WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2023 – 11:44 pm GMT

PDB ID	:	7PA1
Title	:	Structure of N-acetylglucosamine kinase from Plesiomonas shigelloides in complex with AMP-PNP in the absence of N-acetylglucoseamine substrate
Authors	:	Roy, S.; Isupov, M.N.; Harmer, N.J.; Ames, J.R.
Deposited on	:	2021-07-28
Resolution	:	2.20 Å(reported)

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

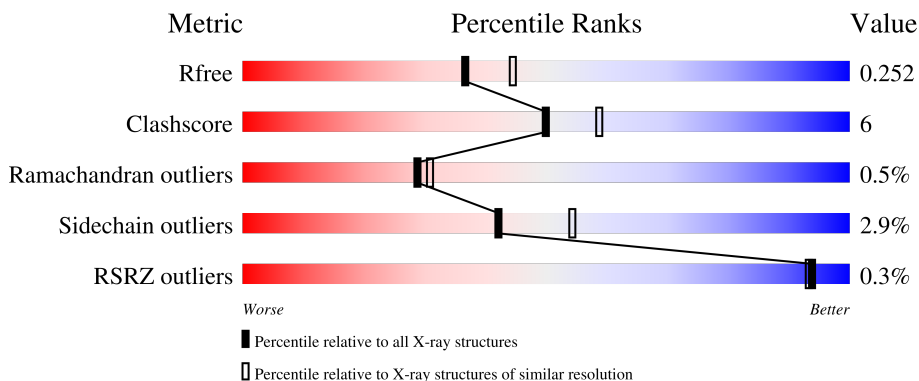|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		6
Ramachandran outliers		0.5%
Sidechain outliers		2.9%
RSRZ outliers		0.3%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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 <=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	66% · 6% · 27%
1	BBB	417	65% · 7% · 27%

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	1004	-	-	X	-
6	EDO	BBB	611	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 4972 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 2339	C 1489	N 406	O 434	S 10	0	4	0
1	BBB	304	Total 2327	C 1480	N 405	O 432	S 10	0	2	0

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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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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
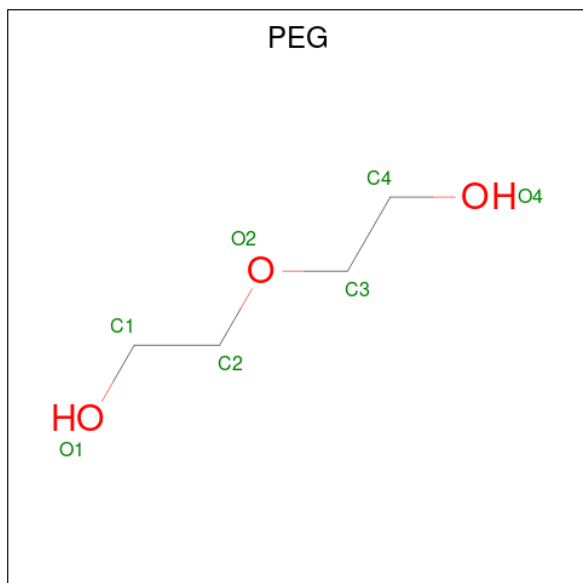
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total 7	C 4	O 3	0	0
2	BBB	1	Total 7	C 4	O 3	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).
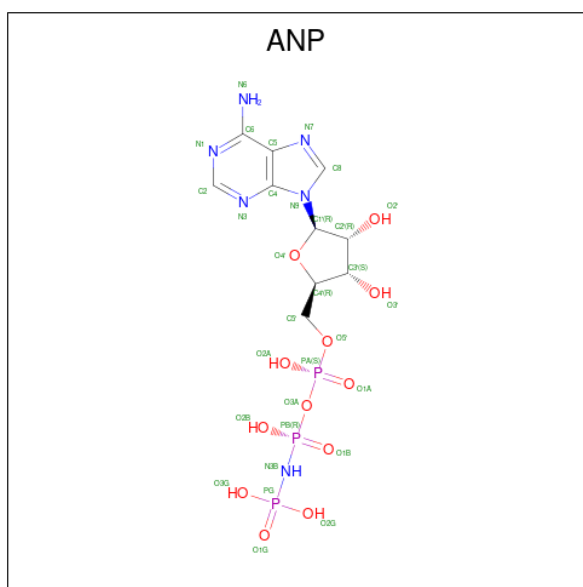
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	BBB	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).
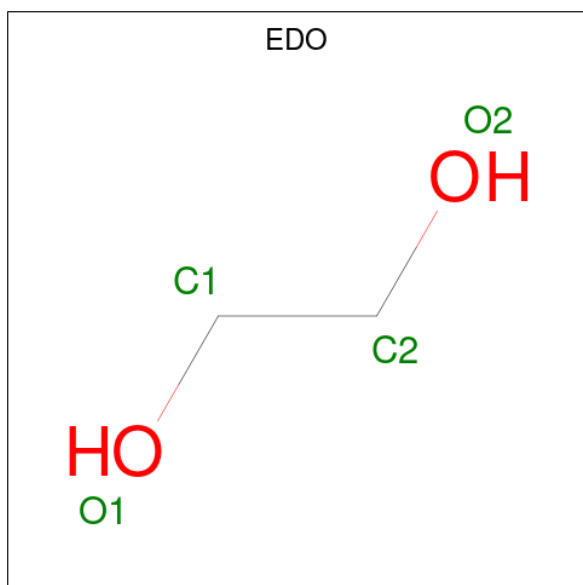
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Zn	0	0
			1	1		
4	BBB	1	Total	Zn	0	0
			1	1		

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

PGE

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	78	Total 78	O 78	0	0
7	BBB	74	Total 74	O 74	0	0

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

Chain AAA:

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

Chain BBB:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	121.27Å 121.27Å 91.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.69 – 2.20 60.63 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.69-2.20) 99.2 (60.63-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.252 0.208 , 0.252	Depositor DCC
R_{free} test set	1846 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4972	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, PGE, ANP, PEG

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	0.44	0/2398	0.76	0/3243
1	BBB	0.44	0/2380	0.78	0/3220
All	All	0.44	0/4778	0.77	0/6463

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 ⓘ

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	2339	0	2337	25	0
1	BBB	2327	0	2318	30	0
2	AAA	7	0	10	1	0
2	BBB	7	0	10	0	0
3	AAA	31	0	13	1	0
3	BBB	31	0	13	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	20	0	28	17	0
5	BBB	20	0	28	2	0
6	AAA	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	24	0	36	7	0
7	AAA	78	0	0	2	0
7	BBB	74	0	0	2	0
All	All	4972	0	4811	56	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 6.

The worst 5 of 56 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:145:HIS:ND1	5:AAA:1004:PGE:H52	1.78	0.98
5:AAA:1004:PGE:H3	1:BBB:141:ASN:HD21	1.32	0.94
1:AAA:145:HIS:ND1	5:AAA:1004:PGE:C5	2.36	0.89
5:AAA:1004:PGE:H3	1:BBB:141:ASN:ND2	1.88	0.88
1:AAA:143:LYS:HG2	5:AAA:1004:PGE:H32	1.57	0.83

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	306/417 (73%)	293 (96%)	10 (3%)	3 (1%)	15	14
1	BBB	304/417 (73%)	291 (96%)	11 (4%)	2 (1%)	22	22
All	All	610/834 (73%)	584 (96%)	21 (3%)	5 (1%)	29	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	34[A]	GLU

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Mol	Chain	Res	Type
1	AAA	34[B]	GLU
1	BBB	34[A]	GLU
1	BBB	34[B]	GLU
1	AAA	289	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	242/340 (71%)	235 (97%)	7 (3%)	42	54
1	BBB	240/340 (71%)	233 (97%)	7 (3%)	42	54
All	All	482/680 (71%)	468 (97%)	14 (3%)	42	54

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	84	MET
1	BBB	148	ARG
1	BBB	294	VAL
1	BBB	181	LYS
1	BBB	197	GLN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#|Z| > 2$
2	PEG	AAA	1001	-	6,6,6	0.22	0	5,5,5	0.16	0
2	PEG	BBB	601	-	6,6,6	0.22	0	5,5,5	0.14	0
5	PGE	AAA	1004	-	9,9,9	0.44	0	8,8,8	0.44	0
6	EDO	BBB	607	-	3,3,3	0.58	0	2,2,2	0.95	0
5	PGE	AAA	1005	-	9,9,9	0.17	0	8,8,8	0.17	0
6	EDO	BBB	610	-	3,3,3	0.26	0	2,2,2	0.24	0
6	EDO	BBB	611	-	3,3,3	0.23	0	2,2,2	0.87	0
6	EDO	AAA	1007	-	3,3,3	0.10	0	2,2,2	0.48	0
6	EDO	AAA	1008	-	3,3,3	0.31	0	2,2,2	0.41	0
6	EDO	BBB	609	-	3,3,3	0.40	0	2,2,2	0.85	0
6	EDO	BBB	606	-	3,3,3	0.29	0	2,2,2	0.51	0
5	PGE	BBB	604	-	9,9,9	0.15	0	8,8,8	0.17	0
6	EDO	AAA	1006	-	3,3,3	0.25	0	2,2,2	0.47	0
6	EDO	BBB	608	-	3,3,3	0.29	0	2,2,2	0.75	0
3	ANP	BBB	602	-	29,33,33	1.21	4 (13%)	31,52,52	1.19	2 (6%)
5	PGE	BBB	605	-	9,9,9	0.24	0	8,8,8	0.22	0
3	ANP	AAA	1002	-	29,33,33	1.23	5 (17%)	31,52,52	1.27	5 (16%)

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	PEG	AAA	1001	-	-	1/4/4/4	-
2	PEG	BBB	601	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	AAA	1004	-	-	4/7/7/7	-
6	EDO	BBB	607	-	-	1/1/1/1	-
5	PGE	AAA	1005	-	-	3/7/7/7	-
6	EDO	BBB	610	-	-	1/1/1/1	-
6	EDO	BBB	611	-	-	0/1/1/1	-
6	EDO	AAA	1007	-	-	0/1/1/1	-
6	EDO	AAA	1008	-	-	1/1/1/1	-
6	EDO	BBB	609	-	-	1/1/1/1	-
6	EDO	BBB	606	-	-	0/1/1/1	-
5	PGE	BBB	604	-	-	3/7/7/7	-
6	EDO	AAA	1006	-	-	1/1/1/1	-
6	EDO	BBB	608	-	-	0/1/1/1	-
3	ANP	BBB	602	-	-	3/14/38/38	0/3/3/3
5	PGE	BBB	605	-	-	2/7/7/7	-
3	ANP	AAA	1002	-	-	5/14/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	602	ANP	PG-O1G	3.98	1.52	1.46
3	AAA	1002	ANP	PG-O1G	3.24	1.51	1.46
3	AAA	1002	ANP	PB-O1B	2.94	1.50	1.46
3	BBB	602	ANP	PB-O1B	2.58	1.50	1.46
3	AAA	1002	ANP	PB-O2B	-2.36	1.50	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	602	ANP	O2B-PB-O1B	4.25	118.83	109.92
3	AAA	1002	ANP	O2B-PB-O1B	3.98	118.27	109.92
3	AAA	1002	ANP	O1G-PG-N3B	-2.83	107.61	111.77
3	BBB	602	ANP	C5-C6-N6	2.68	124.43	120.35
3	AAA	1002	ANP	O2G-PG-O1G	-2.24	107.81	113.45

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1002	ANP	PG-N3B-PB-O1B
3	AAA	1002	ANP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	AAA	1002	ANP	PA-O3A-PB-O2B
3	BBB	602	ANP	PG-N3B-PB-O1B
5	AAA	1005	PGE	C4-C3-O2-C2

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	1001	PEG	1	0
5	AAA	1004	PGE	16	0
6	BBB	607	EDO	1	0
5	AAA	1005	PGE	1	0
6	BBB	610	EDO	1	0
6	BBB	611	EDO	4	0
5	BBB	604	PGE	2	0
6	BBB	608	EDO	1	0
3	AAA	1002	ANP	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 then 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 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP AAA 1002

Bond lengths

Bond angles

Torsions

Rings
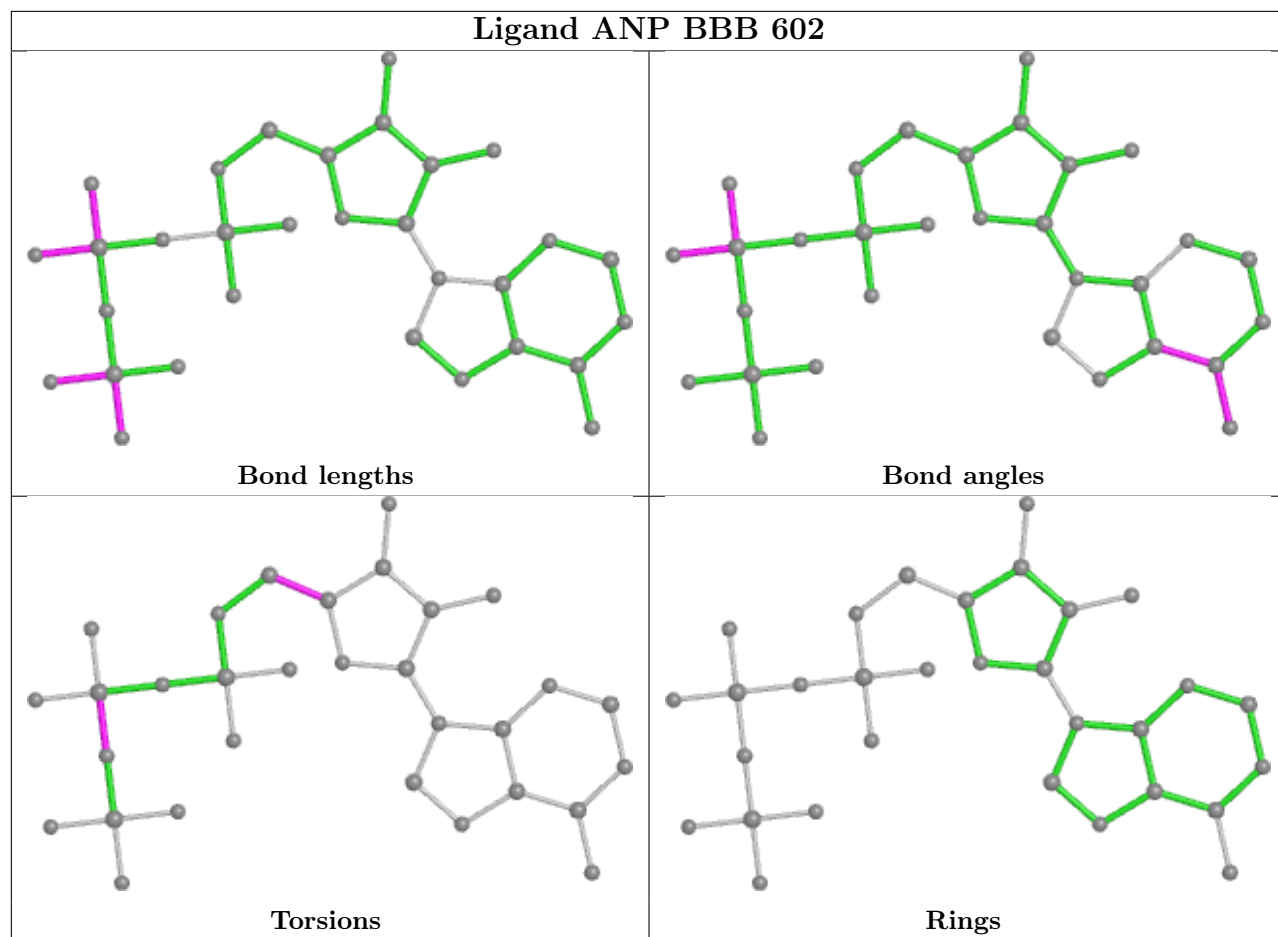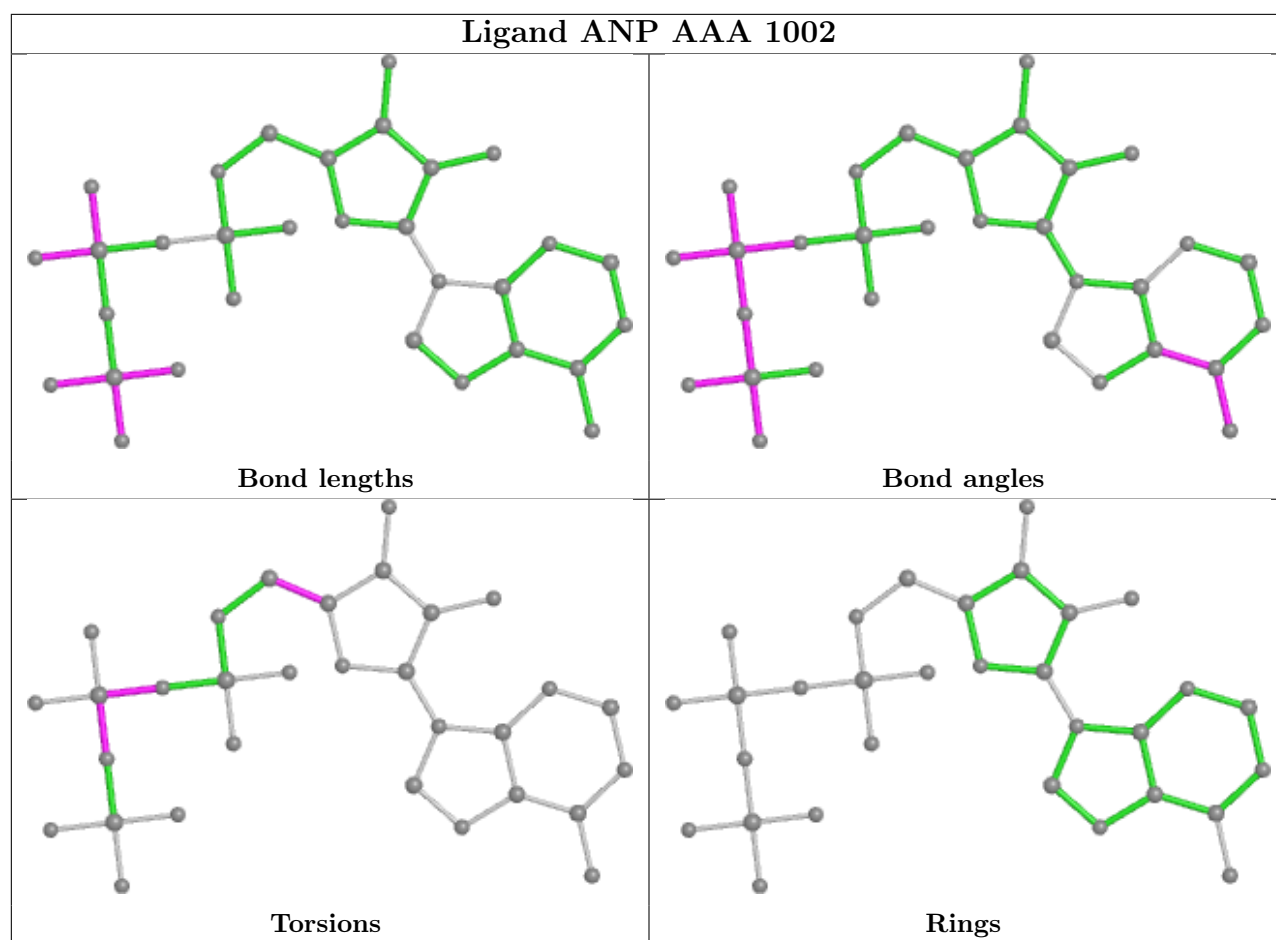
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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^2)	Q<0.9
1	AAA	304/417 (72%)	-0.53	0	100	100	25, 41, 73, 98	0
1	BBB	304/417 (72%)	-0.49	2 (0%)	87	86	23, 40, 75, 110	0
All	All	608/834 (72%)	-0.51	2 (0%)	94	93	23, 41, 75, 110	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	221	ARG	3.3
1	BBB	218[A]	GLN	2.1

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, 95th 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^2)	Q<0.9
6	EDO	BBB	607	4/4	0.60	0.24	48,58,62,69	0
6	EDO	AAA	1007	4/4	0.72	0.20	62,70,76,87	0
2	PEG	BBB	601	7/7	0.76	0.25	60,78,92,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PEG	AAA	1001	7/7	0.80	0.14	55,64,75,94	0
5	PGE	BBB	605	10/10	0.81	0.12	49,64,77,80	0
6	EDO	BBB	608	4/4	0.83	0.23	42,59,75,94	0
5	PGE	AAA	1005	10/10	0.85	0.13	54,77,109,114	0
5	PGE	AAA	1004	10/10	0.86	0.30	50,57,78,91	0
6	EDO	BBB	606	4/4	0.87	0.14	49,54,63,67	0
6	EDO	BBB	611	4/4	0.87	0.20	46,51,55,57	0
6	EDO	BBB	610	4/4	0.89	0.27	58,61,61,72	0
6	EDO	AAA	1006	4/4	0.90	0.14	53,57,60,72	0
6	EDO	BBB	609	4/4	0.91	0.12	36,42,53,56	0
5	PGE	BBB	604	10/10	0.92	0.16	46,56,68,70	0
6	EDO	AAA	1008	4/4	0.92	0.15	36,44,56,61	0
3	ANP	AAA	1002	31/31	0.94	0.13	39,60,117,138	0
3	ANP	BBB	602	31/31	0.95	0.10	49,64,113,133	0
4	ZN	BBB	603	1/1	0.98	0.13	48,48,48,48	0
4	ZN	AAA	1003	1/1	0.99	0.11	53,53,53,53	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.
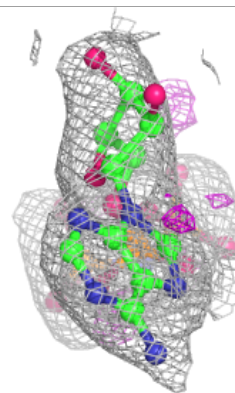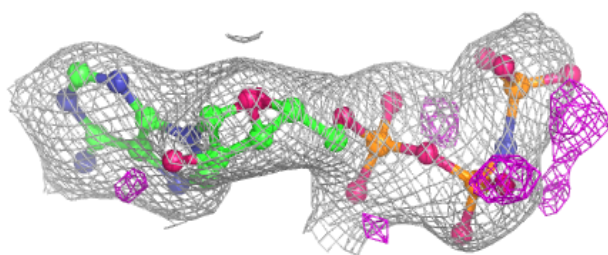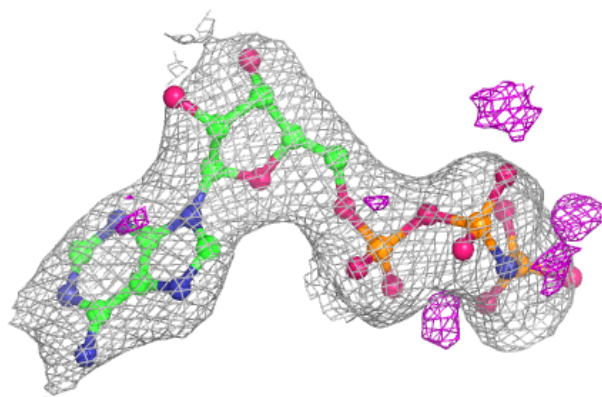

Electron density around ANP AAA 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
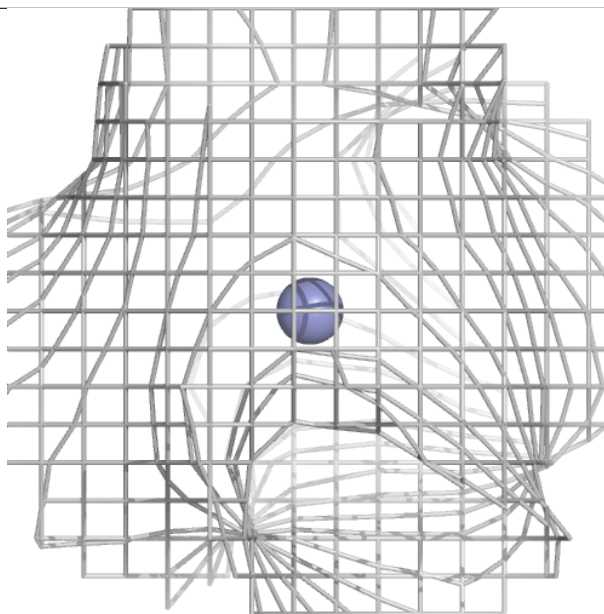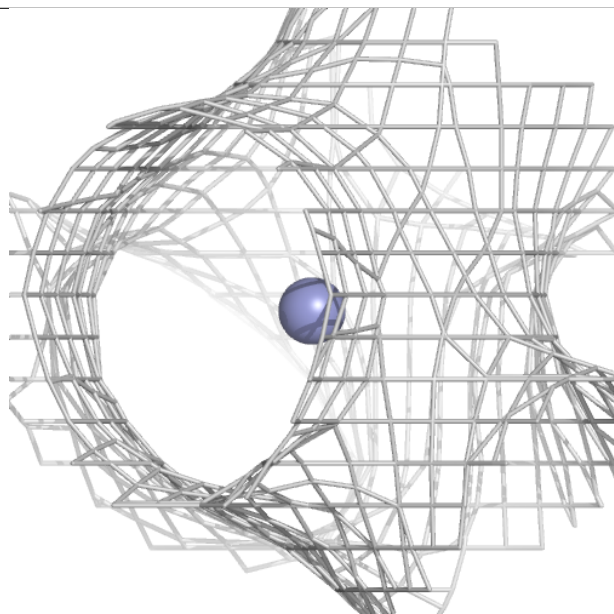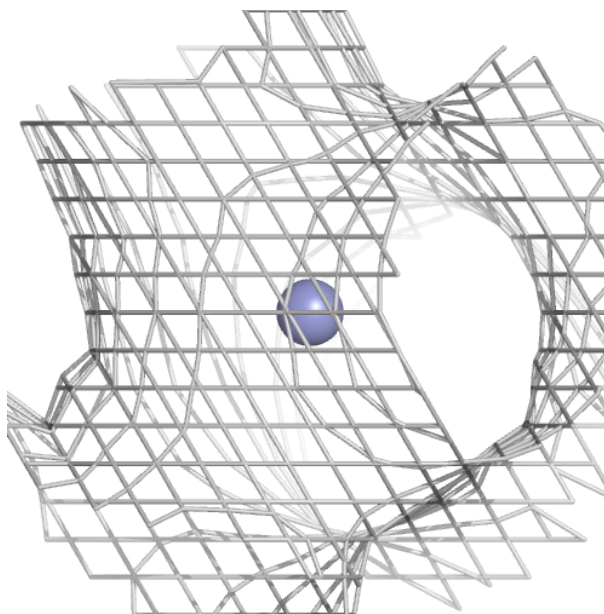mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
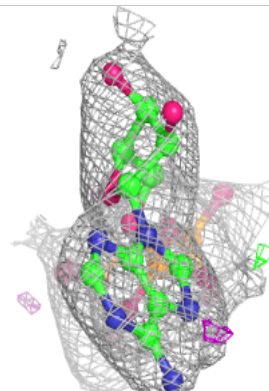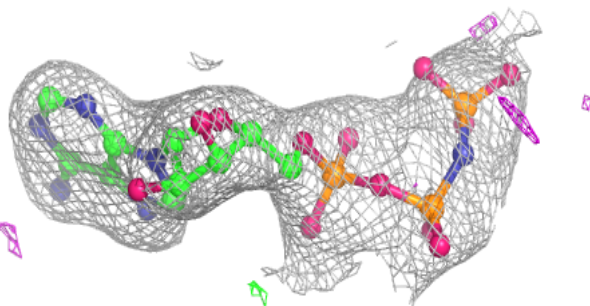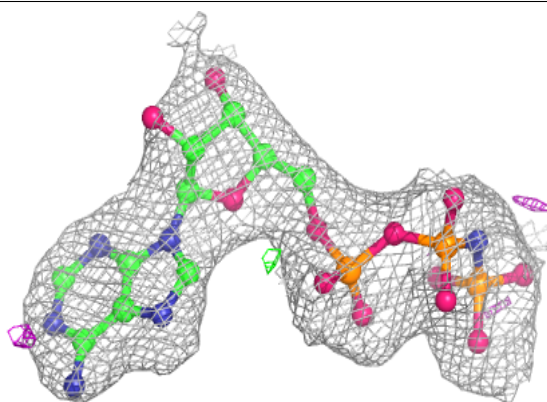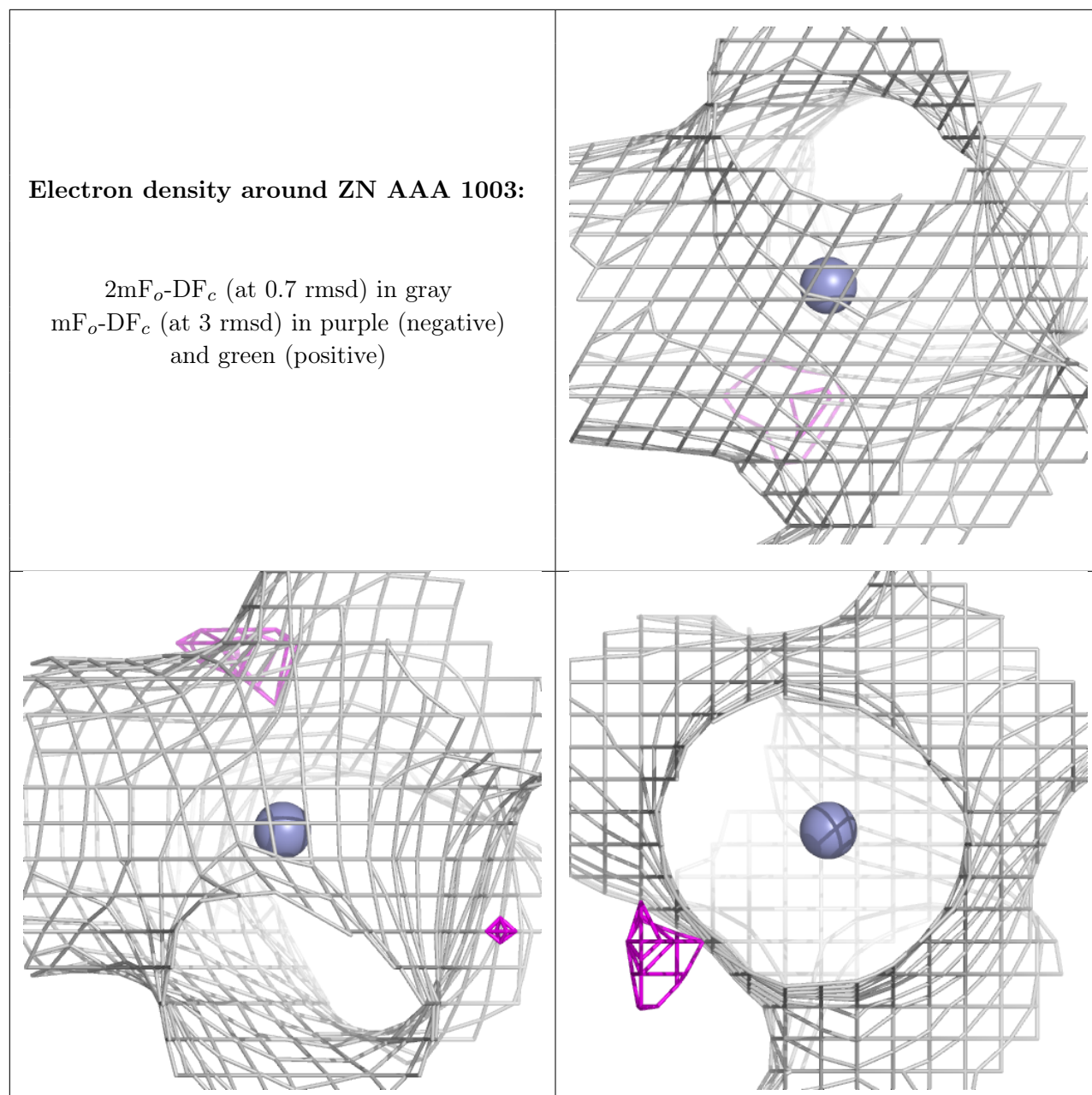
Electron density around ANP BBB 602:

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 BBB 603:

$2mF_o$-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 1003:

$2mF_o$-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.