000	-	37,42,42	0.97	3 (8%)	39,64,64	1.25	3 (7%)
4	SO4	E	1002	-	4,4,4	0.32	0	6,6,6	0.12	0
2	A2N	B	1000	-	37,42,42	1.02	2 (5%)	39,64,64	1.27	4 (10%)
2	A2N	C	1000	-	37,42,42	0.91	2 (5%)	39,64,64	1.38	5 (12%)
2	A2N	F	1000	-	37,42,42	1.13	3 (8%)	39,64,64	1.26	3 (7%)
4	SO4	B	1005	-	4,4,4	0.06	0	6,6,6	0.11	0
4	SO4	B	1011	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	E	1010	-	4,4,4	0.20	0	6,6,6	0.10	0
4	SO4	F	1001	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	B	1006	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	A	1008	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	E	1007	-	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	F	1004	-	4,4,4	0.17	0	6,6,6	0.06	0
4	SO4	F	1009	-	4,4,4	0.51	0	6,6,6	0.16	0
2	A2N	D	1000	-	37,42,42	0.97	2 (5%)	39,64,64	1.39	5 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	C	1003	-	4,4,4	0.28	0	6,6,6	0.10	0
2	A2N	A	1000	-	37,42,42	1.00	2 (5%)	39,64,64	1.26	2 (5%)
4	SO4	D	355	-	4,4,4	0.20	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2N	E	1000	-	-	10/22/58/58	0/4/4/4
2	A2N	B	1000	-	-	10/22/58/58	0/4/4/4
2	A2N	C	1000	-	-	8/22/58/58	0/4/4/4
2	A2N	F	1000	-	-	10/22/58/58	0/4/4/4
2	A2N	D	1000	-	-	9/22/58/58	0/4/4/4
2	A2N	A	1000	-	-	10/22/58/58	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1000	A2N	PBL-OAJ	2.91	1.61	1.50
2	E	1000	A2N	PBL-OAJ	2.85	1.61	1.50
2	F	1000	A2N	OAV-CBC	2.73	1.46	1.43
2	B	1000	A2N	PBL-OAJ	2.55	1.59	1.50
2	C	1000	A2N	OAV-CBC	2.54	1.46	1.43
2	A	1000	A2N	OAV-CBC	2.52	1.46	1.43
2	B	1000	A2N	OAV-CBC	2.47	1.46	1.43
2	D	1000	A2N	OAV-CBC	2.46	1.46	1.43
2	C	1000	A2N	PBL-OAJ	2.45	1.59	1.50
2	A	1000	A2N	PBL-OAJ	2.21	1.58	1.50
2	D	1000	A2N	PBL-OAJ	2.21	1.58	1.50
2	E	1000	A2N	OAV-CBC	2.18	1.45	1.43
2	F	1000	A2N	C2'-C1'	-2.15	1.50	1.53
2	E	1000	A2N	CAA-CAY	2.01	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	A2N	N3-C2-N1	-4.80	121.18	128.68
2	C	1000	A2N	N3-C2-N1	-4.76	121.24	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	A2N	N3-C2-N1	-4.73	121.29	128.68
2	A	1000	A2N	N3-C2-N1	-4.68	121.36	128.68
2	F	1000	A2N	N3-C2-N1	-4.53	121.61	128.68
2	E	1000	A2N	N3-C2-N1	-4.45	121.73	128.68
2	C	1000	A2N	OAC-CAY-NAS	2.68	126.89	121.95
2	A	1000	A2N	PBM-OAX-PBL	-2.66	123.70	132.83
2	E	1000	A2N	PBM-OAX-PBL	-2.64	123.76	132.83
2	D	1000	A2N	OAC-CAY-NAS	2.56	126.66	121.95
2	C	1000	A2N	PBM-OAX-PBL	-2.56	124.06	132.83
2	F	1000	A2N	PBM-OAX-PBL	-2.54	124.11	132.83
2	B	1000	A2N	PBM-OAX-PBL	-2.52	124.17	132.83
2	F	1000	A2N	O4'-C1'-C2'	-2.45	103.35	106.93
2	D	1000	A2N	PBM-OAX-PBL	-2.34	124.81	132.83
2	D	1000	A2N	O4'-C1'-C2'	-2.29	103.58	106.93
2	C	1000	A2N	O4'-C1'-C2'	-2.21	103.69	106.93
2	D	1000	A2N	CAA-CAY-NAS	-2.17	112.42	116.10
2	C	1000	A2N	CAA-CAY-NAS	-2.13	112.50	116.10
2	B	1000	A2N	C4-C5-N7	-2.10	107.21	109.40
2	E	1000	A2N	O4'-C1'-C2'	-2.04	103.95	106.93
2	B	1000	A2N	O4'-C1'-C2'	-2.03	103.96	106.93

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	A2N	CAO-OAU-PBM-OAE
2	A	1000	A2N	CAO-OAU-PBM-OAK
2	A	1000	A2N	CAO-OAU-PBM-OAX
2	B	1000	A2N	OAU-CAO-CBH-OAV
2	B	1000	A2N	CAO-OAU-PBM-OAE
2	B	1000	A2N	CAO-OAU-PBM-OAK
2	B	1000	A2N	CAO-OAU-PBM-OAX
2	C	1000	A2N	OAU-CAO-CBH-OAV
2	C	1000	A2N	CAO-OAU-PBM-OAE
2	C	1000	A2N	CAO-OAU-PBM-OAK
2	C	1000	A2N	CAO-OAU-PBM-OAX
2	D	1000	A2N	OAU-CAO-CBH-OAV
2	D	1000	A2N	CAO-OAU-PBM-OAE
2	D	1000	A2N	CAO-OAU-PBM-OAK
2	D	1000	A2N	CAO-OAU-PBM-OAX
2	E	1000	A2N	CAO-OAU-PBM-OAE
2	E	1000	A2N	CAO-OAU-PBM-OAK

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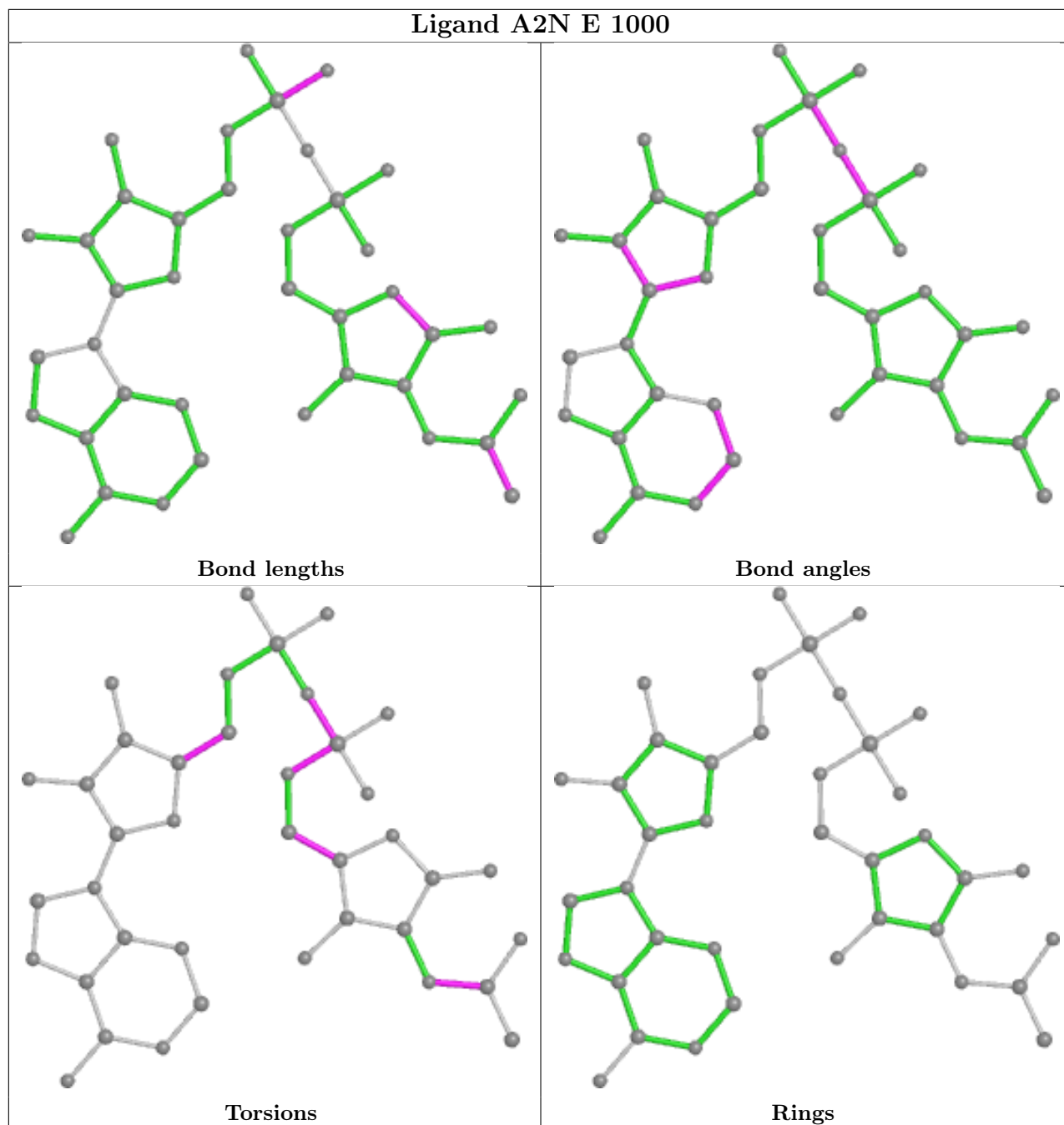
Mol	Chain	Res	Type	Atoms
2	E	1000	A2N	CAO-OAU-PBM-OAX
2	F	1000	A2N	CAO-OAU-PBM-OAE
2	F	1000	A2N	CAO-OAU-PBM-OAK
2	F	1000	A2N	CAO-OAU-PBM-OAX
2	A	1000	A2N	OAU-CAO-CBH-OAV
2	B	1000	A2N	OAU-CAO-CBH-CBF
2	C	1000	A2N	OAU-CAO-CBH-CBF
2	D	1000	A2N	OAU-CAO-CBH-CBF
2	E	1000	A2N	OAU-CAO-CBH-OAV
2	E	1000	A2N	OAU-CAO-CBH-CBF
2	F	1000	A2N	OAU-CAO-CBH-OAV
2	F	1000	A2N	OAU-CAO-CBH-CBF
2	A	1000	A2N	CAA-CAY-NAS-CBI
2	A	1000	A2N	OAC-CAY-NAS-CBI
2	B	1000	A2N	CAA-CAY-NAS-CBI
2	B	1000	A2N	OAC-CAY-NAS-CBI
2	E	1000	A2N	CAA-CAY-NAS-CBI
2	E	1000	A2N	OAC-CAY-NAS-CBI
2	F	1000	A2N	CAA-CAY-NAS-CBI
2	F	1000	A2N	OAC-CAY-NAS-CBI
2	A	1000	A2N	OAU-CAO-CBH-CBF
2	A	1000	A2N	PBL-OAX-PBM-OAE
2	B	1000	A2N	PBL-OAX-PBM-OAE
2	C	1000	A2N	PBL-OAX-PBM-OAE
2	D	1000	A2N	PBL-OAX-PBM-OAE
2	E	1000	A2N	PBL-OAX-PBM-OAE
2	F	1000	A2N	PBL-OAX-PBM-OAE
2	E	1000	A2N	PBL-OAX-PBM-OAK
2	D	1000	A2N	PBM-OAX-PBL-O5'
2	A	1000	A2N	O4'-C4'-C5'-O5'
2	D	1000	A2N	O4'-C4'-C5'-O5'
2	F	1000	A2N	O4'-C4'-C5'-O5'
2	A	1000	A2N	PBL-OAX-PBM-OAK
2	B	1000	A2N	PBL-OAX-PBM-OAK
2	C	1000	A2N	PBL-OAX-PBM-OAK
2	D	1000	A2N	PBL-OAX-PBM-OAK
2	F	1000	A2N	PBL-OAX-PBM-OAK
2	B	1000	A2N	O4'-C4'-C5'-O5'
2	C	1000	A2N	O4'-C4'-C5'-O5'
2	E	1000	A2N	O4'-C4'-C5'-O5'

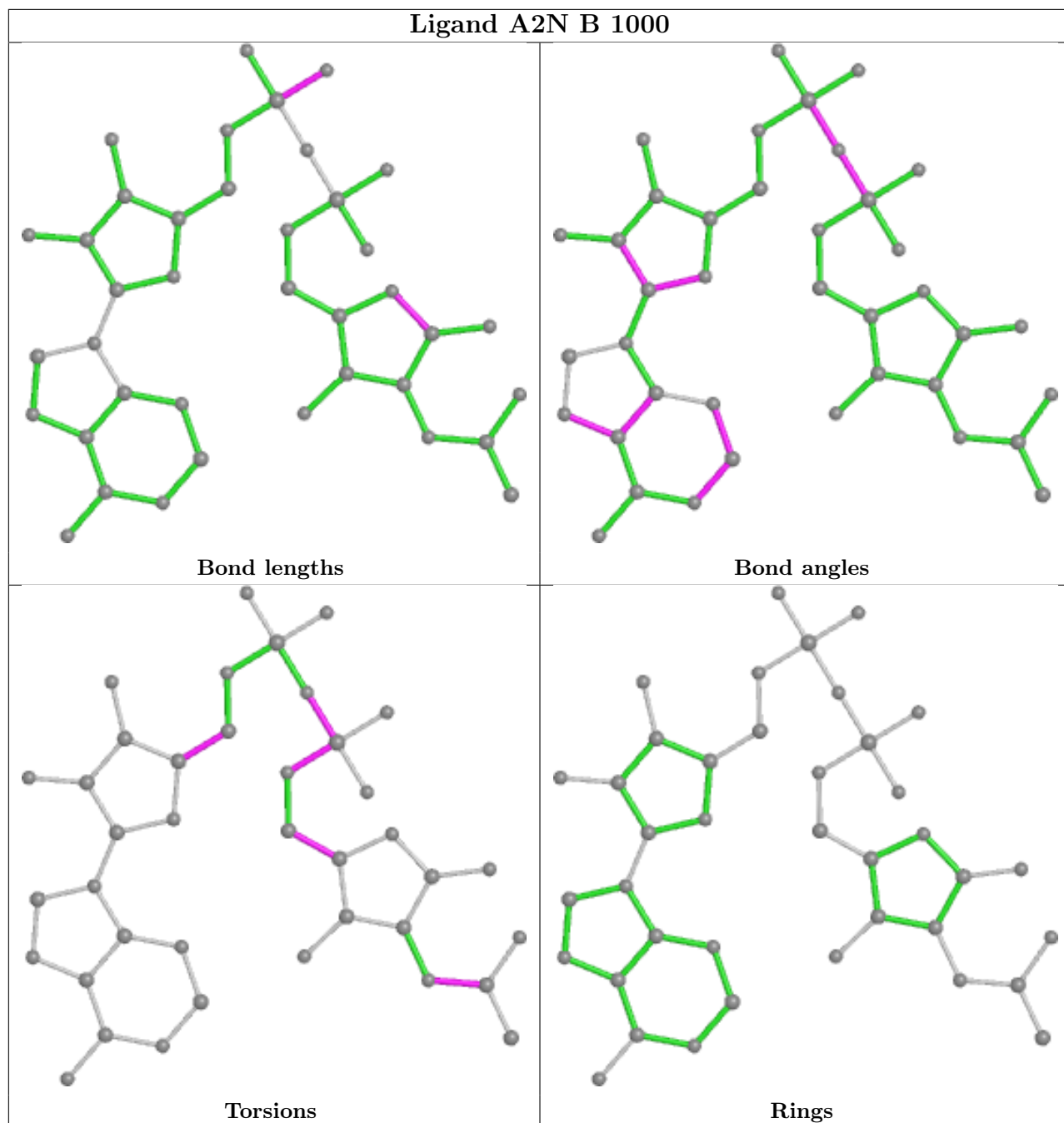
There are no ring outliers.

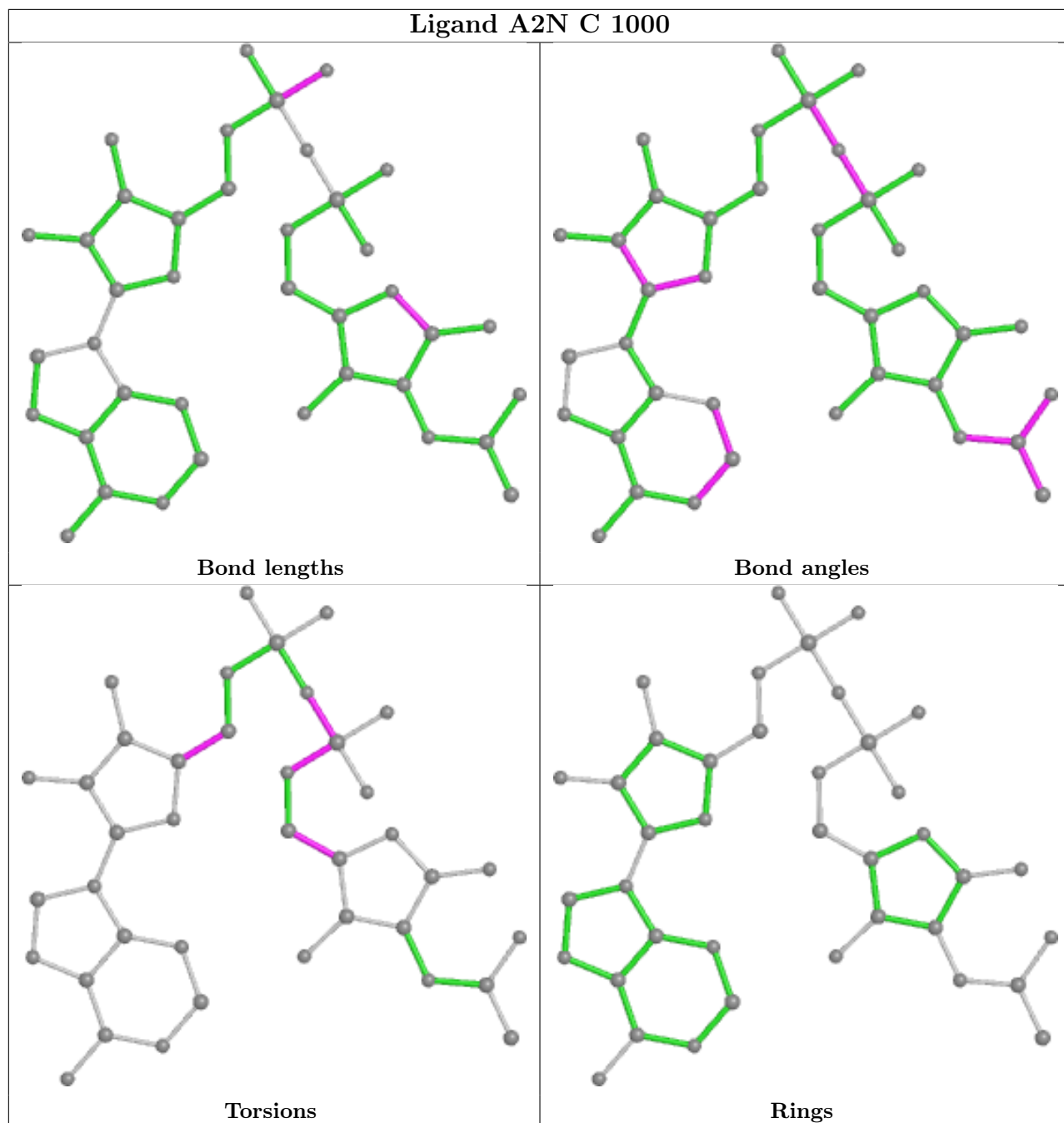
6 monomers are involved in 13 short contacts:

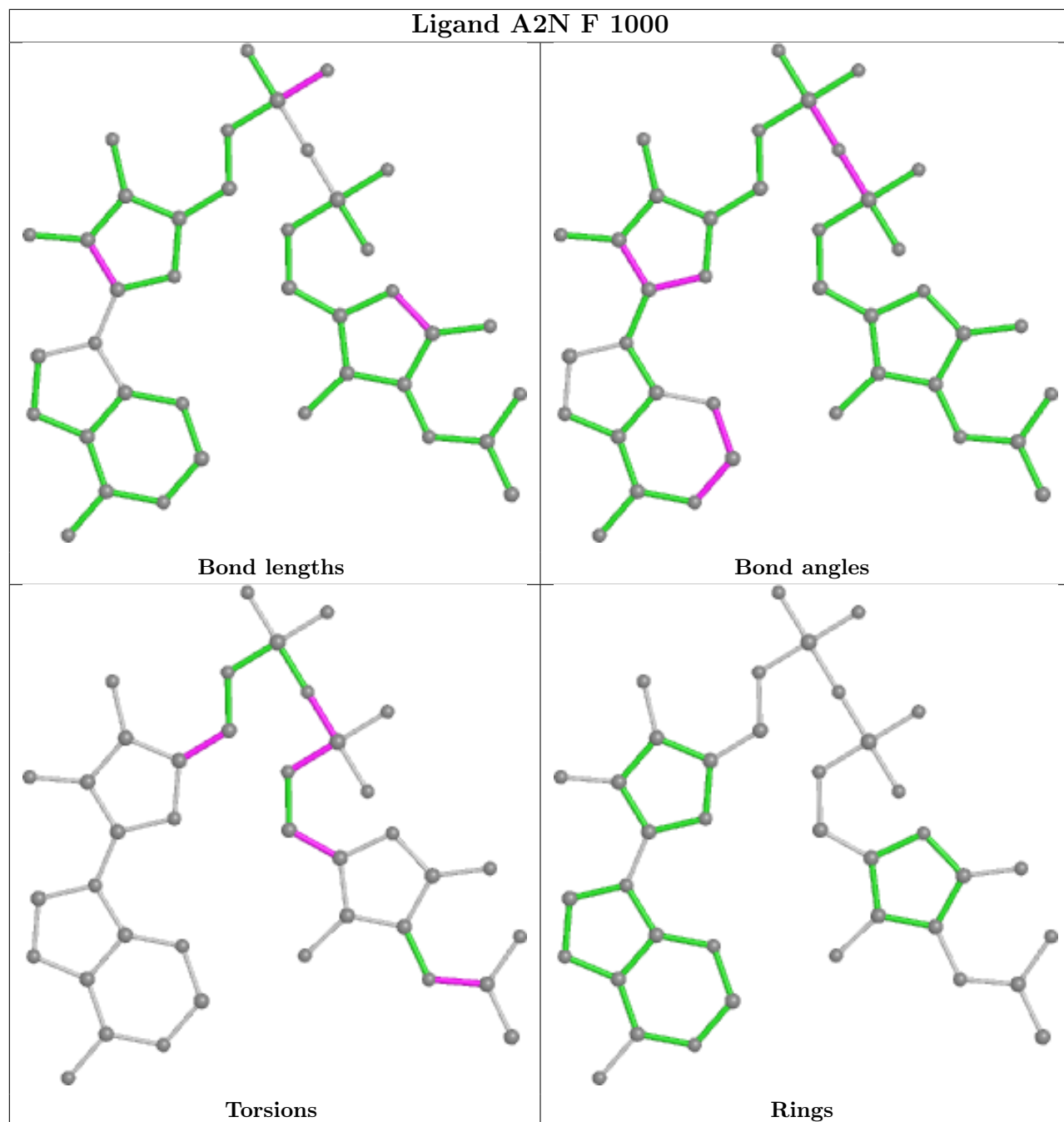
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1000	A2N	3	0
2	B	1000	A2N	2	0
2	C	1000	A2N	1	0
2	F	1000	A2N	3	0
2	D	1000	A2N	2	0
2	A	1000	A2N	2	0

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.

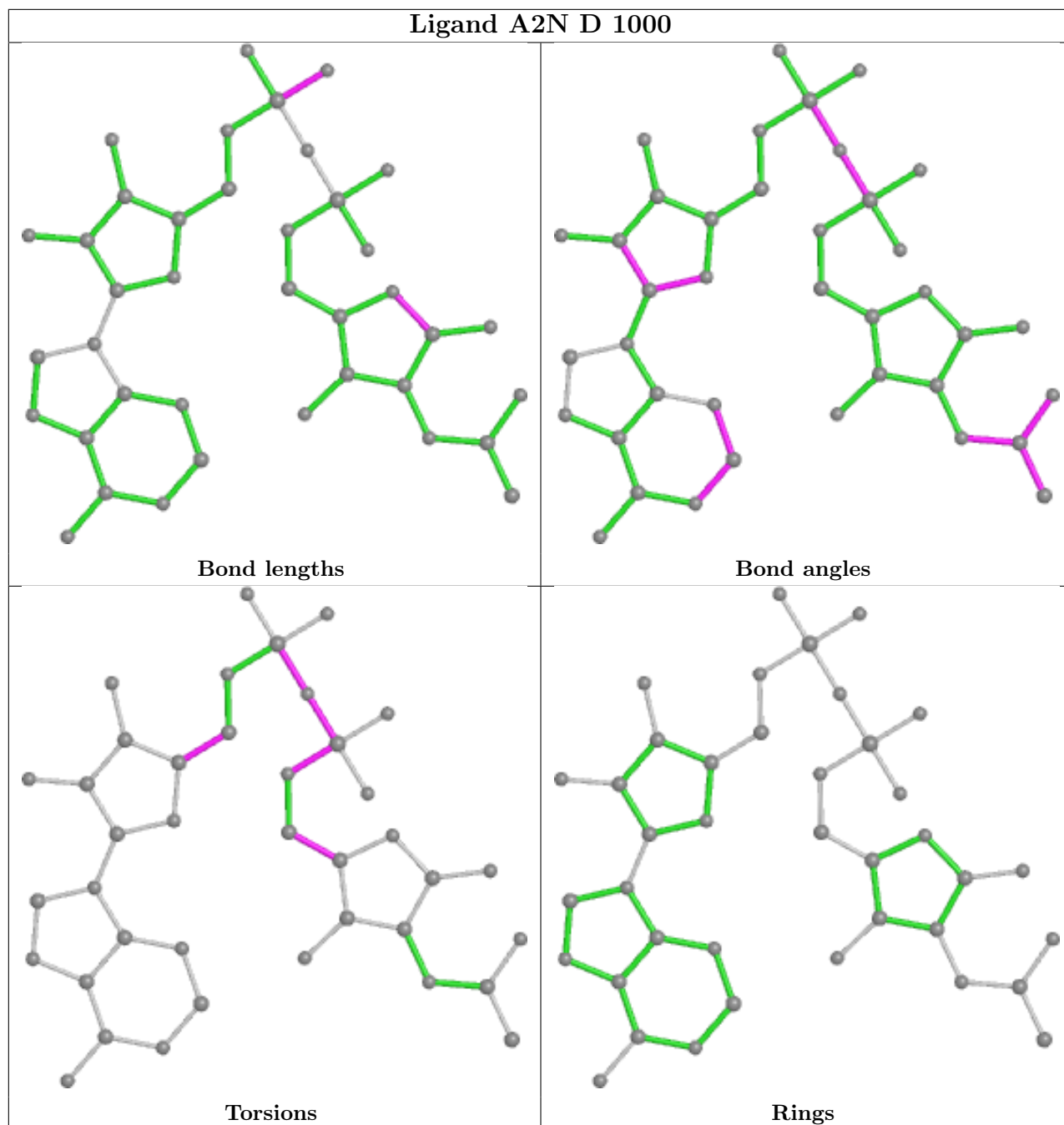


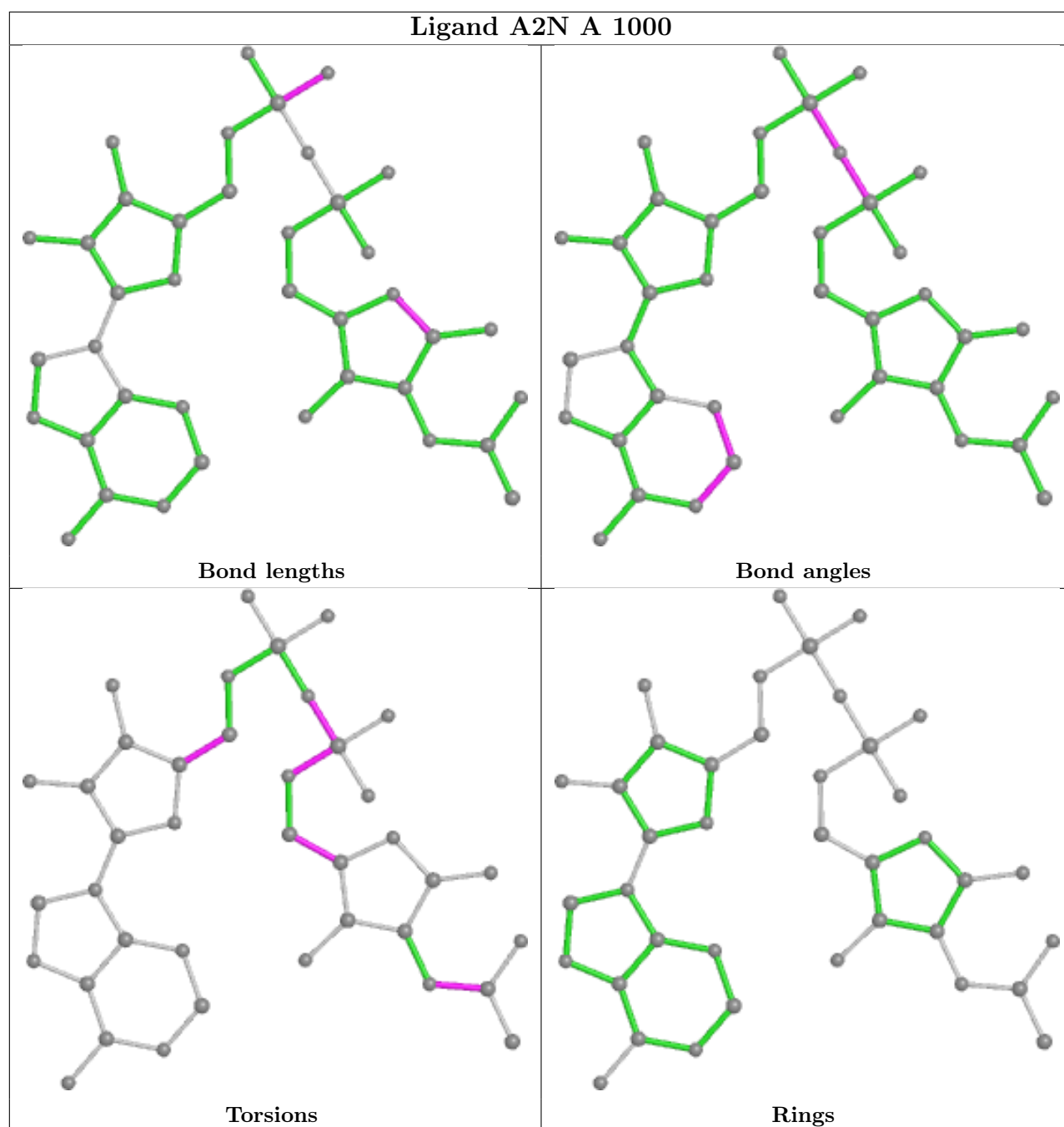












## 5.7 Other polymers [i](#)

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	277/355 (78%)	0.53	11 (3%) 38 44	17, 31, 50, 77	0
1	B	280/355 (78%)	0.61	15 (5%) 25 31	18, 33, 55, 90	0
1	C	276/355 (77%)	0.61	22 (7%) 12 15	18, 33, 53, 82	0
1	D	276/355 (77%)	0.60	20 (7%) 15 19	19, 33, 54, 77	0
1	E	278/355 (78%)	0.58	16 (5%) 23 28	22, 36, 57, 81	0
1	F	277/355 (78%)	0.60	13 (4%) 31 36	20, 35, 58, 75	0
All	All	1664/2130 (78%)	0.59	97 (5%) 23 28	17, 33, 55, 90	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	ARG	10.4
1	E	11	ALA	9.7
1	A	11	ALA	9.0
1	F	186	TRP	7.9
1	D	169	ALA	7.0
1	A	174	ALA	6.6
1	F	174	ALA	6.1
1	A	12	ASP	6.0
1	C	33	TRP	5.9
1	D	33	TRP	5.5
1	F	190	LEU	5.3
1	B	167	ALA	5.3
1	B	168	LYS	5.2
1	B	174	ALA	5.0
1	F	33	TRP	5.0
1	D	167	ALA	4.6
1	C	184	LEU	4.6
1	E	12	ASP	4.6
1	A	186	TRP	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	11	ALA	4.4
1	D	163	LEU	4.3
1	B	11	ALA	4.0
1	C	186	TRP	4.0
1	D	179	LEU	3.9
1	C	163	LEU	3.9
1	B	187	GLU	3.9
1	E	186	TRP	3.8
1	F	12	ASP	3.7
1	B	186	TRP	3.5
1	B	33	TRP	3.4
1	C	192	ASP	3.3
1	D	189	SER	3.3
1	E	33	TRP	3.3
1	B	12	ASP	3.2
1	D	168	LYS	3.2
1	C	156	GLY	3.1
1	F	175	CYS	3.1
1	F	185	ASP	3.1
1	C	167	ALA	3.0
1	E	167	ALA	2.9
1	D	180	ARG	2.9
1	B	37	ARG	2.9
1	A	247	HIS	2.9
1	D	140	ALA	2.8
1	E	187	GLU	2.8
1	F	184	LEU	2.8
1	E	193	ARG	2.8
1	B	286	PRO	2.8
1	D	77	ALA	2.7
1	D	159	ALA	2.6
1	D	193	ARG	2.6
1	D	218	ARG	2.6
1	D	166	VAL	2.6
1	A	41	GLN	2.6
1	C	215	LEU	2.6
1	D	164	CYS	2.6
1	A	33	TRP	2.5
1	C	157	LEU	2.5
1	E	74	ARG	2.5
1	F	187	GLU	2.5
1	B	14	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	203	ARG	2.5
1	C	229	ARG	2.4
1	A	284	LEU	2.4
1	F	188	ASP	2.4
1	C	12	ASP	2.4
1	C	28	LEU	2.4
1	C	162	ARG	2.4
1	E	163	LEU	2.4
1	C	13	LYS	2.3
1	E	153	GLY	2.3
1	A	175	CYS	2.3
1	E	166	VAL	2.3
1	E	174	ALA	2.3
1	D	43	SER	2.3
1	D	161	GLY	2.3
1	A	15	LYS	2.3
1	E	184	LEU	2.3
1	E	155	MET	2.2
1	B	26	GLU	2.2
1	C	285	PRO	2.2
1	A	40	TRP	2.2
1	C	278	ARG	2.2
1	B	175	CYS	2.1
1	C	218	ARG	2.1
1	E	142	CYS	2.1
1	C	165	THR	2.1
1	C	30	ARG	2.1
1	B	290	PRO	2.1
1	D	176	ARG	2.1
1	F	183	ILE	2.0
1	F	219	PRO	2.0
1	D	165	THR	2.0
1	C	175	CYS	2.0
1	C	40	TRP	2.0
1	C	230	ARG	2.0
1	E	14	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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( $\text{\AA}^2$ )	Q<0.9
5	UNX	F	355	1/1	0.30	0.25	30,30,30,30	0
5	UNX	C	356	1/1	0.33	0.35	30,30,30,30	0
5	UNX	D	356	1/1	0.53	0.59	30,30,30,30	0
5	UNX	D	357	1/1	0.54	0.55	30,30,30,30	0
5	UNX	D	358	1/1	0.55	0.22	30,30,30,30	0
5	UNX	B	357	1/1	0.55	0.21	30,30,30,30	0
4	SO4	F	1001	5/5	0.57	0.68	75,80,81,81	0
5	UNX	C	366	1/1	0.57	0.33	30,30,30,30	0
5	UNX	F	357	1/1	0.57	0.31	30,30,30,30	0
5	UNX	C	359	1/1	0.60	0.55	30,30,30,30	0
5	UNX	F	356	1/1	0.62	0.27	30,30,30,30	0
5	UNX	E	358	1/1	0.63	0.51	30,30,30,30	0
5	UNX	A	355	1/1	0.63	0.46	30,30,30,30	0
5	UNX	F	359	1/1	0.65	0.27	30,30,30,30	0
5	UNX	C	358	1/1	0.67	0.26	30,30,30,30	0
5	UNX	F	362	1/1	0.68	0.21	30,30,30,30	0
5	UNX	B	358	1/1	0.70	0.89	30,30,30,30	0
5	UNX	C	364	1/1	0.72	0.20	30,30,30,30	0
5	UNX	C	363	1/1	0.75	0.60	30,30,30,30	0
5	UNX	C	365	1/1	0.76	0.42	30,30,30,30	0
5	UNX	B	359	1/1	0.77	0.55	30,30,30,30	0
5	UNX	F	361	1/1	0.78	0.32	30,30,30,30	0
5	UNX	C	361	1/1	0.79	0.18	30,30,30,30	0
5	UNX	F	360	1/1	0.79	0.21	30,30,30,30	0
4	SO4	E	1010	5/5	0.81	0.45	64,68,69,70	0
5	UNX	B	355	1/1	0.81	0.58	30,30,30,30	0
4	SO4	F	1004	5/5	0.82	0.21	63,68,68,69	0
5	UNX	C	360	1/1	0.82	0.30	30,30,30,30	0
5	UNX	A	356	1/1	0.83	0.48	30,30,30,30	0
5	UNX	C	357	1/1	0.83	0.67	30,30,30,30	0
5	UNX	C	362	1/1	0.83	0.41	30,30,30,30	0
4	SO4	A	1008	5/5	0.85	0.15	48,52,53,54	0

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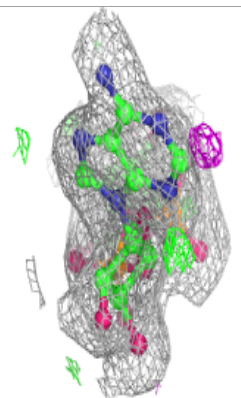
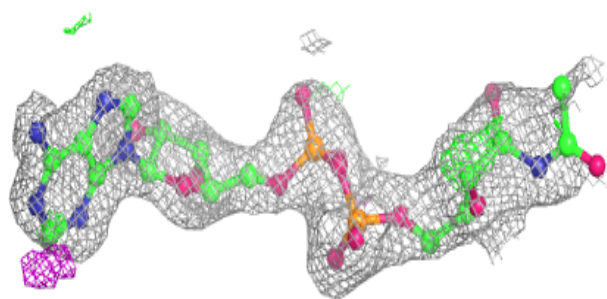
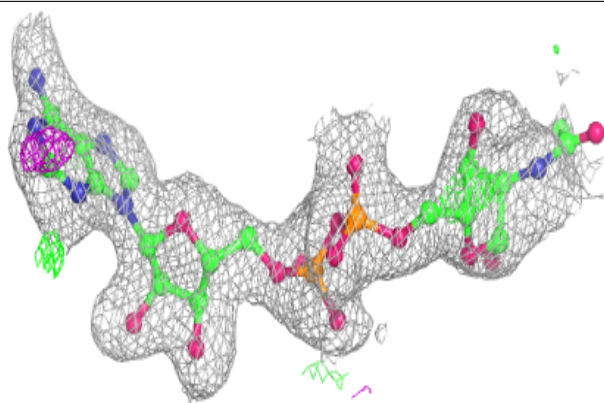
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	354	1/1	0.85	0.13	59,59,59,59	0
5	UNX	B	356	1/1	0.86	0.29	30,30,30,30	0
5	UNX	E	357	1/1	0.87	0.29	30,30,30,30	0
5	UNX	C	355	1/1	0.88	0.10	30,30,30,30	0
5	UNX	E	355	1/1	0.89	0.20	30,30,30,30	0
5	UNX	F	358	1/1	0.89	0.45	30,30,30,30	0
4	SO4	B	1006	5/5	0.90	0.16	51,56,56,57	0
4	SO4	B	1011	5/5	0.91	0.17	61,66,66,67	0
5	UNX	E	356	1/1	0.91	0.14	30,30,30,30	0
4	SO4	C	1003	5/5	0.91	0.15	57,61,61,62	0
4	SO4	B	1005	5/5	0.91	0.20	52,57,57,58	0
4	SO4	E	1007	5/5	0.92	0.17	60,65,65,66	0
5	UNX	A	357	1/1	0.92	0.27	30,30,30,30	0
3	ZN	E	354	1/1	0.93	0.09	57,57,57,57	0
2	A2N	E	1000	39/39	0.93	0.16	11,37,105,157	0
2	A2N	B	1000	39/39	0.93	0.16	21,32,99,138	0
2	A2N	A	1000	39/39	0.94	0.15	11,28,101,119	0
2	A2N	F	1000	39/39	0.94	0.15	8,34,117,144	0
2	A2N	C	1000	39/39	0.94	0.14	14,26,112,149	0
4	SO4	F	1009	5/5	0.95	0.14	39,43,44,45	0
3	ZN	A	354	1/1	0.95	0.09	47,47,47,47	0
4	SO4	E	1002	5/5	0.95	0.16	43,47,48,48	0
3	ZN	D	354	1/1	0.97	0.04	46,46,46,46	0
2	A2N	D	1000	39/39	0.97	0.14	10,25,109,164	0
4	SO4	D	355	5/5	0.98	0.13	35,39,41,41	0
3	ZN	C	354	1/1	0.98	0.12	49,49,49,49	0
3	ZN	F	354	1/1	0.99	0.03	40,40,40,40	0

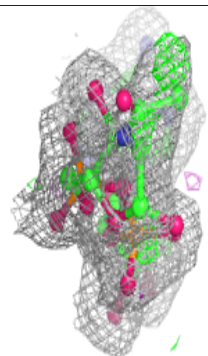
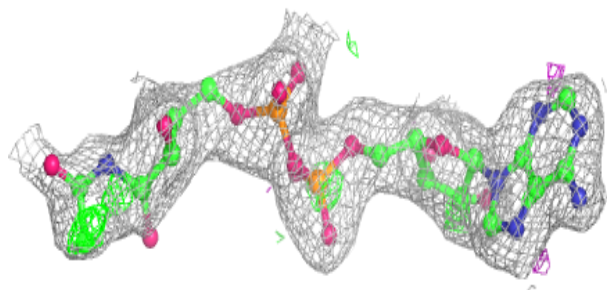
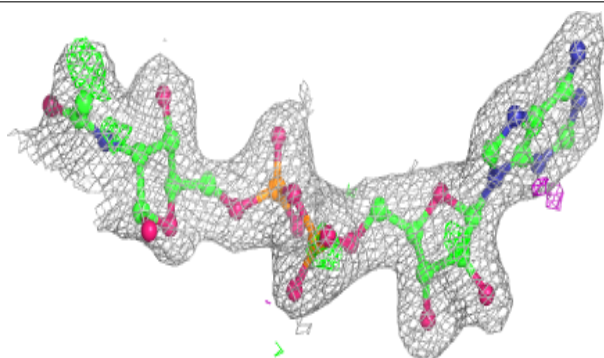
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A2N E 1000:**

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

**Electron density around A2N B 1000:**

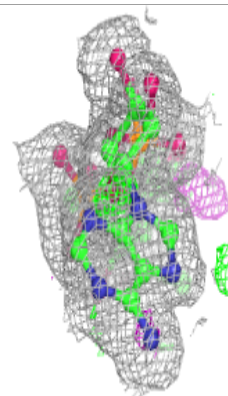
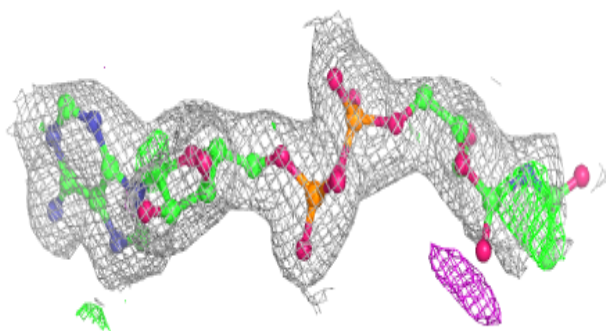
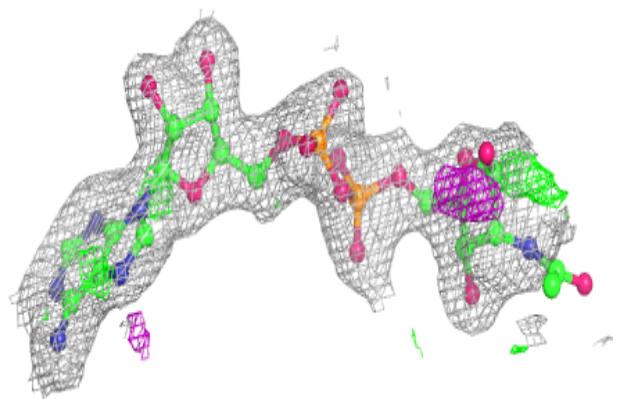
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



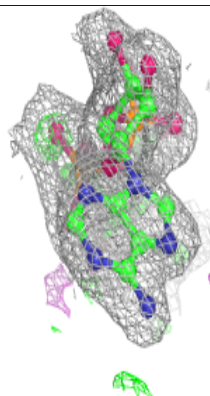
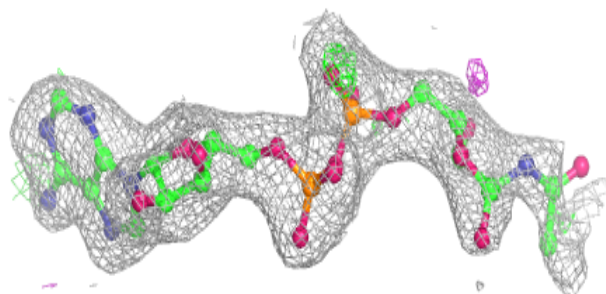
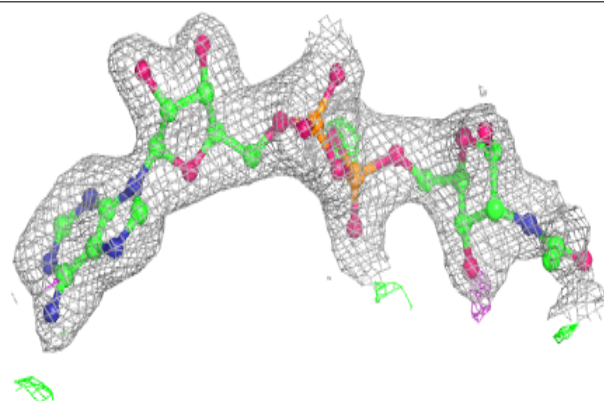


**Electron density around A2N A 1000:**

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

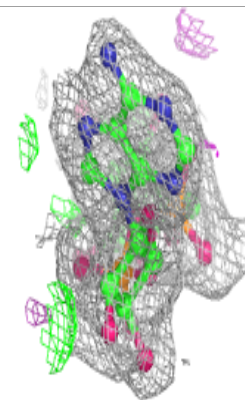
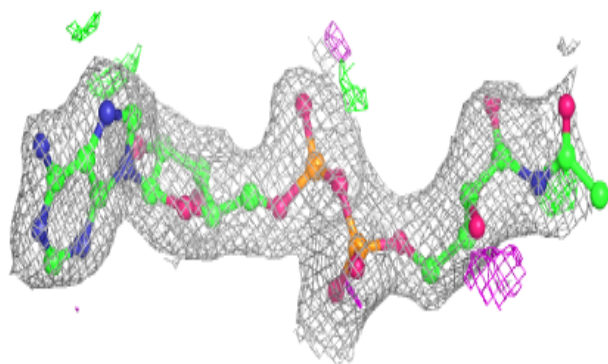
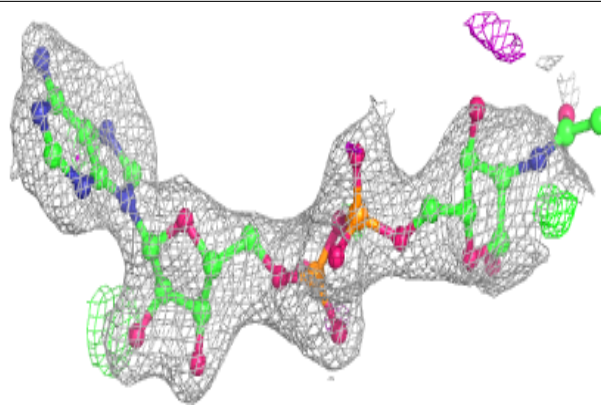
**Electron density around A2N F 1000:**

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

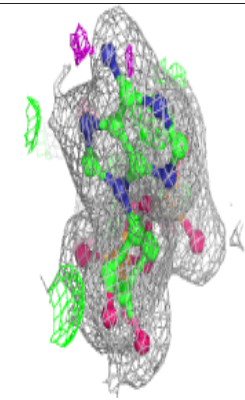
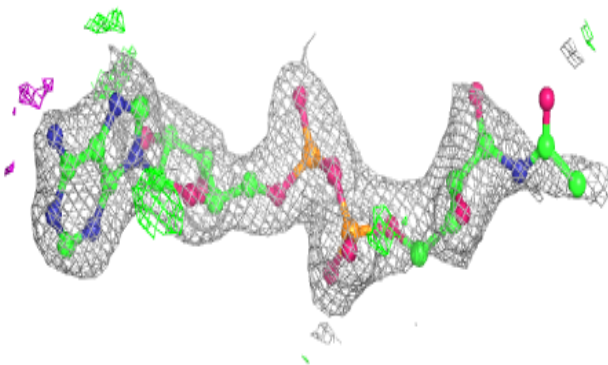
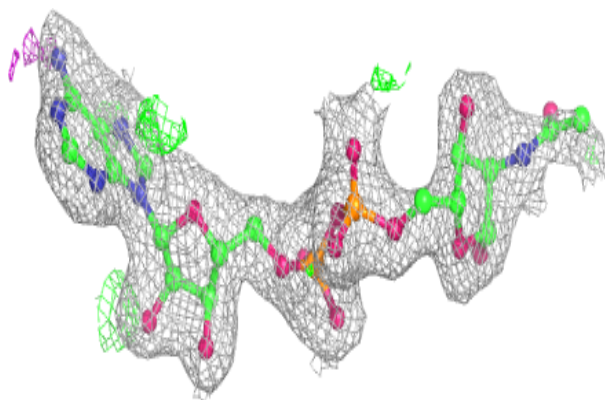


**Electron density around A2N C 1000:**

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

**Electron density around A2N D 1000:**

$2mF_o-DF_c$  (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.