



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:52 AM EDT

PDB ID : 6VO6  
Title : Crystal Structure of Cj1427, an Essential NAD-dependent Dehydrogenase from *Campylobacter jejuni*, in the Presence of NADH and GDP  
Authors : Anderson, T.K.; Spencer, K.D.; Thoden, J.B.; Huddleston, J.P.; Raushel, F.M.; Holden, H.M.  
Deposited on : 2020-01-30  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

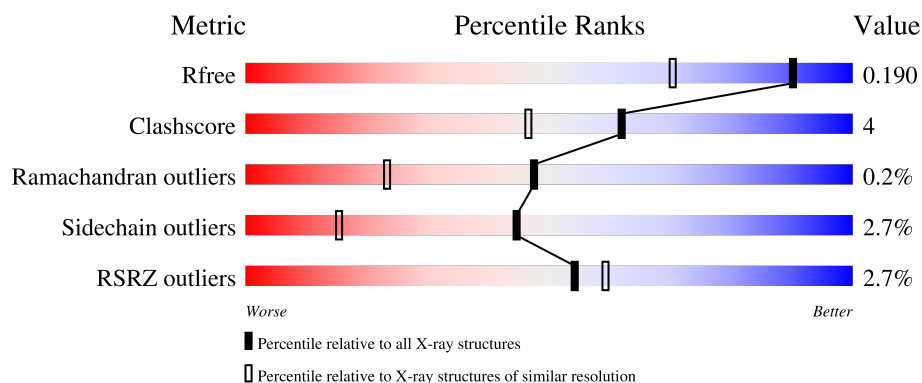
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	321	 2% 88% 7% .
1	B	321	 2% 88% 8% ..
1	C	321	 5% 83% 7% . 7%
1	D	321	 2% 89% 6% ..

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11506 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 Putative sugar-nucleotide epimerase/dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	4	0
			2472	1587	416	453	16			
1	B	310	Total	C	N	O	S	0	10	0
			2532	1624	429	464	15			
1	C	297	Total	C	N	O	S	0	4	0
			2397	1540	407	435	15			
1	D	311	Total	C	N	O	S	0	2	0
			2497	1603	421	458	15			

There are 32 discrepancies between the modelled and reference sequences:

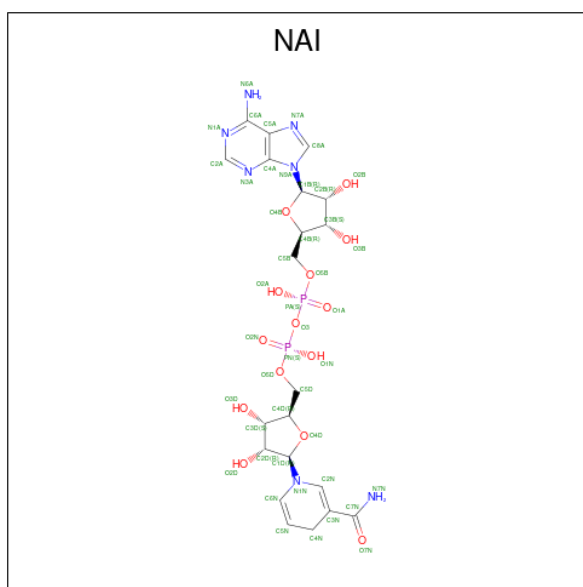
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	LEU	-	expression tag	UNP Q0P8I7
A	315	GLU	-	expression tag	UNP Q0P8I7
A	316	HIS	-	expression tag	UNP Q0P8I7
A	317	HIS	-	expression tag	UNP Q0P8I7
A	318	HIS	-	expression tag	UNP Q0P8I7
A	319	HIS	-	expression tag	UNP Q0P8I7
A	320	HIS	-	expression tag	UNP Q0P8I7
A	321	HIS	-	expression tag	UNP Q0P8I7
B	314	LEU	-	expression tag	UNP Q0P8I7
B	315	GLU	-	expression tag	UNP Q0P8I7
B	316	HIS	-	expression tag	UNP Q0P8I7
B	317	HIS	-	expression tag	UNP Q0P8I7
B	318	HIS	-	expression tag	UNP Q0P8I7
B	319	HIS	-	expression tag	UNP Q0P8I7
B	320	HIS	-	expression tag	UNP Q0P8I7
B	321	HIS	-	expression tag	UNP Q0P8I7
C	314	LEU	-	expression tag	UNP Q0P8I7
C	315	GLU	-	expression tag	UNP Q0P8I7
C	316	HIS	-	expression tag	UNP Q0P8I7
C	317	HIS	-	expression tag	UNP Q0P8I7
C	318	HIS	-	expression tag	UNP Q0P8I7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	319	HIS	-	expression tag	UNP Q0P8I7
C	320	HIS	-	expression tag	UNP Q0P8I7
C	321	HIS	-	expression tag	UNP Q0P8I7
D	314	LEU	-	expression tag	UNP Q0P8I7
D	315	GLU	-	expression tag	UNP Q0P8I7
D	316	HIS	-	expression tag	UNP Q0P8I7
D	317	HIS	-	expression tag	UNP Q0P8I7
D	318	HIS	-	expression tag	UNP Q0P8I7
D	319	HIS	-	expression tag	UNP Q0P8I7
D	320	HIS	-	expression tag	UNP Q0P8I7
D	321	HIS	-	expression tag	UNP Q0P8I7

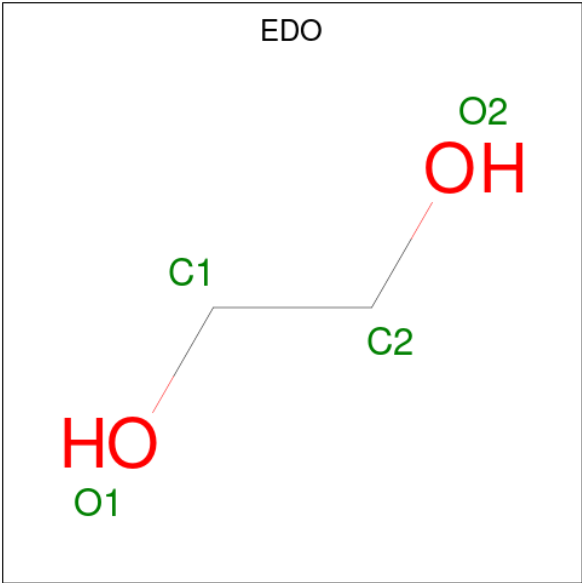
- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
3	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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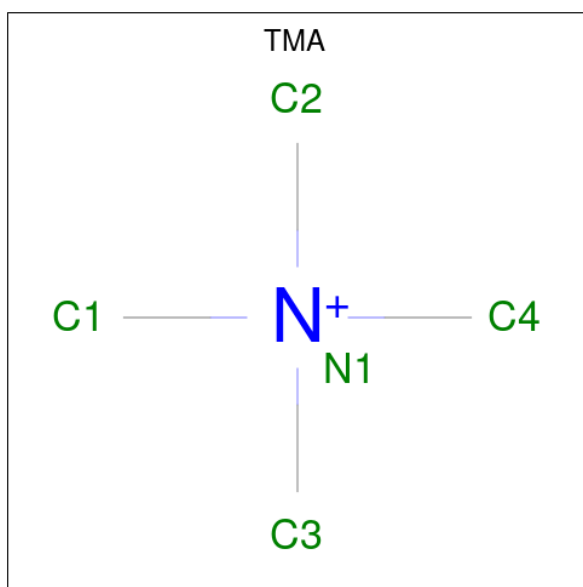
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is TETRAMETHYLAMMONIUM ION (three-letter code: TMA) (formula: C<sub>4</sub>H<sub>12</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	4	1		
6	B	1	Total	C	N	0	0
			5	4	1		
6	B	1	Total	C	N	0	0
			5	4	1		
6	C	1	Total	C	N	0	0
			5	4	1		
6	D	1	Total	C	N	0	0
			5	4	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	298	Total	O	0	0
			298	298		
8	B	337	Total	O	0	0
			337	337		
8	C	299	Total	O	0	0
			299	299		

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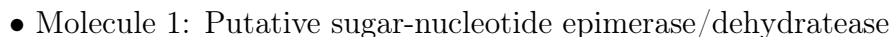
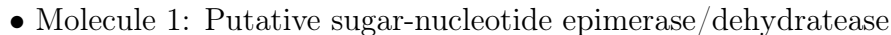
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	363	Total 363	O 363	0	0





- Molecule 1: Putative sugar-nucleotide epimerase/dehydratase



GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.61Å 84.34Å 135.45Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	35.14 – 1.50 35.11 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.14-1.50) 97.5 (35.11-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.163 , 0.189 0.164 , 0.190	Depositor DCC
$R_{free}$ test set	11613 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: GDP, NAI, CL, EDO, TMA, NA

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	0.75	0/2533	0.91	1/3415 (0.0%)
1	B	0.78	2/2613 (0.1%)	0.95	5/3522 (0.1%)
1	C	0.80	2/2455 (0.1%)	0.95	5/3308 (0.2%)
1	D	0.78	0/2554	0.97	6/3443 (0.2%)
All	All	0.78	4/10155 (0.0%)	0.95	17/13688 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308[A]	ARG	C-O	6.02	1.34	1.23
1	B	308[B]	ARG	C-O	6.02	1.34	1.23
1	C	200	GLU	CD-OE1	-5.36	1.19	1.25
1	C	200	GLU	CD-OE2	-5.06	1.20	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308[A]	ARG	N-CA-C	7.09	130.14	111.00
1	B	308[B]	ARG	N-CA-C	7.09	130.14	111.00
1	D	123	TYR	CB-CG-CD1	5.88	124.53	121.00
1	C	308[A]	ARG	CA-C-O	5.86	132.41	120.10
1	C	308[B]	ARG	CA-C-O	5.86	132.41	120.10
1	B	216	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	D	299	ARG	CG-CD-NE	5.75	123.86	111.80
1	C	238	ALA	CB-CA-C	5.74	118.71	110.10
1	D	216	PHE	CB-CG-CD1	5.74	124.82	120.80
1	A	203	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	D	190	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	D	299	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	299	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	175	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	308[A]	ARG	N-CA-C	5.04	124.61	111.00
1	C	308[B]	ARG	N-CA-C	5.04	124.61	111.00
1	B	307	ASN	CB-CA-C	5.03	120.47	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	2472	0	2496	15	0
1	B	2532	0	2572	22	0
1	C	2397	0	2431	35	0
1	D	2497	0	2520	19	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
3	A	28	0	12	0	0
3	D	28	0	12	2	0
4	A	16	0	24	0	0
4	B	16	0	23	3	0
4	C	12	0	18	0	0
4	D	8	0	12	0	0
5	A	1	0	0	0	0
6	A	5	0	12	0	0
6	B	10	0	24	3	0
6	C	5	0	12	0	0
6	D	5	0	12	0	0
7	D	1	0	0	0	0
8	A	298	0	0	2	0
8	B	337	0	0	11	0
8	C	299	0	0	10	0
8	D	363	0	0	3	0
All	All	11506	0	10288	91	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 (91) 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:402:GDP:H5'	8:D:501:HOH:O	1.48	1.11
1:C:88[A]:ARG:HE	1:C:89:ASN:ND2	1.50	1.08
1:B:255[A]:ASP:OD2	8:B:502:HOH:O	1.78	1.01
1:C:204:ARG:O	1:C:239:ASN:HA	1.66	0.95
1:C:88[A]:ARG:HE	1:C:89:ASN:HD21	0.97	0.93
1:C:292:ASP:OD1	8:C:501:HOH:O	1.89	0.90
1:C:88[A]:ARG:NE	1:C:89:ASN:HD21	1.73	0.85
1:B:198:PHE:CD2	6:B:407:TMA:H21	2.13	0.83
1:C:168:THR:HG22	8:C:534:HOH:O	1.77	0.82
1:C:28:GLU:OE1	8:C:502:HOH:O	1.97	0.82
1:C:238:ALA:HA	8:C:647:HOH:O	1.80	0.82
1:B:247[A]:GLU:OE2	8:B:503:HOH:O	1.97	0.81
1:B:111:SER:HA	4:B:404:EDO:H21	1.64	0.78
1:B:224:ASP:OD1	8:B:504:HOH:O	2.06	0.73
1:A:59[A]:MET:SD	1:A:96:ILE:HD13	2.29	0.73
1:A:59[A]:MET:SD	1:A:96:ILE:CD1	2.79	0.71
1:D:62:ASN:HD22	1:D:65:ARG:NH1	1.90	0.69
3:D:402:GDP:O2B	8:D:501:HOH:O	2.12	0.67
1:D:166:LEU:CD2	1:D:233:MET:HE3	2.26	0.66
1:D:166:LEU:CD2	1:D:233:MET:CE	2.73	0.66
1:B:120:ASN:C	1:B:120:ASN:HD22	1.99	0.64
1:B:251:LYS:NZ	1:B:291:GLU:OE2	2.21	0.62
1:D:62:ASN:ND2	1:D:65:ARG:HH12	1.98	0.61
4:B:402:EDO:H21	8:B:610:HOH:O	2.00	0.61
1:C:88[B]:ARG:NH2	8:C:503:HOH:O	2.33	0.61
1:C:62:ASN:HD22	1:C:65:ARG:HH12	1.48	0.61
1:C:203:ARG:HH11	1:C:203:ARG:HG3	1.65	0.60
1:C:295:LYS:NZ	8:C:505:HOH:O	2.35	0.60
1:A:120:ASN:HD22	1:A:120:ASN:C	2.05	0.59
4:B:403:EDO:H22	8:B:540:HOH:O	2.03	0.59
1:D:62:ASN:HD22	1:D:65:ARG:HH12	1.49	0.59
1:B:123:TYR:O	8:B:505:HOH:O	2.17	0.59
1:C:166:LEU:CD2	1:C:233:MET:CE	2.84	0.56
1:D:62:ASN:ND2	1:D:65:ARG:NH1	2.54	0.55
1:D:166:LEU:HD21	1:D:233:MET:CE	2.36	0.55
1:D:201:HIS:HE1	8:D:756:HOH:O	1.89	0.55
1:D:120:ASN:C	1:D:120:ASN:HD22	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:THR:HG21	1:C:181:LEU:HB3	1.89	0.54
1:B:55:ASN:OD1	1:C:88[A]:ARG:NH2	2.36	0.54
1:B:4[C]:LYS:HD3	8:B:508:HOH:O	2.07	0.53
1:D:166:LEU:HD22	1:D:233:MET:HE3	1.91	0.53
1:C:88[A]:ARG:NE	1:C:89:ASN:ND2	2.35	0.53
1:C:166:LEU:HD21	1:C:233:MET:HE3	1.92	0.52
1:B:308[B]:ARG:HG2	1:D:308:ARG:HE	1.75	0.52
1:C:166:LEU:CD2	1:C:233:MET:HE2	2.40	0.51
1:D:166:LEU:CD2	1:D:233:MET:HE2	2.39	0.51
1:D:166:LEU:HD21	1:D:233:MET:HE3	1.92	0.51
1:A:61:GLU:HG3	8:A:692:HOH:O	2.11	0.51
1:C:238:ALA:HB3	8:C:573:HOH:O	2.11	0.50
1:A:59[A]:MET:SD	1:A:96:ILE:HD11	2.50	0.50
1:B:198:PHE:CZ	6:B:407:TMA:H31	2.46	0.50
1:C:166:LEU:HD21	1:C:233:MET:CE	2.43	0.49
1:A:64:ILE:HG13	1:A:103:MET:HE1	1.95	0.48
1:D:80:LEU:HD13	1:D:96:ILE:HG21	1.95	0.48
1:D:92:LEU:O	1:D:96:ILE:HG22	2.13	0.48
1:C:166:LEU:CD2	1:C:233:MET:HE3	2.43	0.48
1:C:94:LYS:HD2	8:C:664:HOH:O	2.13	0.48
1:A:85:LEU:HD22	1:C:311:ASN:HB3	1.96	0.47
1:C:62:ASN:ND2	1:C:65:ARG:HH12	2.12	0.47
1:B:198:PHE:CG	6:B:407:TMA:H21	2.51	0.46
1:B:166:LEU:CD2	1:B:233:MET:CE	2.93	0.46
1:A:305:LYS:O	1:C:308[A]:ARG:HD2	2.16	0.45
1:C:272:TYR:N	8:C:514:HOH:O	2.50	0.45
1:A:166:LEU:CD2	1:A:233:MET:CE	2.95	0.45
1:C:307:ASN:ND2	1:C:307:ASN:C	2.70	0.45
1:C:307:ASN:ND2	1:C:307:ASN:O	2.50	0.45
1:B:120:ASN:C	1:B:120:ASN:ND2	2.67	0.45
1:B:4[B]:LYS:NZ	8:B:515:HOH:O	2.50	0.44
1:B:193:LYS:HE3	8:B:683:HOH:O	2.18	0.43
1:C:102:LYS:HG3	1:C:154:TYR:CZ	2.54	0.43
1:A:150:HIS:HD2	8:A:637:HOH:O	2.02	0.43
1:A:65:ARG:HG3	1:A:107:PHE:CD1	2.53	0.43
1:D:83:ALA:N	1:D:84:PRO:CD	2.82	0.42
1:B:309:PHE:N	8:B:501:HOH:O	1.77	0.42
1:A:166:LEU:CD2	1:A:233:MET:HE2	2.50	0.42
1:B:166:LEU:CD2	1:B:233:MET:HE3	2.49	0.42
1:D:89:ASN:OD1	1:D:89:ASN:N	2.53	0.42
1:C:252:TYR:OH	1:C:291:GLU:OE1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308[B]:ARG:HH11	1:C:308[B]:ARG:HD3	1.72	0.41
1:A:120:ASN:C	1:A:120:ASN:ND2	2.71	0.41
1:B:88:ARG:NH1	8:B:509:HOH:O	2.46	0.41
1:C:55:ASN:C	1:C:55:ASN:HD22	2.24	0.41
1:D:169:VAL:HA	1:D:207:ILE:O	2.21	0.41
1:B:83:ALA:N	1:B:84:PRO:CD	2.84	0.41
1:C:83:ALA:HB3	1:C:84:PRO:HD3	2.03	0.40
1:C:292:ASP:HA	8:C:501:HOH:O	2.20	0.40
1:D:91:LYS:N	1:D:91:LYS:HD3	2.35	0.40
1:A:59[B]:MET:SD	1:A:100:ALA:HB2	2.61	0.40
1:C:83:ALA:N	1:C:84:PRO:CD	2.85	0.40
1:A:169:VAL:HA	1:A:207:ILE:O	2.22	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	307/321 (96%)	300 (98%)	7 (2%)	0	100	100
1	B	318/321 (99%)	309 (97%)	9 (3%)	0	100	100
1	C	295/321 (92%)	284 (96%)	9 (3%)	2 (1%)	22	6
1	D	311/321 (97%)	303 (97%)	8 (3%)	0	100	100
All	All	1231/1284 (96%)	1196 (97%)	33 (3%)	2 (0%)	47	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	238	ALA
1	C	262	ASN



### 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	270/280 (96%)	262 (97%)	8 (3%)	41	12
1	B	279/280 (100%)	270 (97%)	9 (3%)	39	10
1	C	262/280 (94%)	254 (97%)	8 (3%)	40	11
1	D	272/280 (97%)	265 (97%)	7 (3%)	46	16
All	All	1083/1120 (97%)	1051 (97%)	32 (3%)	44	12

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24[A]	GLU
1	A	24[B]	GLU
1	A	55	ASN
1	A	91	LYS
1	A	120	ASN
1	A	175	ARG
1	A	205	ASN
1	A	272	TYR
1	B	38	ASP
1	B	103	MET
1	B	120	ASN
1	B	131	MET
1	B	148	LYS
1	B	150[A]	HIS
1	B	150[B]	HIS
1	B	175	ARG
1	B	205	ASN
1	C	55	ASN
1	C	88[A]	ARG
1	C	88[B]	ARG
1	C	175	ARG
1	C	203	ARG
1	C	225	LYS
1	C	239	ASN

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Mol	Chain	Res	Type
1	C	307	ASN
1	D	55	ASN
1	D	89	ASN
1	D	91	LYS
1	D	120	ASN
1	D	175	ARG
1	D	205	ASN
1	D	272	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	120	ASN
1	A	150	HIS
1	A	153	GLN
1	A	205	ASN
1	B	89	ASN
1	B	120	ASN
1	B	205	ASN
1	C	55	ASN
1	C	62	ASN
1	C	89	ASN
1	C	307	ASN
1	D	55	ASN
1	D	62	ASN
1	D	120	ASN
1	D	150	HIS
1	D	201	HIS
1	D	205	ASN

### 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 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	$\# Z  > 2$
6	TMA	B	406	-	4,4,4	0.37	0	6,6,6	0.05	0
2	NAI	C	401	-	43,48,48	1.38	5 (11%)	50,73,73	1.00	2 (4%)
3	GDP	D	402	-	25,30,30	1.43	1 (4%)	30,47,47	1.51	7 (23%)
4	EDO	C	404	-	3,3,3	0.51	0	2,2,2	0.35	0
4	EDO	A	405	-	3,3,3	0.28	0	2,2,2	0.06	0
3	GDP	A	402	-	25,30,30	1.13	3 (12%)	30,47,47	0.95	1 (3%)
6	TMA	B	407	-	4,4,4	0.21	0	6,6,6	0.20	0
6	TMA	A	408	-	4,4,4	0.34	0	6,6,6	0.09	0
4	EDO	B	404	-	3,3,3	0.80	0	2,2,2	0.78	0
4	EDO	B	403	-	3,3,3	0.27	0	2,2,2	0.56	0
4	EDO	B	405	-	3,3,3	0.61	0	2,2,2	1.22	0
6	TMA	C	405	-	4,4,4	0.33	0	6,6,6	0.09	0
4	EDO	A	403	-	3,3,3	0.18	0	2,2,2	0.14	0
4	EDO	B	402	-	3,3,3	0.09	0	2,2,2	0.27	0
4	EDO	C	403	-	3,3,3	0.41	0	2,2,2	0.60	0
4	EDO	D	405	-	3,3,3	0.29	0	2,2,2	0.09	0
4	EDO	A	404	-	3,3,3	0.15	0	2,2,2	0.06	0
4	EDO	A	406	-	3,3,3	0.10	0	2,2,2	0.07	0
2	NAI	A	401	-	43,48,48	1.05	2 (4%)	50,73,73	0.82	1 (2%)
4	EDO	D	404	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	C	402	-	3,3,3	0.42	0	2,2,2	0.32	0
2	NAI	B	401	-	43,48,48	1.15	4 (9%)	50,73,73	0.95	1 (2%)
6	TMA	D	406	-	4,4,4	0.23	0	6,6,6	0.12	0
2	NAI	D	401	-	43,48,48	1.02	2 (4%)	50,73,73	1.06	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	C	401	-	-	2/25/72/72	0/5/5/5
3	GDP	D	402	-	-	2/12/32/32	0/3/3/3
4	EDO	C	404	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
3	GDP	A	402	-	-	1/12/32/32	0/3/3/3
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
2	NAI	A	401	-	-	4/25/72/72	0/5/5/5
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	C	402	-	-	0/1/1/1	-
2	NAI	B	401	-	-	4/25/72/72	0/5/5/5
2	NAI	D	401	-	-	5/25/72/72	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	GDP	O4'-C1'	5.13	1.47	1.40
2	C	401	NAI	C4N-C5N	-4.34	1.37	1.49
2	C	401	NAI	PN-O3	3.98	1.63	1.59
2	A	401	NAI	C4N-C3N	-3.93	1.42	1.50
2	D	401	NAI	C4N-C3N	-3.84	1.42	1.50
2	B	401	NAI	C4N-C5N	-3.39	1.40	1.49
2	C	401	NAI	PA-O3	3.12	1.62	1.59
2	A	401	NAI	C4N-C5N	-2.95	1.41	1.49
2	B	401	NAI	PN-O3	2.90	1.62	1.59
2	C	401	NAI	C4N-C3N	-2.54	1.45	1.50
2	D	401	NAI	C4N-C5N	-2.52	1.42	1.49
3	A	402	GDP	C6-N1	-2.46	1.34	1.37
2	B	401	NAI	C1B-N9A	-2.39	1.44	1.49
2	B	401	NAI	C4N-C3N	-2.29	1.45	1.50
3	A	402	GDP	O3'-C3'	2.11	1.48	1.43
2	C	401	NAI	PN-O1N	-2.02	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	GDP	PB-O2B	-2.01	1.47	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	GDP	O4'-C1'-N9	-3.50	104.11	108.75
3	A	402	GDP	C8-N7-C5	3.05	107.74	102.55
3	D	402	GDP	O2A-PA-O1A	2.76	125.30	112.44
3	D	402	GDP	O3A-PA-O1A	-2.65	102.73	110.70
3	D	402	GDP	C4'-O4'-C1'	-2.60	107.54	109.92
3	D	402	GDP	O6-C6-N1	2.60	123.70	120.62
2	D	401	NAI	C4A-C5A-N7A	2.59	112.07	109.34
2	D	401	NAI	O7N-C7N-C3N	-2.51	116.18	120.90
2	D	401	NAI	C3N-C2N-N1N	-2.47	119.58	123.20
2	D	401	NAI	C4B-O4B-C1B	-2.43	107.70	109.92
3	D	402	GDP	O2B-PB-O1B	2.41	120.21	110.83
3	D	402	GDP	O6-C6-C5	-2.13	120.10	124.32
2	C	401	NAI	O4B-C1B-N9A	-2.09	105.97	108.75
2	D	401	NAI	O4B-C1B-N9A	-2.09	105.97	108.75
2	B	401	NAI	C4B-O4B-C1B	-2.06	108.04	109.92
2	A	401	NAI	O4B-C1B-N9A	-2.04	106.04	108.75
2	C	401	NAI	O3-PA-O1A	-2.02	104.64	110.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	C5B-O5B-PA-O1A
2	B	401	NAI	C5D-O5D-PN-O2N
2	C	401	NAI	C5D-O5D-PN-O2N
2	D	401	NAI	C5B-O5B-PA-O1A
2	D	401	NAI	C5D-O5D-PN-O2N
2	A	401	NAI	O4D-C1D-N1N-C6N
4	B	403	EDO	O1-C1-C2-O2
2	D	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	O4D-C1D-N1N-C6N
2	C	401	NAI	O4D-C1D-N1N-C6N
2	B	401	NAI	C5D-O5D-PN-O3
2	D	401	NAI	C5B-O5B-PA-O2A
2	D	401	NAI	C5B-O5B-PA-O3
4	C	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C2N-C3N-C7N-N7N
3	D	402	GDP	PB-O3A-PA-O2A
4	B	405	EDO	O1-C1-C2-O2
2	A	401	NAI	O4B-C4B-C5B-O5B
4	A	405	EDO	O1-C1-C2-O2
4	C	404	EDO	O1-C1-C2-O2
3	D	402	GDP	PB-O3A-PA-O1A
3	A	402	GDP	PB-O3A-PA-O2A

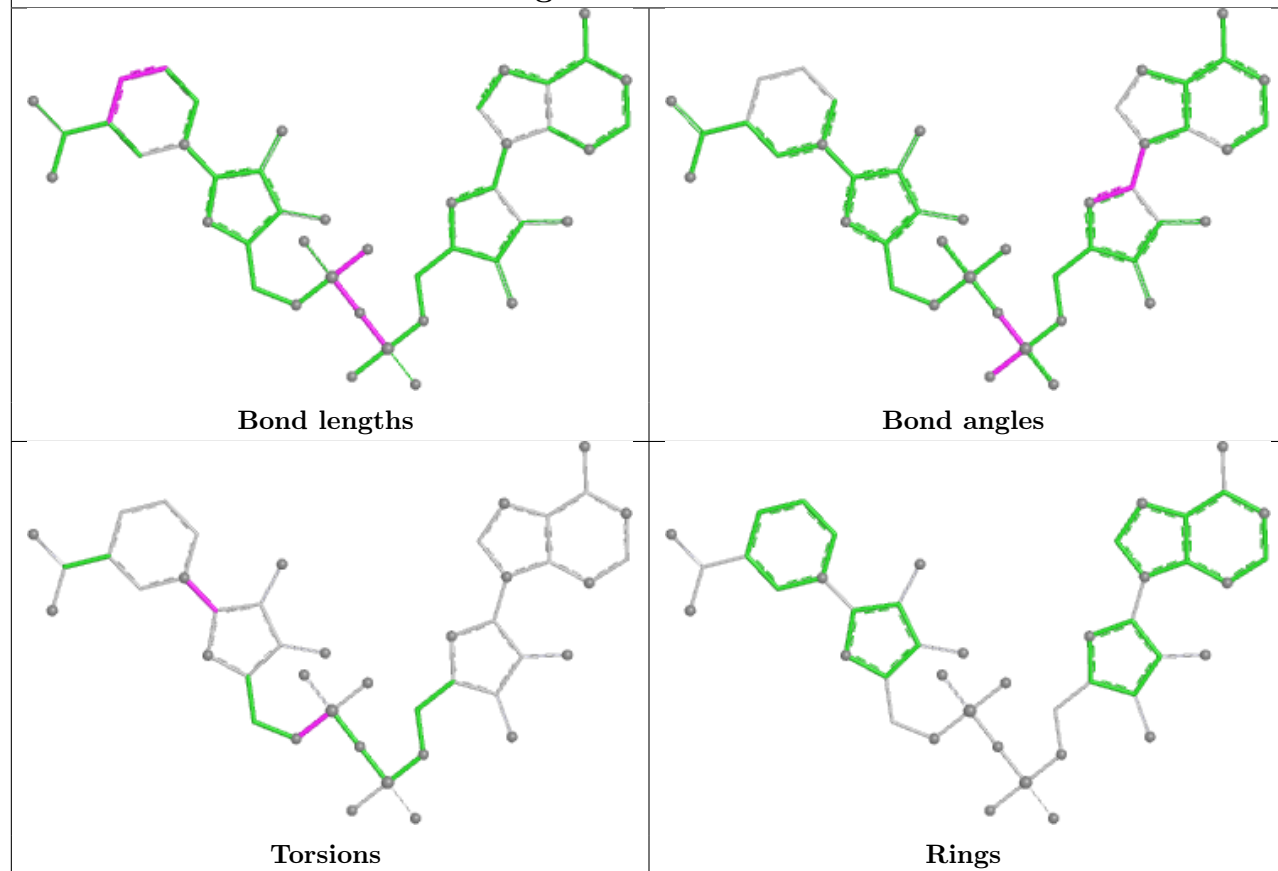
There are no ring outliers.

5 monomers are involved in 8 short contacts:

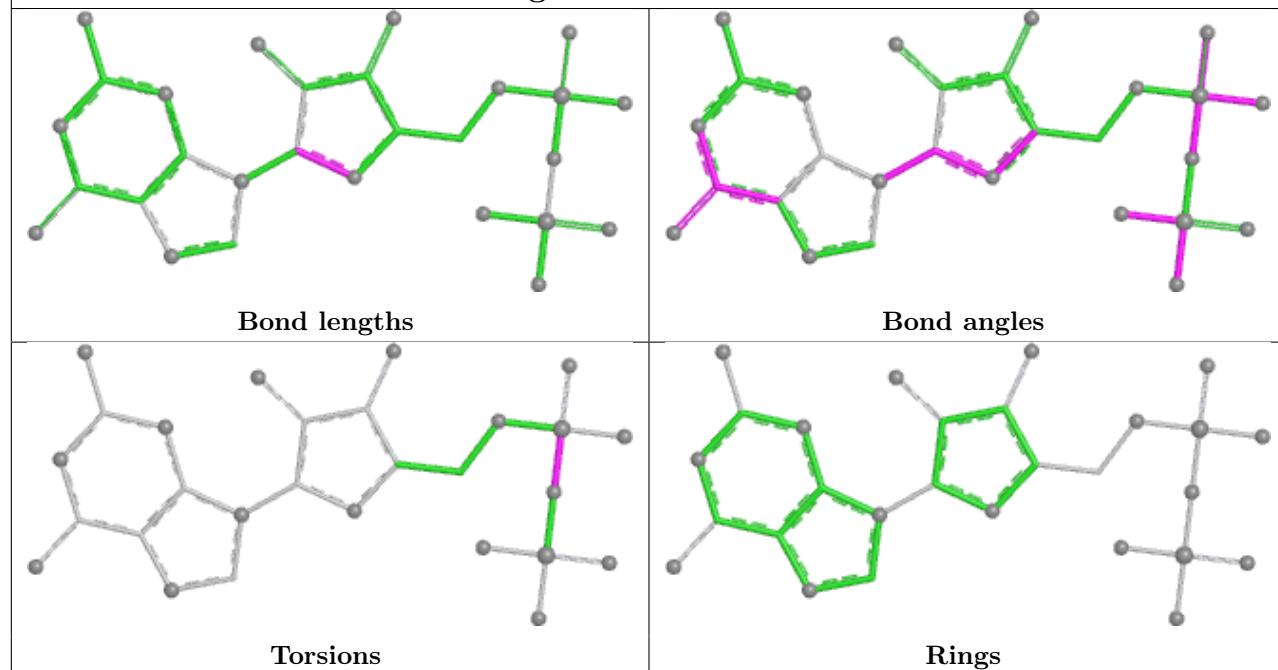
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	GDP	2	0
6	B	407	TMA	3	0
4	B	404	EDO	1	0
4	B	403	EDO	1	0
4	B	402	EDO	1	0

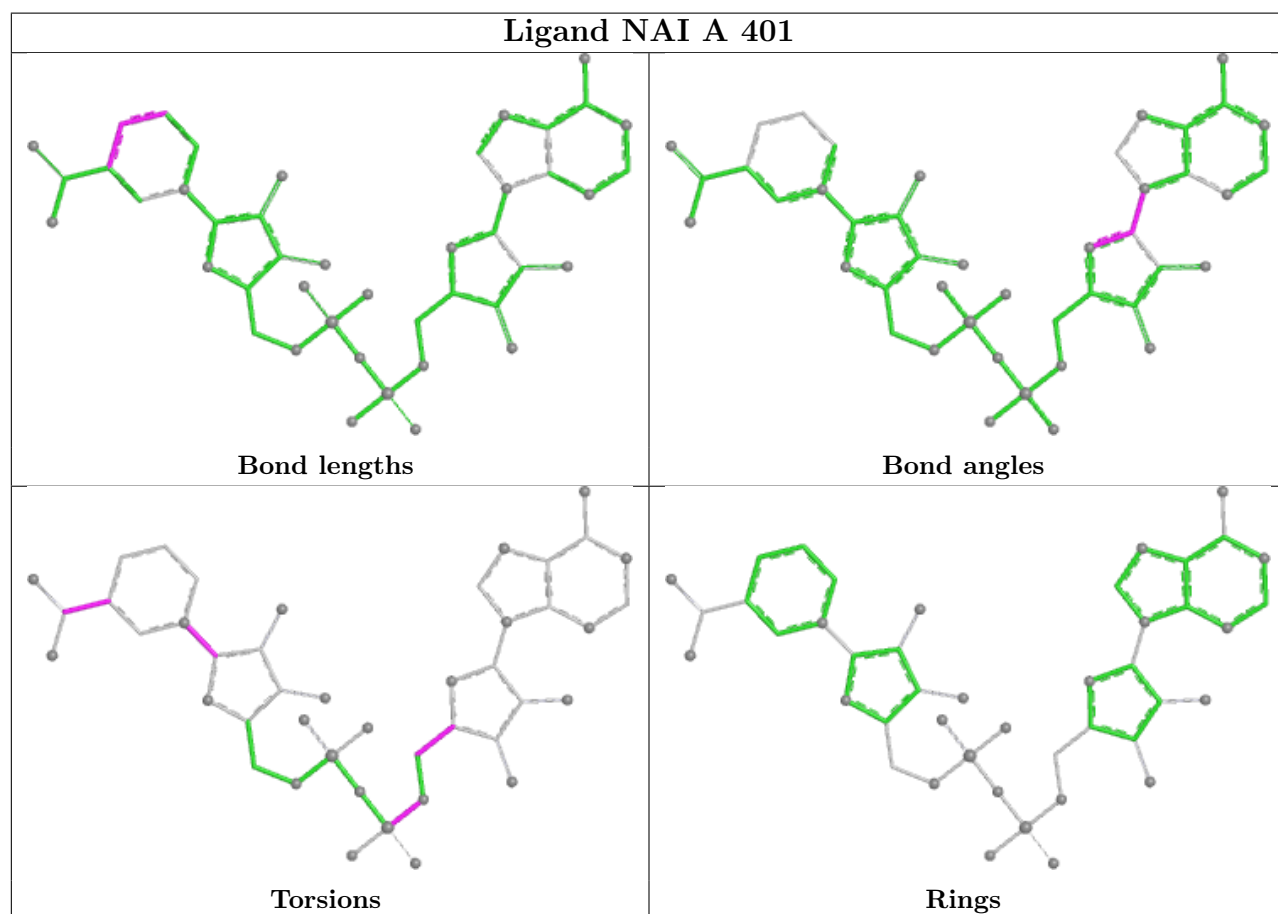
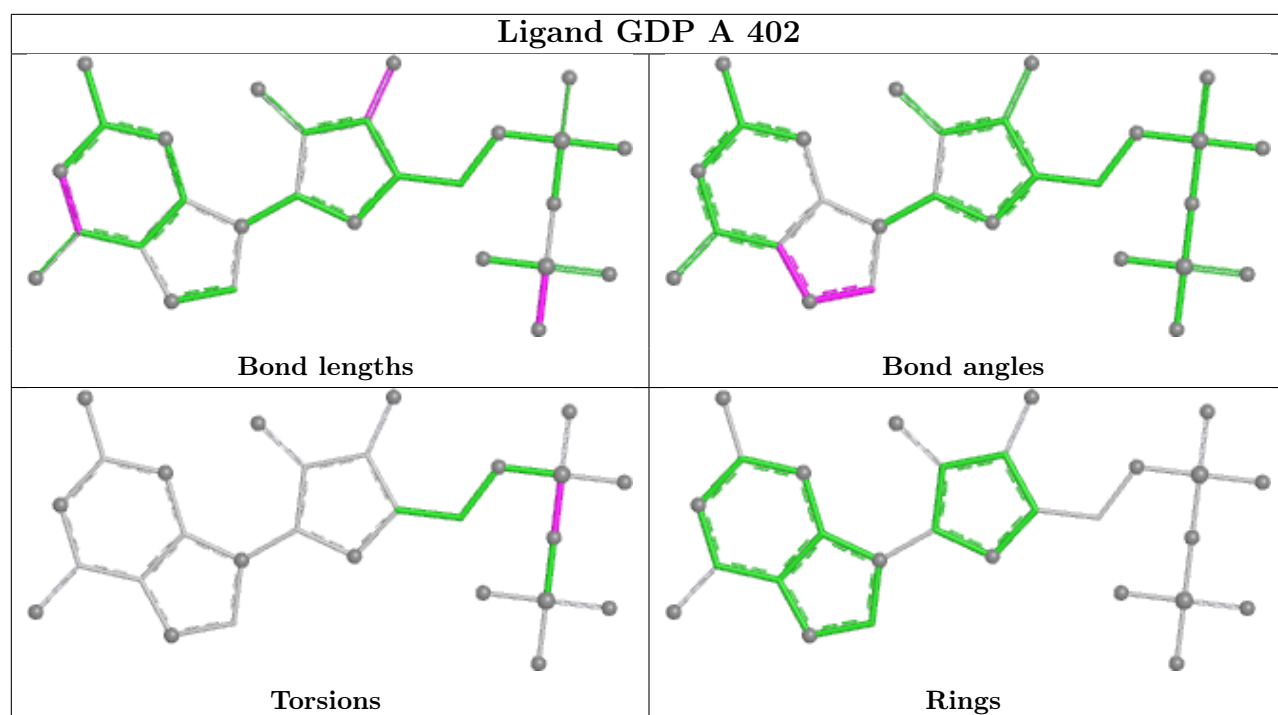
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C 401

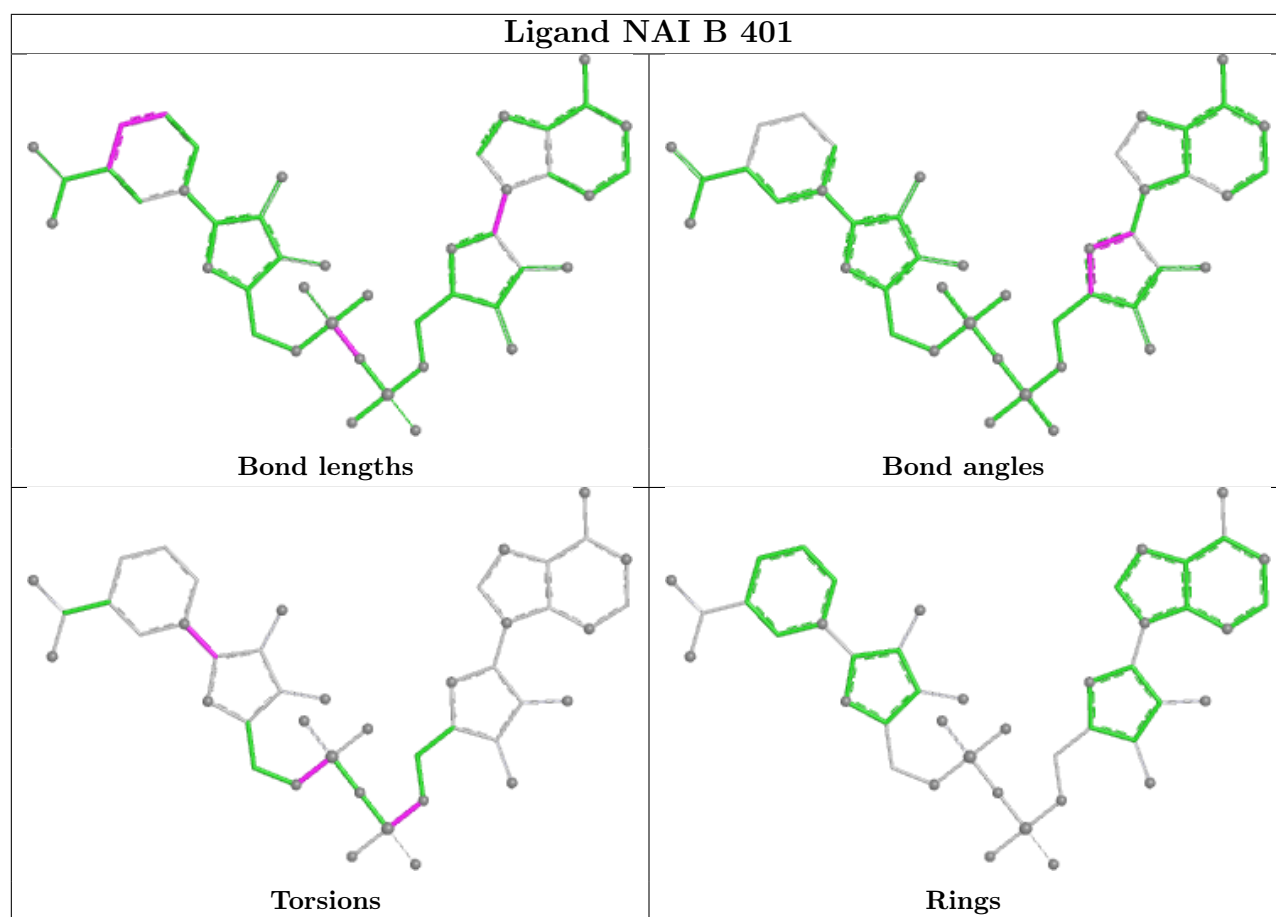


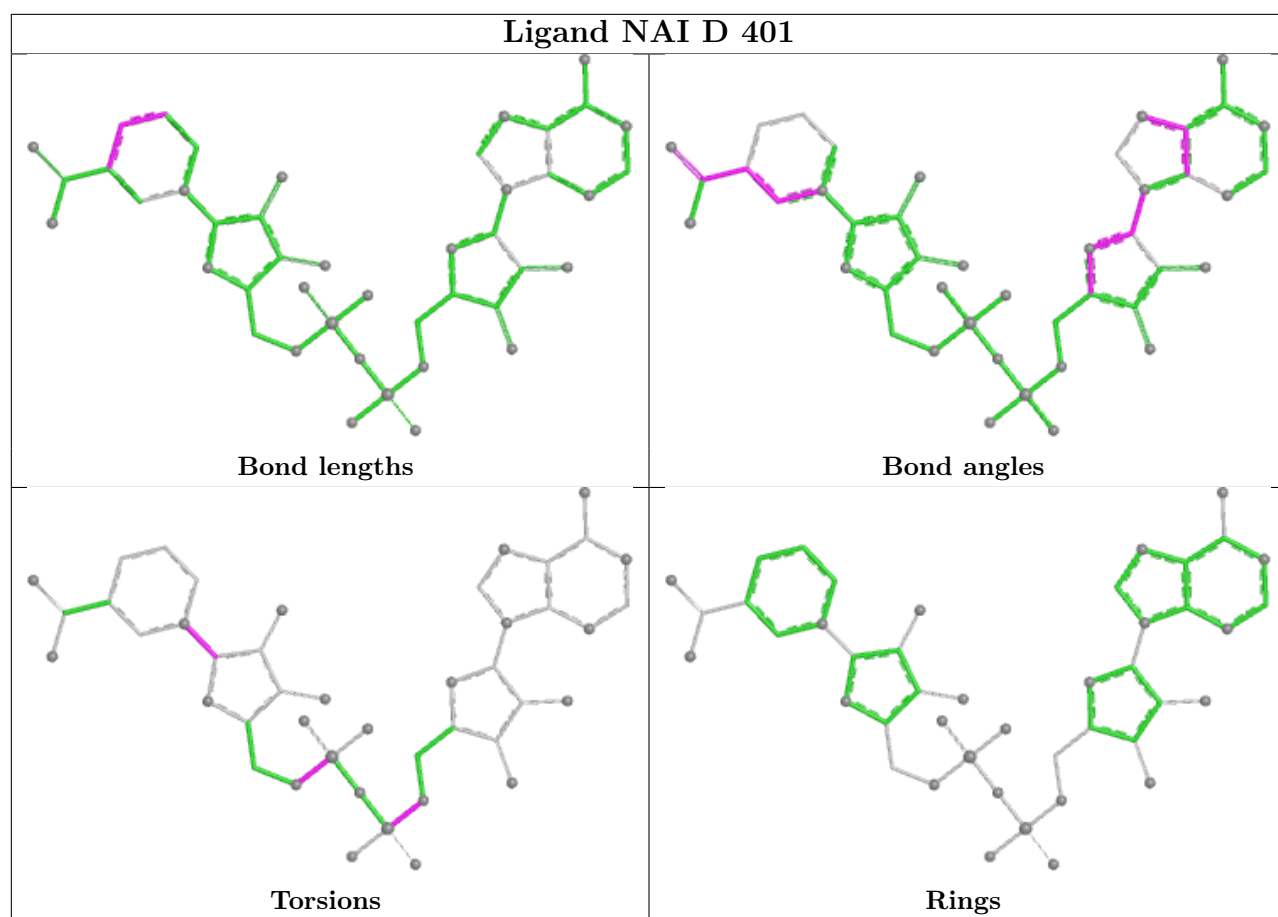
## Ligand GDP D 402











## 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	307/321 (95%)	-0.12	5 (1%) 72 77	11, 20, 32, 60	0
1	B	310/321 (96%)	-0.26	5 (1%) 72 77	11, 17, 29, 46	0
1	C	297/321 (92%)	0.11	15 (5%) 28 30	10, 18, 42, 65	0
1	D	311/321 (96%)	-0.10	8 (2%) 56 61	10, 17, 32, 52	0
All	All	1225/1284 (95%)	-0.09	33 (2%) 54 59	10, 18, 34, 65	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	263	ILE	7.7
1	C	141	ILE	7.7
1	C	202	PHE	7.4
1	C	262	ASN	6.5
1	C	201	HIS	6.2
1	B	141	ILE	5.9
1	C	310	ALA	5.1
1	C	138	LEU	5.0
1	C	272	TYR	4.0
1	D	89	ASN	3.6
1	B	125	ILE	3.6
1	B	270	ARG	3.5
1	D	312	PHE	3.5
1	D	88	ARG	3.3
1	C	238	ALA	3.2
1	A	88	ARG	3.1
1	A	130	ALA	3.0
1	D	2	SER	3.0
1	C	88[A]	ARG	2.8
1	C	137	PRO	2.7
1	A	125	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	199	GLU	2.6
1	C	198	PHE	2.6
1	A	2	SER	2.5
1	D	115	ILE	2.5
1	B	139	ARG	2.4
1	D	75	ILE	2.3
1	C	261	ALA	2.2
1	A	262	ASN	2.1
1	B	308[A]	ARG	2.1
1	D	164	PHE	2.1
1	C	139	ARG	2.0
1	D	85	LEU	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.

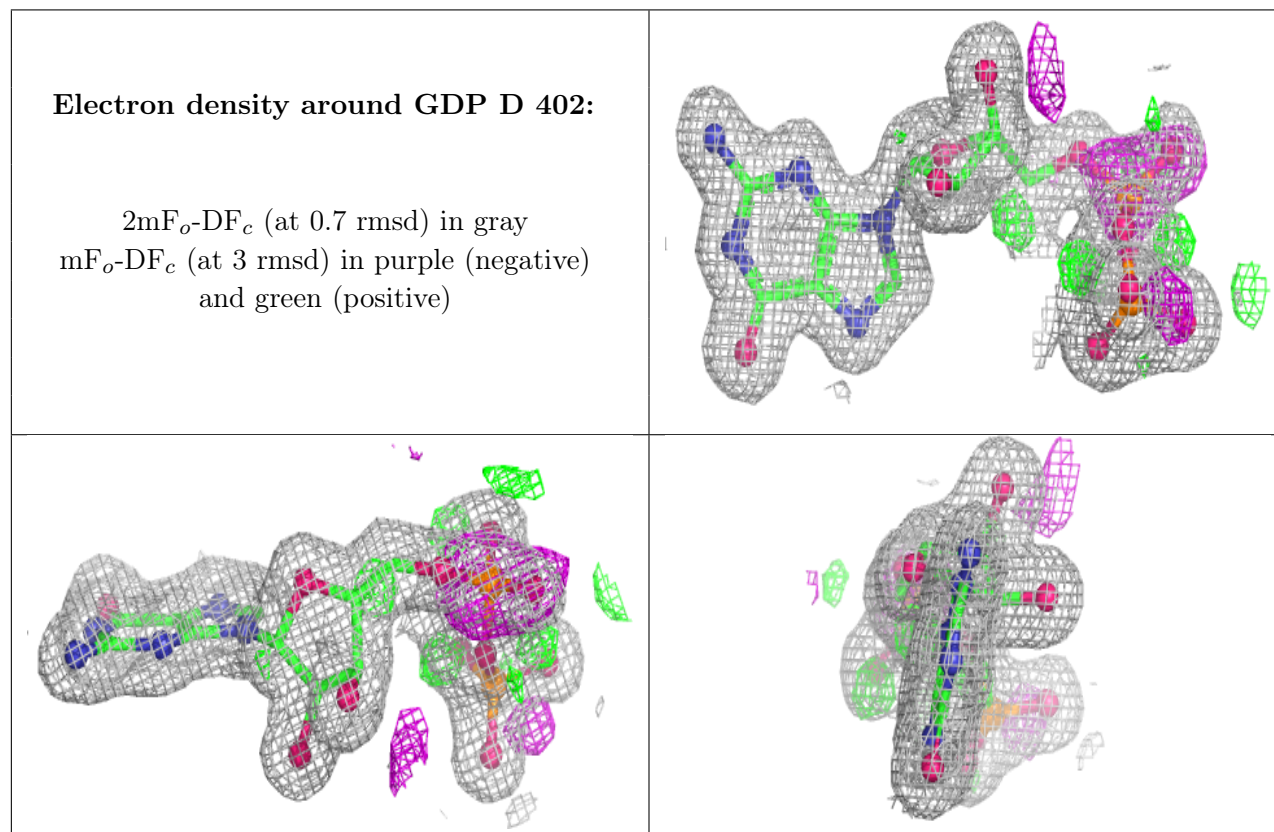
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	405	4/4	0.74	0.18	35,36,37,37	0
4	EDO	D	405	4/4	0.81	0.17	28,31,34,37	0
4	EDO	A	406	4/4	0.84	0.26	44,52,52,54	0
6	TMA	A	408	5/5	0.84	0.17	51,54,56,56	0
6	TMA	B	406	5/5	0.86	0.18	63,67,68,69	0
6	TMA	B	407	5/5	0.87	0.25	38,43,49,49	0
6	TMA	D	406	5/5	0.87	0.16	30,35,35,36	0
4	EDO	C	404	4/4	0.90	0.23	28,28,30,33	0
4	EDO	B	402	4/4	0.90	0.11	35,37,37,40	0
6	TMA	C	405	5/5	0.91	0.16	43,47,48,49	0
4	EDO	B	404	4/4	0.91	0.23	28,28,28,30	0

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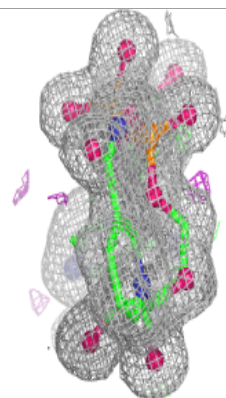
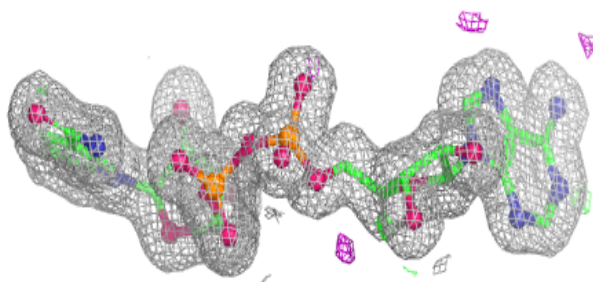
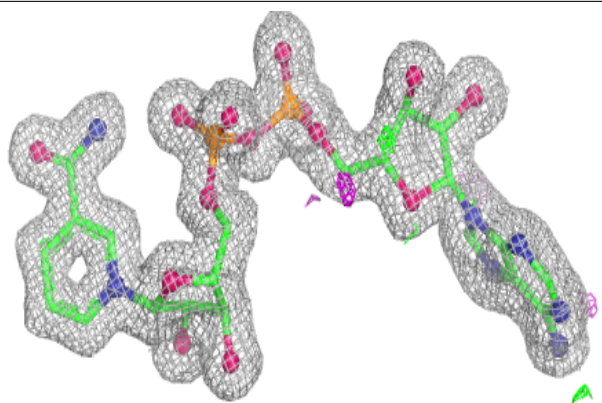
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	403	4/4	0.93	0.12	25,29,33,34	0
4	EDO	A	405	4/4	0.93	0.28	32,33,34,37	0
4	EDO	C	402	4/4	0.94	0.14	24,25,27,29	0
4	EDO	B	403	4/4	0.95	0.11	22,26,30,34	0
4	EDO	A	404	4/4	0.95	0.17	33,38,42,44	0
3	GDP	D	402	28/28	0.96	0.07	13,16,20,21	0
4	EDO	D	404	4/4	0.96	0.09	16,16,16,17	0
4	EDO	A	403	4/4	0.97	0.06	20,21,21,21	0
2	NAI	D	401	44/44	0.98	0.08	10,12,15,18	0
3	GDP	A	402	28/28	0.98	0.06	14,16,19,20	0
2	NAI	A	401	44/44	0.98	0.08	12,13,16,18	0
5	CL	A	407	1/1	0.99	0.03	21,21,21,21	0
2	NAI	B	401	44/44	0.99	0.06	10,12,13,14	0
2	NAI	C	401	44/44	0.99	0.07	11,12,13,14	0
7	NA	D	403	1/1	0.99	0.07	17,17,17,17	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.

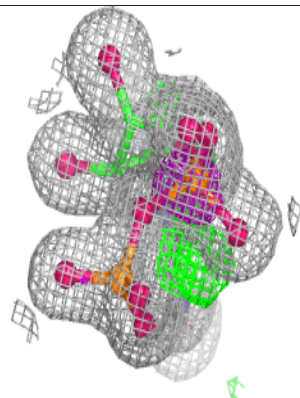
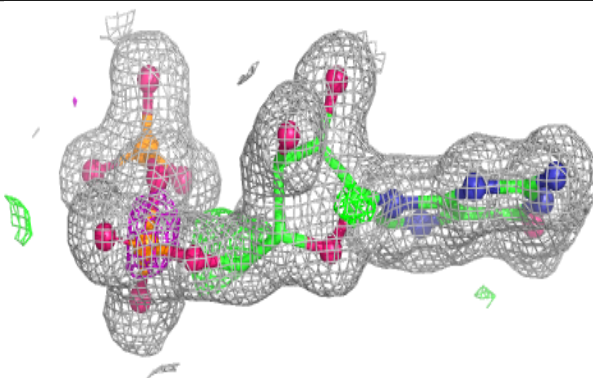
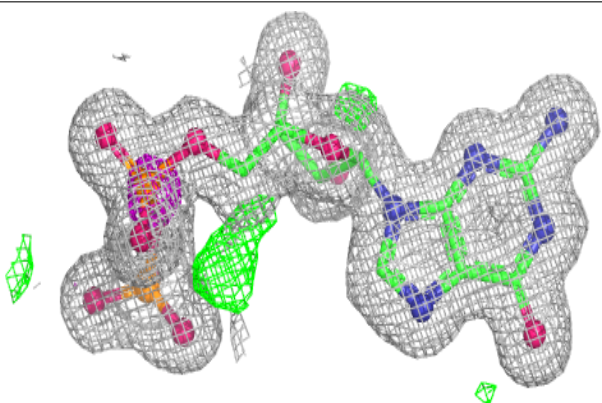


**Electron density around NAI D 401:**

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

**Electron density around GDP A 402:**

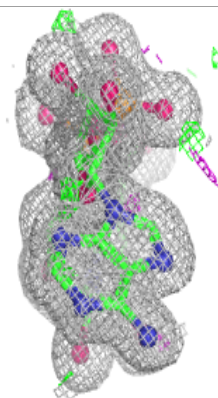
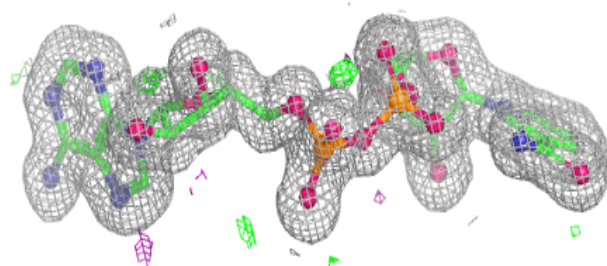
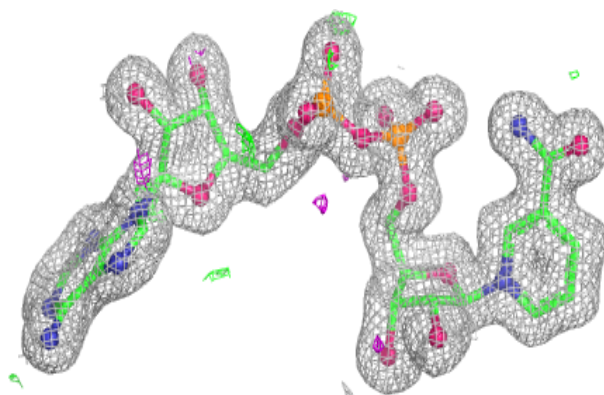
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



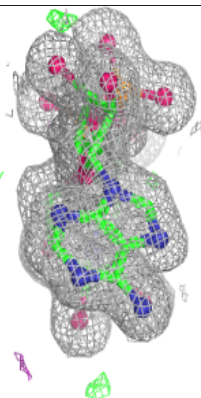
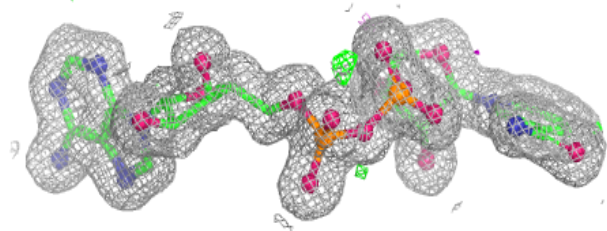
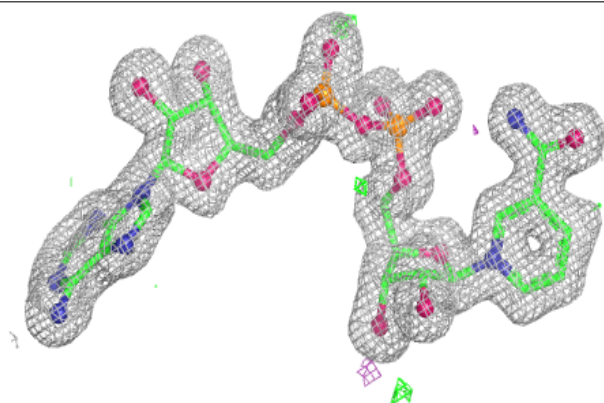


**Electron density around NAI A 401:**

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

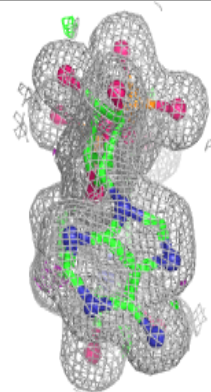
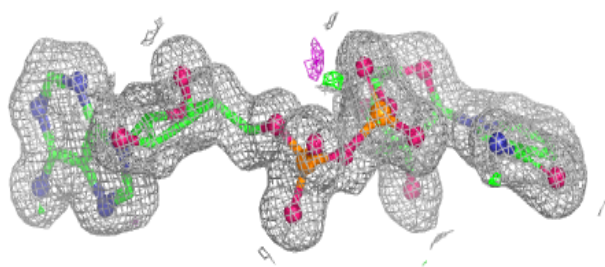
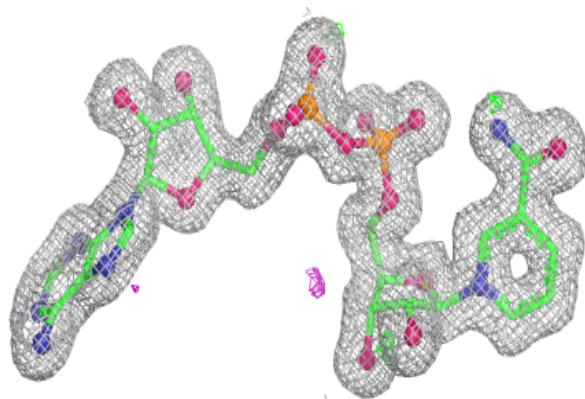
**Electron density around NAI B 401:**

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



**Electron density around NAI C 401:**

$2mF_o-DF_c$  (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.