wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2024 – 03:39 pm GMT

PDB ID	:	8OH8
Title	:	Crystal structure of the cysteine-rich Gallus gallus urate oxidase in complex with the 8-azaxanthine inhibitor under reducing conditions (space group P 21 21 21)
Authors	:	Di Palma, M.; Chegkazi, M.; Bui, S.; Mori, G.; Percudani, R.; Steiner, R.A.
Deposited on	:	2023-03-20
Resolution	:	2.12 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:

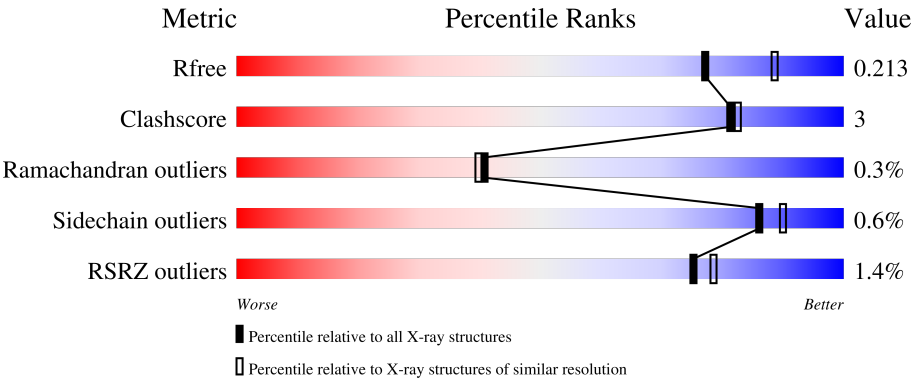
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	82% 5% 13%
1	BBB	343	82% 6% 12%
1	CCC	343	% 80% 7% 13%
1	DDD	343	4% 83% . 13%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10403 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	4	0
			2427	1542	415	446	24			
1	BBB	303	Total	C	N	O	S	0	5	0
			2478	1572	427	454	25			
1	CCC	297	Total	C	N	O	S	0	6	0
			2445	1554	422	446	23			
1	DDD	298	Total	C	N	O	S	0	6	0
			2449	1554	423	448	24			

There are 92 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

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	ALA	-	expression tag	UNP A0A8V0ZED1
AAA	0	SER	-	expression tag	UNP A0A8V0ZED1
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

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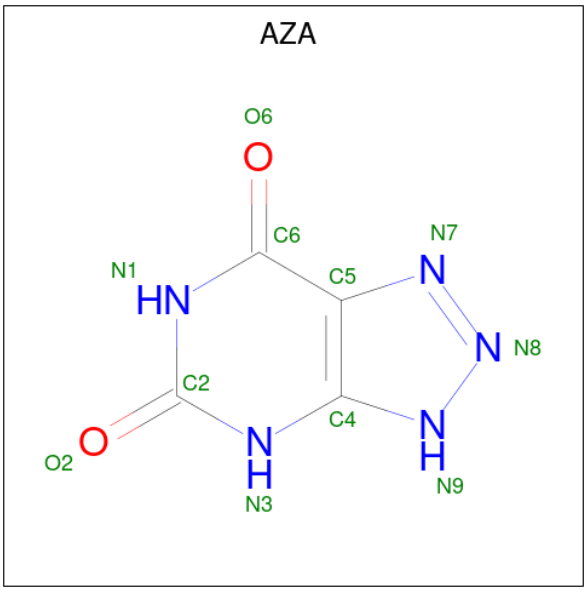
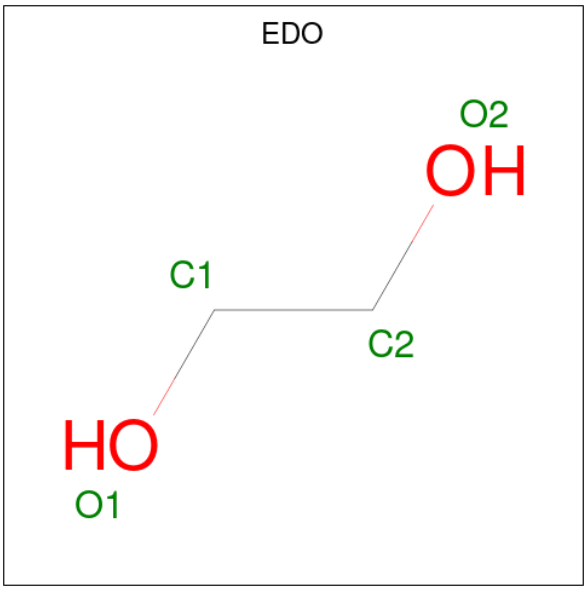
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-5	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-4	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-3	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-2	MET	-	expression tag	UNP A0A8V0ZED1
CCC	-1	ALA	-	expression tag	UNP A0A8V0ZED1
CCC	0	SER	-	expression tag	UNP A0A8V0ZED1
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 2 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
2	AAA	1	Total C N O 11 4 5 2	0	0
2	BBB	1	Total C N O 11 4 5 2	0	0
2	CCC	1	Total C N O 11 4 5 2	0	0
2	DDD	1	Total C N O 11 4 5 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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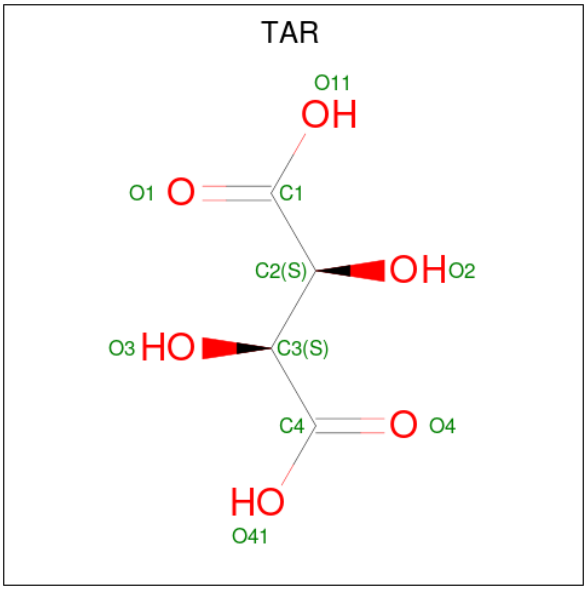
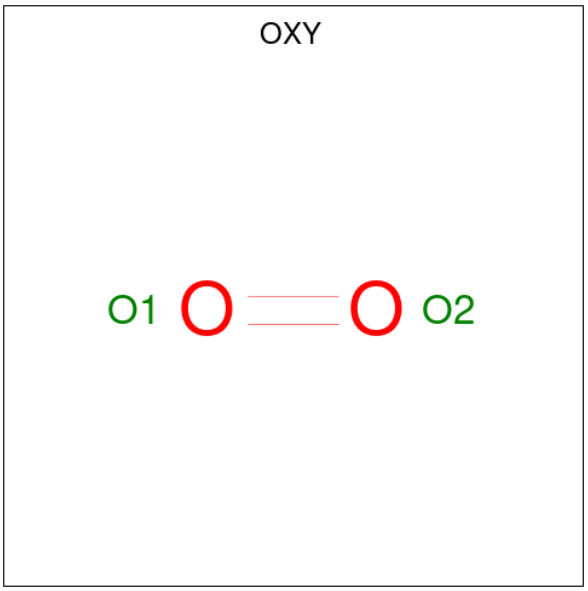
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	DDD	1	Total C O 4 2 2	0	0

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



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

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total O 2 2	0	0
5	CCC	1	Total O 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	DDD	2	Total Cl 2 2	0	0

- Molecule 7 is water.

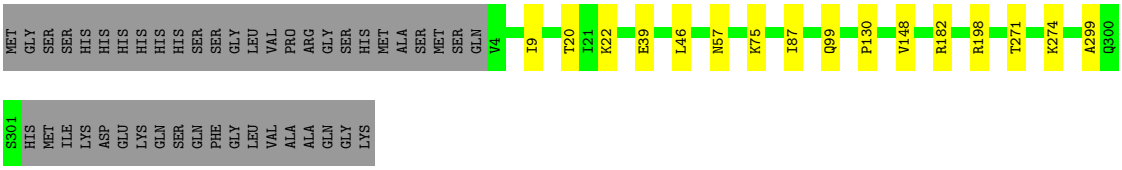
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	122	Total O 123 123	0	1
7	BBB	108	Total O 110 110	0	2
7	CCC	105	Total O 109 109	0	4
7	DDD	99	Total O 100 100	0	1

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.

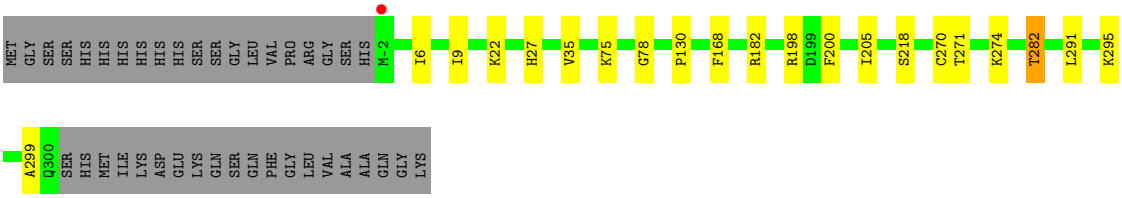
• Molecule 1: Uricase

Chain AAA:



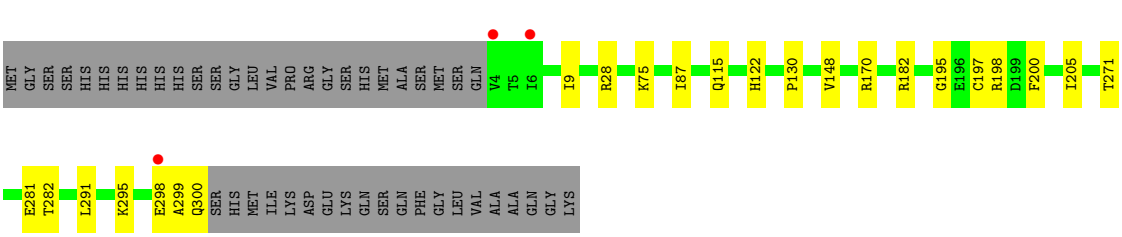
• Molecule 1: Uricase

Chain BBB:



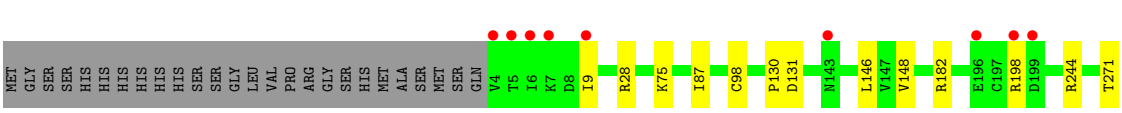
• Molecule 1: Uricase

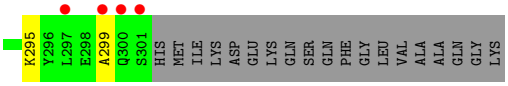
Chain CCC:



• Molecule 1: Uricase

Chain DDD:




K295
Y296
L297
E298
A299
Q300
S301
HIS
MET
ILE
LYS
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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.22Å 124.40Å 125.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.88 – 2.12 66.88 – 2.12	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.88-2.12) 100.0 (66.88-2.12)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.214 0.190 , 0.213	Depositor DCC
R_{free} test set	4571 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10403	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: CL, OXY, EDO, AZA, TAR

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	0/2480	0.82	0/3354
1	BBB	0.65	0/2532	0.81	1/3422 (0.0%)
1	CCC	0.66	0/2499	0.78	0/3378
1	DDD	0.66	0/2502	0.79	0/3382
All	All	0.66	0/10013	0.80	1/13536 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	270	CYS	CB-CA-C	-5.67	99.07	110.40

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	2427	0	2397	14	0
1	BBB	2478	0	2450	19	0
1	CCC	2445	0	2418	20	0
1	DDD	2449	0	2421	11	0
2	AAA	11	0	3	1	0
2	BBB	11	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	11	0	3	1	0
2	DDD	11	0	3	1	0
3	AAA	28	0	42	1	0
3	BBB	24	0	36	2	0
3	CCC	12	0	18	0	0
3	DDD	28	0	42	0	0
4	AAA	10	0	4	0	0
4	DDD	10	0	4	0	0
5	BBB	2	0	0	0	0
5	CCC	2	0	0	0	0
6	DDD	2	0	0	0	0
7	AAA	123	0	0	0	0
7	BBB	110	0	0	2	0
7	CCC	109	0	0	1	0
7	DDD	100	0	0	3	0
All	All	10403	0	9844	51	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 3.

The worst 5 of 51 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:CCC:198[B]:ARG:HG3	1:CCC:198[B]:ARG:NH2	1.56	1.05
1:CCC:198[B]:ARG:HH21	1:CCC:198[B]:ARG:CG	1.73	1.02
1:BBB:27[B]:HIS:HE1	7:BBB:636:HOH:O	1.40	1.01
1:BBB:27[B]:HIS:CE1	7:BBB:636:HOH:O	2.17	0.95
1:CCC:198[B]:ARG:HG3	1:CCC:198[B]:ARG:HH21	0.77	0.86

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	300/343 (88%)	288 (96%)	11 (4%)	1 (0%)	41	40
1	BBB	306/343 (89%)	295 (96%)	10 (3%)	1 (0%)	41	40
1	CCC	301/343 (88%)	291 (97%)	9 (3%)	1 (0%)	41	40
1	DDD	302/343 (88%)	292 (97%)	9 (3%)	1 (0%)	41	40
All	All	1209/1372 (88%)	1166 (96%)	39 (3%)	4 (0%)	41	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	299	ALA
1	BBB	299	ALA
1	CCC	299	ALA
1	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	275/308 (89%)	275 (100%)	0	100	100
1	BBB	280/308 (91%)	277 (99%)	3 (1%)	73	79
1	CCC	276/308 (90%)	273 (99%)	3 (1%)	73	79
1	DDD	277/308 (90%)	276 (100%)	1 (0%)	91	94
All	All	1108/1232 (90%)	1101 (99%)	7 (1%)	86	90

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	170	ARG
1	CCC	282	THR
1	DDD	295	LYS
1	CCC	295	LYS
1	BBB	295	LYS

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 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
3	EDO	AAA	404	-	3,3,3	0.13	0	2,2,2	0.08	0
2	AZA	CCC	401	-	9,12,12	1.33	1 (11%)	4,17,17	7.91	2 (50%)
2	AZA	DDD	401	-	9,12,12	1.64	2 (22%)	4,17,17	8.12	2 (50%)
3	EDO	AAA	408	-	3,3,3	0.13	0	2,2,2	0.31	0
2	AZA	BBB	502	-	9,12,12	1.48	1 (11%)	4,17,17	8.02	2 (50%)
2	AZA	AAA	401	-	9,12,12	1.48	2 (22%)	4,17,17	7.96	3 (75%)
3	EDO	CCC	405	-	3,3,3	0.05	0	2,2,2	0.18	0
3	EDO	BBB	507	-	3,3,3	0.12	0	2,2,2	0.28	0
3	EDO	AAA	405	-	3,3,3	0.10	0	2,2,2	0.16	0
3	EDO	CCC	403	-	3,3,3	0.10	0	2,2,2	0.11	0
3	EDO	DDD	403	-	3,3,3	0.11	0	2,2,2	0.15	0
5	OXY	BBB	501	-	1,1,1	0.14	0	-		
3	EDO	CCC	404	-	3,3,3	0.08	0	2,2,2	0.18	0
3	EDO	BBB	506	-	3,3,3	0.09	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	BBB	503	-	3,3,3	0.16	0	2,2,2	0.14	0
3	EDO	AAA	407	-	3,3,3	0.08	0	2,2,2	0.22	0
3	EDO	DDD	407	-	3,3,3	0.08	0	2,2,2	0.18	0
3	EDO	AAA	406	-	3,3,3	0.16	0	2,2,2	0.18	0
3	EDO	DDD	405	-	3,3,3	0.07	0	2,2,2	0.22	0
3	EDO	AAA	403	-	3,3,3	0.07	0	2,2,2	0.22	0
5	OXY	CCC	402	-	1,1,1	0.13	0	-		
4	TAR	DDD	409	-	9,9,9	1.09	0	12,12,12	0.98	0
3	EDO	DDD	402	-	3,3,3	0.17	0	2,2,2	0.28	0
4	TAR	AAA	409	-	9,9,9	1.07	0	12,12,12	1.06	0
3	EDO	AAA	402	-	3,3,3	0.12	0	2,2,2	0.19	0
3	EDO	BBB	505	-	3,3,3	0.11	0	2,2,2	0.28	0
3	EDO	BBB	504	-	3,3,3	0.15	0	2,2,2	0.04	0
3	EDO	BBB	508	-	3,3,3	0.08	0	2,2,2	0.20	0
3	EDO	DDD	404	-	3,3,3	0.07	0	2,2,2	0.01	0
3	EDO	DDD	408	-	3,3,3	0.11	0	2,2,2	0.28	0
3	EDO	DDD	406	-	3,3,3	0.17	0	2,2,2	0.22	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
3	EDO	AAA	404	-	-	0/1/1/1	-
2	AZA	CCC	401	-	-	-	0/2/2/2
2	AZA	DDD	401	-	-	-	0/2/2/2
3	EDO	AAA	408	-	-	0/1/1/1	-
2	AZA	BBB	502	-	-	-	0/2/2/2
2	AZA	AAA	401	-	-	-	0/2/2/2
3	EDO	CCC	405	-	-	0/1/1/1	-
3	EDO	BBB	507	-	-	0/1/1/1	-
3	EDO	AAA	405	-	-	1/1/1/1	-
3	EDO	CCC	403	-	-	0/1/1/1	-
3	EDO	DDD	403	-	-	1/1/1/1	-
3	EDO	CCC	404	-	-	1/1/1/1	-
3	EDO	BBB	506	-	-	1/1/1/1	-
3	EDO	BBB	503	-	-	0/1/1/1	-
3	EDO	AAA	407	-	-	1/1/1/1	-
3	EDO	DDD	407	-	-	1/1/1/1	-
3	EDO	AAA	406	-	-	0/1/1/1	-
3	EDO	DDD	405	-	-	0/1/1/1	-
3	EDO	AAA	403	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TAR	DDD	409	-	-	8/12/12/12	-
3	EDO	DDD	402	-	-	0/1/1/1	-
4	TAR	AAA	409	-	-	9/12/12/12	-
3	EDO	AAA	402	-	-	0/1/1/1	-
3	EDO	BBB	505	-	-	0/1/1/1	-
3	EDO	BBB	504	-	-	0/1/1/1	-
3	EDO	BBB	508	-	-	0/1/1/1	-
3	EDO	DDD	404	-	-	0/1/1/1	-
3	EDO	DDD	408	-	-	0/1/1/1	-
3	EDO	DDD	406	-	-	0/1/1/1	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	502	AZA	C6-N1	3.80	1.39	1.33
2	AAA	401	AZA	C6-N1	3.53	1.39	1.33
2	DDD	401	AZA	C6-N1	3.42	1.39	1.33
2	CCC	401	AZA	C6-N1	3.41	1.39	1.33
2	DDD	401	AZA	C5-C6	3.17	1.46	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	401	AZA	C2-N1-C6	14.13	127.07	115.14
2	BBB	502	AZA	C2-N1-C6	14.06	127.02	115.14
2	AAA	401	AZA	C2-N1-C6	14.03	126.99	115.14
2	CCC	401	AZA	C2-N1-C6	13.92	126.89	115.14
2	DDD	401	AZA	C5-C6-N1	-7.57	113.07	123.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	409	TAR	C1-C2-C3-O3
4	AAA	409	TAR	C1-C2-C3-C4
4	AAA	409	TAR	O2-C2-C3-O3
4	AAA	409	TAR	O2-C2-C3-C4
4	DDD	409	TAR	C1-C2-C3-O3

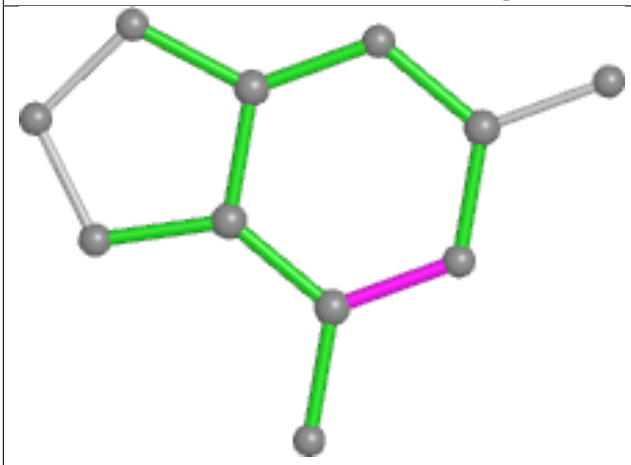
There are no ring outliers.

8 monomers are involved in 7 short contacts:

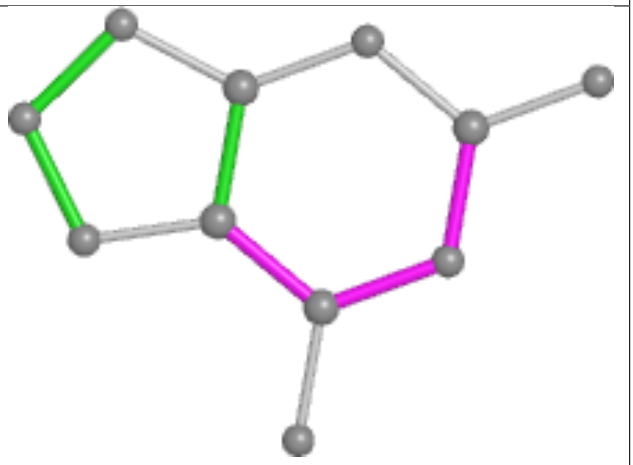
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	401	AZA	1	0
2	DDD	401	AZA	1	0
2	BBB	502	AZA	1	0
2	AAA	401	AZA	1	0
3	BBB	506	EDO	1	0
3	AAA	406	EDO	1	0
3	AAA	403	EDO	1	0
3	BBB	505	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

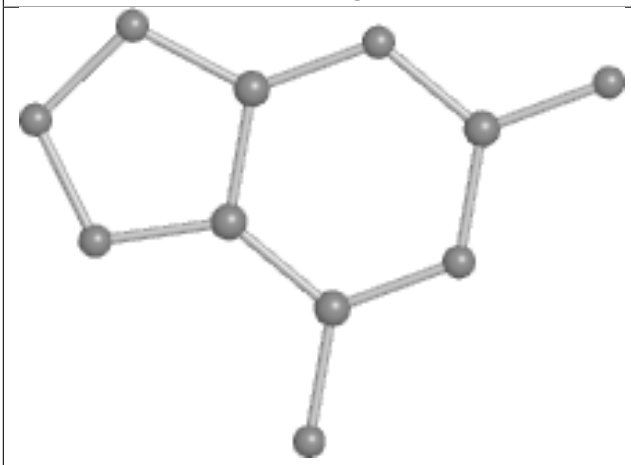
Ligand AZA CCC 401



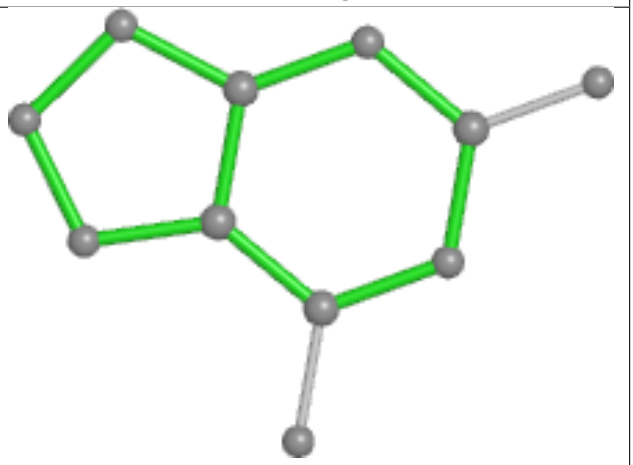
Bond lengths



Bond angles

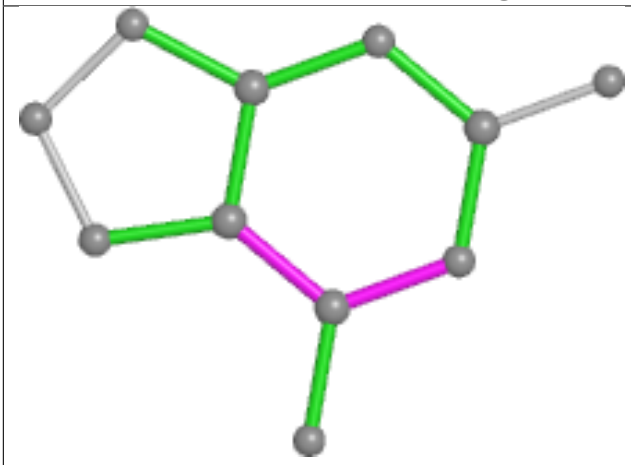


Torsions

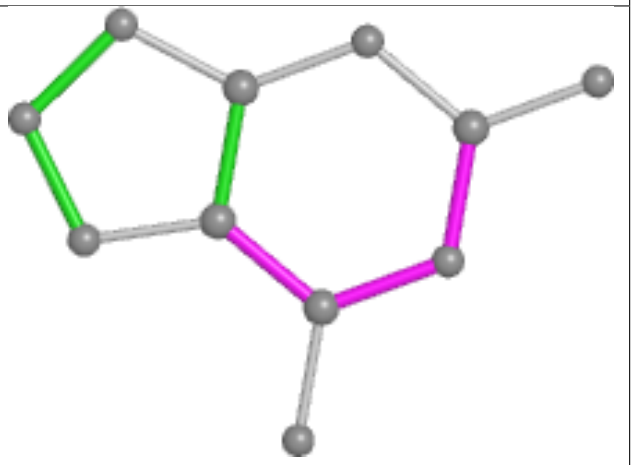


Rings

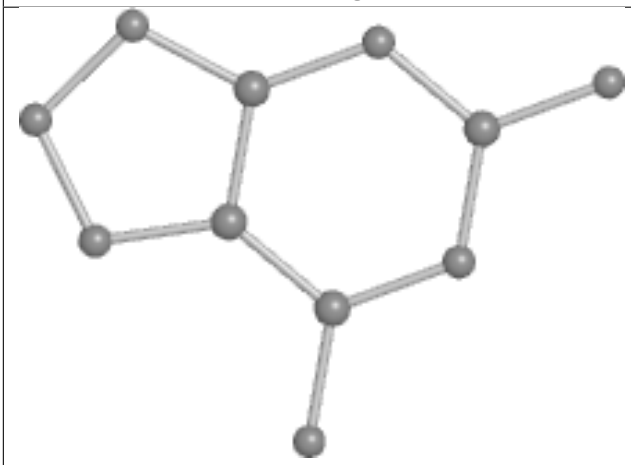
Ligand AZA DDD 401



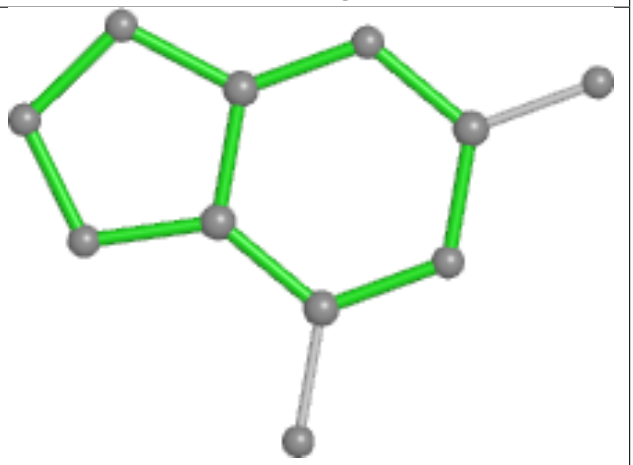
Bond lengths



Bond angles

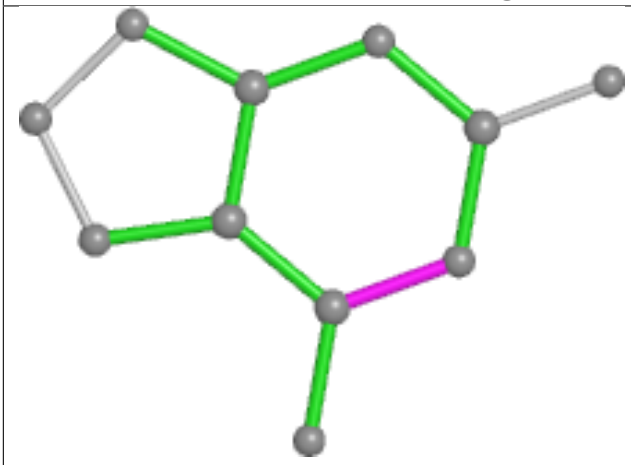


Torsions

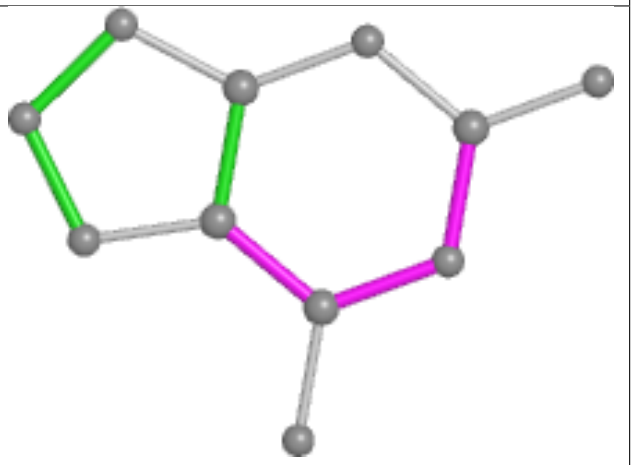


Rings

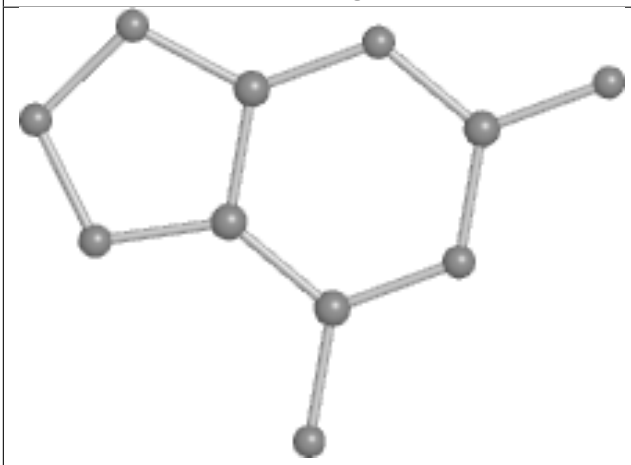
Ligand AZA BBB 502



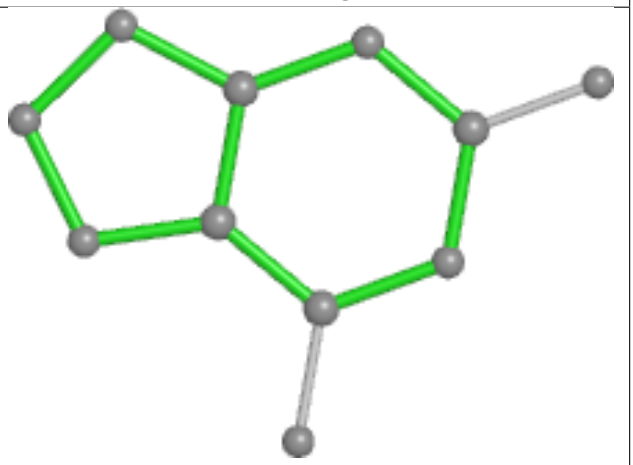
Bond lengths



Bond angles

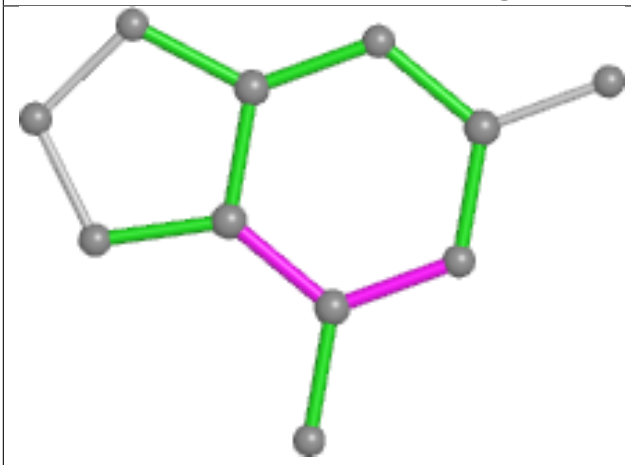


Torsions



Rings

Ligand AZA AAA 401



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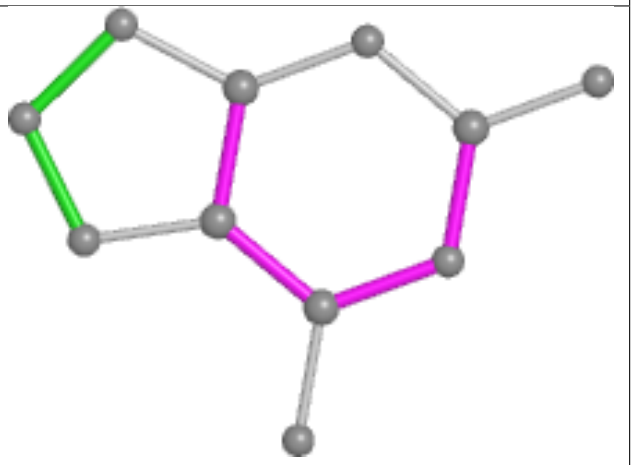
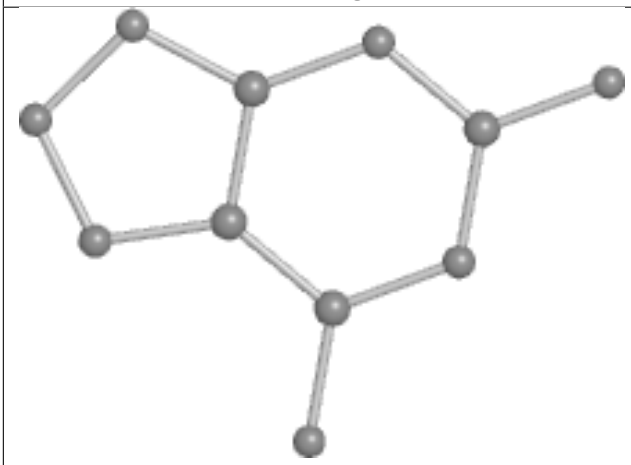
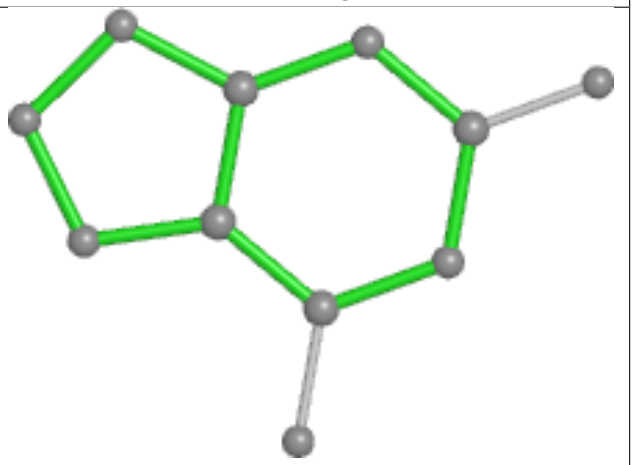


Bond angles

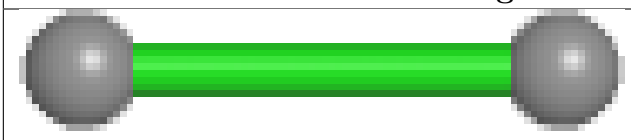


Torsions

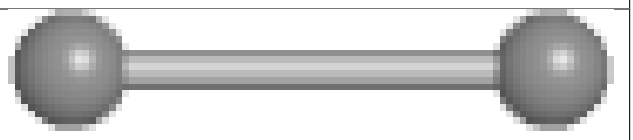


Rings

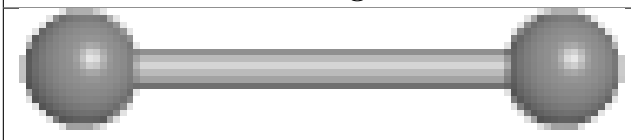
Ligand OXY BBB 501



Bond lengths

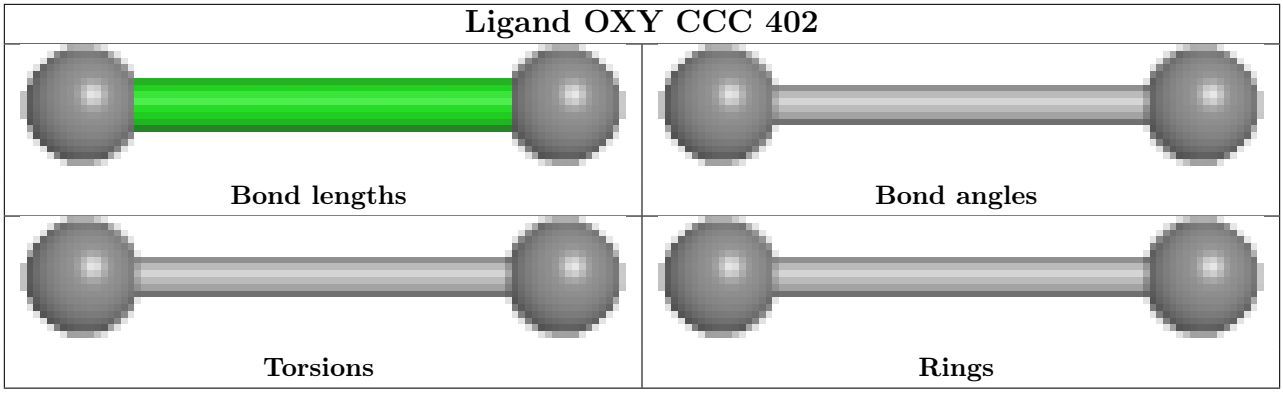


Bond angles



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	298/343 (86%)	-0.07	0 100 100	34, 43, 74, 102	0
1	BBB	303/343 (88%)	-0.17	1 (0%) 94 95	36, 47, 71, 114	0
1	CCC	297/343 (86%)	-0.26	3 (1%) 82 85	34, 46, 78, 107	0
1	DDD	298/343 (86%)	-0.13	13 (4%) 34 40	34, 47, 83, 110	0
All	All	1196/1372 (87%)	-0.16	17 (1%) 75 78	34, 46, 75, 114	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	6	ILE	3.9
1	BBB	-2	MET	3.8
1	DDD	4	VAL	3.0
1	DDD	301	SER	3.0
1	DDD	300	GLN	3.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

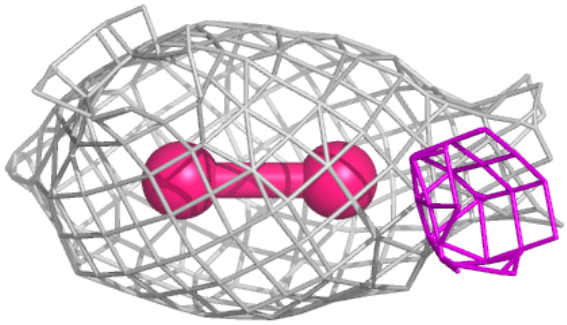
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

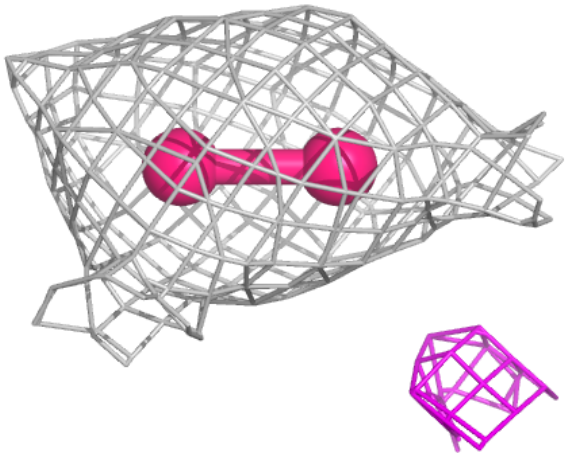
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TAR	AAA	409	10/10	0.67	0.17	73,85,93,93	0
4	TAR	DDD	409	10/10	0.71	0.28	77,86,94,95	0
3	EDO	DDD	405	4/4	0.74	0.20	88,91,92,93	0
3	EDO	DDD	406	4/4	0.81	0.24	63,76,79,80	0
3	EDO	BBB	507	4/4	0.82	0.19	66,75,78,81	0
3	EDO	DDD	407	4/4	0.82	0.23	79,80,85,85	0
6	CL	DDD	411	1/1	0.84	0.09	71,71,71,71	0
3	EDO	AAA	404	4/4	0.88	0.20	49,53,55,65	0
3	EDO	DDD	404	4/4	0.88	0.21	64,68,69,74	0
3	EDO	AAA	403	4/4	0.89	0.15	70,73,74,77	0
3	EDO	BBB	506	4/4	0.90	0.15	68,69,70,71	0
3	EDO	AAA	405	4/4	0.90	0.17	74,75,76,78	0
3	EDO	AAA	406	4/4	0.90	0.23	62,70,70,73	0
5	OXY	CCC	402	2/2	0.91	0.17	50,50,50,51	0
6	CL	DDD	410	1/1	0.92	0.11	52,52,52,52	1
3	EDO	BBB	505	4/4	0.92	0.17	70,70,73,76	0
3	EDO	BBB	508	4/4	0.93	0.16	63,68,70,71	0
3	EDO	BBB	504	4/4	0.94	0.22	57,58,58,67	0
3	EDO	CCC	405	4/4	0.94	0.24	70,70,72,76	0
3	EDO	DDD	403	4/4	0.94	0.20	60,70,70,75	0
3	EDO	AAA	408	4/4	0.94	0.14	60,67,67,71	0
3	EDO	AAA	402	4/4	0.95	0.10	42,43,43,44	0
3	EDO	BBB	503	4/4	0.96	0.14	43,43,47,48	0
3	EDO	DDD	402	4/4	0.96	0.09	42,45,45,46	0
3	EDO	CCC	404	4/4	0.96	0.18	64,65,67,69	0
2	AZA	AAA	401	11/11	0.97	0.10	32,38,43,44	0
3	EDO	AAA	407	4/4	0.97	0.16	54,65,70,80	0
5	OXY	BBB	501	2/2	0.97	0.19	50,50,50,51	0
2	AZA	DDD	401	11/11	0.97	0.09	33,36,38,40	0
3	EDO	CCC	403	4/4	0.97	0.14	47,47,49,51	0
3	EDO	DDD	408	4/4	0.97	0.24	70,73,75,76	0
2	AZA	BBB	502	11/11	0.98	0.08	34,36,38,38	0
2	AZA	CCC	401	11/11	0.98	0.09	34,36,41,42	0

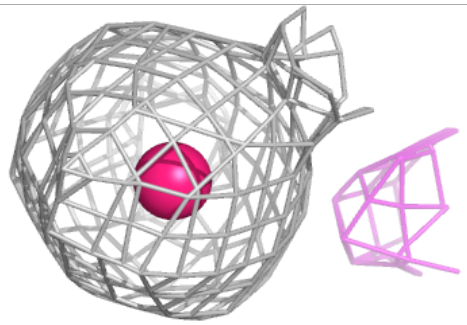
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OXY CCC 402:

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

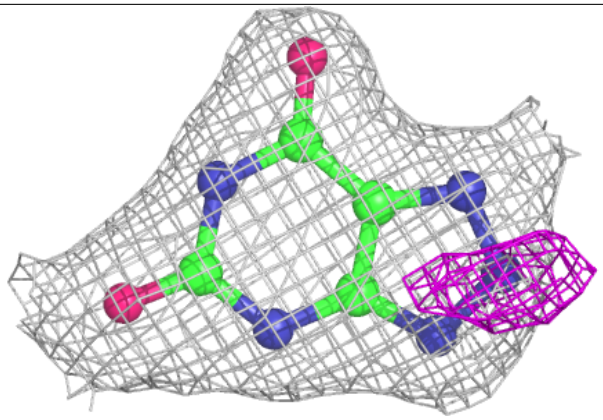


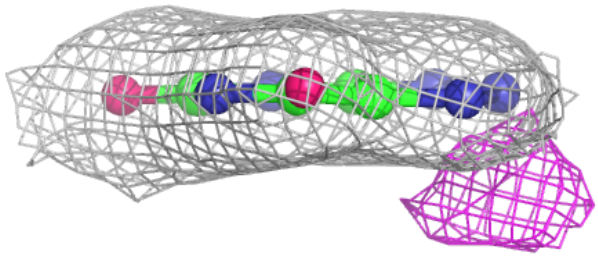


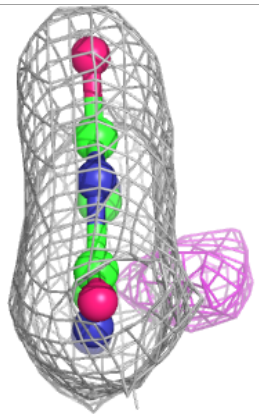


Electron density around AZA AAA 401:

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

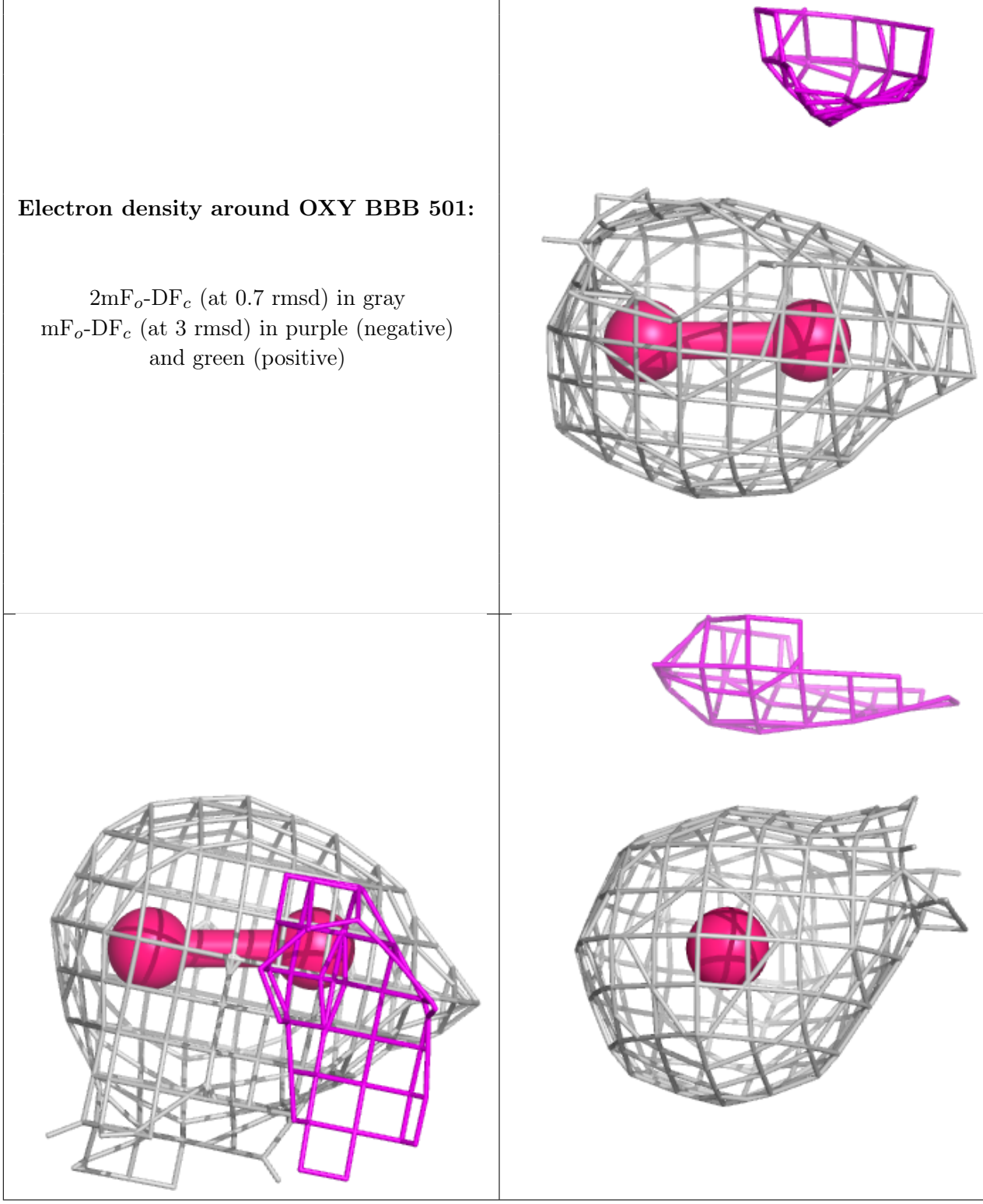






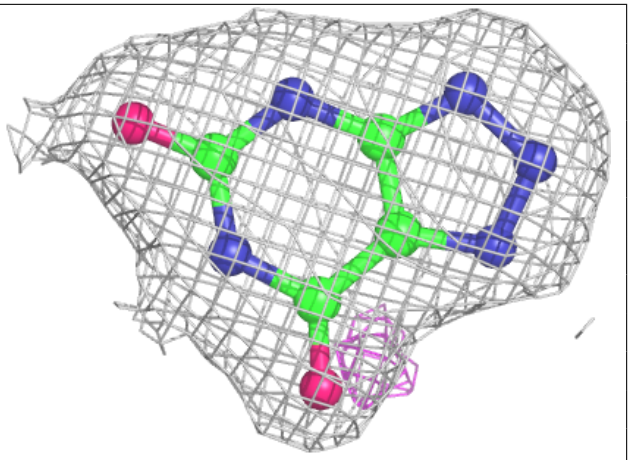
Electron density around OXY BBB 501:

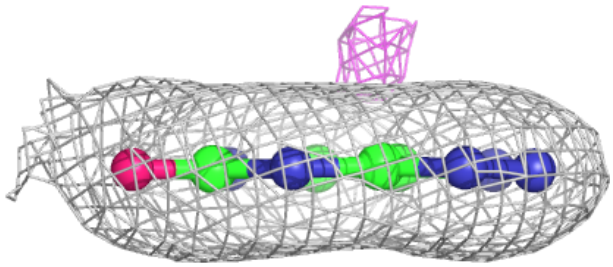
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

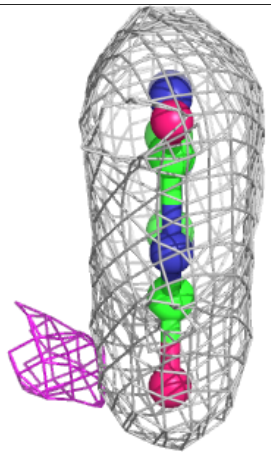


Electron density around AZA DDD 401:

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

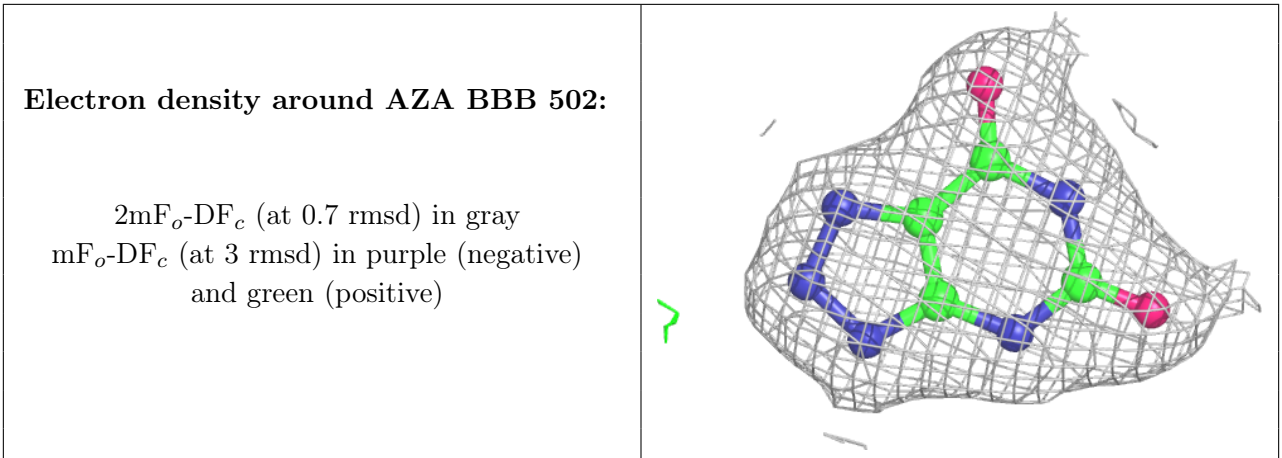


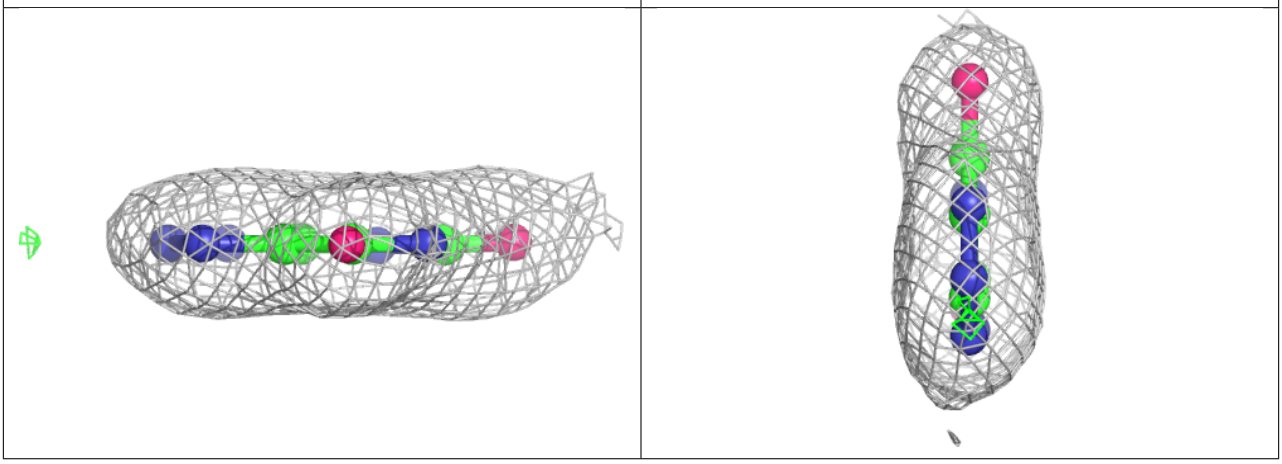




Electron density around AZA BBB 502:

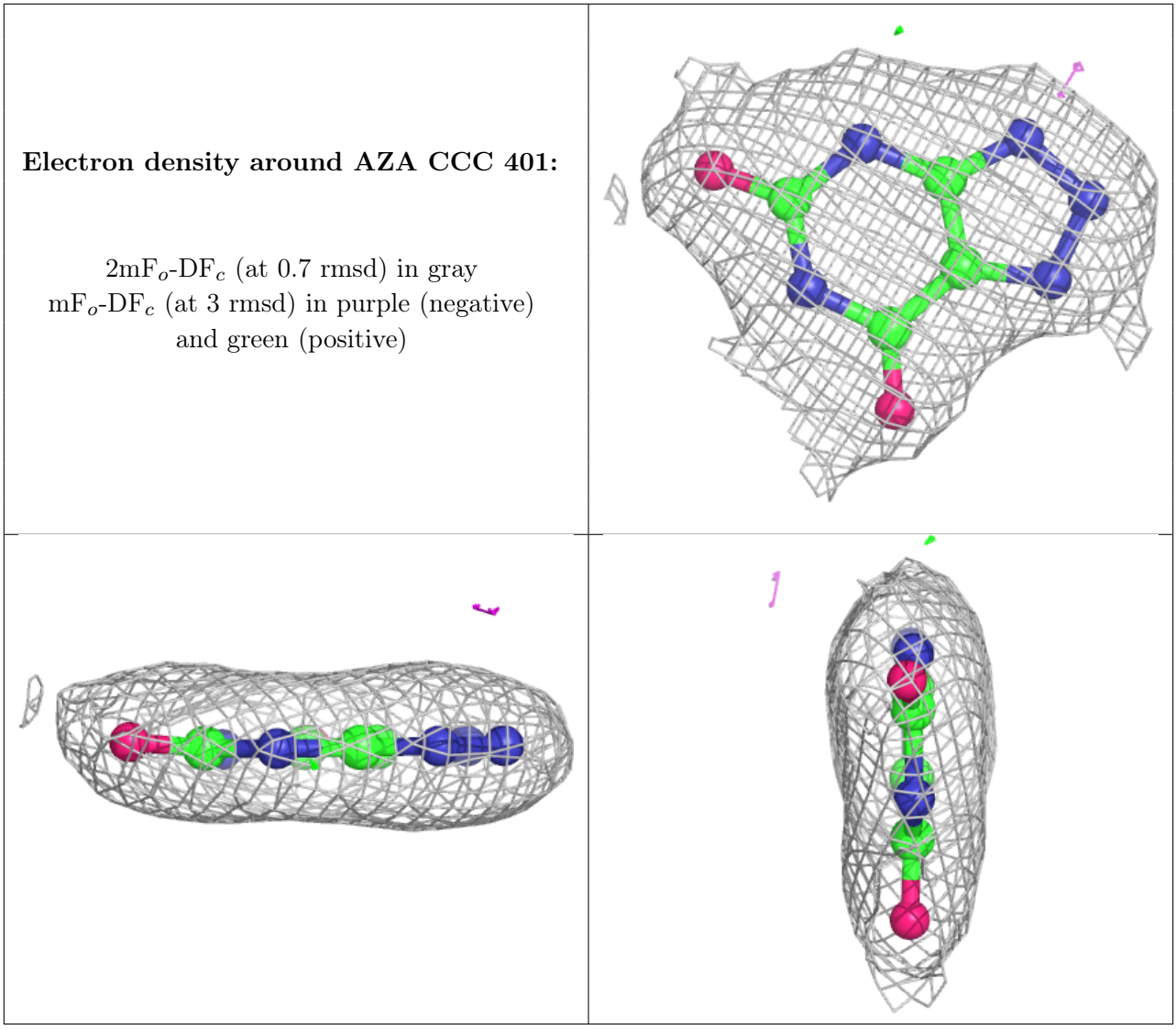
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around AZA CCC 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.