



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:53 am BST

PDB ID : 4R68  
Title : Lactate Dehydrogenase in complex with inhibitor compound 31  
Authors : Eigenbrot, C.; Ultsch, M.  
Deposited on : 2014-08-22  
Resolution : 2.11 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 : 2.11  
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) : 2.11

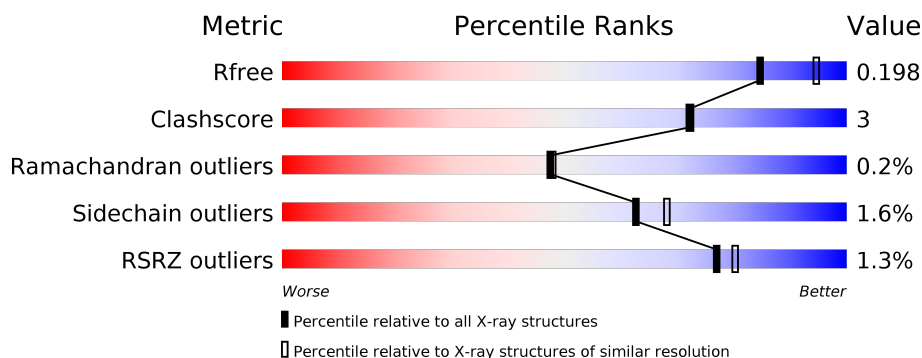
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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 on 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	331	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	331	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	C	331	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	331	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>

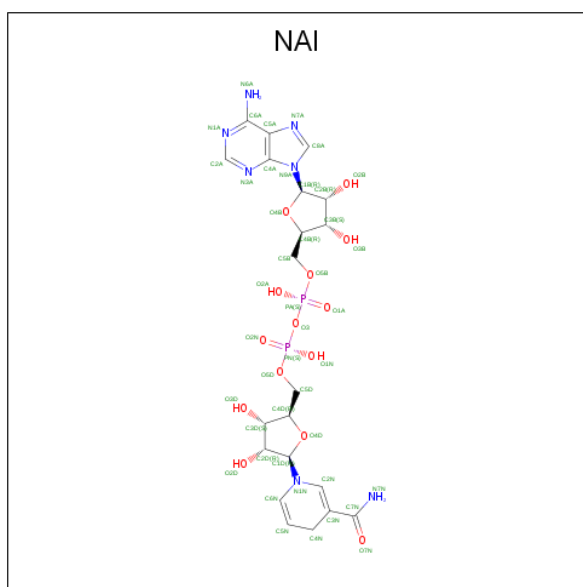


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total 2587	C 1652	N 439	O 482	S 14	0	4	0
1	B	331	Total 2576	C 1644	N 442	O 477	S 13	0	1	0
1	C	323	Total 2506	C 1607	N 424	O 462	S 13	0	1	0
1	D	331	Total 2581	C 1650	N 439	O 478	S 14	0	3	0

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



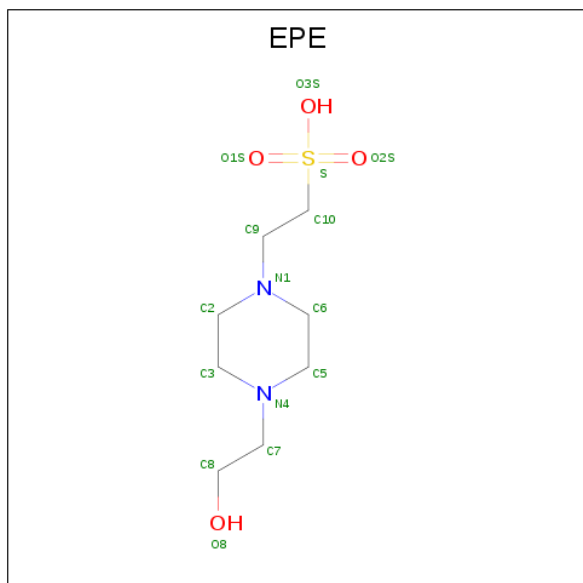
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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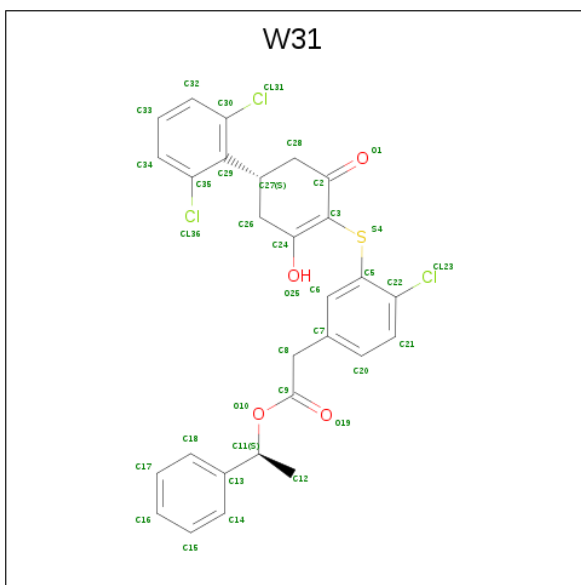
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is (1S)-1-phenylethyl (4-chloro-3-{[(4S)-4-(2,6-dichlorophenyl)-2-hydroxy-6-oxocyclohex-1-en-1-yl]sulfanyl}phenyl)acetate (three-letter code: W31) (formula: C<sub>28</sub>H<sub>23</sub>Cl<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	S	0	0
			36	28	3	4	1		
4	B	1	Total	C	Cl	O	S	0	0
			36	28	3	4	1		
4	C	1	Total	C	Cl	O	S	0	0
			36	28	3	4	1		
4	D	1	Total	C	Cl	O	S	0	0
			36	28	3	4	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

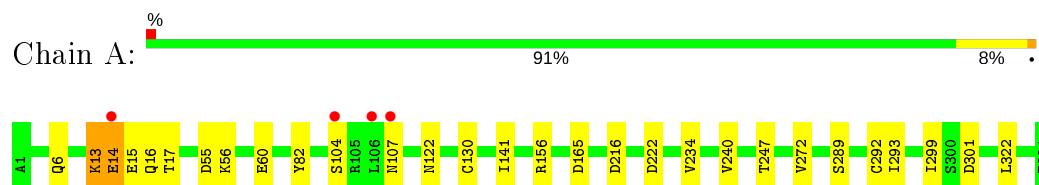
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	233	Total	O		0	0
			233	233			
6	B	247	Total	O		0	0
			247	247			
6	C	200	Total	O		0	0
			200	200			
6	D	257	Total	O		0	0
			257	257			

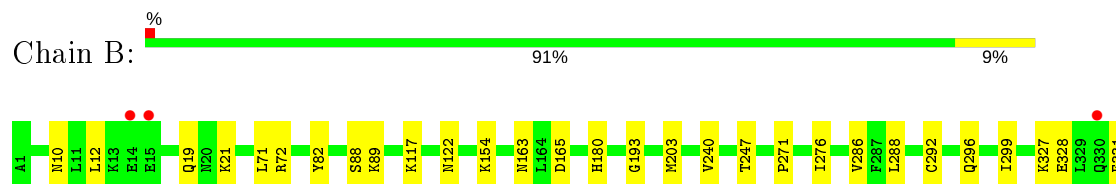
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

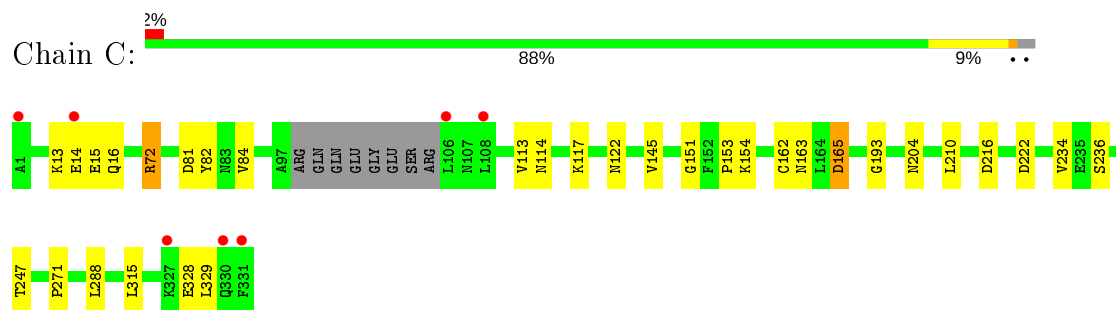
- Molecule 1: L-lactate dehydrogenase A chain



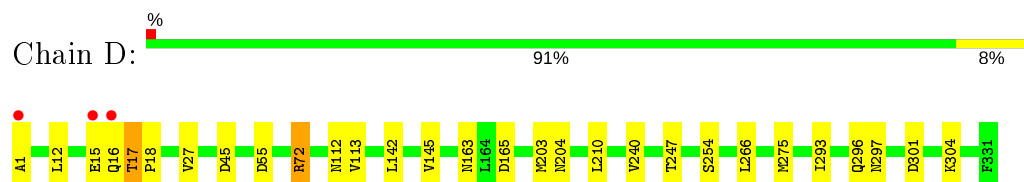
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.64Å 81.07Å 102.48Å 90.00° 98.75° 90.00°	Depositor
Resolution (Å)	57.12 – 2.11 57.13 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.2 (57.12-2.11) 97.2 (57.13-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.155 , 0.197 0.155 , 0.198	Depositor DCC
$R_{free}$ test set	1425 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11572	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 4.75% 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: W31, NAI, EPE, 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	0.35	0/2643	0.54	0/3573
1	B	0.37	0/2623	0.52	0/3546
1	C	0.34	0/2552	0.51	0/3451
1	D	0.36	0/2634	0.52	0/3561
All	All	0.35	0/10452	0.52	0/14131

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	2587	0	2680	18	0
1	B	2576	0	2669	18	0
1	C	2506	0	2606	18	0
1	D	2581	0	2681	18	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	17	1	0
3	C	15	0	17	3	0
3	D	15	0	17	0	0
4	A	36	0	22	1	0
4	B	36	0	22	2	0
4	C	36	0	22	2	0
4	D	36	0	22	1	0
5	D	5	0	0	0	0
6	A	233	0	0	1	0
6	B	247	0	0	2	0
6	C	200	0	0	2	0
6	D	257	0	0	3	0
All	All	11572	0	10896	72	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 3.

All (72) 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:14:GLU:HB3	1:A:15:GLU:HB2	1.67	0.76
1:B:203:MET:SD	6:B:1110:HOH:O	2.43	0.75
1:D:203[A]:MET:HG2	1:D:210:LEU:HD22	1.71	0.73
1:D:112:ASN:HB3	1:D:142:LEU:HD21	1.74	0.69
1:B:276:ILE:HG12	1:B:288:LEU:HB2	1.79	0.64
1:A:107:ASN:HA	6:A:1118:HOH:O	1.99	0.62
1:A:293:ILE:HD12	1:A:301:ASP:HB2	1.82	0.59
1:C:154[B]:LYS:HG3	3:C:802:EPE:O2S	2.02	0.59
1:D:163:ASN:OD1	1:D:254[B]:SER:OG	2.25	0.55
1:C:153:PRO:HA	3:C:802:EPE:H92	1.89	0.54
1:C:114:ASN:HA	1:C:117:LYS:HD3	1.90	0.53
1:A:16:GLN:HB2	1:D:296:GLN:NE2	2.24	0.52
1:D:113:VAL:HG22	1:D:145:VAL:HG21	1.91	0.52
1:C:82:TYR:CG	1:C:122:ASN:HB3	2.45	0.51
1:B:163:ASN:HA	1:B:271:PRO:HG2	1.94	0.50
1:D:15:GLU:HG3	1:D:17:THR:HG22	1.92	0.50
1:C:113:VAL:HG21	1:C:329:LEU:HD13	1.93	0.50
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.94	0.49
4:A:803:W31:H17	4:A:803:W31:CL31	2.49	0.49
1:A:240:VAL:HG11	1:A:247:THR:HG22	1.95	0.49
1:D:293[A]:ILE:HD12	1:D:301:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:CYS:HA	1:C:165:ASP:OD2	2.12	0.49
1:C:81:ASP:O	1:C:84:VAL:HG22	2.13	0.48
1:B:180:HIS:HB2	1:D:266:LEU:O	2.14	0.48
4:C:803:W31:H17	4:C:803:W31:CL31	2.51	0.48
1:B:117:LYS:HD3	1:B:331:PHE:C	2.34	0.48
1:A:55[A]:ASP:OD1	1:A:56:LYS:N	2.46	0.48
1:B:154:LYS:NZ	6:B:1018:HOH:O	2.29	0.48
1:B:276:ILE:HD11	1:B:286:VAL:HG23	1.94	0.47
1:D:55:ASP:HB3	6:D:1147:HOH:O	2.14	0.47
1:C:72:ARG:NH1	6:C:1041:HOH:O	2.47	0.47
1:D:72:ARG:HE	1:D:72:ARG:HB2	1.55	0.47
1:A:56:LYS:NZ	1:A:60:GLU:OE2	2.43	0.46
1:D:240:VAL:HG11	1:D:247:THR:HG22	1.97	0.46
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.50	0.46
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.49	0.46
1:C:151:GLY:HA3	3:C:802:EPE:H81	1.96	0.46
1:A:14:GLU:HB3	1:A:15:GLU:CB	2.42	0.46
1:B:72[B]:ARG:HB2	1:B:72[B]:ARG:HE	1.60	0.45
1:B:10:ASN:ND2	1:B:12:LEU:O	2.45	0.45
1:B:71:LEU:O	1:B:72[A]:ARG:HD3	2.16	0.45
1:C:204:ASN:HA	1:C:210:LEU:HD13	1.98	0.45
1:C:328:GLU:HB2	6:C:1098:HOH:O	2.17	0.44
1:C:247:THR:CG2	2:C:801:NAI:H5N	2.47	0.44
4:D:802:W31:H17	4:D:802:W31:CL31	2.55	0.44
1:B:19:GLN:O	1:B:89:LYS:HE2	2.18	0.43
1:C:113:VAL:HG22	1:C:145:VAL:HG21	1.99	0.43
1:D:1:ALA:N	6:D:1101:HOH:O	2.51	0.43
1:A:16:GLN:NE2	1:D:297:ASN:OD1	2.41	0.43
1:B:327:LYS:HE2	1:B:328:GLU:OE2	2.19	0.43
1:B:240:VAL:CG1	1:B:247:THR:HG22	2.48	0.43
3:B:802:EPE:H101	3:B:802:EPE:H61	1.76	0.43
1:A:216:ASP:O	1:A:222:ASP:HB2	2.19	0.42
1:A:6:GLN:O	1:D:304:LYS:HE3	2.19	0.42
1:D:204:ASN:HA	1:D:210:LEU:HD13	2.00	0.42
1:A:272:VAL:O	1:A:289:SER:HA	2.20	0.42
1:C:163:ASN:HA	1:C:271:PRO:HG2	2.02	0.42
1:C:288:LEU:HD13	1:C:315:LEU:HD13	2.01	0.42
1:B:292:CYS:HB3	1:B:299:ILE:HG23	2.02	0.41
4:B:803:W31:CL36	4:B:803:W31:H17	2.57	0.41
1:A:130:CYS:O	1:A:156:ARG:HD2	2.21	0.41
1:A:141:ILE:HG13	1:A:322:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:GLN:OE1	1:C:16:GLN:HB3	2.20	0.41
1:C:216:ASP:O	1:C:222:ASP:HB2	2.20	0.41
1:C:193:GLY:HA2	4:C:803:W31:C20	2.51	0.41
1:D:240:VAL:CG1	1:D:247:THR:HG22	2.50	0.41
1:B:193:GLY:HA2	4:B:803:W31:C20	2.50	0.41
1:D:45:ASP:HA	6:D:1087:HOH:O	2.20	0.40
1:A:104:SER:OG	1:A:107:ASN:ND2	2.55	0.40
1:B:21:LYS:HB3	1:B:88:SER:HA	2.02	0.40
1:A:13:LYS:HA	1:A:13:LYS:HD3	1.88	0.40
1:D:17:THR:HA	1:D:18:PRO:HD3	1.80	0.40

There are no symmetry-related clashes.

## 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	333/331 (101%)	323 (97%)	10 (3%)	0	100	100
1	B	330/331 (100%)	324 (98%)	6 (2%)	0	100	100
1	C	320/331 (97%)	313 (98%)	6 (2%)	1 (0%)	41	40
1	D	332/331 (100%)	323 (97%)	8 (2%)	1 (0%)	41	40
All	All	1315/1324 (99%)	1283 (98%)	30 (2%)	2 (0%)	47	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	GLU
1	D	27	VAL

### 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	291/287 (101%)	286 (98%)	5 (2%)	60	66
1	B	288/287 (100%)	287 (100%)	1 (0%)	92	95
1	C	281/287 (98%)	275 (98%)	6 (2%)	53	57
1	D	290/287 (101%)	284 (98%)	6 (2%)	53	57
All	All	1150/1148 (100%)	1132 (98%)	18 (2%)	62	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	14	GLU
1	A	17	THR
1	A	165	ASP
1	A	234	VAL
1	B	165	ASP
1	C	13	LYS
1	C	15	GLU
1	C	72	ARG
1	C	165	ASP
1	C	234	VAL
1	C	236	SER
1	D	12	LEU
1	D	16	GLN
1	D	17	THR
1	D	72	ARG
1	D	165	ASP
1	D	275	MET

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

Mol	Chain	Res	Type
1	A	107	ASN

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Mol	Chain	Res	Type
1	C	110	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EPE	A	802	-	15,15,15	0.81	1 (6%)	18,20,20	1.99	6 (33%)
2	NAI	C	801	-	42,48,48	2.04	12 (28%)	47,73,73	1.27	6 (12%)
2	NAI	B	801	-	42,48,48	1.95	11 (26%)	47,73,73	1.39	10 (21%)
2	NAI	D	801	-	42,48,48	1.98	10 (23%)	47,73,73	1.24	4 (8%)
5	SO4	D	804	-	4,4,4	0.21	0	6,6,6	0.22	0
3	EPE	D	803	-	15,15,15	0.94	1 (6%)	18,20,20	1.91	5 (27%)
2	NAI	A	801	-	42,48,48	2.03	11 (26%)	47,73,73	1.28	6 (12%)
4	W31	D	802	-	39,39,39	0.64	0	48,55,55	1.35	6 (12%)
3	EPE	B	802	-	15,15,15	0.86	1 (6%)	18,20,20	2.01	6 (33%)
4	W31	A	803	-	39,39,39	0.59	0	48,55,55	1.62	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	W31	B	803	-	39,39,39	0.72	0	48,55,55	1.57	9 (18%)
4	W31	C	803	-	39,39,39	0.58	0	48,55,55	1.49	9 (18%)
3	EPE	C	802	-	15,15,15	0.84	1 (6%)	18,20,20	2.35	7 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	802	-	-	5/9/19/19	0/1/1/1
2	NAI	C	801	-	-	5/25/72/72	0/5/5/5
2	NAI	B	801	-	-	3/25/72/72	0/5/5/5
2	NAI	D	801	-	-	6/25/72/72	0/5/5/5
3	EPE	D	803	-	-	5/9/19/19	0/1/1/1
2	NAI	A	801	-	-	5/25/72/72	0/5/5/5
4	W31	D	802	-	-	8/20/36/36	0/4/4/4
3	EPE	B	802	-	-	2/9/19/19	0/1/1/1
4	W31	A	803	-	-	9/20/36/36	0/4/4/4
4	W31	B	803	-	-	7/20/36/36	0/4/4/4
4	W31	C	803	-	-	8/20/36/36	0/4/4/4
3	EPE	C	802	-	-	5/9/19/19	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAI	C4N-C3N	-5.01	1.40	1.49
2	C	801	NAI	C6N-C5N	4.97	1.42	1.33
2	D	801	NAI	C6N-C5N	4.75	1.41	1.33
2	D	801	NAI	C4N-C3N	-4.68	1.40	1.49
2	C	801	NAI	C4N-C3N	-4.62	1.40	1.49
2	A	801	NAI	C6N-C5N	4.51	1.41	1.33
2	A	801	NAI	C2B-C3B	-4.49	1.41	1.53
2	B	801	NAI	C2B-C3B	-4.48	1.41	1.53
2	C	801	NAI	C2B-C3B	-4.46	1.41	1.53
2	B	801	NAI	C4N-C3N	-4.42	1.41	1.49
2	B	801	NAI	C6N-C5N	4.41	1.41	1.33
2	D	801	NAI	C2B-C3B	-4.28	1.41	1.53
2	A	801	NAI	C7N-N7N	3.62	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAI	O2D-C2D	-3.57	1.34	1.43
2	B	801	NAI	C7N-N7N	3.54	1.42	1.33
2	D	801	NAI	C7N-N7N	3.51	1.42	1.33
2	A	801	NAI	C6A-N6A	3.39	1.46	1.34
2	C	801	NAI	C7N-N7N	3.37	1.42	1.33
2	C	801	NAI	C6A-N6A	3.29	1.46	1.34
2	D	801	NAI	C6A-N6A	3.26	1.46	1.34
2	C	801	NAI	O2D-C2D	-3.25	1.35	1.43
2	B	801	NAI	C6A-N6A	3.15	1.45	1.34
2	B	801	NAI	O2D-C2D	-3.11	1.35	1.43
3	D	803	EPE	C10-S	3.11	1.81	1.77
2	D	801	NAI	O2D-C2D	-3.09	1.35	1.43
2	C	801	NAI	C4N-C5N	-3.03	1.41	1.48
3	C	802	EPE	C10-S	3.01	1.81	1.77
2	B	801	NAI	C4N-C5N	-2.92	1.41	1.48
2	D	801	NAI	C2B-C1B	-2.90	1.49	1.53
3	B	802	EPE	C10-S	2.90	1.81	1.77
2	A	801	NAI	C4N-C5N	-2.86	1.41	1.48
2	A	801	NAI	C5D-C4D	-2.75	1.43	1.51
2	D	801	NAI	C4N-C5N	-2.72	1.41	1.48
2	B	801	NAI	C5D-C4D	-2.69	1.43	1.51
2	C	801	NAI	C5D-C4D	-2.68	1.43	1.51
2	A	801	NAI	C2B-C1B	-2.68	1.49	1.53
2	C	801	NAI	C2B-C1B	-2.68	1.49	1.53
3	A	802	EPE	C10-S	2.64	1.81	1.77
2	D	801	NAI	C5D-C4D	-2.59	1.43	1.51
2	C	801	NAI	C5B-C4B	-2.36	1.44	1.51
2	D	801	NAI	O4B-C4B	-2.26	1.40	1.45
2	B	801	NAI	C2B-C1B	-2.23	1.50	1.53
2	A	801	NAI	C3D-C4D	-2.13	1.47	1.53
2	B	801	NAI	O4B-C4B	-2.12	1.40	1.45
2	A	801	NAI	O3D-C3D	-2.09	1.38	1.43
2	C	801	NAI	C3D-C4D	-2.08	1.47	1.53
2	B	801	NAI	C3D-C4D	-2.06	1.47	1.53
2	C	801	NAI	O4B-C4B	-2.05	1.40	1.45

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	EPE	C5-N4-C3	6.34	123.10	108.83
4	A	803	W31	O10-C9-C8	5.22	122.13	110.99
3	A	802	EPE	C5-N4-C3	4.69	119.40	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	EPE	C5-N4-C3	4.42	118.78	108.83
2	A	801	NAI	N3A-C2A-N1A	-4.34	121.89	128.68
4	D	802	W31	O10-C9-C8	4.34	120.24	110.99
4	C	803	W31	O10-C9-C8	4.31	120.19	110.99
2	B	801	NAI	N3A-C2A-N1A	-4.26	122.02	128.68
3	B	802	EPE	C5-N4-C3	4.20	118.28	108.83
2	C	801	NAI	N3A-C2A-N1A	-4.17	122.17	128.68
2	D	801	NAI	N3A-C2A-N1A	-4.09	122.28	128.68
4	C	803	W31	O25-C24-C26	4.08	119.97	113.28
3	B	802	EPE	C7-N4-C3	3.90	121.22	111.23
4	B	803	W31	O25-C24-C26	3.88	119.65	113.28
4	B	803	W31	O10-C9-C8	3.80	119.10	110.99
4	B	803	W31	O1-C2-C3	-3.74	117.75	121.95
4	D	802	W31	O25-C24-C26	3.67	119.30	113.28
4	A	803	W31	O25-C24-C26	3.66	119.29	113.28
3	B	802	EPE	C7-N4-C5	3.60	120.44	111.23
3	A	802	EPE	C7-N4-C5	3.58	120.39	111.23
4	B	803	W31	O10-C11-C12	3.52	114.50	106.53
3	A	802	EPE	C7-N4-C3	3.48	120.14	111.23
4	A	803	W31	O1-C2-C3	-3.47	118.05	121.95
3	C	802	EPE	O3S-S-C10	3.42	111.31	105.77
3	D	803	EPE	C7-N4-C3	3.42	119.98	111.23
3	D	803	EPE	C7-N4-C5	3.37	119.85	111.23
2	B	801	NAI	PN-O3-PA	-3.31	121.45	132.83
4	B	803	W31	C27-C28-C2	-3.28	106.19	114.14
4	A	803	W31	C27-C28-C2	-3.24	106.29	114.14
2	B	801	NAI	O4B-C1B-C2B	-3.19	102.27	106.93
4	C	803	W31	C27-C28-C2	-3.06	106.74	114.14
4	D	802	W31	O10-C11-C12	3.00	113.32	106.53
3	B	802	EPE	O1S-S-C10	2.97	110.49	106.92
4	A	803	W31	C29-C30-CL31	2.94	123.33	120.49
2	C	801	NAI	PN-O3-PA	-2.86	123.01	132.83
2	D	801	NAI	PN-O3-PA	-2.83	123.10	132.83
3	C	802	EPE	O1S-S-C10	2.82	110.31	106.92
3	A	802	EPE	O3S-S-C10	2.81	110.31	105.77
3	C	802	EPE	C7-N4-C3	2.80	118.38	111.23
4	A	803	W31	O10-C11-C12	2.77	112.80	106.53
3	C	802	EPE	C6-C5-N4	2.75	116.28	110.64
4	C	803	W31	O10-C11-C12	2.72	112.70	106.53
2	B	801	NAI	O4D-C1D-N1N	2.66	113.26	108.06
4	C	803	W31	C35-C29-C30	2.66	117.98	114.91
4	C	803	W31	C29-C30-CL31	2.65	123.05	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	NAI	C4A-C5A-N7A	-2.65	106.64	109.40
2	C	801	NAI	O4B-C1B-C2B	-2.62	103.10	106.93
3	B	802	EPE	O3S-S-C10	2.59	109.95	105.77
4	D	802	W31	C27-C28-C2	-2.58	107.90	114.14
3	B	802	EPE	C6-N1-C2	2.53	114.52	108.83
2	A	801	NAI	O5B-C5B-C4B	2.52	117.68	108.99
3	D	803	EPE	O3S-S-C10	2.49	109.80	105.77
2	A	801	NAI	C4A-C5A-N7A	-2.47	106.82	109.40
3	C	802	EPE	C7-N4-C5	2.47	117.56	111.23
2	C	801	NAI	C4A-C5A-N7A	-2.45	106.84	109.40
3	A	802	EPE	O1S-S-C10	2.41	109.82	106.92
2	B	801	NAI	O5D-C5D-C4D	2.35	117.07	108.99
2	A	801	NAI	O4D-C1D-N1N	2.32	112.60	108.06
4	A	803	W31	C35-C29-C30	2.32	117.58	114.91
2	A	801	NAI	PN-O3-PA	-2.31	124.89	132.83
2	D	801	NAI	O5D-C5D-C4D	2.30	116.92	108.99
4	C	803	W31	O1-C2-C3	-2.29	119.37	121.95
4	D	802	W31	C28-C27-C29	2.28	117.78	112.41
2	B	801	NAI	O4D-C1D-C2D	-2.25	101.73	106.64
3	D	803	EPE	O2S-S-C10	2.24	109.61	106.92
4	B	803	W31	C28-C27-C29	2.23	117.66	112.41
4	A	803	W31	O10-C9-O19	-2.21	118.36	123.70
3	A	802	EPE	C6-N1-C2	2.21	113.79	108.83
2	A	801	NAI	O5D-C5D-C4D	2.20	116.58	108.99
4	B	803	W31	C35-C29-C30	2.19	117.44	114.91
2	B	801	NAI	O7N-C7N-N7N	-2.19	117.76	122.88
2	B	801	NAI	O5B-C5B-C4B	2.18	116.51	108.99
4	D	802	W31	O10-C9-O19	-2.15	118.51	123.70
2	B	801	NAI	C4A-C5A-N7A	-2.14	107.17	109.40
2	B	801	NAI	C3N-C7N-N7N	2.11	121.42	117.67
4	B	803	W31	C29-C35-CL36	2.10	122.52	120.49
4	A	803	W31	C5-S4-C3	-2.08	100.16	102.81
3	C	802	EPE	C2-C3-N4	2.07	114.89	110.64
4	C	803	W31	O10-C9-O19	-2.07	118.71	123.70
2	C	801	NAI	C5B-C4B-C3B	-2.06	107.47	115.18
4	C	803	W31	C12-C11-C13	-2.04	108.55	112.56
4	B	803	W31	O10-C9-O19	-2.03	118.81	123.70
2	C	801	NAI	O5D-C5D-C4D	2.02	115.94	108.99

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	EPE	C9-C10-S-O1S
3	A	802	EPE	C9-C10-S-O3S
3	D	803	EPE	C8-C7-N4-C3
3	D	803	EPE	C9-C10-S-O1S
4	D	802	W31	C12-C11-O10-C9
4	D	802	W31	C13-C11-O10-C9
4	D	802	W31	C8-C9-O10-C11
4	A	803	W31	C12-C11-O10-C9
4	A	803	W31	C13-C11-O10-C9
4	A	803	W31	C8-C9-O10-C11
4	B	803	W31	C12-C11-O10-C9
4	B	803	W31	C8-C9-O10-C11
4	C	803	W31	C12-C11-O10-C9
4	C	803	W31	C8-C9-O10-C11
3	C	802	EPE	C8-C7-N4-C3
4	D	802	W31	O19-C9-O10-C11
4	B	803	W31	O19-C9-O10-C11
3	B	802	EPE	N4-C7-C8-O8
4	A	803	W31	O19-C9-O10-C11
4	C	803	W31	O19-C9-O10-C11
3	A	802	EPE	C8-C7-N4-C3
3	C	802	EPE	C9-C10-S-O3S
4	A	803	W31	C12-C11-C13-C18
3	D	803	EPE	C9-C10-S-O3S
4	C	803	W31	C13-C11-O10-C9
4	A	803	W31	C12-C11-C13-C14
4	C	803	W31	C12-C11-C13-C14
2	D	801	NAI	C2D-C1D-N1N-C2N
2	C	801	NAI	C2D-C1D-N1N-C2N
2	C	801	NAI	O4D-C1D-N1N-C2N
3	A	802	EPE	C9-C10-S-O2S
3	D	803	EPE	C9-C10-S-O2S
3	C	802	EPE	C9-C10-S-O1S
3	C	802	EPE	C9-C10-S-O2S
4	C	803	W31	C12-C11-C13-C18
2	A	801	NAI	O4D-C1D-N1N-C2N
4	C	803	W31	O10-C11-C13-C14
2	D	801	NAI	O4D-C1D-N1N-C2N
4	B	803	W31	C12-C11-C13-C14
2	A	801	NAI	C2D-C1D-N1N-C2N
4	D	802	W31	C12-C11-C13-C14
2	B	801	NAI	O4D-C1D-N1N-C2N
3	A	802	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
2	B	801	NAI	C2D-C1D-N1N-C2N
2	D	801	NAI	C2D-C1D-N1N-C6N
3	D	803	EPE	C10-C9-N1-C2
4	D	802	W31	O10-C11-C13-C14
4	B	803	W31	O10-C11-C13-C14
4	B	803	W31	O10-C11-C13-C18
2	B	801	NAI	O4B-C4B-C5B-O5B
4	D	802	W31	C12-C11-C13-C18
4	B	803	W31	C12-C11-C13-C18
2	D	801	NAI	O4D-C1D-N1N-C6N
2	C	801	NAI	C2D-C1D-N1N-C6N
4	D	802	W31	O10-C11-C13-C18
4	C	803	W31	O10-C11-C13-C18
2	C	801	NAI	O4D-C1D-N1N-C6N
2	A	801	NAI	O4D-C1D-N1N-C6N
4	A	803	W31	C7-C8-C9-O10
2	D	801	NAI	C5D-O5D-PN-O3
4	A	803	W31	O10-C11-C13-C14
4	A	803	W31	O10-C11-C13-C18
2	A	801	NAI	O4B-C4B-C5B-O5B
3	B	802	EPE	C8-C7-N4-C5
2	C	801	NAI	O4B-C4B-C5B-O5B
2	D	801	NAI	O4B-C4B-C5B-O5B
2	A	801	NAI	C2D-C1D-N1N-C6N
3	C	802	EPE	C8-C7-N4-C5

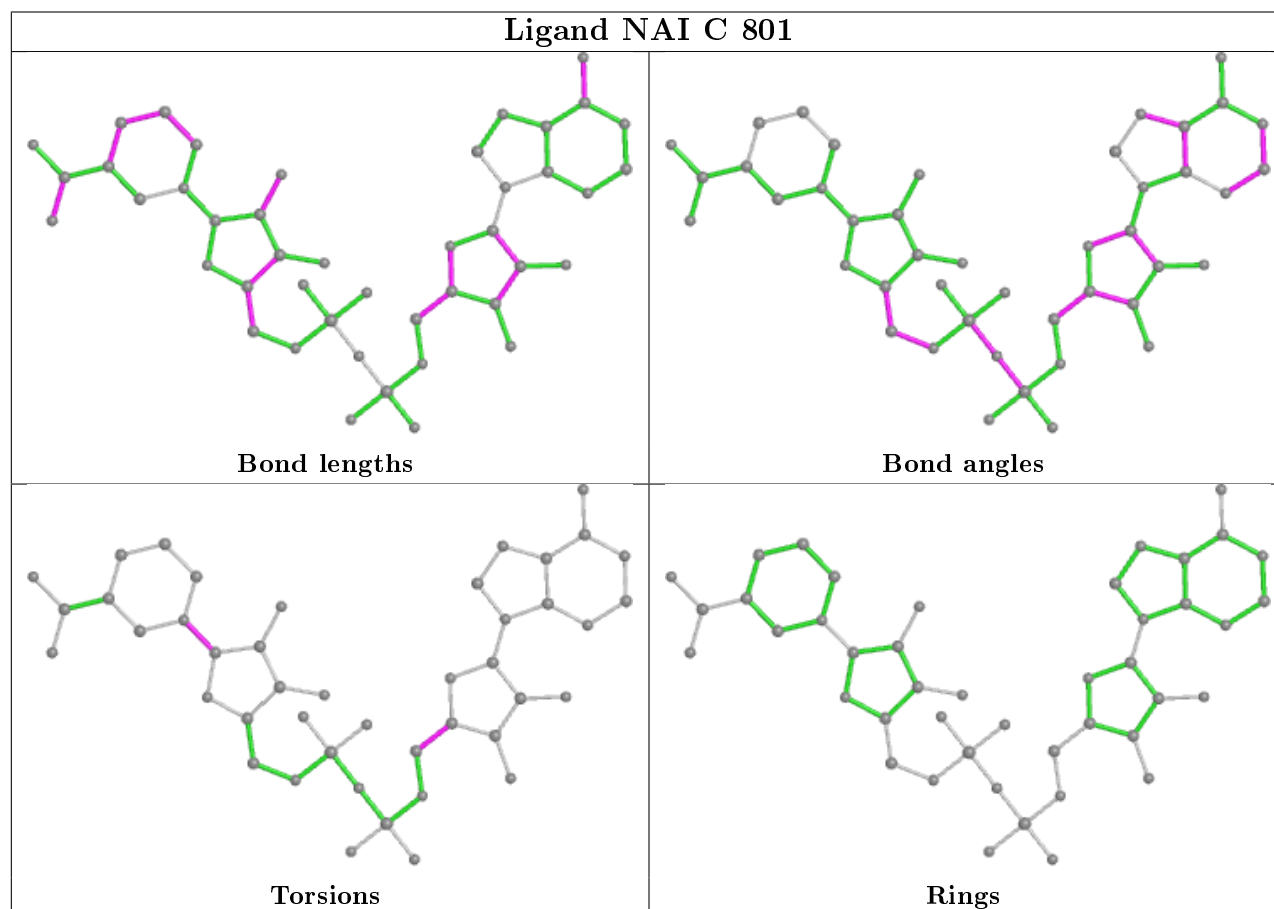
There are no ring outliers.

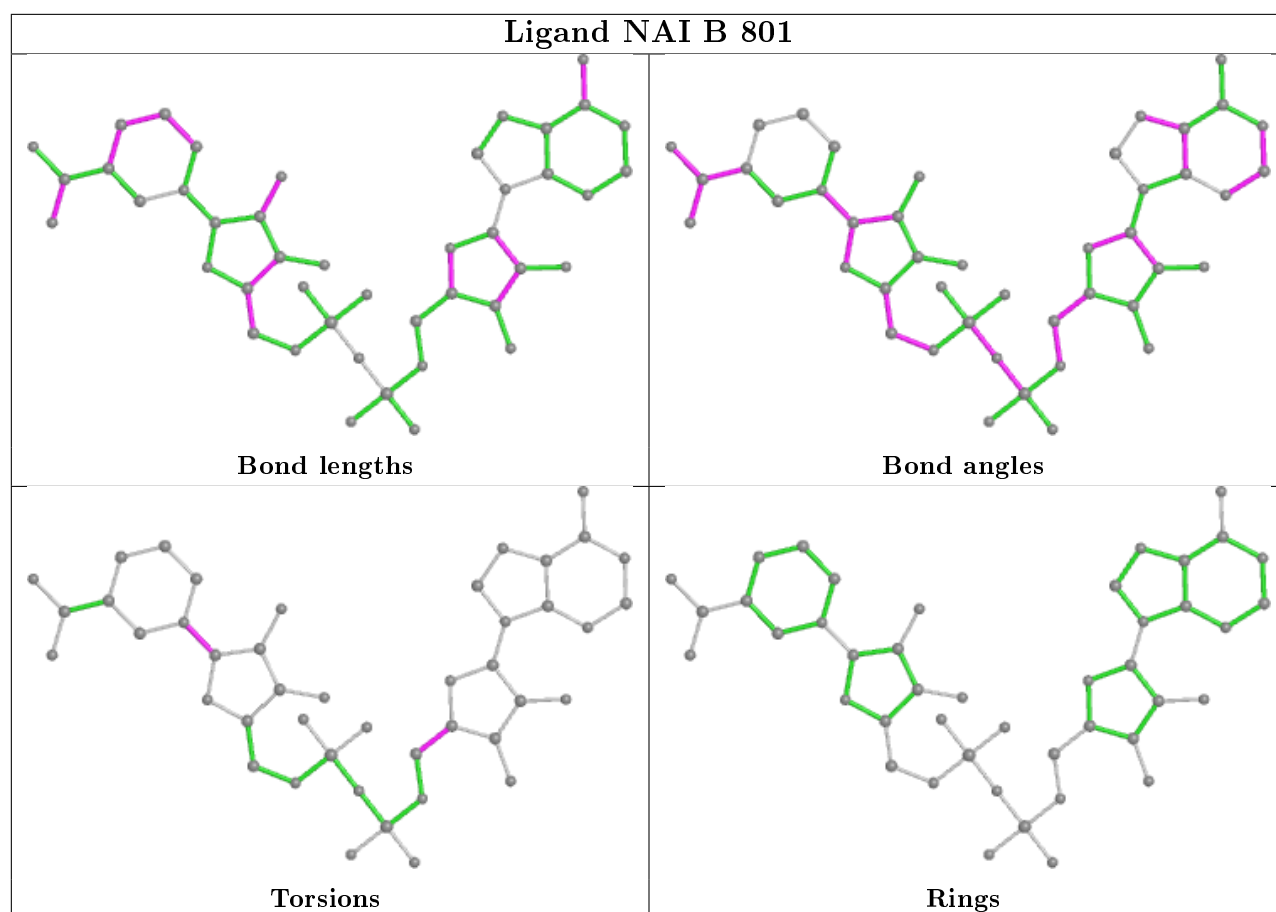
7 monomers are involved in 11 short contacts:

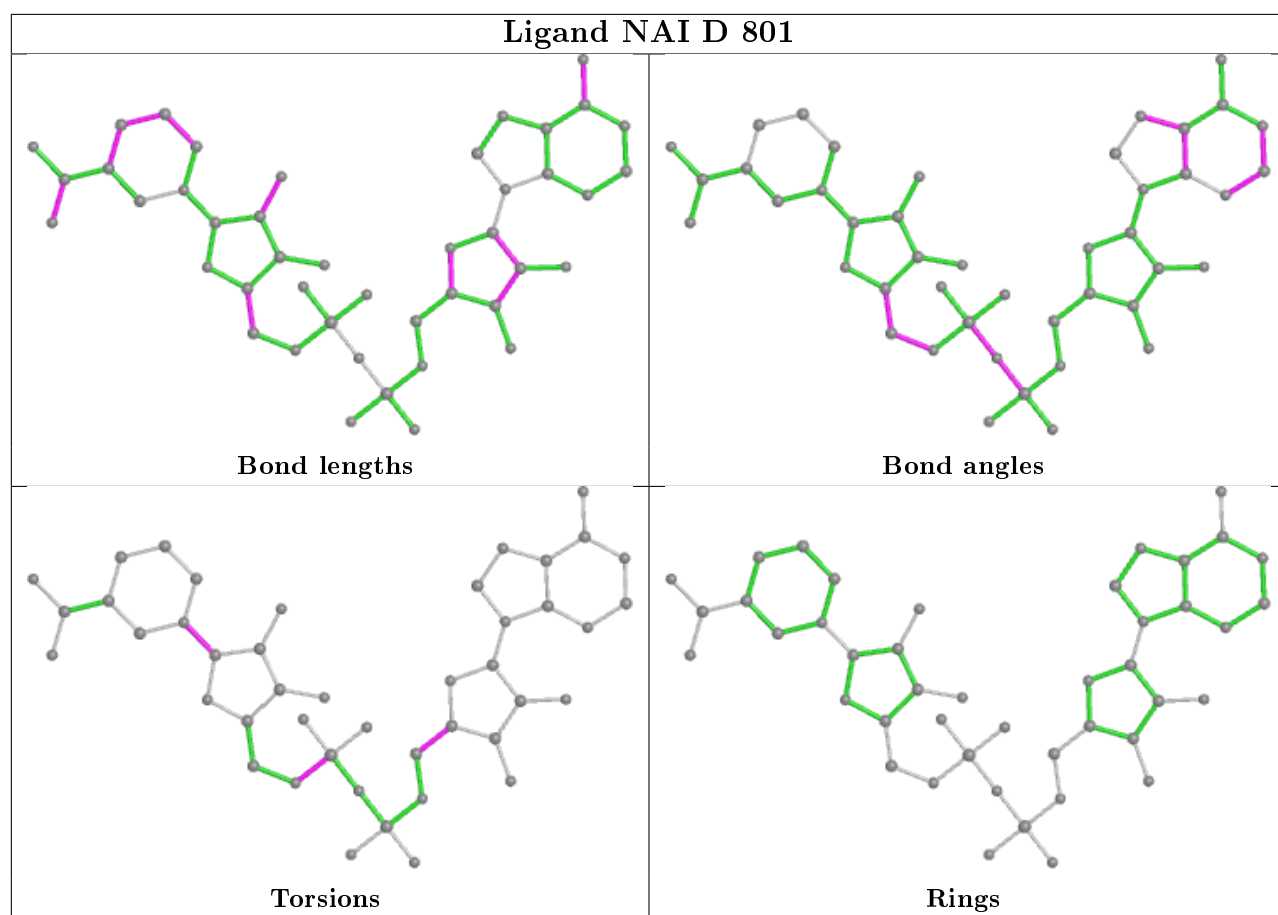
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	NAI	1	0
4	D	802	W31	1	0
3	B	802	EPE	1	0
4	A	803	W31	1	0
4	B	803	W31	2	0
4	C	803	W31	2	0
3	C	802	EPE	3	0

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

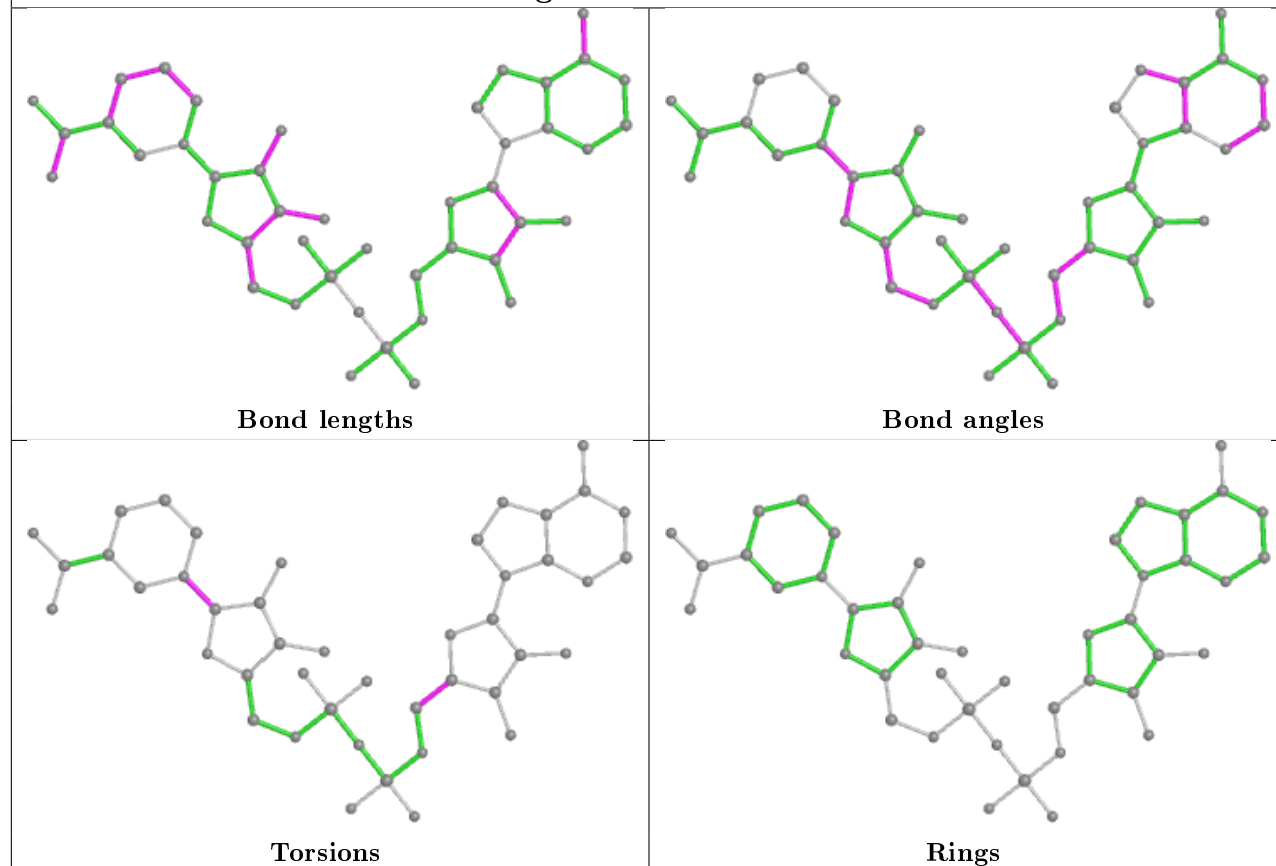
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



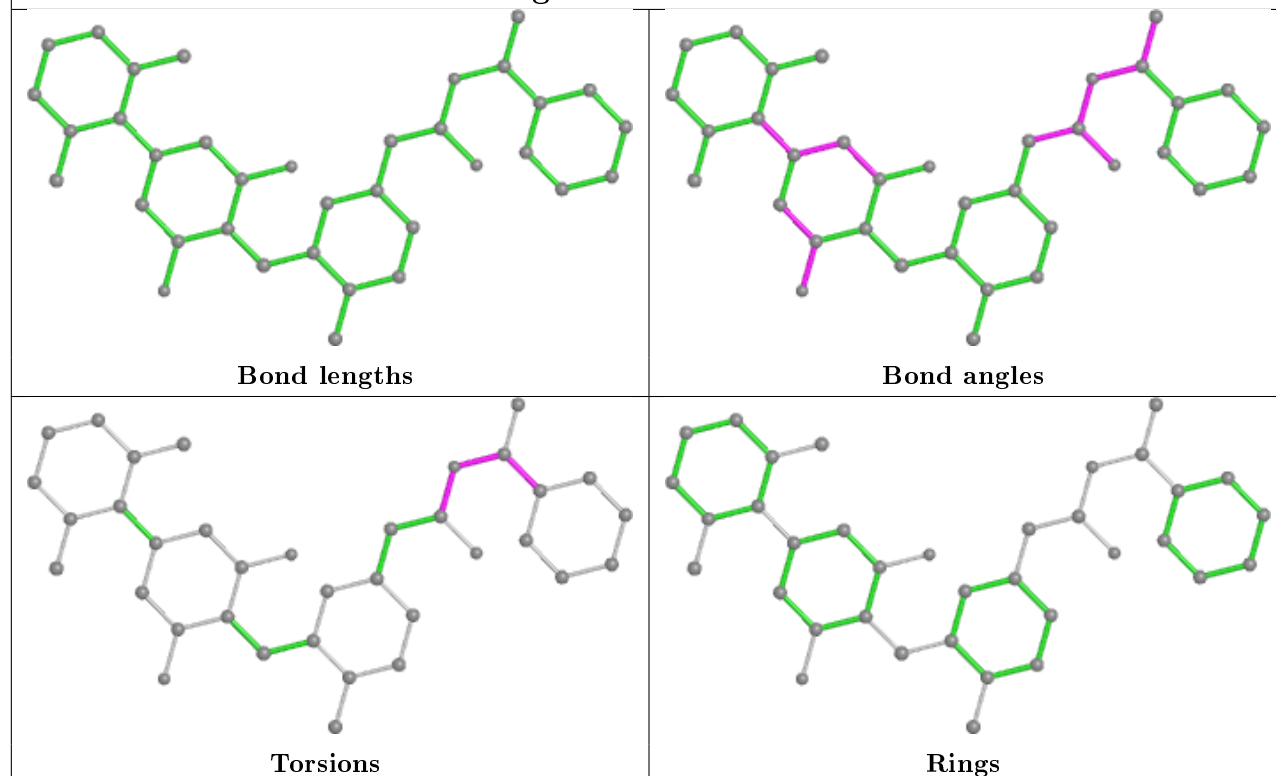




## Ligand NAI A 801

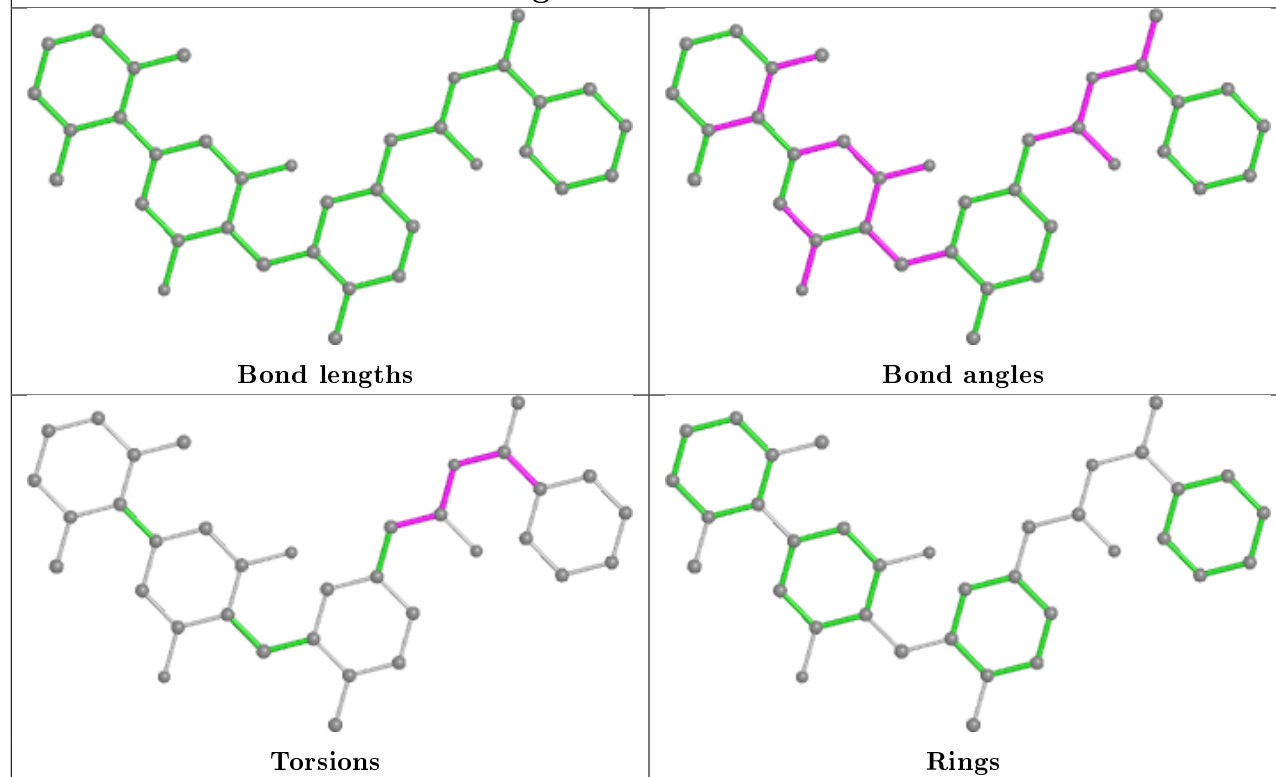


## Ligand W31 D 802

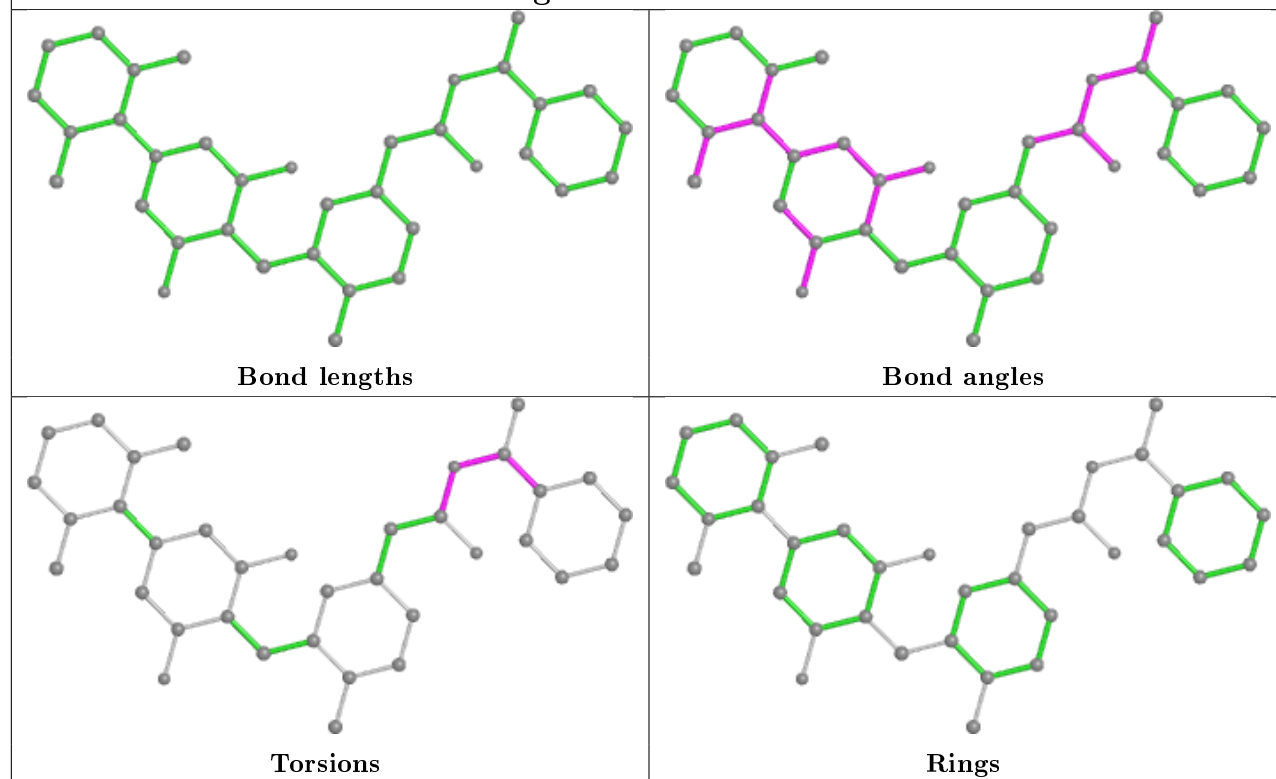


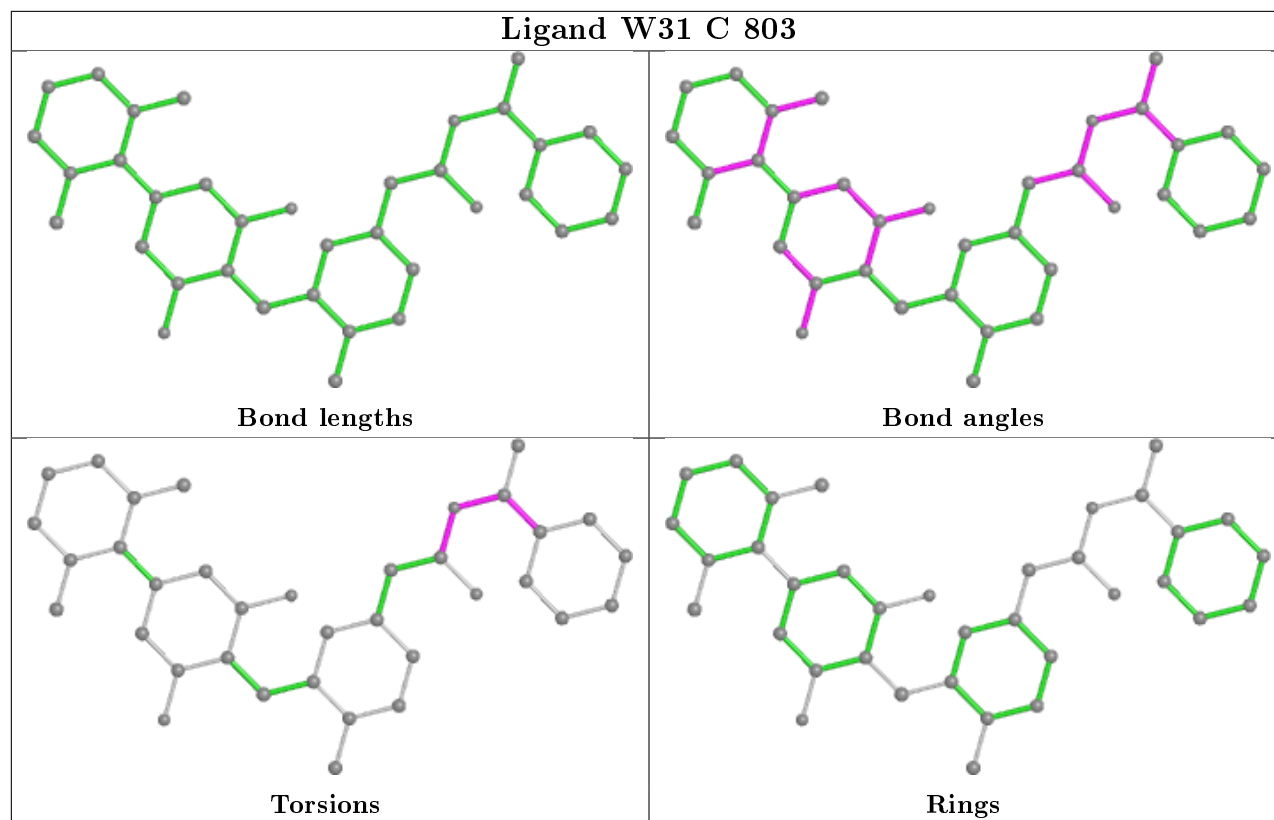


## Ligand W31 A 803



## Ligand W31 B 803





## 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	331/331 (100%)	-0.40	4 (1%) 79 82	14, 22, 46, 66	0
1	B	331/331 (100%)	-0.43	3 (0%) 84 86	14, 21, 35, 88	0
1	C	323/331 (97%)	-0.32	7 (2%) 62 66	16, 24, 44, 79	0
1	D	331/331 (100%)	-0.49	3 (0%) 84 86	13, 21, 37, 75	0
All	All	1316/1324 (99%)	-0.41	17 (1%) 77 80	13, 22, 42, 88	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	GLU	3.7
1	D	16	GLN	3.4
1	A	104	SER	3.0
1	B	15	GLU	2.8
1	A	106	LEU	2.7
1	C	106	LEU	2.6
1	C	108	LEU	2.5
1	D	1	ALA	2.3
1	C	331	PHE	2.3
1	D	15	GLU	2.3
1	C	330	GLN	2.2
1	B	330	GLN	2.2
1	B	14	GLU	2.1
1	A	107	ASN	2.0
1	C	14	GLU	2.0
1	C	1	ALA	2.0
1	C	327	LYS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

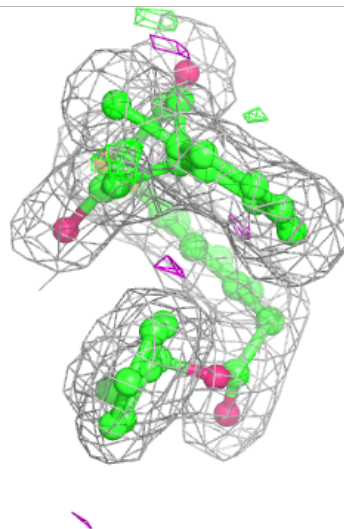
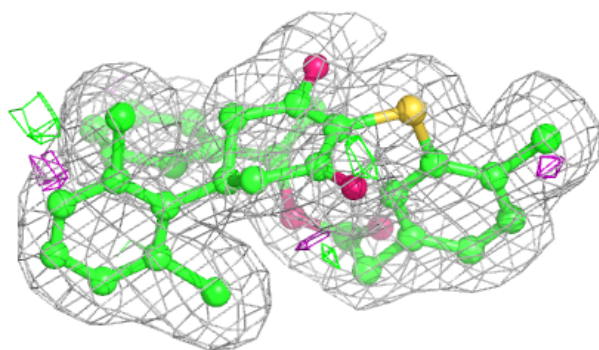
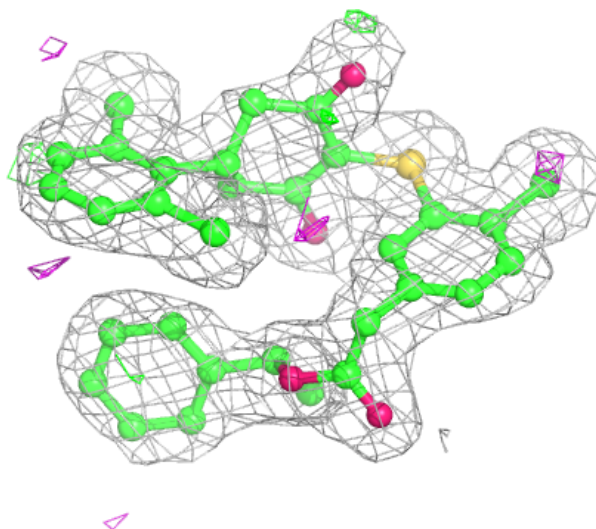
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EPE	A	802	15/15	0.84	0.25	30,41,46,46	15
3	EPE	B	802	15/15	0.89	0.24	32,53,60,65	0
3	EPE	C	802	15/15	0.90	0.20	33,37,45,49	15
5	SO4	D	804	5/5	0.91	0.18	18,25,29,36	5
3	EPE	D	803	15/15	0.94	0.12	22,28,48,49	0
4	W31	D	802	36/36	0.97	0.09	15,18,25,25	0
2	NAI	C	801	44/44	0.97	0.09	17,24,27,29	0
4	W31	A	803	36/36	0.97	0.10	13,20,25,29	0
4	W31	C	803	36/36	0.97	0.09	18,23,31,31	0
2	NAI	B	801	44/44	0.97	0.08	12,18,21,23	0
4	W31	B	803	36/36	0.98	0.09	13,20,24,29	0
2	NAI	A	801	44/44	0.98	0.08	15,19,23,27	0
2	NAI	D	801	44/44	0.98	0.08	13,18,21,23	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.

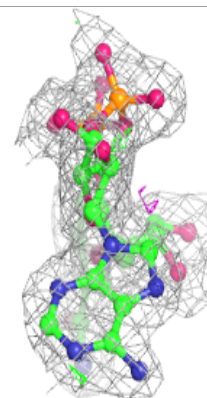
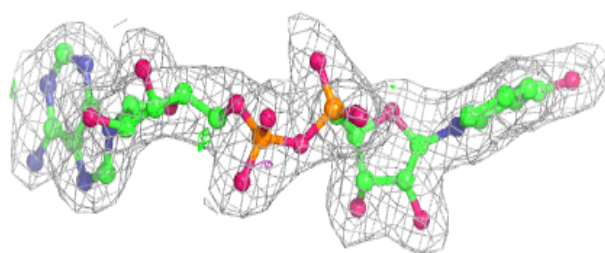
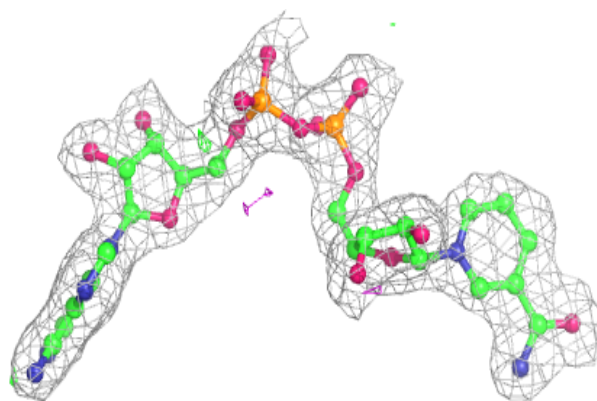
**Electron density around W31 D 802:**

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

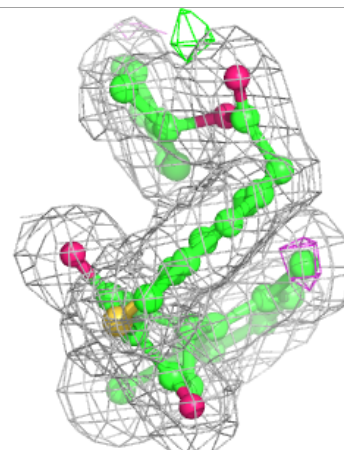
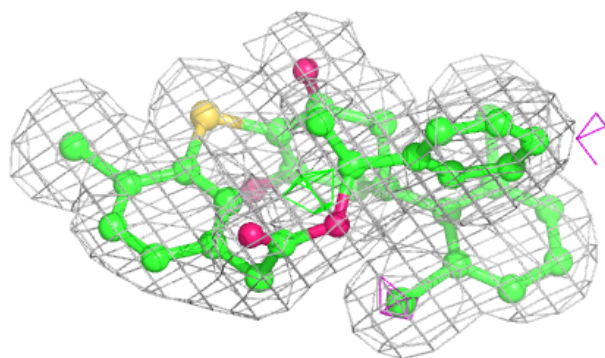
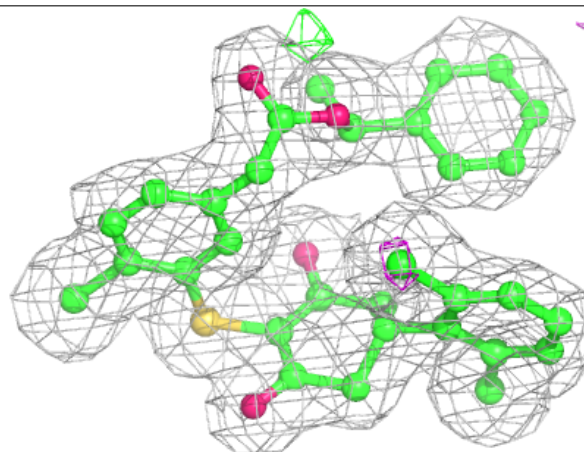


**Electron density around NAI C 801:**

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

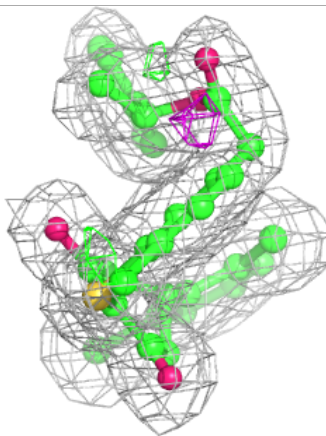
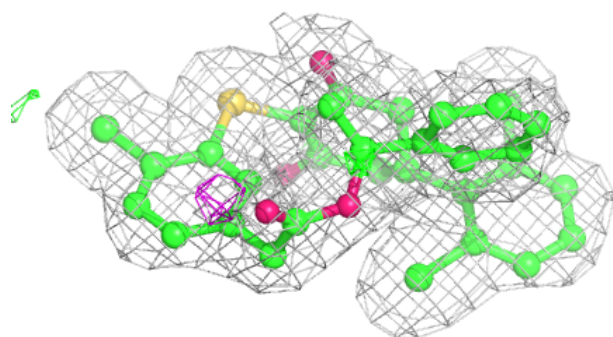
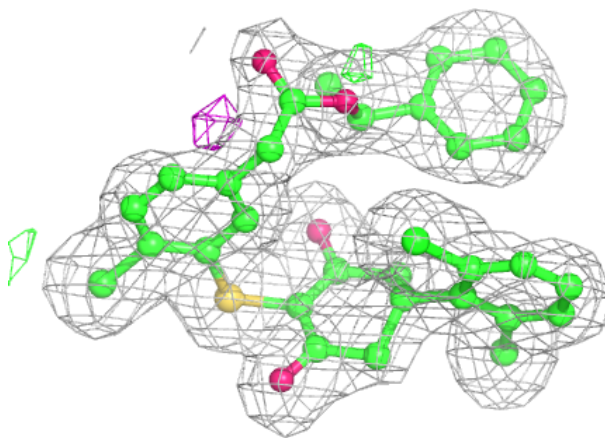
**Electron density around W31 A 803:**

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



**Electron density around W31 C 803:**

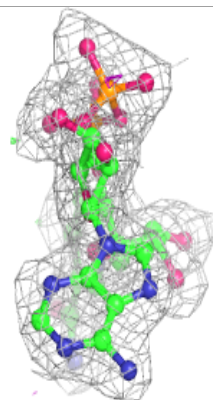
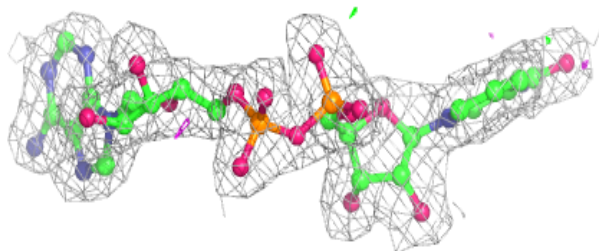
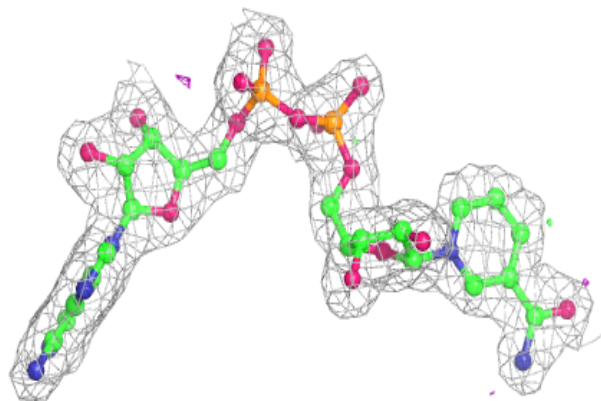
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around NAI B 801:**

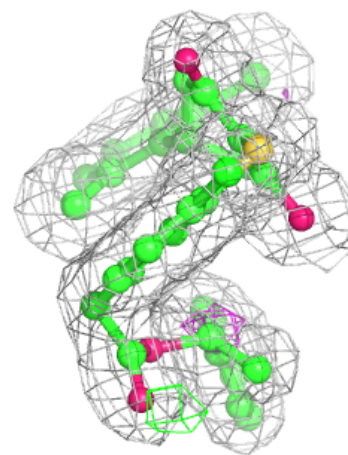
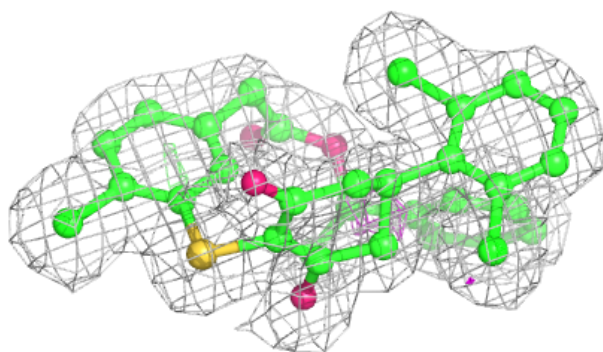
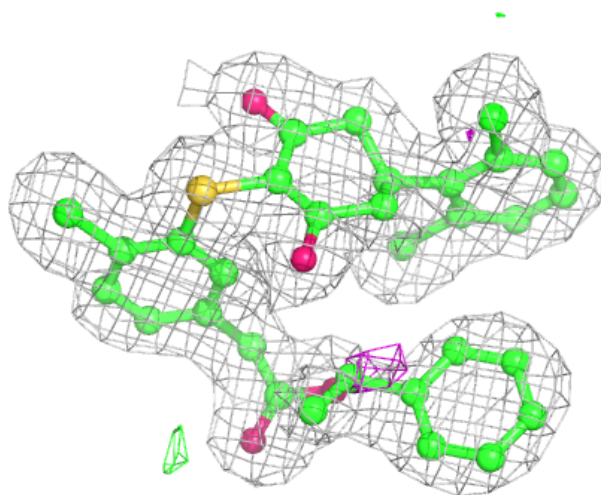
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





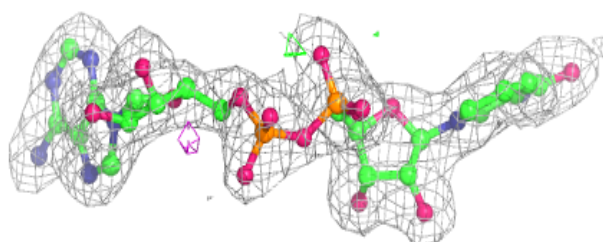
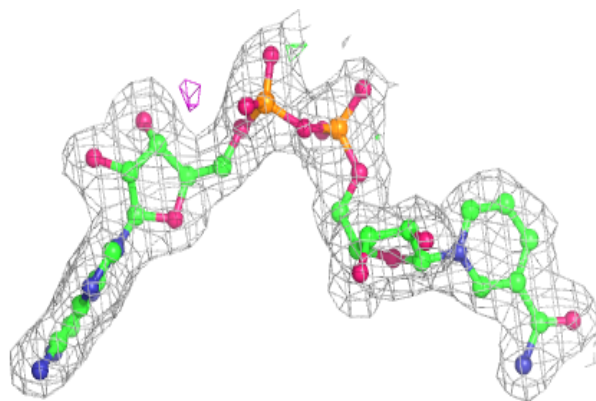
**Electron density around W31 B 803:**

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

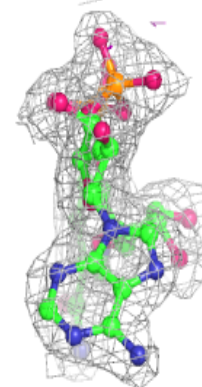
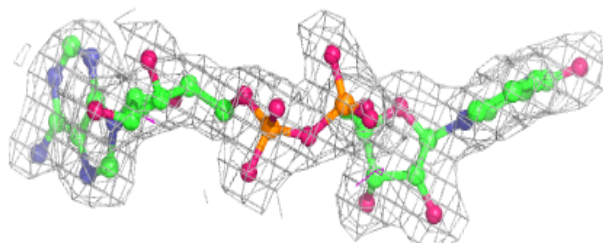
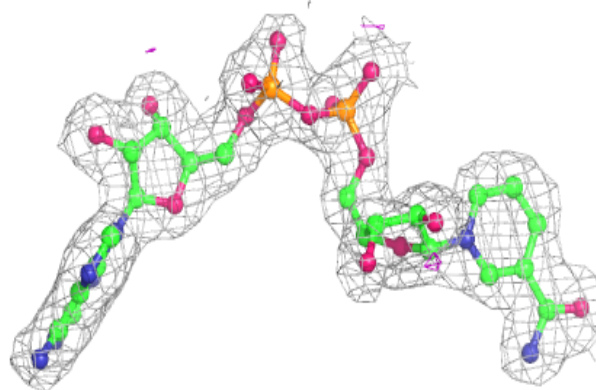


**Electron density around NAI A 801:**

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

**Electron density around NAI D 801:**

$2mF_o-DF_c$  (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.