Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:05 pm GMT

PDB ID	:	7P7W
Title	:	N-acetylglucosamine kinase from Plesiomonas shigelloides compexed with alpha-N-acetylglucosamine and ADP
Authors	:	Roy, S.; Isupov, M.N.; Harmer, N.J.; Ames, J.R.
Deposited on	:	2021-07-20
Resolution	:	1.57 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*
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.

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

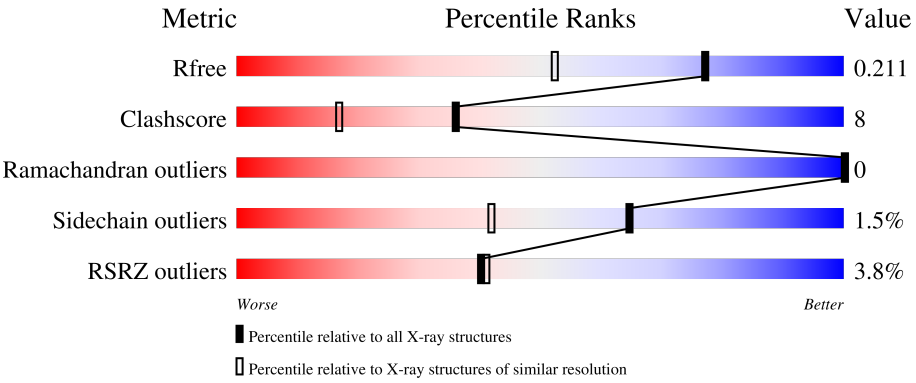
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	5% 64% 9% 27%
1	BBB	417	66% 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
3	GOL	AAA	502	-	-	X	-
3	GOL	BBB	1005	-	-	X	-
4	IMD	BBB	1004	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5811 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	28	0
			2472	1598	422	439	13			
1	BBB	306	Total	C	N	O	S	0	28	0
			2504	1612	431	450	11			

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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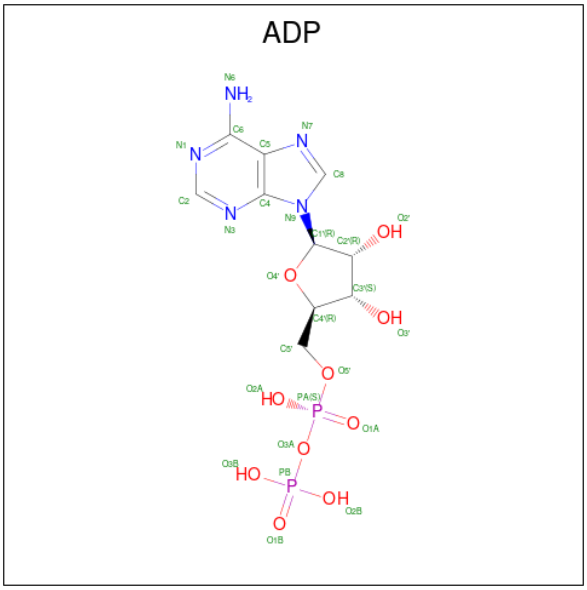
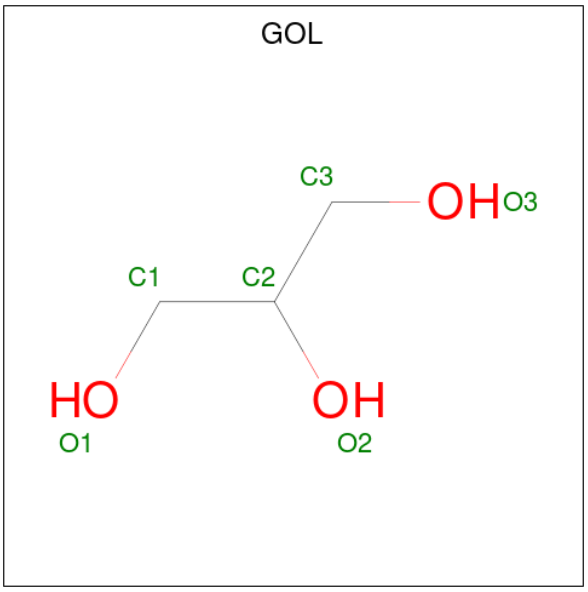
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-109	HIS	-	expression tag	UNP Q12306
BBB	-108	HIS	-	expression tag	UNP Q12306
BBB	-107	HIS	-	expression tag	UNP Q12306
BBB	-106	GLY	-	expression tag	UNP Q12306
BBB	-10	SER	-	linker	UNP Q12306
BBB	-9	SER	-	linker	UNP Q12306
BBB	-8	GLY	-	linker	UNP Q12306
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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



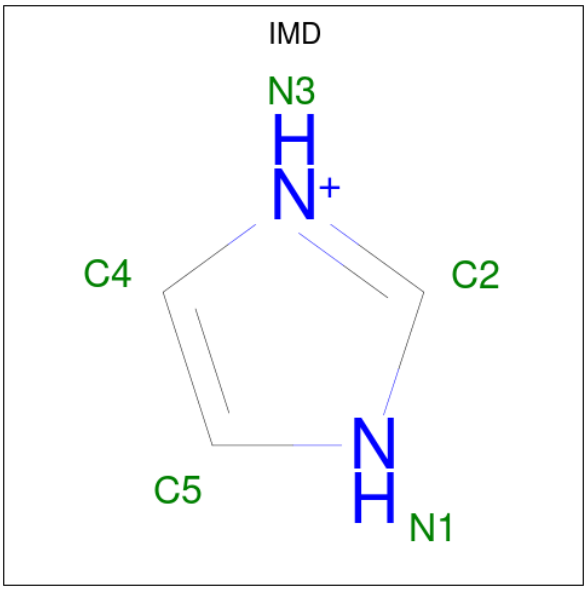
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	BBB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0
3	BBB	1	Total C O 6 3 3	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C N 5 3 2	0	0

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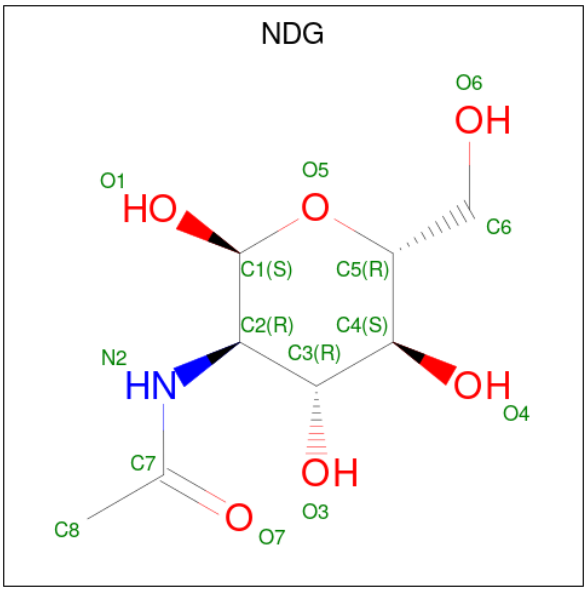
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C N 5 3 2	0	0
4	BBB	1	Total C N 5 3 2	0	0
4	BBB	1	Total C N 5 3 2	0	0

- Molecule 5 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).

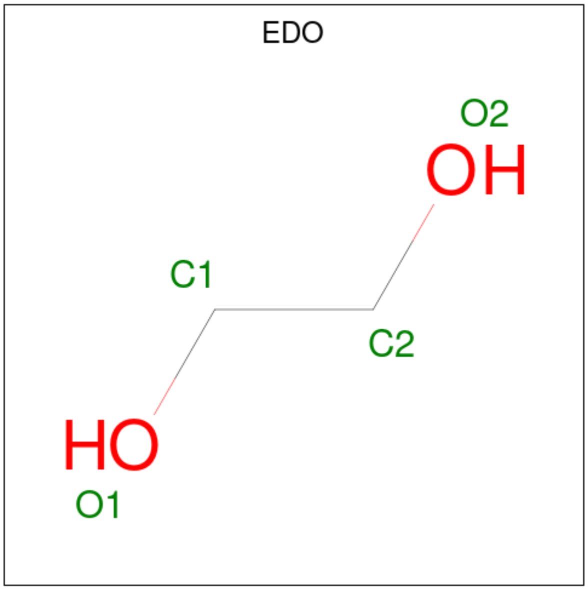


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C N O 15 8 1 6	0	0
5	BBB	1	Total C N O 15 8 1 6	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- 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 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	AAA	1	Total C O 4 2 2	0	0
7	BBB	1	Total C O 4 2 2	0	0
7	BBB	1	Total C O 4 2 2	0	0

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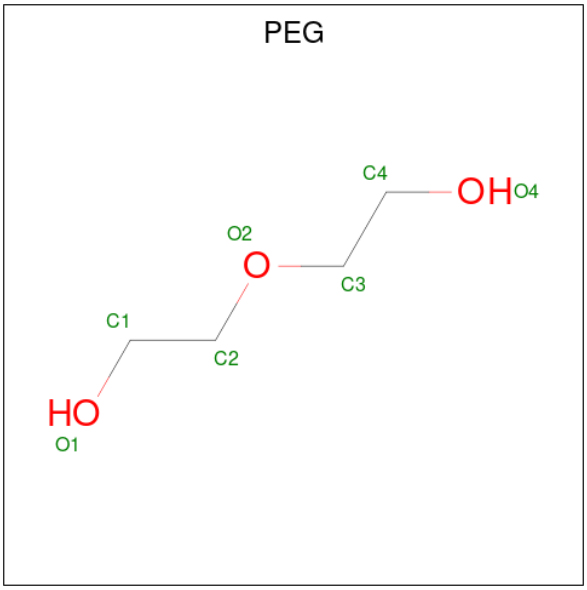
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	BBB	1	Total C O 4 2 2	0	0
7	BBB	1	Total C O 4 2 2	0	0
7	BBB	1	Total C O 4 2 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

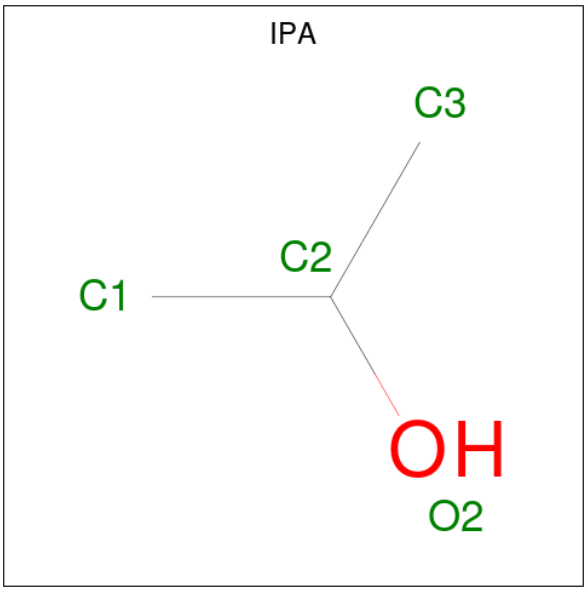


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total C O 7 4 3	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 10 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	BBB	1	Total C O 4 3 1	0	0

- Molecule 11 is water.

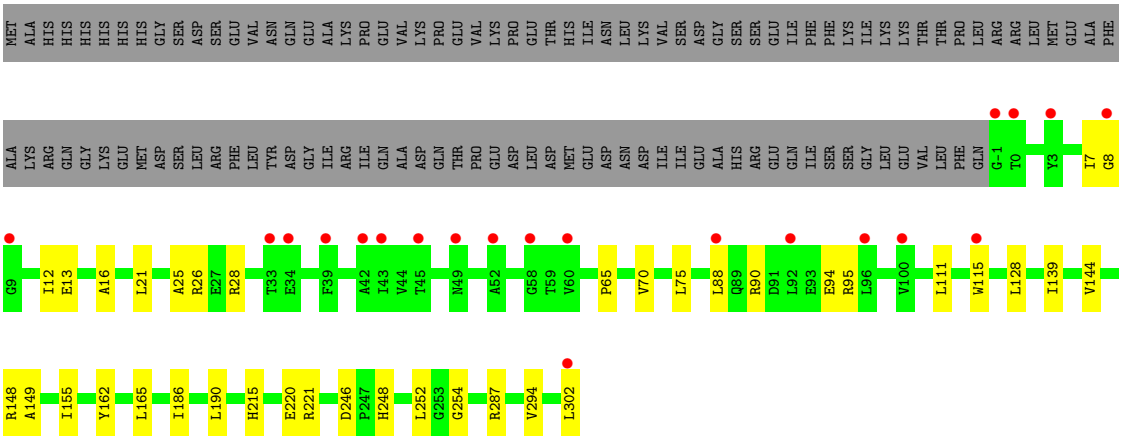
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	AAA	301	Total O 301 301	0	0
11	BBB	327	Total O 327 327	0	0

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.

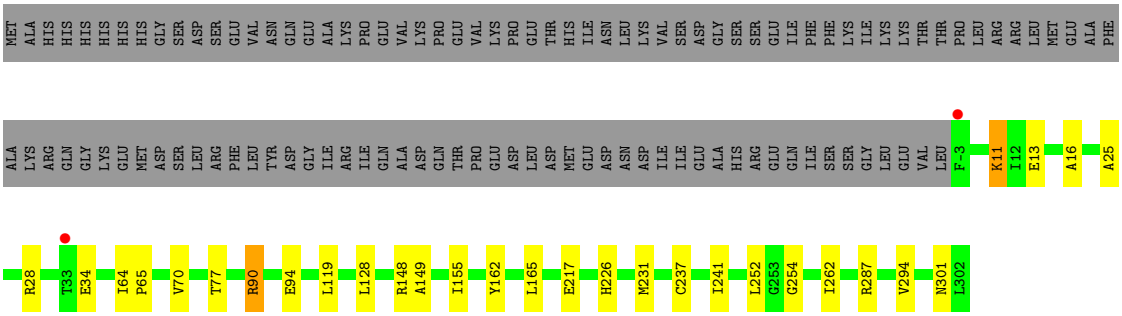
• Molecule 1: Ubiquitin-like protein SMT3,N-acetyl-D-glucosamine kinase

Chain AAA:



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

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.10Å 115.10Å 120.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.68 – 1.57 99.68 – 1.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.68-1.57) 100.0 (99.68-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.211 0.186 , 0.211	Depositor DCC
R_{free} test set	6471 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5811	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: EDO, ZN, NDG, IMD, GOL, K, PEG, ADP, IPA

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	0.37	0/2605	0.67	0/3520
1	BBB	0.35	0/2630	0.68	0/3554
All	All	0.36	0/5235	0.68	0/7074

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	2472	0	2569	47	0
1	BBB	2504	0	2576	33	0
2	AAA	27	0	12	1	0
2	BBB	27	0	12	0	0
3	AAA	12	0	16	7	0
3	BBB	6	0	8	8	0
4	AAA	10	0	10	2	0
4	BBB	10	0	10	5	0
5	AAA	15	0	12	0	0
5	BBB	15	0	12	0	0
6	AAA	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	2	0	0	0	0
7	AAA	48	0	72	3	0
7	BBB	20	0	30	1	0
8	AAA	7	0	10	0	0
9	AAA	1	0	0	0	0
9	BBB	1	0	0	0	0
10	BBB	4	0	8	0	0
11	AAA	301	0	0	6	0
11	BBB	327	0	0	5	0
All	All	5811	0	5357	84	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 8.

All (84) 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:95[B]:ARG:NH1	11:AAA:601:HOH:O	1.61	1.25
1:AAA:254:GLY:H	3:AAA:502:GOL:H12	1.15	1.08
4:BBB:1004:IMD:C5	3:BBB:1005:GOL:H12	1.96	0.96
1:AAA:254:GLY:H	3:AAA:502:GOL:C1	1.83	0.91
1:BBB:217[A]:GLU:OE1	11:BBB:1101:HOH:O	1.91	0.89
1:AAA:75[B]:LEU:HD11	1:AAA:88:LEU:HB2	1.55	0.88
4:BBB:1004:IMD:H5	3:BBB:1005:GOL:H12	1.55	0.88
1:AAA:254:GLY:N	3:AAA:502:GOL:H12	1.94	0.83
1:AAA:111:LEU:HD21	1:AAA:144[B]:VAL:HG23	1.65	0.79
1:BBB:64:ILE:CG1	1:BBB:65[B]:PRO:HD2	2.12	0.79
1:AAA:111:LEU:CD2	1:AAA:144[B]:VAL:HG23	2.14	0.78
3:AAA:502:GOL:H31	4:AAA:503:IMD:H4	1.65	0.77
1:BBB:254:GLY:H	3:BBB:1005:GOL:H32	1.50	0.75
1:BBB:231[B]:MET:HE2	1:BBB:262:ILE:HA	1.69	0.73
1:BBB:64:ILE:HG12	1:BBB:65[B]:PRO:HD2	1.70	0.73
1:BBB:65[A]:PRO:O	1:BBB:77[A]:THR:HG22	1.89	0.72
1:BBB:231[B]:MET:HE3	11:BBB:1284:HOH:O	1.89	0.72
4:BBB:1004:IMD:C5	3:BBB:1005:GOL:C1	2.67	0.72
1:BBB:128[A]:LEU:CD1	1:BBB:155:ILE:HD11	2.20	0.71
1:BBB:128[B]:LEU:HD22	1:BBB:155:ILE:HD11	1.73	0.68
3:AAA:502:GOL:H11	11:AAA:827:HOH:O	1.94	0.67
1:AAA:28[B]:ARG:HD2	11:AAA:709:HOH:O	1.94	0.67
4:BBB:1004:IMD:C4	3:BBB:1005:GOL:H12	2.24	0.66
1:AAA:220:GLU:HB2	7:AAA:515:EDO:H11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BBB:1004:IMD:H5	3:BBB:1005:GOL:C1	2.24	0.65
1:AAA:128[A]:LEU:CD1	1:AAA:155:ILE:HD11	2.25	0.65
1:AAA:111:LEU:HG	1:AAA:144[B]:VAL:CG2	2.27	0.65
1:AAA:139:ILE:CD1	1:AAA:144[B]:VAL:HG22	2.26	0.65
1:AAA:75[B]:LEU:HD11	1:AAA:88:LEU:CB	2.28	0.64
1:BBB:64:ILE:HG13	1:BBB:65[B]:PRO:HD2	1.79	0.64
1:AAA:13:GLU:CG	1:AAA:294[B]:VAL:HG11	2.32	0.60
1:BBB:254:GLY:N	3:BBB:1005:GOL:H32	2.16	0.60
1:BBB:254:GLY:H	3:BBB:1005:GOL:C3	2.15	0.59
1:BBB:226:HIS:HD2	11:BBB:1276:HOH:O	1.85	0.59
1:AAA:128[B]:LEU:HD22	1:AAA:155:ILE:HD11	1.86	0.57
1:AAA:111:LEU:HG	1:AAA:144[B]:VAL:HG21	1.86	0.56
3:AAA:502:GOL:H31	4:AAA:503:IMD:C4	2.35	0.56
1:BBB:90:ARG:O	1:BBB:94[B]:GLU:HG3	2.06	0.56
1:AAA:13:GLU:CG	1:AAA:294[A]:VAL:HG21	2.37	0.54
1:AAA:165[B]:LEU:HD11	1:BBB:162:TYR:HB2	1.89	0.54
1:AAA:221:ARG:HH12	3:AAA:505:GOL:H31	1.74	0.53
1:AAA:111:LEU:HD21	1:AAA:144[B]:VAL:CG2	2.37	0.52
1:BBB:70[B]:VAL:HG11	1:BBB:149:ALA:HA	1.91	0.51
1:BBB:16:ALA:HB3	1:BBB:25:ALA:HB3	1.94	0.50
1:AAA:139:ILE:HD13	1:AAA:144[B]:VAL:HG22	1.93	0.49
1:AAA:13:GLU:HG2	1:AAA:294[B]:VAL:HG11	1.94	0.49
1:AAA:111:LEU:CG	1:AAA:144[B]:VAL:CG2	2.90	0.49
1:AAA:13:GLU:HG3	1:AAA:294[A]:VAL:HG21	1.95	0.49
1:BBB:13:GLU:HG2	1:BBB:294:VAL:HG21	1.95	0.49
1:AAA:186[B]:ILE:HD13	1:AAA:190:LEU:HD12	1.94	0.48
1:AAA:13:GLU:HG3	1:AAA:294[B]:VAL:HG11	1.94	0.48
1:BBB:119:LEU:HG	1:BBB:287[A]:ARG:HH12	1.79	0.48
1:AAA:28[B]:ARG:HD3	11:AAA:612:HOH:O	2.14	0.48
11:AAA:637:HOH:O	7:BBB:1013:EDO:H11	2.14	0.47
1:BBB:64:ILE:CG1	1:BBB:65[B]:PRO:CD	2.89	0.47
1:AAA:8:GLY:HA3	2:AAA:501:ADP:O1B	2.14	0.47
1:AAA:248:HIS:HA	1:BBB:148[B]:ARG:HB2	1.97	0.47
1:AAA:128[A]:LEU:HD23	1:AAA:252:LEU:HD22	1.97	0.47
1:AAA:115[A]:TRP:HB3	11:AAA:655:HOH:O	2.15	0.46
1:AAA:111:LEU:CG	1:AAA:144[B]:VAL:HG21	2.44	0.46
1:AAA:7:ILE:O	1:AAA:65:PRO:HD3	2.15	0.46
1:AAA:111:LEU:CD2	1:AAA:144[B]:VAL:CG2	2.89	0.44
1:BBB:301:ASN:ND2	11:BBB:1110:HOH:O	2.50	0.44
1:AAA:246:ASP:OD1	1:BBB:148[A]:ARG:HB3	2.17	0.44
1:AAA:13:GLU:HG2	1:AAA:294[A]:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:64:ILE:HG13	1:BBB:65[B]:PRO:CD	2.48	0.44
1:AAA:162:TYR:HB2	1:BBB:165[A]:LEU:HD11	2.00	0.43
1:BBB:28[B]:ARG:NH2	11:BBB:1103:HOH:O	2.41	0.43
1:BBB:128[A]:LEU:HD23	1:BBB:252:LEU:HD22	1.99	0.43
1:BBB:128[B]:LEU:CD2	1:BBB:155:ILE:HD11	2.44	0.43
1:AAA:7:ILE:HG12	1:AAA:12:ILE:HG12	2.00	0.43
1:AAA:220:GLU:CB	7:AAA:515:EDO:H11	2.48	0.42
1:AAA:165[B]:LEU:HD13	1:BBB:165[B]:LEU:HD23	2.02	0.42
1:AAA:16:ALA:HB3	1:AAA:25:ALA:HB3	2.03	0.41
1:BBB:128[A]:LEU:HD23	1:BBB:252:LEU:CD2	2.50	0.41
1:AAA:128[B]:LEU:CD2	1:AAA:155:ILE:HD11	2.50	0.41
1:AAA:90[B]:ARG:NH2	1:AAA:90[B]:ARG:HG3	2.35	0.41
1:AAA:215:HIS:CG	7:AAA:515:EDO:H12	2.56	0.41
1:AAA:21:LEU:HD21	1:AAA:302:LEU:HD21	2.02	0.40
1:BBB:11:LYS:HD2	1:BBB:28[B]:ARG:NH2	2.36	0.40
1:BBB:231[B]:MET:CE	1:BBB:262:ILE:HA	2.44	0.40
1:AAA:70[B]:VAL:HG11	1:AAA:149:ALA:HA	2.04	0.40
1:AAA:128[A]:LEU:HD23	1:AAA:252:LEU:CD2	2.51	0.40
1:BBB:237:CYS:O	1:BBB:241[B]:ILE:HG12	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	
1	AAA	330/417 (79%)	324 (98%)	6 (2%)	0	100	100
1	BBB	332/417 (80%)	327 (98%)	5 (2%)	0	100	100
All	All	662/834 (79%)	651 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	265/340 (78%)	259 (98%)	6 (2%)	50 23
1	BBB	267/340 (78%)	264 (99%)	3 (1%)	73 55
All	All	532/680 (78%)	523 (98%)	9 (2%)	65 36

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	26	ARG
1	AAA	94[A]	GLU
1	AAA	94[B]	GLU
1	AAA	148	ARG
1	AAA	287[A]	ARG
1	AAA	287[B]	ARG
1	BBB	11	LYS
1	BBB	34	GLU
1	BBB	90	ARG

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.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 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	AAA	516	-	3,3,3	0.18	0	2,2,2	0.24	0
2	ADP	BBB	1002	-	24,29,29	0.67	0	29,45,45	0.92	1 (3%)
7	EDO	AAA	517	-	3,3,3	0.11	0	2,2,2	0.43	0
7	EDO	AAA	512	-	3,3,3	0.15	0	2,2,2	0.26	0
3	GOL	AAA	505	-	5,5,5	0.09	0	5,5,5	0.37	0
7	EDO	AAA	511	-	3,3,3	0.06	0	2,2,2	0.17	0
7	EDO	BBB	1009	-	3,3,3	0.12	0	2,2,2	0.06	0
7	EDO	AAA	509	-	3,3,3	0.48	0	2,2,2	0.16	0
7	EDO	AAA	514	-	3,3,3	0.09	0	2,2,2	0.18	0
3	GOL	BBB	1005	-	5,5,5	0.13	0	5,5,5	0.40	0
7	EDO	AAA	513	-	3,3,3	0.03	0	2,2,2	0.17	0
7	EDO	BBB	1013	-	3,3,3	0.07	0	2,2,2	0.16	0
4	IMD	BBB	1004	-	3,5,5	0.30	0	4,5,5	0.63	0
7	EDO	AAA	519	-	3,3,3	0.07	0	2,2,2	0.32	0
4	IMD	AAA	504	-	3,5,5	0.27	0	4,5,5	0.68	0
4	IMD	BBB	1003	-	3,5,5	0.27	0	4,5,5	0.55	0
10	IPA	BBB	1001	-	3,3,3	0.10	0	3,3,3	0.30	0
5	NDG	BBB	1006	-	15,15,15	0.34	0	21,21,21	0.74	0
7	EDO	BBB	1011	-	3,3,3	0.09	0	2,2,2	0.10	0
8	PEG	AAA	521	-	6,6,6	0.15	0	5,5,5	0.11	0
7	EDO	AAA	520	-	3,3,3	0.11	0	2,2,2	0.18	0
7	EDO	BBB	1010	-	3,3,3	0.06	0	2,2,2	0.17	0
7	EDO	AAA	515	-	3,3,3	0.12	0	2,2,2	0.40	0
3	GOL	AAA	502	-	5,5,5	0.11	0	5,5,5	0.60	0
5	NDG	AAA	506	-	15,15,15	0.33	0	21,21,21	1.70	2 (9%)
7	EDO	AAA	518	-	3,3,3	0.10	0	2,2,2	0.22	0
2	ADP	AAA	501	-	24,29,29	0.60	0	29,45,45	1.01	2 (6%)
4	IMD	AAA	503	-	3,5,5	0.27	0	4,5,5	0.65	0
7	EDO	AAA	510	-	3,3,3	0.08	0	2,2,2	0.28	0
7	EDO	BBB	1012	-	3,3,3	0.06	0	2,2,2	0.29	0

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	AAA	516	-	-	0/1/1/1	-
2	ADP	BBB	1002	-	-	6/12/32/32	0/3/3/3
7	EDO	AAA	517	-	-	1/1/1/1	-
7	EDO	AAA	512	-	-	1/1/1/1	-
3	GOL	AAA	505	-	-	4/4/4/4	-
7	EDO	AAA	511	-	-	1/1/1/1	-
7	EDO	BBB	1009	-	-	1/1/1/1	-
7	EDO	AAA	509	-	-	0/1/1/1	-
7	EDO	AAA	514	-	-	0/1/1/1	-
3	GOL	BBB	1005	-	-	4/4/4/4	-
7	EDO	AAA	513	-	-	1/1/1/1	-
7	EDO	BBB	1013	-	-	1/1/1/1	-
4	IMD	BBB	1004	-	-	-	0/1/1/1
7	EDO	AAA	519	-	-	0/1/1/1	-
4	IMD	AAA	504	-	-	-	0/1/1/1
4	IMD	BBB	1003	-	-	-	0/1/1/1
5	NDG	BBB	1006	-	-	0/6/26/26	0/1/1/1
7	EDO	BBB	1011	-	-	1/1/1/1	-
8	PEG	AAA	521	-	-	1/4/4/4	-
7	EDO	AAA	520	-	-	0/1/1/1	-
7	EDO	BBB	1010	-	-	1/1/1/1	-
7	EDO	AAA	515	-	-	1/1/1/1	-
3	GOL	AAA	502	-	-	3/4/4/4	-
5	NDG	AAA	506	-	-	0/6/26/26	0/1/1/1
7	EDO	AAA	518	-	-	1/1/1/1	-
2	ADP	AAA	501	-	-	1/12/32/32	0/3/3/3
4	IMD	AAA	503	-	-	-	0/1/1/1
7	EDO	AAA	510	-	-	1/1/1/1	-
7	EDO	BBB	1012	-	-	1/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AAA	506	NDG	O5-C1-C2	6.74	116.29	109.52
5	AAA	506	NDG	C1-C2-N2	2.59	113.73	110.73
2	AAA	501	ADP	C5-C6-N6	2.41	124.01	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	1002	ADP	C5-C6-N6	2.22	123.73	120.35
2	AAA	501	ADP	PA-O3A-PB	2.09	140.00	132.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	1002	ADP	PB-O3A-PA-O5'
2	BBB	1002	ADP	C5'-O5'-PA-O2A
3	AAA	505	GOL	O1-C1-C2-O2
3	AAA	505	GOL	O1-C1-C2-C3
3	BBB	1005	GOL	O1-C1-C2-C3
3	BBB	1005	GOL	C1-C2-C3-O3
3	AAA	505	GOL	C1-C2-C3-O3
8	AAA	521	PEG	O2-C3-C4-O4
7	AAA	511	EDO	O1-C1-C2-O2
7	AAA	518	EDO	O1-C1-C2-O2
7	BBB	1010	EDO	O1-C1-C2-O2
3	BBB	1005	GOL	O1-C1-C2-O2
3	AAA	502	GOL	O1-C1-C2-O2
3	BBB	1005	GOL	O2-C2-C3-O3
7	AAA	512	EDO	O1-C1-C2-O2
2	AAA	501	ADP	PB-O3A-PA-O5'
2	BBB	1002	ADP	PA-O3A-PB-O3B
2	BBB	1002	ADP	C5'-O5'-PA-O3A
2	BBB	1002	ADP	C5'-O5'-PA-O1A
7	AAA	515	EDO	O1-C1-C2-O2
7	AAA	510	EDO	O1-C1-C2-O2
7	AAA	513	EDO	O1-C1-C2-O2
7	AAA	517	EDO	O1-C1-C2-O2
7	BBB	1011	EDO	O1-C1-C2-O2
3	AAA	505	GOL	O2-C2-C3-O3
3	AAA	502	GOL	O1-C1-C2-C3
7	BBB	1009	EDO	O1-C1-C2-O2
2	BBB	1002	ADP	C3'-C4'-C5'-O5'
7	BBB	1012	EDO	O1-C1-C2-O2
7	BBB	1013	EDO	O1-C1-C2-O2
3	AAA	502	GOL	O2-C2-C3-O3

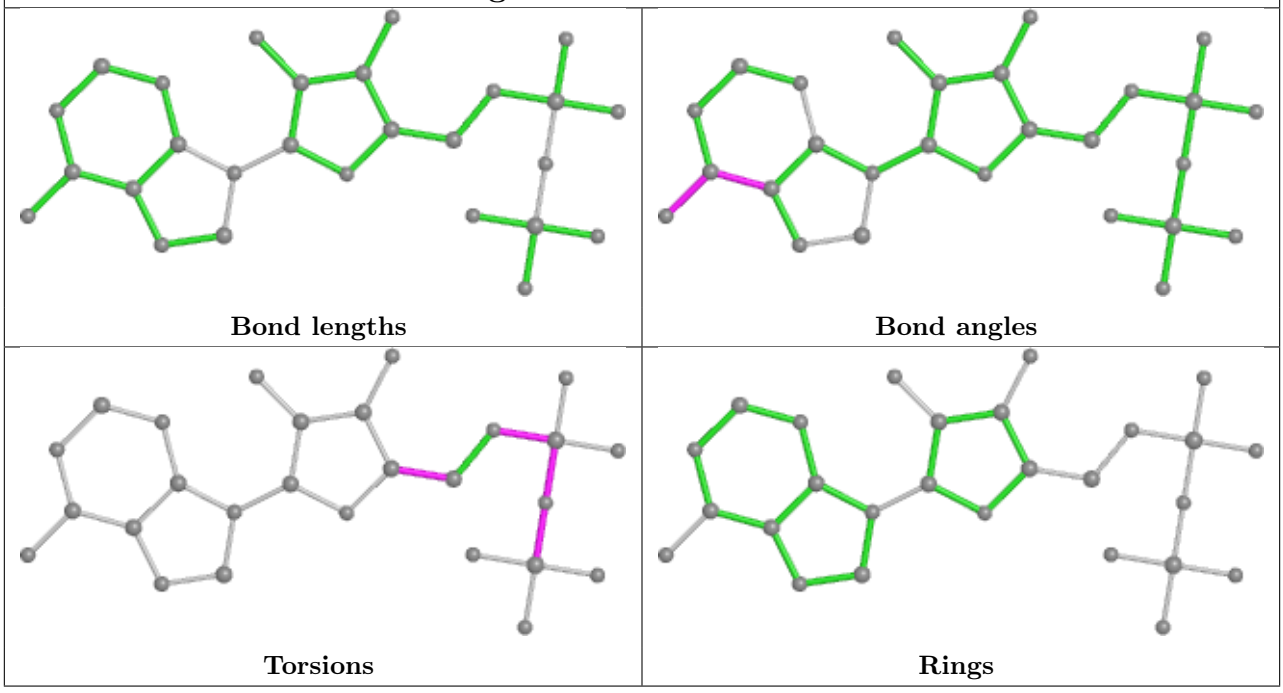
There are no ring outliers.

8 monomers are involved in 20 short contacts:

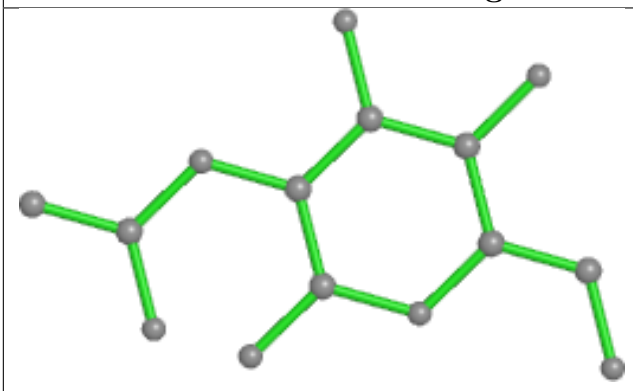
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	505	GOL	1	0
3	BBB	1005	GOL	8	0
7	BBB	1013	EDO	1	0
4	BBB	1004	IMD	5	0
7	AAA	515	EDO	3	0
3	AAA	502	GOL	6	0
2	AAA	501	ADP	1	0
4	AAA	503	IMD	2	0

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 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.

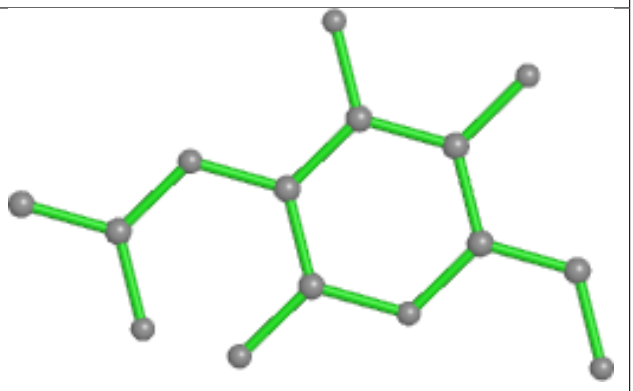
Ligand ADP BBB 1002



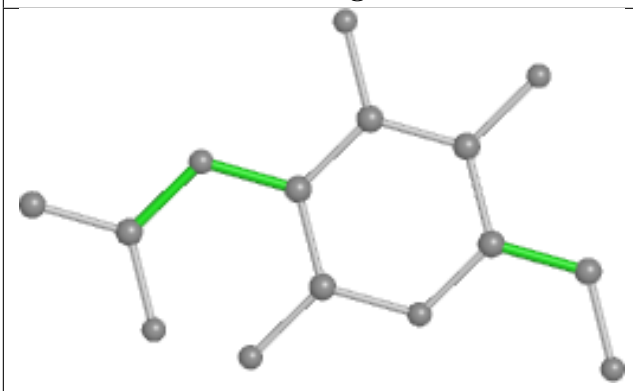
Ligand NDG BBB 1006



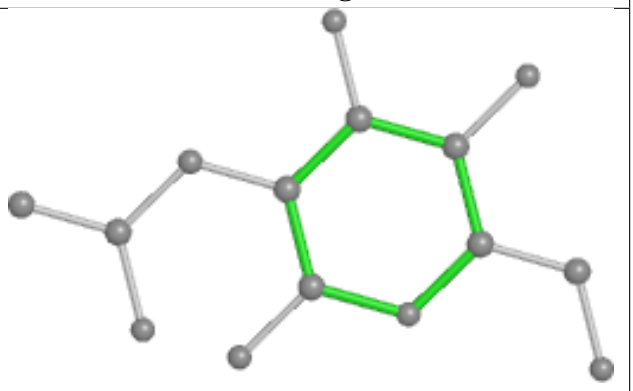
Bond lengths



Bond angles

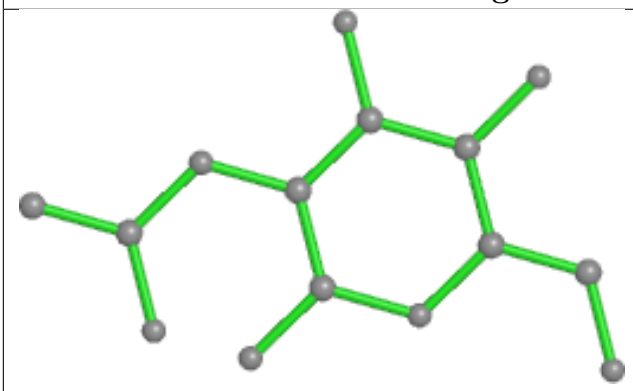


Torsions

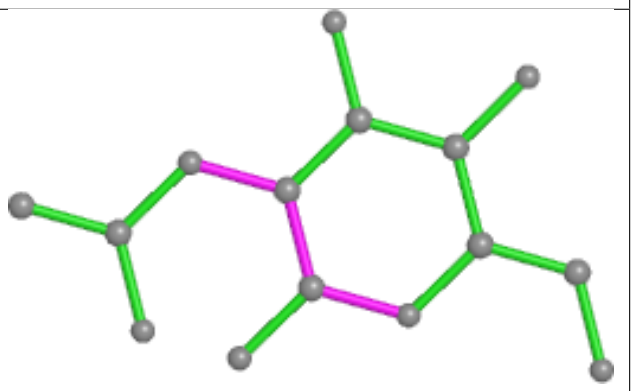


Rings

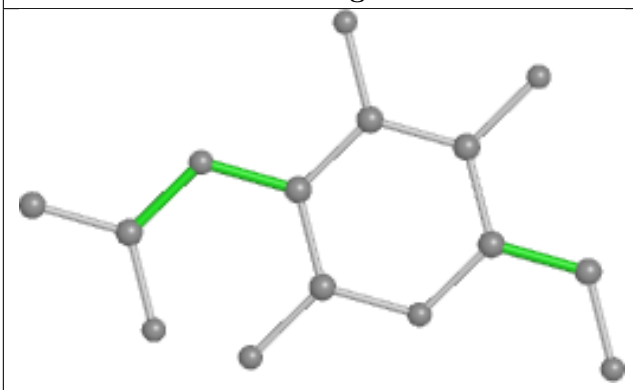
Ligand NDG AAA 506



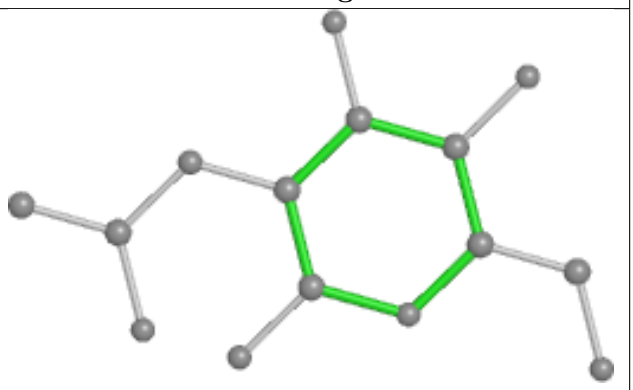
Bond lengths



Bond angles

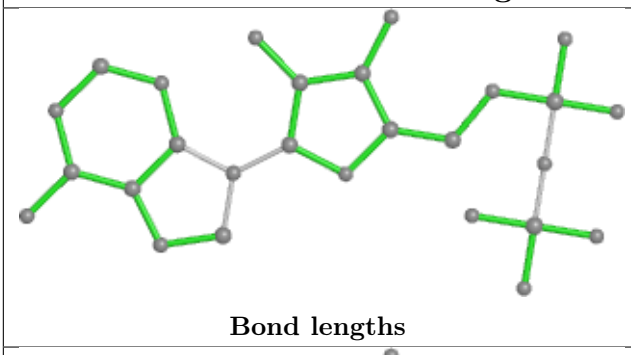


Torsions

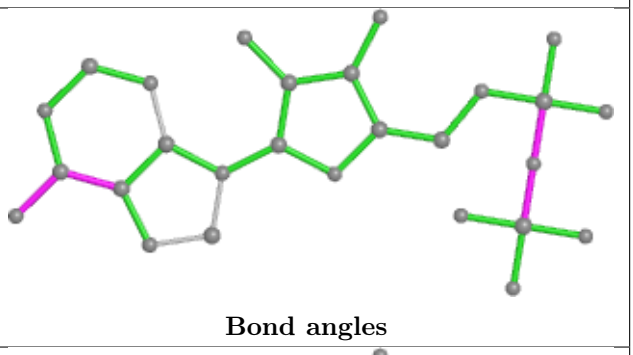


Rings

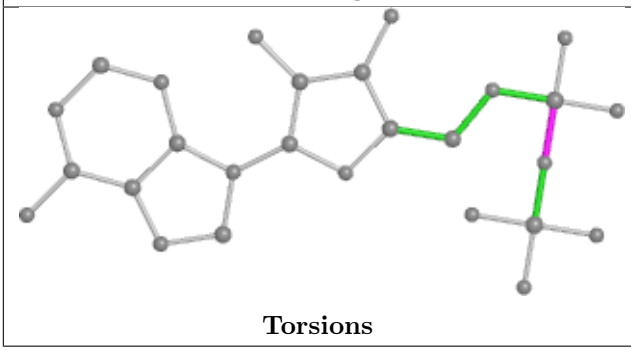
Ligand ADP AAA 501



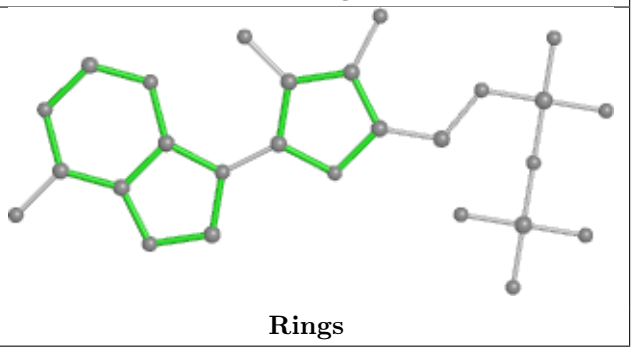
Bond lengths



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, 95^{th} 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%)	0.13	21 (6%) 16 17	16, 25, 46, 85	0
1	BBB	306/417 (73%)	-0.24	2 (0%) 87 88	17, 24, 40, 82	0
All	All	610/834 (73%)	-0.06	23 (3%) 40 41	16, 24, 44, 85	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	-1	GLY	7.6
1	AAA	115[A]	TRP	5.5
1	AAA	88	LEU	4.3
1	AAA	42	ALA	3.9
1	AAA	58	GLY	3.9
1	AAA	60	VAL	3.8
1	AAA	39	PHE	3.5
1	BBB	-3	PHE	3.5
1	AAA	0	THR	3.2
1	AAA	34	GLU	3.0
1	AAA	9	GLY	3.0
1	AAA	92	LEU	2.8
1	AAA	43	ILE	2.8
1	AAA	33	THR	2.7
1	AAA	96	LEU	2.6
1	BBB	33	THR	2.4
1	AAA	3	TYR	2.4
1	AAA	100	VAL	2.4
1	AAA	302	LEU	2.3
1	AAA	49	ASN	2.3
1	AAA	52	ALA	2.3
1	AAA	45	THR	2.2
1	AAA	8	GLY	2.1

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

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

6.3 Carbohydrates (i)

There are no 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^{th} 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
7	EDO	AAA	512	4/4	0.65	0.11	44,51,53,54	0
4	IMD	BBB	1004	5/5	0.72	0.34	79,86,98,99	0
7	EDO	BBB	1013	4/4	0.72	0.14	39,40,42,44	4
3	GOL	BBB	1005	6/6	0.77	0.29	29,42,46,50	6
7	EDO	AAA	519	4/4	0.78	0.13	49,50,57,57	0
3	GOL	AAA	505	6/6	0.80	0.16	49,58,66,68	0
7	EDO	AAA	518	4/4	0.81	0.09	55,59,60,66	0
7	EDO	AAA	510	4/4	0.82	0.21	50,54,63,70	0
7	EDO	BBB	1011	4/4	0.83	0.16	59,61,67,67	0
7	EDO	AAA	520	4/4	0.85	0.11	58,59,61,65	0
7	EDO	BBB	1009	4/4	0.85	0.18	50,51,61,70	0
2	ADP	BBB	1002	27/27	0.86	0.11	25,32,57,62	0
7	EDO	AAA	514	4/4	0.87	0.12	47,68,70,71	0
8	PEG	AAA	521	7/7	0.88	0.14	39,45,61,62	0
7	EDO	BBB	1010	4/4	0.89	0.08	40,53,57,58	0
7	EDO	AAA	511	4/4	0.89	0.16	65,73,74,97	0
7	EDO	AAA	517	4/4	0.89	0.12	52,55,56,62	0
7	EDO	AAA	513	4/4	0.89	0.18	53,60,67,83	0
4	IMD	AAA	504	5/5	0.90	0.14	45,49,50,53	0
7	EDO	BBB	1012	4/4	0.90	0.12	59,61,63,65	0
3	GOL	AAA	502	6/6	0.91	0.16	25,34,43,44	6
7	EDO	AAA	515	4/4	0.91	0.25	34,44,49,70	0
4	IMD	AAA	503	5/5	0.91	0.17	47,50,54,59	0
10	IPA	BBB	1001	4/4	0.91	0.15	54,56,58,65	0
6	ZN	BBB	1008	1/1	0.92	0.05	41,41,41,41	1
4	IMD	BBB	1003	5/5	0.92	0.08	40,43,45,47	0
7	EDO	AAA	516	4/4	0.93	0.18	41,49,52,62	0

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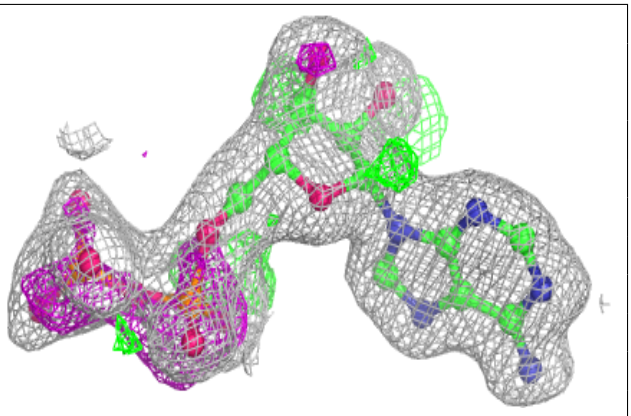
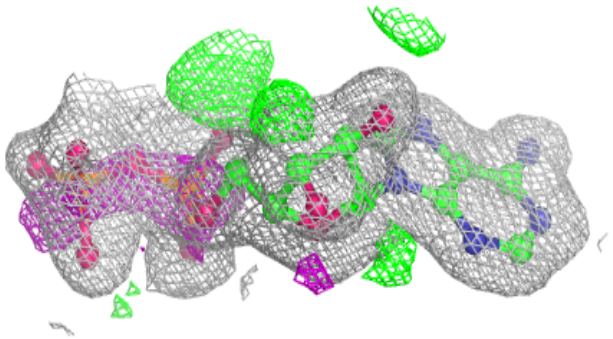
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NDG	AAA	506	15/15	0.93	0.09	25,27,34,35	0
5	NDG	BBB	1006	15/15	0.94	0.09	22,25,32,32	0
2	ADP	AAA	501	27/27	0.94	0.09	22,27,38,45	0
7	EDO	AAA	509	4/4	0.97	0.29	35,36,39,42	0
6	ZN	AAA	508	1/1	0.99	0.05	37,37,37,37	1
9	K	AAA	522	1/1	0.99	0.10	26,26,26,26	1
6	ZN	BBB	1007	1/1	0.99	0.13	20,20,20,20	0
9	K	BBB	1014	1/1	1.00	0.10	25,25,25,25	1
6	ZN	AAA	507	1/1	1.00	0.12	22,22,22,22	0

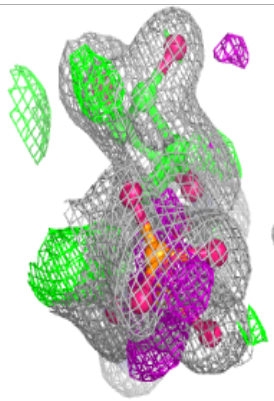
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP BBB 1002:

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

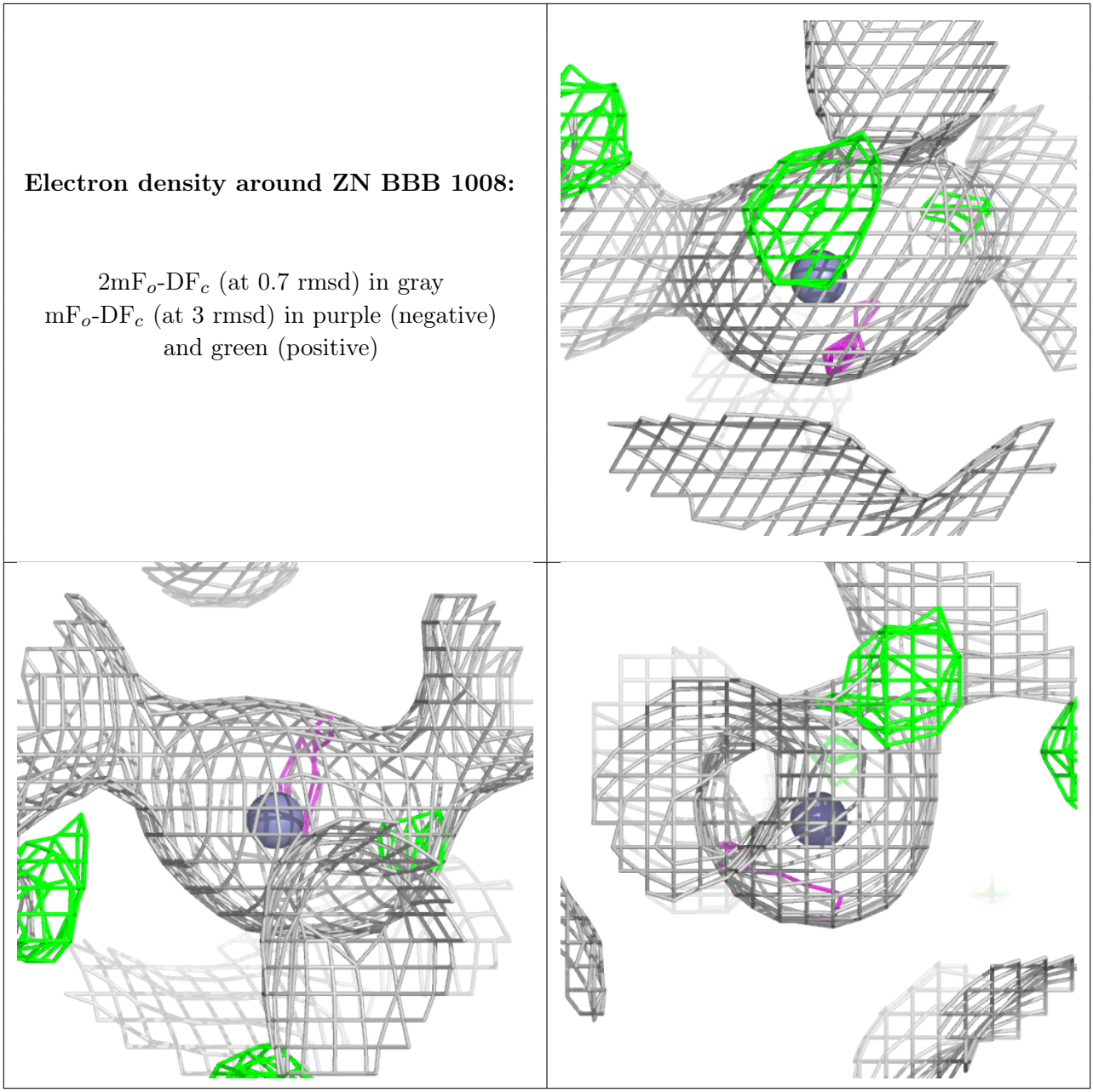






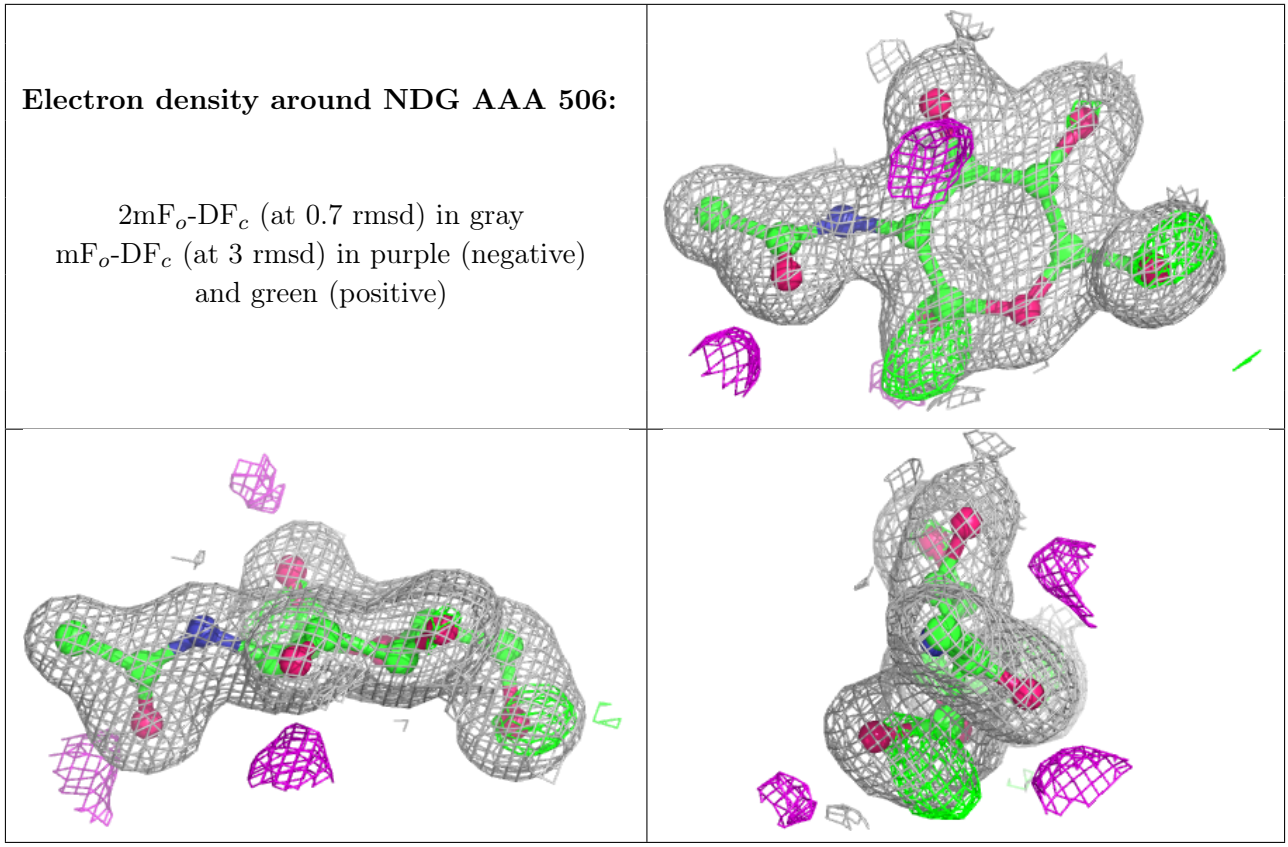
Electron density around ZN BBB 1008:

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



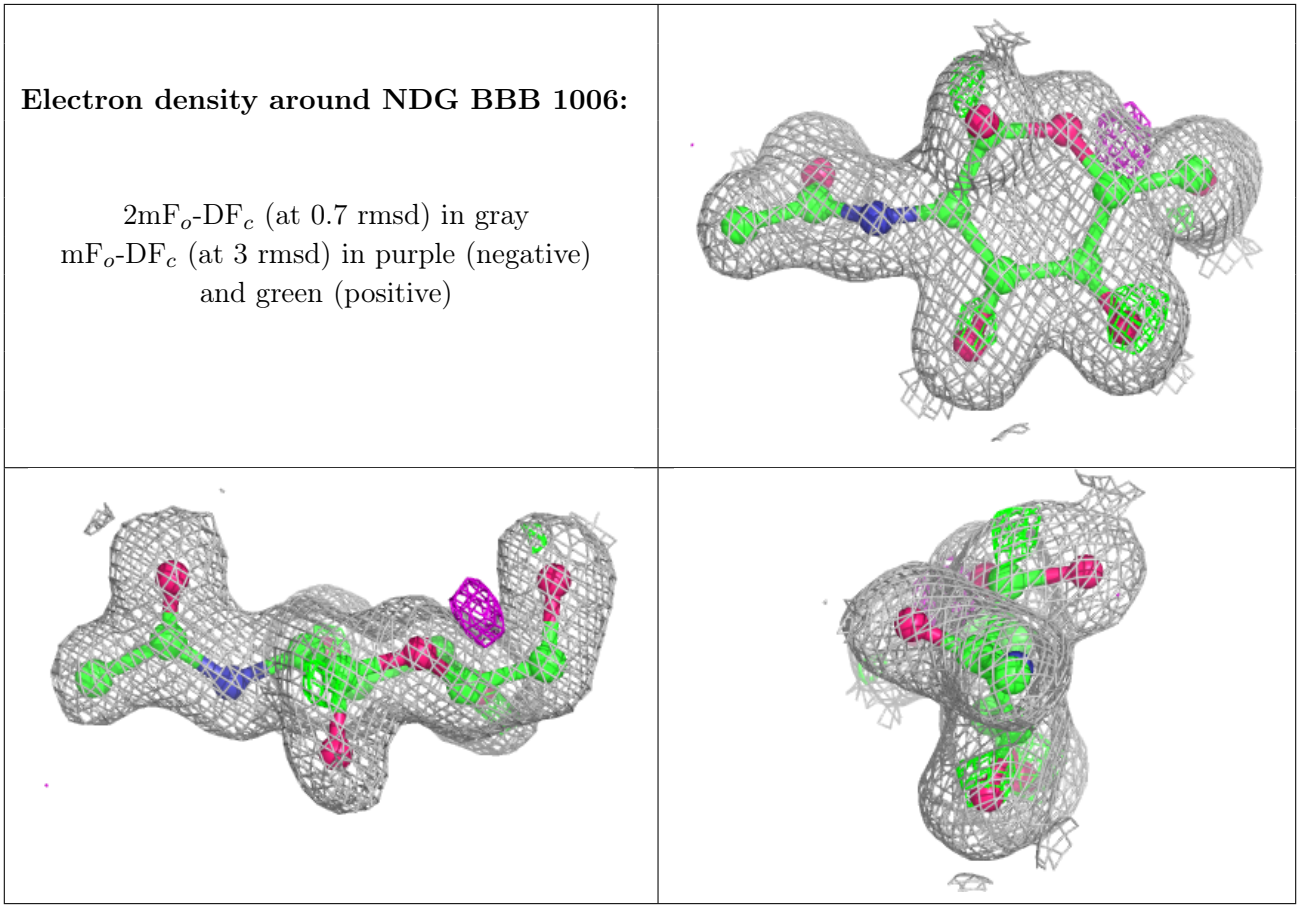
Electron density around NDG AAA 506:

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



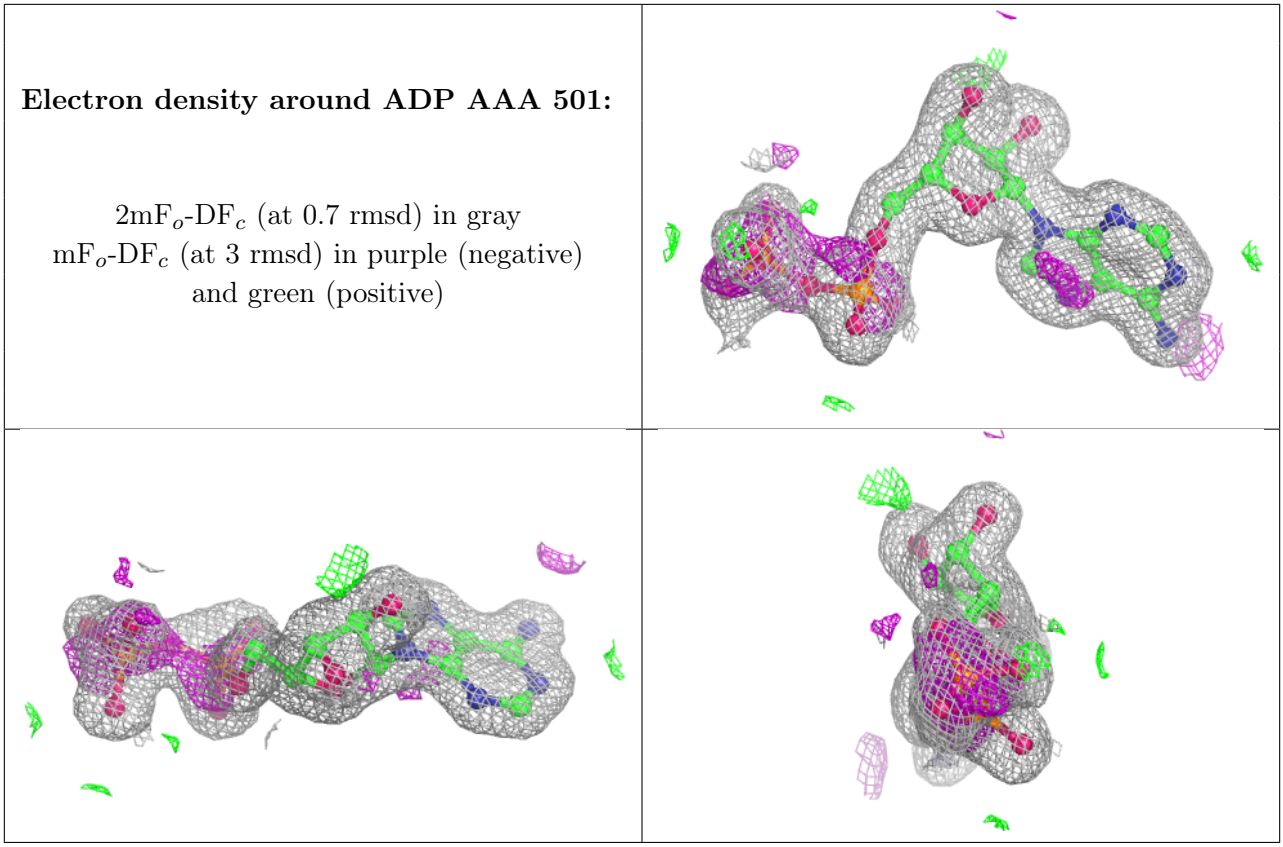
Electron density around NDG BBB 1006:

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



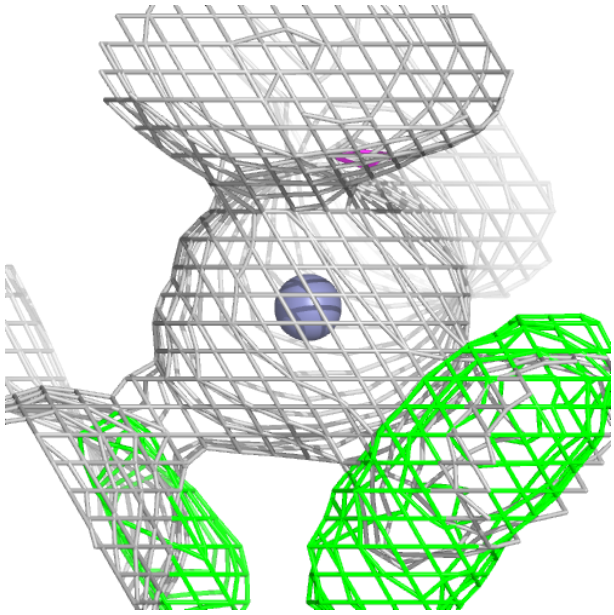
Electron density around ADP AAA 501:

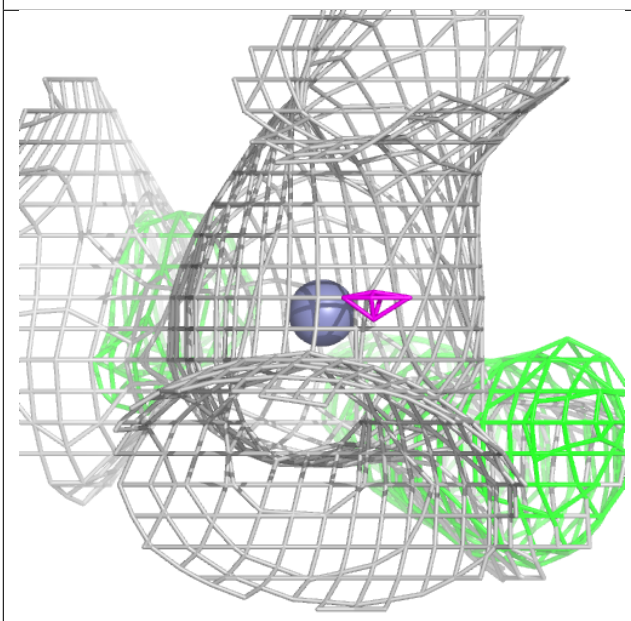
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

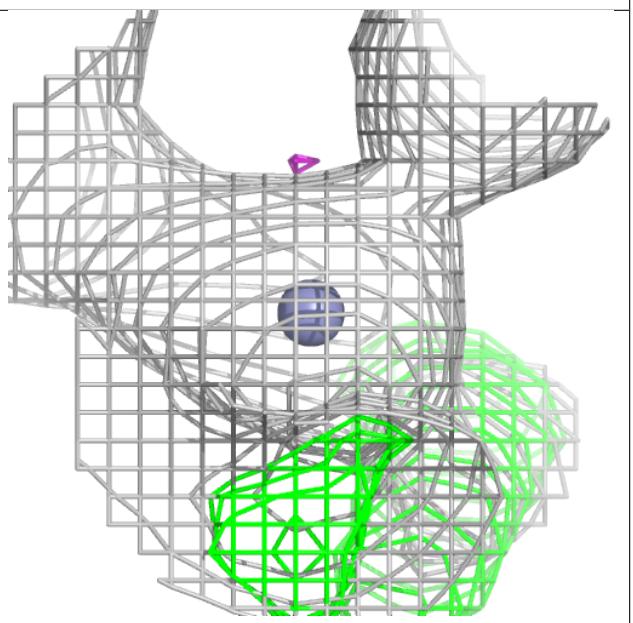


Electron density around ZN AAA 508:

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

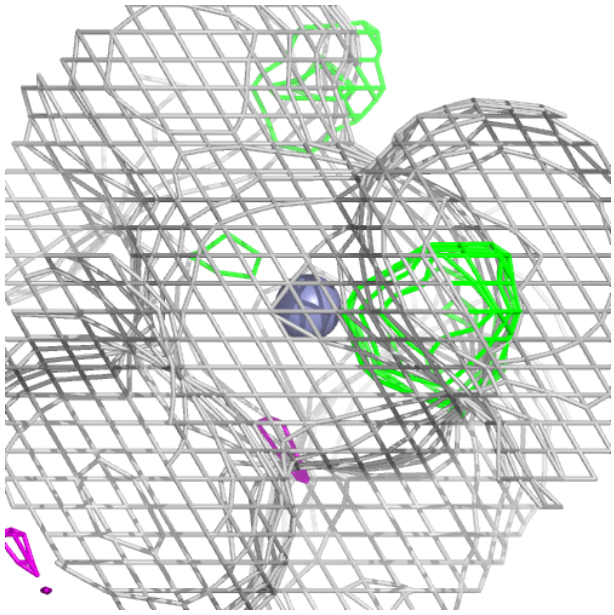


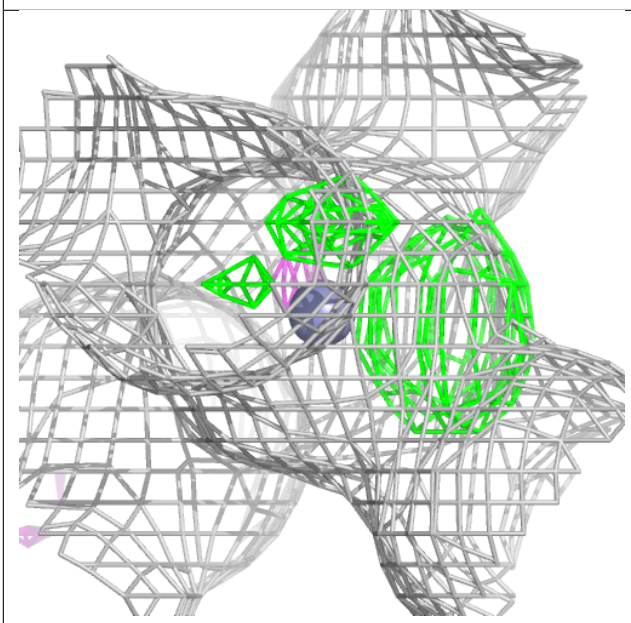


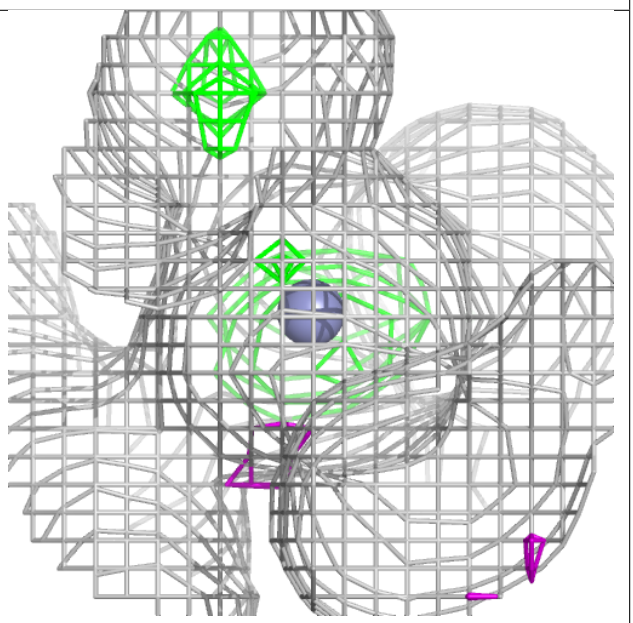


Electron density around ZN BBB 1007:

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

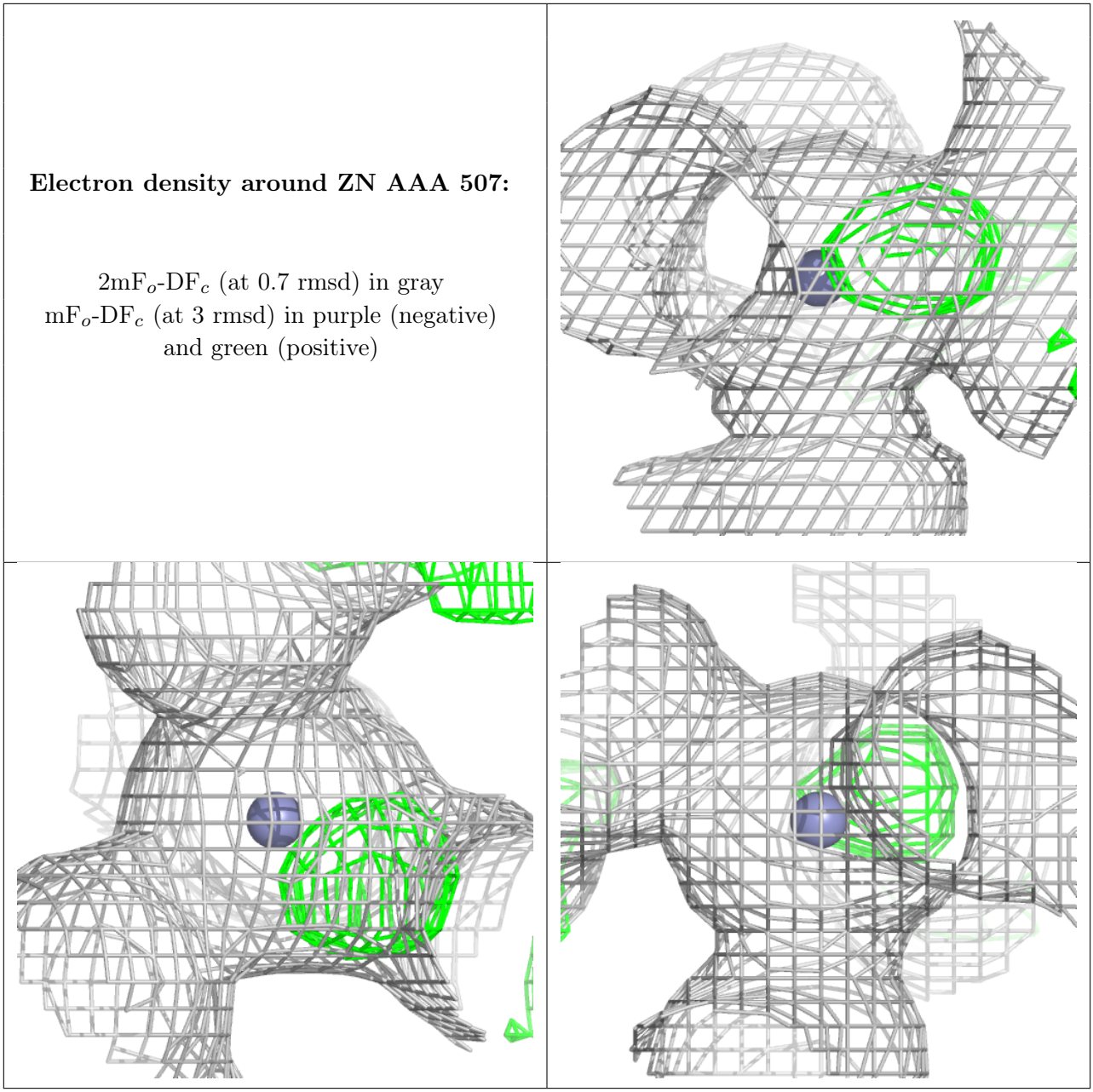






Electron density around ZN AAA 507:

$2mF_o$-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.