



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2022 – 06:44 pm BST

PDB ID : 7P9P  
Title : N-acetylglucosamine kinase from Plesiomonas shigelloides complexed with alpha-N-acetylglucosamine and AMP-PNP inhibitor  
Authors : Roy, S.; Isupov, M.N.; Harmer, N.J.; Ames, J.R.  
Deposited on : 2021-07-27  
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

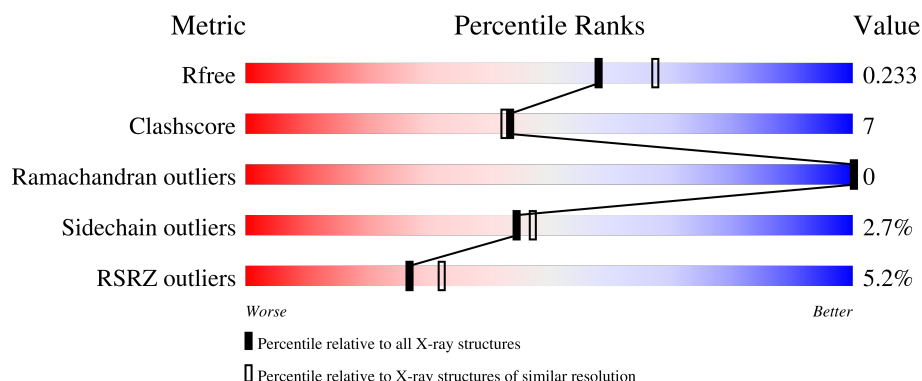
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

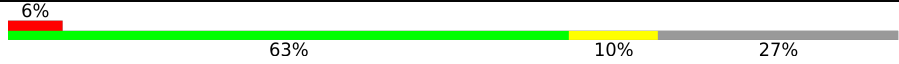
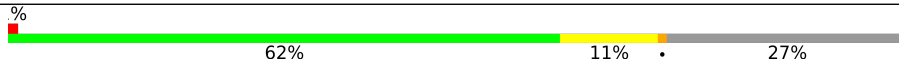
The reported resolution of this entry is 2.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	AAA	417	
1	BBB	417	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PGE	AAA	404	-	-	X	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5228 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 Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	304	Total	C	N	O	S	0	5	0
			2352	1498	411	433	10			
1	BBB	306	Total	C	N	O	S	0	8	0
			2389	1527	418	434	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-114	MET	-	initiating methionine	UNP Q12306
AAA	-113	ALA	-	expression tag	UNP Q12306
AAA	-112	HIS	-	expression tag	UNP Q12306
AAA	-111	HIS	-	expression tag	UNP Q12306
AAA	-110	HIS	-	expression tag	UNP Q12306
AAA	-109	HIS	-	expression tag	UNP Q12306
AAA	-108	HIS	-	expression tag	UNP Q12306
AAA	-107	HIS	-	expression tag	UNP Q12306
AAA	-106	GLY	-	expression tag	UNP Q12306
AAA	-10	SER	-	linker	UNP Q12306
AAA	-9	SER	-	linker	UNP Q12306
AAA	-8	GLY	-	linker	UNP Q12306
AAA	-7	LEU	-	linker	UNP Q12306
AAA	-6	GLU	-	linker	UNP Q12306
AAA	-5	VAL	-	linker	UNP Q12306
AAA	-4	LEU	-	linker	UNP Q12306
AAA	-3	PHE	-	linker	UNP Q12306
AAA	-2	GLN	-	linker	UNP Q12306
AAA	-1	GLY	-	linker	UNP Q12306
AAA	0	THR	-	linker	UNP Q12306
BBB	-114	MET	-	initiating methionine	UNP Q12306
BBB	-113	ALA	-	expression tag	UNP Q12306
BBB	-112	HIS	-	expression tag	UNP Q12306
BBB	-111	HIS	-	expression tag	UNP Q12306
BBB	-110	HIS	-	expression tag	UNP Q12306

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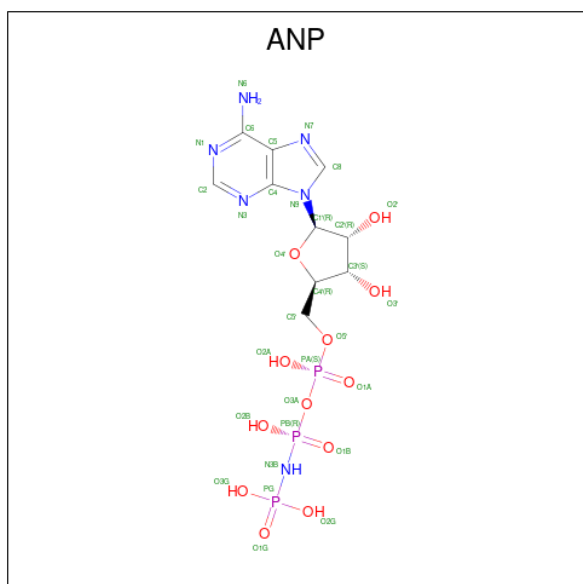
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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-109	HIS	-	expression tag	UNP Q12306
BBB	-108	HIS	-	expression tag	UNP Q12306
BBB	-107	HIS	-	expression tag	UNP Q12306
BBB	-106	GLY	-	expression tag	UNP Q12306
BBB	-10	SER	-	linker	UNP Q12306
BBB	-9	SER	-	linker	UNP Q12306
BBB	-8	GLY	-	linker	UNP Q12306
BBB	-7	LEU	-	linker	UNP Q12306
BBB	-6	GLU	-	linker	UNP Q12306
BBB	-5	VAL	-	linker	UNP Q12306
BBB	-4	LEU	-	linker	UNP Q12306
BBB	-3	PHE	-	linker	UNP Q12306
BBB	-2	GLN	-	linker	UNP Q12306
BBB	-1	GLY	-	linker	UNP Q12306
BBB	0	THR	-	linker	UNP Q12306

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total	Zn	0	0
			2	2		
2	BBB	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	
			31	10	6	12	3	0
3	BBB	1	Total	C	N	O	P	
			62	20	12	24	6	1

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



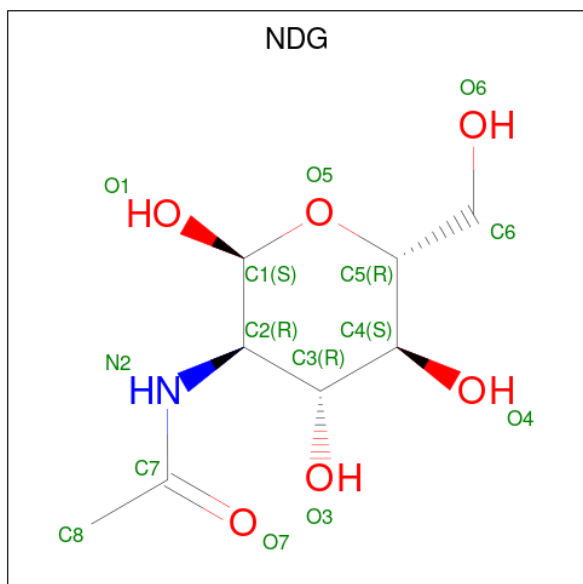
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O		
			7	4	3	0	0
4	AAA	1	Total	C	O		
			7	4	3	0	0
4	AAA	1	Total	C	O		
			7	4	3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			10	6	4		
5	BBB	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



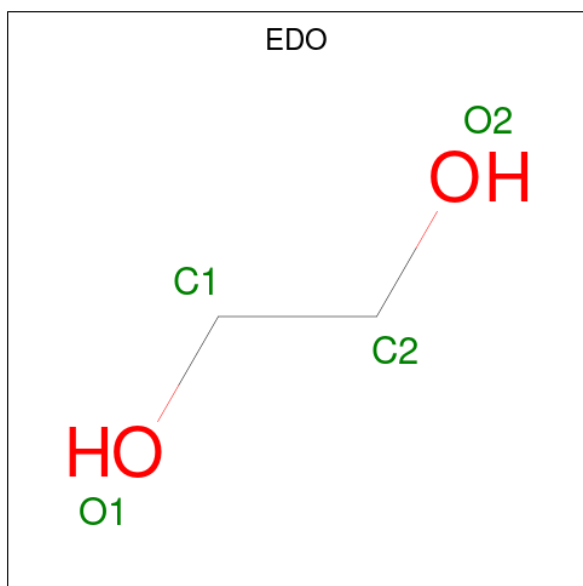
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	BBB	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	AAA	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		
7	BBB	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total	K	0	0
			1	1		
8	BBB	1	Total	K	0	0
			1	1		

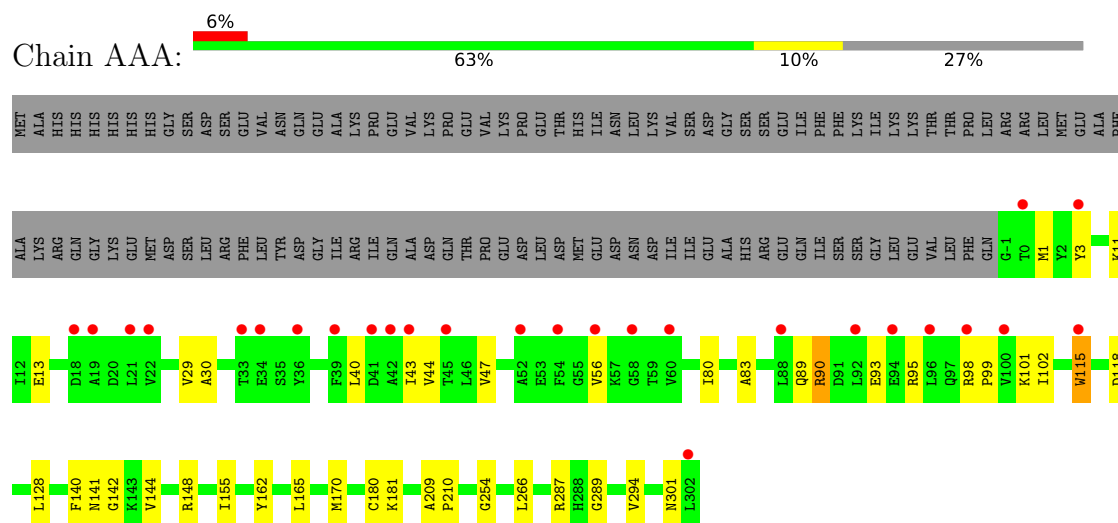
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	130	Total	O	0	0
			130	130		
9	BBB	127	Total	O	0	0
			127	127		

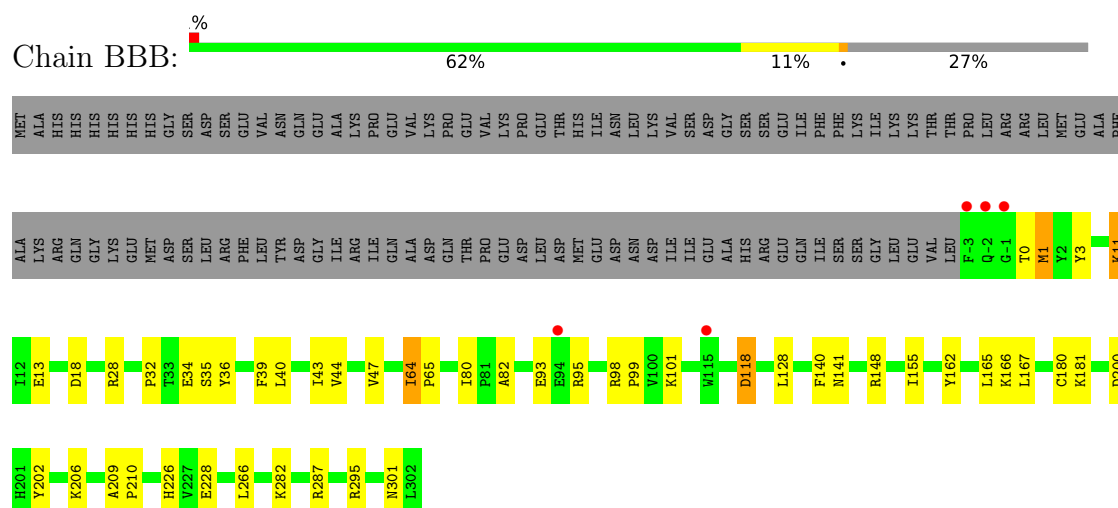
### 3 Residue-property plots

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: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase



- Molecule 1: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.20Å 115.20Å 120.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.11 – 2.11 57.60 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.11-2.11) 100.0 (57.60-2.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.191 , 0.233 0.192 , 0.233	Depositor DCC
$R_{free}$ test set	2795 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: ZN, K, ANP, PEG, PGE, EDO, NDG

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	AAA	0.43	0/2413	0.75	0/3265
1	BBB	0.41	0/2463	0.75	0/3331
All	All	0.42	0/4876	0.75	0/6596

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2352	0	2347	32	0
1	BBB	2389	0	2405	37	0
2	AAA	2	0	0	0	0
2	BBB	2	0	0	0	0
3	AAA	31	0	13	0	0
3	BBB	62	0	26	0	0
4	AAA	21	0	30	0	0
5	AAA	10	0	14	8	0
5	BBB	10	0	14	2	0
6	AAA	15	0	12	0	0
6	BBB	15	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AAA	28	0	42	1	0
7	BBB	32	0	48	2	0
8	AAA	1	0	0	0	0
8	BBB	1	0	0	0	0
9	AAA	130	0	0	3	0
9	BBB	127	0	0	3	0
All	All	5228	0	4963	67	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 (67) 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)
5:AAA:404:PGE:H22	1:BBB:140:PHE:HB2	1.51	0.91
1:AAA:140:PHE:HB2	5:AAA:404:PGE:H52	1.52	0.89
1:BBB:282:LYS:HD2	9:BBB:678:HOH:O	1.81	0.79
1:BBB:1:MET:HE2	1:BBB:18:ASP:HA	1.66	0.77
1:BBB:64:ILE:HG13	1:BBB:65:PRO:HD2	1.73	0.69
1:AAA:118:ASP:OD2	1:AAA:287[B]:ARG:NH2	2.22	0.67
1:AAA:287[B]:ARG:HG2	1:AAA:287[B]:ARG:HH11	1.61	0.66
1:AAA:287[B]:ARG:HG2	1:AAA:287[B]:ARG:NH1	2.10	0.65
5:AAA:404:PGE:C4	1:BBB:141:ASN:HD22	2.12	0.63
1:AAA:140:PHE:HB3	5:AAA:404:PGE:H2	1.80	0.62
1:AAA:141:ASN:HD22	5:AAA:404:PGE:C3	2.12	0.62
1:BBB:118:ASP:HB3	1:BBB:287[B]:ARG:HH21	1.65	0.62
1:AAA:13:GLU:HG3	1:AAA:294:VAL:HG21	1.82	0.62
1:BBB:11:LYS:HD2	1:BBB:28:ARG:NH1	2.17	0.60
1:AAA:162:TYR:HB2	1:BBB:165[A]:LEU:HD11	1.83	0.60
1:BBB:1:MET:HG2	1:BBB:3:TYR:HE1	1.68	0.59
1:BBB:64:ILE:HG13	1:BBB:65:PRO:CD	2.32	0.59
1:AAA:128:LEU:CD1	1:AAA:155:ILE:HD11	2.34	0.58
1:BBB:34:GLU:HG2	1:BBB:35:SER:N	2.18	0.57
1:BBB:128:LEU:CD1	1:BBB:155:ILE:HD11	2.35	0.57
1:BBB:34:GLU:HG2	1:BBB:35:SER:H	1.72	0.55
1:BBB:226:HIS:HD2	9:BBB:683:HOH:O	1.89	0.55
1:BBB:128:LEU:HD13	1:BBB:155:ILE:HD11	1.90	0.54
1:AAA:98:ARG:HB2	1:AAA:99:PRO:HD2	1.89	0.54
1:BBB:98:ARG:HB2	1:BBB:99:PRO:HD2	1.90	0.54
5:AAA:404:PGE:H42	1:BBB:141:ASN:HD22	1.71	0.53
1:BBB:1:MET:HG2	1:BBB:3:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:32:PRO:HG2	1:BBB:39:PHE:HA	1.91	0.52
1:AAA:289:GLY:HA2	9:AAA:574:HOH:O	2.09	0.51
5:AAA:404:PGE:H5	1:BBB:140:PHE:HB3	1.92	0.51
1:BBB:166:LYS:HE2	9:BBB:606:HOH:O	2.11	0.51
1:BBB:228:GLU:HG3	5:BBB:503:PGE:H22	1.93	0.49
1:AAA:180:CYS:O	1:AAA:181:LYS:HB2	2.13	0.49
1:AAA:209:ALA:HB3	1:AAA:210:PRO:HD3	1.95	0.49
1:BBB:209:ALA:HB3	1:BBB:210:PRO:HD3	1.95	0.48
1:AAA:140:PHE:HB2	5:AAA:404:PGE:C5	2.35	0.48
1:AAA:80:ILE:HG22	1:AAA:83:ALA:H	1.78	0.48
1:BBB:101:LYS:HE3	1:BBB:301:ASN:ND2	2.28	0.47
1:AAA:128:LEU:HD13	1:AAA:155:ILE:HD11	1.96	0.47
1:BBB:202:TYR:CZ	7:BBB:506:EDO:H21	2.50	0.47
1:AAA:43:ILE:O	1:AAA:47:VAL:HG23	2.15	0.46
1:BBB:43:ILE:O	1:BBB:47:VAL:HG23	2.15	0.46
1:BBB:180:CYS:O	1:BBB:181:LYS:HB2	2.16	0.45
1:AAA:165:LEU:HD11	1:BBB:162:TYR:HB2	1.99	0.45
1:AAA:266:LEU:HD23	1:AAA:266:LEU:HA	1.86	0.44
1:AAA:101:LYS:HE3	1:AAA:301:ASN:ND2	2.32	0.44
1:BBB:36:TYR:HB2	1:BBB:82:ALA:O	2.18	0.44
1:BBB:93:GLU:HG2	1:BBB:98:ARG:O	2.18	0.44
1:BBB:167:LEU:HD11	5:BBB:503:PGE:H3	1.98	0.44
1:AAA:80:ILE:HG22	1:AAA:80:ILE:O	2.17	0.44
1:AAA:93:GLU:HG2	1:AAA:98:ARG:O	2.17	0.44
1:AAA:90:ARG:NE	1:AAA:90:ARG:HA	2.32	0.44
1:BBB:266:LEU:HD23	1:BBB:266:LEU:HA	1.85	0.43
1:AAA:29:VAL:HG12	1:AAA:30:ALA:O	2.19	0.43
1:BBB:40:LEU:O	1:BBB:44:VAL:HG23	2.19	0.43
1:BBB:202:TYR:CE2	7:BBB:506:EDO:H21	2.53	0.43
1:BBB:295[B]:ARG:HE	1:BBB:295[B]:ARG:HB3	1.69	0.42
1:AAA:144:VAL:HG12	9:AAA:541:HOH:O	2.18	0.42
1:BBB:13:GLU:HG3	1:BBB:28:ARG:HG2	2.02	0.42
1:AAA:40:LEU:O	1:AAA:44:VAL:HG23	2.18	0.42
1:AAA:1:MET:HG2	1:AAA:3:TYR:HE1	1.86	0.41
1:AAA:115[A]:TRP:HZ3	1:AAA:142:GLY:CA	2.34	0.41
1:AAA:170:MET:HB2	1:AAA:170:MET:HE2	1.94	0.41
1:AAA:89:GLN:HB2	1:AAA:102:ILE:HG13	2.03	0.40
1:BBB:200:ASP:OD2	1:BBB:206:LYS:HE2	2.21	0.40
1:AAA:56:VAL:HB	9:AAA:526:HOH:O	2.20	0.40
1:AAA:254:GLY:H	7:AAA:410:EDO:H12	1.86	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	AAA	307/417 (74%)	295 (96%)	12 (4%)	0	100	100
1	BBB	312/417 (75%)	301 (96%)	11 (4%)	0	100	100
All	All	619/834 (74%)	596 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	243/340 (72%)	237 (98%)	6 (2%)	47	50
1	BBB	248/340 (73%)	240 (97%)	8 (3%)	39	40
All	All	491/680 (72%)	477 (97%)	14 (3%)	44	44

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	11	LYS
1	AAA	90	ARG
1	AAA	95	ARG
1	AAA	115[A]	TRP
1	AAA	115[B]	TRP
1	AAA	148	ARG
1	BBB	0	THR
1	BBB	1	MET

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Mol	Chain	Res	Type
1	BBB	11	LYS
1	BBB	64	ILE
1	BBB	80	ILE
1	BBB	95	ARG
1	BBB	118	ASP
1	BBB	148	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 6 are monoatomic - leaving 25 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	$\# Z  > 2$
7	EDO	BBB	512	-	3,3,3	0.08	0	2,2,2	0.19	0
7	EDO	AAA	414	-	3,3,3	0.22	0	2,2,2	0.69	0
5	PGE	AAA	404	-	9,9,9	0.57	0	8,8,8	0.55	0
6	NDG	AAA	407	-	15,15,15	0.37	0	21,21,21	1.45	2 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	BBB	508	-	3,3,3	0.25	0	2,2,2	0.45	0
7	EDO	AAA	412	-	3,3,3	0.15	0	2,2,2	0.36	0
7	EDO	AAA	408	-	3,3,3	0.66	0	2,2,2	1.14	0
7	EDO	BBB	511	-	3,3,3	0.26	0	2,2,2	0.59	0
7	EDO	BBB	510	-	3,3,3	0.34	0	2,2,2	0.68	0
7	EDO	BBB	505	-	3,3,3	0.32	0	2,2,2	0.62	0
4	PEG	AAA	403	-	6,6,6	0.39	0	5,5,5	0.29	0
6	NDG	BBB	504	-	15,15,15	0.36	0	21,21,21	0.89	0
7	EDO	BBB	509	-	3,3,3	0.15	0	2,2,2	0.36	0
4	PEG	AAA	405	-	6,6,6	0.15	0	5,5,5	0.09	0
7	EDO	AAA	411	-	3,3,3	0.10	0	2,2,2	0.24	0
7	EDO	BBB	506	-	3,3,3	0.14	0	2,2,2	0.30	0
7	EDO	BBB	507	-	3,3,3	0.10	0	2,2,2	0.08	0
5	PGE	BBB	503	-	9,9,9	0.18	0	8,8,8	0.26	0
3	ANP	BBB	501[A]	-	29,33,33	1.14	4 (13%)	31,52,52	1.25	4 (12%)
4	PEG	AAA	406	-	6,6,6	0.15	0	5,5,5	0.10	0
7	EDO	AAA	410	-	3,3,3	0.27	0	2,2,2	0.07	0
7	EDO	AAA	409	-	3,3,3	0.19	0	2,2,2	0.20	0
7	EDO	AAA	413	-	3,3,3	0.12	0	2,2,2	0.11	0
3	ANP	AAA	402	-	29,33,33	1.16	4 (13%)	31,52,52	1.72	4 (12%)
3	ANP	BBB	501[B]	-	29,33,33	1.26	4 (13%)	31,52,52	1.18	3 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	BBB	512	-	-	1/1/1/1	-
7	EDO	AAA	414	-	-	0/1/1/1	-
5	PGE	AAA	404	-	-	3/7/7/7	-
6	NDG	AAA	407	-	-	0/6/26/26	0/1/1/1
7	EDO	BBB	508	-	-	1/1/1/1	-
7	EDO	AAA	412	-	-	1/1/1/1	-
7	EDO	AAA	408	-	-	0/1/1/1	-
7	EDO	BBB	511	-	-	0/1/1/1	-
7	EDO	BBB	510	-	-	0/1/1/1	-
7	EDO	BBB	505	-	-	0/1/1/1	-
4	PEG	AAA	403	-	-	3/4/4/4	-
6	NDG	BBB	504	-	-	0/6/26/26	0/1/1/1
7	EDO	BBB	509	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	AAA	405	-	-	3/4/4/4	-
7	EDO	AAA	411	-	-	0/1/1/1	-
7	EDO	BBB	506	-	-	1/1/1/1	-
7	EDO	BBB	507	-	-	0/1/1/1	-
5	PGE	BBB	503	-	-	4/7/7/7	-
3	ANP	BBB	501[A]	-	-	2/14/38/38	0/3/3/3
4	PEG	AAA	406	-	-	1/4/4/4	-
7	EDO	AAA	410	-	-	0/1/1/1	-
7	EDO	AAA	409	-	-	0/1/1/1	-
7	EDO	AAA	413	-	-	1/1/1/1	-
3	ANP	AAA	402	-	-	4/14/38/38	0/3/3/3
3	ANP	BBB	501[B]	-	-	3/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	501[B]	ANP	PG-O1G	3.65	1.51	1.46
3	BBB	501[B]	ANP	PB-O1B	3.04	1.51	1.46
3	AAA	402	ANP	PG-O2G	-2.88	1.49	1.56
3	BBB	501[A]	ANP	PG-O1G	2.75	1.50	1.46
3	BBB	501[A]	ANP	PB-O1B	2.58	1.50	1.46
3	AAA	402	ANP	PB-O2B	-2.40	1.50	1.56
3	BBB	501[B]	ANP	PB-O2B	-2.39	1.50	1.56
3	AAA	402	ANP	PB-O1B	2.35	1.49	1.46
3	BBB	501[A]	ANP	PB-O2B	-2.34	1.50	1.56
3	BBB	501[B]	ANP	PG-O3G	-2.10	1.51	1.56
3	BBB	501[A]	ANP	PG-O3G	-2.05	1.51	1.56
3	AAA	402	ANP	PG-O1G	2.03	1.49	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	402	ANP	O2G-PG-O1G	-5.94	98.52	113.45
6	AAA	407	NDG	O5-C1-C2	4.62	114.16	109.52
3	AAA	402	ANP	O2B-PB-O1B	4.13	118.59	109.92
3	BBB	501[B]	ANP	O2B-PB-O1B	4.06	118.43	109.92
3	AAA	402	ANP	O1B-PB-N3B	-3.91	106.01	111.77
3	BBB	501[A]	ANP	O2B-PB-O1B	3.73	117.74	109.92
3	BBB	501[A]	ANP	O1G-PG-N3B	-3.62	106.43	111.77
6	AAA	407	NDG	C1-C2-N2	3.41	114.68	110.73
3	AAA	402	ANP	O1G-PG-N3B	-2.89	107.52	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	501[A]	ANP	O2G-PG-O1G	-2.56	107.01	113.45
3	BBB	501[B]	ANP	O1B-PB-N3B	2.43	115.34	111.77
3	BBB	501[B]	ANP	C5-C6-N6	2.27	123.80	120.35
3	BBB	501[A]	ANP	C5-C6-N6	2.18	123.67	120.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

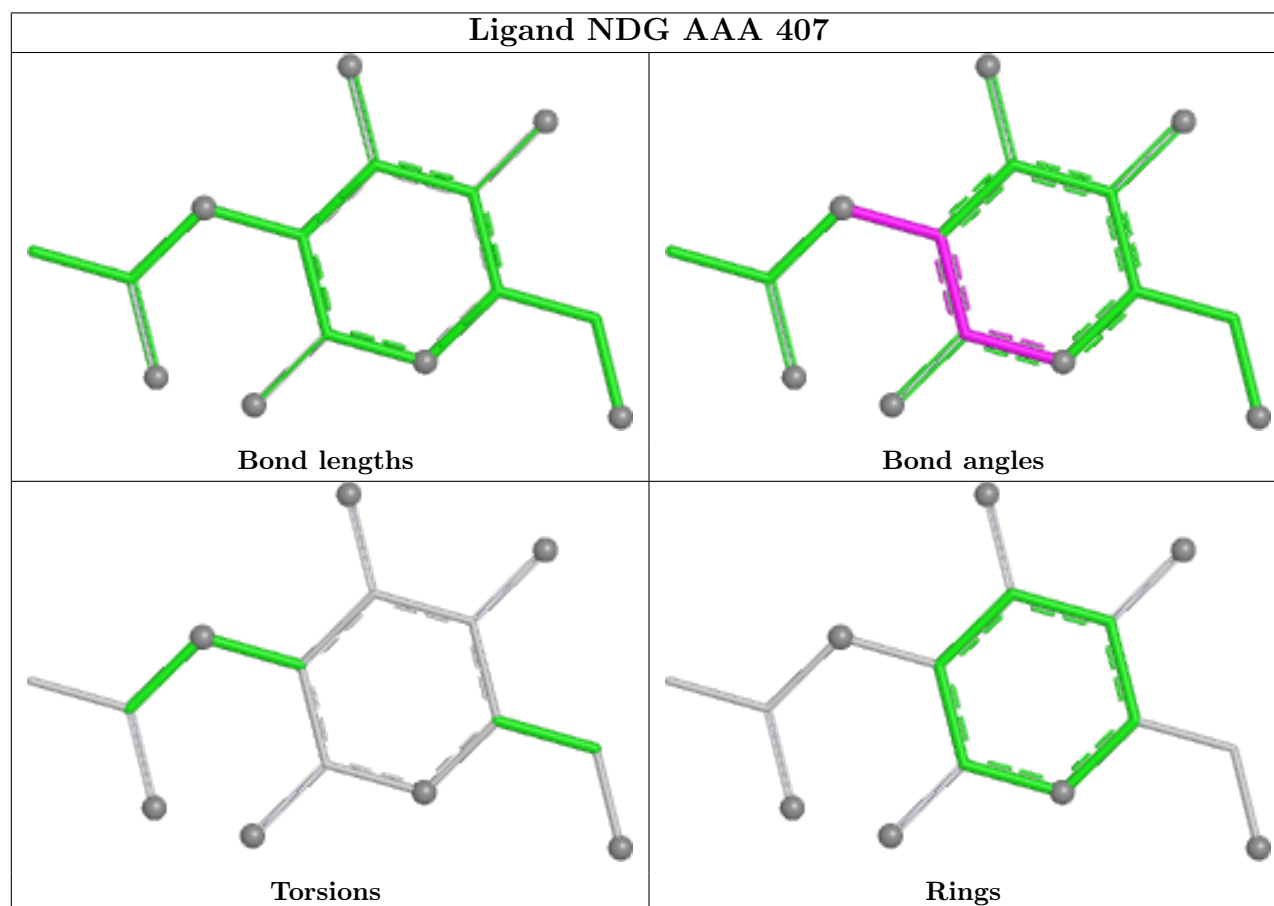
Mol	Chain	Res	Type	Atoms
3	AAA	402	ANP	PB-N3B-PG-O1G
3	AAA	402	ANP	PG-N3B-PB-O1B
3	AAA	402	ANP	PA-O3A-PB-O1B
3	AAA	402	ANP	PA-O3A-PB-O2B
3	BBB	501[A]	ANP	PB-N3B-PG-O1G
3	BBB	501[A]	ANP	PA-O3A-PB-O1B
3	BBB	501[B]	ANP	PB-N3B-PG-O1G
5	BBB	503	PGE	O2-C3-C4-O3
5	AAA	404	PGE	O2-C3-C4-O3
4	AAA	406	PEG	O2-C3-C4-O4
7	AAA	412	EDO	O1-C1-C2-O2
7	BBB	506	EDO	O1-C1-C2-O2
5	BBB	503	PGE	O3-C5-C6-O4
4	AAA	403	PEG	O2-C3-C4-O4
7	BBB	508	EDO	O1-C1-C2-O2
5	BBB	503	PGE	C3-C4-O3-C5
5	BBB	503	PGE	C1-C2-O2-C3
4	AAA	405	PEG	C4-C3-O2-C2
4	AAA	405	PEG	O1-C1-C2-O2
3	BBB	501[B]	ANP	PB-O3A-PA-O2A
7	AAA	413	EDO	O1-C1-C2-O2
7	BBB	512	EDO	O1-C1-C2-O2
4	AAA	405	PEG	O2-C3-C4-O4
5	AAA	404	PGE	C6-C5-O3-C4
4	AAA	403	PEG	O1-C1-C2-O2
5	AAA	404	PGE	C3-C4-O3-C5
3	BBB	501[B]	ANP	PB-O3A-PA-O1A
7	BBB	509	EDO	O1-C1-C2-O2
4	AAA	403	PEG	C1-C2-O2-C3

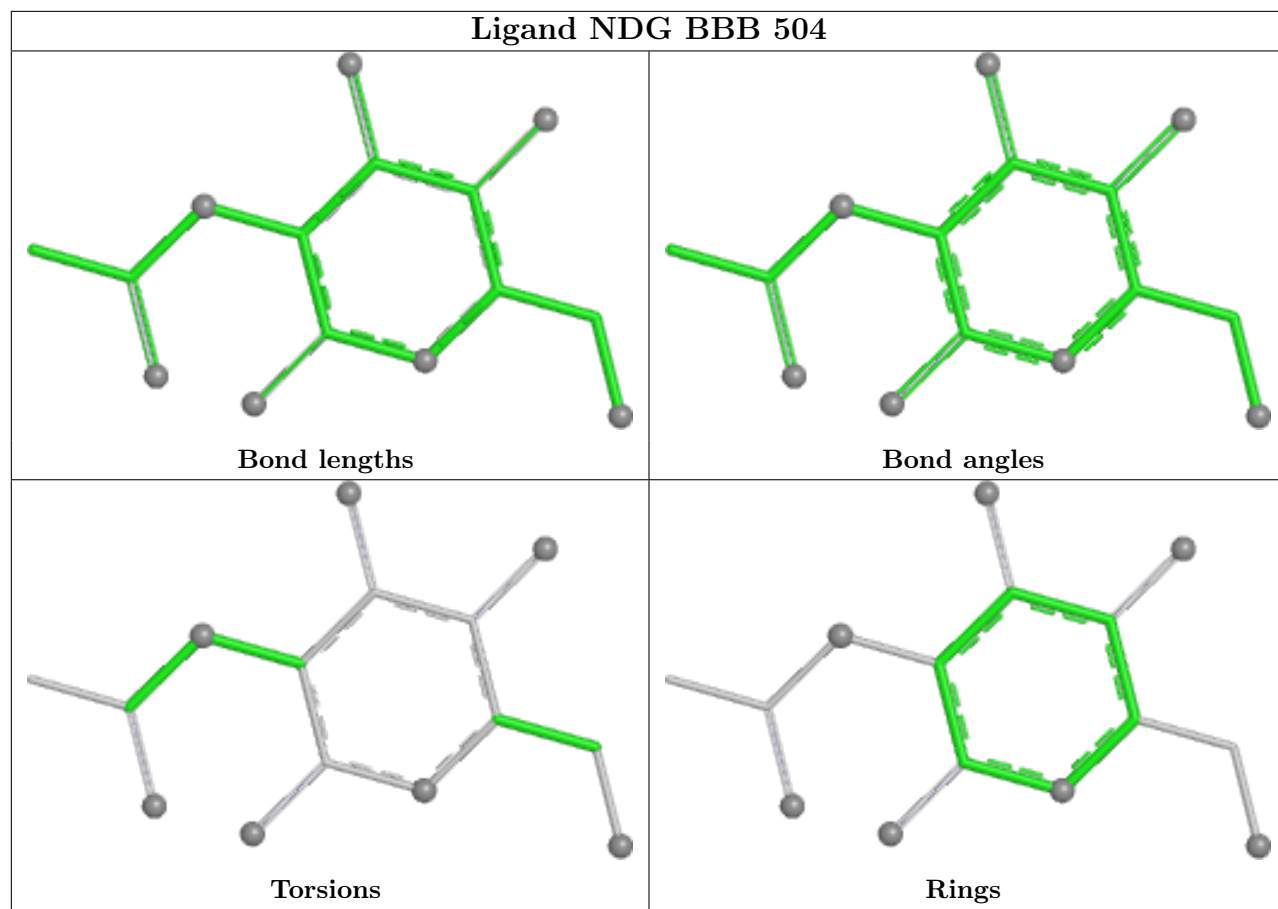
There are no ring outliers.

4 monomers are involved in 13 short contacts:

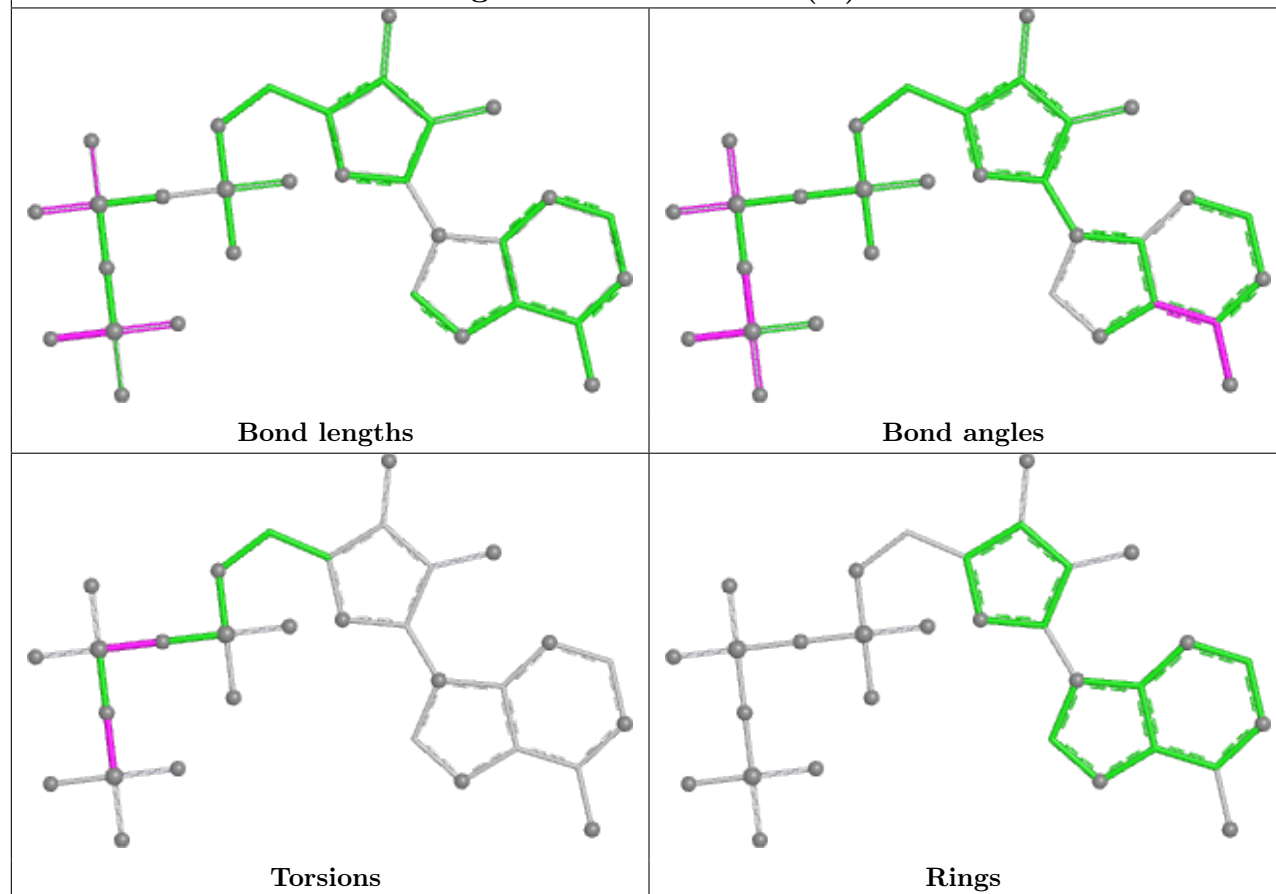
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	404	PGE	8	0
7	BBB	506	EDO	2	0
5	BBB	503	PGE	2	0
7	AAA	410	EDO	1	0

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.

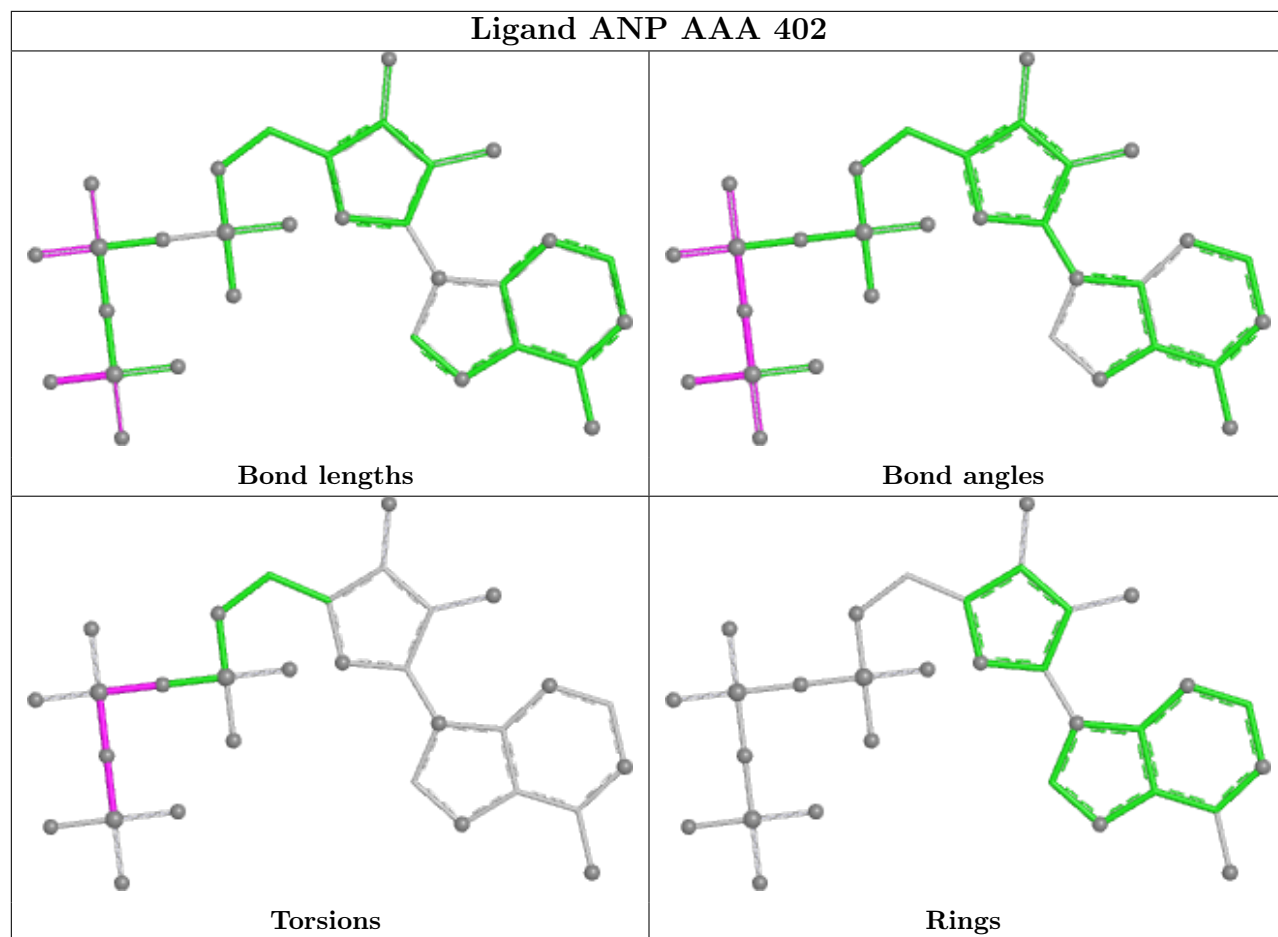


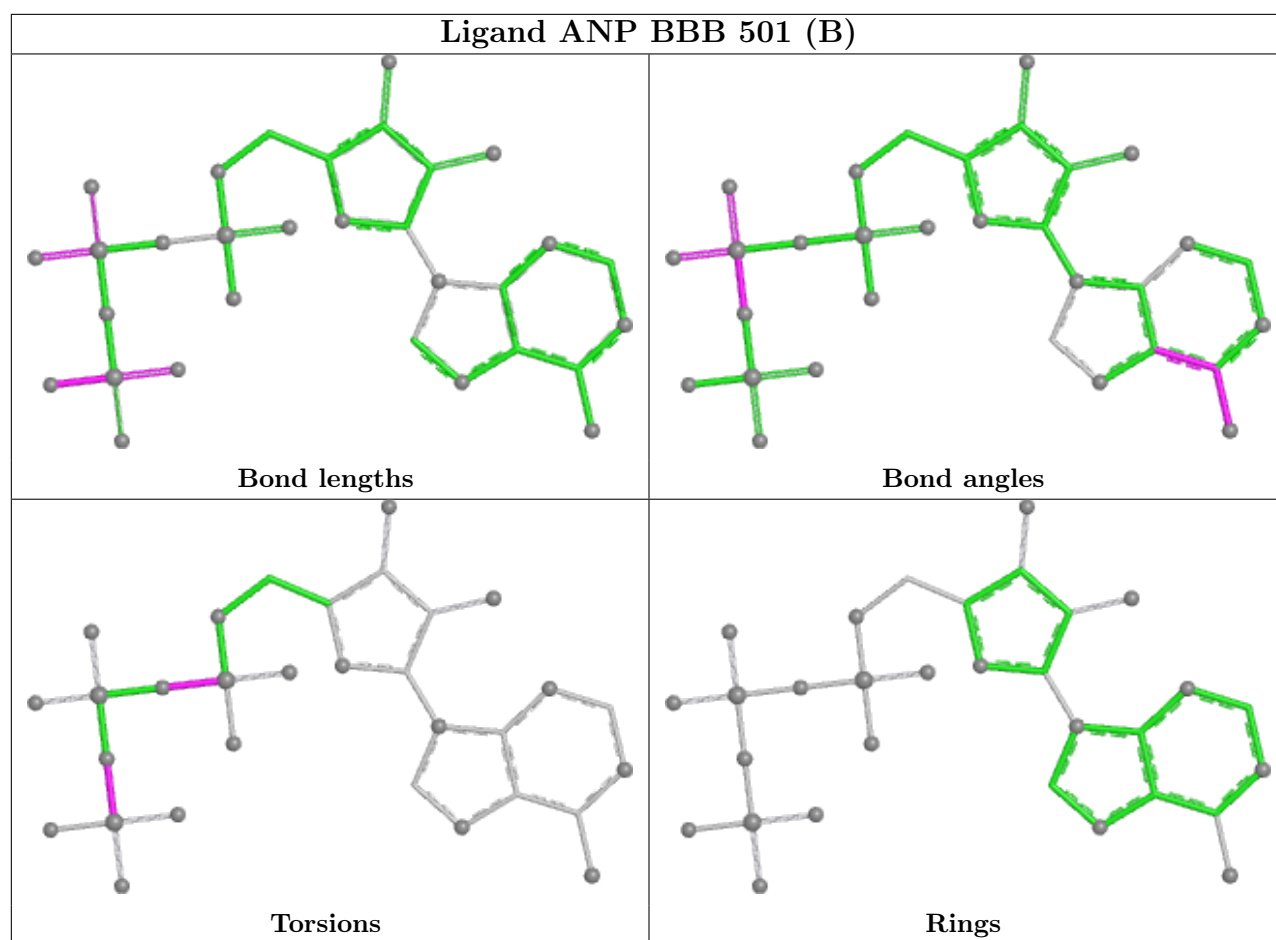


## Ligand ANP BBB 501 (A)



## Ligand ANP AAA 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	AAA	304/417 (72%)	0.22	27 (8%) <span>9</span> <span>12</span>	30, 43, 84, 124	0
1	BBB	306/417 (73%)	-0.14	5 (1%) <span>72</span> <span>76</span>	30, 42, 70, 106	0
All	All	610/834 (73%)	0.04	32 (5%) <span>27</span> <span>32</span>	30, 43, 82, 124	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	33	THR	6.8
1	AAA	34	GLU	6.0
1	BBB	-3	PHE	5.9
1	BBB	-2	GLN	4.5
1	AAA	60	VAL	4.4
1	AAA	88	LEU	4.4
1	AAA	39	PHE	4.2
1	AAA	92	LEU	4.2
1	AAA	42	ALA	3.9
1	AAA	36	TYR	3.5
1	AAA	43	ILE	3.5
1	AAA	52	ALA	3.5
1	AAA	100	VAL	3.0
1	AAA	96	LEU	3.0
1	BBB	-1	GLY	2.8
1	AAA	98	ARG	2.8
1	AAA	302	LEU	2.6
1	AAA	58	GLY	2.6
1	AAA	0	THR	2.5
1	AAA	18	ASP	2.5
1	AAA	45	THR	2.4
1	BBB	115[A]	TRP	2.4
1	AAA	21	LEU	2.4
1	BBB	94	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	19	ALA	2.3
1	AAA	115[A]	TRP	2.2
1	AAA	56	VAL	2.2
1	AAA	54	PHE	2.2
1	AAA	41	ASP	2.1
1	AAA	3	TYR	2.1
1	AAA	94	GLU	2.0
1	AAA	22	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	EDO	BBB	509	4/4	0.68	0.31	75,83,88,100	0
7	EDO	BBB	505	4/4	0.71	0.27	55,69,72,82	0
5	PGE	AAA	404	10/10	0.71	0.53	42,49,56,57	10
7	EDO	BBB	512	4/4	0.72	0.24	81,85,85,86	0
4	PEG	AAA	403	7/7	0.75	0.30	45,61,67,72	7
7	EDO	AAA	408	4/4	0.77	0.30	48,57,68,79	0
7	EDO	BBB	510	4/4	0.78	0.24	61,65,73,77	0
7	EDO	AAA	409	4/4	0.79	0.19	60,78,83,92	0
7	EDO	AAA	412	4/4	0.80	0.29	67,73,80,81	0
4	PEG	AAA	406	7/7	0.83	0.27	61,68,77,89	7
7	EDO	BBB	507	4/4	0.84	0.12	61,66,71,82	0
5	PGE	BBB	503	10/10	0.85	0.17	53,66,80,84	10
7	EDO	AAA	411	4/4	0.86	0.25	66,67,74,78	0
7	EDO	AAA	414	4/4	0.87	0.17	72,73,79,83	0
7	EDO	BBB	506	4/4	0.88	0.26	66,69,73,76	0

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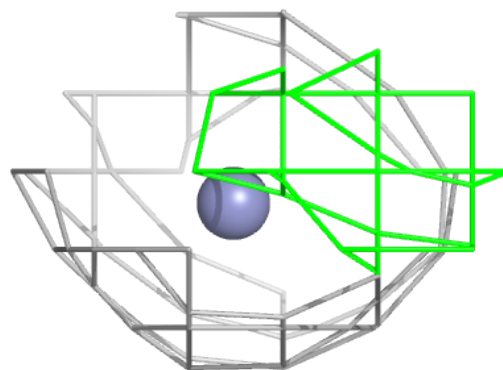
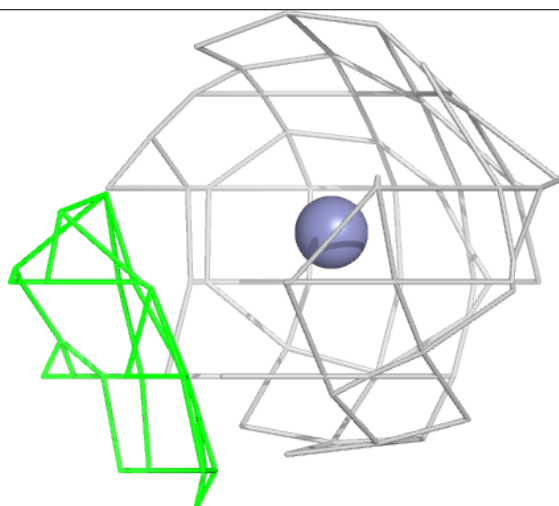
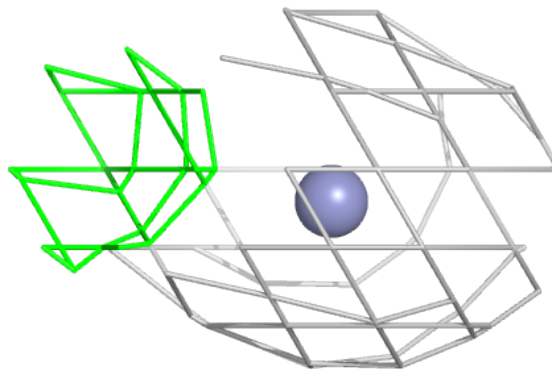
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	AAA	410	4/4	0.88	0.16	55,63,67,68	0
7	EDO	BBB	508	4/4	0.88	0.17	68,68,68,69	0
2	ZN	BBB	514	1/1	0.91	0.07	62,62,62,62	1
2	ZN	AAA	416	1/1	0.91	0.14	55,55,55,55	1
7	EDO	AAA	413	4/4	0.93	0.25	70,76,89,99	0
6	NDG	AAA	407	15/15	0.93	0.13	56,63,69,72	0
4	PEG	AAA	405	7/7	0.93	0.15	48,61,72,80	7
8	K	AAA	415	1/1	0.93	0.11	56,56,56,56	0
7	EDO	BBB	511	4/4	0.94	0.16	58,58,68,75	0
3	ANP	BBB	501[B]	31/31	0.95	0.15	36,49,78,83	31
6	NDG	BBB	504	15/15	0.95	0.19	50,62,68,71	0
3	ANP	BBB	501[A]	31/31	0.95	0.15	34,44,79,86	31
3	ANP	AAA	402	31/31	0.97	0.10	36,45,106,117	0
8	K	BBB	513	1/1	0.99	0.05	45,45,45,45	0
2	ZN	AAA	401	1/1	1.00	0.07	46,46,46,46	0
2	ZN	BBB	502	1/1	1.00	0.13	40,40,40,40	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.

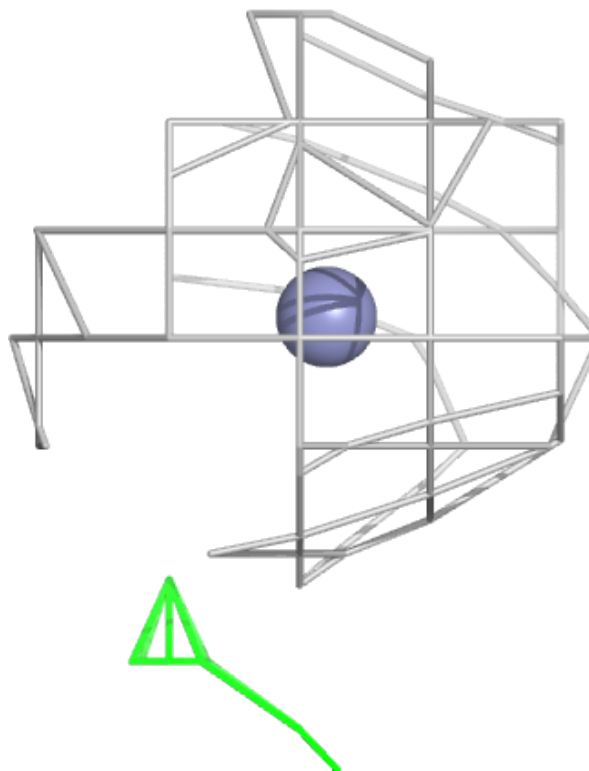
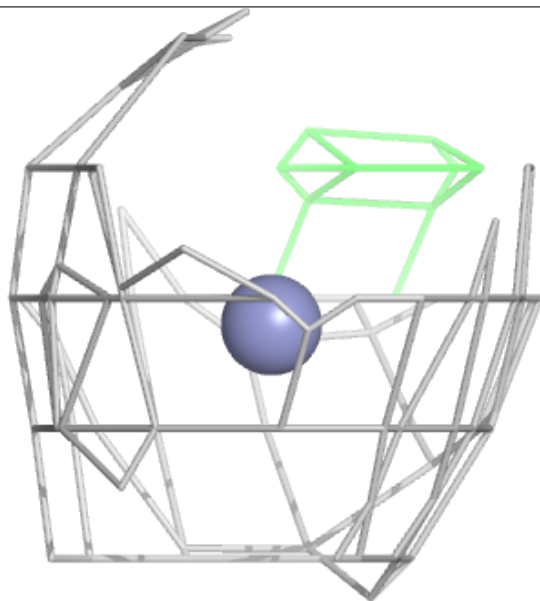
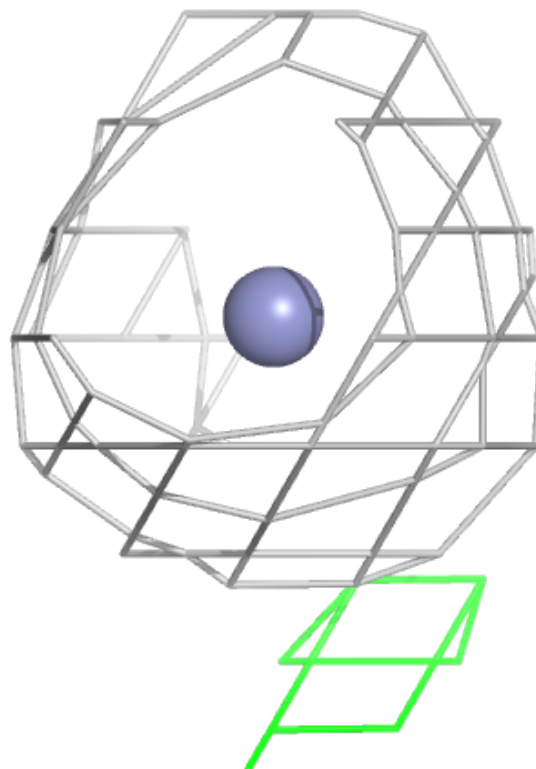
**Electron density around ZN BBB 514:**

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



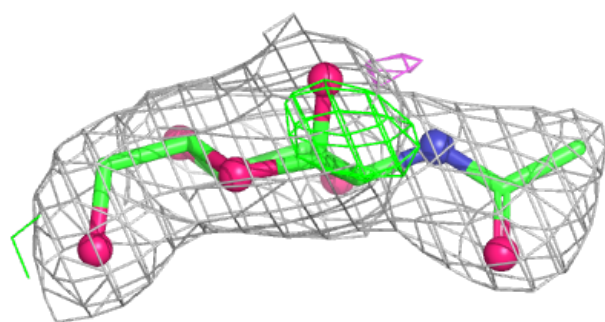
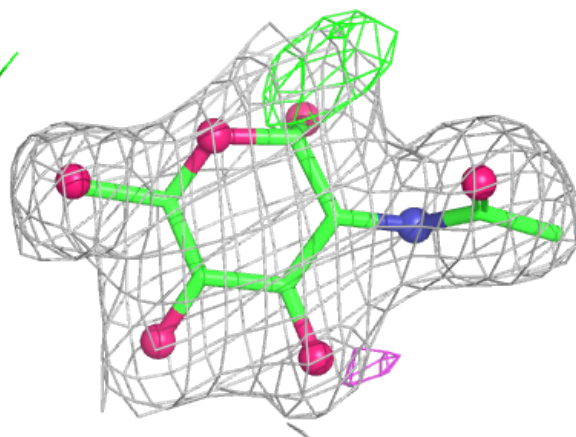
**Electron density around ZN AAA 416:**

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

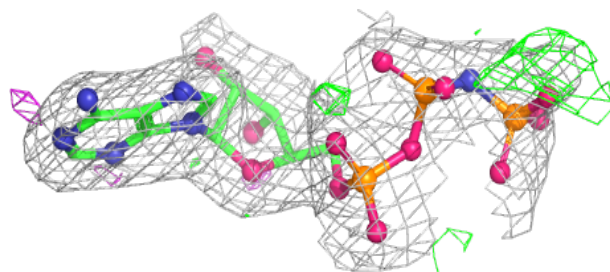
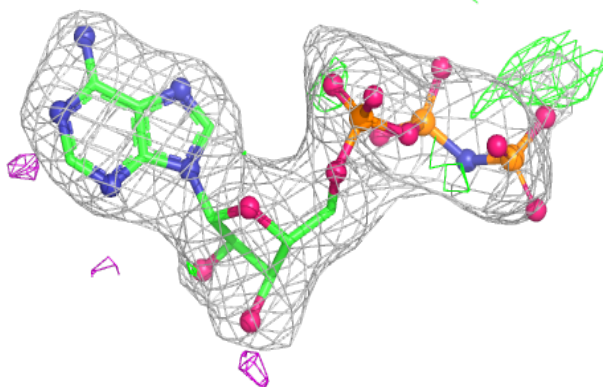


**Electron density around NDG AAA 407:**

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

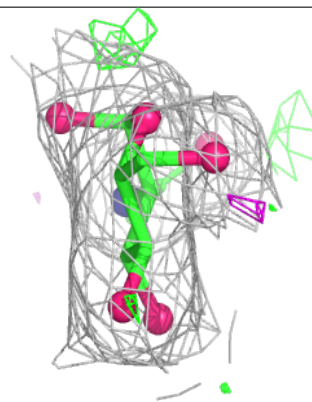
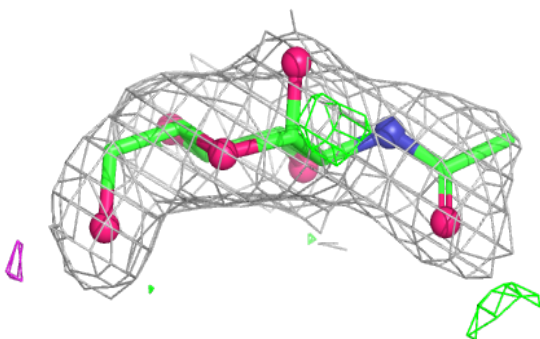
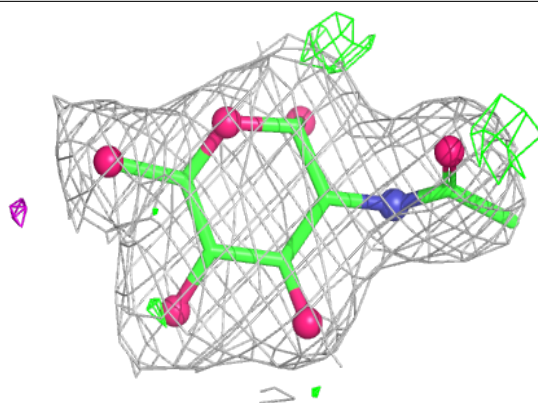
**Electron density around ANP BBB 501 (B):**

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

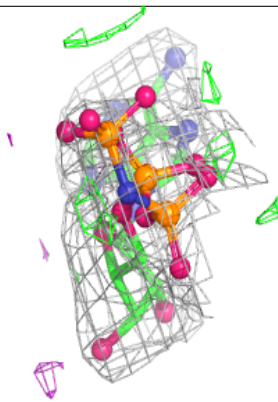
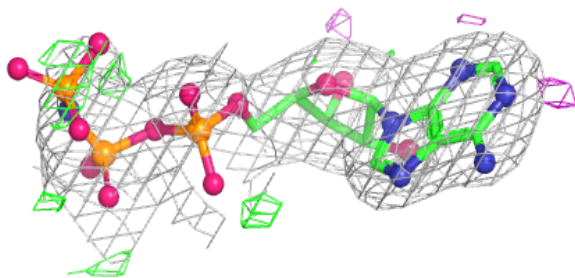
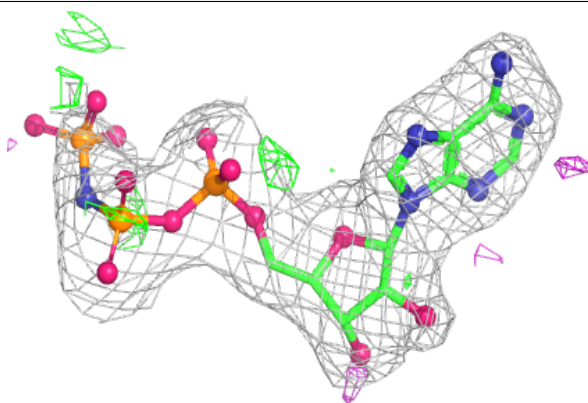


**Electron density around NDG BBB 504:**

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

**Electron density around ANP BBB 501 (A):**

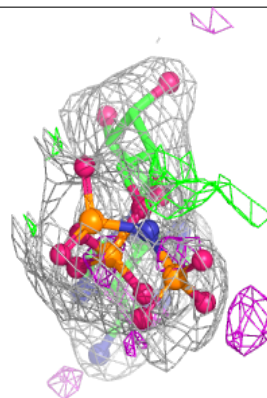
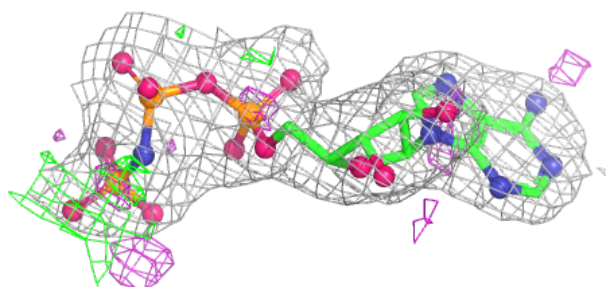
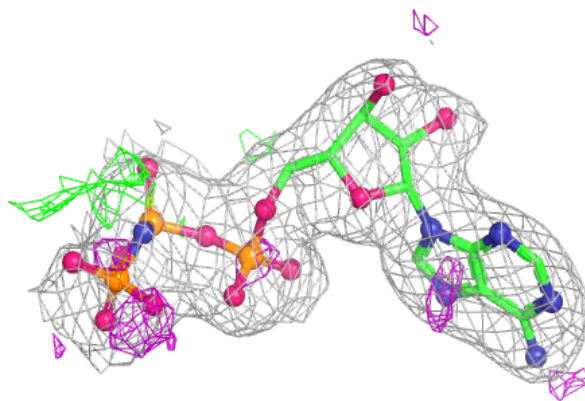
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ANP AAA 402:**

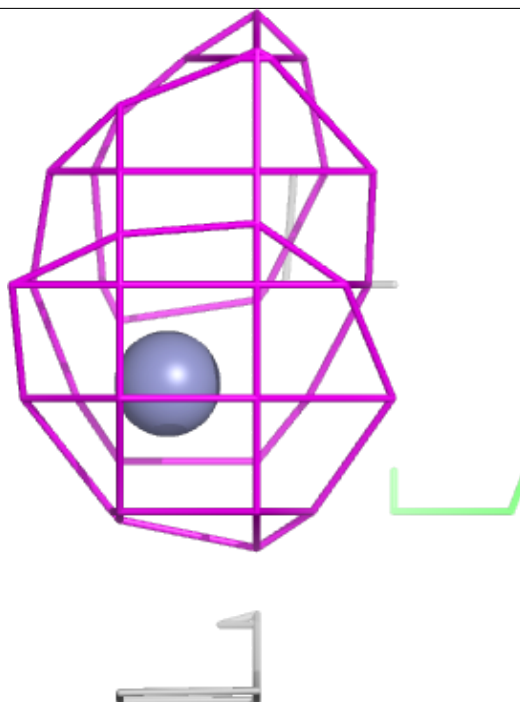
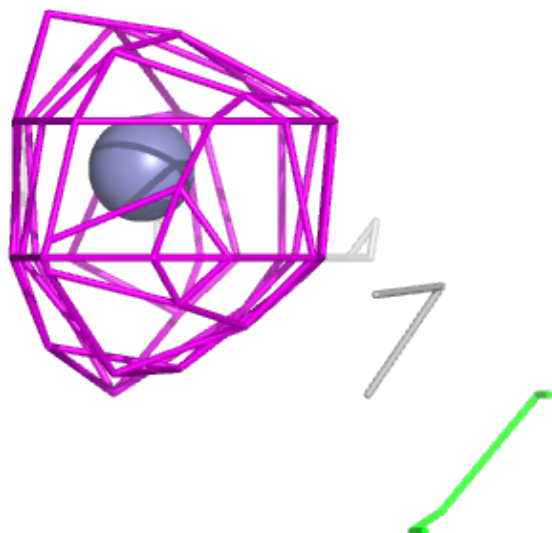
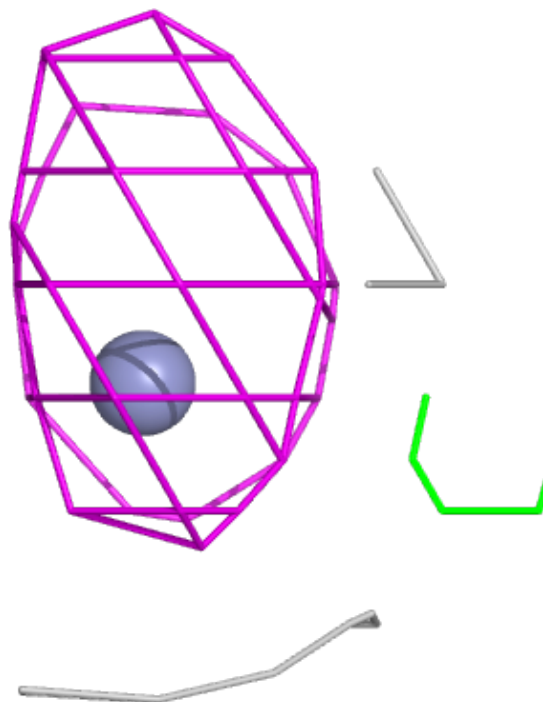
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

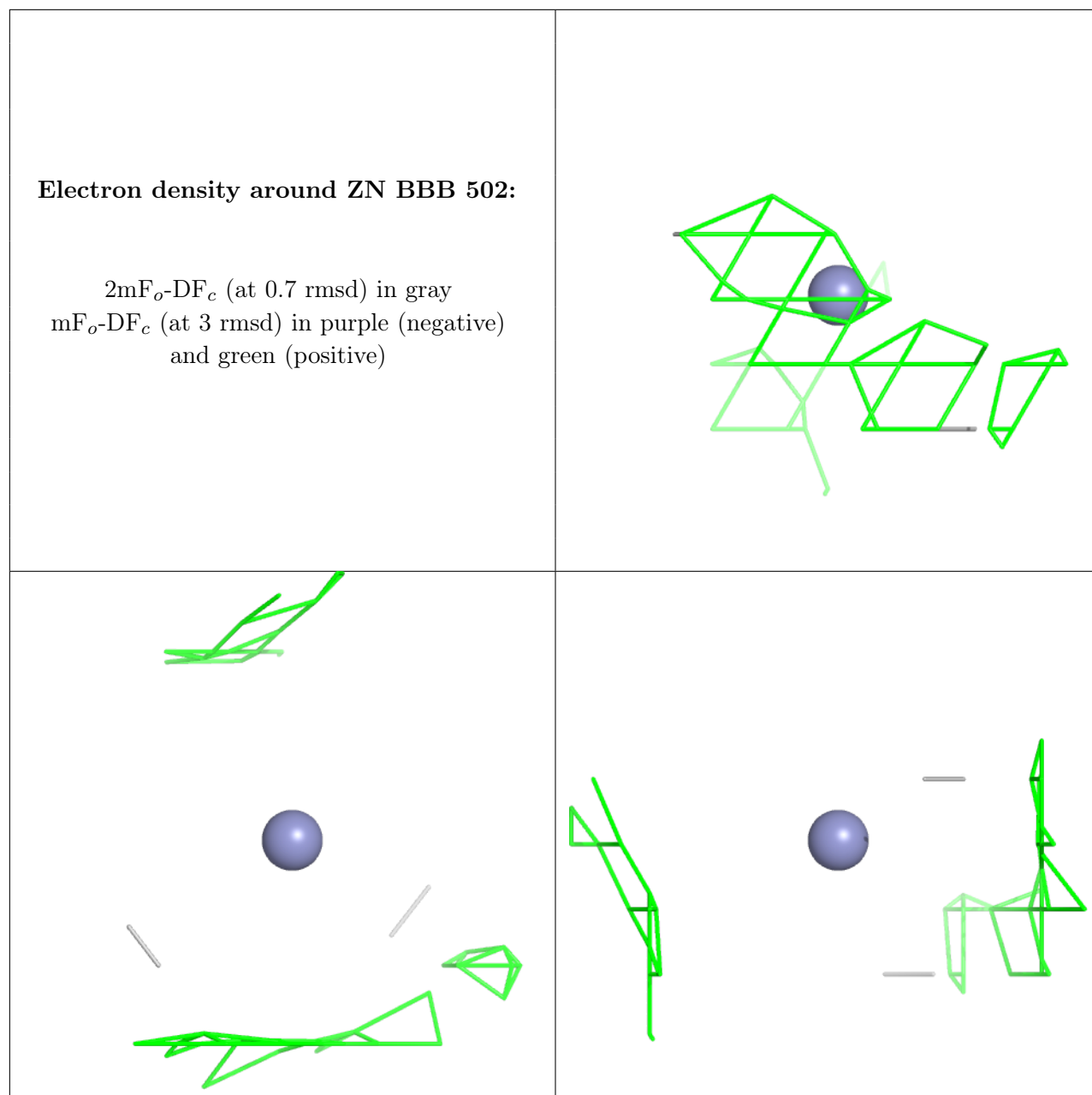




**Electron density around ZN AAA 401:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.