wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2024 – 03:47 pm GMT

PDB ID	:	8OFK
Title	:	Crystal structure of the cysteine-rich Gallus gallus urate oxidase in complex with the 8-azaxanthine inhibitor under reducing conditions (space group C 2 2 21)
Authors	:	Di Palma, M.; Chegkazi, M.; Bui, S.; Mori, G.; Percudani, R.; Steiner, R.A.
Deposited on	:	2023-03-15
Resolution	:	1.71 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:

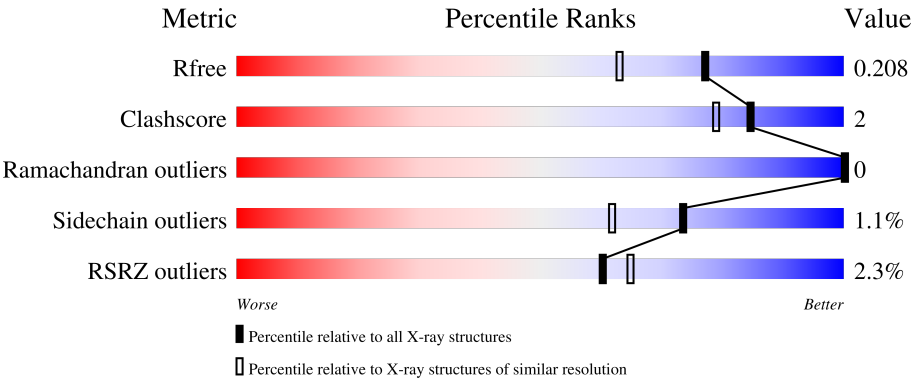
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	83% · 13%
1	BBB	343	2% 85% · 13%
1	CCC	343	83% · 13%
1	DDD	343	3% 83% · 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11102 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	300	Total	C	N	O	S	0	10	0
			2491	1582	425	458	26			
1	BBB	300	Total	C	N	O	S	0	13	0
			2516	1596	432	460	28			
1	CCC	298	Total	C	N	O	S	0	8	0
			2461	1563	422	451	25			
1	DDD	299	Total	C	N	O	S	0	11	0
			2497	1581	433	458	25			

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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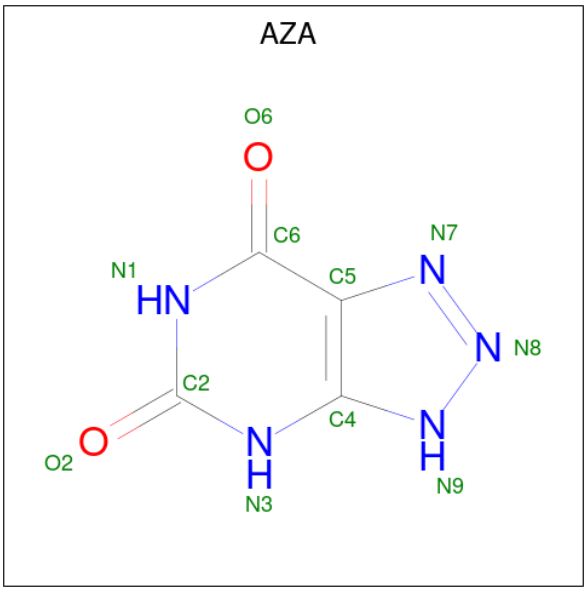
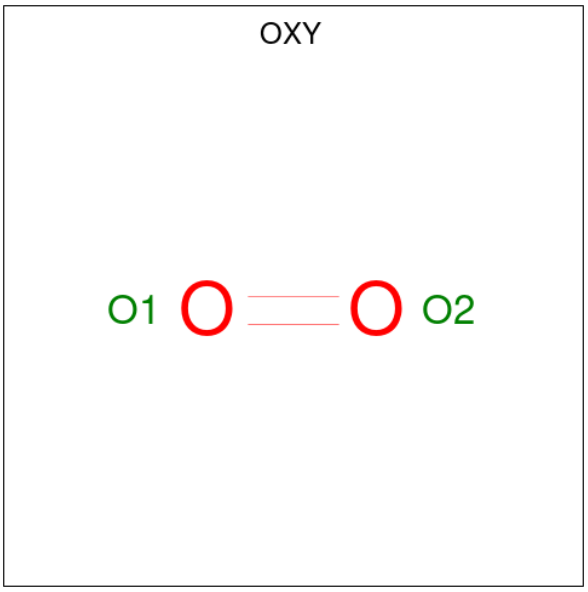
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-5	GLY	-	expression tag	UNP A0A8V0ZED1
CCC	-4	SER	-	expression tag	UNP A0A8V0ZED1
CCC	-3	HIS	-	expression tag	UNP A0A8V0ZED1
CCC	-2	MET	-	expression tag	UNP A0A8V0ZED1
CCC	-1	ALA	-	expression tag	UNP A0A8V0ZED1
CCC	0	SER	-	expression tag	UNP A0A8V0ZED1
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).



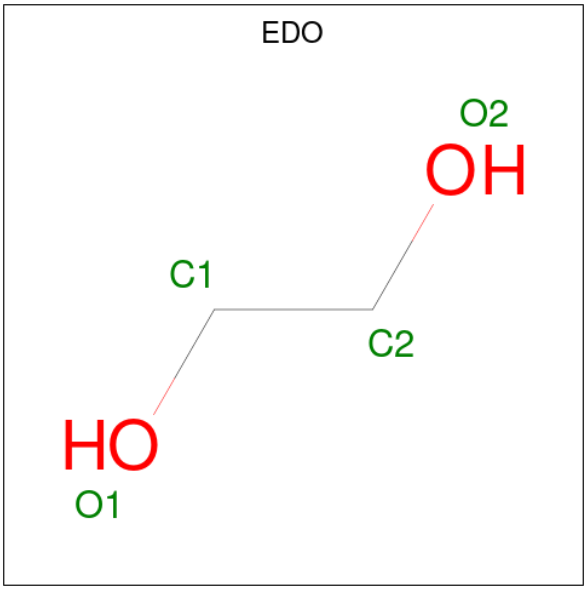
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C N O 11 4 5 2	0	0
2	BBB	1	Total C N O 11 4 5 2	0	0
2	CCC	1	Total C N O 11 4 5 2	0	0
2	DDD	1	Total C N O 11 4 5 2	0	0

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	3	Total Cl 3 3	0	0
5	BBB	5	Total Cl 5 5	0	0
5	CCC	1	Total Cl 1 1	0	0
5	DDD	3	Total Cl 3 3	0	0

- Molecule 6 is water.

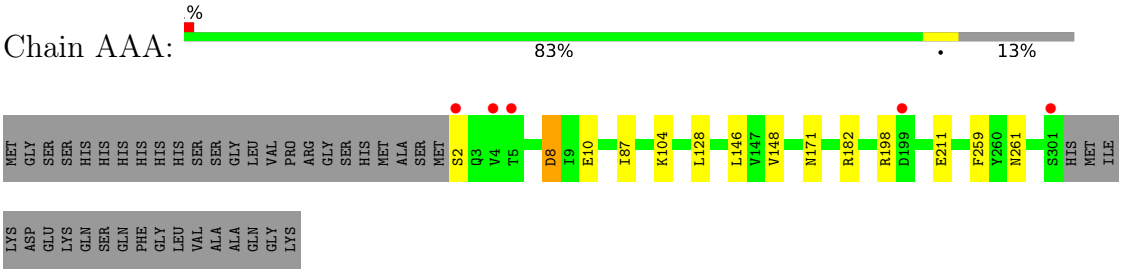
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	269	Total O 274 274	0	5
6	BBB	261	Total O 265 265	0	4
6	CCC	210	Total O 215 215	0	5
6	DDD	193	Total O 199 199	0	6

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.

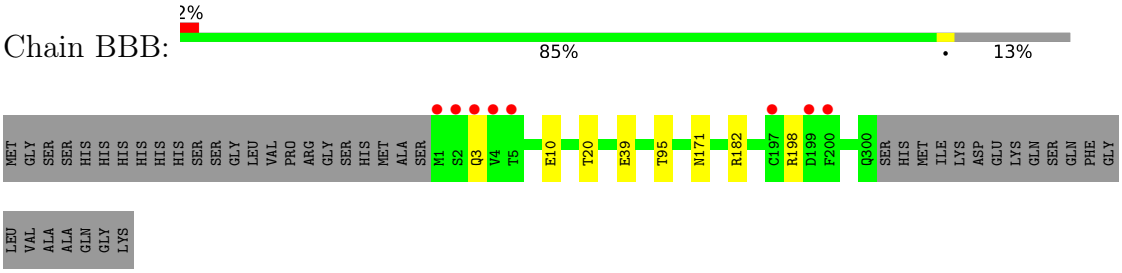
• Molecule 1: Uricase

Chain AAA:



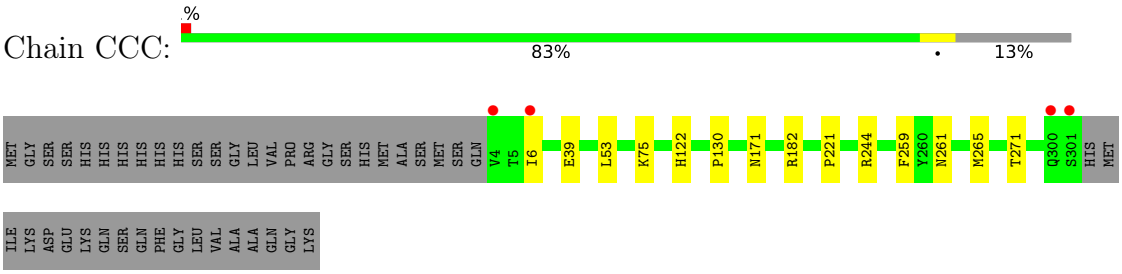
• Molecule 1: Uricase

Chain BBB:



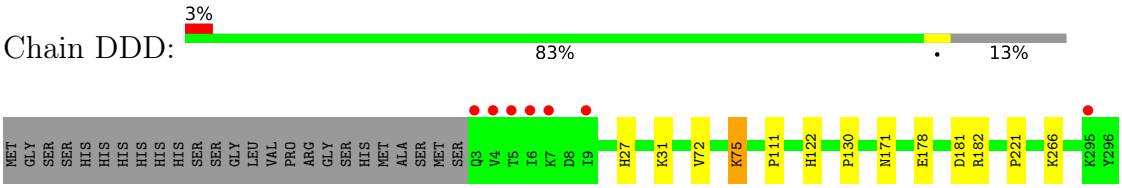
• Molecule 1: Uricase

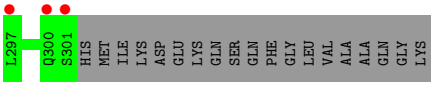
Chain CCC:



• Molecule 1: Uricase

Chain DDD:




L297
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	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.19Å 125.47Å 238.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.50 – 1.71 81.50 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (81.50-1.71) 98.0 (81.50-1.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.201 0.188 , 0.208	Depositor DCC
R_{free} test set	8247 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11102	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, OXY, AZA, CL

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	0.66	0/2546	0.76	0/3442
1	BBB	0.66	0/2570	0.75	0/3470
1	CCC	0.63	0/2514	0.74	0/3397
1	DDD	0.63	0/2552	0.74	0/3451
All	All	0.65	0/10182	0.75	0/13760

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	2491	0	2447	19	0
1	BBB	2516	0	2483	6	0
1	CCC	2461	0	2434	13	0
1	DDD	2497	0	2453	13	0
2	AAA	11	0	3	1	0
2	BBB	11	0	3	2	0
2	CCC	11	0	3	1	0
2	DDD	11	0	3	2	0
3	AAA	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	2	0	0	1	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	AAA	28	0	42	2	0
4	BBB	28	0	42	0	0
4	CCC	32	0	48	1	0
4	DDD	32	0	48	3	0
5	AAA	3	0	0	0	0
5	BBB	5	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	3	0	0	0	0
6	AAA	274	0	0	5	0
6	BBB	265	0	0	3	0
6	CCC	215	0	0	1	0
6	DDD	199	0	0	1	0
All	All	11102	0	10009	46	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 46 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:198[B]:ARG:CG	1:AAA:198[B]:ARG:HH11	1.42	1.30
1:AAA:198[B]:ARG:HH11	1:AAA:198[B]:ARG:HG3	1.01	1.10
1:DDD:181[B]:ASP:O	6:DDD:502:HOH:O	1.74	1.04
1:AAA:198[B]:ARG:HH11	1:AAA:198[B]:ARG:HG2	1.33	0.91
1:AAA:198[B]:ARG:HG3	1:AAA:198[B]:ARG:NH1	1.63	0.91

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	308/343 (90%)	301 (98%)	7 (2%)	0	100	100
1	BBB	311/343 (91%)	305 (98%)	6 (2%)	0	100	100
1	CCC	304/343 (89%)	298 (98%)	6 (2%)	0	100	100
1	DDD	308/343 (90%)	304 (99%)	4 (1%)	0	100	100
All	All	1231/1372 (90%)	1208 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	282/308 (92%)	278 (99%)	4 (1%)	67	52
1	BBB	285/308 (92%)	283 (99%)	2 (1%)	84	76
1	CCC	279/308 (91%)	277 (99%)	2 (1%)	84	76
1	DDD	283/308 (92%)	279 (99%)	4 (1%)	67	52
All	All	1129/1232 (92%)	1117 (99%)	12 (1%)	73	62

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	171	ASN
1	DDD	75	LYS
1	DDD	266	LYS
1	DDD	171	ASN
1	AAA	171	ASN

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 50 ligands modelled in this entry, 12 are monoatomic - leaving 38 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	$\#\|Z\| > 2$
4	EDO	DDD	405	-	3,3,3	0.09	0	2,2,2	0.18	0
3	OXY	AAA	402	-	1,1,1	0.17	0	-		
4	EDO	DDD	410	-	3,3,3	0.28	0	2,2,2	0.39	0
4	EDO	CCC	407	-	3,3,3	0.07	0	2,2,2	0.27	0
4	EDO	AAA	406	-	3,3,3	0.06	0	2,2,2	0.17	0
4	EDO	DDD	406	-	3,3,3	0.13	0	2,2,2	0.27	0
3	OXY	CCC	402	-	1,1,1	0.15	0	-		
4	EDO	BBB	507	-	3,3,3	0.08	0	2,2,2	0.25	0
4	EDO	BBB	506[B]	-	3,3,3	0.08	0	2,2,2	0.29	0
2	AZA	AAA	401	-	9,12,12	1.63	2 (22%)	4,17,17	8.04	3 (75%)
4	EDO	DDD	403	-	3,3,3	0.10	0	2,2,2	0.13	0
2	AZA	DDD	401	-	9,12,12	1.39	1 (11%)	4,17,17	7.87	2 (50%)
3	OXY	BBB	501	-	1,1,1	0.27	0	-		
4	EDO	BBB	508	-	3,3,3	0.24	0	2,2,2	0.71	0
4	EDO	AAA	408	-	3,3,3	0.11	0	2,2,2	0.25	0
3	OXY	DDD	402	-	1,1,1	0.15	0	-		
4	EDO	CCC	408[B]	-	3,3,3	0.08	0	2,2,2	0.19	0
4	EDO	BBB	505	-	3,3,3	0.03	0	2,2,2	0.17	0
2	AZA	CCC	401	-	9,12,12	1.38	1 (11%)	4,17,17	7.94	2 (50%)
4	EDO	BBB	506[A]	-	3,3,3	0.09	0	2,2,2	0.25	0
4	EDO	CCC	403	-	3,3,3	0.06	0	2,2,2	0.07	0
4	EDO	CCC	404[B]	-	3,3,3	0.09	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	BBB	503	-	3,3,3	0.11	0	2,2,2	0.23	0
4	EDO	BBB	504	-	3,3,3	0.13	0	2,2,2	0.06	0
4	EDO	DDD	409	-	3,3,3	0.08	0	2,2,2	0.29	0
4	EDO	AAA	403	-	3,3,3	0.19	0	2,2,2	0.12	0
4	EDO	CCC	408[A]	-	3,3,3	0.09	0	2,2,2	0.19	0
4	EDO	AAA	407	-	3,3,3	0.10	0	2,2,2	0.32	0
4	EDO	DDD	407	-	3,3,3	0.07	0	2,2,2	0.42	0
2	AZA	BBB	502	-	9,12,12	1.27	1 (11%)	4,17,17	7.83	2 (50%)
4	EDO	DDD	404	-	3,3,3	0.07	0	2,2,2	0.25	0
4	EDO	DDD	408	-	3,3,3	0.06	0	2,2,2	0.04	0
4	EDO	CCC	404[A]	-	3,3,3	0.10	0	2,2,2	0.17	0
4	EDO	AAA	409	-	3,3,3	0.08	0	2,2,2	0.24	0
4	EDO	CCC	406	-	3,3,3	0.25	0	2,2,2	0.22	0
4	EDO	AAA	404	-	3,3,3	0.10	0	2,2,2	0.06	0
4	EDO	AAA	405	-	3,3,3	0.51	0	2,2,2	0.30	0
4	EDO	CCC	405	-	3,3,3	0.05	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
4	EDO	DDD	405	-	-	1/1/1/1	-
4	EDO	DDD	410	-	-	1/1/1/1	-
4	EDO	CCC	407	-	-	1/1/1/1	-
4	EDO	AAA	406	-	-	0/1/1/1	-
4	EDO	DDD	406	-	-	1/1/1/1	-
4	EDO	DDD	403	-	-	0/1/1/1	-
4	EDO	BBB	507	-	-	1/1/1/1	-
4	EDO	BBB	506[B]	-	-	1/1/1/1	-
2	AZA	AAA	401	-	-	-	0/2/2/2
2	AZA	DDD	401	-	-	-	0/2/2/2
4	EDO	BBB	508	-	-	0/1/1/1	-
4	EDO	AAA	408	-	-	1/1/1/1	-
4	EDO	CCC	408[B]	-	-	0/1/1/1	-
4	EDO	BBB	505	-	-	1/1/1/1	-
2	AZA	CCC	401	-	-	-	0/2/2/2
4	EDO	BBB	506[A]	-	-	1/1/1/1	-
4	EDO	CCC	403	-	-	0/1/1/1	-
4	EDO	CCC	404[B]	-	-	1/1/1/1	-
4	EDO	BBB	503	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	BBB	504	-	-	0/1/1/1	-
4	EDO	DDD	409	-	-	1/1/1/1	-
4	EDO	AAA	403	-	-	0/1/1/1	-
4	EDO	CCC	408[A]	-	-	0/1/1/1	-
4	EDO	AAA	407	-	-	0/1/1/1	-
4	EDO	DDD	407	-	-	1/1/1/1	-
2	AZA	BBB	502	-	-	-	0/2/2/2
4	EDO	DDD	404	-	-	1/1/1/1	-
4	EDO	DDD	408	-	-	0/1/1/1	-
4	EDO	CCC	404[A]	-	-	1/1/1/1	-
4	EDO	AAA	409	-	-	0/1/1/1	-
4	EDO	CCC	406	-	-	1/1/1/1	-
4	EDO	AAA	404	-	-	0/1/1/1	-
4	EDO	AAA	405	-	-	1/1/1/1	-
4	EDO	CCC	405	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	401	AZA	C6-N1	3.42	1.39	1.33
2	BBB	502	AZA	C6-N1	3.35	1.38	1.33
2	AAA	401	AZA	C5-C6	3.34	1.47	1.41
2	CCC	401	AZA	C6-N1	3.26	1.38	1.33
2	AAA	401	AZA	C6-N1	3.00	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	401	AZA	C2-N1-C6	14.11	127.06	115.14
2	CCC	401	AZA	C2-N1-C6	14.00	126.96	115.14
2	BBB	502	AZA	C2-N1-C6	13.90	126.87	115.14
2	DDD	401	AZA	C2-N1-C6	13.87	126.86	115.14
2	AAA	401	AZA	C5-C6-N1	-7.22	113.56	123.43

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	507	EDO	O1-C1-C2-O2
4	AAA	408	EDO	O1-C1-C2-O2
4	BBB	506[B]	EDO	O1-C1-C2-O2

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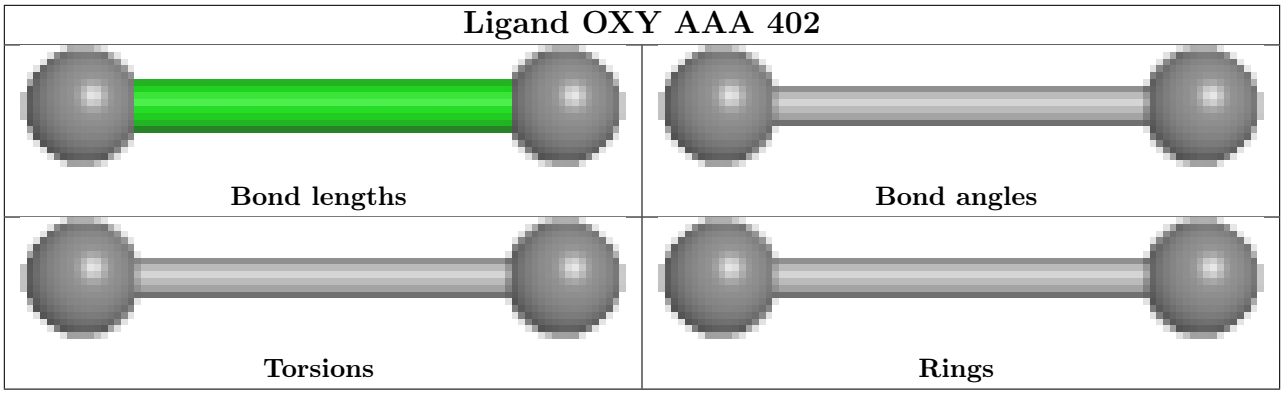
Mol	Chain	Res	Type	Atoms
4	CCC	407	EDO	O1-C1-C2-O2
4	DDD	406	EDO	O1-C1-C2-O2

There are no ring outliers.

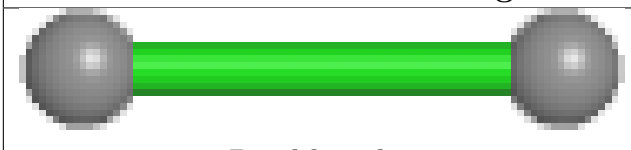
12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	402	OXY	1	0
4	DDD	410	EDO	1	0
4	AAA	406	EDO	1	0
2	AAA	401	AZA	1	0
2	DDD	401	AZA	2	0
3	BBB	501	OXY	1	0
2	CCC	401	AZA	1	0
4	CCC	404[B]	EDO	1	0
4	AAA	407	EDO	1	0
4	DDD	407	EDO	2	0
2	BBB	502	AZA	2	0
4	AAA	405	EDO	1	0

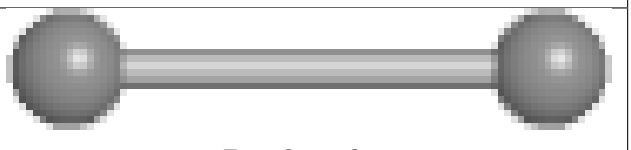
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



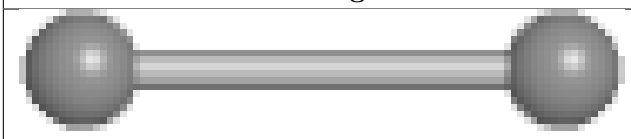
Ligand OXY CCC 402



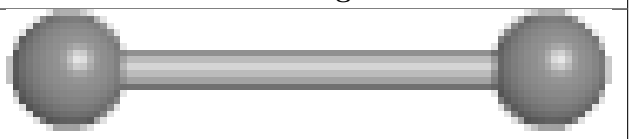
Bond lengths



Bond angles

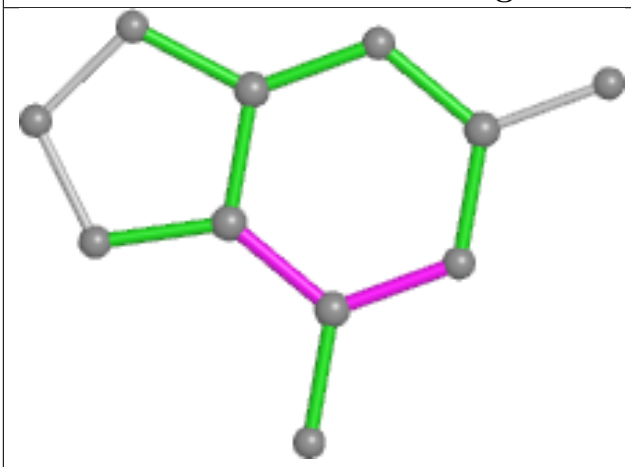


Torsions



Rings

Ligand AZA AAA 401



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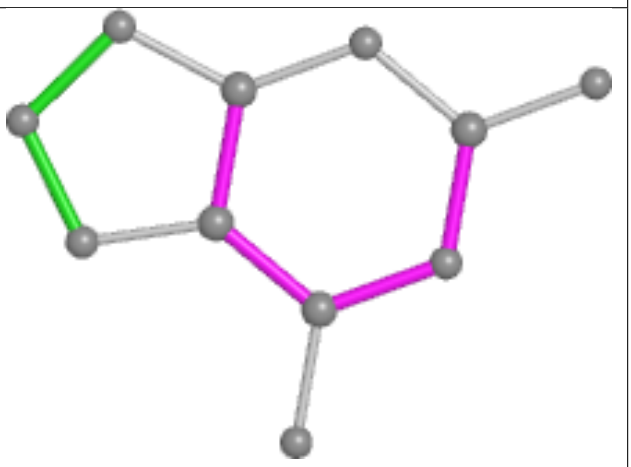

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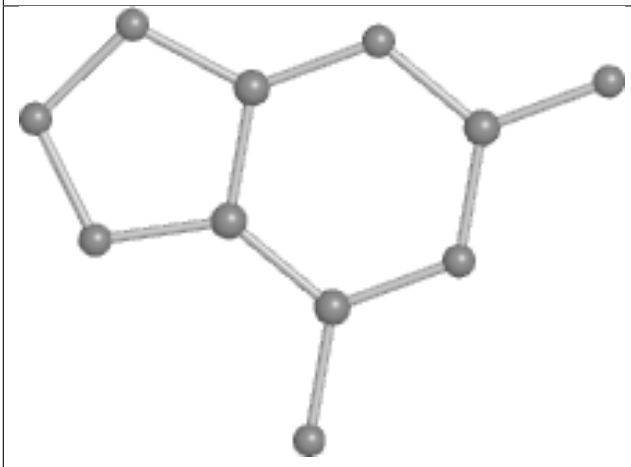
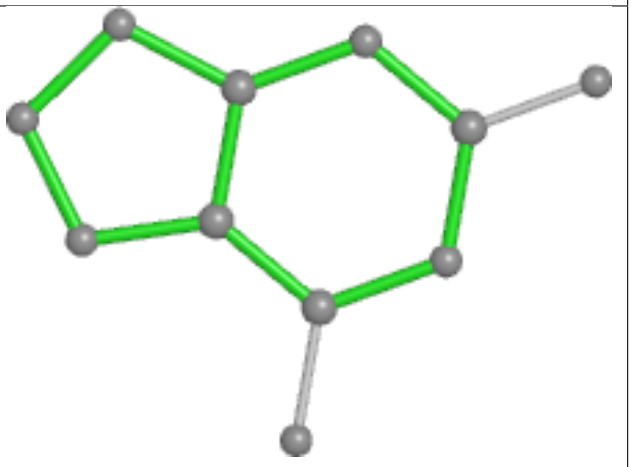
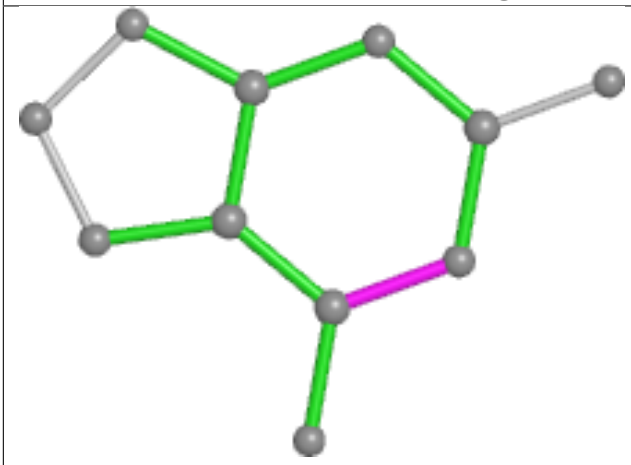


Torsions

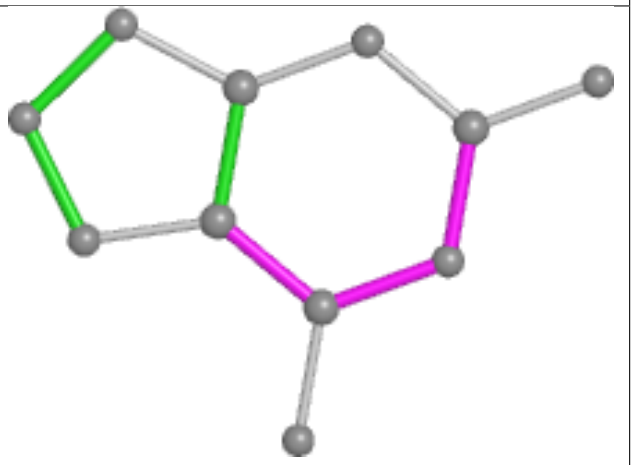


Rings

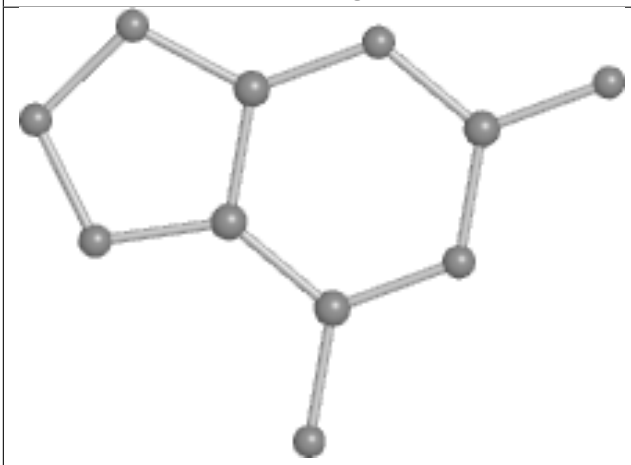
Ligand AZA DDD 401



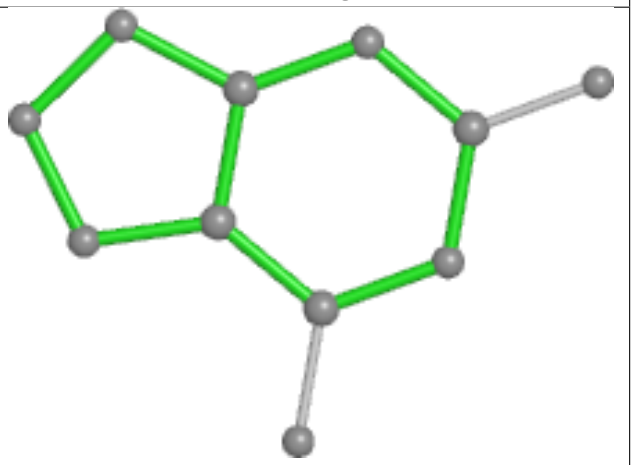
Bond lengths



Bond angles

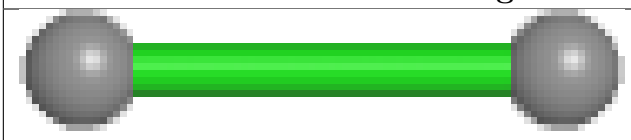


Torsions

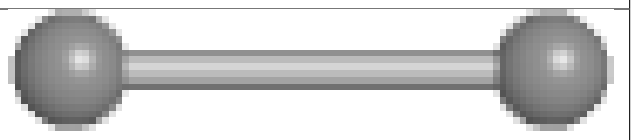


Rings

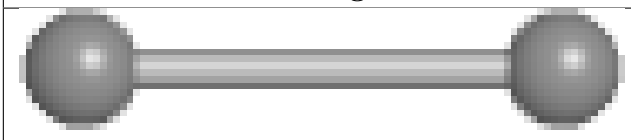
Ligand OXY BBB 501



Bond lengths



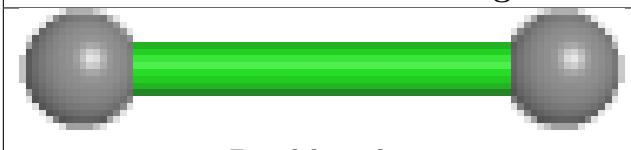
Bond angles



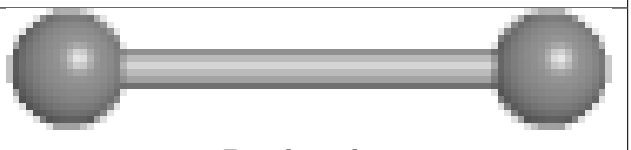
Torsions

Rings

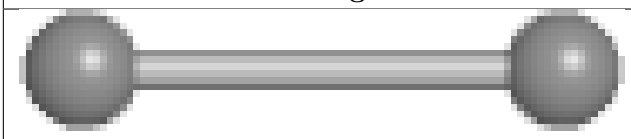
Ligand OXY DDD 402



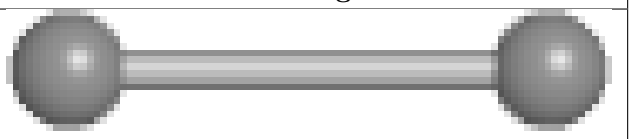
Bond lengths



Bond angles

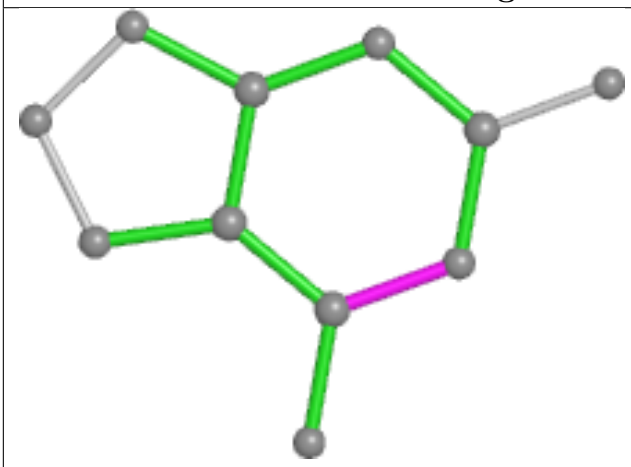


Torsions

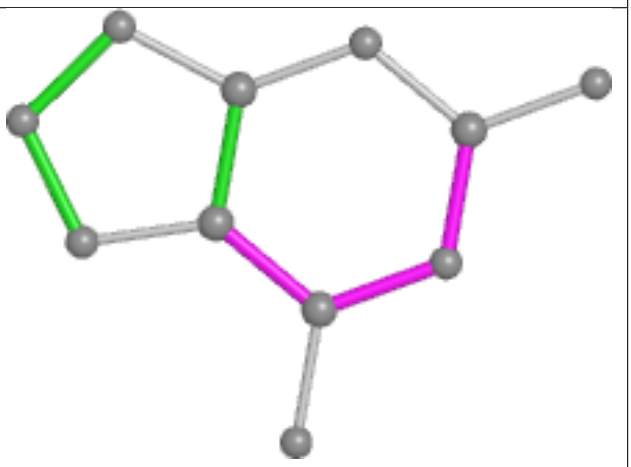


Rings

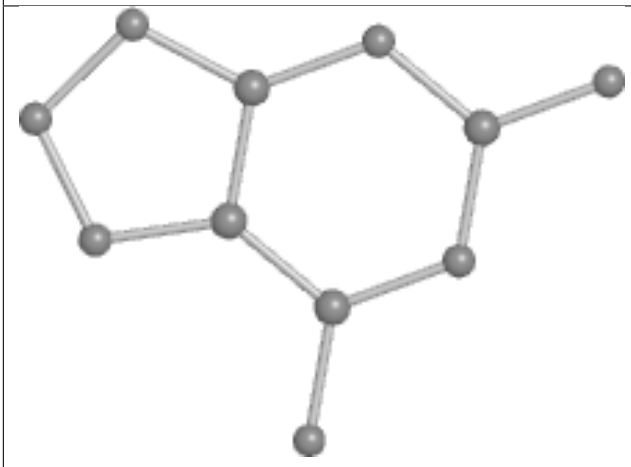
Ligand AZA CCC 401



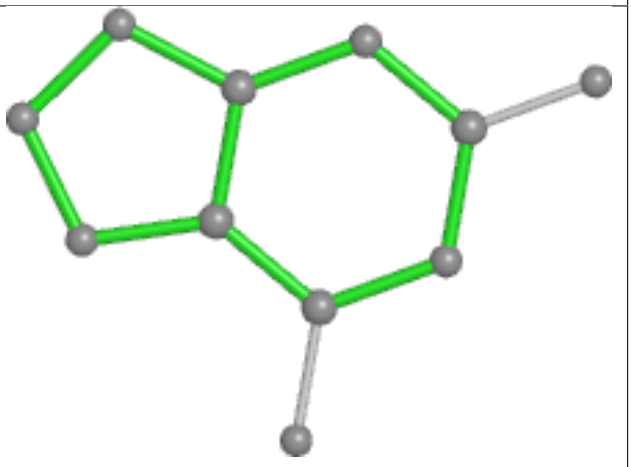
Bond lengths



Bond angles

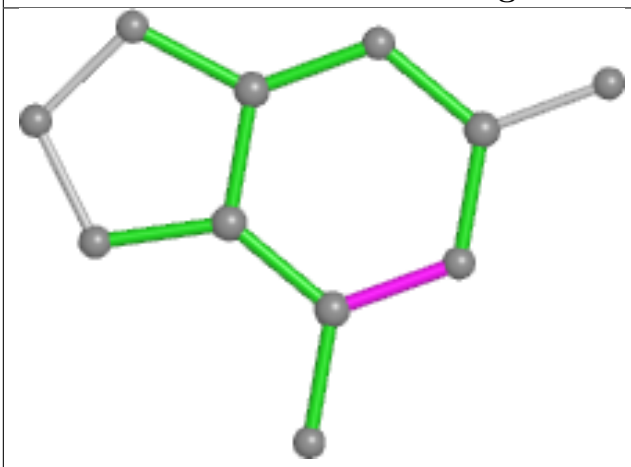


Torsions

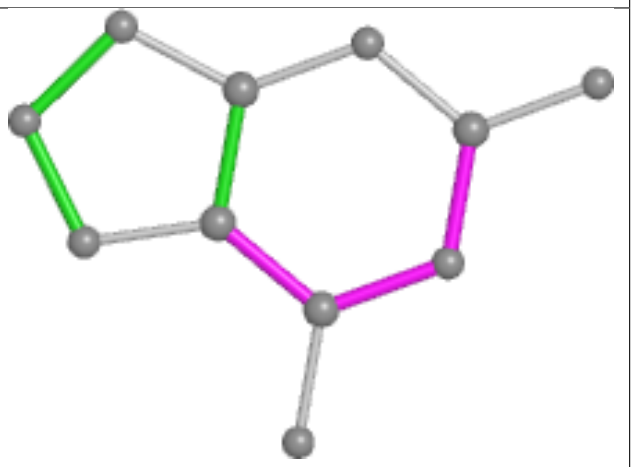


Rings

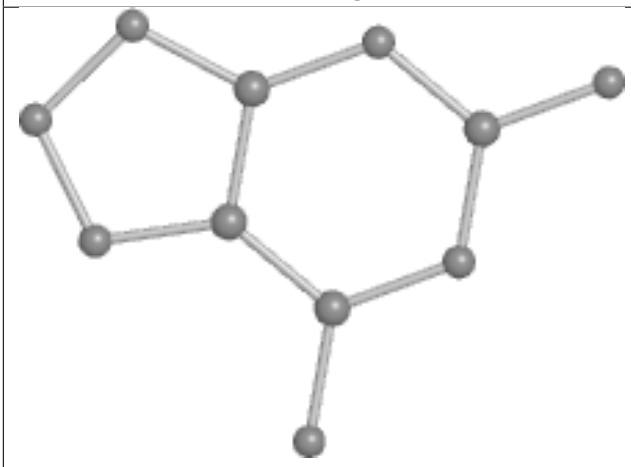
Ligand AZA BBB 502



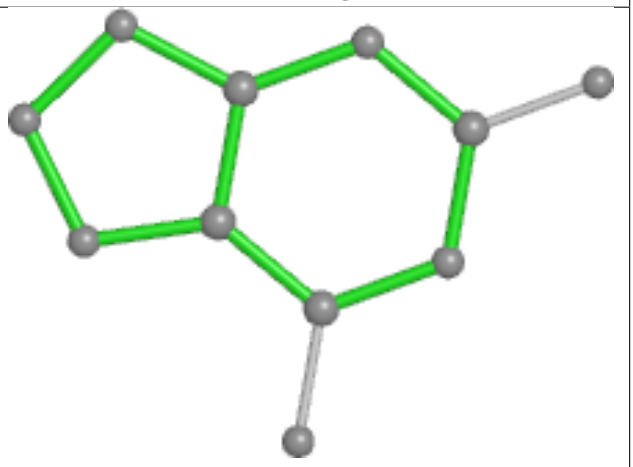
Bond lengths



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	300/343 (87%)	-0.15	5 (1%)	70	74	22, 30, 54, 92	0
1	BBB	300/343 (87%)	-0.09	8 (2%)	54	58	23, 33, 58, 91	0
1	CCC	298/343 (86%)	-0.08	4 (1%)	77	81	27, 37, 59, 89	0
1	DDD	299/343 (87%)	-0.12	10 (3%)	46	51	25, 36, 62, 91	0
All	All	1197/1372 (87%)	-0.11	27 (2%)	60	65	22, 35, 60, 92	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	4	VAL	4.8
1	BBB	4	VAL	4.7
1	DDD	3	GLN	4.0
1	BBB	3	GLN	3.6
1	DDD	6	ILE	3.4

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	EDO	CCC	407	4/4	0.74	0.25	60,63,65,67	0
4	EDO	DDD	404	4/4	0.75	0.12	71,74,74,76	0
4	EDO	AAA	406	4/4	0.79	0.16	56,60,62,63	0
4	EDO	DDD	409	4/4	0.80	0.17	56,61,62,63	0
4	EDO	DDD	410	4/4	0.82	0.15	43,47,49,51	0
4	EDO	BBB	507	4/4	0.84	0.11	62,64,65,65	0
4	EDO	DDD	406	4/4	0.84	0.18	41,46,52,55	0
4	EDO	DDD	407	4/4	0.84	0.22	43,50,52,57	0
4	EDO	CCC	406	4/4	0.84	0.23	35,42,47,51	0
4	EDO	BBB	505	4/4	0.84	0.24	72,74,75,75	0
4	EDO	AAA	409	4/4	0.85	0.31	68,71,72,72	0
4	EDO	AAA	404	4/4	0.85	0.13	45,46,46,51	0
4	EDO	BBB	506[A]	4/4	0.85	0.14	45,48,49,49	4
4	EDO	BBB	506[B]	4/4	0.85	0.14	43,45,45,46	4
4	EDO	DDD	408	4/4	0.86	0.11	50,51,54,56	0
4	EDO	DDD	405	4/4	0.88	0.18	56,57,57,57	0
4	EDO	BBB	504	4/4	0.88	0.14	46,49,49,56	0
4	EDO	AAA	405	4/4	0.88	0.19	31,35,41,47	0
4	EDO	BBB	508	4/4	0.90	0.19	34,37,38,38	0
4	EDO	AAA	408	4/4	0.91	0.17	45,46,49,49	0
4	EDO	CCC	404[A]	4/4	0.92	0.14	33,33,33,35	4
4	EDO	CCC	404[B]	4/4	0.92	0.14	33,37,37,38	4
4	EDO	CCC	405	4/4	0.92	0.17	47,47,48,51	0
5	CL	AAA	411	1/1	0.92	0.08	51,51,51,51	0
5	CL	BBB	509	1/1	0.93	0.11	37,37,37,37	0
5	CL	DDD	412	1/1	0.93	0.04	52,52,52,52	0
4	EDO	CCC	403	4/4	0.94	0.08	32,33,34,34	0
4	EDO	AAA	407	4/4	0.95	0.19	51,51,51,53	0
5	CL	AAA	412	1/1	0.95	0.07	46,46,46,46	0
4	EDO	DDD	403	4/4	0.96	0.07	32,34,35,36	0
3	OXY	CCC	402	2/2	0.96	0.10	33,33,33,35	0
4	EDO	AAA	403	4/4	0.96	0.07	27,28,30,30	0
4	EDO	BBB	503	4/4	0.96	0.07	33,33,34,35	0
4	EDO	CCC	408[A]	4/4	0.96	0.10	40,41,41,41	4
4	EDO	CCC	408[B]	4/4	0.96	0.10	36,36,36,37	4
2	AZA	CCC	401	11/11	0.97	0.08	29,30,31,32	0
5	CL	BBB	510	1/1	0.97	0.11	35,35,35,35	0
2	AZA	BBB	502	11/11	0.97	0.08	25,26,28,30	0
5	CL	DDD	413	1/1	0.97	0.04	52,52,52,52	0
3	OXY	DDD	402	2/2	0.98	0.08	29,29,29,30	2
2	AZA	DDD	401	11/11	0.98	0.09	27,28,30,31	0
3	OXY	AAA	402	2/2	0.98	0.09	28,28,28,30	0
5	CL	BBB	513	1/1	0.98	0.12	49,49,49,49	0

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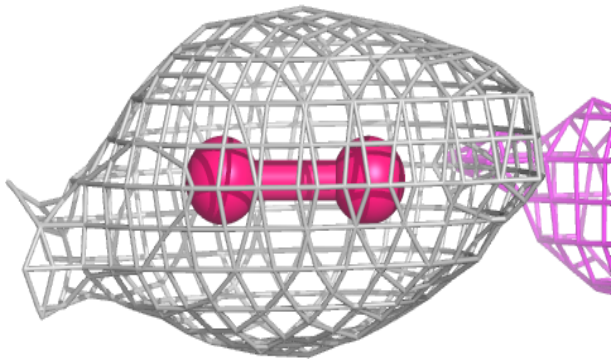
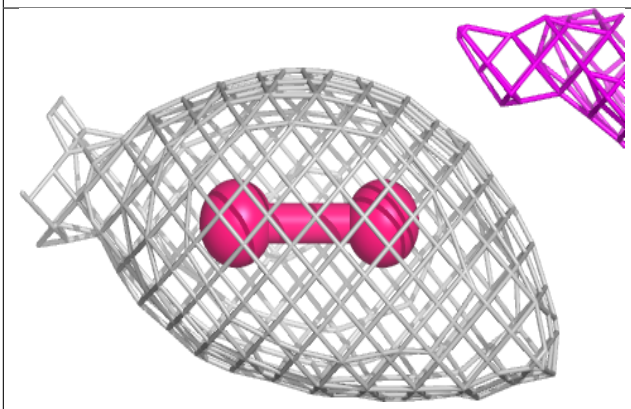
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	AAA	410	1/1	0.98	0.10	35,35,35,35	0
2	AZA	AAA	401	11/11	0.98	0.09	21,22,24,24	0
3	OXY	BBB	501	2/2	0.99	0.07	24,24,24,28	0
5	CL	CCC	409	1/1	0.99	0.14	32,32,32,32	0
5	CL	DDD	411	1/1	0.99	0.13	29,29,29,29	0
5	CL	BBB	511	1/1	0.99	0.13	39,39,39,39	0
5	CL	BBB	512	1/1	0.99	0.09	43,43,43,43	0

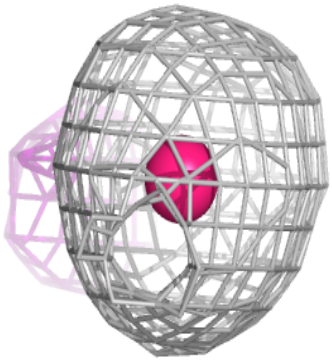
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

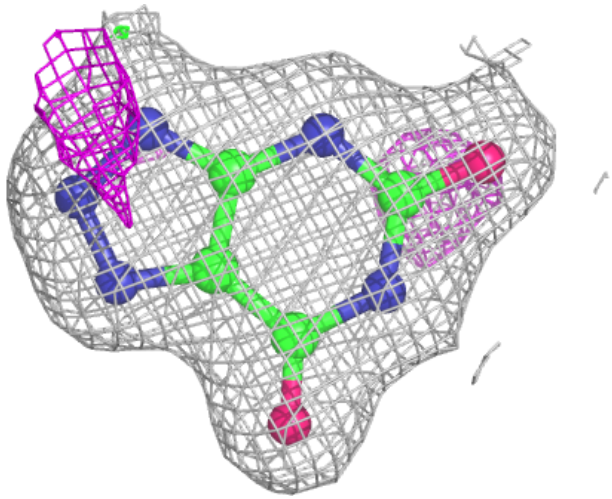


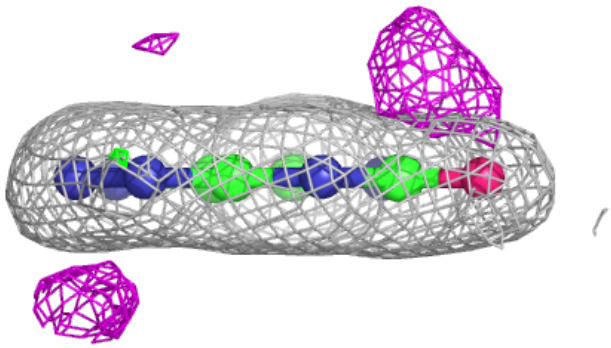


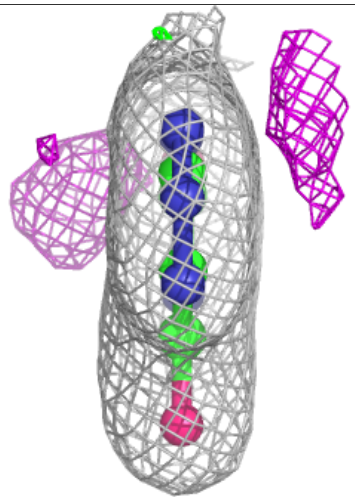


Electron density around AZA CCC 401:

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

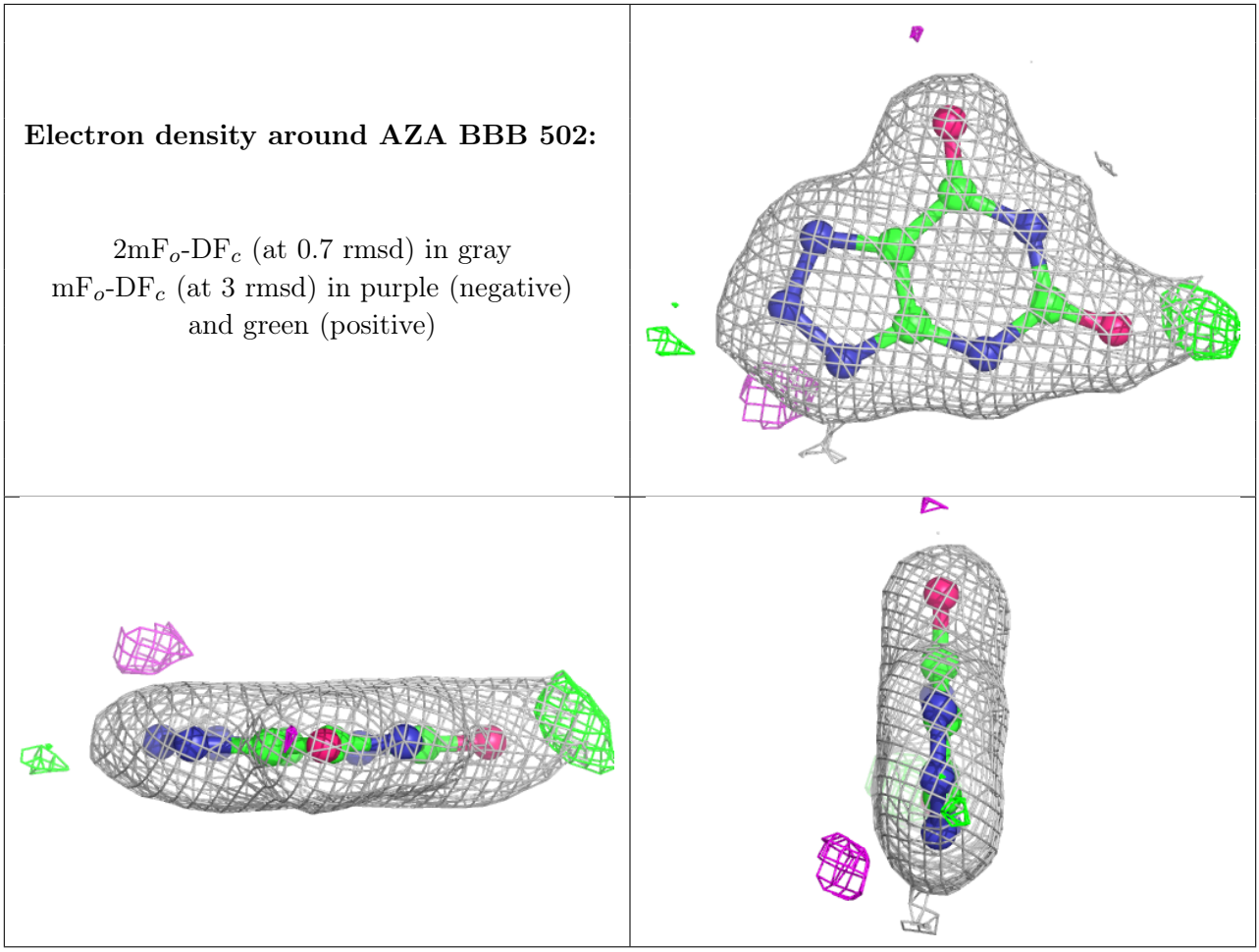






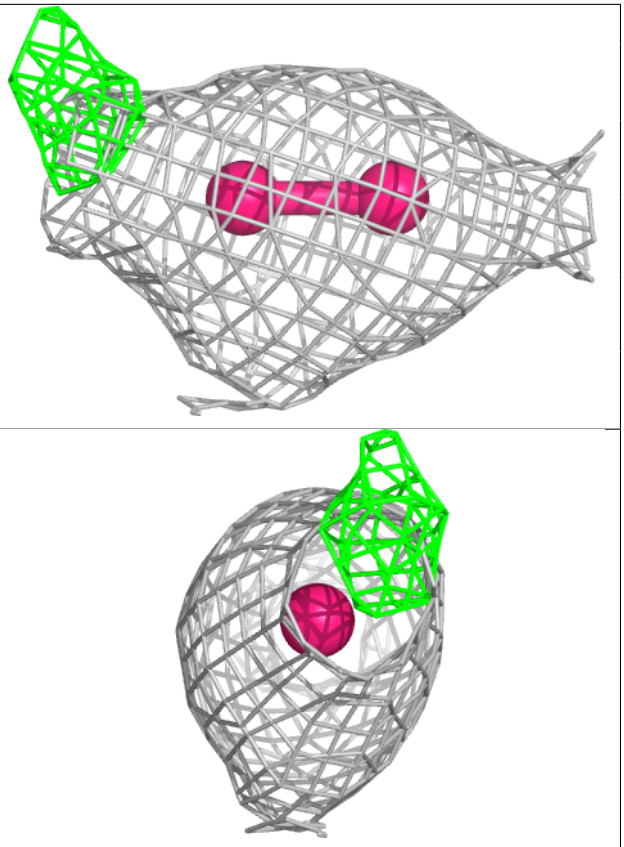
Electron density around AZA BBB 502:

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



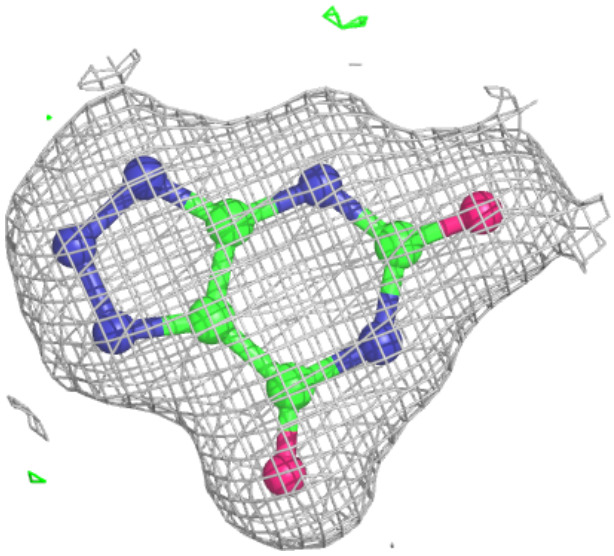
Electron density around OXY DDD 402:

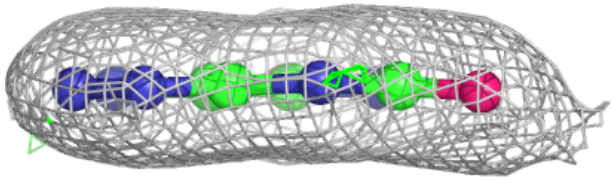
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

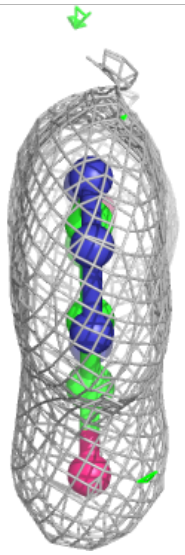


Electron density around AZA DDD 401:

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

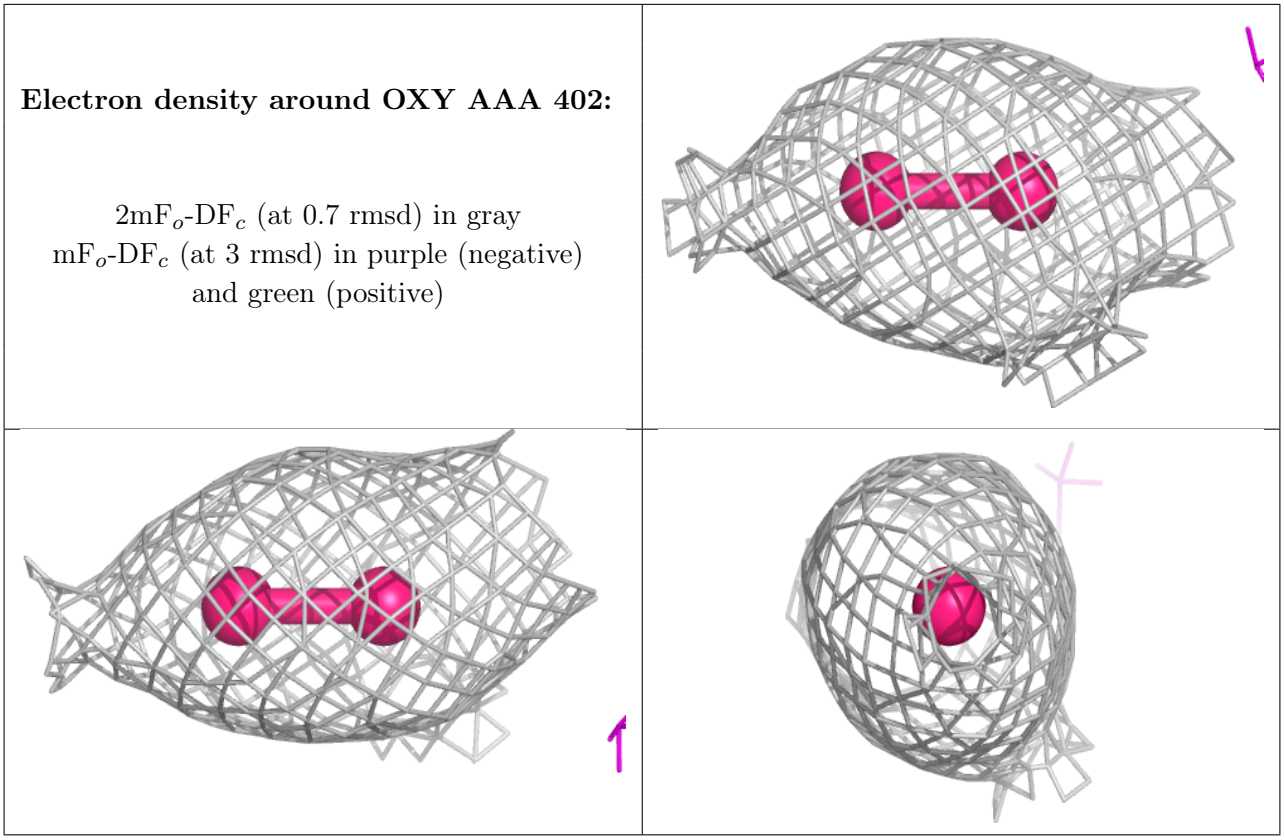






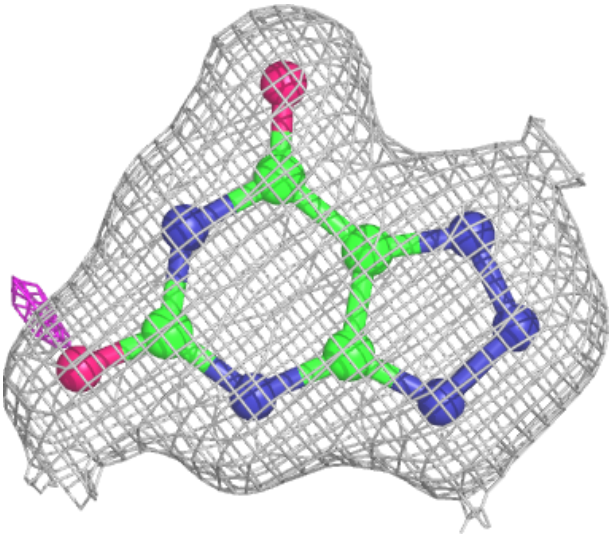
Electron density around OXY AAA 402:

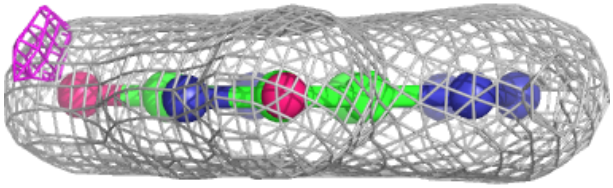
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

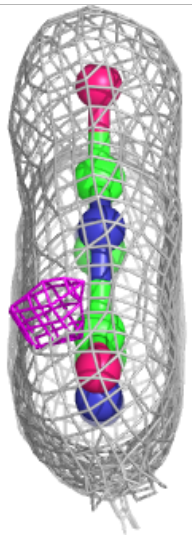


Electron density around AZA AAA 401:

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

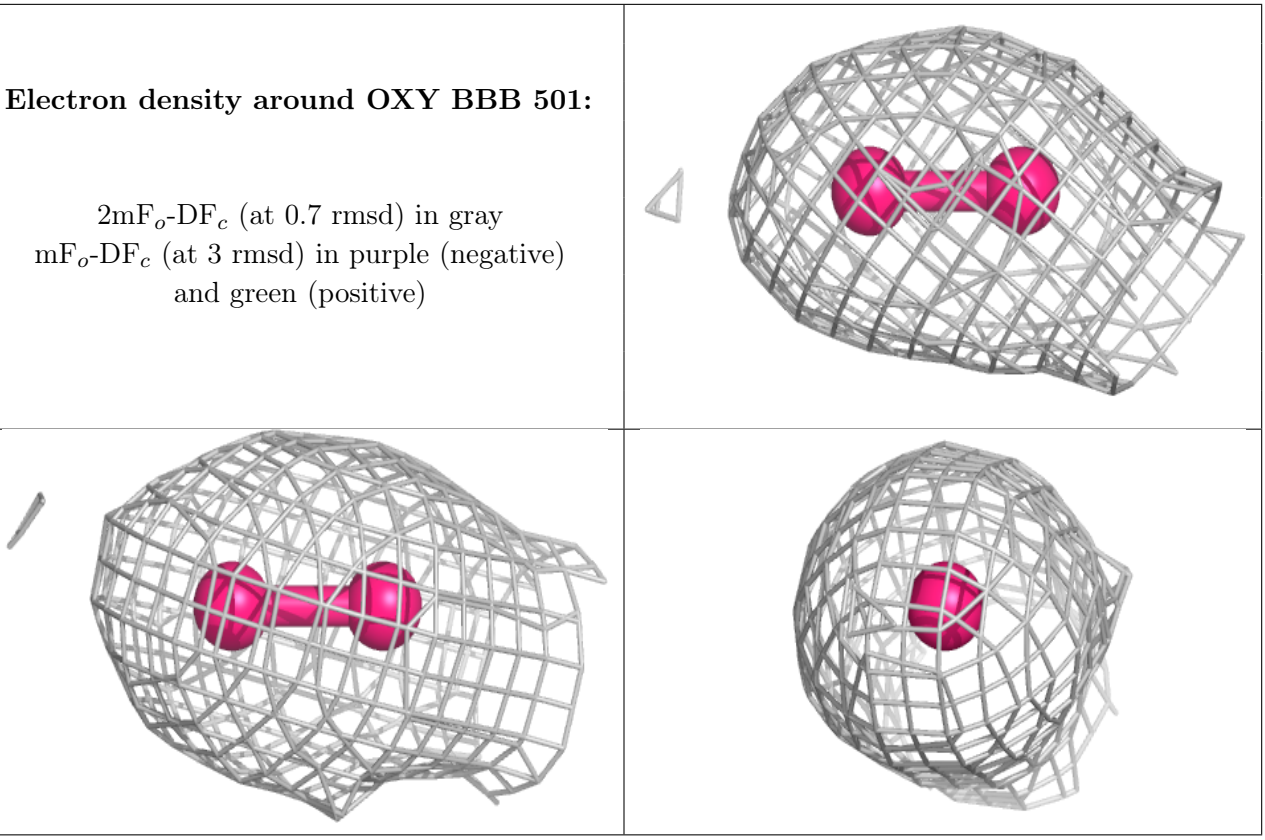






Electron density around OXY BBB 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.