



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 01:28 PM EDT

PDB ID : 2IH4  
Title : Crystal structure of the adenine-specific DNA methyltransferase M.TaqI complexed with the cofactor analog AETA and a 10 bp DNA containing pyrrolo-dC at the target base partner position  
Authors : Lenz, T.; Scheidig, A.J.; Weinhold, E.  
Deposited on : 2006-09-25  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

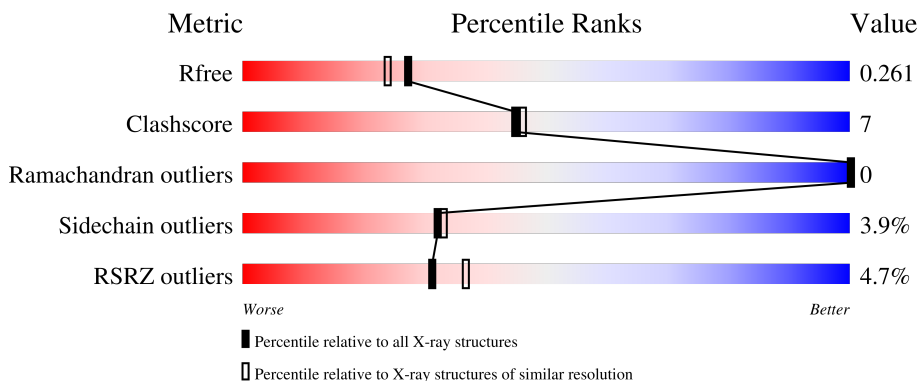
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



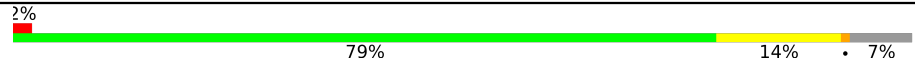

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	10	
1	E	10	
2	C	10	
2	F	10	

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Mol	Chain	Length	Quality of chain
3	A	421	 2% 79% 14% • 7%
3	D	421	 6% 79% 14% • 7%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7741 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 DNA chain called 5'-D(\*GP\*TP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	10	202	98	34	61	9	0	0	0
1	E	10	202	98	34	61	9	0	0	0

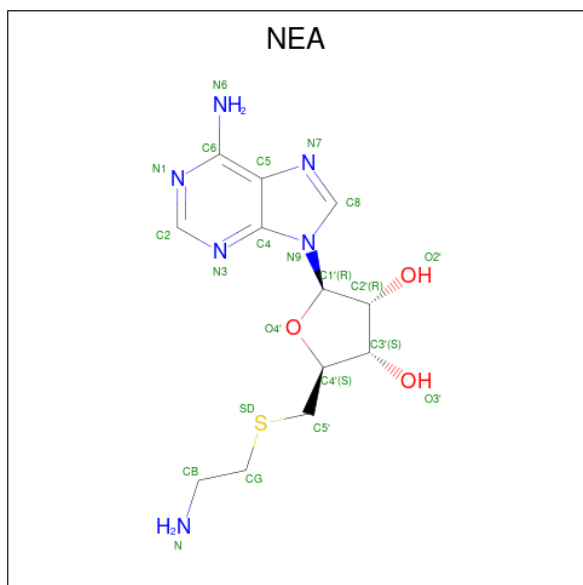
- Molecule 2 is a DNA chain called 5'-D(\*GP\*AP\*CP\*AP\*(4PC)P\*CP\*GP\*(6MA)P\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	10	205	100	42	54	9	0	0	0
2	F	10	205	100	42	54	9	0	0	0

- Molecule 3 is a protein called Modification methylase TaqI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	393	3189	2087	548	548	6	0	0	0
3	D	393	3189	2087	548	548	6	0	0	0

- Molecule 4 is 5'-DEOXY-5'-[2-(AMINO)ETHYLTHIO]ADENOSINE (three-letter code: NEA) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
4	A	1	Total	22	12	6	3	1	0	0
4	D	1	Total	22	12	6	3	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			
5	A	1	Total	6	3	3	0	0
5	D	1	Total	6	3	3	0	0

- Molecule 6 is water.

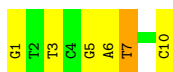
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	36	Total O 36 36	0	0
6	C	24	Total O 24 24	0	0
6	E	21	Total O 21 21	0	0
6	F	12	Total O 12 12	0	0
6	A	222	Total O 222 222	0	0
6	D	178	Total O 178 178	0	0

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


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5'-D(\*GP\*TP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*C)-3'

Chain B: 



- Molecule 1: 5'-D(\*GP\*TP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*C)-3'

Chain E: 



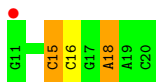
- Molecule 2: 5'-D(\*GP\*AP\*CP\*AP\*(4PC)P\*CP\*GP\*(6MA)P\*AP\*C)-3'

Chain C: 




- Molecule 2: 5'-D(\*GP\*AP\*CP\*AP\*(4PC)P\*CP\*GP\*(6MA)P\*AP\*C)-3'

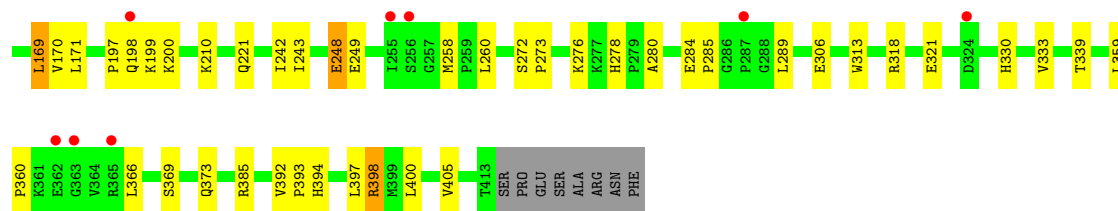
Chain F: 



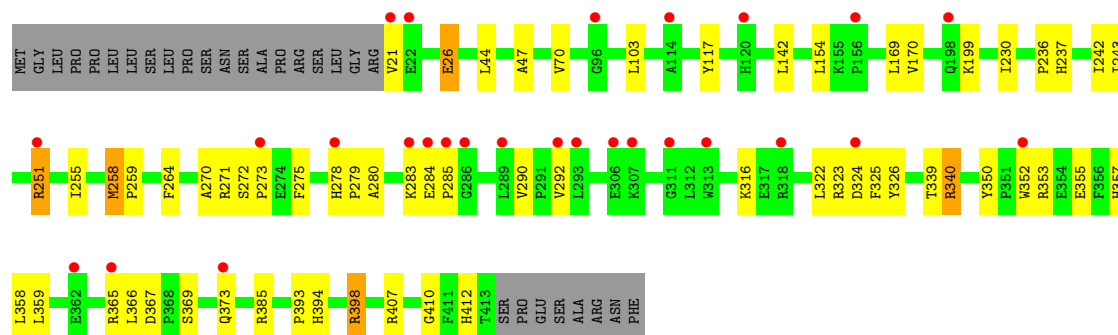
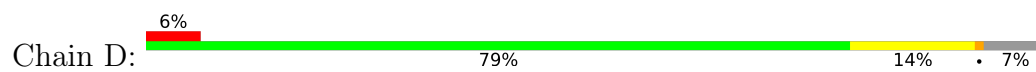
- Molecule 3: Modification methylase TaqI

Chain A: 





• Molecule 3: Modification methylase TaqI





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.20Å 66.58Å 111.31Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.99-2.10) 93.5 (19.99-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.206 , 0.265 0.205 , 0.261	Depositor DCC
$R_{free}$ test set	2370 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.646	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.062 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7741	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: NEA, 6MA, GOL, 4PC

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	B	0.84	0/225	1.73	8/346 (2.3%)
1	E	0.71	0/225	1.46	3/346 (0.9%)
2	C	0.80	0/179	1.57	4/269 (1.5%)
2	F	0.61	0/179	1.21	0/269
3	A	0.41	0/3293	0.59	2/4475 (0.0%)
3	D	0.40	0/3293	0.57	0/4475
All	All	0.45	0/7394	0.76	17/10180 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	DC	O4'-C4'-C3'	-9.88	100.07	106.00
1	B	3	DT	O4'-C1'-N1	-8.65	101.94	108.00
2	C	11	DG	O4'-C1'-N9	8.39	113.87	108.00
2	C	20	DC	O4'-C1'-N1	7.62	113.34	108.00
1	B	7	DT	C6-C5-C7	-7.48	118.41	122.90
1	B	3	DT	C6-C5-C7	-7.30	118.52	122.90
2	C	11	DG	P-O3'-C3'	6.93	128.01	119.70
1	E	10	DC	O4'-C4'-C3'	-6.63	101.85	104.50
1	B	1	DG	P-O3'-C3'	6.43	127.42	119.70
1	E	6	DA	O4'-C1'-N9	-6.29	103.60	108.00
1	E	1	DG	P-O3'-C3'	6.14	127.07	119.70
3	A	103	LEU	CA-CB-CG	5.90	128.86	115.30
1	B	10	DC	O4'-C1'-N1	5.53	111.87	108.00
3	A	169	LEU	CA-CB-CG	5.16	127.16	115.30
2	C	11	DG	O4'-C1'-C2'	-5.14	101.79	105.90
1	B	1	DG	O4'-C1'-N9	-5.07	104.45	108.00
1	B	3	DT	N1-C1'-C2'	5.00	122.10	112.60

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	B	202	0	116	6	0
1	E	202	0	116	3	0
2	C	205	0	116	3	0
2	F	205	0	116	5	0
3	A	3189	0	3184	44	0
3	D	3189	0	3184	43	0
4	A	22	0	18	1	0
4	D	22	0	18	2	0
5	A	6	0	8	0	0
5	D	6	0	8	0	0
6	A	222	0	0	2	0
6	B	36	0	0	0	0
6	C	24	0	0	0	0
6	D	178	0	0	2	0
6	E	21	0	0	0	0
6	F	12	0	0	0	0
All	All	7741	0	6884	92	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 7.

All (92) 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:A:66:ARG:HG2	3:A:66:ARG:HH11	1.18	1.08
3:D:251:ARG:HH11	3:D:251:ARG:HG3	1.25	1.01
3:D:340:ARG:HG2	3:D:340:ARG:HH11	1.36	0.88
3:A:360:PRO:HB3	3:A:366:LEU:HD21	1.57	0.86
1:B:5:DG:N7	3:A:394:HIS:HE1	1.76	0.82
3:A:369:SER:O	3:A:373:GLN:HG2	1.80	0.81
3:A:66:ARG:HH11	3:A:66:ARG:CG	1.98	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:DG:N7	3:D:394:HIS:HE1	1.90	0.69
3:A:260:LEU:HD13	3:A:405:VAL:HG21	1.76	0.67
3:D:251:ARG:HG3	3:D:251:ARG:NH1	2.04	0.65
3:D:365:ARG:HB2	3:D:412:HIS:CE1	2.32	0.64
3:A:278:HIS:HD2	3:A:280:ALA:H	1.46	0.64
3:D:272:SER:OG	3:D:273:PRO:HD3	1.99	0.63
3:A:169:LEU:HB3	3:A:243:ILE:HB	1.81	0.62
3:A:42:ARG:HG2	3:A:42:ARG:HH11	1.66	0.60
3:A:66:ARG:HG2	3:A:66:ARG:NH1	1.98	0.60
3:D:169:LEU:HB3	3:D:243:ILE:HB	1.85	0.59
2:F:15:4PC:H2"	2:F:16:DC:C2	2.40	0.57
3:D:407:ARG:HG2	6:D:2167:HOH:O	2.05	0.56
3:A:74:PRO:HA	3:A:87:LEU:HD21	1.86	0.56
3:A:102:ILE:HD12	3:A:154:LEU:HD13	1.88	0.56
3:D:251:ARG:HH11	3:D:251:ARG:CG	2.08	0.56
3:A:318:ARG:HD2	3:A:321:GLU:OE2	2.07	0.55
3:A:285:PRO:HG3	3:A:313:TRP:CZ2	2.42	0.54
3:A:69:GLY:HA3	3:A:79:LEU:HD11	1.89	0.53
1:E:2:DT:H72	3:D:271:ARG:HG2	1.90	0.53
2:C:15:4PC:H162	3:A:393:PRO:HG2	1.90	0.53
3:A:330:HIS:HE1	6:A:2161:HOH:O	1.92	0.53
3:D:325:PHE:HB2	3:D:359:LEU:HD11	1.91	0.53
3:A:111:VAL:HA	3:A:119:ILE:HB	1.91	0.52
3:D:340:ARG:HH11	3:D:340:ARG:CG	2.14	0.52
3:A:276:LYS:NZ	6:A:2163:HOH:O	2.41	0.52
3:A:272:SER:OG	3:A:273:PRO:HD3	2.09	0.52
3:A:278:HIS:CD2	3:A:280:ALA:H	2.27	0.52
3:A:93:TRP:CZ2	3:A:95:PRO:HB3	2.45	0.51
1:B:7:DT:H73	3:A:200:LYS:O	2.10	0.51
3:D:270:ALA:HB3	3:D:275:PHE:CE2	2.46	0.50
3:D:290:VAL:HG21	3:D:316:LYS:HB2	1.93	0.50
3:D:44:LEU:HD11	3:D:70:VAL:HG23	1.94	0.50
3:D:275:PHE:CE1	3:D:322:LEU:HD13	2.47	0.50
3:D:272:SER:HB3	3:D:353:ARG:HD2	1.94	0.50
3:D:284:GLU:HG3	3:D:285:PRO:HD2	1.94	0.49
3:A:80:PRO:HG2	3:A:82:TRP:CZ2	2.49	0.48
3:A:171:LEU:HD21	3:A:392:VAL:HG11	1.95	0.48
3:A:360:PRO:CB	3:A:366:LEU:HD21	2.38	0.48
3:D:340:ARG:HG2	3:D:340:ARG:NH1	2.15	0.48
2:F:15:4PC:H162	3:D:393:PRO:CG	2.44	0.47
3:A:170:VAL:HG12	3:A:242:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:258:MET:HG3	3:D:259:PRO:HD2	1.98	0.46
3:D:170:VAL:HA	3:D:242:ILE:HG23	1.96	0.46
1:B:6:DA:N3	3:A:199:LYS:HD3	2.31	0.46
3:D:283:LYS:HD3	6:D:2154:HOH:O	2.15	0.46
3:D:270:ALA:HB3	3:D:275:PHE:HE2	1.80	0.46
3:D:369:SER:O	3:D:373:GLN:HG2	2.16	0.45
2:C:17:DG:C8	2:C:18:6MA:H13	2.51	0.45
3:A:66:ARG:CG	3:A:66:ARG:NH1	2.67	0.45
2:F:18:6MA:N3	3:D:117:TYR:OH	2.49	0.45
2:F:15:4PC:H162	3:D:393:PRO:HG2	2.00	0.44
1:B:6:DA:H1'	3:A:199:LYS:HD3	1.98	0.44
3:A:154:LEU:HB3	3:A:210:LYS:HD2	1.99	0.44
1:E:9:DT:C4	1:E:10:DC:N4	2.86	0.44
3:A:197:PRO:C	3:A:198:GLN:HG2	2.38	0.44
3:A:397:LEU:HD23	3:A:398:ARG:NH1	2.33	0.43
3:D:278:HIS:CD2	3:D:280:ALA:H	2.35	0.43
3:D:264:PHE:CD1	3:D:358:LEU:HB3	2.54	0.43
2:C:15:4PC:H2''	2:C:16:DC:C2	2.53	0.43
3:A:47:ALA:HB1	4:A:1001:NEA:O4'	2.19	0.43
2:F:15:4PC:C16	3:D:393:PRO:HG3	2.49	0.43
3:A:170:VAL:HG12	3:A:242:ILE:CG2	2.49	0.43
1:B:6:DA:H3'	1:B:7:DT:C5'	2.49	0.42
3:A:248:GLU:HG3	3:A:249:GLU:N	2.34	0.42
3:D:47:ALA:HB1	4:D:1002:NEA:O4'	2.20	0.42
3:A:150:ALA:HB1	3:A:160:LEU:HD13	2.02	0.42
3:A:278:HIS:HE1	3:A:321:GLU:OE1	2.03	0.42
3:A:42:ARG:HG2	3:A:42:ARG:NH1	2.32	0.42
1:B:5:DG:N7	3:A:394:HIS:CE1	2.69	0.42
3:D:398:ARG:N	3:D:398:ARG:HD2	2.33	0.42
3:A:260:LEU:HD13	3:A:405:VAL:CG2	2.48	0.41
3:D:367:ASP:HB3	3:D:410:GLY:HA2	2.03	0.41
3:D:251:ARG:O	3:D:255:ILE:HG23	2.20	0.41
3:D:323:ARG:HB2	3:D:326:TYR:CE2	2.55	0.41
3:D:26:GLU:CD	3:D:26:GLU:H	2.24	0.41
3:D:236:PRO:HG2	3:D:237:HIS:CD2	2.55	0.41
3:A:273:PRO:HA	3:A:276:LYS:HD2	2.03	0.41
3:A:289:LEU:HB3	3:A:313:TRP:HB3	2.01	0.41
3:A:333:VAL:HG11	3:A:400:LEU:HD13	2.03	0.41
3:D:278:HIS:HA	3:D:279:PRO:HD3	1.84	0.41
3:D:352:TRP:CG	3:D:357:HIS:HE1	2.39	0.41
3:D:292:VAL:HG12	3:D:353:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:21:VAL:HG13	4:D:1002:NEA:HG1	2.02	0.40
3:D:290:VAL:HG13	3:D:350:TYR:CE2	2.56	0.40
3:D:355:GLU:OE1	3:D:355:GLU:HA	2.22	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	
3	A	391/421 (93%)	375 (96%)	16 (4%)	0	100	100
3	D	391/421 (93%)	375 (96%)	16 (4%)	0	100	100
All	All	782/842 (93%)	750 (96%)	32 (4%)	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	
3	A	332/356 (93%)	320 (96%)	12 (4%)	35	36
3	D	332/356 (93%)	318 (96%)	14 (4%)	30	30
All	All	664/712 (93%)	638 (96%)	26 (4%)	32	33

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	66	ARG
3	A	103	LEU
3	A	143	TYR
3	A	221	GLN
3	A	248	GLU
3	A	258	MET
3	A	284	GLU
3	A	306	GLU
3	A	339	THR
3	A	359	LEU
3	A	385	ARG
3	A	398	ARG
3	D	26	GLU
3	D	103	LEU
3	D	142	LEU
3	D	154	LEU
3	D	199	LYS
3	D	230	ILE
3	D	251	ARG
3	D	258	MET
3	D	324	ASP
3	D	339	THR
3	D	340	ARG
3	D	366	LEU
3	D	385	ARG
3	D	398	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	221	GLN
3	A	278	HIS
3	A	394	HIS
3	A	412	HIS
3	D	221	GLN
3	D	237	HIS
3	D	278	HIS
3	D	394	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
2	6MA	C	18	1,2	18,24,25	0.79	1 (5%)	15,34,37	0.99	1 (6%)
2	6MA	F	18	1,2	18,24,25	0.74	0	15,34,37	1.01	1 (6%)
2	4PC	C	15	2	21,24,25	1.02	2 (9%)	27,35,38	1.51	4 (14%)
2	4PC	F	15	2	21,24,25	1.04	2 (9%)	27,35,38	1.45	4 (14%)

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	6MA	C	18	1,2	-	1/5/23/24	0/3/3/3
2	6MA	F	18	1,2	-	1/5/23/24	0/3/3/3
2	4PC	C	15	2	-	1/7/21/22	0/3/3/3
2	4PC	F	15	2	-	3/7/21/22	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	15	4PC	C14-C5	-3.05	1.34	1.42
2	C	15	4PC	C14-C5	-2.76	1.35	1.42
2	C	18	6MA	C8-N7	-2.17	1.30	1.34
2	C	15	4PC	C4-N17	-2.14	1.33	1.37
2	F	15	4PC	C4-N17	-2.12	1.33	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	15	4PC	C14-C15-N17	4.37	109.98	107.32
2	F	15	4PC	C14-C15-N17	4.01	109.76	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	4PC	C16-C15-C14	-3.53	126.32	131.97
2	F	18	6MA	C2-N1-C6	3.52	119.61	116.59
2	C	15	4PC	C16-C15-C14	-3.44	126.46	131.97
2	C	18	6MA	C2-N1-C6	3.18	119.32	116.59
2	C	15	4PC	O4'-C1'-N1	2.85	112.96	107.86
2	F	15	4PC	O2-C2-N3	-2.68	117.97	122.33
2	F	15	4PC	O4'-C1'-N1	2.39	112.13	107.86
2	C	15	4PC	C2'-C1'-N1	2.28	119.03	113.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	15	4PC	C2'-C1'-N1-C2
2	F	15	4PC	C2'-C1'-N1-C6
2	F	15	4PC	C4'-C5'-O5'-P
2	F	18	6MA	O4'-C4'-C5'-O5'
2	C	15	4PC	C4'-C5'-O5'-P
2	C	18	6MA	N1-C6-N6-C1

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	18	6MA	1	0
2	F	18	6MA	1	0
2	C	15	4PC	2	0
2	F	15	4PC	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
5	GOL	A	2002	-	5,5,5	0.44	0	5,5,5	0.17	0
4	NEA	A	1001	-	21,24,24	1.23	2 (9%)	21,34,34	1.69	2 (9%)
5	GOL	D	2001	-	5,5,5	0.39	0	5,5,5	0.16	0
4	NEA	D	1002	-	21,24,24	1.17	2 (9%)	21,34,34	1.65	2 (9%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	2002	-	-	0/4/4/4	-
4	NEA	A	1001	-	-	1/5/25/25	0/3/3/3
5	GOL	D	2001	-	-	1/4/4/4	-
4	NEA	D	1002	-	-	0/5/25/25	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NEA	C2-N3	4.10	1.38	1.32
4	D	1002	NEA	C2-N3	4.06	1.38	1.32
4	A	1001	NEA	C2-N1	2.61	1.38	1.33
4	D	1002	NEA	C2-N1	2.54	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	NEA	N3-C2-N1	-5.84	119.56	128.68
4	A	1001	NEA	N3-C2-N1	-5.73	119.72	128.68
4	A	1001	NEA	C5'-SD-CG	-3.91	90.53	102.27
4	D	1002	NEA	C5'-SD-CG	-2.71	94.14	102.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

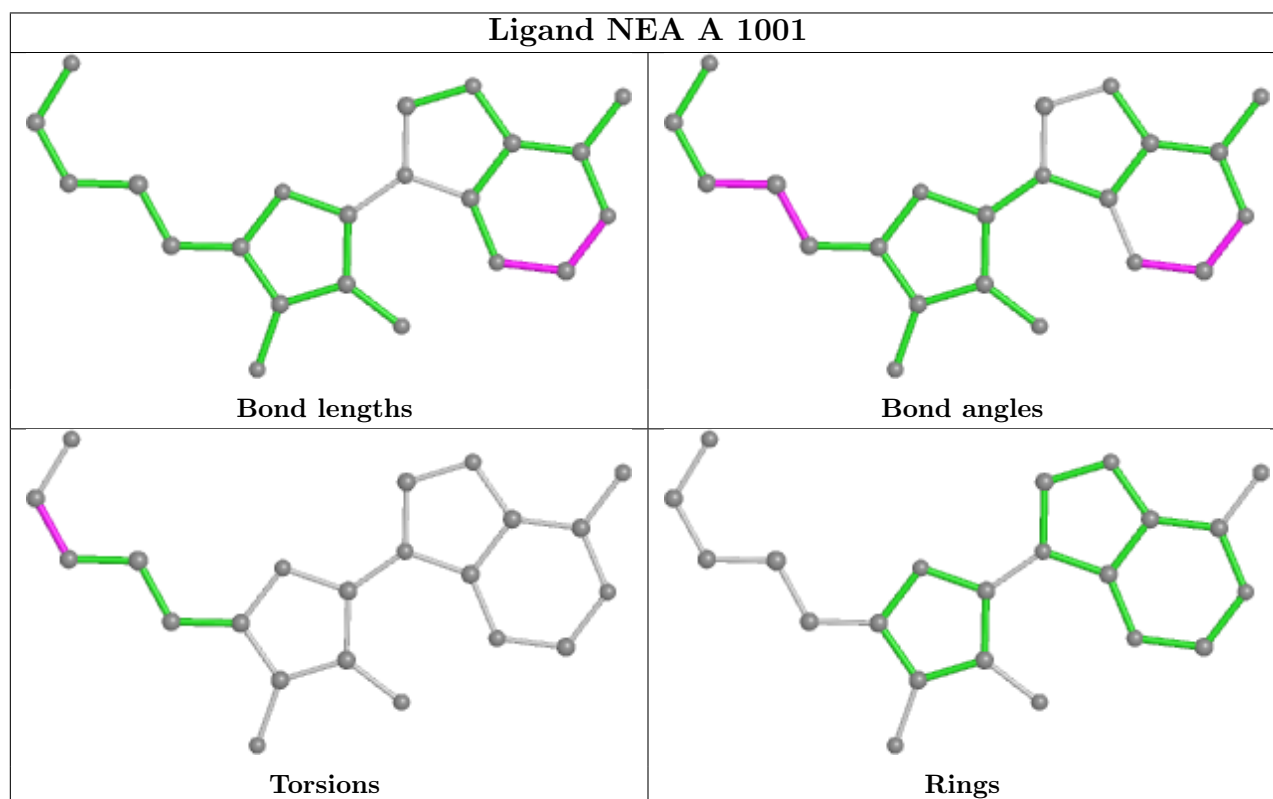
Mol	Chain	Res	Type	Atoms
4	A	1001	NEA	N-CB-CG-SD
5	D	2001	GOL	O1-C1-C2-C3

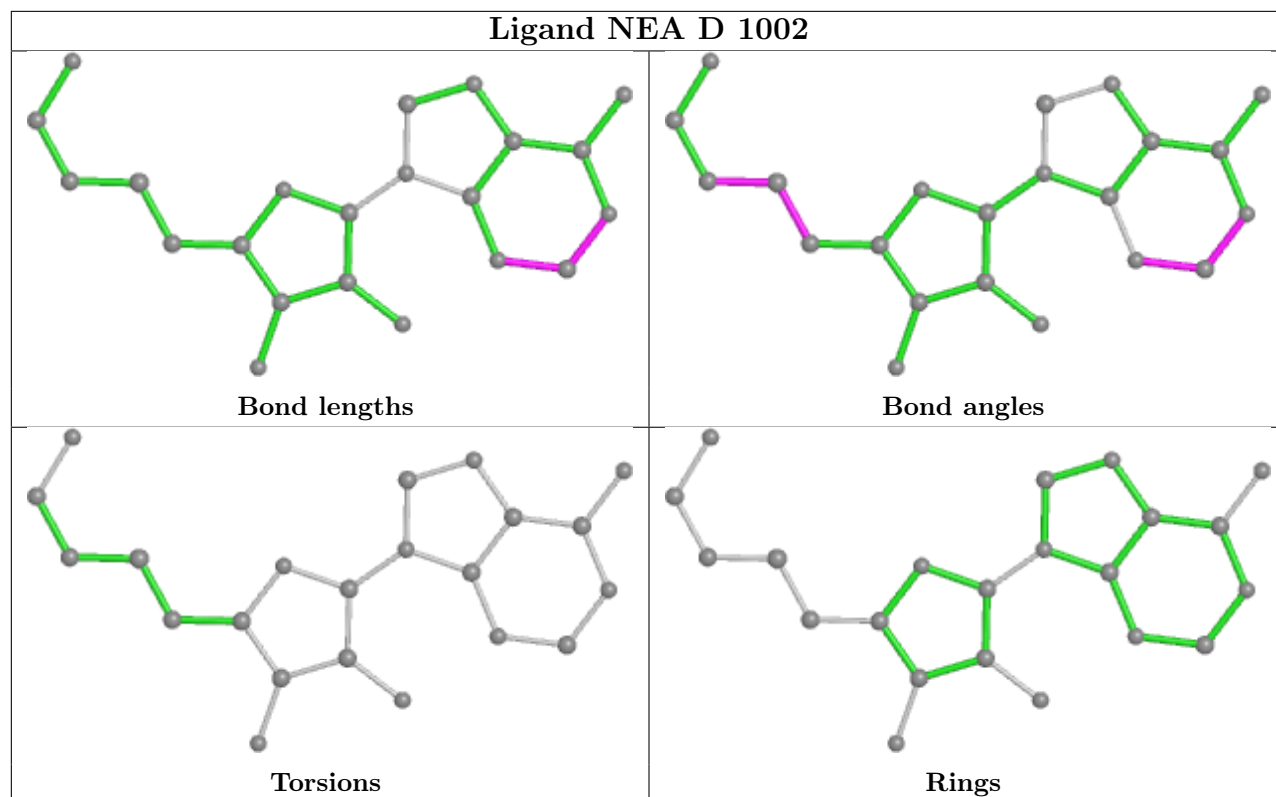
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	NEA	1	0
4	D	1002	NEA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	10/10 (100%)	-0.69	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	10, 16, 21, 28	0
1	E	10/10 (100%)	0.43	1 (10%) <span style="border: 1px solid red; padding: 2px;">7</span> <span style="border: 1px solid red; padding: 2px;">9</span>	20, 36, 62, 69	0
2	C	8/10 (80%)	-0.36	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	12, 15, 26, 27	0
2	F	8/10 (80%)	0.74	1 (12%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">5</span>	42, 44, 58, 64	0
3	A	393/421 (93%)	-0.01	10 (2%) <span style="border: 1px solid blue; padding: 2px;">57</span> <span style="border: 1px solid blue; padding: 2px;">62</span>	9, 19, 29, 34	0
3	D	393/421 (93%)	0.31	27 (6%) <span style="border: 1px solid red; padding: 2px;">16</span> <span style="border: 1px solid red; padding: 2px;">21</span>	13, 23, 41, 47	0
All	All	822/882 (93%)	0.15	39 (4%) <span style="border: 1px solid red; padding: 2px;">31</span> <span style="border: 1px solid red; padding: 2px;">37</span>	9, 21, 39, 69	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	286	GLY	4.0
3	D	293	LEU	3.7
3	A	96	GLY	3.7
3	D	21	VAL	3.5
3	D	289	LEU	3.4
3	A	122	PHE	3.3
3	D	156	PRO	2.9
3	D	313	TRP	2.9
3	A	287	PRO	2.9
3	D	198	GLN	2.7
3	D	284	GLU	2.7
2	F	11	DG	2.7
3	A	198	GLN	2.6
3	D	22	GLU	2.6
3	D	324	ASP	2.5
3	D	273	PRO	2.4
1	E	10	DC	2.4
3	D	365	ARG	2.4
3	D	96	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	311	GLY	2.4
3	D	292	VAL	2.3
3	D	362	GLU	2.3
3	A	324	ASP	2.3
3	D	283	LYS	2.3
3	D	278	HIS	2.2
3	D	251	ARG	2.2
3	D	318	ARG	2.2
3	D	352	TRP	2.2
3	A	255	ILE	2.2
3	D	307	LYS	2.2
3	A	363	GLY	2.2
3	D	285	PRO	2.2
3	A	365	ARG	2.2
3	A	256	SER	2.1
3	A	362	GLU	2.1
3	D	114	ALA	2.1
3	D	373	GLN	2.1
3	D	120	HIS	2.0
3	D	306	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	6MA	F	18	22/23	0.85	0.17	41,47,48,49	0
2	4PC	F	15	22/23	0.93	0.14	37,40,40,40	0
2	6MA	C	18	22/23	0.95	0.10	10,12,17,19	0
2	4PC	C	15	22/23	0.97	0.10	13,14,17,19	0

## 6.3 Carbohydrates [i](#)

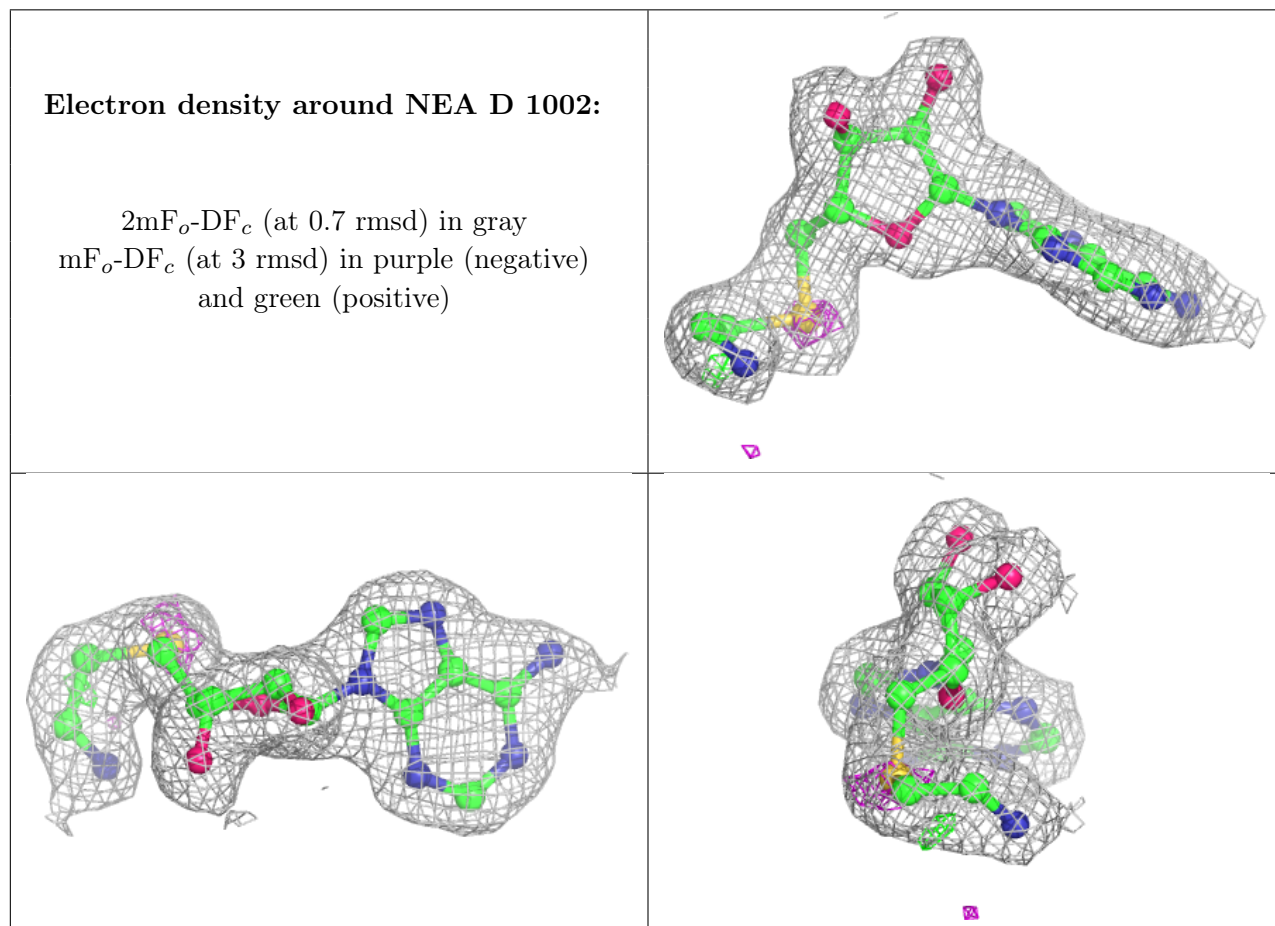
There are no monosaccharides in this entry.

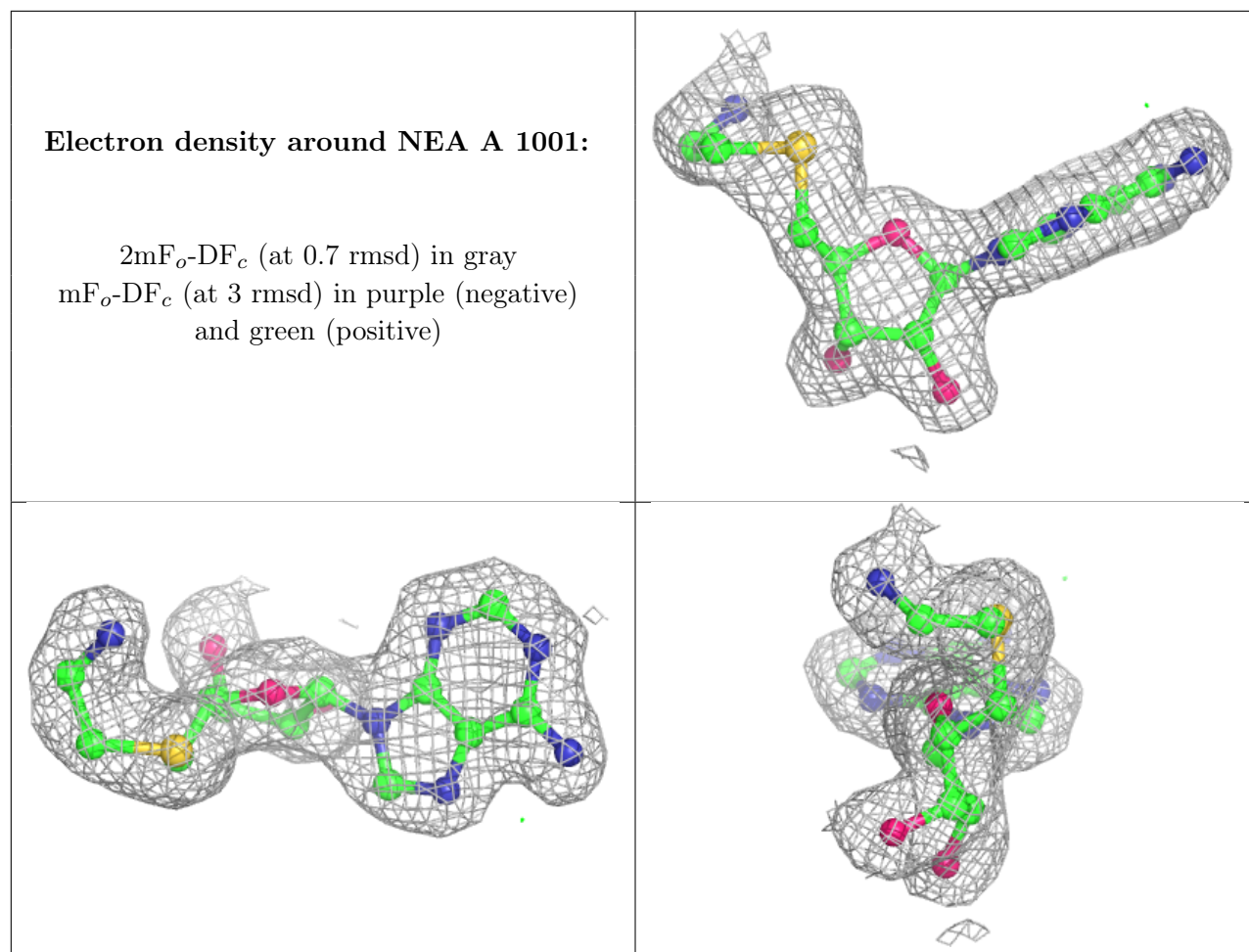
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NEA	D	1002	22/22	0.92	0.11	17,20,22,22	0
5	GOL	A	2002	6/6	0.92	0.14	20,22,23,24	0
5	GOL	D	2001	6/6	0.92	0.13	25,27,27,28	0
4	NEA	A	1001	22/22	0.95	0.09	13,15,17,18	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.