wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2024 – 03:29 pm GMT

PDB ID	:	8OIW
Title	:	Crystal structure of the cysteine-rich Gallus gallus urate oxidase in complex with the 8-azaxanthine inhibitor under oxidising conditions (space group P 21 21 21)
Authors	:	Di Palma, M.; Chegkazi, M.; Bui, S.; Mori, G.; Percudani, R.; Steiner, R.A.
Deposited on	:	2023-03-23
Resolution	:	1.89 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:

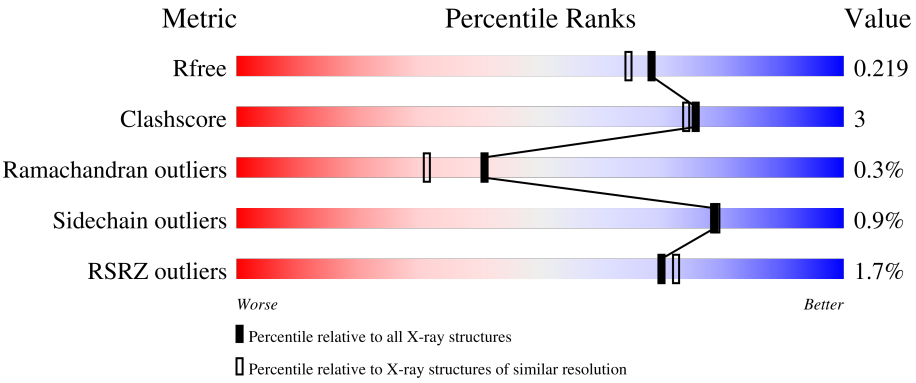
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	80% 6% 13%
2	BBB	343	83% 5% 12%
2	CCC	343	82% 5% 13%
2	DDD	343	81% 6% 13%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10503 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
			Total	C	N	O	S			
1	AAA	297	2432	1542	415	450	25	0	5	0

There are 23 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

- Molecule 2 is a protein called Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	303	Total	C	N	O	S	0	4	0
			2466	1561	423	457	25			
2	CCC	298	Total	C	N	O	S	0	6	0
			2446	1548	418	454	26			
2	DDD	297	Total	C	N	O	S	0	6	0
			2441	1546	417	453	25			

There are 69 discrepancies between the modelled and reference sequences:

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

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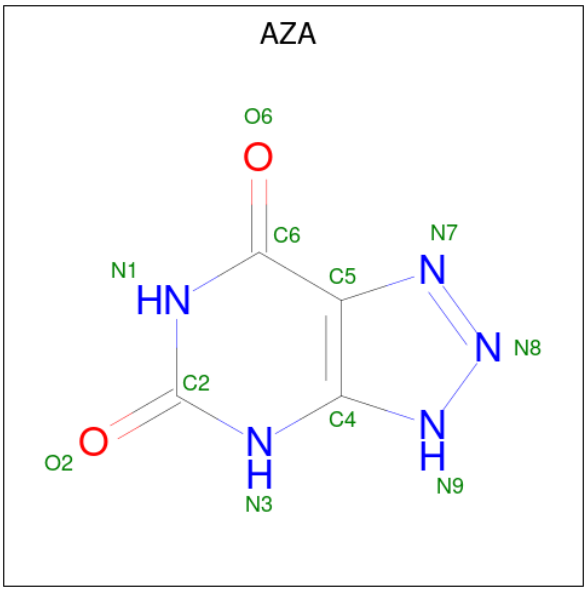
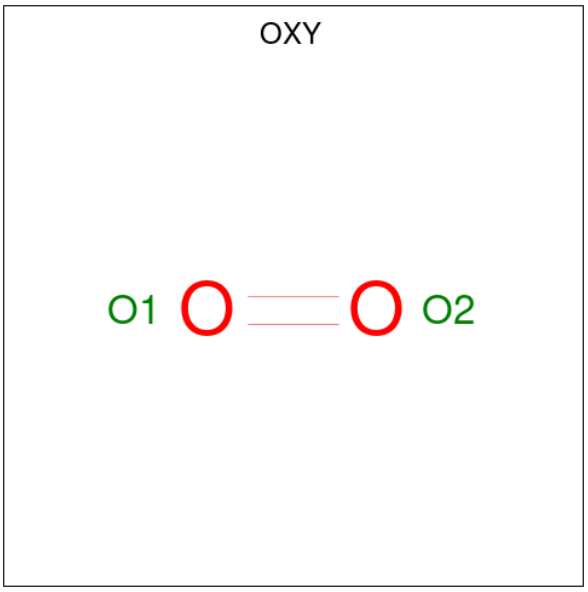
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-12	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-11	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-10	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-9	LEU	-	expression tag	UNP A0A8V0ZED1
CCC	-8	VAL	-	expression tag	UNP A0A8V0ZED1
CCC	-7	PRO	-	expression tag	UNP A0A8V0ZED1
CCC	-6	ARG	-	expression tag	UNP A0A8V0ZED1
CCC	-5	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-4	SER	-	expression tag	UNP A0A8V0ZED1
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 3 is 8-AZAXANTHINE (three-letter code: AZA) (formula: $C_4H_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



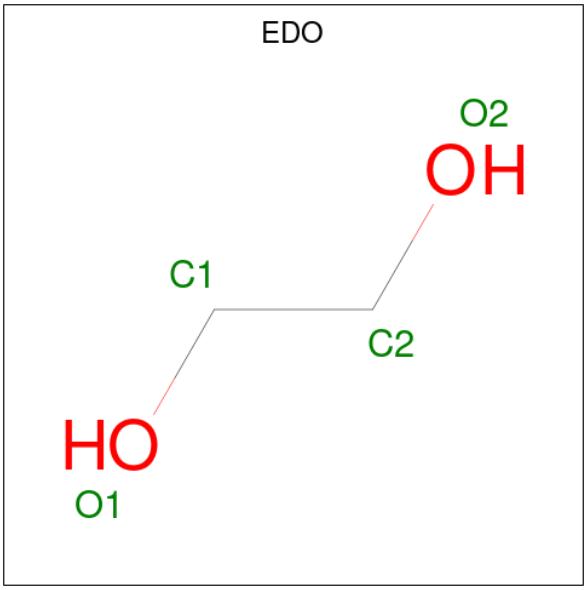
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C N O 11 4 5 2	0	0
3	BBB	1	Total C N O 11 4 5 2	0	0
3	CCC	1	Total C N O 11 4 5 2	0	0
3	DDD	1	Total C N O 11 4 5 2	0	0

- 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	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

- 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	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0

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

- Molecule 7 is water.

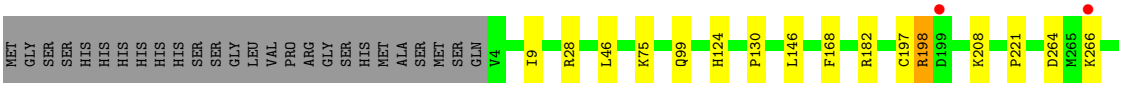
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	153	Total O 153 153	0	0
7	BBB	153	Total O 155 155	0	2
7	CCC	156	Total O 156 156	0	0
7	DDD	135	Total O 136 136	0	1

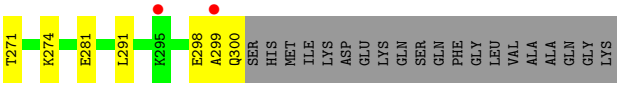
3 Residue-property plots (i)

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

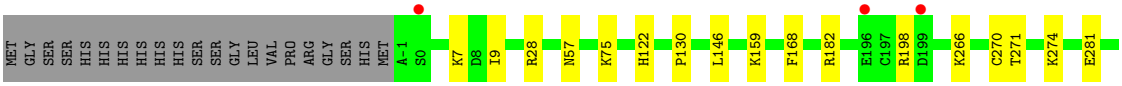
Chain AAA:

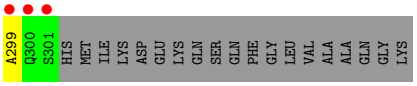




- Molecule 2: Uricase

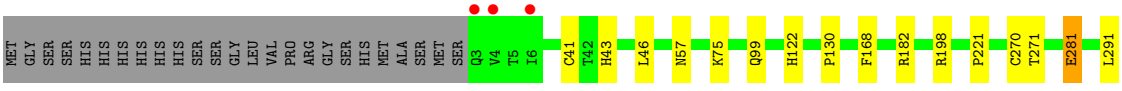
Chain BBB:





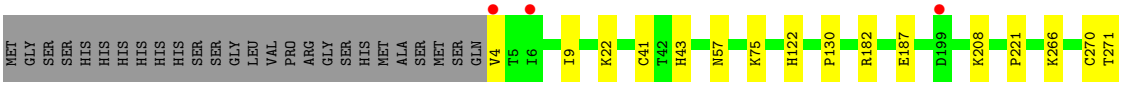
- Molecule 2: Uricase

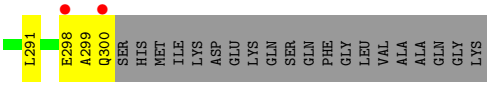
Chain CCC:



- Molecule 2: Uricase

Chain DDD:




L291
E298
A299
Q300
SER
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	101.78Å 124.86Å 128.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.89 – 1.89 78.89 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.7 (78.89-1.89) 97.7 (78.89-1.89)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.188 , 0.214 0.195 , 0.219	Depositor DCC
R_{free} test set	6236 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10503	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, CSO, AZA, CSD, CL, 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	0.63	0/2461	0.78	0/3327
2	BBB	0.64	0/2498	0.77	0/3377
2	CCC	0.63	0/2471	0.77	0/3344
2	DDD	0.64	0/2470	0.77	0/3341
All	All	0.63	0/9900	0.77	0/13389

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	2432	0	2395	21	0
2	BBB	2466	0	2439	18	0
2	CCC	2446	0	2409	23	0
2	DDD	2441	0	2400	19	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	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
5	AAA	12	0	18	0	0
5	BBB	12	0	18	0	0
5	CCC	16	0	24	0	0
5	DDD	16	0	24	3	0
6	AAA	4	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	3	0	0	0	0
6	DDD	2	0	0	0	0
7	AAA	153	0	0	2	0
7	BBB	155	0	0	2	0
7	CCC	156	0	0	9	0
7	DDD	136	0	0	2	0
All	All	10503	0	9739	61	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 61 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)
2:CCC:198[A]:ARG:CZ	7:CCC:501:HOH:O	1.99	1.09
4:AAA:402:OXY:O1	7:AAA:501:HOH:O	1.91	0.88
2:CCC:198[B]:ARG:NH1	7:CCC:502:HOH:O	2.10	0.84
2:CCC:198[A]:ARG:NE	7:CCC:501:HOH:O	2.05	0.78
2:CCC:198[B]:ARG:NE	7:CCC:501:HOH:O	2.14	0.78

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	297/343 (87%)	287 (97%)	9 (3%)	1 (0%)	41	31
2	BBB	302/343 (88%)	291 (96%)	10 (3%)	1 (0%)	41	31
2	CCC	298/343 (87%)	288 (97%)	9 (3%)	1 (0%)	41	31
2	DDD	298/343 (87%)	288 (97%)	9 (3%)	1 (0%)	41	31
All	All	1195/1372 (87%)	1154 (97%)	37 (3%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	299	ALA
2	DDD	299	ALA
2	CCC	299	ALA
2	BBB	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	272/305 (89%)	268 (98%)	4 (2%)	65	62
2	BBB	276/305 (90%)	274 (99%)	2 (1%)	84	84
2	CCC	273/305 (90%)	271 (99%)	2 (1%)	84	84
2	DDD	273/305 (90%)	270 (99%)	3 (1%)	73	73
All	All	1094/1220 (90%)	1083 (99%)	11 (1%)	78	76

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	281	GLU
2	DDD	208	LYS
2	DDD	270	CYS
2	DDD	266	LYS
2	BBB	266	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)

13 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	$\#\|Z\| > 2$
2	CSD	CCC	141	2	3,7,8	0.81	0	1,8,10	1.10	0
2	CSD	CCC	197[A]	2	3,7,8	0.90	0	1,8,10	0.51	0
2	CSD	DDD	197	2	3,7,8	0.71	0	1,8,10	0.49	0
1	CSO	AAA	197	1	3,6,7	0.75	0	0,6,8	-	-
2	CSD	CCC	197[B]	2	3,7,8	0.78	0	1,8,10	0.45	0
2	CSD	DDD	141	2	3,7,8	0.58	0	1,8,10	0.63	0
2	CSD	DDD	41	2	3,7,8	0.72	0	1,8,10	0.06	0
2	CSD	BBB	141	2	3,7,8	0.65	0	1,8,10	0.52	0
2	CSD	CCC	41	2	3,7,8	0.63	0	1,8,10	0.06	0
1	CSD	AAA	41	1	3,7,8	0.72	0	1,8,10	0.47	0
1	CSD	AAA	141	1	3,7,8	0.64	0	1,8,10	0.40	0
2	CSD	BBB	197	2	3,7,8	0.77	0	1,8,10	0.43	0
2	CSD	BBB	41	2	3,7,8	0.67	0	1,8,10	0.32	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
2	CSD	CCC	141	2	-	1/2/6/8	-
2	CSD	CCC	197[A]	2	-	1/2/6/8	-
2	CSD	DDD	197	2	-	1/2/6/8	-
1	CSO	AAA	197	1	-	1/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	CCC	197[B]	2	-	1/2/6/8	-
2	CSD	DDD	141	2	-	1/2/6/8	-
2	CSD	DDD	41	2	-	1/2/6/8	-
2	CSD	BBB	141	2	-	1/2/6/8	-
2	CSD	CCC	41	2	-	1/2/6/8	-
1	CSD	AAA	41	1	-	1/2/6/8	-
1	CSD	AAA	141	1	-	1/2/6/8	-
2	CSD	BBB	197	2	-	1/2/6/8	-
2	CSD	BBB	41	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 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
2	BBB	41	CSD	CA-CB-SG-OD1
2	BBB	141	CSD	CA-CB-SG-OD1
2	BBB	197	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	197	CSO	1	0
2	DDD	41	CSD	1	0
2	CCC	41	CSD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 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	405	-	3,3,3	0.06	0	2,2,2	0.22	0
5	EDO	CCC	404	-	3,3,3	0.04	0	2,2,2	0.11	0
5	EDO	BBB	404	-	3,3,3	0.08	0	2,2,2	0.23	0
5	EDO	DDD	403	-	3,3,3	0.01	0	2,2,2	0.08	0
4	OXY	AAA	402	-	1,1,1	0.11	0	-		
3	AZA	CCC	402	-	9,12,12	1.61	2 (22%)	4,17,17	7.99	3 (75%)
5	EDO	CCC	406	-	3,3,3	0.11	0	2,2,2	0.11	0
5	EDO	DDD	404	-	3,3,3	0.12	0	2,2,2	0.31	0
4	OXY	CCC	401	-	1,1,1	0.13	0	-		
3	AZA	BBB	401	-	9,12,12	1.36	1 (11%)	4,17,17	8.15	2 (50%)
5	EDO	CCC	403	-	3,3,3	0.11	0	2,2,2	0.08	0
3	AZA	DDD	401	-	9,12,12	1.29	1 (11%)	4,17,17	7.74	2 (50%)
5	EDO	BBB	403	-	3,3,3	0.09	0	2,2,2	0.22	0
5	EDO	CCC	405	-	3,3,3	0.07	0	2,2,2	0.17	0
5	EDO	AAA	404	-	3,3,3	0.08	0	2,2,2	0.19	0
4	OXY	AAA	403	-	1,1,1	0.12	0	-		
5	EDO	BBB	405	-	3,3,3	0.08	0	2,2,2	0.16	0
5	EDO	AAA	406	-	3,3,3	0.05	0	2,2,2	0.13	0
3	AZA	AAA	401	-	9,12,12	1.23	1 (11%)	4,17,17	7.97	2 (50%)
5	EDO	DDD	405	-	3,3,3	0.12	0	2,2,2	0.29	0
4	OXY	BBB	402	-	1,1,1	0.14	0	-		
5	EDO	DDD	402	-	3,3,3	0.17	0	2,2,2	0.17	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	BBB	405	-	-	0/1/1/1	-
5	EDO	DDD	403	-	-	1/1/1/1	-
3	AZA	BBB	401	-	-	-	0/2/2/2
5	EDO	AAA	406	-	-	0/1/1/1	-
3	AZA	CCC	402	-	-	-	0/2/2/2
5	EDO	CCC	406	-	-	0/1/1/1	-
5	EDO	CCC	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AZA	AAA	401	-	-	-	0/2/2/2
5	EDO	AAA	405	-	-	1/1/1/1	-
5	EDO	BBB	403	-	-	0/1/1/1	-
3	AZA	DDD	401	-	-	-	0/2/2/2
5	EDO	DDD	404	-	-	1/1/1/1	-
5	EDO	DDD	405	-	-	1/1/1/1	-
5	EDO	CCC	404	-	-	1/1/1/1	-
5	EDO	CCC	405	-	-	1/1/1/1	-
5	EDO	AAA	404	-	-	0/1/1/1	-
5	EDO	DDD	402	-	-	0/1/1/1	-
5	EDO	BBB	404	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	401	AZA	C6-N1	3.78	1.39	1.33
3	DDD	401	AZA	C6-N1	3.49	1.39	1.33
3	CCC	402	AZA	C6-N1	3.47	1.39	1.33
3	AAA	401	AZA	C6-N1	3.29	1.38	1.33
3	CCC	402	AZA	C5-C6	2.97	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})
3	BBB	401	AZA	C2-N1-C6	14.34	127.25	115.14
3	AAA	401	AZA	C2-N1-C6	14.20	127.13	115.14
3	CCC	402	AZA	C2-N1-C6	14.04	127.00	115.14
3	DDD	401	AZA	C2-N1-C6	13.66	126.67	115.14
3	BBB	401	AZA	C5-C6-N1	-7.50	113.17	123.43

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

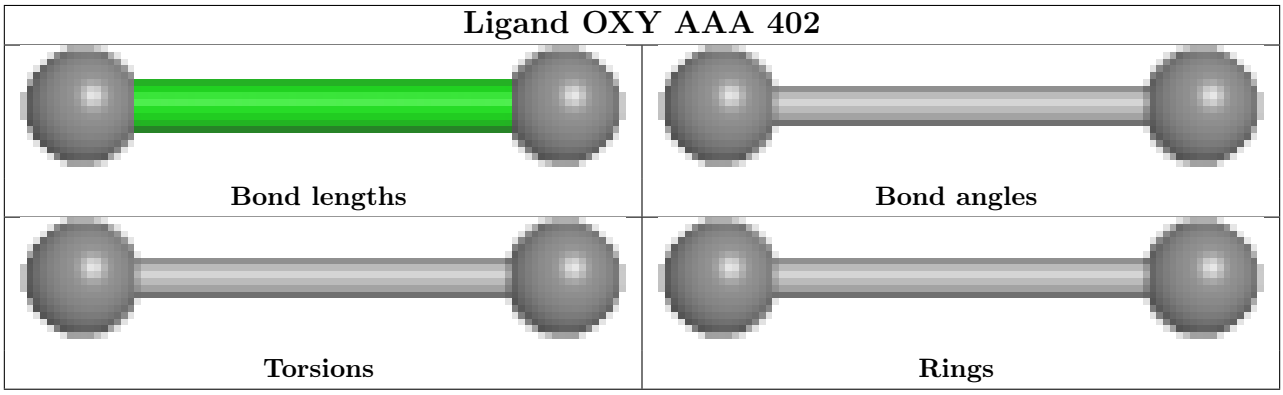
Mol	Chain	Res	Type	Atoms
5	CCC	405	EDO	O1-C1-C2-O2
5	DDD	404	EDO	O1-C1-C2-O2
5	AAA	405	EDO	O1-C1-C2-O2
5	DDD	405	EDO	O1-C1-C2-O2
5	CCC	404	EDO	O1-C1-C2-O2

There are no ring outliers.

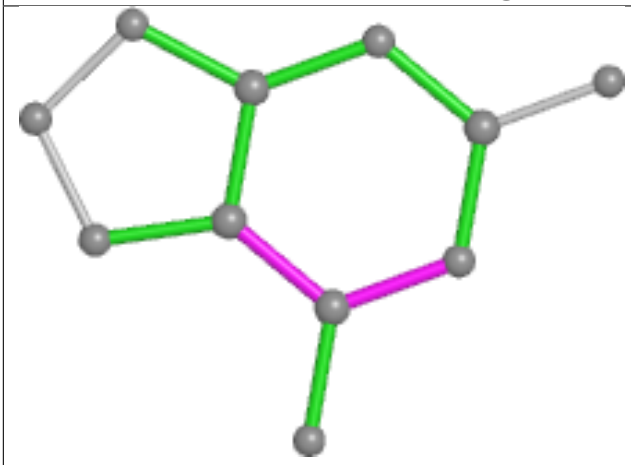
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	402	OXY	1	0
3	CCC	402	AZA	1	0
5	DDD	404	EDO	1	0
3	BBB	401	AZA	1	0
3	DDD	401	AZA	1	0
3	AAA	401	AZA	1	0
5	DDD	405	EDO	2	0

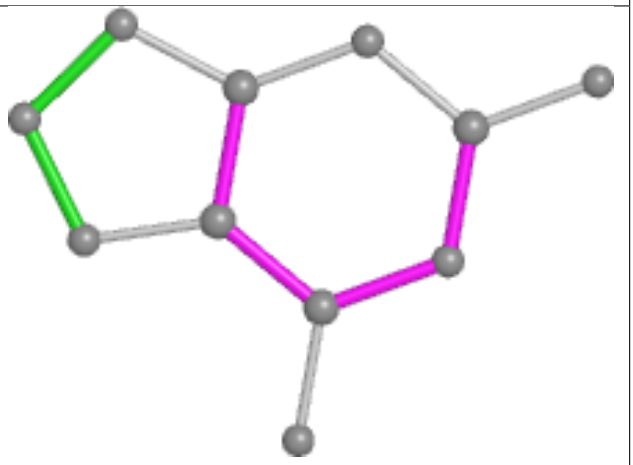
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



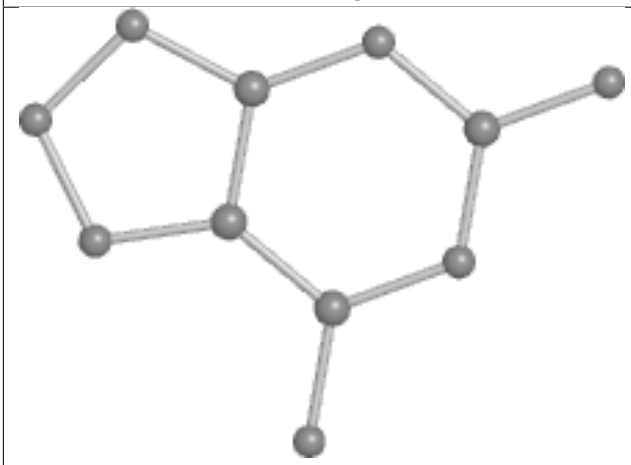
Ligand AZA CCC 402



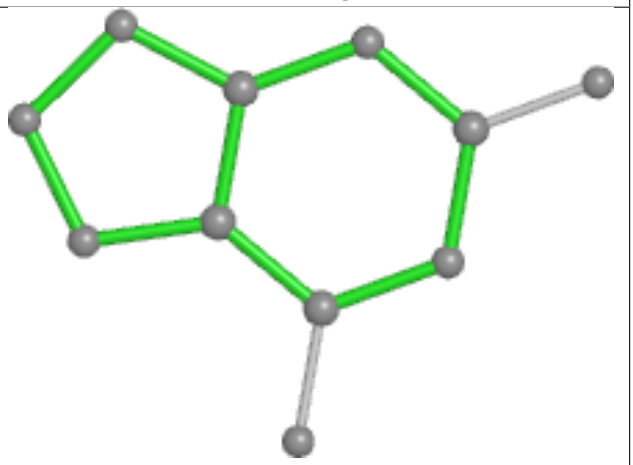
Bond lengths



Bond angles

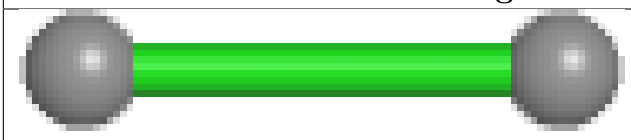


Torsions

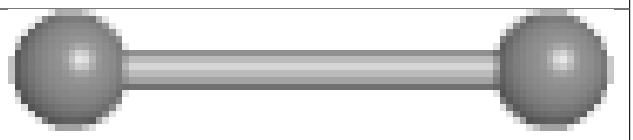


Rings

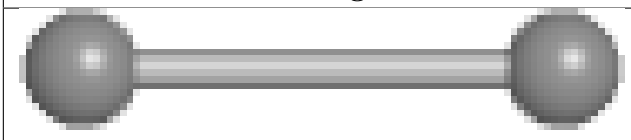
Ligand OXY CCC 401



Bond lengths



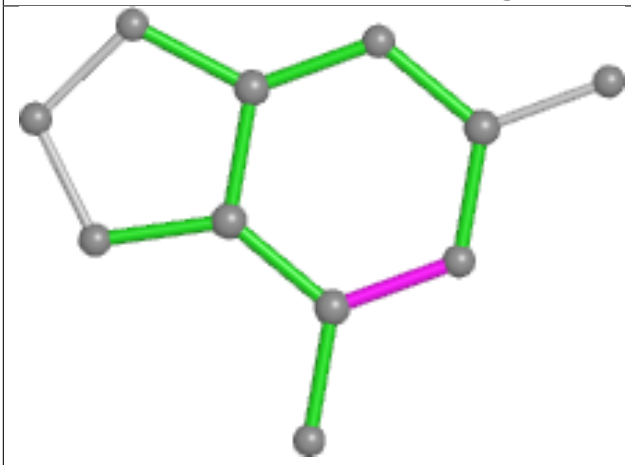
Bond angles



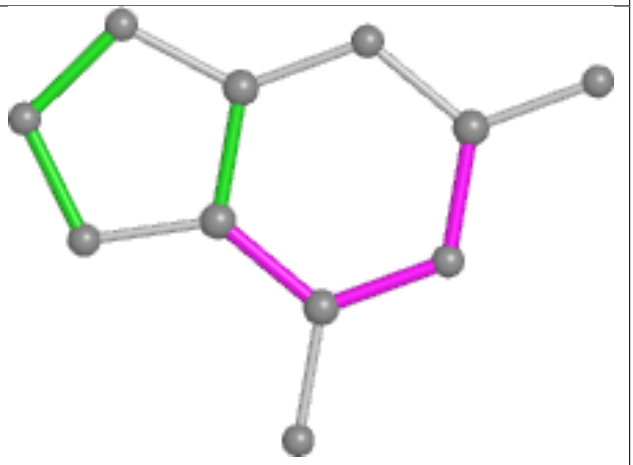
Torsions

Rings

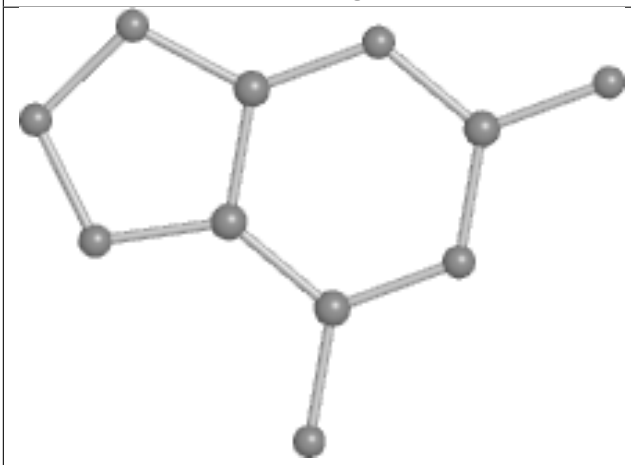
Ligand AZA BBB 401



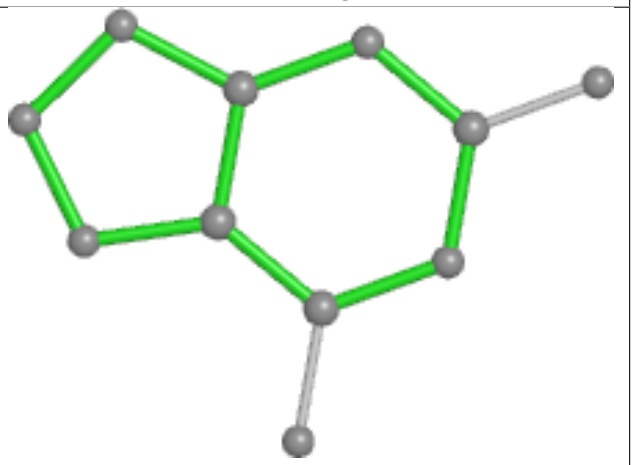
Bond lengths



Bond angles

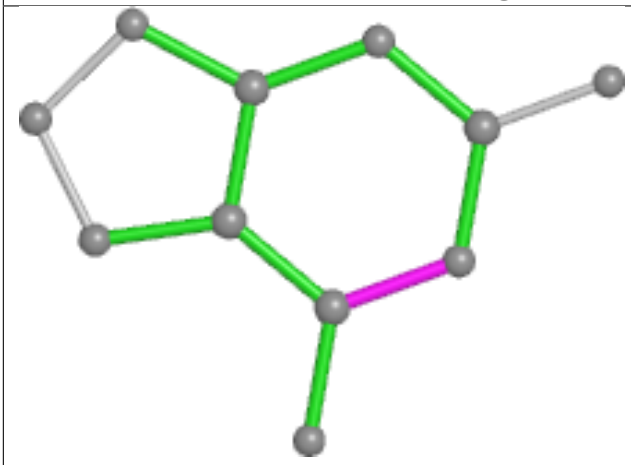


Torsions

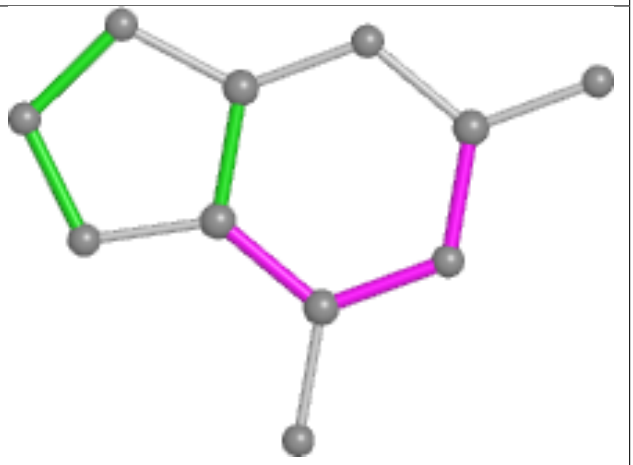


Rings

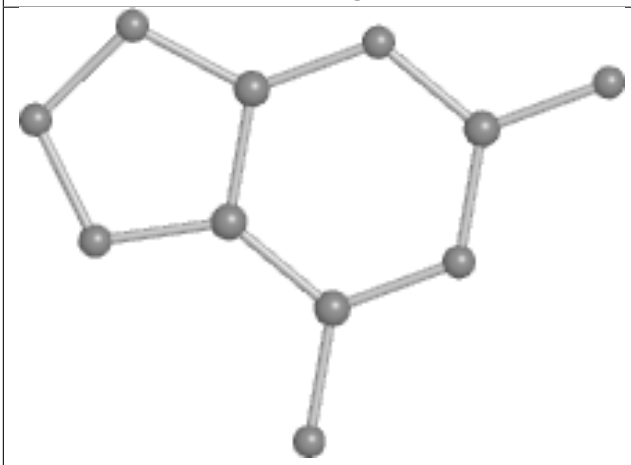
Ligand AZA DDD 401



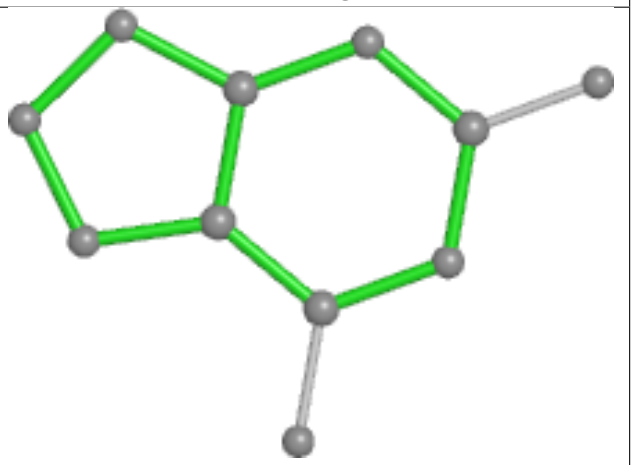
Bond lengths



Bond angles

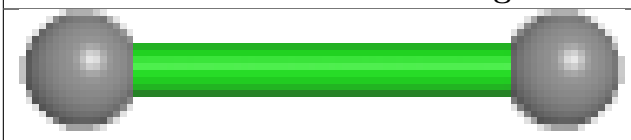


Torsions

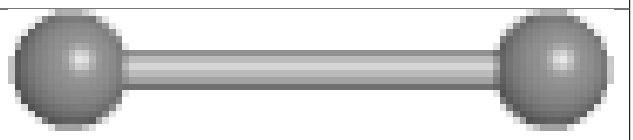


Rings

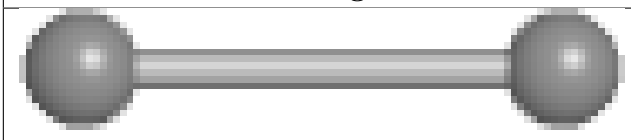
Ligand OXY AAA 403



Bond lengths



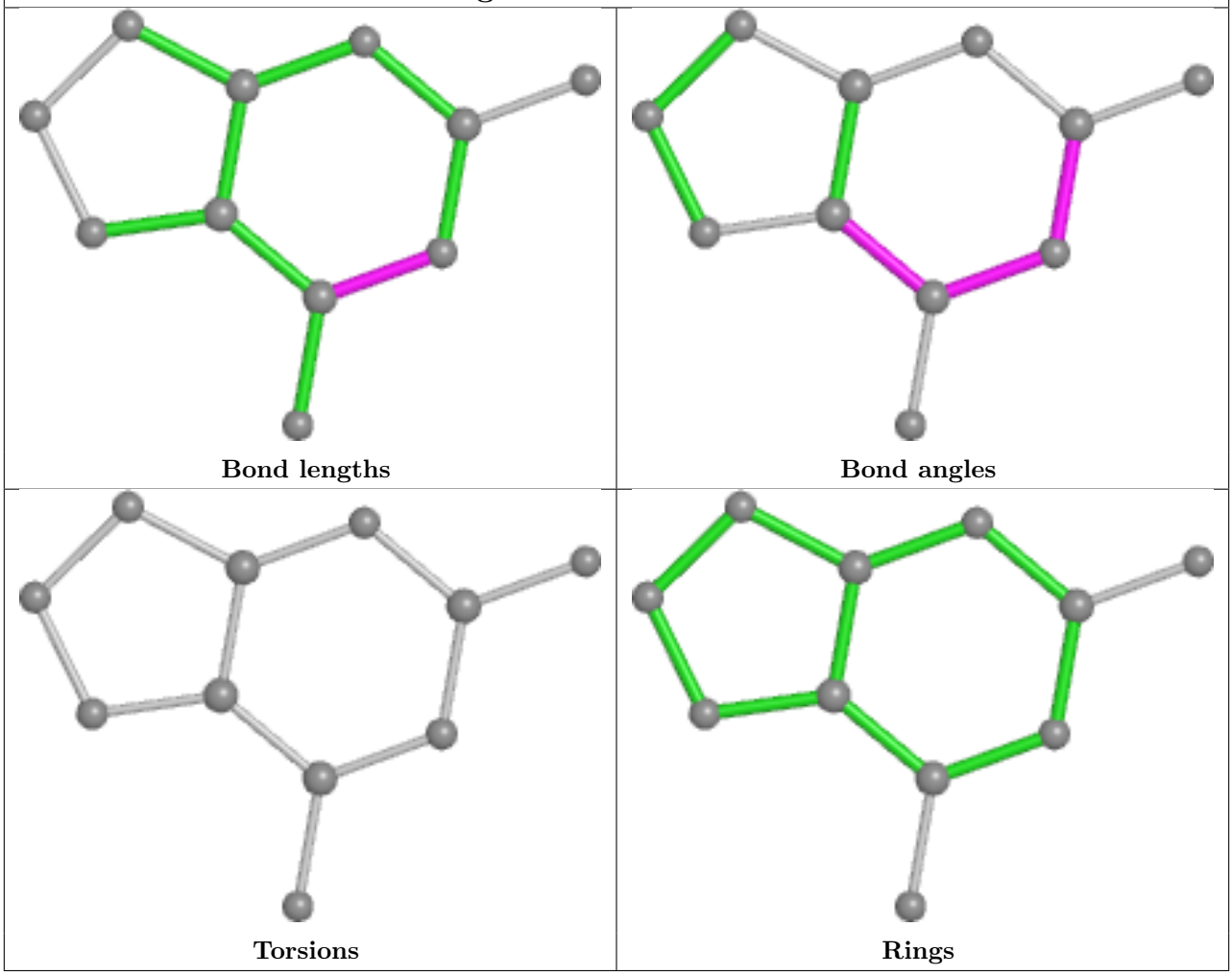
Bond angles



Torsions

Rings

Ligand AZA AAA 401



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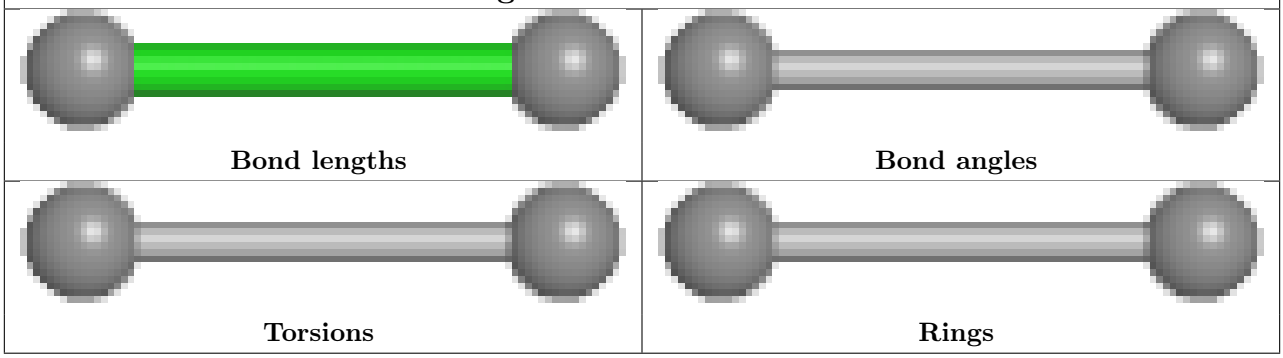

5.7 Other polymers (i)

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%)	0.08	4 (1%)	75	77	31, 40, 67, 101	0
2	BBB	300/343 (87%)	0.12	6 (2%)	65	68	30, 41, 67, 112	0
2	CCC	295/343 (86%)	0.16	5 (1%)	70	72	30, 39, 67, 108	0
2	DDD	294/343 (85%)	0.08	5 (1%)	70	72	33, 42, 70, 99	0
All	All	1183/1372 (86%)	0.11	20 (1%)	70	72	30, 41, 68, 112	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	301	SER	7.4
2	CCC	3	GLN	6.2
2	CCC	4	VAL	4.9
1	AAA	199	ASP	4.4
2	BBB	0	SER	3.3

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	0.73	0.12	79,82,92,92	0
2	CSD	BBB	197	8/9	0.83	0.17	64,68,79,81	0
1	CSO	AAA	197	7/8	0.85	0.17	68,70,76,81	0
2	CSD	CCC	197[B]	8/9	0.89	0.12	55,56,58,59	8
2	CSD	CCC	197[A]	8/9	0.89	0.12	55,57,58,59	8
2	CSD	CCC	41	8/9	0.95	0.12	33,34,47,49	0
1	CSD	AAA	41	8/9	0.96	0.10	32,35,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CSD	BBB	141	8/9	0.96	0.10	37,39,48,51	0
2	CSD	DDD	41	8/9	0.96	0.11	35,37,45,48	0
2	CSD	CCC	141	8/9	0.96	0.12	37,38,49,52	0
1	CSD	AAA	141	8/9	0.97	0.09	38,40,56,57	0
2	CSD	BBB	41	8/9	0.97	0.10	31,35,43,45	0
2	CSD	DDD	141	8/9	0.98	0.09	41,43,53,55	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	0.61	0.17	70,70,71,76	0
5	EDO	BBB	404	4/4	0.72	0.15	71,73,76,76	0
5	EDO	AAA	405	4/4	0.72	0.16	74,77,77,77	0
5	EDO	AAA	406	4/4	0.81	0.17	70,70,72,73	0
5	EDO	DDD	404	4/4	0.84	0.22	52,61,65,67	0
5	EDO	CCC	406	4/4	0.87	0.17	51,52,55,62	0
5	EDO	CCC	404	4/4	0.88	0.12	66,66,67,68	0
5	EDO	BBB	405	4/4	0.88	0.13	71,72,74,74	0
5	EDO	DDD	403	4/4	0.89	0.15	59,60,61,63	0
5	EDO	DDD	405	4/4	0.89	0.17	61,68,72,75	0
4	OXY	CCC	401	2/2	0.91	0.14	48,48,48,49	0
5	EDO	CCC	403	4/4	0.94	0.12	41,42,42,43	0
6	CL	CCC	408	1/1	0.94	0.07	56,56,56,56	0
6	CL	AAA	409	1/1	0.95	0.07	68,68,68,68	0
6	CL	AAA	410	1/1	0.95	0.09	59,59,59,59	0
6	CL	AAA	408	1/1	0.95	0.07	71,71,71,71	0
6	CL	DDD	406	1/1	0.95	0.10	48,48,48,48	0
5	EDO	DDD	402	4/4	0.96	0.11	37,39,39,39	0
5	EDO	AAA	404	4/4	0.96	0.13	43,44,44,44	0
5	EDO	BBB	403	4/4	0.96	0.13	40,40,41,41	0
3	AZA	AAA	401	11/11	0.97	0.09	31,31,34,34	0
3	AZA	BBB	401	11/11	0.97	0.10	30,32,33,33	0

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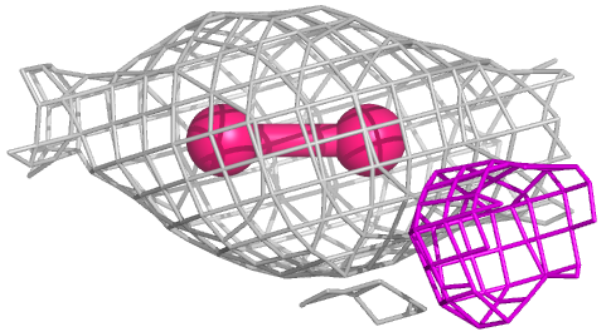
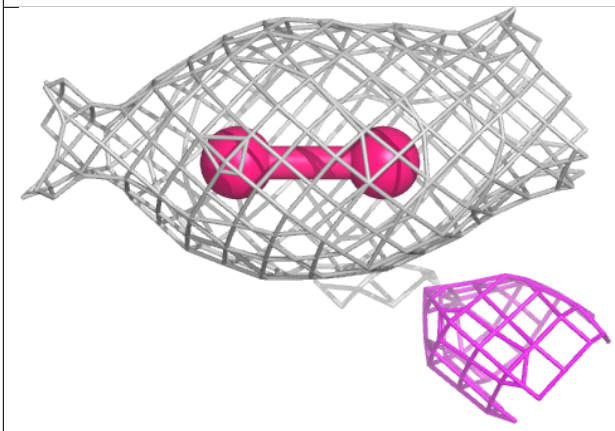
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	AZA	CCC	402	11/11	0.97	0.09	32,34,35,37	0
3	AZA	DDD	401	11/11	0.97	0.10	33,34,37,39	0
4	OXY	BBB	402	2/2	0.97	0.10	42,42,42,44	0
6	CL	BBB	406	1/1	0.98	0.14	41,41,41,41	0
4	OXY	AAA	403	2/2	0.98	0.10	40,40,40,43	0
6	CL	CCC	409	1/1	0.98	0.11	47,47,47,47	0
4	OXY	AAA	402	2/2	0.98	0.13	22,22,22,24	2
6	CL	CCC	407	1/1	0.99	0.11	46,46,46,46	0
6	CL	AAA	407	1/1	0.99	0.16	34,34,34,34	0
6	CL	DDD	407	1/1	0.99	0.07	51,51,51,51	0

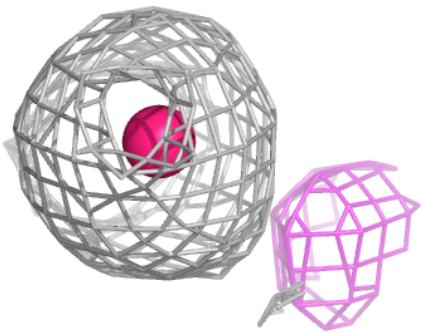
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OXY CCC 401:

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

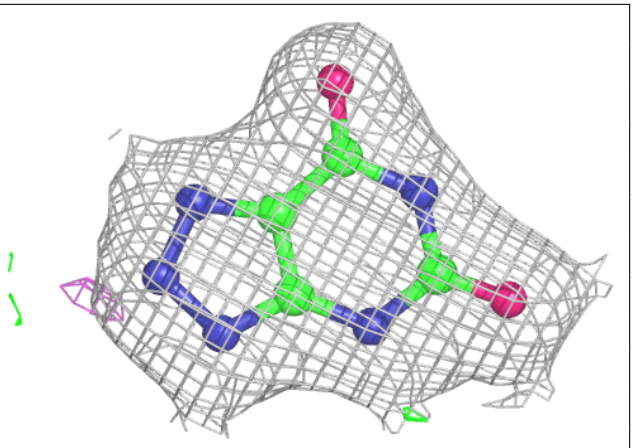


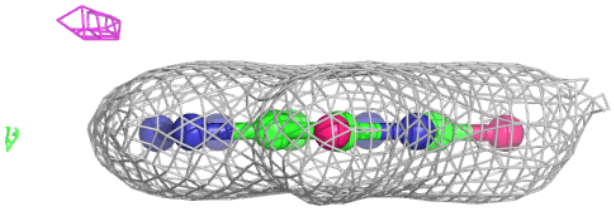


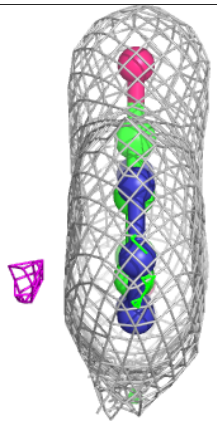


Electron density around AZA AAA 401:

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

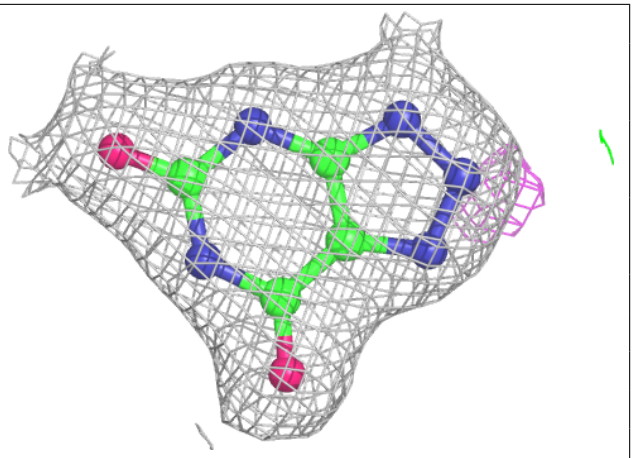


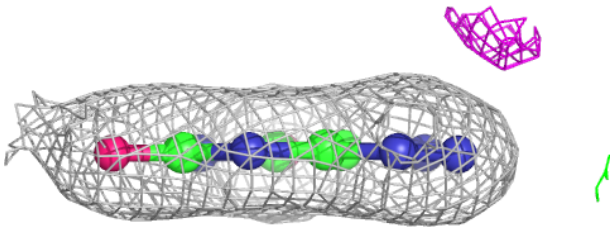


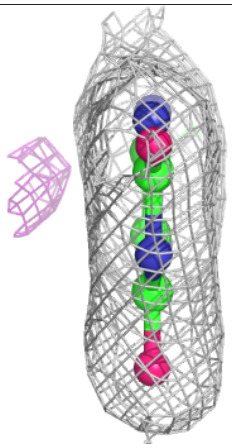


Electron density around AZA BBB 401:

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

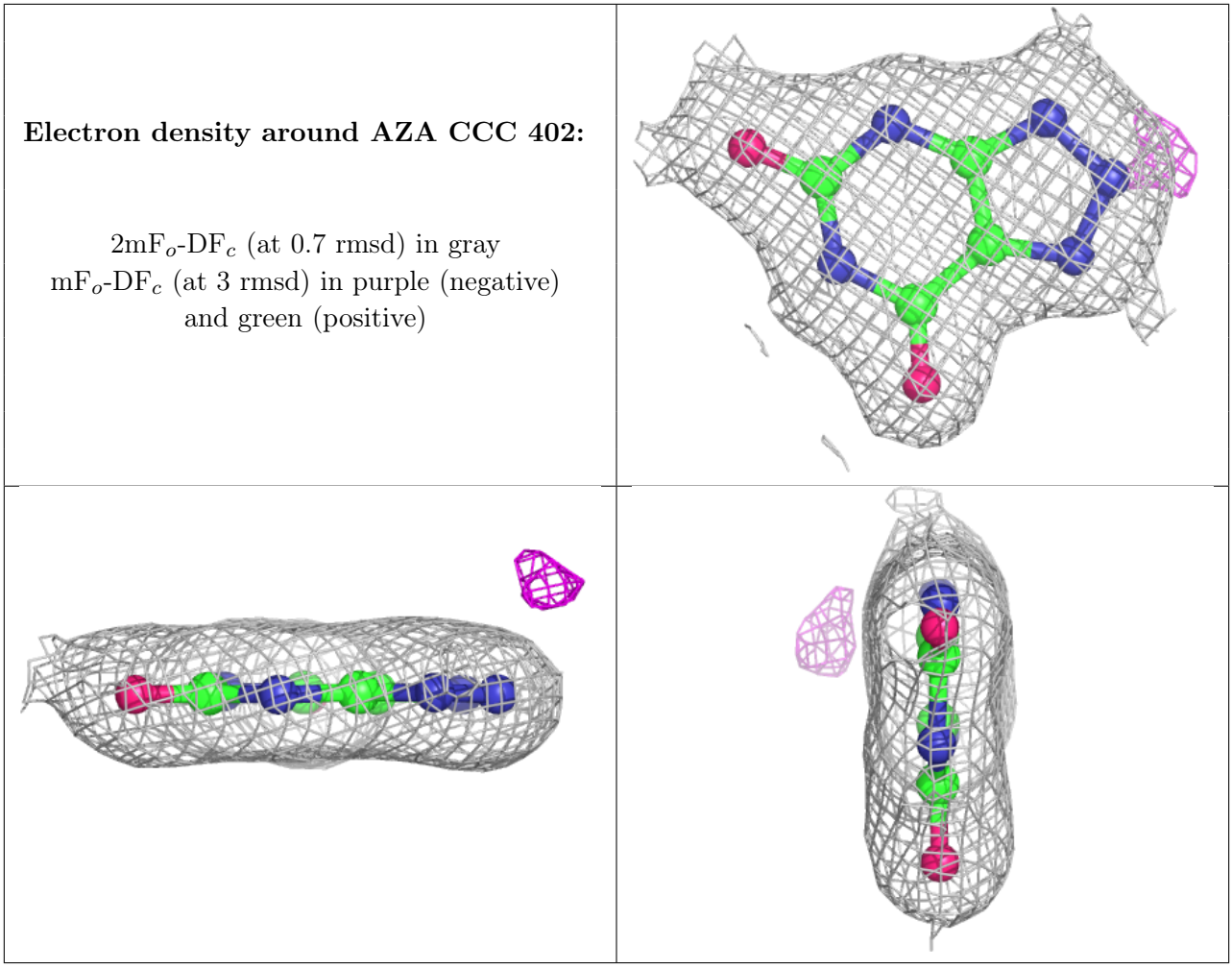






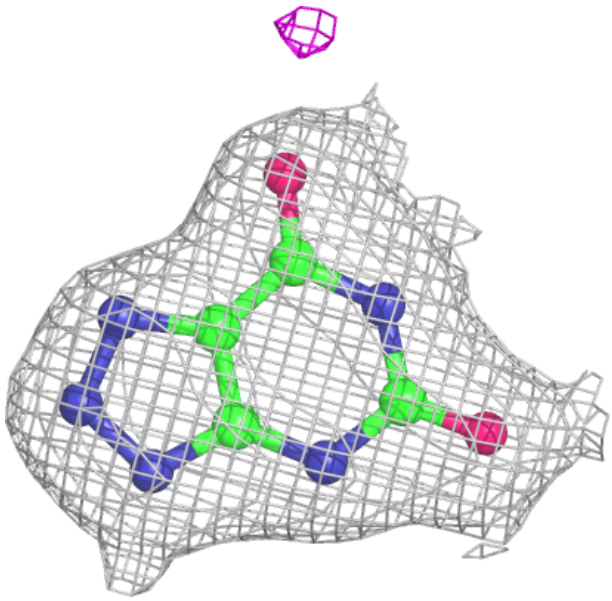
Electron density around AZA CCC 402:

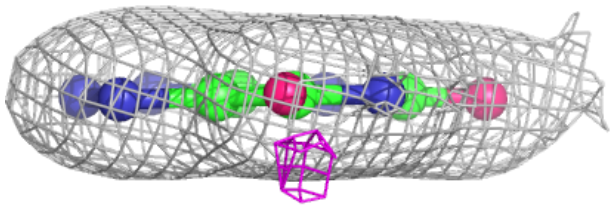
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

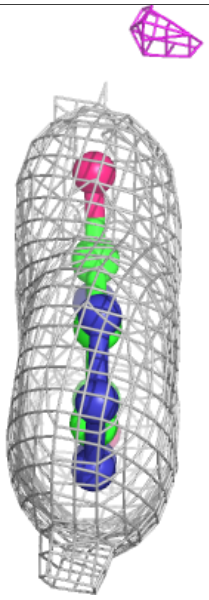


Electron density around AZA DDD 401:

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

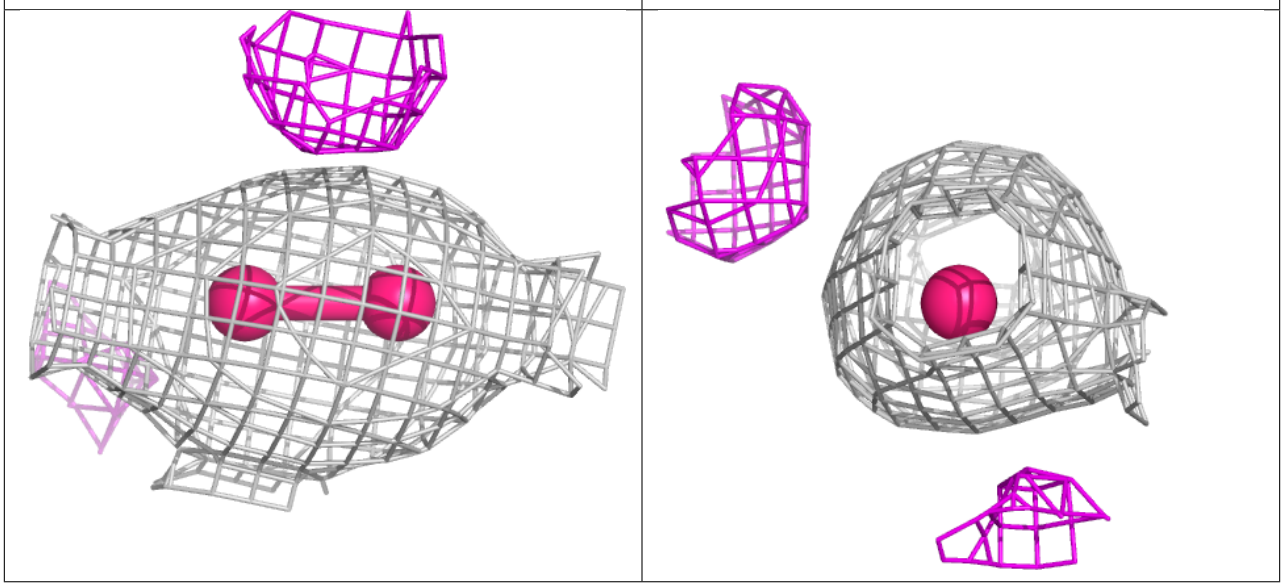






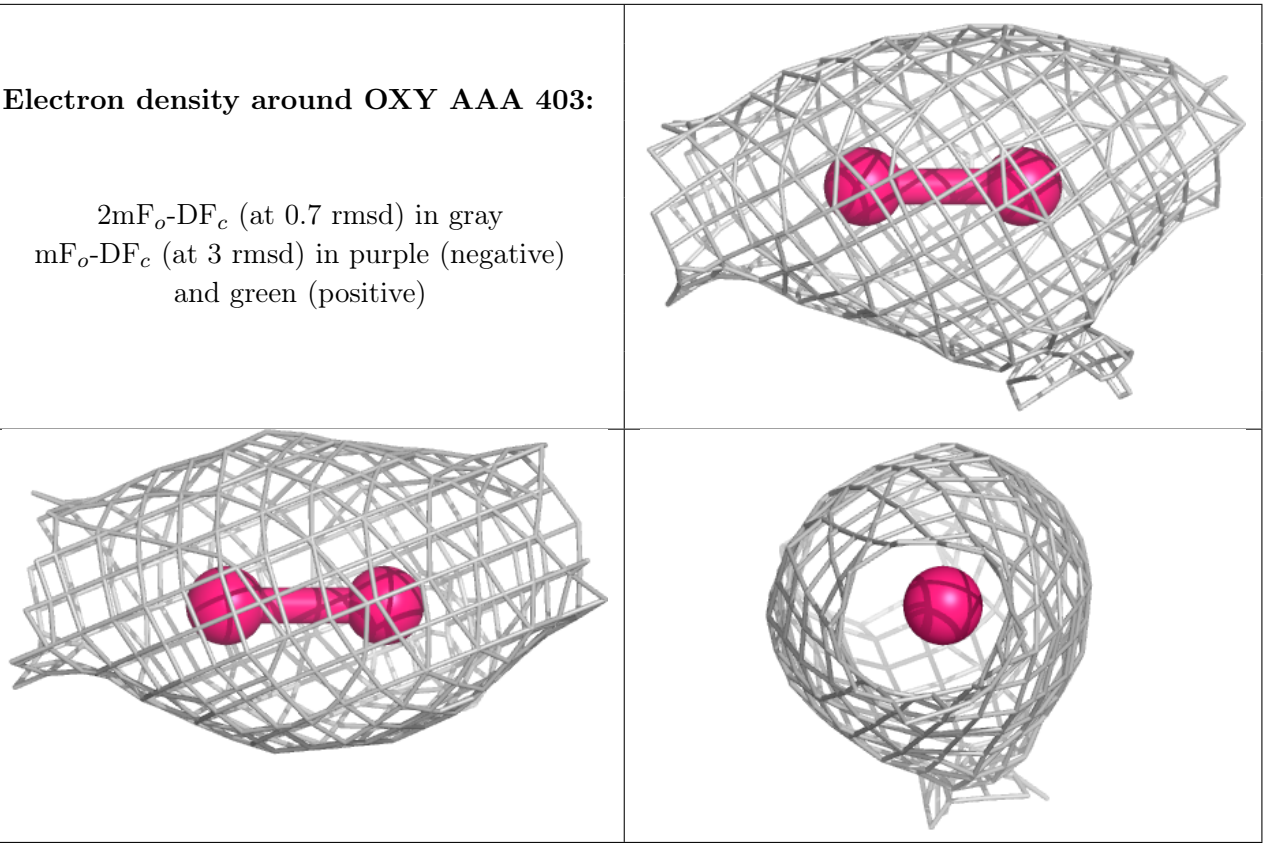
Electron density around OXY BBB 402:

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



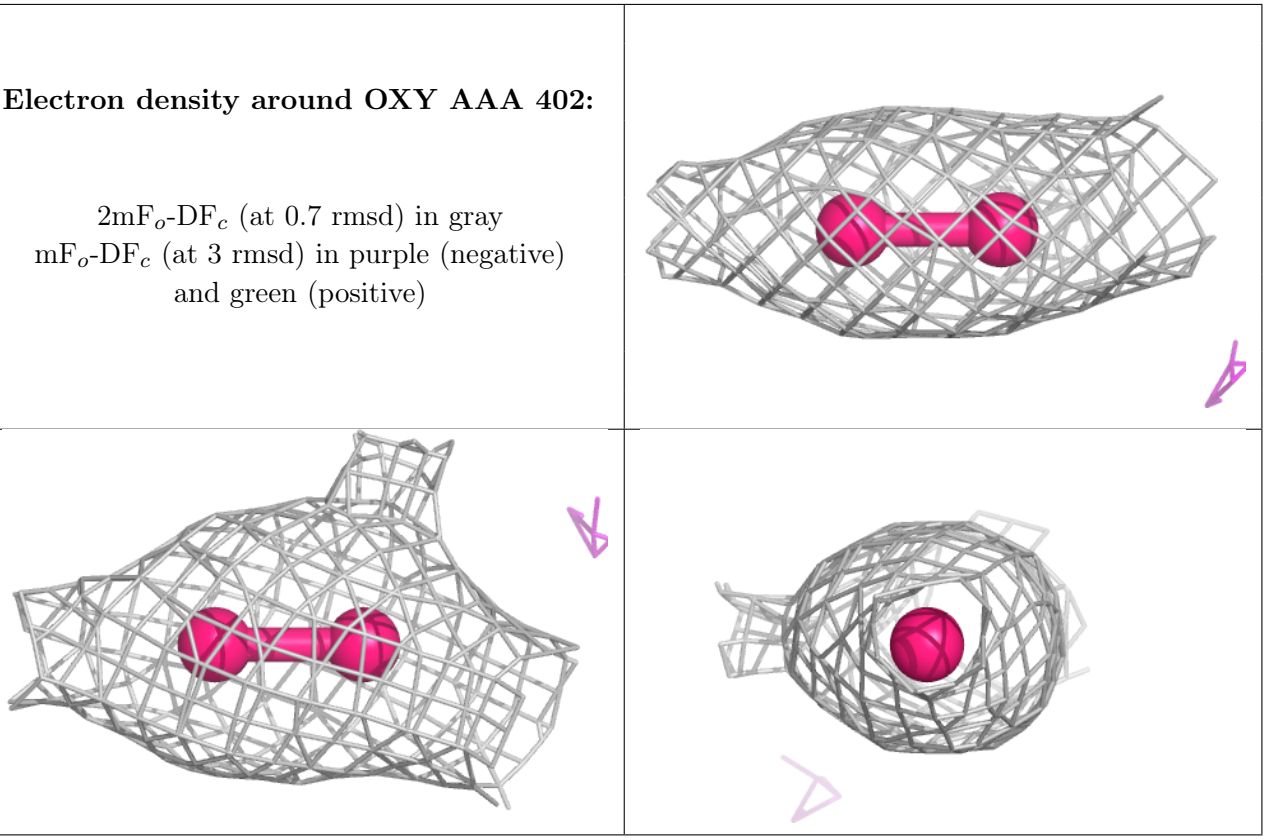
Electron density around OXY AAA 403:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.