wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2024 – 03:45 pm GMT

PDB ID	:	8OIH
Title	:	Crystal structure of the cysteine-rich Gallus gallus urate oxidase in complex with the 8-azaxanthine inhibitor under oxidising conditions (space group C 2 2 21)
Authors	:	Di Palma, M.; Chegkazi, M.; Bui, S.; Mori, G.; Percudani, R.; Steiner, R.A.
Deposited on	:	2023-03-22
Resolution	:	1.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

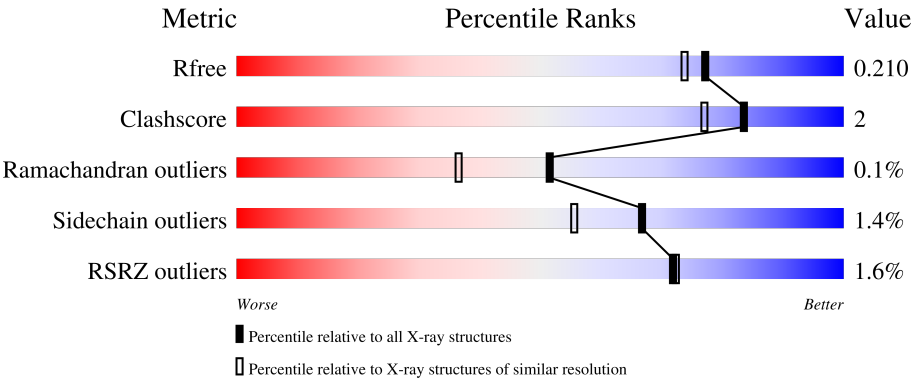
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	343	84% · 13%
1	BBB	343	81% 6% 13%
1	CCC	343	81% 6% · 13%
2	DDD	343	83% · 12%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10860 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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	298	Total	C	N	O	S	0	9	0
			2475	1561	421	467	26			
1	BBB	298	Total	C	N	O	S	0	10	0
			2485	1572	421	467	25			
1	CCC	299	Total	C	N	O	S	0	6	0
			2462	1556	420	461	25			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-22	MET	-	initiating methionine	UNP A0A8V0ZED1
AAA	-21	GLY	-	expression tag	UNP A0A8V0ZED1
AAA	-20	SER	-	expression tag	UNP A0A8V0ZED1
AAA	-19	SER	-	expression tag	UNP A0A8V0ZED1
AAA	-18	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-17	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-16	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-15	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-14	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-13	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-12	SER	-	expression tag	UNP A0A8V0ZED1
AAA	-11	SER	-	expression tag	UNP A0A8V0ZED1
AAA	-10	GLY	-	expression tag	UNP A0A8V0ZED1
AAA	-9	LEU	-	expression tag	UNP A0A8V0ZED1
AAA	-8	VAL	-	expression tag	UNP A0A8V0ZED1
AAA	-7	PRO	-	expression tag	UNP A0A8V0ZED1
AAA	-6	ARG	-	expression tag	UNP A0A8V0ZED1
AAA	-5	GLY	-	expression tag	UNP A0A8V0ZED1
AAA	-4	SER	-	expression tag	UNP A0A8V0ZED1
AAA	-3	HIS	-	expression tag	UNP A0A8V0ZED1
AAA	-2	MET	-	expression tag	UNP A0A8V0ZED1
AAA	-1	ALA	-	expression tag	UNP A0A8V0ZED1
AAA	0	SER	-	expression tag	UNP A0A8V0ZED1

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-22	MET	-	initiating methionine	UNP A0A8V0ZED1
BBB	-21	GLY	-	expression tag	UNP A0A8V0ZED1
BBB	-20	SER	-	expression tag	UNP A0A8V0ZED1
BBB	-19	SER	-	expression tag	UNP A0A8V0ZED1
BBB	-18	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-17	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-16	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-15	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-14	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-13	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-12	SER	-	expression tag	UNP A0A8V0ZED1
BBB	-11	SER	-	expression tag	UNP A0A8V0ZED1
BBB	-10	GLY	-	expression tag	UNP A0A8V0ZED1
BBB	-9	LEU	-	expression tag	UNP A0A8V0ZED1
BBB	-8	VAL	-	expression tag	UNP A0A8V0ZED1
BBB	-7	PRO	-	expression tag	UNP A0A8V0ZED1
BBB	-6	ARG	-	expression tag	UNP A0A8V0ZED1
BBB	-5	GLY	-	expression tag	UNP A0A8V0ZED1
BBB	-4	SER	-	expression tag	UNP A0A8V0ZED1
BBB	-3	HIS	-	expression tag	UNP A0A8V0ZED1
BBB	-2	MET	-	expression tag	UNP A0A8V0ZED1
BBB	-1	ALA	-	expression tag	UNP A0A8V0ZED1
BBB	0	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-22	MET	-	initiating methionine	UNP A0A8V0ZED1
CCC	-21	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-20	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-19	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-18	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-17	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-16	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-15	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-14	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-13	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-12	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-11	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-10	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-9	LEU	-	expression tag	UNP A0A8V0ZED1
CCC	-8	VAL	-	expression tag	UNP A0A8V0ZED1
CCC	-7	PRO	-	expression tag	UNP A0A8V0ZED1
CCC	-6	ARG	-	expression tag	UNP A0A8V0ZED1
CCC	-5	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-4	SER	-	expression tag	UNP A0A8V0ZED1

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-3	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-2	MET	-	expression tag	UNP A0A8V0ZED1
CCC	-1	ALA	-	expression tag	UNP A0A8V0ZED1
CCC	0	SER	-	expression tag	UNP A0A8V0ZED1

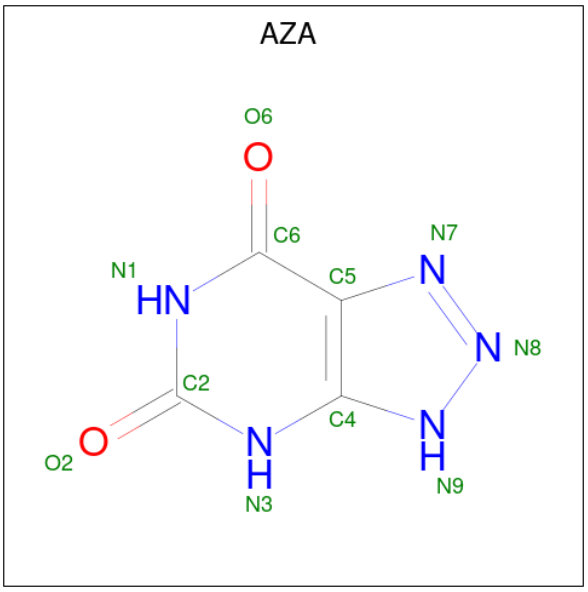
- Molecule 2 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	DDD	301	Total	C	N	O	S	0	5	0
			2467	1557	418	467	25			

There are 23 discrepancies between the modelled and reference sequences:

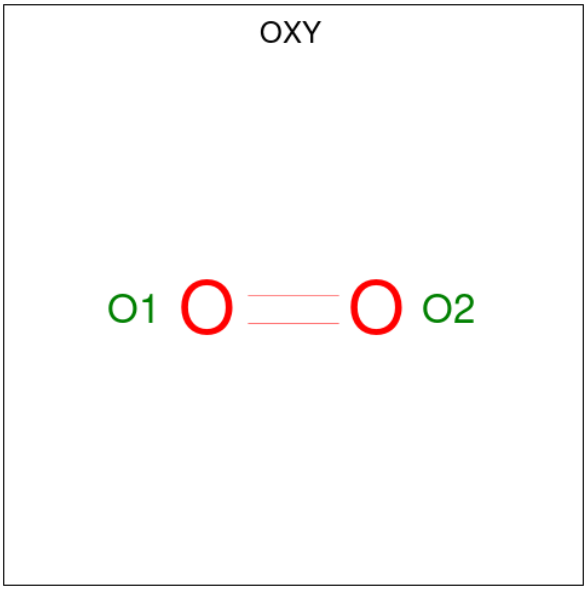
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-22	MET	-	initiating methionine	UNP A0A8V0ZED1
DDD	-21	GLY	-	expression tag	UNP A0A8V0ZED1
DDD	-20	SER	-	expression tag	UNP A0A8V0ZED1
DDD	-19	SER	-	expression tag	UNP A0A8V0ZED1
DDD	-18	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-17	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-16	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-15	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-14	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-13	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-12	SER	-	expression tag	UNP A0A8V0ZED1
DDD	-11	SER	-	expression tag	UNP A0A8V0ZED1
DDD	-10	GLY	-	expression tag	UNP A0A8V0ZED1
DDD	-9	LEU	-	expression tag	UNP A0A8V0ZED1
DDD	-8	VAL	-	expression tag	UNP A0A8V0ZED1
DDD	-7	PRO	-	expression tag	UNP A0A8V0ZED1
DDD	-6	ARG	-	expression tag	UNP A0A8V0ZED1
DDD	-5	GLY	-	expression tag	UNP A0A8V0ZED1
DDD	-4	SER	-	expression tag	UNP A0A8V0ZED1
DDD	-3	HIS	-	expression tag	UNP A0A8V0ZED1
DDD	-2	MET	-	expression tag	UNP A0A8V0ZED1
DDD	-1	ALA	-	expression tag	UNP A0A8V0ZED1
DDD	0	SER	-	expression tag	UNP A0A8V0ZED1

- Molecule 3 is 8-AZAXANTHINE (three-letter code: AZA) (formula: $C_4H_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



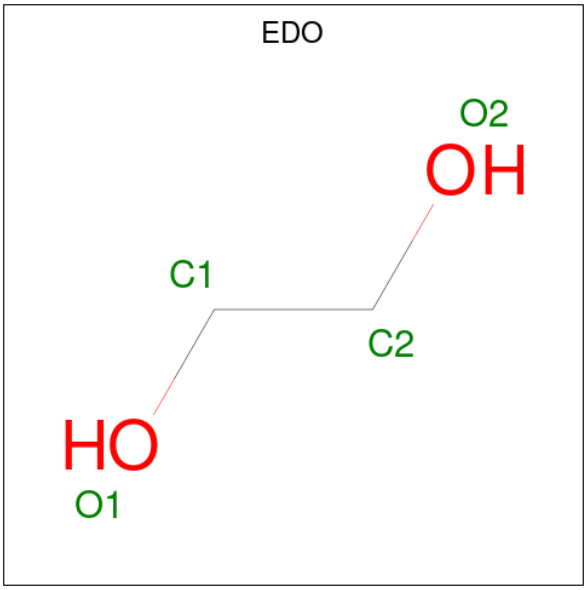
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C N O 11 4 5 2	0	0
3	BBB	1	Total C N O 11 4 5 2	0	0
3	CCC	1	Total C N O 11 4 5 2	0	0
3	DDD	1	Total C N O 11 4 5 2	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O 2 2	0	0
4	BBB	1	Total O 2 2	0	0
4	CCC	1	Total O 2 2	0	0
4	DDD	1	Total O 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	1
			8	4	4		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	1
			8	4	4		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	1
			8	4	4		
5	CCC	1	Total	C	O	0	0
			4	2	2		
5	CCC	1	Total	C	O	0	0
			4	2	2		
5	CCC	1	Total	C	O	0	0
			4	2	2		
5	CCC	1	Total	C	O	0	0
			4	2	2		
5	CCC	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total C O 8 4 4	0	1
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	3	Total Cl 3 3	0	0
6	BBB	2	Total Cl 2 2	0	0
6	CCC	4	Total Cl 4 4	0	0
6	DDD	3	Total Cl 3 3	0	0

- Molecule 7 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total Br 1 1	0	0
7	BBB	1	Total Br 1 1	0	0

- Molecule 8 is water.

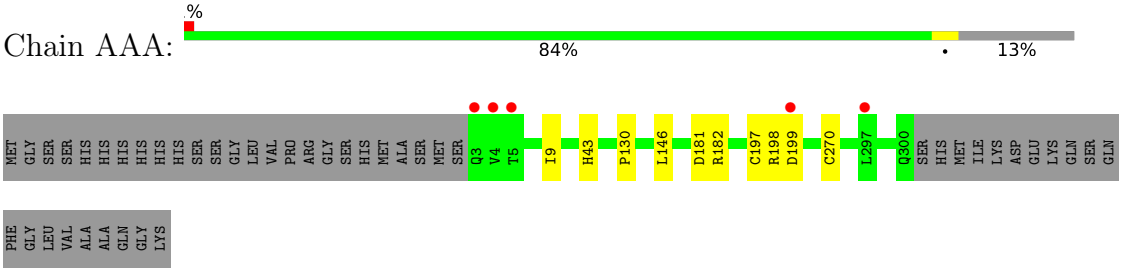
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	203	Total O 205 205	0	2
8	BBB	185	Total O 187 187	0	2
8	CCC	182	Total O 183 183	0	1
8	DDD	177	Total O 178 178	0	1

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.

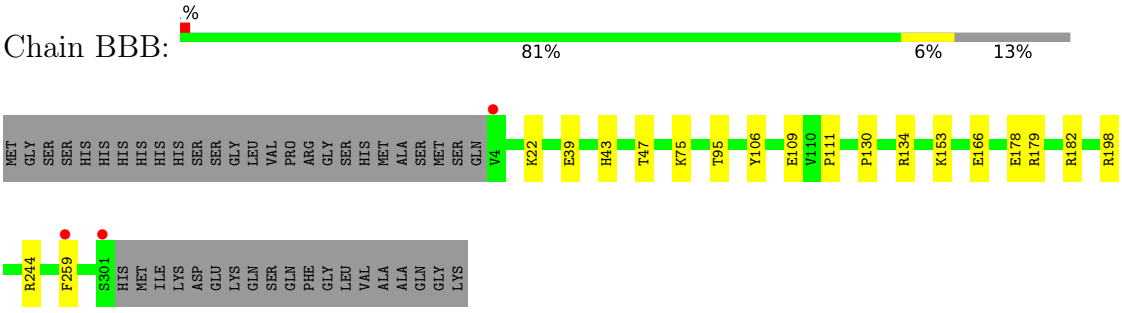
• Molecule 1: Uricase

Chain AAA:



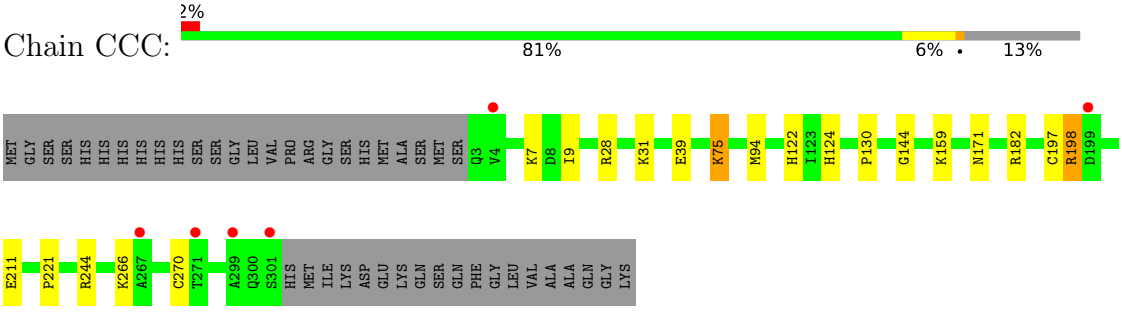
• Molecule 1: Uricase

Chain BBB:



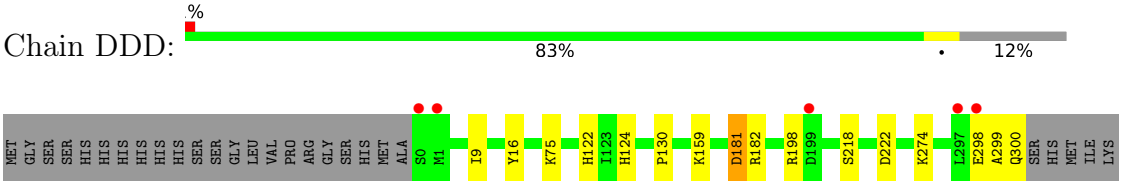
• Molecule 1: Uricase

Chain CCC:



• Molecule 2: Uricase

Chain DDD:



ASP
GLU
LYS
GLN
SER
GLN
PHE
GLY
LEU
VAL
ALA
ALA
GLN
GLY
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	106.51Å 125.99Å 240.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.06 – 1.86 77.06 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (77.06-1.86) 99.9 (77.06-1.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.206 0.180 , 0.210	Depositor DCC
R_{free} test set	6736 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10860	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: CSD, AZA, CL, EDO, BR, OXY

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	0.68	0/2482	0.81	0/3360
1	BBB	0.69	0/2503	0.79	0/3387
1	CCC	0.73	0/2476	0.80	0/3350
2	DDD	0.68	0/2473	0.79	0/3347
All	All	0.70	0/9934	0.80	0/13444

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CCC	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	144	GLY	Mainchain

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	2475	0	2419	13	0
1	BBB	2485	0	2432	14	0
1	CCC	2462	0	2417	13	0
2	DDD	2467	0	2417	12	0
3	AAA	11	0	3	1	0
3	BBB	11	0	3	1	0
3	CCC	11	0	3	1	0
3	DDD	11	0	3	1	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	2	0	0	0	0
5	AAA	48	0	72	1	0
5	BBB	60	0	90	5	0
5	CCC	28	0	42	2	0
5	DDD	16	0	24	0	0
6	AAA	3	0	0	1	0
6	BBB	2	0	0	0	0
6	CCC	4	0	0	0	0
6	DDD	3	0	0	0	0
7	AAA	1	0	0	0	0
7	BBB	1	0	0	0	0
8	AAA	205	0	0	5	0
8	BBB	187	0	0	4	0
8	CCC	183	0	0	2	0
8	DDD	178	0	0	0	0
All	All	10860	0	9925	48	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 2.

The worst 5 of 48 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:BBB:406[B]:EDO:O2	8:BBB:635[B]:HOH:O	1.80	0.98
1:AAA:197[B]:CSD:C	1:AAA:198[B]:ARG:HG2	2.08	0.82
1:AAA:197[B]:CSD:O	1:AAA:198[B]:ARG:HG2	1.83	0.78
1:CCC:130:PRO:O	2:DDD:130:PRO:HD2	1.88	0.72
1:AAA:181[B]:ASP:O	8:AAA:501:HOH:O	2.08	0.71

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	299/343 (87%)	291 (97%)	8 (3%)	0	100	100
1	BBB	301/343 (88%)	294 (98%)	7 (2%)	0	100	100
1	CCC	298/343 (87%)	294 (99%)	4 (1%)	0	100	100
2	DDD	298/343 (87%)	290 (97%)	7 (2%)	1 (0%)	41	26
All	All	1196/1372 (87%)	1169 (98%)	26 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	DDD	299	ALA

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	273/304 (90%)	271 (99%)	2 (1%)	84	79
1	BBB	276/304 (91%)	275 (100%)	1 (0%)	91	89
1	CCC	273/304 (90%)	263 (96%)	10 (4%)	34	17
2	DDD	273/303 (90%)	268 (98%)	5 (2%)	59	45
All	All	1095/1215 (90%)	1077 (98%)	18 (2%)	67	49

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	DDD	75	LYS
2	DDD	198	ARG
2	DDD	181[B]	ASP
1	CCC	171	ASN
2	DDD	16	TYR

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)

22 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSD	AAA	197[A]	1	3,7,8	0.77	0	1,8,10	0.34	0
1	CSD	AAA	197[B]	1	3,7,8	0.76	0	1,8,10	0.05	0
1	CSD	AAA	204[A]	1	3,7,8	0.77	0	1,8,10	0.92	0
1	CSD	AAA	204[B]	1	3,7,8	0.77	0	1,8,10	0.61	0
1	CSD	AAA	41	1	3,7,8	0.79	0	1,8,10	1.77	0
1	CSD	BBB	141	1	3,7,8	0.52	0	1,8,10	0.65	0
1	CSD	BBB	197	1	3,7,8	0.69	0	1,8,10	0.28	0
2	CSD	DDD	141	2	3,7,8	0.61	0	1,8,10	0.65	0
1	CSD	CCC	204[A]	1	3,7,8	0.92	0	1,8,10	0.41	0
1	CSD	CCC	204[B]	1	3,7,8	0.85	0	1,8,10	0.65	0
2	CSD	DDD	98	2	3,7,8	0.70	0	1,8,10	1.03	0
2	CSD	DDD	204[A]	2	3,7,8	0.75	0	1,8,10	0.43	0
2	CSD	DDD	204[B]	2	3,7,8	0.91	0	1,8,10	0.31	0
2	CSD	DDD	197	2	3,7,8	0.71	0	1,8,10	0.31	0
1	CSD	CCC	41	1	3,7,8	0.70	0	1,8,10	0.50	0
1	CSD	AAA	141	1	3,7,8	0.67	0	1,8,10	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSD	BBB	204[B]	1	3,7,8	0.84	0	1,8,10	0.30	0
1	CSD	BBB	204[A]	1	3,7,8	0.75	0	1,8,10	0.86	0
1	CSD	CCC	197	1	3,7,8	0.77	0	1,8,10	0.62	0
1	CSD	CCC	141	1	3,7,8	0.67	0	1,8,10	1.14	0
2	CSD	DDD	41	2	3,7,8	0.79	0	1,8,10	0.26	0
1	CSD	BBB	41	1	3,7,8	0.56	0	1,8,10	0.44	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
1	CSD	AAA	197[A]	1	-	1/2/6/8	-
1	CSD	AAA	197[B]	1	-	1/2/6/8	-
1	CSD	AAA	204[A]	1	-	0/2/6/8	-
1	CSD	AAA	204[B]	1	-	1/2/6/8	-
1	CSD	AAA	41	1	-	1/2/6/8	-
1	CSD	BBB	141	1	-	1/2/6/8	-
1	CSD	BBB	197	1	-	0/2/6/8	-
2	CSD	DDD	141	2	-	1/2/6/8	-
1	CSD	CCC	204[A]	1	-	1/2/6/8	-
1	CSD	CCC	204[B]	1	-	0/2/6/8	-
2	CSD	DDD	98	2	-	0/2/6/8	-
2	CSD	DDD	204[A]	2	-	0/2/6/8	-
2	CSD	DDD	204[B]	2	-	1/2/6/8	-
2	CSD	DDD	197	2	-	1/2/6/8	-
1	CSD	CCC	41	1	-	2/2/6/8	-
1	CSD	AAA	141	1	-	1/2/6/8	-
1	CSD	BBB	204[B]	1	-	0/2/6/8	-
1	CSD	BBB	204[A]	1	-	0/2/6/8	-
1	CSD	CCC	197	1	-	1/2/6/8	-
1	CSD	CCC	141	1	-	0/2/6/8	-
2	CSD	DDD	41	2	-	1/2/6/8	-
1	CSD	BBB	41	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	41	CSD	CA-CB-SG-OD1
1	AAA	141	CSD	CA-CB-SG-OD1
1	AAA	197[A]	CSD	N-CA-CB-SG
1	AAA	197[B]	CSD	CA-CB-SG-OD1
1	AAA	204[B]	CSD	CA-CB-SG-OD1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	197[B]	CSD	3	0
1	CCC	197	CSD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 14 are monoatomic - leaving 46 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	$\#\|Z\| > 2$
5	EDO	AAA	403	-	3,3,3	0.07	0	2,2,2	0.04	0
5	EDO	AAA	405	-	3,3,3	0.05	0	2,2,2	0.14	0
5	EDO	BBB	401	-	3,3,3	0.10	0	2,2,2	0.14	0
4	OXY	AAA	402	-	1,1,1	0.04	0	-		
5	EDO	CCC	401	-	3,3,3	0.12	0	2,2,2	0.12	0
4	OXY	BBB	414	-	1,1,1	0.08	0	-		
3	AZA	AAA	401	-	9,12,12	1.36	1 (11%)	4,17,17	7.71	2 (50%)
5	EDO	AAA	412	-	3,3,3	0.15	0	2,2,2	0.27	0
5	EDO	BBB	409	-	3,3,3	0.26	0	2,2,2	0.26	0
5	EDO	BBB	403	-	3,3,3	0.15	0	2,2,2	0.26	0
5	EDO	BBB	402	-	3,3,3	0.11	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OXY	DDD	406	-	1,1,1	0.01	0	-		
5	EDO	AAA	408	-	3,3,3	0.12	0	2,2,2	0.16	0
5	EDO	BBB	410	-	3,3,3	0.03	0	2,2,2	0.02	0
5	EDO	AAA	406	-	3,3,3	0.09	0	2,2,2	0.42	0
3	AZA	DDD	405	-	9,12,12	1.30	1 (11%)	4,17,17	8.11	2 (50%)
5	EDO	CCC	403	-	3,3,3	0.06	0	2,2,2	0.11	0
5	EDO	BBB	405	-	3,3,3	0.22	0	2,2,2	0.09	0
5	EDO	CCC	405	-	3,3,3	0.08	0	2,2,2	0.19	0
3	AZA	BBB	413	-	9,12,12	1.43	2 (22%)	4,17,17	8.15	2 (50%)
5	EDO	DDD	401	-	3,3,3	0.07	0	2,2,2	0.24	0
5	EDO	AAA	409	-	3,3,3	0.17	0	2,2,2	0.44	0
5	EDO	BBB	406[A]	-	3,3,3	0.13	0	2,2,2	0.25	0
5	EDO	CCC	404	-	3,3,3	0.10	0	2,2,2	0.24	0
5	EDO	BBB	406[B]	-	3,3,3	0.10	0	2,2,2	0.22	0
3	AZA	CCC	407	-	9,12,12	1.28	1 (11%)	4,17,17	7.79	2 (50%)
5	EDO	AAA	414	-	3,3,3	0.07	0	2,2,2	0.11	0
5	EDO	AAA	404	-	3,3,3	0.08	0	2,2,2	0.19	0
5	EDO	AAA	407	-	3,3,3	0.17	0	2,2,2	0.47	0
5	EDO	DDD	403	-	3,3,3	0.08	0	2,2,2	0.23	0
5	EDO	CCC	406[A]	-	3,3,3	0.09	0	2,2,2	0.25	0
5	EDO	CCC	406[B]	-	3,3,3	0.05	0	2,2,2	0.19	0
5	EDO	AAA	411	-	3,3,3	0.17	0	2,2,2	0.26	0
4	OXY	CCC	408	-	1,1,1	0.12	0	-		
5	EDO	AAA	410	-	3,3,3	0.09	0	2,2,2	0.18	0
5	EDO	AAA	413	-	3,3,3	0.15	0	2,2,2	0.28	0
5	EDO	BBB	407	-	3,3,3	0.16	0	2,2,2	0.33	0
5	EDO	BBB	411	-	3,3,3	0.27	0	2,2,2	0.26	0
5	EDO	BBB	404	-	3,3,3	0.05	0	2,2,2	0.23	0
5	EDO	BBB	408[A]	-	3,3,3	0.19	0	2,2,2	0.24	0
5	EDO	BBB	408[B]	-	3,3,3	0.01	0	2,2,2	0.17	0
5	EDO	BBB	412[A]	-	3,3,3	0.08	0	2,2,2	0.25	0
5	EDO	CCC	402	-	3,3,3	0.10	0	2,2,2	0.13	0
5	EDO	BBB	412[B]	-	3,3,3	0.09	0	2,2,2	0.32	0
5	EDO	DDD	402	-	3,3,3	0.08	0	2,2,2	0.22	0
5	EDO	DDD	404	-	3,3,3	0.14	0	2,2,2	0.09	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
5	EDO	AAA	403	-	-	0/1/1/1	-
5	EDO	AAA	405	-	-	0/1/1/1	-
5	EDO	BBB	401	-	-	1/1/1/1	-
5	EDO	CCC	401	-	-	0/1/1/1	-
5	EDO	AAA	412	-	-	0/1/1/1	-
3	AZA	AAA	401	-	-	-	0/2/2/2
5	EDO	BBB	409	-	-	1/1/1/1	-
5	EDO	BBB	403	-	-	0/1/1/1	-
5	EDO	BBB	402	-	-	0/1/1/1	-
5	EDO	AAA	408	-	-	1/1/1/1	-
5	EDO	BBB	410	-	-	0/1/1/1	-
5	EDO	AAA	406	-	-	0/1/1/1	-
5	EDO	CCC	403	-	-	0/1/1/1	-
5	EDO	CCC	405	-	-	1/1/1/1	-
5	EDO	BBB	405	-	-	0/1/1/1	-
3	AZA	DDD	405	-	-	-	0/2/2/2
3	AZA	BBB	413	-	-	-	0/2/2/2
5	EDO	DDD	401	-	-	1/1/1/1	-
5	EDO	AAA	409	-	-	1/1/1/1	-
5	EDO	BBB	406[A]	-	-	0/1/1/1	-
5	EDO	CCC	404	-	-	1/1/1/1	-
5	EDO	BBB	406[B]	-	-	1/1/1/1	-
5	EDO	AAA	414	-	-	1/1/1/1	-
3	AZA	CCC	407	-	-	-	0/2/2/2
5	EDO	AAA	404	-	-	0/1/1/1	-
5	EDO	AAA	407	-	-	1/1/1/1	-
5	EDO	DDD	403	-	-	0/1/1/1	-
5	EDO	CCC	406[A]	-	-	0/1/1/1	-
5	EDO	CCC	406[B]	-	-	1/1/1/1	-
5	EDO	AAA	411	-	-	0/1/1/1	-
5	EDO	AAA	410	-	-	1/1/1/1	-
5	EDO	AAA	413	-	-	0/1/1/1	-
5	EDO	BBB	407	-	-	0/1/1/1	-
5	EDO	BBB	411	-	-	0/1/1/1	-
5	EDO	BBB	404	-	-	1/1/1/1	-
5	EDO	BBB	408[A]	-	-	1/1/1/1	-
5	EDO	BBB	408[B]	-	-	0/1/1/1	-
5	EDO	BBB	412[A]	-	-	0/1/1/1	-
5	EDO	CCC	402	-	-	0/1/1/1	-
5	EDO	BBB	412[B]	-	-	1/1/1/1	-
5	EDO	DDD	402	-	-	0/1/1/1	-
5	EDO	DDD	404	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	401	AZA	C6-N1	3.66	1.39	1.33
3	CCC	407	AZA	C6-N1	3.47	1.39	1.33
3	DDD	405	AZA	C6-N1	3.37	1.38	1.33
3	BBB	413	AZA	C6-N1	3.29	1.38	1.33
3	BBB	413	AZA	C5-C6	2.21	1.45	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DDD	405	AZA	C2-N1-C6	14.26	127.18	115.14
3	BBB	413	AZA	C2-N1-C6	14.23	127.16	115.14
3	CCC	407	AZA	C2-N1-C6	13.84	126.83	115.14
3	AAA	401	AZA	C2-N1-C6	13.61	126.63	115.14
3	BBB	413	AZA	C5-C6-N1	-7.61	113.03	123.43

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	DDD	401	EDO	O1-C1-C2-O2
5	AAA	407	EDO	O1-C1-C2-O2
5	AAA	409	EDO	O1-C1-C2-O2
5	BBB	401	EDO	O1-C1-C2-O2
5	BBB	404	EDO	O1-C1-C2-O2

There are no ring outliers.

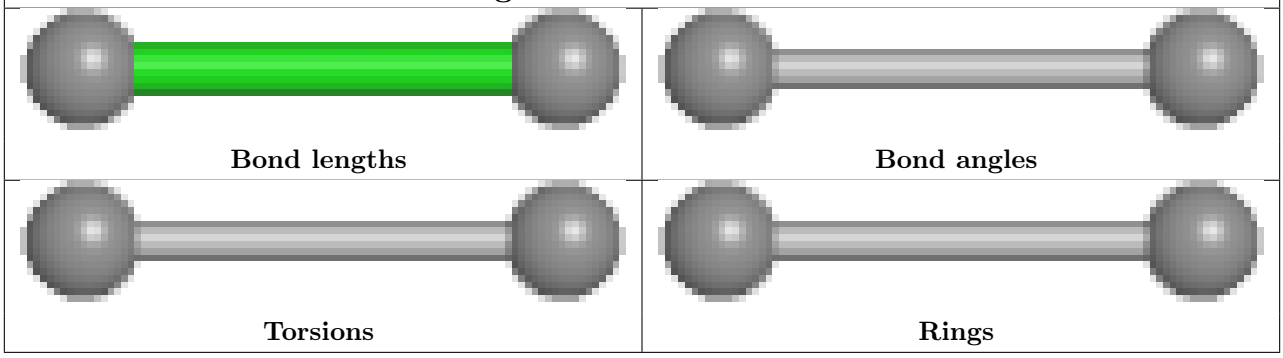
11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	401	AZA	1	0
5	BBB	409	EDO	1	0
3	DDD	405	AZA	1	0
5	CCC	405	EDO	1	0
3	BBB	413	AZA	1	0
5	BBB	406[B]	EDO	1	0
3	CCC	407	AZA	1	0
5	AAA	407	EDO	1	0
5	CCC	406[B]	EDO	1	0
5	AAA	411	EDO	1	0
5	BBB	411	EDO	3	0

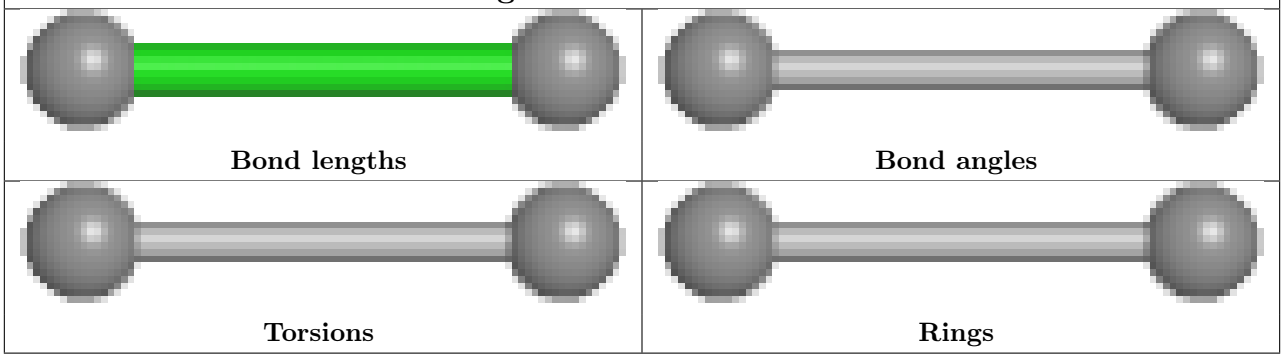
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

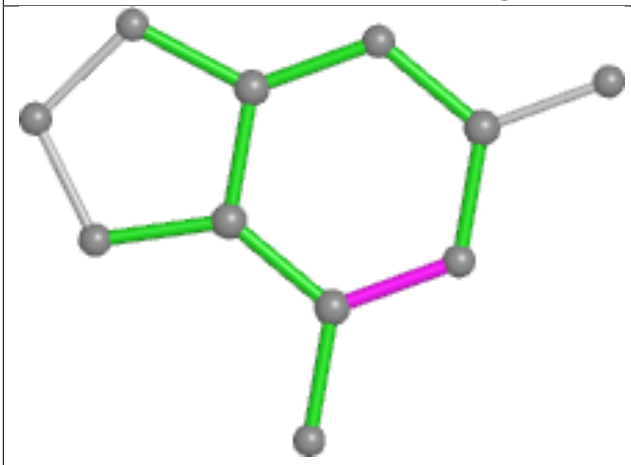
Ligand OXY AAA 402



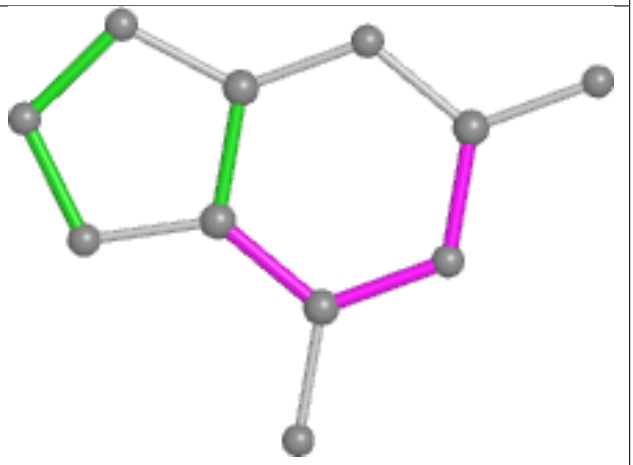
Ligand OXY BBB 414



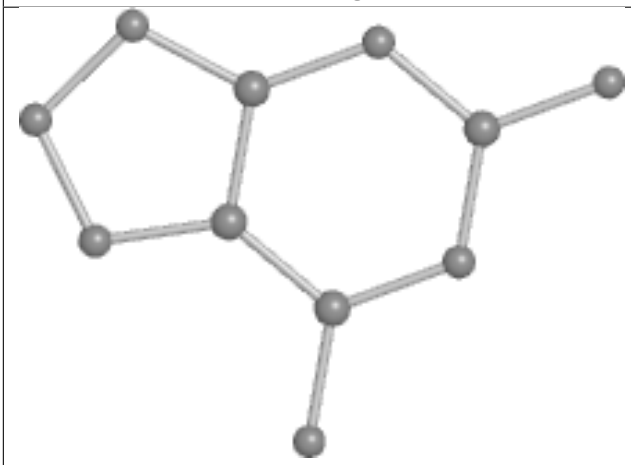
Ligand AZA AAA 401



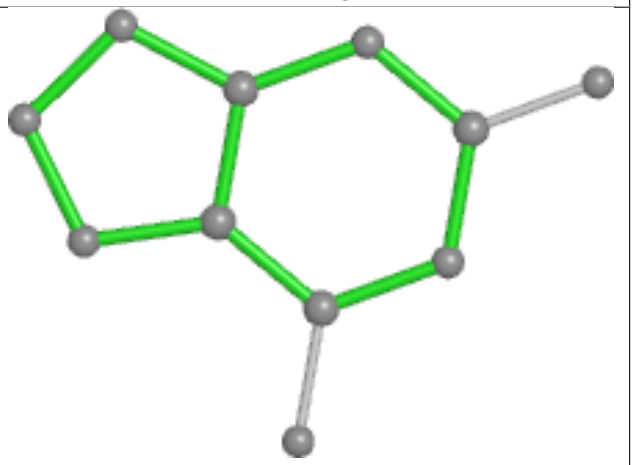
Bond lengths



Bond angles

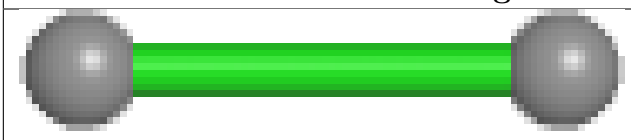


Torsions

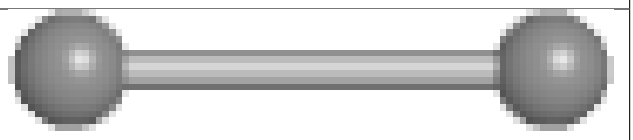


Rings

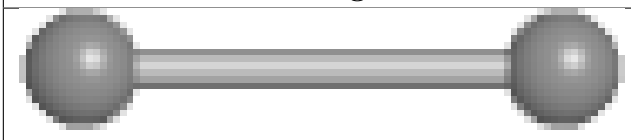
Ligand OXY DDD 406



Bond lengths



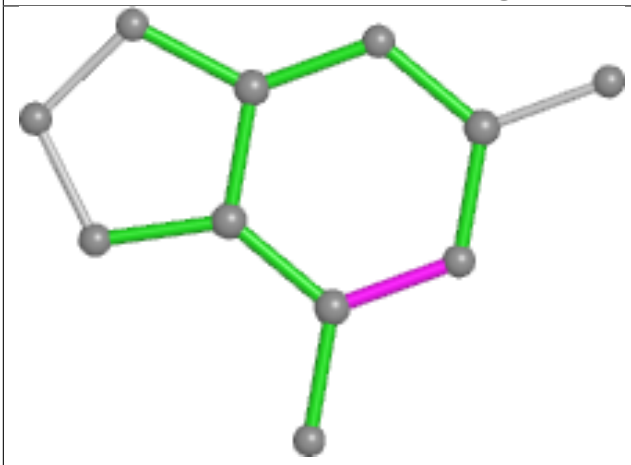
Bond angles



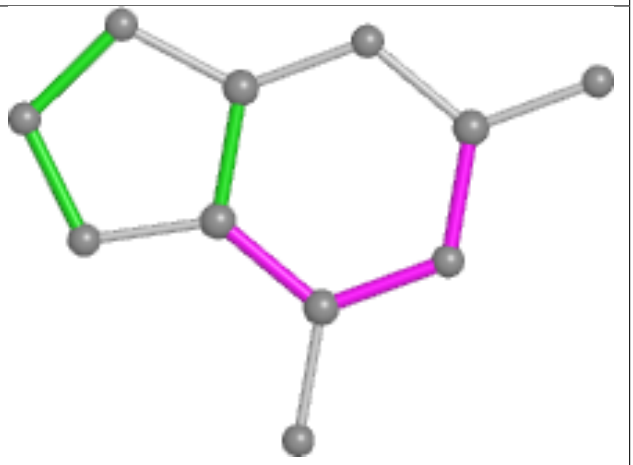
Torsions

Rings

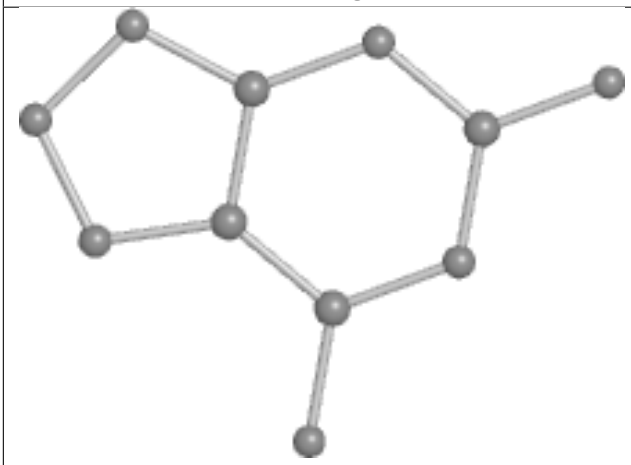
Ligand AZA DDD 405



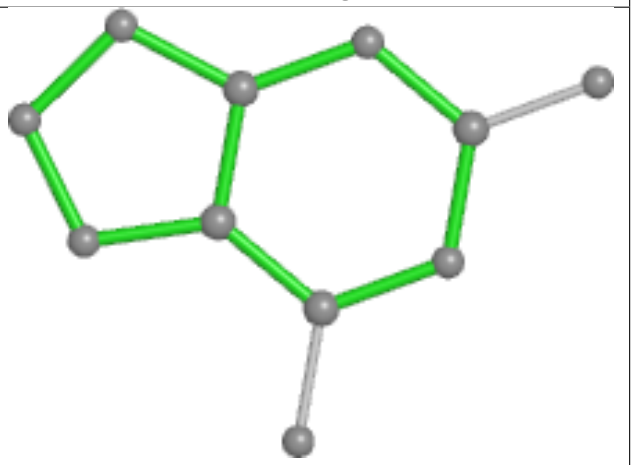
Bond lengths



Bond angles

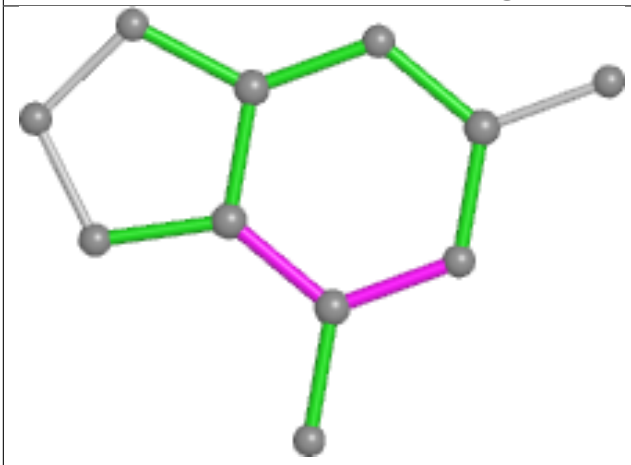


Torsions

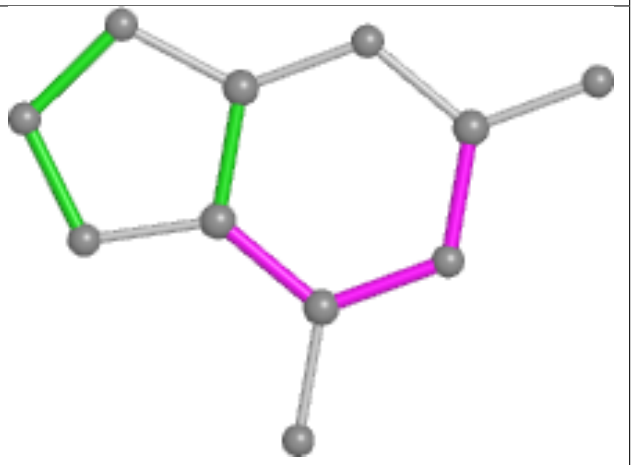


Rings

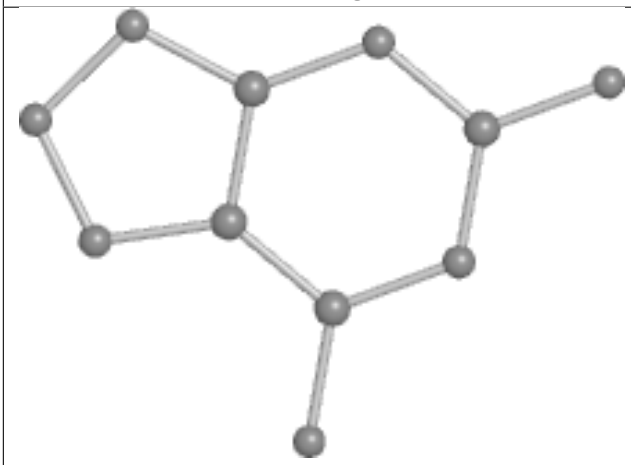
Ligand AZA BBB 413



Bond lengths



Bond angles



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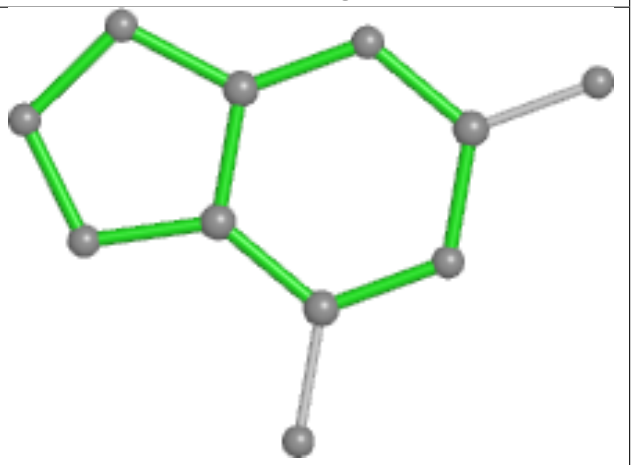
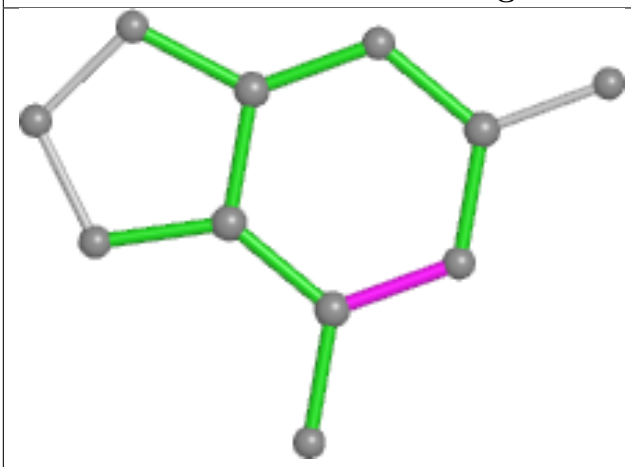
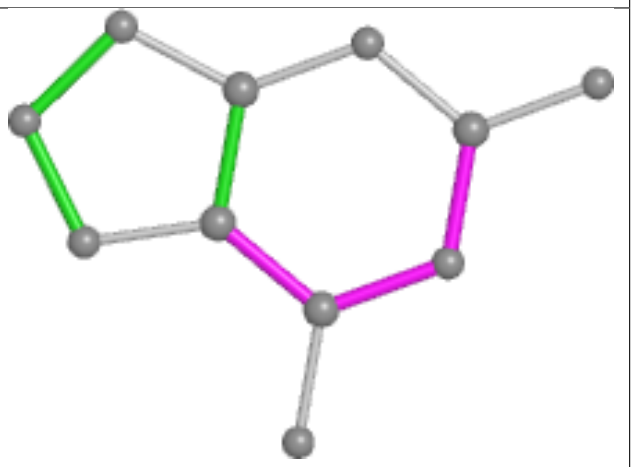


Rings

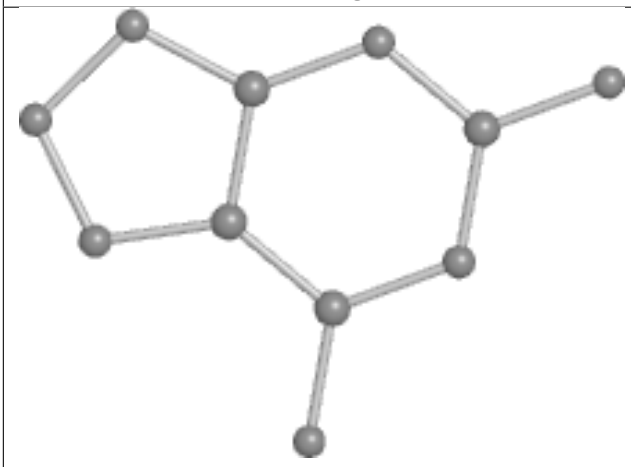
Ligand AZA CCC 407



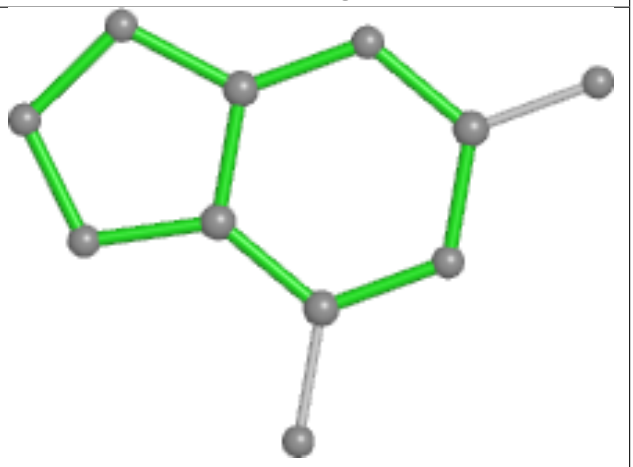
Bond lengths



Bond angles

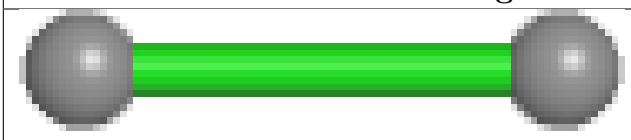


Torsions

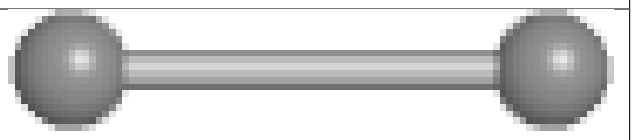


Rings

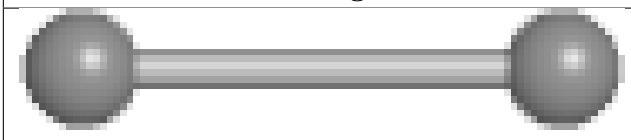
Ligand OXY CCC 408



Bond lengths



Bond angles



Torsions

Rings

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^{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	294/343 (85%)	-0.09	5 (1%)	70	70	32, 41, 66, 100	0
1	BBB	294/343 (85%)	-0.02	3 (1%)	82	82	33, 43, 68, 102	0
1	CCC	295/343 (86%)	0.04	6 (2%)	65	64	33, 45, 74, 116	0
2	DDD	296/343 (86%)	-0.01	5 (1%)	70	70	36, 49, 73, 110	0
All	All	1179/1372 (85%)	-0.02	19 (1%)	72	72	32, 45, 71, 116	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	4	VAL	4.8
1	AAA	4	VAL	4.2
1	AAA	3	GLN	3.7
1	CCC	271	THR	3.1
1	BBB	259[A]	PHE	2.8

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

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
2	CSD	DDD	197	8/9	0.74	0.17	87,89,98,99	0
1	CSD	CCC	197	8/9	0.75	0.20	59,63,84,86	0
2	CSD	DDD	98	8/9	0.89	0.13	46,50,68,70	0
1	CSD	BBB	197	8/9	0.89	0.13	63,68,83,85	0
1	CSD	AAA	197[A]	8/9	0.90	0.15	63,65,66,66	8
1	CSD	AAA	197[B]	8/9	0.90	0.15	63,64,65,65	8
1	CSD	CCC	204[A]	8/9	0.91	0.13	38,41,43,45	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	CCC	204[B]	8/9	0.91	0.13	41,45,59,59	8
1	CSD	BBB	204[B]	8/9	0.94	0.14	43,46,57,58	8
1	CSD	CCC	41	8/9	0.94	0.15	38,39,49,53	0
1	CSD	CCC	141	8/9	0.94	0.10	49,52,65,69	0
1	CSD	BBB	204[A]	8/9	0.94	0.14	42,44,50,52	8
2	CSD	DDD	41	8/9	0.95	0.10	36,39,47,52	0
1	CSD	AAA	204[A]	8/9	0.95	0.12	44,47,51,53	8
1	CSD	AAA	204[B]	8/9	0.95	0.12	45,48,58,60	8
2	CSD	DDD	204[A]	8/9	0.95	0.10	54,56,62,63	8
2	CSD	DDD	204[B]	8/9	0.95	0.10	55,57,64,67	8
1	CSD	AAA	141	8/9	0.96	0.08	39,43,52,55	0
2	CSD	DDD	141	8/9	0.96	0.07	51,54,59,62	0
1	CSD	BBB	41	8/9	0.96	0.11	34,36,47,52	0
1	CSD	BBB	141	8/9	0.96	0.08	46,49,61,63	0
1	CSD	AAA	41	8/9	0.96	0.10	34,35,46,50	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	EDO	CCC	405	4/4	0.76	0.31	72,73,73,75	0
5	EDO	CCC	403	4/4	0.77	0.27	84,86,87,88	0
5	EDO	BBB	408[B]	4/4	0.79	0.21	66,69,73,77	4
5	EDO	AAA	414	4/4	0.79	0.28	62,70,70,71	0
5	EDO	BBB	408[A]	4/4	0.79	0.21	45,46,47,47	4
5	EDO	BBB	401	4/4	0.80	0.15	79,86,86,88	0
5	EDO	BBB	407	4/4	0.81	0.17	43,50,58,62	0
5	EDO	DDD	403	4/4	0.81	0.20	79,83,83,83	0
5	EDO	AAA	412	4/4	0.83	0.28	67,69,70,71	0
5	EDO	AAA	413	4/4	0.83	0.20	57,67,68,70	0
5	EDO	BBB	409	4/4	0.84	0.24	45,53,60,61	0
5	EDO	AAA	407	4/4	0.85	0.28	48,55,58,61	0
5	EDO	CCC	406[A]	4/4	0.86	0.25	53,56,57,58	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	CCC	406[B]	4/4	0.86	0.25	59,60,61,62	4
5	EDO	BBB	410	4/4	0.86	0.14	82,85,86,86	0
5	EDO	BBB	412[B]	4/4	0.87	0.30	46,46,47,47	4
5	EDO	BBB	404	4/4	0.87	0.16	75,76,78,79	0
5	EDO	AAA	406	4/4	0.87	0.19	47,58,62,63	0
5	EDO	AAA	408	4/4	0.87	0.24	57,66,71,78	0
5	EDO	BBB	411	4/4	0.87	0.28	39,47,47,57	0
5	EDO	BBB	412[A]	4/4	0.87	0.30	50,54,54,55	4
4	OXY	DDD	406	2/2	0.88	0.13	43,43,43,51	0
5	EDO	AAA	409	4/4	0.88	0.22	50,61,66,70	0
5	EDO	DDD	404	4/4	0.88	0.17	68,69,70,74	0
6	CL	CCC	410	1/1	0.88	0.08	75,75,75,75	0
5	EDO	AAA	411	4/4	0.89	0.19	52,55,59,63	0
5	EDO	BBB	403	4/4	0.89	0.11	57,63,65,68	0
6	CL	DDD	408	1/1	0.89	0.08	58,58,58,58	0
5	EDO	AAA	410	4/4	0.90	0.18	67,75,76,77	0
5	EDO	CCC	404	4/4	0.90	0.34	55,64,64,66	0
5	EDO	BBB	405	4/4	0.90	0.15	38,39,39,39	0
6	CL	DDD	409	1/1	0.90	0.07	64,64,64,64	0
5	EDO	CCC	401	4/4	0.91	0.14	51,52,53,54	0
5	EDO	CCC	402	4/4	0.91	0.15	42,43,44,45	0
5	EDO	AAA	403	4/4	0.91	0.10	53,56,58,62	0
4	OXY	BBB	414	2/2	0.91	0.14	48,48,48,50	0
5	EDO	DDD	401	4/4	0.92	0.14	64,66,67,70	0
5	EDO	BBB	402	4/4	0.92	0.15	57,57,57,59	0
4	OXY	AAA	402	2/2	0.93	0.09	38,38,38,40	0
6	CL	AAA	416	1/1	0.94	0.10	55,55,55,55	0
5	EDO	AAA	404	4/4	0.94	0.23	49,54,58,59	0
6	CL	CCC	412	1/1	0.94	0.05	65,65,65,65	0
5	EDO	BBB	406[A]	4/4	0.94	0.12	39,43,43,44	4
5	EDO	BBB	406[B]	4/4	0.94	0.12	49,51,52,52	4
6	CL	DDD	407	1/1	0.95	0.10	52,52,52,52	0
5	EDO	AAA	405	4/4	0.95	0.10	38,41,41,42	0
6	CL	BBB	416	1/1	0.95	0.07	69,69,69,69	0
6	CL	BBB	415	1/1	0.96	0.10	60,60,60,60	0
6	CL	AAA	415	1/1	0.96	0.12	62,62,62,62	0
6	CL	CCC	409	1/1	0.96	0.10	51,51,51,51	0
3	AZA	DDD	405	11/11	0.96	0.10	37,39,43,44	0
5	EDO	DDD	402	4/4	0.97	0.10	45,48,49,50	0
3	AZA	CCC	407	11/11	0.97	0.09	32,35,38,39	0
4	OXY	CCC	408	2/2	0.97	0.08	40,40,40,45	0
6	CL	CCC	411	1/1	0.97	0.19	56,56,56,56	0

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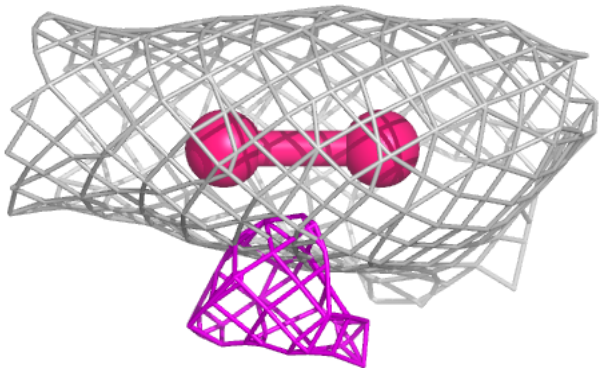
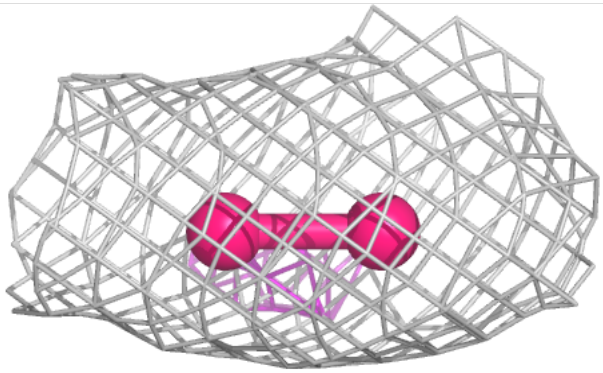
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AZA	AAA	401	11/11	0.98	0.11	31,34,37,38	0
3	AZA	BBB	413	11/11	0.98	0.10	33,35,37,37	0
6	CL	AAA	417	1/1	0.98	0.07	60,60,60,60	0
7	BR	AAA	418	1/1	0.99	0.06	48,48,48,48	1
7	BR	BBB	417	1/1	0.99	0.05	52,52,52,52	1

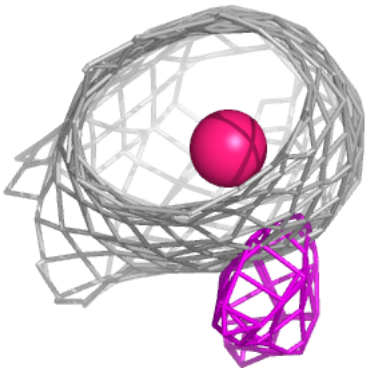
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OXY DDD 406:

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

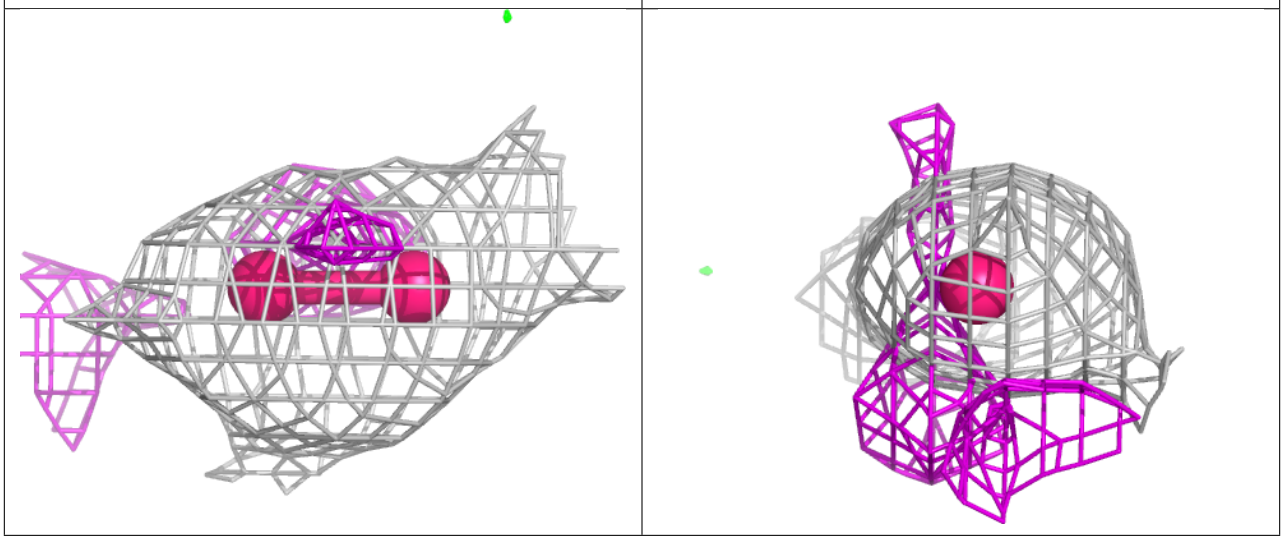






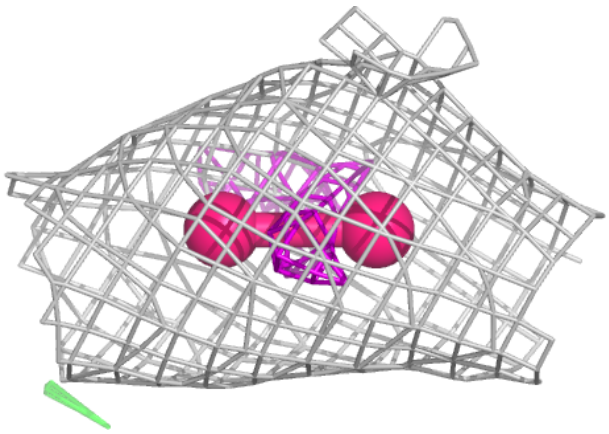
Electron density around OXY BBB 414:

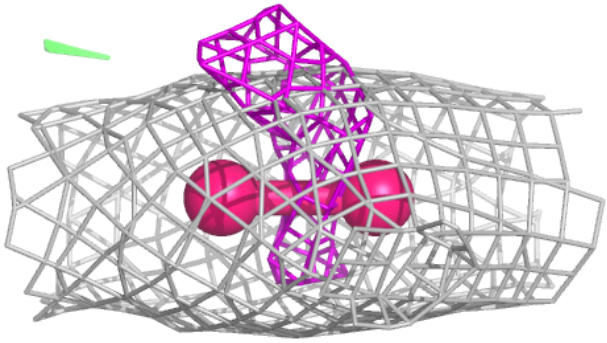
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

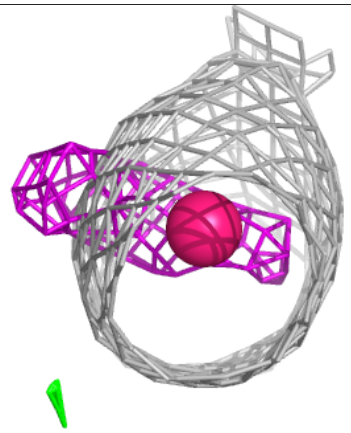


Electron density around OXY AAA 402:

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

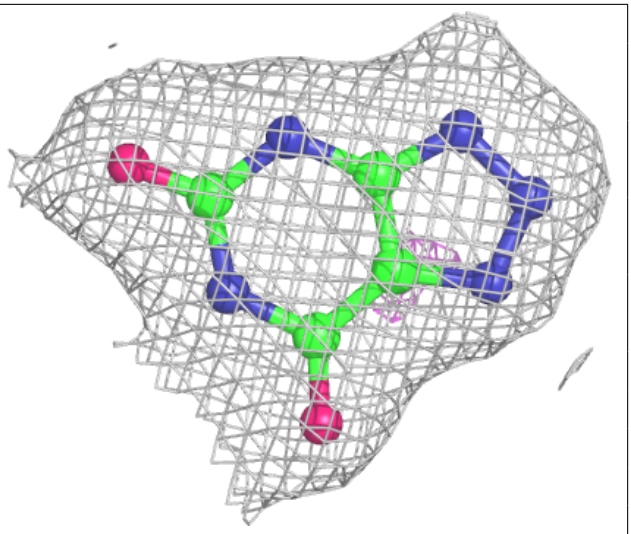


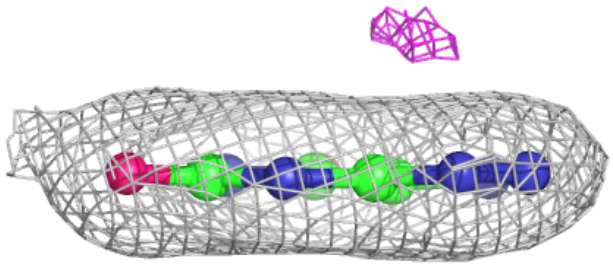


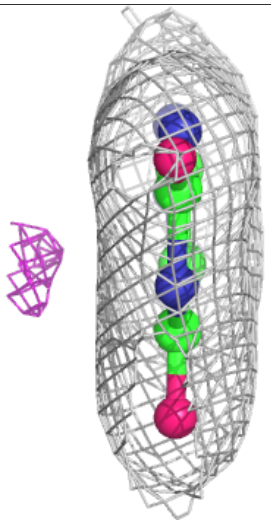


Electron density around AZA DDD 405:

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

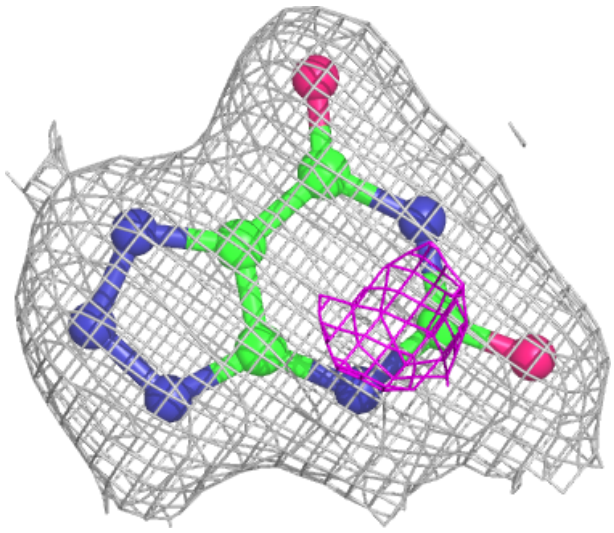


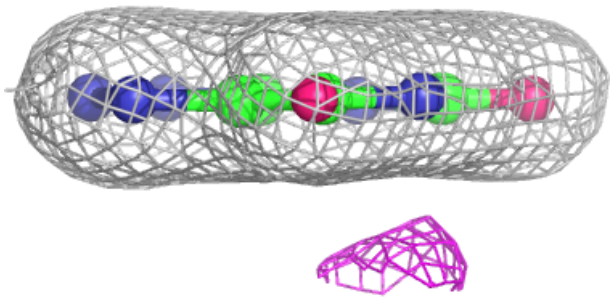


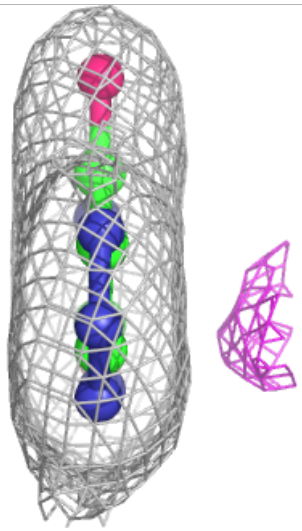


Electron density around AZA CCC 407:

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

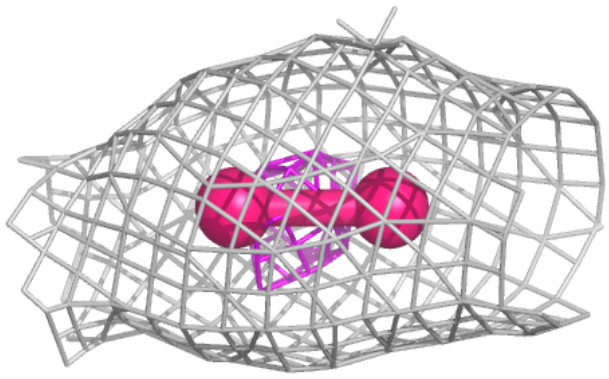


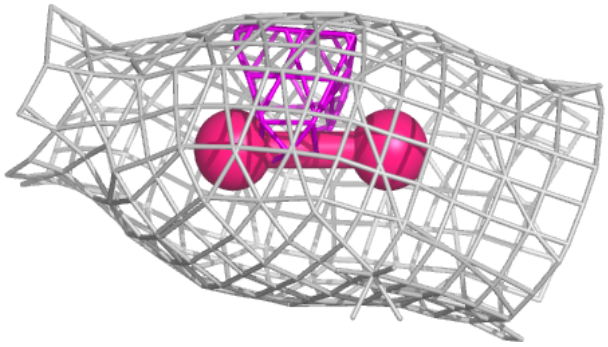


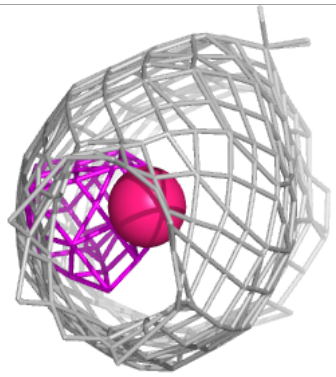


Electron density around OXY CCC 408:

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

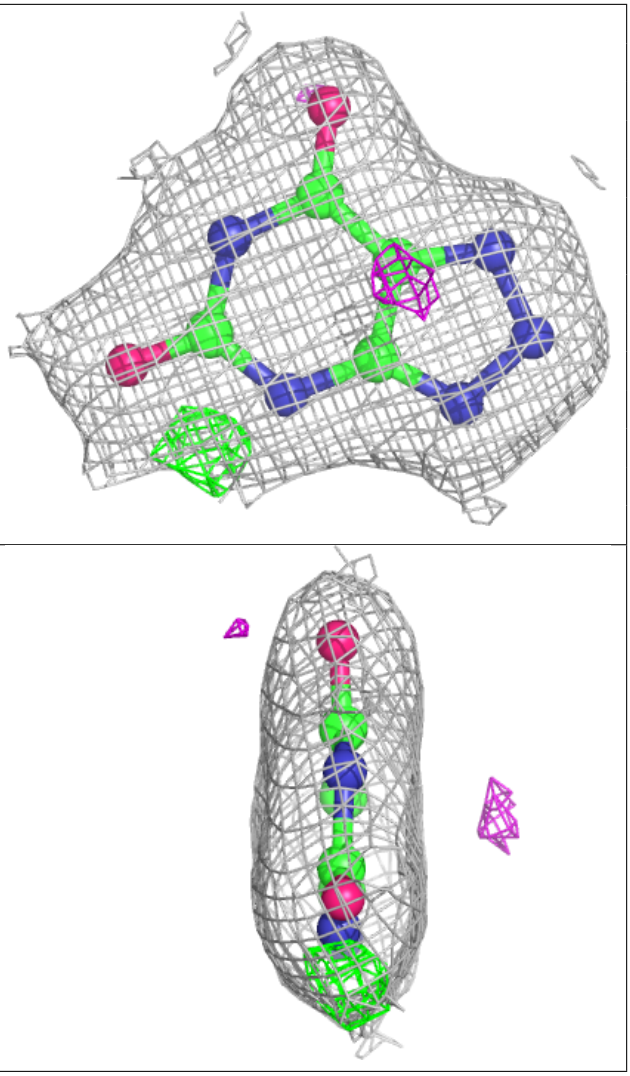






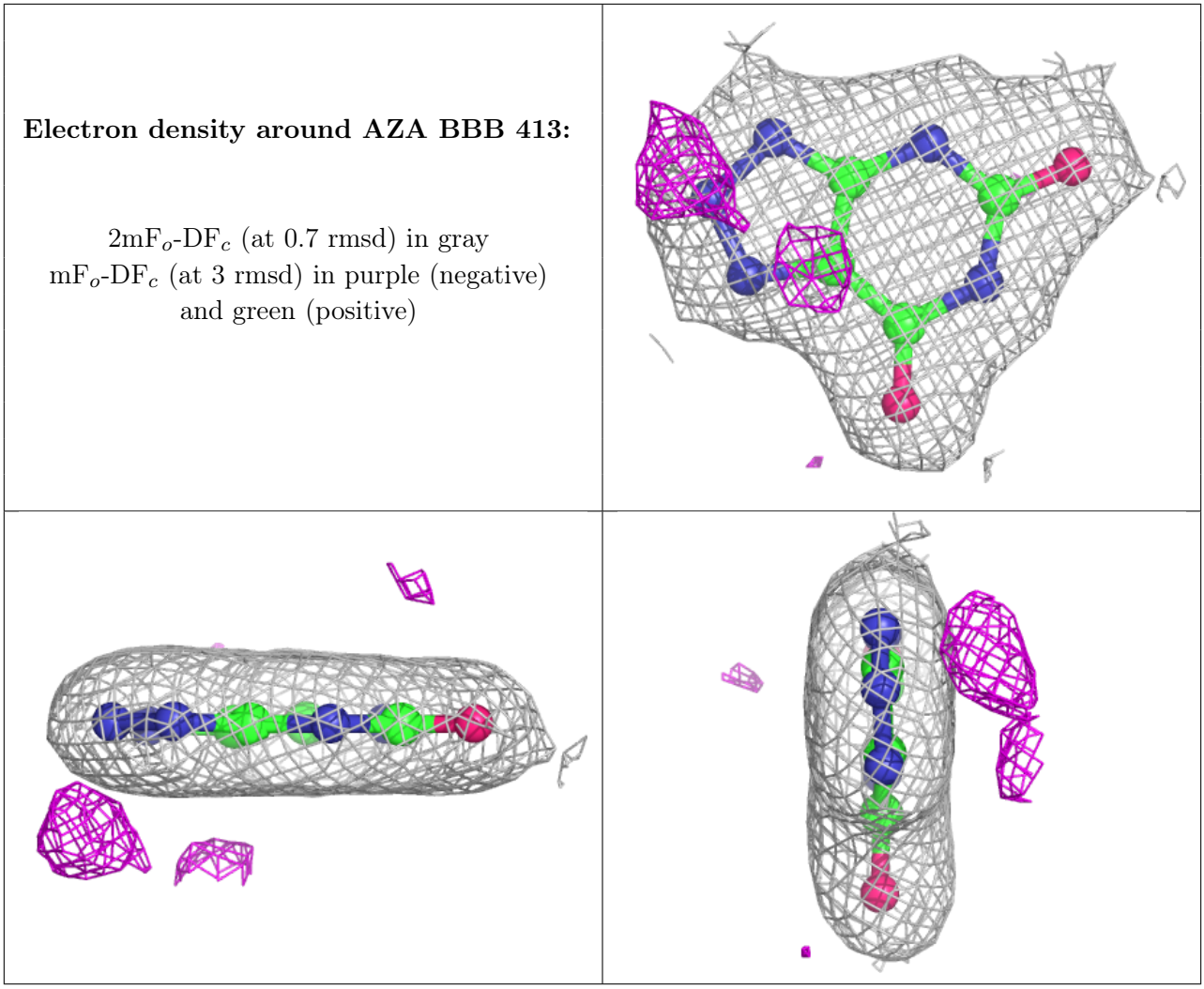
Electron density around AZA AAA 401:

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



Electron density around AZA BBB 413:

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



6.5 Other polymers (i)

There are no such residues in this entry.