



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 12:15 AM EST

PDB ID : 6X9C  
Title : Structure of proline utilization A with L-proline bound in the L-glutamate-gamma-mma-semialdehyde dehydrogenase active site  
Authors : Tanner, J.J.; Campbell, A.C.  
Deposited on : 2020-06-02  
Resolution : 1.44 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 : 2.16  
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) : 2.16

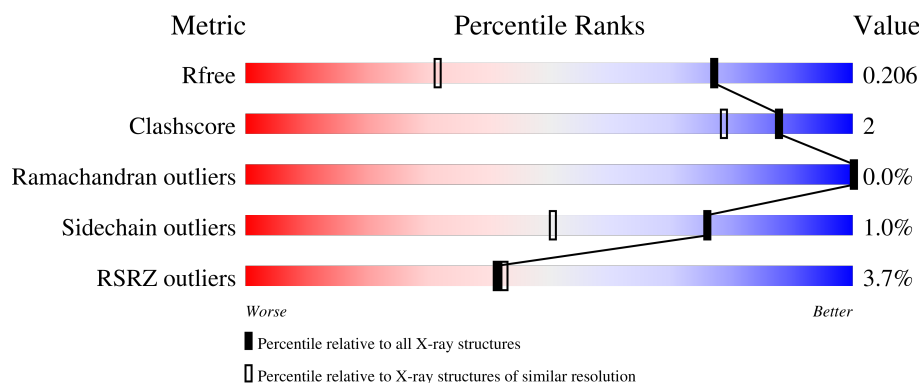
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.44 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	1235	<div> <div>3%</div> <div>94%</div> <div>• •</div> </div>
1	B	1235	<div> <div>4%</div> <div>92%</div> <div>6% •</div> </div>

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 20266 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.

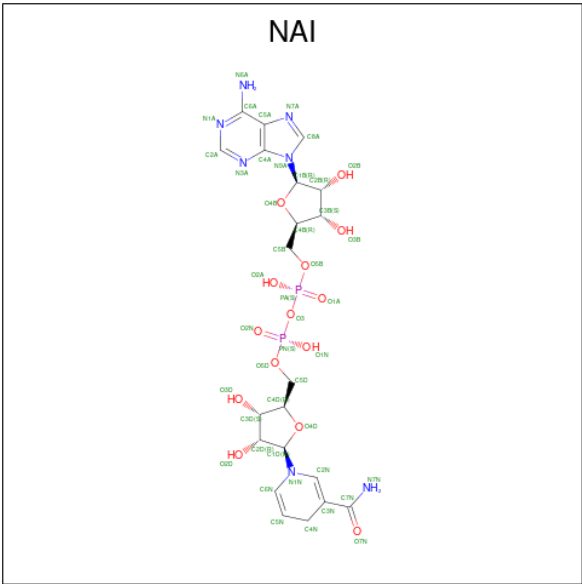
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1209	Total	C	N	O	S	0	9	0
			8980	5661	1602	1685	32			
1	B	1208	Total	C	N	O	S	0	15	0
			8985	5666	1601	1687	31			

There are 4 discrepancies between the modelled and reference sequences:

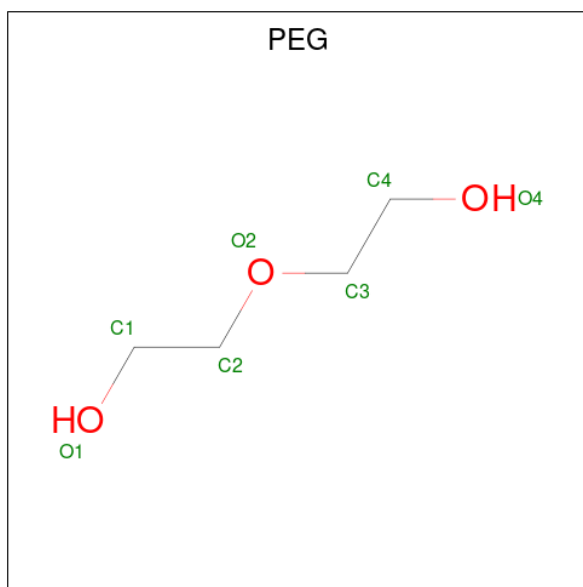
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



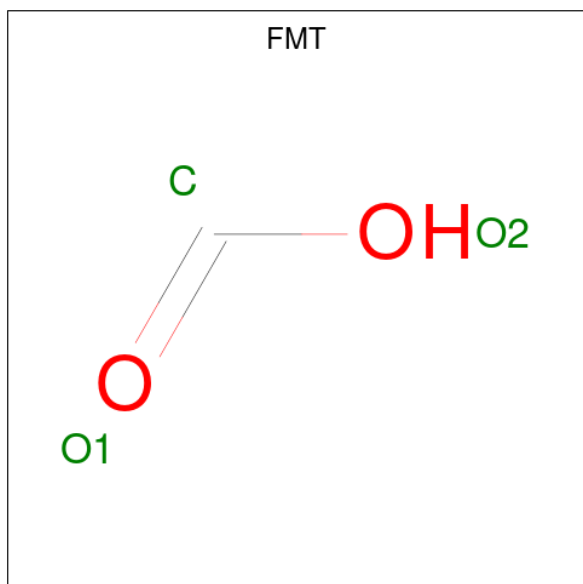
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			44	21	7	14	2	
2	B	1	Total	C	N	O	P	
			88	42	14	28	4	
								0
								1

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



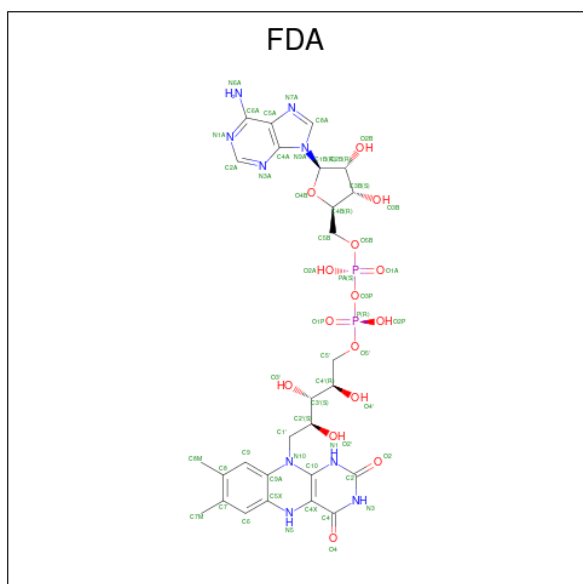
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			7	4	3	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula:  $C_{27}H_{35}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).

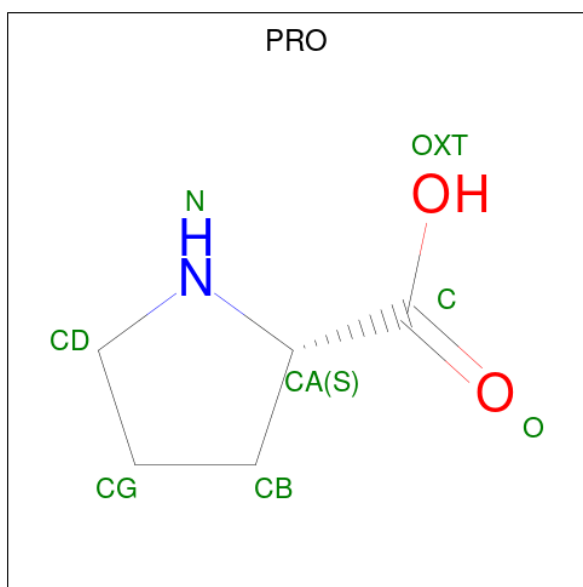


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

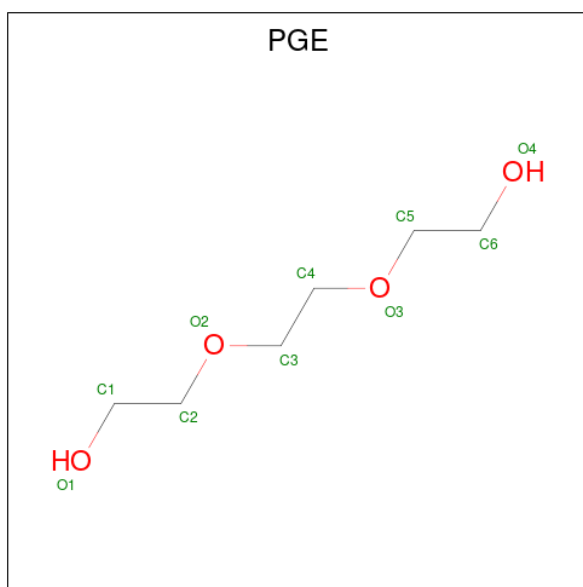
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		

- Molecule 8 is PROLINE (three-letter code: PRO) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			8	5	1	2		
8	A	1	Total	C	N	O	0	0
			8	5	1	2		
8	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

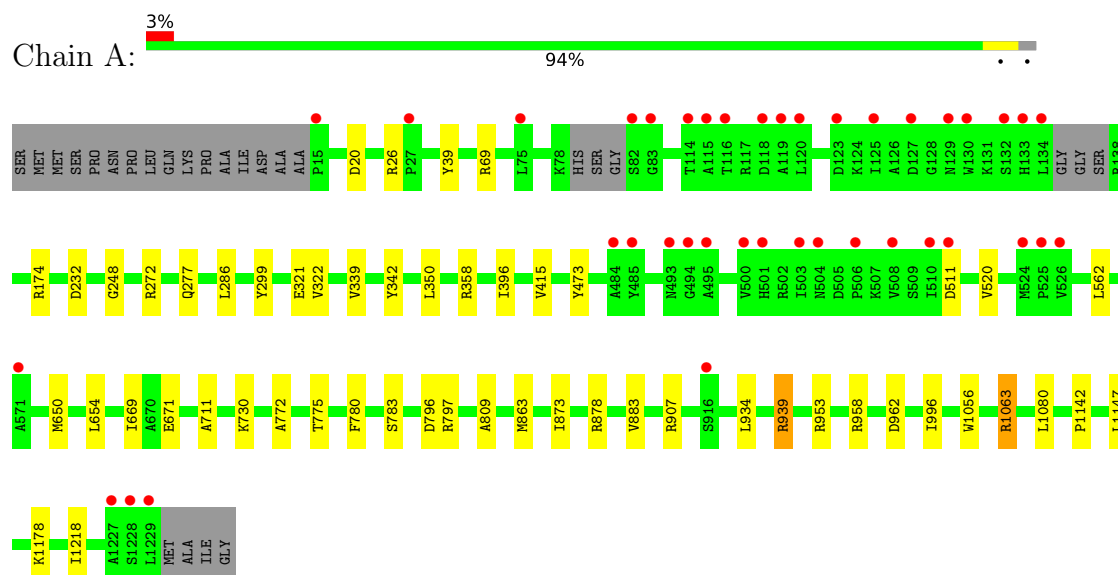
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1024	Total 1024	O 1024	0	0
10	B	968	Total 968	O 968	0	2



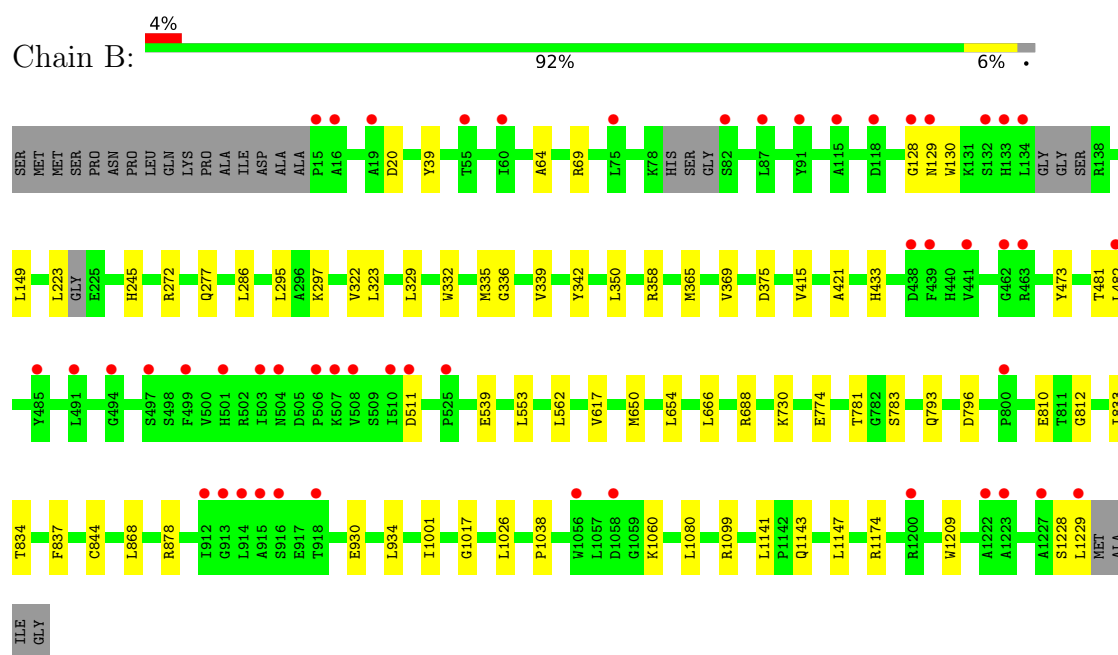
### 3 Residue-property plots [i](#)

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: Bifunctional protein PutA



#### • Molecule 1: Bifunctional protein PutA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.08Å 102.25Å 127.12Å 90.00° 106.48° 90.00°	Depositor
Resolution (Å)	48.46 – 1.44 48.46 – 1.44	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.46-1.44) 92.1 (48.46-1.44)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.44Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.180 , 0.205 0.180 , 0.206	Depositor DCC
$R_{free}$ test set	20729 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: FDA, MG, PGE, FMT, NAI, SO4, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/9165	0.54	1/12477 (0.0%)
1	B	0.32	0/9186	0.55	0/12508
All	All	0.32	0/18351	0.54	1/24985 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ARG	NE-CZ-NH1	5.70	123.15	120.30

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	8980	0	9005	30	0
1	B	8985	0	9008	43	0
2	A	44	0	27	1	0
2	B	88	0	54	6	0
3	A	7	0	10	0	0
4	A	3	0	1	0	0
5	A	53	0	33	2	0
5	B	53	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	15	0	0	1	0
6	B	10	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	16	0	14	0	0
8	B	8	0	7	0	0
9	B	10	0	14	0	0
10	A	1024	0	0	4	0
10	B	968	0	0	6	0
All	All	20266	0	18206	73	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 (73) 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:B:473:TYR:HB2	5:B:1303:FDA:HM72	1.71	0.72
1:A:473:TYR:HB2	5:A:1304:FDA:HM72	1.75	0.68
1:B:539:GLU:OE1	10:B:1401:HOH:O	2.11	0.68
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.78	0.66
1:B:20:ASP:OD2	1:B:878:ARG:NH2	2.30	0.64
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.79	0.64
1:A:796:ASP:HA	1:A:1178:LYS:NZ	2.12	0.64
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.82	0.61
1:B:1174[B]:ARG:NH1	10:B:1404:HOH:O	2.33	0.60
1:A:20:ASP:OD2	1:A:878:ARG:NH1	2.33	0.60
1:B:844:CYS:SG	2:B:1301[B]:NAI:H42N	2.43	0.59
1:B:339[A]:VAL:HG21	1:B:350:LEU:HD21	1.86	0.57
1:A:339[A]:VAL:HG21	1:A:350:LEU:HD21	1.85	0.57
1:A:939:ARG:NH2	10:A:1407:HOH:O	2.36	0.56
1:B:650:MET:O	1:B:654:LEU:HG	2.05	0.56
1:A:1147:LEU:HD22	1:B:1147:LEU:HD13	1.88	0.55
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.87	0.55
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.88	0.55
1:B:796:ASP:OD1	1:B:1174[B]:ARG:NH2	2.39	0.55
1:A:1063:ARG:HD2	10:A:1441:HOH:O	2.07	0.54
1:A:650:MET:O	1:A:654:LEU:HG	2.07	0.54
1:B:1099[B]:ARG:HD2	1:B:1209:TRP:O	2.08	0.53
1:B:834[A]:THR:HG22	1:B:1001:ILE:HD11	1.91	0.53
1:B:69:ARG:NH2	1:B:511:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:THR:HG21	2:B:1301[B]:NAI:H4N	1.91	0.51
1:B:245:HIS:CE1	1:B:295:LEU:HD11	2.47	0.50
1:B:783:SER:HB3	2:B:1301[A]:NAI:O4D	2.12	0.49
1:A:775:THR:HB	1:A:797:ARG:HH22	1.78	0.49
1:B:128:GLY:O	1:B:130:TRP:N	2.46	0.48
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.49	0.47
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.95	0.47
1:B:844:CYS:SG	2:B:1301[B]:NAI:C4N	3.02	0.47
1:B:617:VAL:HG12	1:B:774:GLU:HB2	1.97	0.47
1:A:562:LEU:HD11	1:A:654:LEU:HD12	1.97	0.46
1:A:783:SER:HB3	2:A:1301:NAI:O4D	2.15	0.46
1:A:1080[B]:LEU:HD12	10:A:2023:HOH:O	2.16	0.45
1:B:1017:GLY:HA2	10:B:2097:HOH:O	2.15	0.45
1:B:369:VAL:HG12	1:B:421:ALA:HB3	1.98	0.45
1:A:358:ARG:HG3	1:A:415:VAL:HG11	1.98	0.45
5:A:1304:FDA:O4'	5:A:1304:FDA:H9	2.17	0.45
1:A:396:ILE:HD11	1:A:520:VAL:HB	2.00	0.44
1:A:780:PHE:O	1:A:809:ALA:HA	2.17	0.44
1:B:837:PHE:CE2	1:B:868:LEU:HD21	2.52	0.44
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	2.00	0.44
1:B:358:ARG:HG2	1:B:415:VAL:HG11	2.00	0.43
1:A:958:ARG:NH1	1:A:962:ASP:OD2	2.44	0.43
1:A:671:GLU:HG3	1:A:711:ALA:HB2	2.00	0.43
1:B:323:LEU:HD13	1:B:335:MET:HE3	2.00	0.42
1:B:223:LEU:HD13	1:B:482:LEU:HA	2.01	0.42
1:A:863:MET:HB2	1:A:863:MET:HE2	1.88	0.42
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.54	0.42
1:A:26:ARG:HH22	1:A:322:VAL:HG23	1.84	0.42
1:B:297:LYS:HD2	1:B:329:LEU:HA	2.00	0.42
1:A:772:ALA:O	1:A:797:ARG:NH2	2.53	0.42
1:B:375[B]:ASP:OD1	1:B:1229:LEU:HB3	2.20	0.42
1:B:562:LEU:HD11	1:B:654:LEU:HD12	2.01	0.42
1:B:553:LEU:HD12	1:B:666:LEU:HD13	2.00	0.42
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.55	0.41
1:A:232:ASP:OD2	10:A:1401:HOH:O	2.22	0.41
1:A:654:LEU:HD21	1:A:669:ILE:HA	2.03	0.41
1:A:69:ARG:NH2	1:A:511:ASP:OD1	2.53	0.41
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.03	0.41
1:B:812:GLY:H	2:B:1301[B]:NAI:H71N	1.67	0.41
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.20	0.41
1:B:688[B]:ARG:NH1	10:B:1418:HOH:O	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080[A]:LEU:HD12	10:B:1982:HOH:O	2.20	0.41
1:B:323:LEU:HB3	1:B:335:MET:HE3	2.02	0.41
1:B:336:GLY:HA2	1:B:365:MET:O	2.21	0.41
1:B:781:THR:CG2	2:B:1301[B]:NAI:H4N	2.51	0.40
1:B:793:GLN:HG2	10:B:1716:HOH:O	2.21	0.40
1:A:953:ARG:N	6:A:1307:SO4:O4	2.36	0.40
1:B:1060:LYS:HB2	1:B:1060:LYS:HE3	1.86	0.40
1:B:149:LEU:HA	1:B:149:LEU:HD23	1.92	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	1212/1235 (98%)	1193 (98%)	19 (2%)	0	100	100
1	B	1215/1235 (98%)	1193 (98%)	21 (2%)	1 (0%)	51	24
All	All	2427/2470 (98%)	2386 (98%)	40 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ASN

### 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	903/951 (95%)	895 (99%)	8 (1%)	78	54
1	B	904/951 (95%)	893 (99%)	11 (1%)	71	43
All	All	1807/1902 (95%)	1788 (99%)	19 (1%)	76	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	321	GLU
1	A	342	TYR
1	A	730	LYS
1	A	907	ARG
1	A	934	LEU
1	A	939	ARG
1	A	1063	ARG
1	B	39	TYR
1	B	342	TYR
1	B	481	THR
1	B	730	LYS
1	B	810[A]	GLU
1	B	810[B]	GLU
1	B	833	ILE
1	B	930	GLU
1	B	934	LEU
1	B	1141	LEU
1	B	1228	SER

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
5	FDA	A	1304	-	51,58,58	2.73	18 (35%)	60,89,89	1.73	8 (13%)
3	PEG	A	1302	-	6,6,6	0.49	0	5,5,5	0.26	0
8	PRO	B	1307	-	5,8,8	0.66	0	6,10,10	1.15	0
6	SO4	B	1305	-	4,4,4	0.15	0	6,6,6	0.09	0
9	PGE	B	1302	-	9,9,9	0.52	0	8,8,8	0.29	0
6	SO4	A	1306	-	4,4,4	0.14	0	6,6,6	0.12	0
2	NAI	B	1301[A]	7	42,48,48	1.37	4 (9%)	47,73,73	1.44	7 (14%)
6	SO4	A	1305	-	4,4,4	0.12	0	6,6,6	0.29	0
4	FMT	A	1303	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAI	B	1301[B]	-	42,48,48	1.33	4 (9%)	47,73,73	1.59	10 (21%)
6	SO4	A	1307	-	4,4,4	0.16	0	6,6,6	0.16	0
2	NAI	A	1301	7	42,48,48	1.30	3 (7%)	47,73,73	1.45	7 (14%)
8	PRO	A	1309	-	5,8,8	0.51	0	6,10,10	1.10	0
6	SO4	B	1304	-	4,4,4	0.24	0	6,6,6	0.21	0
5	FDA	B	1303	-	51,58,58	2.83	18 (35%)	60,89,89	1.83	10 (16%)
8	PRO	A	1310	-	5,8,8	0.58	0	6,10,10	1.06	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
5	FDA	A	1304	-	-	7/30/50/50	0/6/6/6
3	PEG	A	1302	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PRO	B	1307	-	-	0/0/11/11	0/1/1/1
9	PGE	B	1302	-	-	2/7/7/7	-
2	NAI	B	1301[A]	7	-	4/25/72/72	0/5/5/5
8	PRO	A	1310	-	-	0/0/11/11	0/1/1/1
2	NAI	B	1301[B]	-	-	8/25/72/72	0/5/5/5
2	NAI	A	1301	7	-	3/25/72/72	0/5/5/5
8	PRO	A	1309	-	-	0/0/11/11	0/1/1/1
5	FDA	B	1303	-	-	8/30/50/50	0/6/6/6

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1303	FDA	C10-N1	9.00	1.44	1.33
5	B	1303	FDA	C4X-N5	8.50	1.45	1.33
5	A	1304	FDA	C4X-N5	8.15	1.44	1.33
5	A	1304	FDA	C10-N1	8.13	1.43	1.33
5	A	1304	FDA	C5X-N5	6.60	1.46	1.35
5	B	1303	FDA	C5X-N5	5.91	1.45	1.35
5	B	1303	FDA	C9A-N10	5.27	1.45	1.38
5	B	1303	FDA	C4-C4X	4.87	1.49	1.41
5	B	1303	FDA	O4-C4	4.60	1.36	1.24
5	A	1304	FDA	O4-C4	4.57	1.36	1.24
2	B	1301[A]	NAI	PA-O5B	4.47	1.77	1.59
5	A	1304	FDA	C4-C4X	4.43	1.49	1.41
5	A	1304	FDA	C6-C5X	4.25	1.48	1.41
5	B	1303	FDA	C6-C5X	4.22	1.48	1.41
5	B	1303	FDA	C4-N3	4.21	1.40	1.33
5	A	1304	FDA	C4-N3	4.20	1.40	1.33
5	A	1304	FDA	C9A-N10	4.18	1.44	1.38
5	A	1304	FDA	C9-C9A	3.85	1.48	1.40
2	B	1301[B]	NAI	PN-O5D	3.82	1.74	1.59
2	B	1301[A]	NAI	PN-O5D	3.79	1.74	1.59
2	B	1301[B]	NAI	PA-O5B	3.61	1.73	1.59
5	B	1303	FDA	C9-C9A	3.55	1.47	1.40
2	A	1301	NAI	PA-O5B	3.45	1.73	1.59
5	B	1303	FDA	C9A-C5X	-3.40	1.35	1.42
5	B	1303	FDA	C2B-C1B	-3.37	1.48	1.53
2	A	1301	NAI	PN-O5D	3.31	1.72	1.59
5	A	1304	FDA	C2A-N3A	3.06	1.37	1.32
5	B	1303	FDA	C2A-N3A	3.05	1.37	1.32
5	A	1304	FDA	C9A-C5X	-2.96	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1304	FDA	C2B-C1B	-2.89	1.49	1.53
5	B	1303	FDA	C6A-N6A	2.77	1.44	1.34
5	A	1304	FDA	C6A-N6A	2.68	1.43	1.34
5	A	1304	FDA	PA-O5B	-2.60	1.48	1.59
5	A	1304	FDA	O2'-C2'	-2.51	1.38	1.43
5	B	1303	FDA	C2-N1	2.47	1.43	1.38
5	A	1304	FDA	O4B-C4B	-2.44	1.39	1.45
5	A	1304	FDA	C2-N1	2.32	1.42	1.38
2	B	1301[B]	NAI	C7N-N7N	2.24	1.39	1.33
2	B	1301[B]	NAI	C2A-N1A	2.23	1.38	1.33
2	B	1301[A]	NAI	C2A-N1A	2.21	1.38	1.33
2	B	1301[A]	NAI	C7N-N7N	2.20	1.39	1.33
5	A	1304	FDA	P-O1P	2.20	1.58	1.50
5	B	1303	FDA	PA-O2A	-2.17	1.45	1.55
2	A	1301	NAI	C2A-N3A	2.14	1.35	1.32
5	B	1303	FDA	O4B-C4B	-2.12	1.40	1.45
5	B	1303	FDA	P-O1P	2.08	1.58	1.50
5	B	1303	FDA	PA-O5B	-2.08	1.50	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1303	FDA	C1'-N10-C9A	6.27	123.23	118.29
5	A	1304	FDA	C1'-N10-C9A	5.94	122.97	118.29
5	A	1304	FDA	C4-N3-C2	5.82	120.05	115.14
5	B	1303	FDA	N3A-C2A-N1A	-5.66	119.83	128.68
5	A	1304	FDA	N3A-C2A-N1A	-5.43	120.20	128.68
2	B	1301[A]	NAI	PN-O3-PA	-5.38	114.36	132.83
5	B	1303	FDA	C4-N3-C2	5.36	119.67	115.14
2	B	1301[B]	NAI	PN-O3-PA	-4.74	116.56	132.83
2	A	1301	NAI	PN-O3-PA	-4.61	117.01	132.83
5	B	1303	FDA	C9A-N10-C10	-3.90	116.80	121.91
5	A	1304	FDA	C9A-N10-C10	-3.83	116.90	121.91
2	B	1301[B]	NAI	C3N-C2N-N1N	-3.35	118.31	123.10
2	B	1301[A]	NAI	C3N-C2N-N1N	-3.13	118.64	123.10
5	B	1303	FDA	C4X-C4-N3	-3.07	119.23	123.43
5	B	1303	FDA	C5X-C9A-N10	3.04	119.92	117.72
2	A	1301	NAI	O2A-PA-O1A	3.02	127.18	112.24
2	A	1301	NAI	O1N-PN-O2N	2.96	126.85	112.24
5	A	1304	FDA	C5X-C9A-N10	2.87	119.80	117.72
2	B	1301[B]	NAI	O5B-PA-O1A	-2.85	97.92	109.07
2	B	1301[B]	NAI	O1N-PN-O2N	2.77	125.93	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301[A]	NAI	O5D-PN-O2N	-2.75	98.31	109.07
2	A	1301	NAI	PN-O5D-C5D	-2.73	105.65	121.68
2	A	1301	NAI	C3N-C2N-N1N	-2.72	119.22	123.10
5	B	1303	FDA	C10-C4X-N5	-2.67	119.42	121.26
5	A	1304	FDA	C4X-C4-N3	-2.61	119.86	123.43
2	B	1301[B]	NAI	O2A-PA-O1A	2.60	125.11	112.24
2	B	1301[A]	NAI	O2A-PA-O1A	2.60	125.07	112.24
5	B	1303	FDA	C1B-N9A-C4A	-2.48	122.29	126.64
2	A	1301	NAI	O5D-PN-O2N	-2.44	99.52	109.07
2	B	1301[B]	NAI	PA-O5B-C5B	-2.43	107.45	121.68
2	B	1301[B]	NAI	O7N-C7N-N7N	-2.37	117.34	122.88
2	B	1301[A]	NAI	PN-O5D-C5D	-2.32	108.06	121.68
2	B	1301[B]	NAI	O4D-C1D-C2D	-2.27	101.69	106.64
5	B	1303	FDA	C2A-N1A-C6A	2.22	122.55	118.75
5	B	1303	FDA	P-O3P-PA	2.21	140.42	132.83
5	A	1304	FDA	C1B-N9A-C4A	-2.21	122.76	126.64
5	A	1304	FDA	C4-C4X-N5	2.18	121.09	118.60
2	B	1301[A]	NAI	C2D-C3D-C4D	-2.18	98.41	102.64
2	B	1301[B]	NAI	PN-O5D-C5D	-2.17	108.97	121.68
2	B	1301[B]	NAI	O5D-PN-O2N	-2.08	100.93	109.07
2	B	1301[A]	NAI	PA-O5B-C5B	-2.07	109.51	121.68
2	A	1301	NAI	PA-O5B-C5B	-2.07	109.54	121.68

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1304	FDA	C5'-O5'-P-O2P
2	B	1301[A]	NAI	C5B-O5B-PA-O1A
2	B	1301[A]	NAI	O4D-C1D-N1N-C2N
2	B	1301[B]	NAI	C5B-O5B-PA-O3
2	A	1301	NAI	C5B-O5B-PA-O1A
2	A	1301	NAI	O4D-C1D-N1N-C2N
2	B	1301[B]	NAI	O4D-C1D-N1N-C2N
9	B	1302	PGE	O2-C3-C4-O3
5	A	1304	FDA	C2'-C3'-C4'-O4'
5	B	1303	FDA	C2'-C3'-C4'-O4'
5	A	1304	FDA	P-O3P-PA-O5B
5	B	1303	FDA	P-O3P-PA-O5B
5	B	1303	FDA	PA-O3P-P-O5'
9	B	1302	PGE	C1-C2-O2-C3
2	B	1301[B]	NAI	C4D-C5D-O5D-PN

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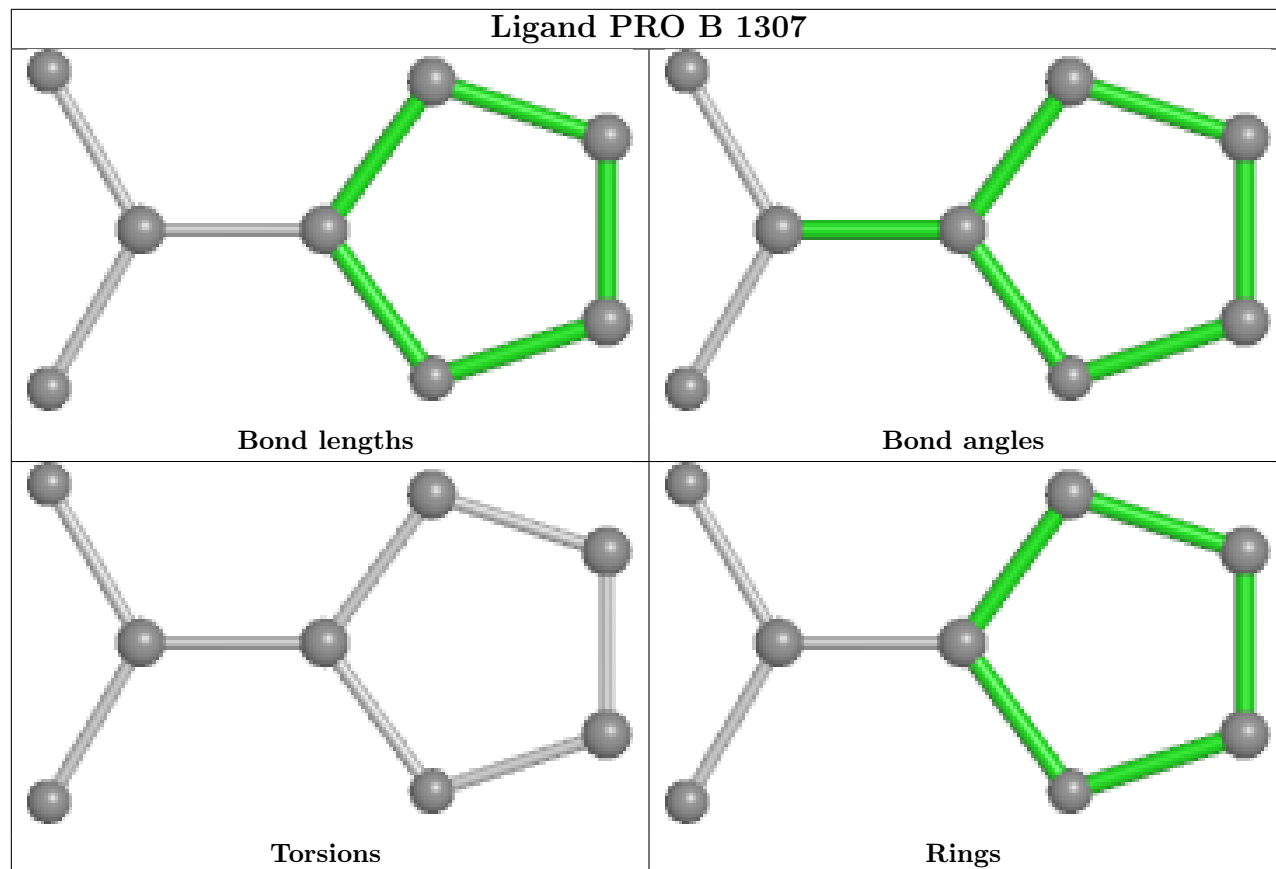
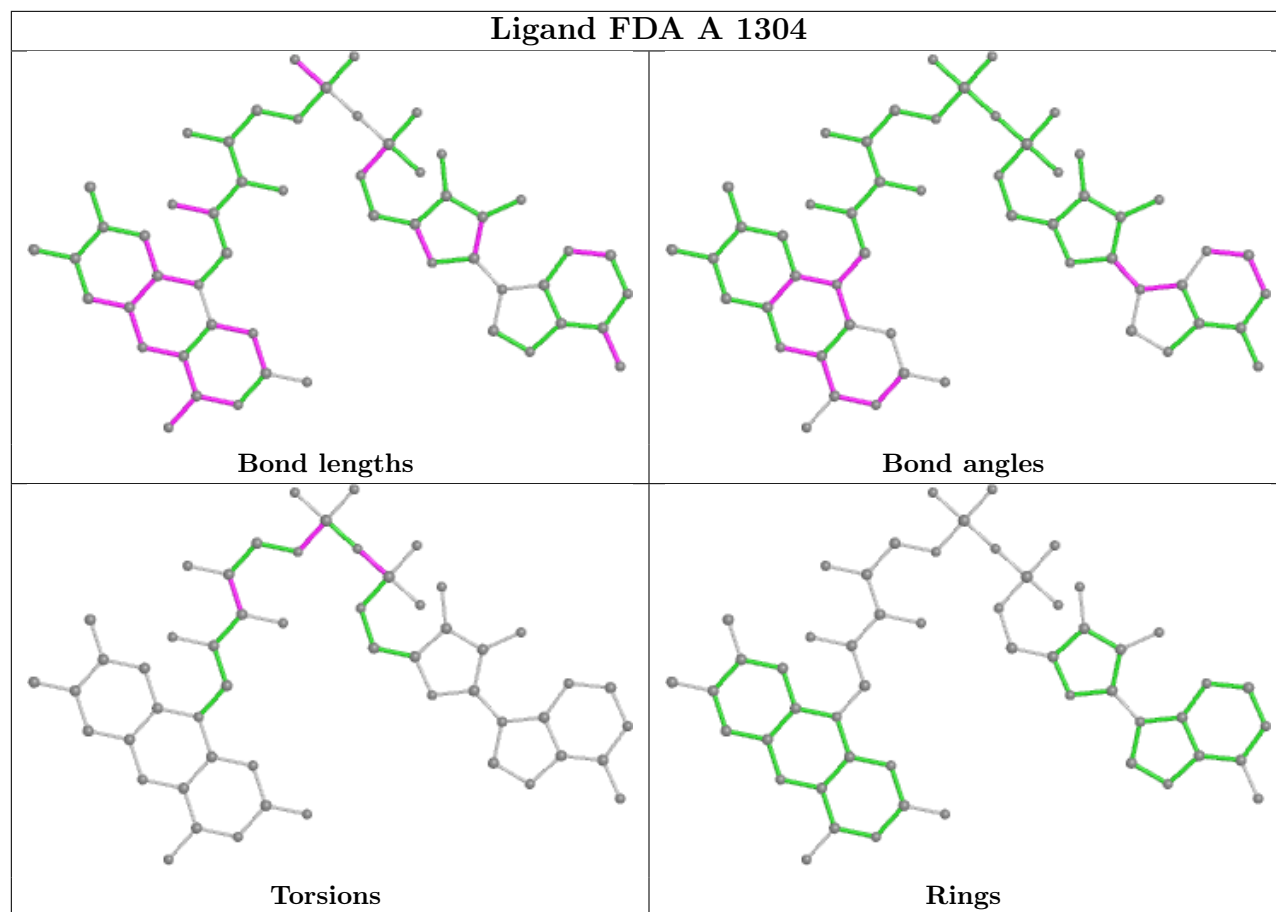
Mol	Chain	Res	Type	Atoms
2	B	1301[A]	NAI	C5B-O5B-PA-O3
5	B	1303	FDA	C5B-O5B-PA-O3P
5	B	1303	FDA	C4'-C5'-O5'-P
5	A	1304	FDA	C5'-O5'-P-O1P
2	B	1301[A]	NAI	C5B-O5B-PA-O2A
2	B	1301[B]	NAI	C5B-O5B-PA-O1A
2	B	1301[B]	NAI	C5B-O5B-PA-O2A
2	A	1301	NAI	C5B-O5B-PA-O2A
2	B	1301[B]	NAI	O4B-C4B-C5B-O5B
5	A	1304	FDA	C2'-C3'-C4'-C5'
5	B	1303	FDA	P-O3P-PA-O1A
2	B	1301[B]	NAI	C3D-C4D-C5D-O5D
2	B	1301[B]	NAI	PN-O3-PA-O2A
5	A	1304	FDA	O3'-C3'-C4'-O4'
5	B	1303	FDA	O3'-C3'-C4'-O4'
5	B	1303	FDA	C3B-C4B-C5B-O5B
5	A	1304	FDA	O3'-C3'-C4'-C5'

There are no ring outliers.

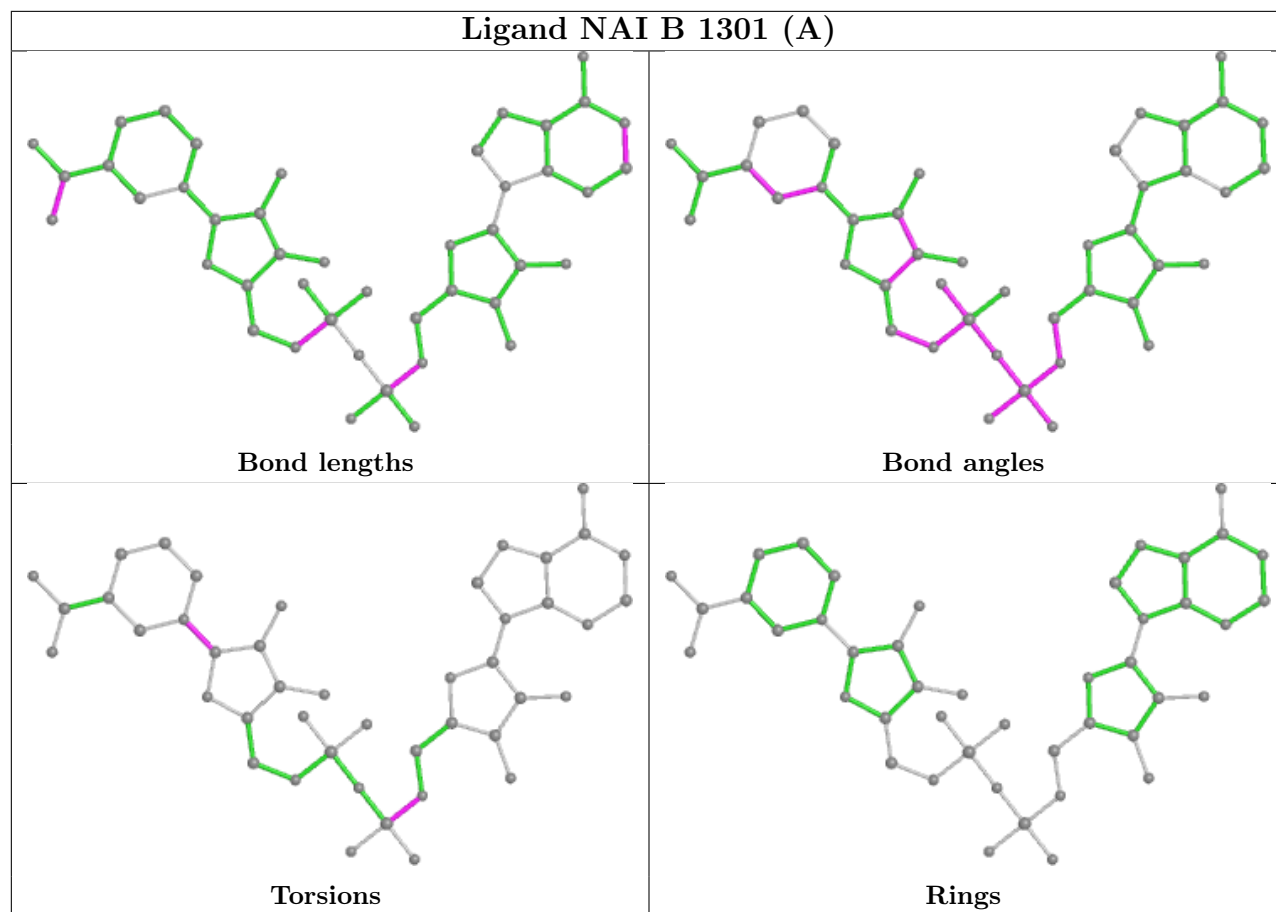
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1304	FDA	2	0
2	B	1301[A]	NAI	1	0
2	B	1301[B]	NAI	5	0
6	A	1307	SO4	1	0
2	A	1301	NAI	1	0
5	B	1303	FDA	1	0

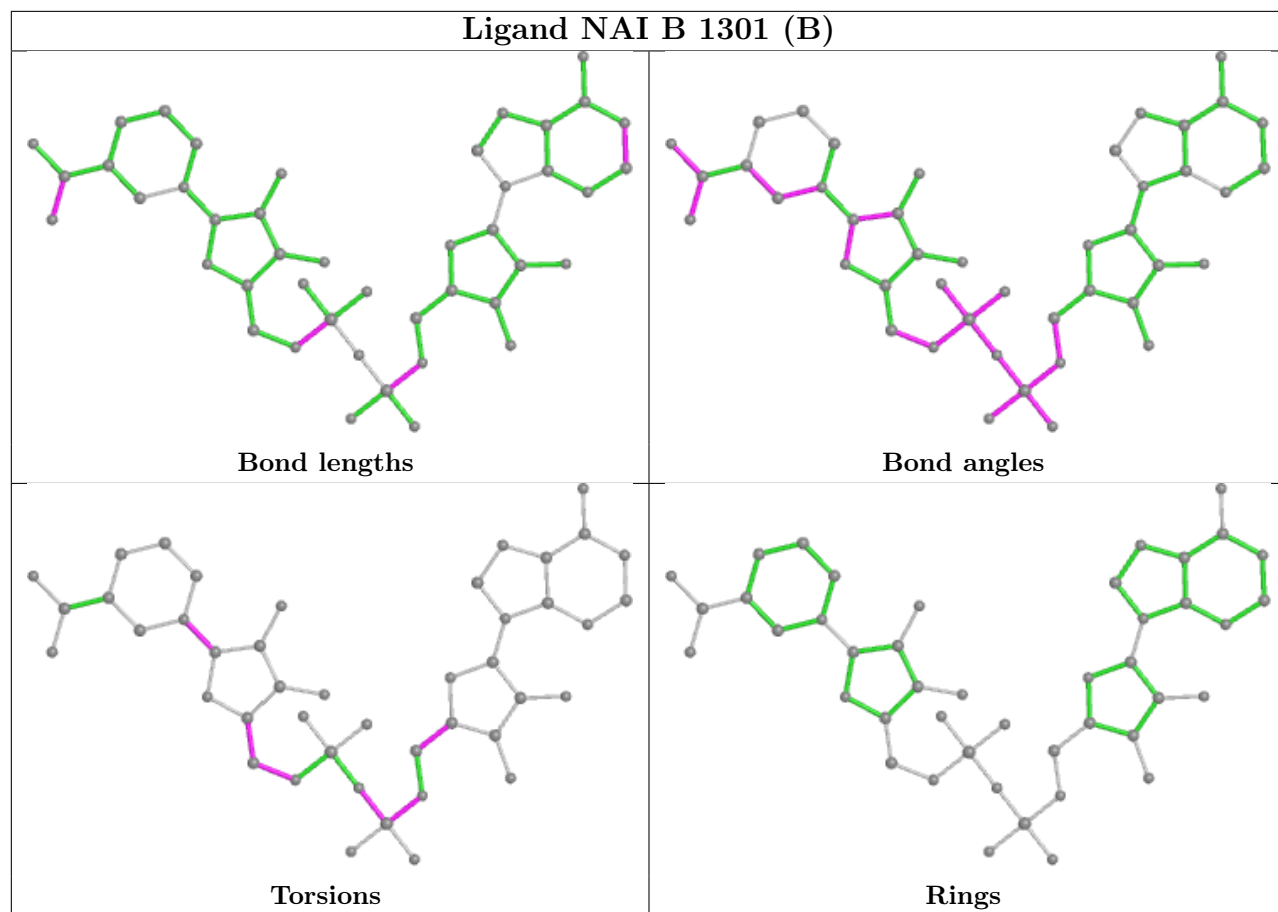
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

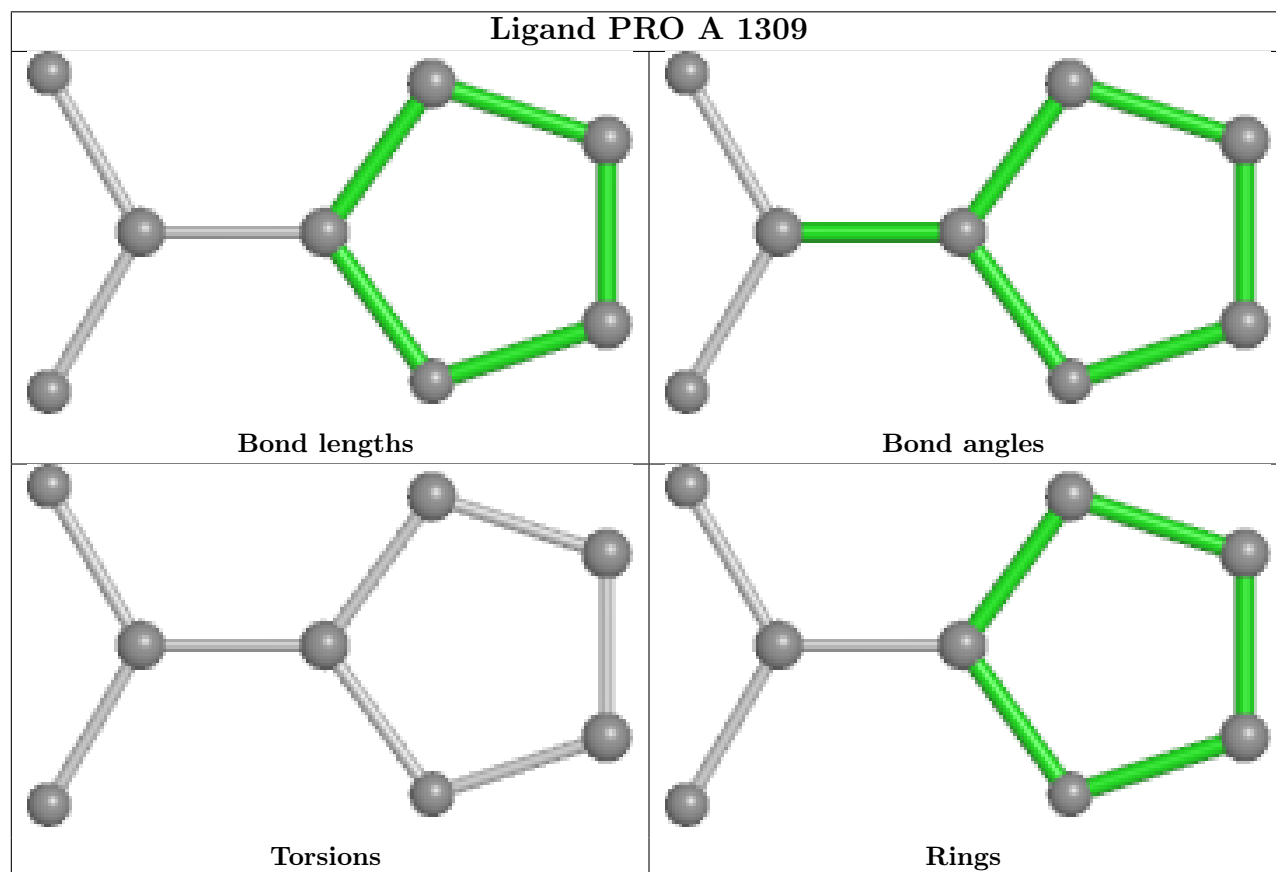
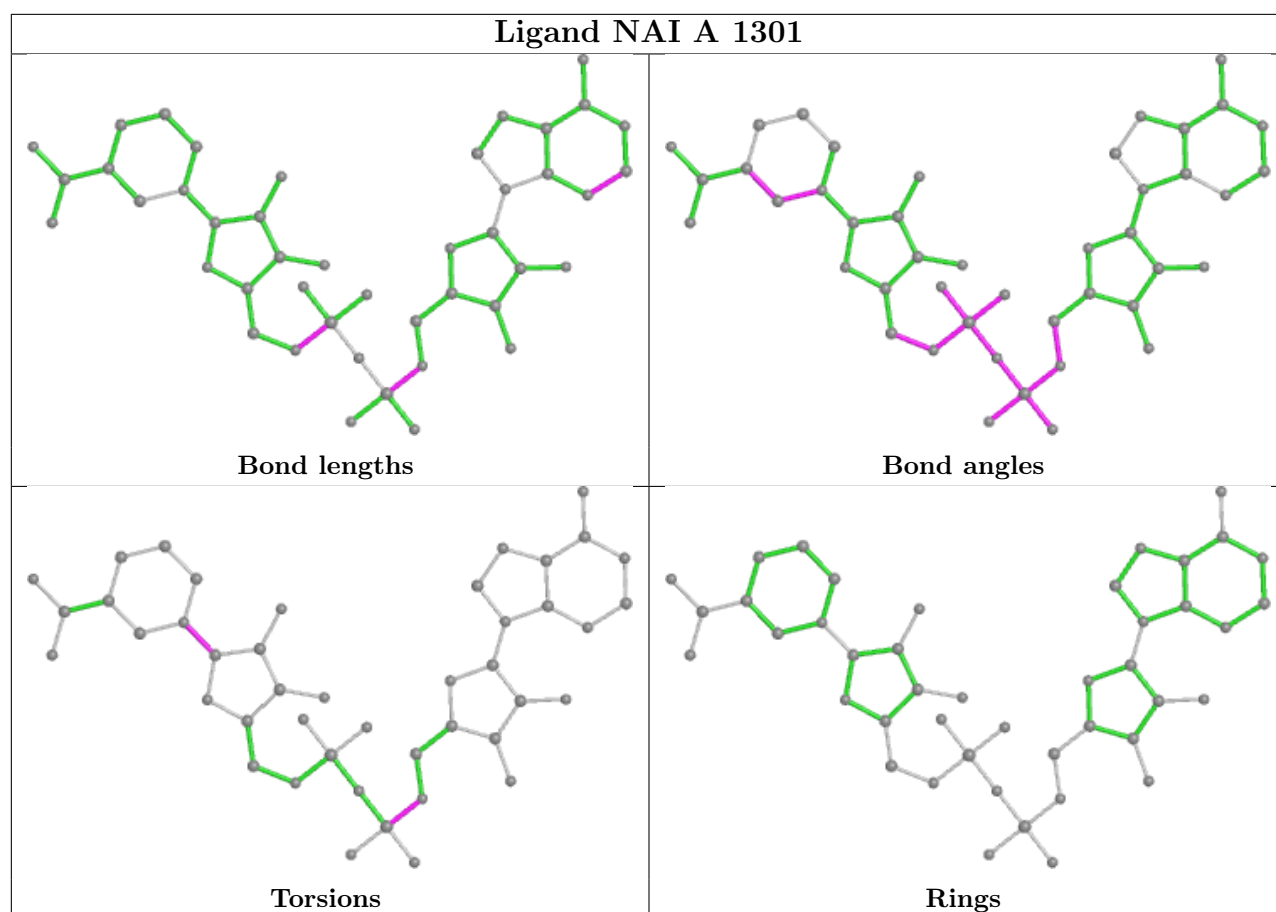


## Ligand NAI B 1301 (A)

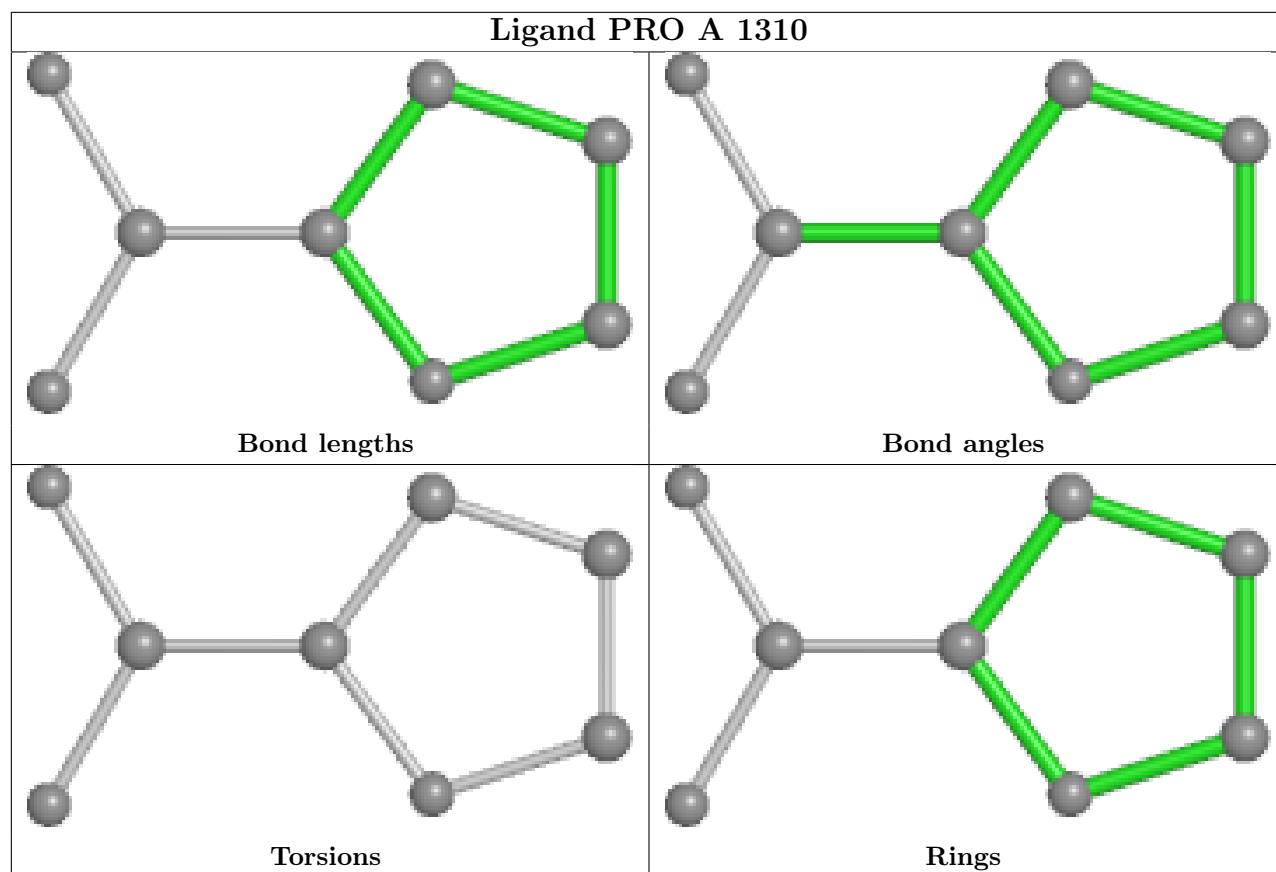
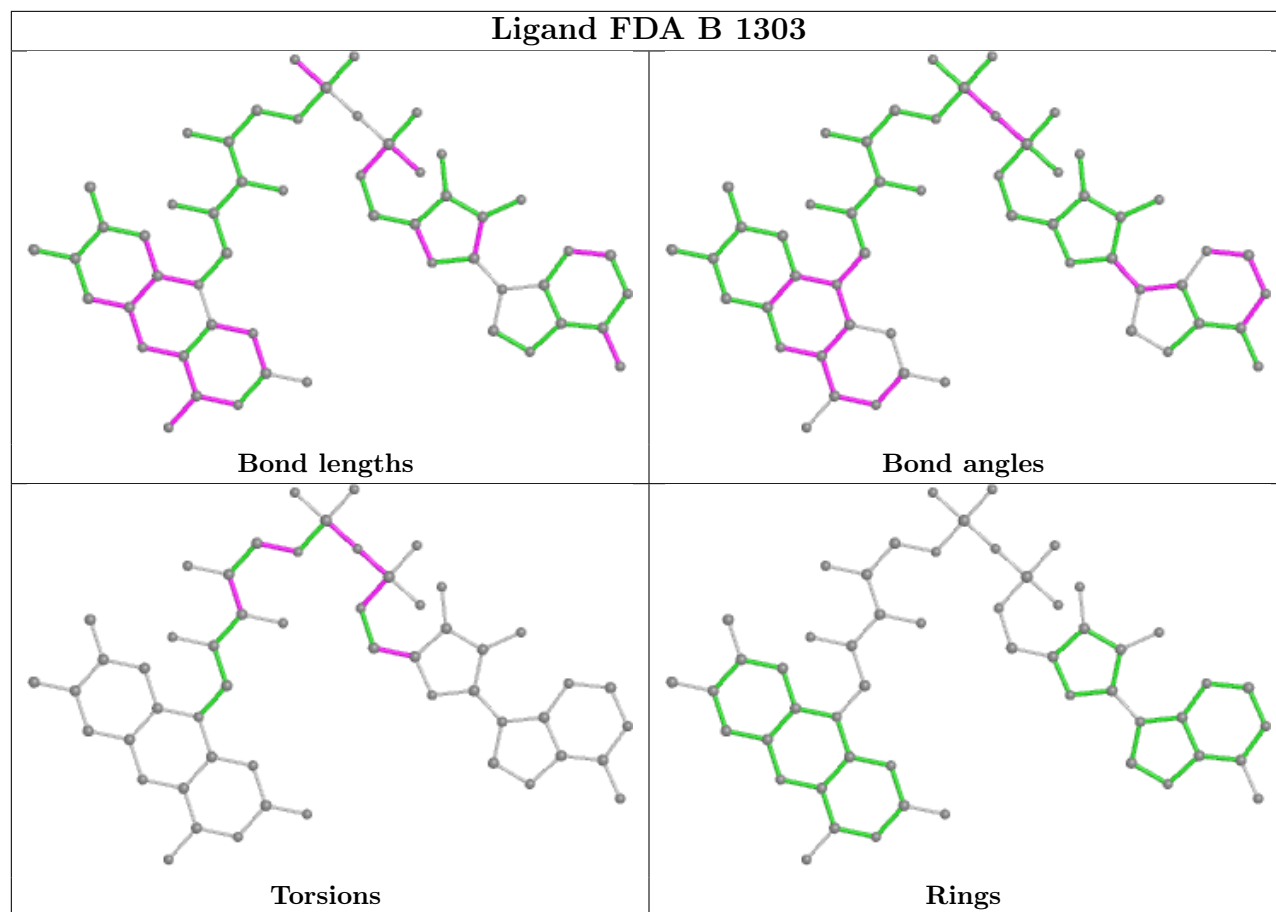


## Ligand NAI B 1301 (B)









## 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	1209/1235 (97%)	0.06	40 (3%) 46 47	13, 22, 41, 67	0
1	B	1208/1235 (97%)	0.18	50 (4%) 37 38	13, 23, 44, 70	0
All	All	2417/2470 (97%)	0.12	90 (3%) 41 42	13, 22, 43, 70	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	PRO	6.3
1	A	506	PRO	6.1
1	A	127	ASP	4.4
1	B	1227	ALA	4.3
1	B	128	GLY	3.8
1	A	493	ASN	3.8
1	B	912	ILE	3.6
1	A	134	LEU	3.5
1	A	120	LEU	3.5
1	B	19	ALA	3.4
1	A	500	VAL	3.4
1	B	485	TYR	3.3
1	B	16	ALA	3.2
1	B	506	PRO	3.2
1	B	439	PHE	3.2
1	A	114	THR	3.1
1	A	1227	ALA	3.1
1	B	1200	ARG	3.1
1	A	115	ALA	3.1
1	B	511	ASP	3.1
1	A	133	HIS	3.0
1	A	501	HIS	3.0
1	B	497	SER	3.0
1	B	441	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	115	ALA	2.9
1	A	75	LEU	2.9
1	B	438	ASP	2.9
1	A	82	SER	2.9
1	A	504	ASN	2.8
1	A	494	GLY	2.8
1	B	510	ILE	2.8
1	A	130	TRP	2.7
1	B	507	LYS	2.7
1	B	129	ASN	2.7
1	A	1229	LEU	2.7
1	A	116	THR	2.6
1	B	918	THR	2.6
1	B	914	LEU	2.6
1	A	508	VAL	2.6
1	A	495	ALA	2.6
1	B	55	THR	2.6
1	B	913	GLY	2.6
1	B	87	LEU	2.6
1	B	482	LEU	2.5
1	A	916	SER	2.5
1	B	118	ASP	2.5
1	A	1228	SER	2.5
1	A	485	TYR	2.5
1	B	132	SER	2.5
1	A	525	PRO	2.5
1	A	129	ASN	2.4
1	B	508	VAL	2.4
1	B	916	SER	2.4
1	A	27	PRO	2.4
1	A	503	ILE	2.4
1	A	132	SER	2.4
1	B	1058	ASP	2.4
1	B	75	LEU	2.4
1	B	800	PRO	2.4
1	B	503	ILE	2.4
1	B	1229	LEU	2.3
1	B	462	GLY	2.3
1	B	499	PHE	2.3
1	A	511	ASP	2.3
1	B	91	TYR	2.3
1	B	60	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	119	ALA	2.2
1	A	571	ALA	2.2
1	A	125	ILE	2.2
1	A	510	ILE	2.2
1	B	1056	TRP	2.2
1	A	123	ASP	2.2
1	B	504	ASN	2.2
1	B	491	LEU	2.2
1	B	133	HIS	2.2
1	B	134	LEU	2.1
1	A	526	VAL	2.1
1	A	83	GLY	2.1
1	B	82	SER	2.1
1	A	484	ALA	2.1
1	B	1223	ALA	2.1
1	B	915	ALA	2.1
1	B	1222	ALA	2.1
1	A	15	PRO	2.1
1	A	524	MET	2.0
1	B	494	GLY	2.0
1	B	463	ARG	2.0
1	B	525	PRO	2.0
1	A	118	ASP	2.0
1	B	501	HIS	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](#)

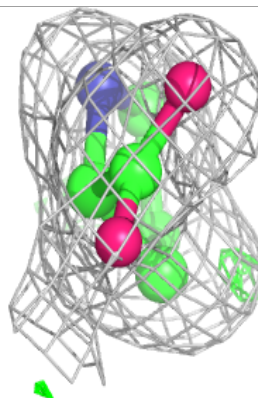
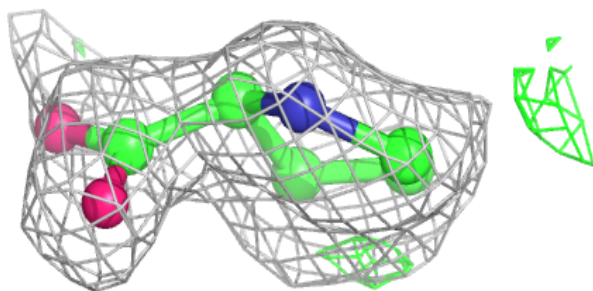
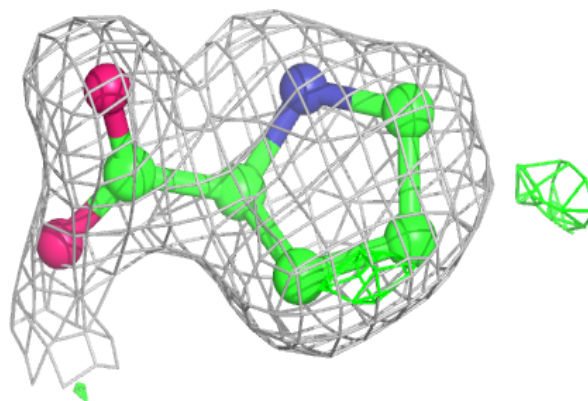
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	PRO	A	1310	8/8	0.80	0.12	30,39,49,54	0
9	PGE	B	1302	10/10	0.86	0.14	38,45,55,55	0
6	SO4	B	1305	5/5	0.89	0.22	68,70,76,77	0
3	PEG	A	1302	7/7	0.90	0.10	28,32,44,44	0
6	SO4	A	1307	5/5	0.91	0.23	48,57,66,68	0
7	MG	A	1308	1/1	0.91	0.10	36,36,36,36	0
2	NAI	A	1301	44/44	0.92	0.11	19,24,30,30	0
6	SO4	A	1306	5/5	0.92	0.13	54,57,61,66	0
8	PRO	A	1309	8/8	0.94	0.14	18,25,29,31	8
2	NAI	B	1301[A]	44/44	0.95	0.12	12,17,21,23	44
2	NAI	B	1301[B]	44/44	0.95	0.12	7,16,18,21	44
5	FDA	B	1303	53/53	0.95	0.08	15,20,24,26	0
8	PRO	B	1307	8/8	0.95	0.13	19,25,31,33	8
5	FDA	A	1304	53/53	0.96	0.08	16,19,23,28	0
7	MG	B	1306	1/1	0.97	0.10	23,23,23,23	0
4	FMT	A	1303	3/3	0.97	0.09	20,20,35,35	0
6	SO4	A	1305	5/5	0.99	0.06	18,19,21,24	0
6	SO4	B	1304	5/5	0.99	0.05	17,17,20,21	0

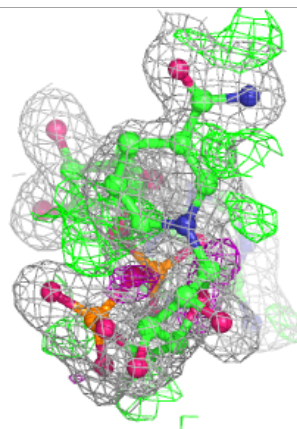
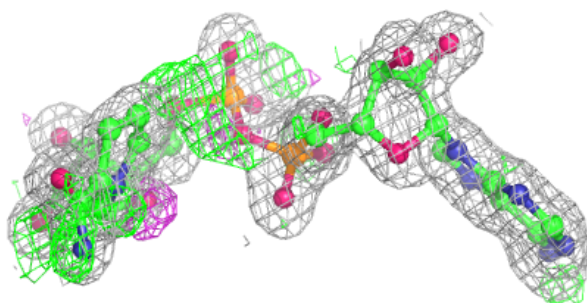
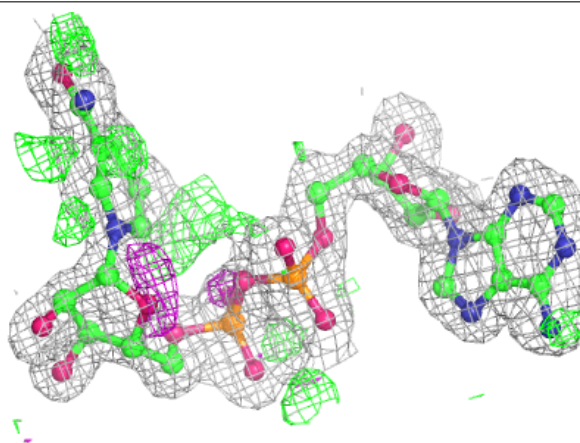
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PRO A 1310:**

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

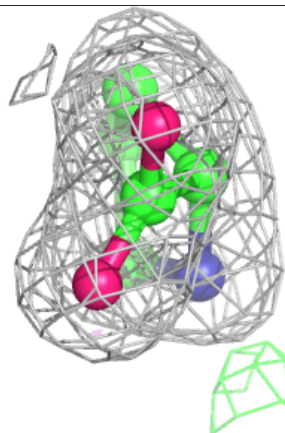
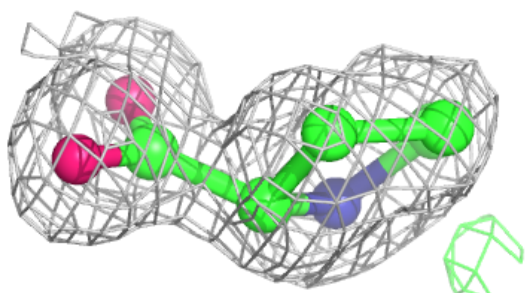
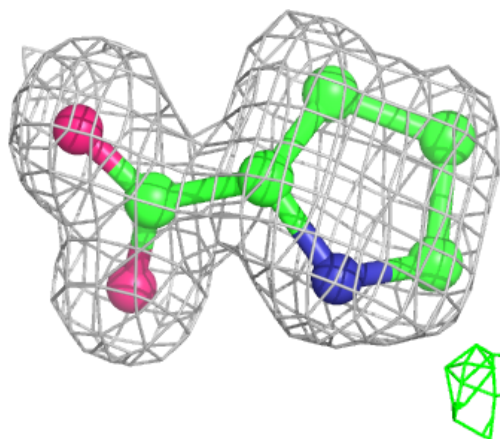
**Electron density around NAI A 1301:**

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

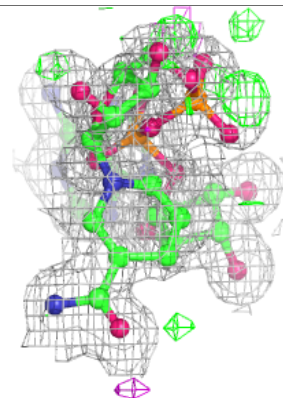
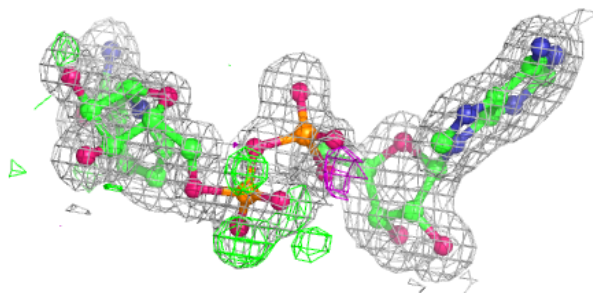
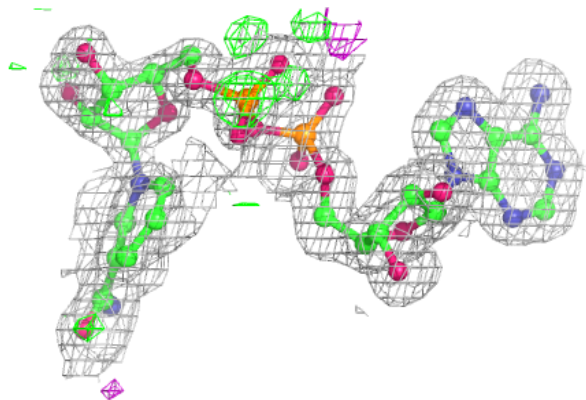


**Electron density around PRO A 1309:**

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

**Electron density around NAI B 1301 (A):**

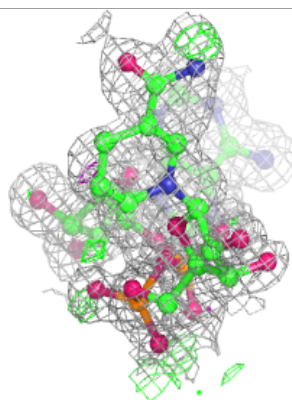
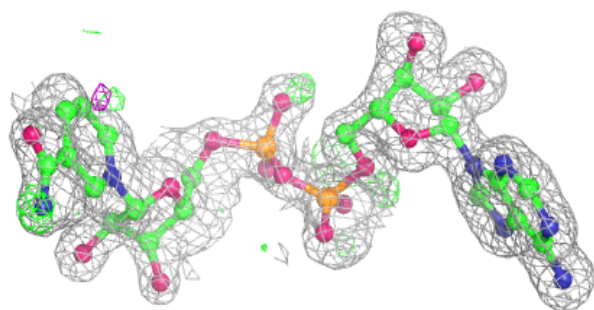
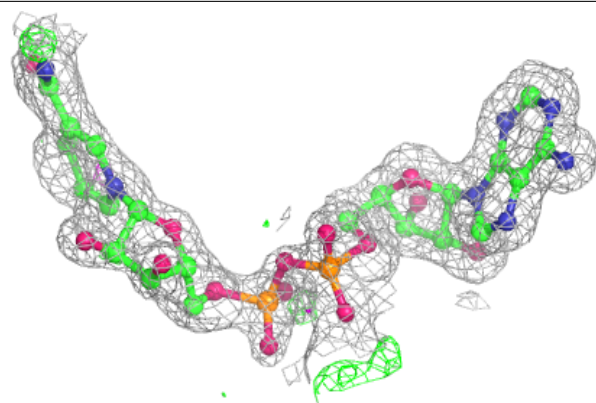
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



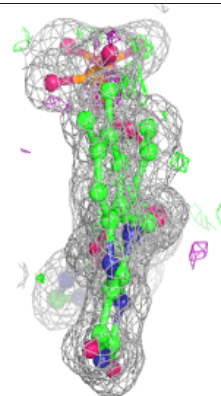
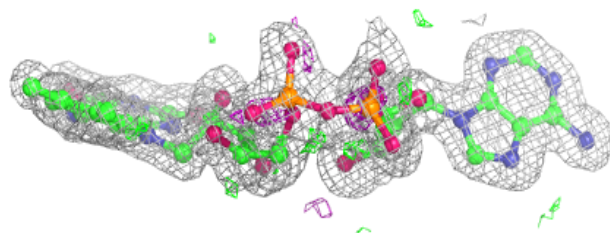
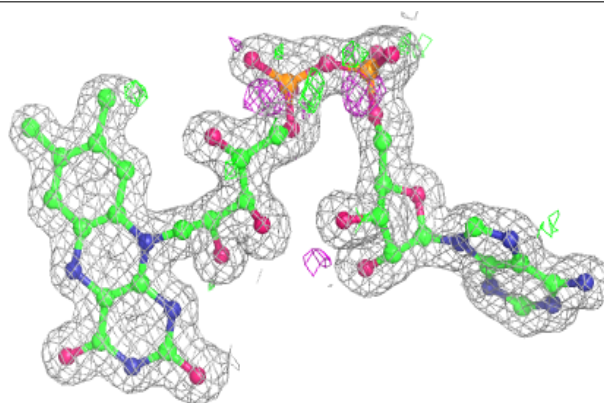


**Electron density around NAI B 1301 (B):**

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

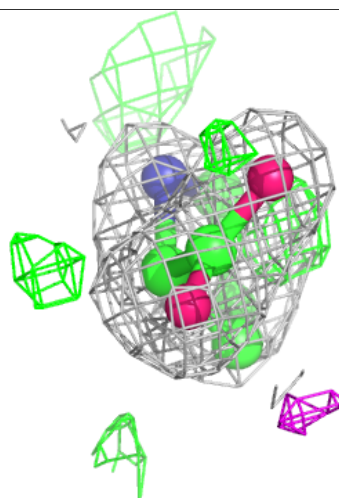
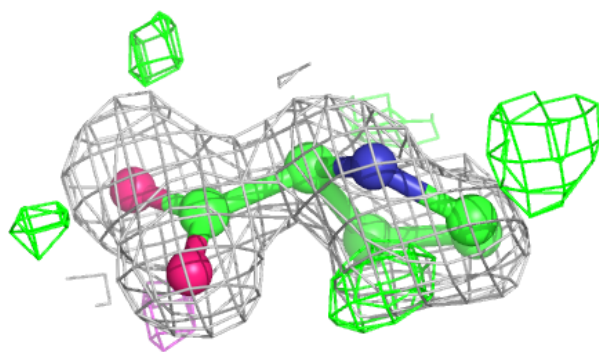
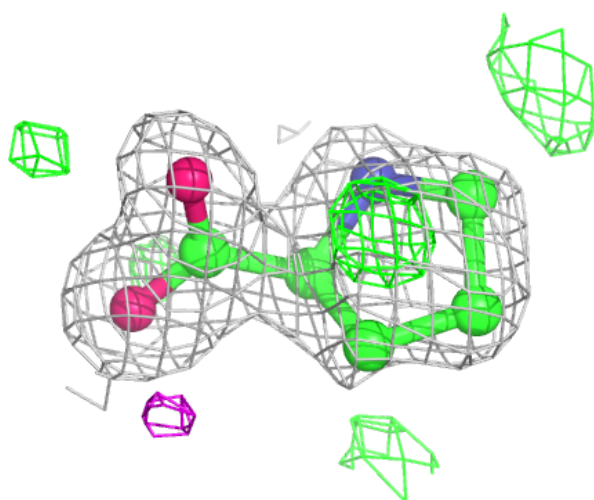
**Electron density around FDA B 1303:**

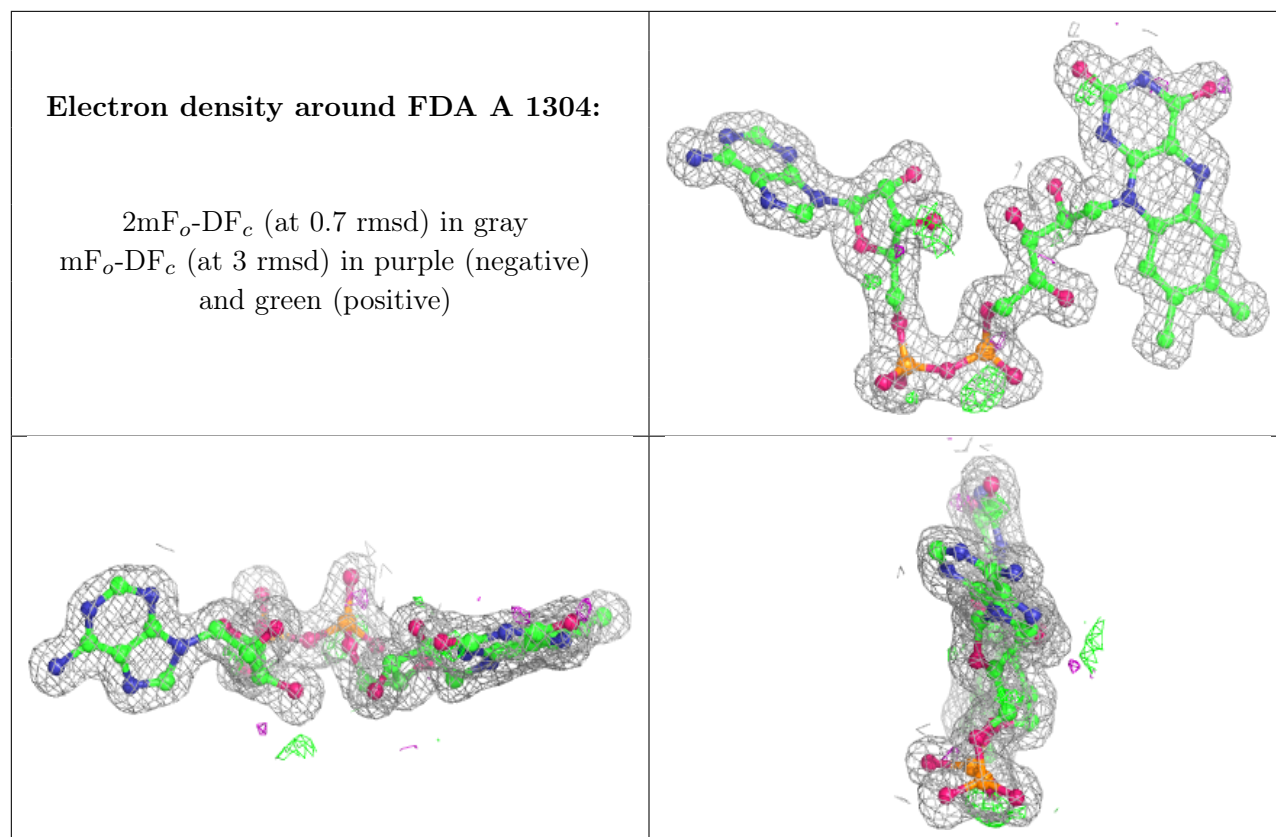
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PRO B 1307:**

$2mF_o-DF_c$  (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.