



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:31 pm BST

PDB ID : 3VZS  
Title : Crystal structure of PhaB from *Ralstonia eutropha* in complex with Acetoacetyl-CoA and NADP  
Authors : Ikeda, K.; Tanaka, Y.; Tanaka, I.; Yao, M.  
Deposited on : 2012-10-15  
Resolution : 2.14 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 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

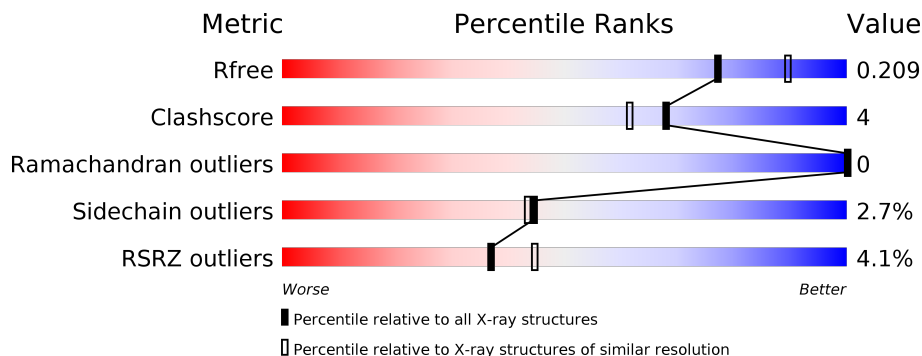
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	257	
1	B	257	
1	C	257	
1	D	257	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8469 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 Acetoacetyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	Total 1835	C 1149	N 324	O 353	S 9	0	0	0
1	B	249	Total 1872	C 1170	N 333	O 360	S 9	0	0	0
1	C	244	Total 1835	C 1149	N 324	O 353	S 9	0	0	0
1	D	249	Total 1872	C 1170	N 333	O 360	S 9	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

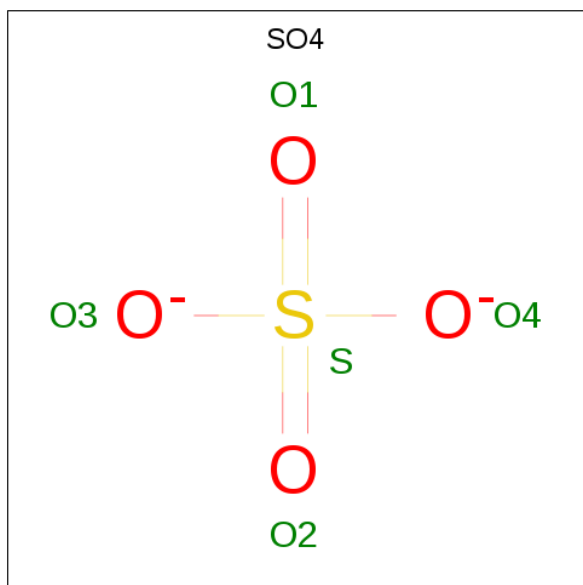
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P14697
A	-9	ARG	-	EXPRESSION TAG	UNP P14697
A	-8	GLY	-	EXPRESSION TAG	UNP P14697
A	-7	SER	-	EXPRESSION TAG	UNP P14697
A	-6	HIS	-	EXPRESSION TAG	UNP P14697
A	-5	HIS	-	EXPRESSION TAG	UNP P14697
A	-4	HIS	-	EXPRESSION TAG	UNP P14697
A	-3	HIS	-	EXPRESSION TAG	UNP P14697
A	-2	HIS	-	EXPRESSION TAG	UNP P14697
A	-1	HIS	-	EXPRESSION TAG	UNP P14697
A	0	GLY	-	EXPRESSION TAG	UNP P14697
A	1	SER	-	EXPRESSION TAG	UNP P14697
B	-10	MET	-	EXPRESSION TAG	UNP P14697
B	-9	ARG	-	EXPRESSION TAG	UNP P14697
B	-8	GLY	-	EXPRESSION TAG	UNP P14697
B	-7	SER	-	EXPRESSION TAG	UNP P14697
B	-6	HIS	-	EXPRESSION TAG	UNP P14697
B	-5	HIS	-	EXPRESSION TAG	UNP P14697
B	-4	HIS	-	EXPRESSION TAG	UNP P14697
B	-3	HIS	-	EXPRESSION TAG	UNP P14697
B	-2	HIS	-	EXPRESSION TAG	UNP P14697

*Continued on next page...*

*Continued from previous page...*

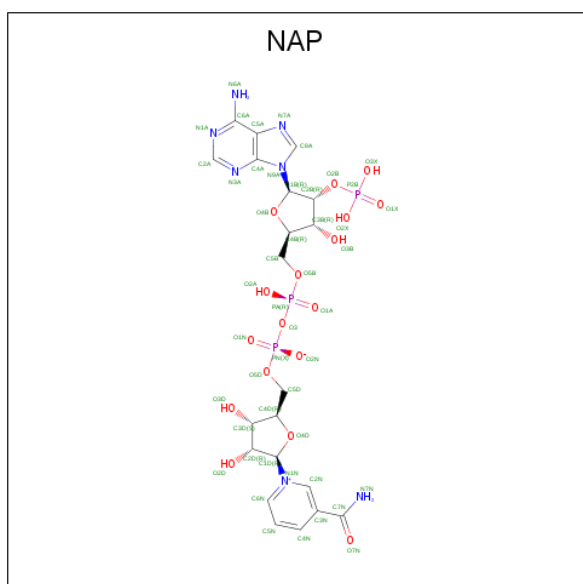
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	EXPRESSION TAG	UNP P14697
B	0	GLY	-	EXPRESSION TAG	UNP P14697
B	1	SER	-	EXPRESSION TAG	UNP P14697
C	-10	MET	-	EXPRESSION TAG	UNP P14697
C	-9	ARG	-	EXPRESSION TAG	UNP P14697
C	-8	GLY	-	EXPRESSION TAG	UNP P14697
C	-7	SER	-	EXPRESSION TAG	UNP P14697
C	-6	HIS	-	EXPRESSION TAG	UNP P14697
C	-5	HIS	-	EXPRESSION TAG	UNP P14697
C	-4	HIS	-	EXPRESSION TAG	UNP P14697
C	-3	HIS	-	EXPRESSION TAG	UNP P14697
C	-2	HIS	-	EXPRESSION TAG	UNP P14697
C	-1	HIS	-	EXPRESSION TAG	UNP P14697
C	0	GLY	-	EXPRESSION TAG	UNP P14697
C	1	SER	-	EXPRESSION TAG	UNP P14697
D	-10	MET	-	EXPRESSION TAG	UNP P14697
D	-9	ARG	-	EXPRESSION TAG	UNP P14697
D	-8	GLY	-	EXPRESSION TAG	UNP P14697
D	-7	SER	-	EXPRESSION TAG	UNP P14697
D	-6	HIS	-	EXPRESSION TAG	UNP P14697
D	-5	HIS	-	EXPRESSION TAG	UNP P14697
D	-4	HIS	-	EXPRESSION TAG	UNP P14697
D	-3	HIS	-	EXPRESSION TAG	UNP P14697
D	-2	HIS	-	EXPRESSION TAG	UNP P14697
D	-1	HIS	-	EXPRESSION TAG	UNP P14697
D	0	GLY	-	EXPRESSION TAG	UNP P14697
D	1	SER	-	EXPRESSION TAG	UNP P14697

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



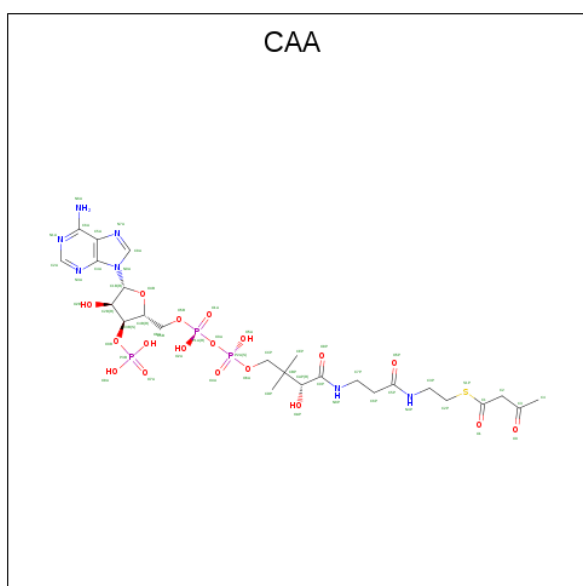
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula:  $C_{25}H_{40}N_7O_{18}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
4	B	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
4	C	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
4	D	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total 182	O 182	0	0
5	B	162	Total 162	O 162	0	0

*Continued on next page...*

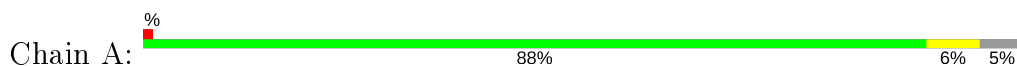
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	C	145	Total 145	O 145	0	0
5	D	138	Total 138	O 138	0	0

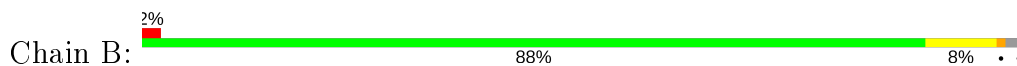
### 3 Residue-property plots [i](#)

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.

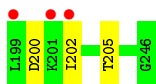
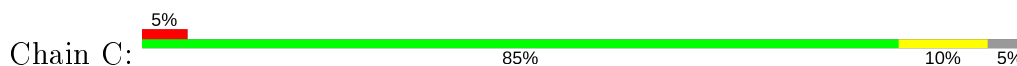
- Molecule 1: Acetoacetyl-CoA reductase



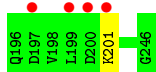
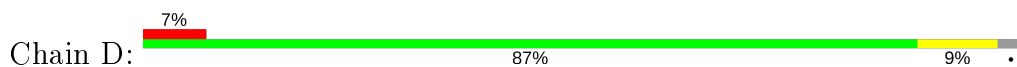
- Molecule 1: Acetoacetyl-CoA reductase



- Molecule 1: Acetoacetyl-CoA reductase



- Molecule 1: Acetoacetyl-CoA reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.40Å 123.44Å 260.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.12 – 2.14 35.12 – 2.14	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.12-2.14) 96.6 (35.12-2.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.05 (at 2.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.165 , 0.209 0.166 , 0.209	Depositor DCC
$R_{free}$ test set	2950 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.044 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: NAP, CAA, 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	0.21	0/1864	0.40	0/2520
1	B	0.21	0/1903	0.42	1/2573 (0.0%)
1	C	0.21	0/1864	0.39	0/2520
1	D	0.21	0/1903	0.41	0/2573
All	All	0.21	0/7534	0.40	1/10186 (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	B	160	LEU	CA-CB-CG	5.14	127.13	115.30

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	1835	0	1829	11	0
1	B	1872	0	1861	12	0
1	C	1835	0	1829	17	0
1	D	1872	0	1861	15	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	48	0	24	4	0
3	B	48	0	24	1	0
3	C	48	0	24	2	0
3	D	48	0	24	5	0
4	A	54	0	36	1	0
4	B	54	0	36	2	0
4	C	54	0	36	0	0
4	D	54	0	36	1	0
5	A	182	0	0	0	0
5	B	162	0	0	1	0
5	C	145	0	0	0	0
5	D	138	0	0	0	0
All	All	8469	0	7620	59	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 4.

All (59) 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)
3:D:302:NAP:H71N	4:D:303:CAA:H4'1	1.45	0.81
4:A:303:CAA:H8A	4:A:303:CAA:H51A	1.71	0.71
1:A:195:ARG:H	1:A:195:ARG:HE	1.39	0.71
1:D:51:LEU:N	1:D:52:GLY:HA2	2.14	0.62
1:B:195:ARG:HD2	1:B:195:ARG:H	1.65	0.62
1:A:84:VAL:HG22	1:A:134:ARG:HB2	1.82	0.61
1:D:139:SER:HB2	1:D:160:LEU:HD22	1.83	0.58
1:B:139:SER:HB2	1:B:160:LEU:HD11	1.86	0.58
4:B:303:CAA:O7A	4:B:303:CAA:H4B	2.04	0.57
1:C:44:TRP:HE3	1:C:45:LEU:HD12	1.69	0.57
1:A:195:ARG:H	1:A:195:ARG:NE	2.02	0.56
1:D:186:ILE:H	3:D:302:NAP:H4N	1.70	0.56
1:B:147:GLN:HE21	4:B:303:CAA:H62	1.71	0.56
1:A:139:SER:HB2	1:A:160:LEU:HD22	1.88	0.56
1:C:84:VAL:HG22	1:C:134:ARG:HB2	1.88	0.55
1:B:22:ARG:NH2	5:B:550:HOH:O	2.32	0.54
1:D:183:PRO:HB2	3:D:302:NAP:N7N	2.23	0.54
1:D:191:VAL:HA	1:D:194:ILE:HG13	1.90	0.53
1:A:183:PRO:HB2	3:A:302:NAP:N7N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:SER:HA	1:B:157:LYS:HD2	1.91	0.52
1:C:139:SER:HB2	1:C:160:LEU:HD22	1.92	0.52
1:D:15:ILE:HG13	1:D:186:ILE:HD11	1.92	0.51
1:C:188:THR:OG1	3:C:302:NAP:H6N	2.11	0.51
1:C:45:LEU:HD11	1:C:57:ALA:HB2	1.91	0.51
1:C:139:SER:HA	1:C:157:LYS:HD2	1.94	0.50
1:D:15:ILE:H	1:D:15:ILE:HD12	1.75	0.50
1:C:191:VAL:HA	1:C:194:ILE:HG13	1.95	0.48
1:D:51:LEU:H	1:D:52:GLY:HA2	1.79	0.48
1:D:139:SER:HA	1:D:157:LYS:HD2	1.95	0.47
1:B:84:VAL:HG22	1:B:134:ARG:HB2	1.95	0.47
1:A:139:SER:HA	1:A:157:LYS:HD2	1.97	0.47
1:A:191:VAL:HA	1:A:194:ILE:HG13	1.98	0.46
1:B:185:TYR:CE2	1:B:202:ILE:HD13	2.50	0.46
1:B:201:LYS:HB2	1:B:201:LYS:HE3	1.83	0.45
1:D:186:ILE:H	3:D:302:NAP:C4N	2.28	0.45
3:A:302:NAP:H2N	3:A:302:NAP:H2D	1.74	0.45
1:B:139:SER:OG	1:B:140:SER:N	2.50	0.45
1:D:5:ILE:HD13	1:D:79:VAL:HG12	1.98	0.45
1:A:202:ILE:O	1:A:205:THR:OG1	2.28	0.44
1:D:183:PRO:HB2	3:D:302:NAP:H72N	1.81	0.44
1:B:186:ILE:HG12	3:B:302:NAP:H4N	1.98	0.44
1:C:202:ILE:O	1:C:205:THR:OG1	2.33	0.44
1:C:113:LEU:HD12	1:C:116:LEU:HD12	2.00	0.43
1:D:181:VAL:O	1:D:183:PRO:HD3	2.18	0.43
1:C:112:ASN:HD22	1:C:157:LYS:HE2	1.82	0.43
1:C:111:THR:HG23	1:C:112:ASN:OD1	2.19	0.42
1:A:38:SER:HA	1:A:39:PRO:HD3	1.83	0.42
1:B:181:VAL:O	1:B:183:PRO:HD3	2.19	0.42
1:B:93:ARG:HG2	1:B:104:ASP:HA	2.00	0.42
1:C:113:LEU:HA	1:C:113:LEU:HD12	1.89	0.41
1:A:188:THR:OG1	3:A:302:NAP:H6N	2.21	0.41
1:C:183:PRO:HB2	3:C:302:NAP:O7N	2.20	0.41
1:D:21:GLN:HB2	1:D:53:PHE:CZ	2.55	0.41
1:D:201:LYS:HE3	1:D:201:LYS:HB2	1.79	0.41
1:A:40:ARG:NH2	3:A:302:NAP:O2X	2.41	0.41
1:C:107:ALA:O	1:C:111:THR:HG22	2.21	0.40
1:C:91:ILE:HG12	1:C:111:THR:HG21	2.03	0.40
1:C:139:SER:OG	1:C:140:SER:N	2.54	0.40
1:C:124:ILE:HD11	1:C:171:VAL:HG11	2.03	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	242/257 (94%)	236 (98%)	6 (2%)	0	100	100
1	B	247/257 (96%)	242 (98%)	5 (2%)	0	100	100
1	C	242/257 (94%)	239 (99%)	3 (1%)	0	100	100
1	D	247/257 (96%)	239 (97%)	8 (3%)	0	100	100
All	All	978/1028 (95%)	956 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/204 (95%)	190 (98%)	3 (2%)	62	65
1	B	197/204 (97%)	191 (97%)	6 (3%)	41	39
1	C	193/204 (95%)	191 (99%)	2 (1%)	76	79
1	D	197/204 (97%)	187 (95%)	10 (5%)	24	19
All	All	780/816 (96%)	759 (97%)	21 (3%)	44	43

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

Mol	Chain	Res	Type
1	A	29	ARG
1	A	69	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	195	ARG
1	B	98	ARG
1	B	113	LEU
1	B	195	ARG
1	B	197	ASP
1	B	220	ILE
1	B	243	LEU
1	C	190	MET
1	C	200	ASP
1	D	-2	HIS
1	D	40	ARG
1	D	41	ARG
1	D	84	VAL
1	D	116	LEU
1	D	134	ARG
1	D	145	LYS
1	D	147	GLN
1	D	186	ILE
1	D	195	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	147	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAP	A	302	-	45,52,52	2.17	13 (28%)	56,80,80	1.31	7 (12%)
3	NAP	B	302	-	45,52,52	2.17	13 (28%)	56,80,80	1.36	9 (16%)
4	CAA	B	303	-	47,56,56	1.78	8 (17%)	60,83,83	1.69	13 (21%)
2	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.04	0
4	CAA	C	303	-	47,56,56	1.78	8 (17%)	60,83,83	1.61	12 (20%)
3	NAP	C	302	-	45,52,52	2.17	13 (28%)	56,80,80	1.37	8 (14%)
2	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.04	0
3	NAP	D	302	-	45,52,52	2.17	13 (28%)	56,80,80	1.36	6 (10%)
2	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	CAA	A	303	-	47,56,56	1.76	8 (17%)	60,83,83	1.56	12 (20%)
2	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	CAA	D	303	-	47,56,56	1.77	8 (17%)	60,83,83	1.60	11 (18%)

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	NAP	A	302	-	-	9/31/67/67	0/5/5/5
3	NAP	B	302	-	-	14/31/67/67	0/5/5/5
4	CAA	B	303	-	-	13/50/71/71	0/3/3/3
4	CAA	D	303	-	-	18/50/71/71	0/3/3/3
4	CAA	C	303	-	-	8/50/71/71	0/3/3/3
3	NAP	C	302	-	-	8/31/67/67	0/5/5/5
3	NAP	D	302	-	-	9/31/67/67	0/5/5/5
4	CAA	A	303	-	-	15/50/71/71	0/3/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	NAP	O4D-C1D	8.75	1.53	1.41
3	C	302	NAP	O4D-C1D	8.58	1.53	1.41
3	D	302	NAP	O4D-C1D	8.52	1.53	1.41
3	B	302	NAP	O4D-C1D	8.49	1.52	1.41
4	B	303	CAA	C5P-N4P	6.27	1.47	1.33
4	D	303	CAA	C5P-N4P	6.20	1.47	1.33
4	A	303	CAA	C5P-N4P	6.17	1.47	1.33
4	C	303	CAA	C5P-N4P	6.15	1.47	1.33
3	B	302	NAP	C7N-N7N	5.78	1.44	1.33
3	C	302	NAP	C7N-N7N	5.76	1.44	1.33
3	D	302	NAP	C7N-N7N	5.72	1.43	1.33
3	A	302	NAP	C7N-N7N	5.63	1.43	1.33
4	C	303	CAA	C2B-C3B	-5.48	1.40	1.52
4	B	303	CAA	C2B-C3B	-5.35	1.41	1.52
4	A	303	CAA	C2B-C3B	-5.27	1.41	1.52
4	D	303	CAA	C2B-C3B	-5.21	1.41	1.52
4	D	303	CAA	C9P-N8P	4.74	1.44	1.33
4	B	303	CAA	C9P-N8P	4.71	1.43	1.33
4	C	303	CAA	C9P-N8P	4.71	1.43	1.33
4	A	303	CAA	C9P-N8P	4.62	1.43	1.33
3	C	302	NAP	O4B-C1B	3.99	1.46	1.41
3	B	302	NAP	O4B-C1B	3.94	1.46	1.41
3	D	302	NAP	O4B-C1B	3.89	1.46	1.41
3	B	302	NAP	C6A-N6A	3.82	1.48	1.34
3	C	302	NAP	C6A-N6A	3.82	1.48	1.34
3	D	302	NAP	C6A-N6A	3.80	1.47	1.34
3	A	302	NAP	C6A-N6A	3.79	1.47	1.34
3	A	302	NAP	O4B-C1B	3.78	1.46	1.41
4	C	303	CAA	C2B-C1B	-3.71	1.48	1.53
4	D	303	CAA	C2B-C1B	-3.43	1.48	1.53
4	A	303	CAA	C2B-C1B	-3.27	1.48	1.53
3	D	302	NAP	C2D-C3D	-3.23	1.44	1.53
3	B	302	NAP	C2D-C3D	-3.15	1.44	1.53
3	C	302	NAP	C3B-C2B	-3.13	1.46	1.52
3	A	302	NAP	C2D-C3D	-3.13	1.44	1.53
3	B	302	NAP	C3B-C2B	-3.12	1.46	1.52
3	D	302	NAP	C3B-C2B	-3.11	1.46	1.52
3	A	302	NAP	C3B-C2B	-3.11	1.46	1.52
3	C	302	NAP	C2D-C3D	-3.10	1.44	1.53
3	B	302	NAP	O2D-C2D	-3.07	1.35	1.43
4	B	303	CAA	C2B-C1B	-3.06	1.49	1.53
3	C	302	NAP	O2D-C2D	-3.03	1.35	1.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	NAP	O2D-C2D	-3.02	1.35	1.43
3	D	302	NAP	O2D-C2D	-3.01	1.35	1.43
4	B	303	CAA	O4B-C4B	-2.86	1.38	1.45
4	D	303	CAA	O4B-C4B	-2.77	1.38	1.45
4	A	303	CAA	O4B-C4B	-2.73	1.38	1.45
4	B	303	CAA	C3B-C4B	-2.61	1.45	1.52
4	C	303	CAA	O4B-C4B	-2.61	1.39	1.45
4	B	303	CAA	C2A-N3A	2.61	1.36	1.32
4	D	303	CAA	C2A-N3A	2.58	1.36	1.32
4	A	303	CAA	C2A-N3A	2.53	1.36	1.32
4	C	303	CAA	C2A-N3A	2.52	1.36	1.32
4	A	303	CAA	C3B-C4B	-2.46	1.46	1.52
4	B	303	CAA	C6A-N6A	2.46	1.43	1.34
3	C	302	NAP	O3B-C3B	-2.42	1.37	1.43
3	B	302	NAP	O3B-C3B	-2.40	1.37	1.43
4	C	303	CAA	C6A-N6A	2.40	1.42	1.34
4	D	303	CAA	C6A-N6A	2.39	1.42	1.34
4	C	303	CAA	C3B-C4B	-2.39	1.46	1.52
4	A	303	CAA	C6A-N6A	2.39	1.42	1.34
3	D	302	NAP	O3D-C3D	-2.39	1.37	1.43
3	A	302	NAP	O3B-C3B	-2.38	1.37	1.43
3	D	302	NAP	O3B-C3B	-2.38	1.37	1.43
4	D	303	CAA	C3B-C4B	-2.38	1.46	1.52
3	D	302	NAP	C2A-N3A	2.37	1.35	1.32
3	C	302	NAP	O3D-C3D	-2.37	1.37	1.43
3	A	302	NAP	O3D-C3D	-2.36	1.37	1.43
3	A	302	NAP	C2A-N3A	2.35	1.35	1.32
3	B	302	NAP	C2A-N3A	2.35	1.35	1.32
3	B	302	NAP	O3D-C3D	-2.32	1.37	1.43
3	C	302	NAP	C2A-N3A	2.31	1.35	1.32
3	D	302	NAP	O4B-C4B	-2.30	1.39	1.45
3	D	302	NAP	O4D-C4D	-2.29	1.39	1.45
3	A	302	NAP	O4B-C4B	-2.29	1.39	1.45
3	C	302	NAP	O4B-C4B	-2.26	1.39	1.45
3	B	302	NAP	O4B-C4B	-2.24	1.40	1.45
3	C	302	NAP	O4D-C4D	-2.22	1.40	1.45
3	B	302	NAP	O4D-C4D	-2.20	1.40	1.45
3	A	302	NAP	O4D-C4D	-2.18	1.40	1.45
3	D	302	NAP	C3B-C4B	-2.16	1.47	1.53
3	B	302	NAP	C3B-C4B	-2.14	1.47	1.53
3	C	302	NAP	C3B-C4B	-2.14	1.47	1.53
3	A	302	NAP	C3B-C4B	-2.10	1.47	1.53

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	303	CAA	O6A-CCP-CBP	4.85	118.35	110.55
4	D	303	CAA	C2-C1-S1P	4.82	119.70	113.69
3	D	302	NAP	N3A-C2A-N1A	-4.61	121.47	128.68
3	A	302	NAP	N3A-C2A-N1A	-4.61	121.47	128.68
3	B	302	NAP	N3A-C2A-N1A	-4.55	121.56	128.68
3	C	302	NAP	N3A-C2A-N1A	-4.55	121.57	128.68
4	A	303	CAA	C2-C1-S1P	4.46	119.25	113.69
4	B	303	CAA	O1-C1-S1P	-4.46	116.82	122.61
4	B	303	CAA	O1-C1-C2	-4.39	115.74	123.35
4	C	303	CAA	O6A-CCP-CBP	4.11	117.15	110.55
4	C	303	CAA	C2-C1-S1P	4.04	118.73	113.69
4	D	303	CAA	N3A-C2A-N1A	-3.97	122.47	128.68
4	C	303	CAA	N3A-C2A-N1A	-3.95	122.50	128.68
4	A	303	CAA	N3A-C2A-N1A	-3.86	122.64	128.68
4	B	303	CAA	C2-C1-S1P	3.86	118.50	113.69
3	B	302	NAP	C3N-C7N-N7N	3.78	122.29	117.75
3	A	302	NAP	C3N-C7N-N7N	3.75	122.25	117.75
4	B	303	CAA	N3A-C2A-N1A	-3.72	122.86	128.68
4	B	303	CAA	O6A-CCP-CBP	3.60	116.34	110.55
4	C	303	CAA	O1-C1-S1P	-3.60	117.94	122.61
3	C	302	NAP	C3N-C7N-N7N	3.55	122.01	117.75
4	A	303	CAA	P2A-O3A-P1A	-3.55	120.65	132.83
3	D	302	NAP	C3N-C7N-N7N	3.55	122.00	117.75
4	B	303	CAA	C4A-C5A-N7A	-3.51	105.74	109.40
4	B	303	CAA	C2P-C3P-N4P	3.26	119.26	112.42
4	C	303	CAA	P2A-O3A-P1A	-3.25	121.67	132.83
4	B	303	CAA	P2A-O3A-P1A	-3.23	121.76	132.83
3	C	302	NAP	PN-O3-PA	-3.17	121.94	132.83
4	D	303	CAA	C4A-C5A-N7A	-3.15	106.12	109.40
3	D	302	NAP	PN-O3-PA	-3.14	122.05	132.83
4	A	303	CAA	O1-C1-S1P	-3.10	118.58	122.61
4	D	303	CAA	O5B-C5B-C4B	3.09	119.64	108.99
4	C	303	CAA	C4A-C5A-N7A	-3.07	106.19	109.40
4	A	303	CAA	C4A-C5A-N7A	-3.06	106.21	109.40
4	A	303	CAA	O6A-CCP-CBP	3.01	115.38	110.55
3	C	302	NAP	O7N-C7N-N7N	-2.90	118.46	122.58
4	C	303	CAA	C6P-C7P-N8P	2.88	117.71	111.90
4	C	303	CAA	O1-C1-C2	-2.86	118.39	123.35
4	D	303	CAA	C6P-C7P-N8P	2.86	117.66	111.90
4	D	303	CAA	P2A-O3A-P1A	-2.85	123.05	132.83
3	C	302	NAP	O5B-C5B-C4B	2.84	118.78	108.99
4	A	303	CAA	O1-C1-C2	-2.81	118.49	123.35

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	NAP	O7N-C7N-N7N	-2.78	118.63	122.58
3	B	302	NAP	PN-O3-PA	-2.75	123.38	132.83
3	D	302	NAP	O5B-C5B-C4B	2.75	118.45	108.99
3	C	302	NAP	O5D-C5D-C4D	2.71	118.31	108.99
3	A	302	NAP	PN-O3-PA	-2.69	123.58	132.83
4	A	303	CAA	C6P-C7P-N8P	2.68	117.31	111.90
4	A	303	CAA	O5B-C5B-C4B	2.66	118.16	108.99
4	C	303	CAA	C2P-C3P-N4P	2.65	117.99	112.42
4	A	303	CAA	C2P-C3P-N4P	2.62	117.92	112.42
4	B	303	CAA	C7P-C6P-C5P	2.61	116.70	112.36
4	D	303	CAA	C7P-C6P-C5P	2.59	116.66	112.36
4	B	303	CAA	O5B-C5B-C4B	2.54	117.74	108.99
3	D	302	NAP	C5N-C4N-C3N	-2.53	117.35	120.34
3	B	302	NAP	O5B-C5B-C4B	2.51	117.64	108.99
4	D	303	CAA	C3B-C2B-C1B	2.51	105.45	99.89
4	C	303	CAA	C7P-C6P-C5P	2.51	116.53	112.36
4	D	303	CAA	C2P-C3P-N4P	2.44	117.54	112.42
3	B	302	NAP	C5N-C4N-C3N	-2.36	117.56	120.34
4	A	303	CAA	C2P-S1P-C1	2.35	109.20	101.87
4	C	303	CAA	O5B-C5B-C4B	2.30	116.92	108.99
3	C	302	NAP	C5N-C4N-C3N	-2.27	117.65	120.34
3	A	302	NAP	C5N-C4N-C3N	-2.25	117.68	120.34
3	B	302	NAP	O7N-C7N-N7N	-2.25	119.39	122.58
4	C	303	CAA	C2P-S1P-C1	2.25	108.86	101.87
3	A	302	NAP	O5B-C5B-C4B	2.24	116.70	108.99
3	B	302	NAP	O5D-C5D-C4D	2.20	116.55	108.99
4	B	303	CAA	C6P-C7P-N8P	2.19	116.32	111.90
4	B	303	CAA	CDP-CBP-CAP	2.18	112.59	108.82
4	A	303	CAA	C7P-C6P-C5P	2.16	115.95	112.36
3	B	302	NAP	O4D-C1D-C2D	-2.13	103.81	106.93
3	D	302	NAP	O7N-C7N-N7N	-2.13	119.55	122.58
3	B	302	NAP	C3D-C2D-C1D	2.08	104.10	100.98
4	B	303	CAA	O4B-C1B-C2B	-2.07	103.91	106.93
3	A	302	NAP	O5D-C5D-C4D	2.05	116.05	108.99
4	D	303	CAA	O1-C1-S1P	-2.02	119.99	122.61
3	C	302	NAP	O4D-C1D-C2D	-2.01	103.99	106.93

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	CAA	C5B-O5B-P1A-O1A

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	303	CAA	C3P-C2P-S1P-C1
4	B	303	CAA	O1-C1-S1P-C2P
4	B	303	CAA	C2-C1-S1P-C2P
4	B	303	CAA	C1-C2-C3-C4
3	A	302	NAP	C5D-O5D-PN-O1N
3	A	302	NAP	C5D-O5D-PN-O2N
3	A	302	NAP	C2D-C1D-N1N-C6N
3	B	302	NAP	C5D-O5D-PN-O1N
3	B	302	NAP	C5D-O5D-PN-O2N
3	B	302	NAP	C2D-C1D-N1N-C2N
3	B	302	NAP	C2D-C1D-N1N-C6N
3	B	302	NAP	C2N-C3N-C7N-O7N
3	B	302	NAP	C2N-C3N-C7N-N7N
3	C	302	NAP	C2D-C1D-N1N-C2N
3	C	302	NAP	C2D-C1D-N1N-C6N
4	C	303	CAA	C4B-C5B-O5B-P1A
4	C	303	CAA	C3P-C2P-S1P-C1
4	C	303	CAA	O1-C1-S1P-C2P
4	C	303	CAA	C2-C1-S1P-C2P
4	C	303	CAA	C1-C2-C3-C4
3	D	302	NAP	C5D-O5D-PN-O3
3	D	302	NAP	C5D-O5D-PN-O1N
3	D	302	NAP	C2D-C1D-N1N-C2N
3	D	302	NAP	C2D-C1D-N1N-C6N
3	D	302	NAP	C2N-C3N-C7N-O7N
3	D	302	NAP	C2N-C3N-C7N-N7N
4	A	303	CAA	C3B-C4B-C5B-O5B
4	A	303	CAA	C5B-O5B-P1A-O1A
4	A	303	CAA	CCP-O6A-P2A-O3A
4	A	303	CAA	CAP-CBP-CCP-O6A
4	A	303	CAA	O1-C1-S1P-C2P
4	A	303	CAA	C2-C1-S1P-C2P
4	D	303	CAA	C3B-O3B-P3B-O7A
4	D	303	CAA	C5B-O5B-P1A-O3A
4	D	303	CAA	CDP-CBP-CCP-O6A
4	D	303	CAA	CEP-CBP-CCP-O6A
4	D	303	CAA	CAP-CBP-CCP-O6A
4	D	303	CAA	C3P-C2P-S1P-C1
4	D	303	CAA	O1-C1-S1P-C2P
4	D	303	CAA	C2-C1-S1P-C2P
3	B	302	NAP	C4N-C3N-C7N-O7N
3	B	302	NAP	C4N-C3N-C7N-N7N

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	303	CAA	C3B-C4B-C5B-O5B
4	B	303	CAA	O4B-C4B-C5B-O5B
3	A	302	NAP	O4D-C4D-C5D-O5D
3	B	302	NAP	O4D-C4D-C5D-O5D
3	C	302	NAP	O4D-C4D-C5D-O5D
4	D	303	CAA	C3B-C4B-C5B-O5B
4	B	303	CAA	C4B-C3B-O3B-P3B
3	D	302	NAP	C4N-C3N-C7N-N7N
3	C	302	NAP	C3D-C4D-C5D-O5D
4	A	303	CAA	O4B-C4B-C5B-O5B
4	D	303	CAA	O4B-C4B-C5B-O5B
3	D	302	NAP	C4N-C3N-C7N-O7N
4	A	303	CAA	C4B-C3B-O3B-P3B
4	A	303	CAA	CDP-CBP-CCP-O6A
4	A	303	CAA	CEP-CBP-CCP-O6A
4	A	303	CAA	C2B-C3B-O3B-P3B
3	B	302	NAP	C3D-C4D-C5D-O5D
3	A	302	NAP	PA-O3-PN-O1N
4	B	303	CAA	C1-C2-C3-O3
4	C	303	CAA	C1-C2-C3-O3
4	D	303	CAA	P1A-O3A-P2A-O6A
4	B	303	CAA	C5B-O5B-P1A-O3A
3	B	302	NAP	C5D-O5D-PN-O3
4	C	303	CAA	C5B-O5B-P1A-O3A
3	A	302	NAP	C3D-C4D-C5D-O5D
3	C	302	NAP	O4B-C4B-C5B-O5B
3	B	302	NAP	PA-O3-PN-O2N
4	D	303	CAA	P2A-O3A-P1A-O1A
4	B	303	CAA	C4B-C5B-O5B-P1A
4	B	303	CAA	C5B-O5B-P1A-O2A
4	A	303	CAA	CCP-O6A-P2A-O4A
4	D	303	CAA	C5B-O5B-P1A-O2A
4	A	303	CAA	C1-C2-C3-C4
4	D	303	CAA	C1-C2-C3-C4
3	C	302	NAP	C3B-C4B-C5B-O5B
4	A	303	CAA	C3P-C2P-S1P-C1
3	C	302	NAP	PA-O3-PN-O1N
3	C	302	NAP	PA-O3-PN-O2N
3	A	302	NAP	C5D-O5D-PN-O3
3	A	302	NAP	C2D-C1D-N1N-C2N
4	A	303	CAA	C5B-O5B-P1A-O3A
4	D	303	CAA	C3B-O3B-P3B-O9A

*Continued on next page...*

*Continued from previous page...*

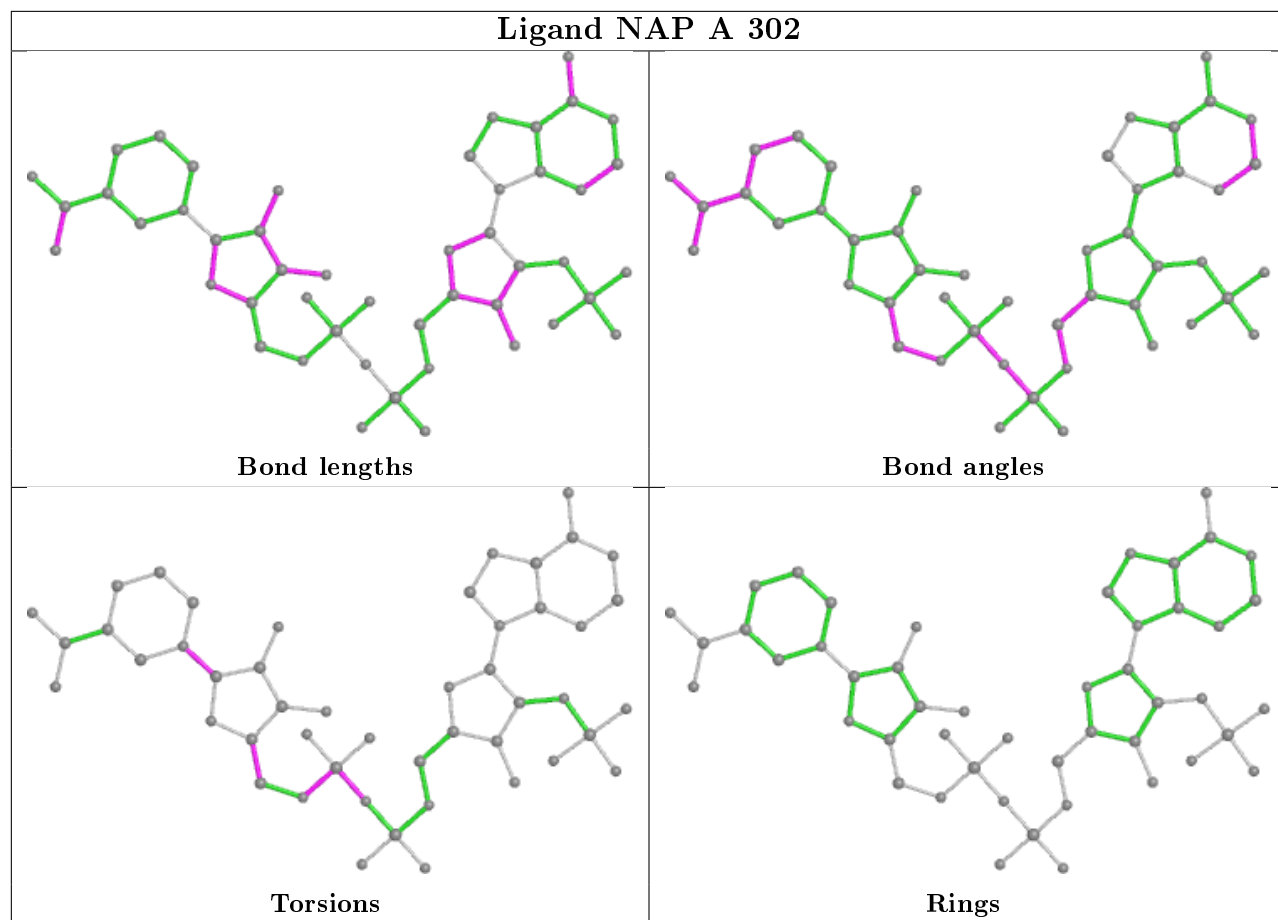
Mol	Chain	Res	Type	Atoms
4	B	303	CAA	P1A-O3A-P2A-O4A
3	A	302	NAP	PA-O3-PN-O2N
3	B	302	NAP	PA-O3-PN-O1N
4	D	303	CAA	P2A-O3A-P1A-O2A
3	B	302	NAP	C5B-O5B-PA-O1A
4	C	303	CAA	CCP-O6A-P2A-O4A
4	D	303	CAA	C5B-O5B-P1A-O1A
4	D	303	CAA	CCP-O6A-P2A-O4A
3	D	302	NAP	O4D-C4D-C5D-O5D

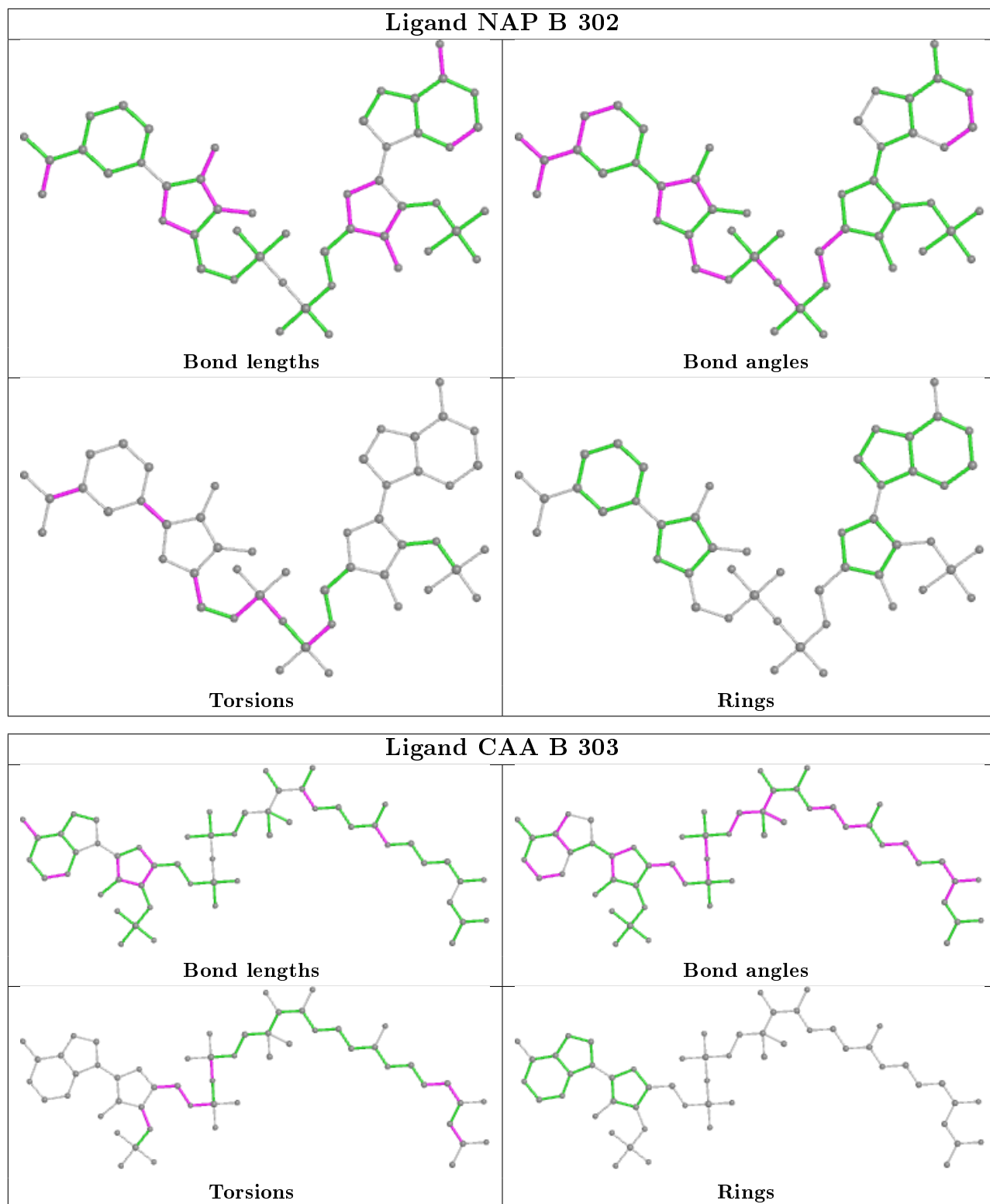
There are no ring outliers.

7 monomers are involved in 15 short contacts:

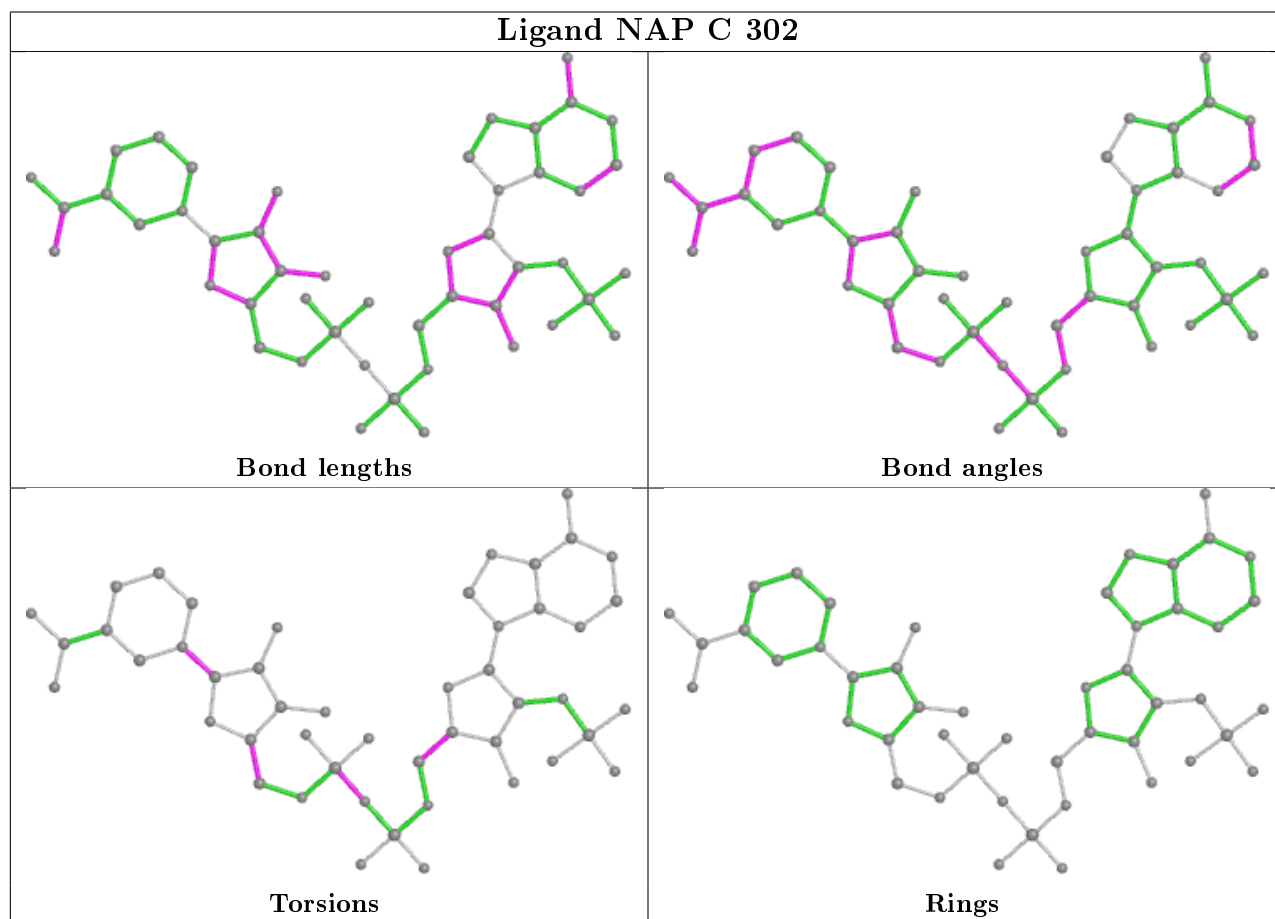
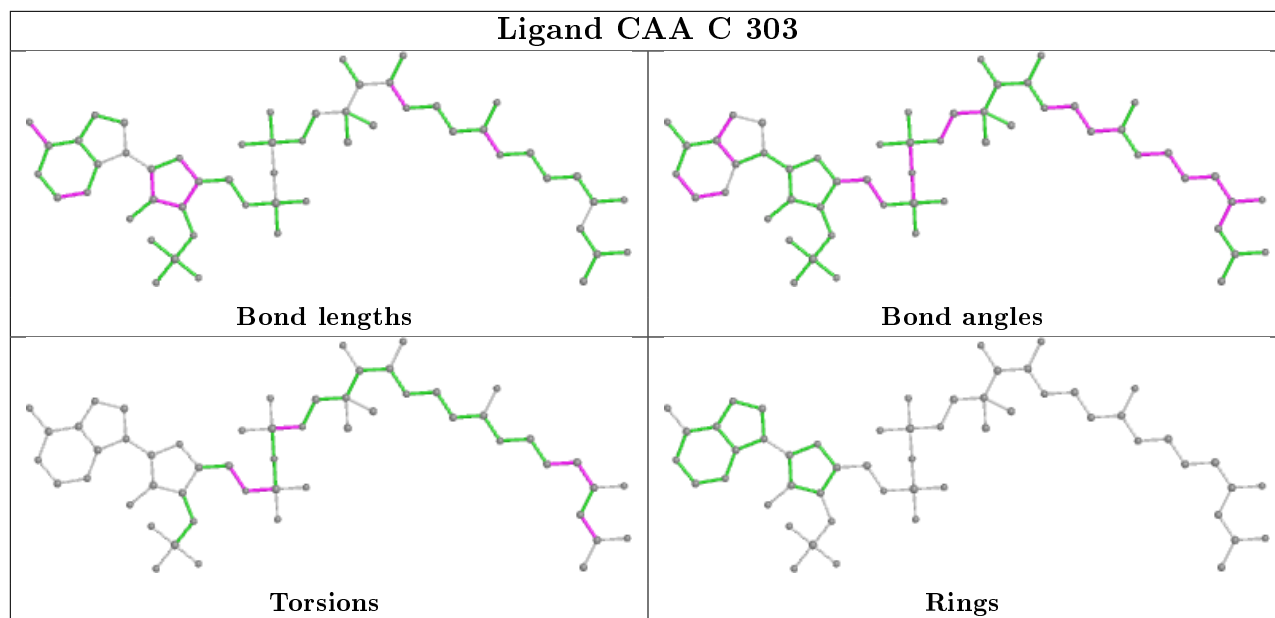
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	NAP	4	0
3	B	302	NAP	1	0
4	B	303	CAA	2	0
3	C	302	NAP	2	0
3	D	302	NAP	5	0
4	A	303	CAA	1	0
4	D	303	CAA	1	0

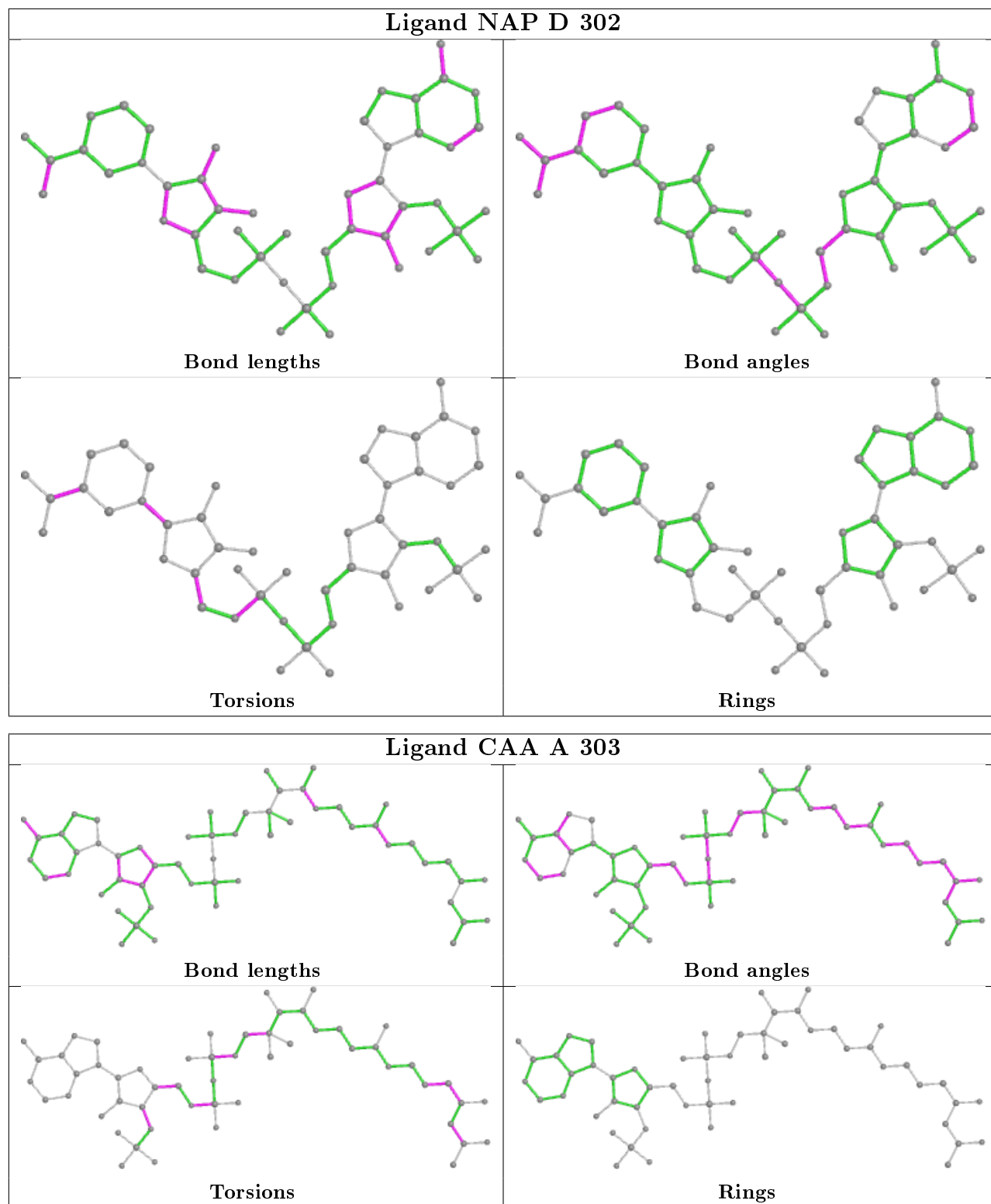
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

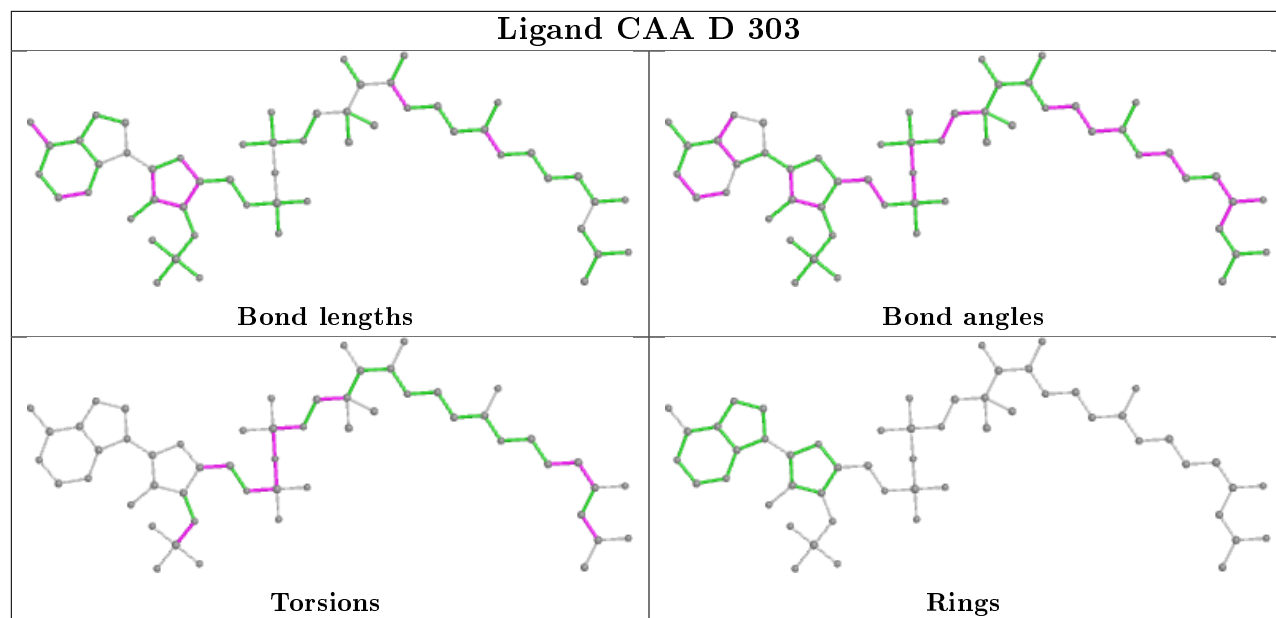












## 5.7 Other polymers [i](#)

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	244/257 (94%)	-0.37	3 (1%) 79 83	5, 12, 29, 54	0
1	B	249/257 (96%)	-0.21	6 (2%) 59 65	7, 13, 33, 59	0
1	C	244/257 (94%)	-0.12	13 (5%) 26 33	6, 13, 45, 69	0
1	D	249/257 (96%)	0.12	18 (7%) 15 19	6, 16, 48, 71	0
All	All	986/1028 (95%)	-0.14	40 (4%) 37 45	5, 13, 41, 71	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	ALA	6.3
1	D	199	LEU	6.1
1	C	195	ARG	5.8
1	D	195	ARG	5.3
1	D	193	ALA	5.0
1	C	199	LEU	5.0
1	A	195	ARG	4.9
1	B	195	ARG	4.5
1	D	197	ASP	4.2
1	D	51	LEU	4.0
1	C	191	VAL	3.7
1	C	198	VAL	3.6
1	D	194	ILE	3.6
1	B	197	ASP	3.3
1	D	42	GLU	3.2
1	A	193	ALA	3.2
1	C	194	ILE	3.1
1	D	43	LYS	3.0
1	C	197	ASP	2.9
1	D	200	ASP	2.9
1	D	50	ALA	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	46	GLU	2.8
1	D	201	LYS	2.8
1	D	-2	HIS	2.6
1	B	194	ILE	2.6
1	C	192	LYS	2.5
1	B	246	GLY	2.5
1	D	190	MET	2.5
1	B	198	VAL	2.4
1	D	191	VAL	2.4
1	C	189	ASP	2.4
1	D	40	ARG	2.3
1	C	201	LYS	2.2
1	D	38	SER	2.2
1	A	197	ASP	2.2
1	C	190	MET	2.2
1	B	193	ALA	2.2
1	C	202	ILE	2.1
1	C	50	ALA	2.1
1	D	41	ARG	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

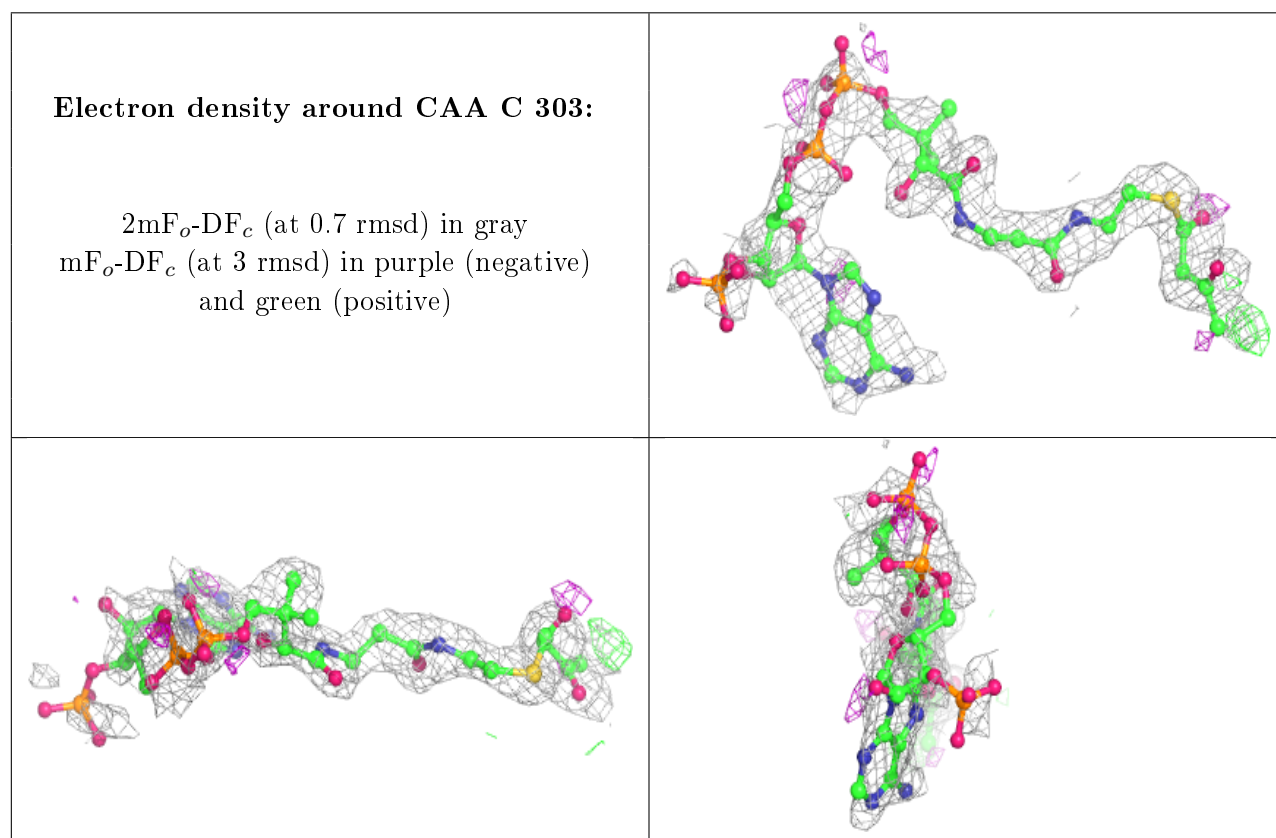
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CAA	C	303	54/54	0.77	0.30	15,56,107,124	0
4	CAA	A	303	54/54	0.77	0.27	9,34,81,114	0
4	CAA	D	303	54/54	0.77	0.29	18,45,97,110	0
3	NAP	C	302	48/48	0.79	0.29	19,47,75,79	0

*Continued on next page...*

Continued from previous page...

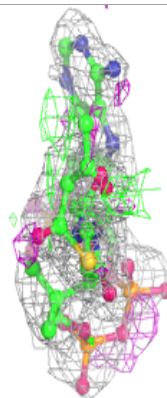
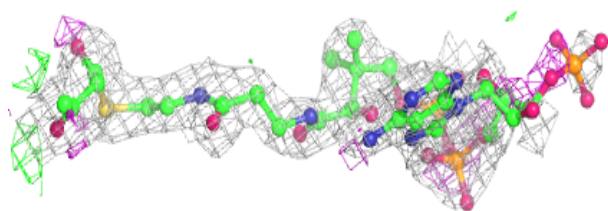
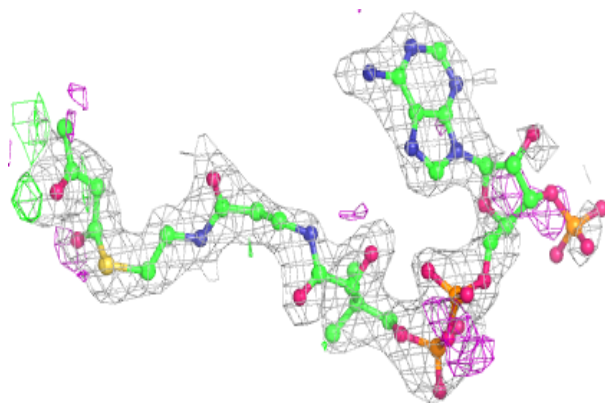
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	D	302	48/48	0.80	0.31	25,54,76,77	0
4	CAA	B	303	54/54	0.84	0.24	13,38,91,113	0
3	NAP	B	302	48/48	0.91	0.19	12,26,57,70	0
2	SO4	C	301	5/5	0.92	0.18	64,69,76,84	0
3	NAP	A	302	48/48	0.93	0.14	13,22,47,60	0
2	SO4	D	301	5/5	0.97	0.14	42,47,49,65	0
2	SO4	A	301	5/5	0.98	0.14	33,35,44,44	0
2	SO4	B	301	5/5	0.98	0.09	33,34,37,47	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.

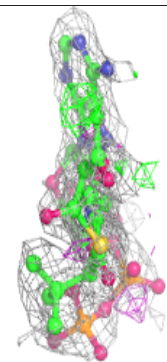
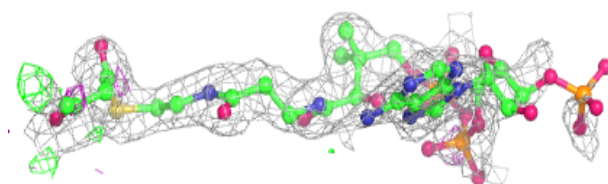
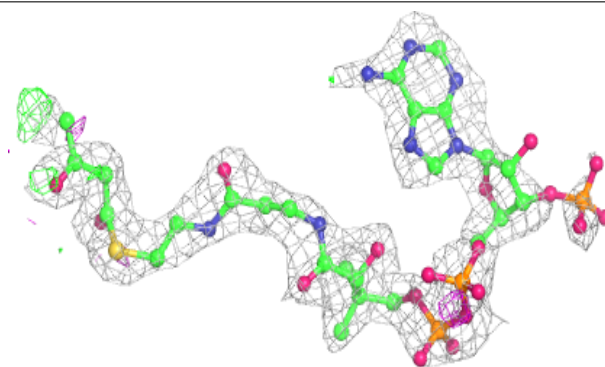


**Electron density around CAA A 303:**

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

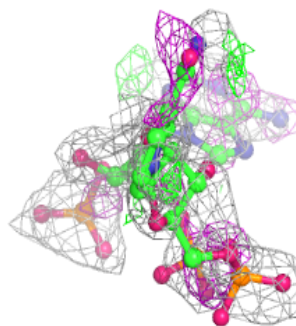
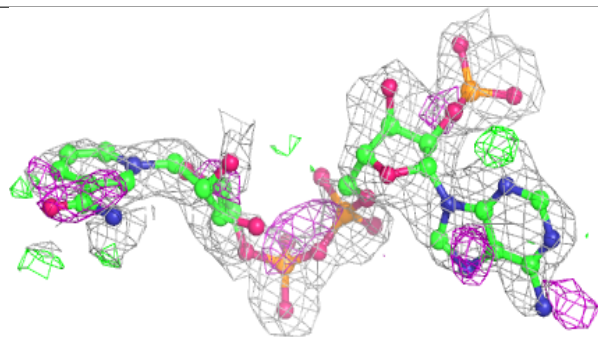
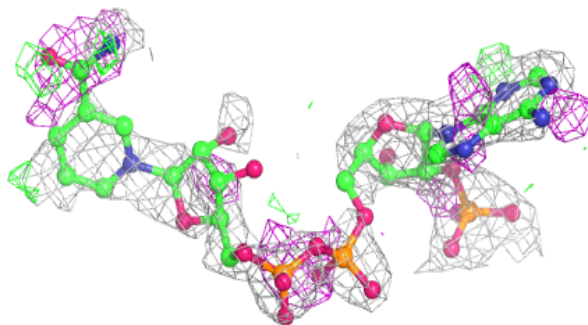
**Electron density around CAA D 303:**

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

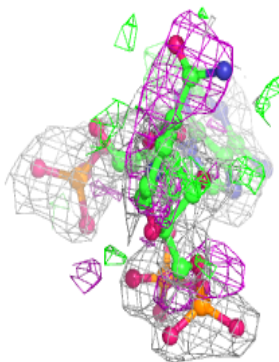
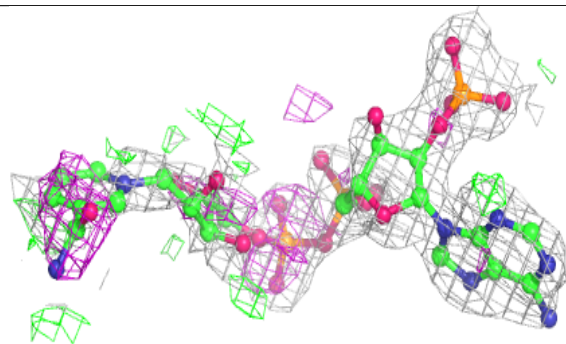
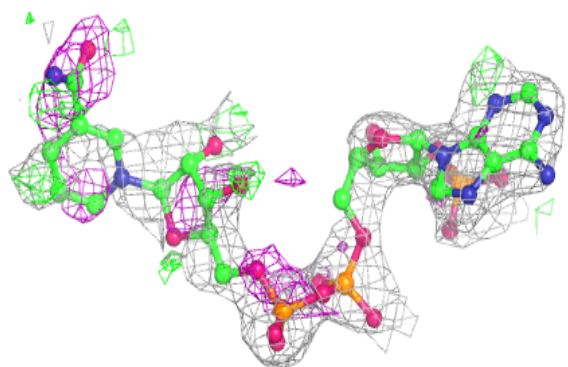


**Electron density around NAP C 302:**

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

**Electron density around NAP D 302:**

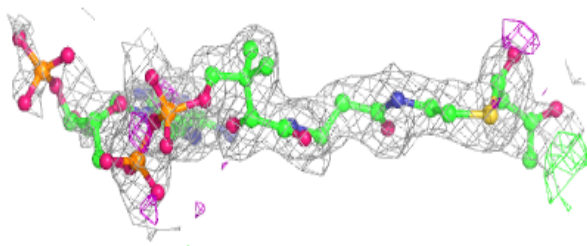
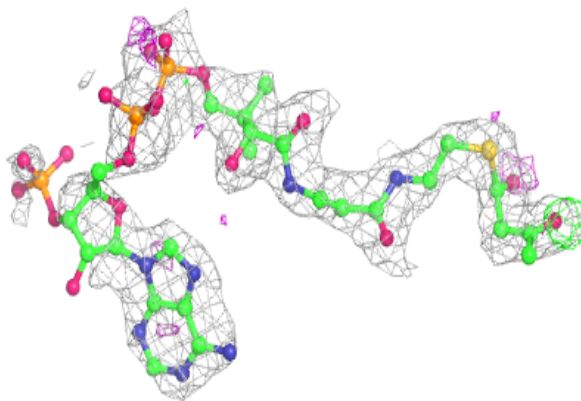
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



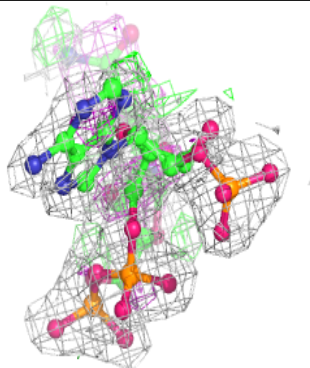
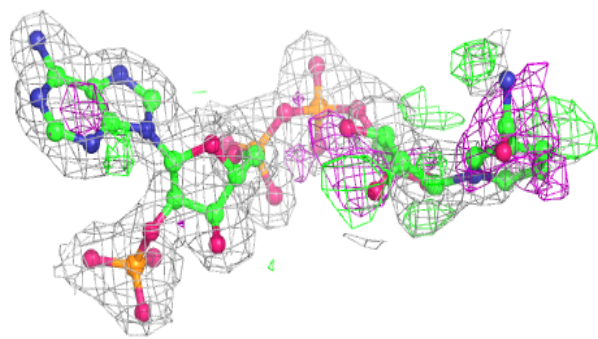
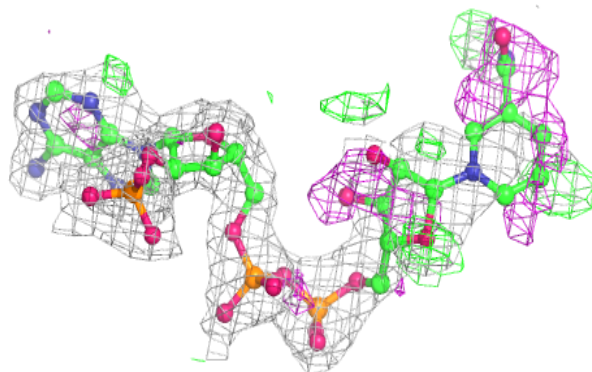


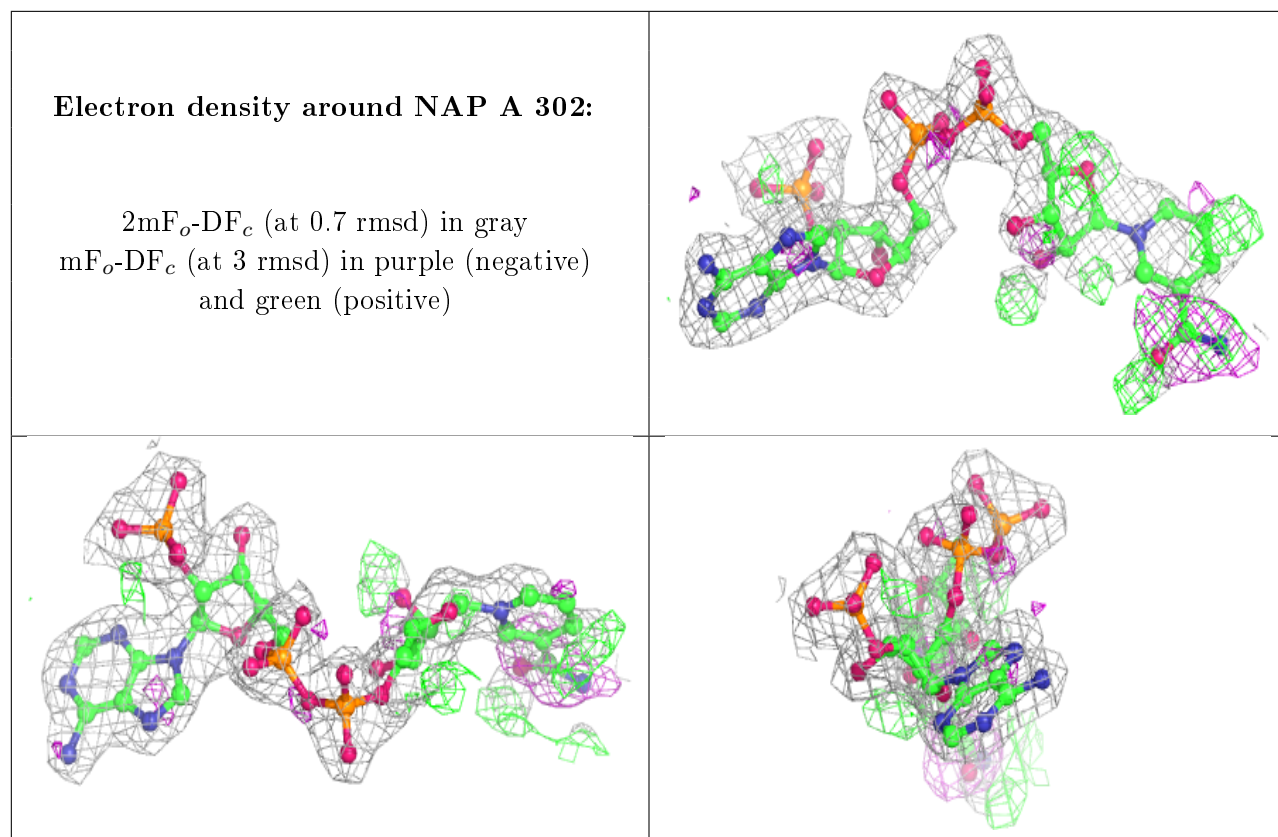
**Electron density around CAA B 303:**

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

**Electron density around NAP B 302:**

$2mF_o-DF_c$  (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.