wwPDB X-ray Structure Validation Summary Report (i)

Sep 30, 2024 – 04:27 PM JST

PDB ID	:	9JFN
Title	:	Arginine decarboxylase in Aspergillus oryzae complexed with agmatine
Authors	:	Mikami, B.; Yasukawa, K.; Fujiwara, S.; Takita, T.; Mizutani, K.; Odagaki, Y.; Murakami, Y.
Deposited on	:	2024-09-05
Resolution	:	2.15 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:

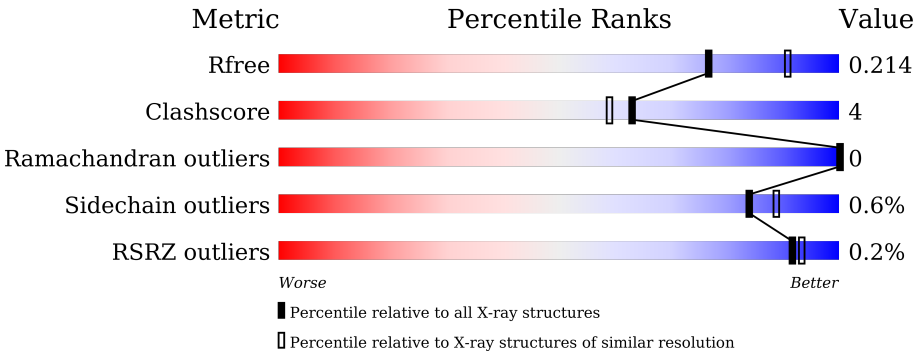
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	A	462	77% 6% 18%
1	B	462	74% 8% 18%
1	C	462	75% 8% 17%
1	D	462	75% 7% 17%
2	E	42	98% .
2	F	42	88% 12%

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Mol	Chain	Length	Quality of chain
2	G	42	90% 10%
2	H	42	90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	C	501	-	-	X	-
3	PEG	C	502	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15402 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 L-tryptophan decarboxylase PsiD-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	11	0
			3040	1934	515	580	11			
1	B	381	Total	C	N	O	S	0	10	0
			3031	1929	509	582	11			
1	C	382	Total	C	N	O	S	4	13	0
			3062	1950	516	585	11			
1	D	382	Total	C	N	O	S	0	9	0
			3038	1930	515	582	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q2UAM5
A	-18	GLY	-	expression tag	UNP Q2UAM5
A	-17	SER	-	expression tag	UNP Q2UAM5
A	-16	SER	-	expression tag	UNP Q2UAM5
A	-15	HIS	-	expression tag	UNP Q2UAM5
A	-14	HIS	-	expression tag	UNP Q2UAM5
A	-13	HIS	-	expression tag	UNP Q2UAM5
A	-12	HIS	-	expression tag	UNP Q2UAM5
A	-11	HIS	-	expression tag	UNP Q2UAM5
A	-10	HIS	-	expression tag	UNP Q2UAM5
A	-9	SER	-	expression tag	UNP Q2UAM5
A	-8	SER	-	expression tag	UNP Q2UAM5
A	-7	GLY	-	expression tag	UNP Q2UAM5
A	-6	LEU	-	expression tag	UNP Q2UAM5
A	-5	VAL	-	expression tag	UNP Q2UAM5
A	-4	PRO	-	expression tag	UNP Q2UAM5
A	-3	ARG	-	expression tag	UNP Q2UAM5
A	-2	GLY	-	expression tag	UNP Q2UAM5
A	-1	SER	-	expression tag	UNP Q2UAM5
A	0	HIS	-	expression tag	UNP Q2UAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q2UAM5
B	-18	GLY	-	expression tag	UNP Q2UAM5
B	-17	SER	-	expression tag	UNP Q2UAM5
B	-16	SER	-	expression tag	UNP Q2UAM5
B	-15	HIS	-	expression tag	UNP Q2UAM5
B	-14	HIS	-	expression tag	UNP Q2UAM5
B	-13	HIS	-	expression tag	UNP Q2UAM5
B	-12	HIS	-	expression tag	UNP Q2UAM5
B	-11	HIS	-	expression tag	UNP Q2UAM5
B	-10	HIS	-	expression tag	UNP Q2UAM5
B	-9	SER	-	expression tag	UNP Q2UAM5
B	-8	SER	-	expression tag	UNP Q2UAM5
B	-7	GLY	-	expression tag	UNP Q2UAM5
B	-6	LEU	-	expression tag	UNP Q2UAM5
B	-5	VAL	-	expression tag	UNP Q2UAM5
B	-4	PRO	-	expression tag	UNP Q2UAM5
B	-3	ARG	-	expression tag	UNP Q2UAM5
B	-2	GLY	-	expression tag	UNP Q2UAM5
B	-1	SER	-	expression tag	UNP Q2UAM5
B	0	HIS	-	expression tag	UNP Q2UAM5
C	-19	MET	-	initiating methionine	UNP Q2UAM5
C	-18	GLY	-	expression tag	UNP Q2UAM5
C	-17	SER	-	expression tag	UNP Q2UAM5
C	-16	SER	-	expression tag	UNP Q2UAM5
C	-15	HIS	-	expression tag	UNP Q2UAM5
C	-14	HIS	-	expression tag	UNP Q2UAM5
C	-13	HIS	-	expression tag	UNP Q2UAM5
C	-12	HIS	-	expression tag	UNP Q2UAM5
C	-11	HIS	-	expression tag	UNP Q2UAM5
C	-10	HIS	-	expression tag	UNP Q2UAM5
C	-9	SER	-	expression tag	UNP Q2UAM5
C	-8	SER	-	expression tag	UNP Q2UAM5
C	-7	GLY	-	expression tag	UNP Q2UAM5
C	-6	LEU	-	expression tag	UNP Q2UAM5
C	-5	VAL	-	expression tag	UNP Q2UAM5
C	-4	PRO	-	expression tag	UNP Q2UAM5
C	-3	ARG	-	expression tag	UNP Q2UAM5
C	-2	GLY	-	expression tag	UNP Q2UAM5
C	-1	SER	-	expression tag	UNP Q2UAM5
C	0	HIS	-	expression tag	UNP Q2UAM5
D	-19	MET	-	initiating methionine	UNP Q2UAM5
D	-18	GLY	-	expression tag	UNP Q2UAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q2UAM5
D	-16	SER	-	expression tag	UNP Q2UAM5
D	-15	HIS	-	expression tag	UNP Q2UAM5
D	-14	HIS	-	expression tag	UNP Q2UAM5
D	-13	HIS	-	expression tag	UNP Q2UAM5
D	-12	HIS	-	expression tag	UNP Q2UAM5
D	-11	HIS	-	expression tag	UNP Q2UAM5
D	-10	HIS	-	expression tag	UNP Q2UAM5
D	-9	SER	-	expression tag	UNP Q2UAM5
D	-8	SER	-	expression tag	UNP Q2UAM5
D	-7	GLY	-	expression tag	UNP Q2UAM5
D	-6	LEU	-	expression tag	UNP Q2UAM5
D	-5	VAL	-	expression tag	UNP Q2UAM5
D	-4	PRO	-	expression tag	UNP Q2UAM5
D	-3	ARG	-	expression tag	UNP Q2UAM5
D	-2	GLY	-	expression tag	UNP Q2UAM5
D	-1	SER	-	expression tag	UNP Q2UAM5
D	0	HIS	-	expression tag	UNP Q2UAM5

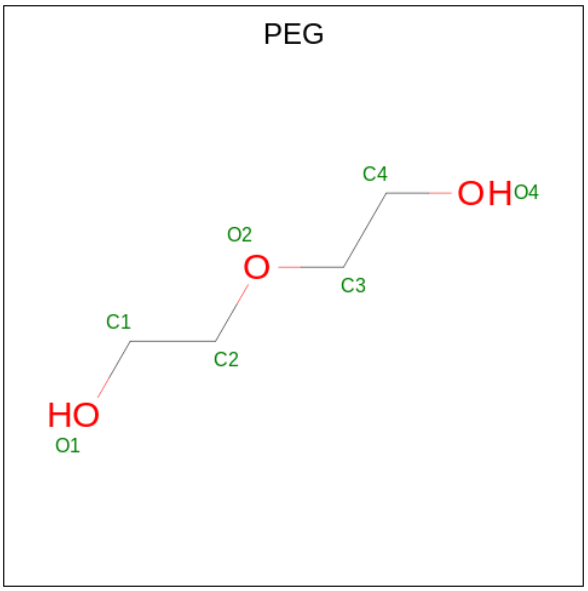
- Molecule 2 is a protein called L-tryptophan decarboxylase PsiD-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			
2	F	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			
2	G	42	Total	C	N	O	S	0	0	0
			327	211	55	60	1			
2	H	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			

There are 4 discrepancies between the modelled and reference sequences:

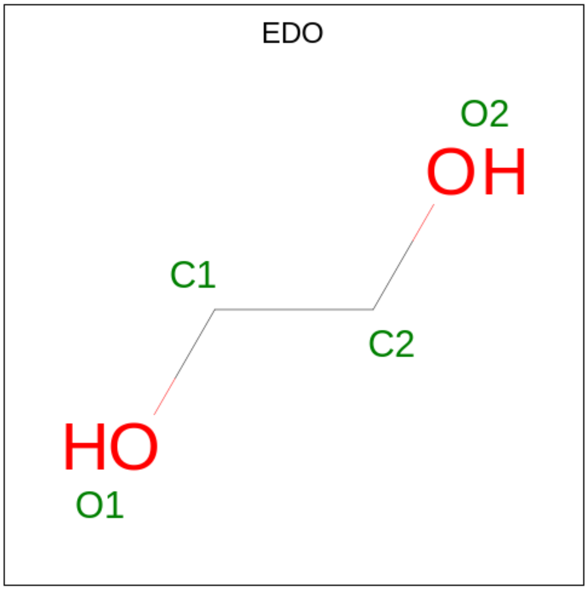
Chain	Residue	Modelled	Actual	Comment	Reference
E	502	PYR	-	modified residue	UNP Q2UAM5
F	502	PYR	-	modified residue	UNP Q2UAM5
G	502	PYR	-	modified residue	UNP Q2UAM5
H	502	PYR	-	modified residue	UNP Q2UAM5

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

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



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

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

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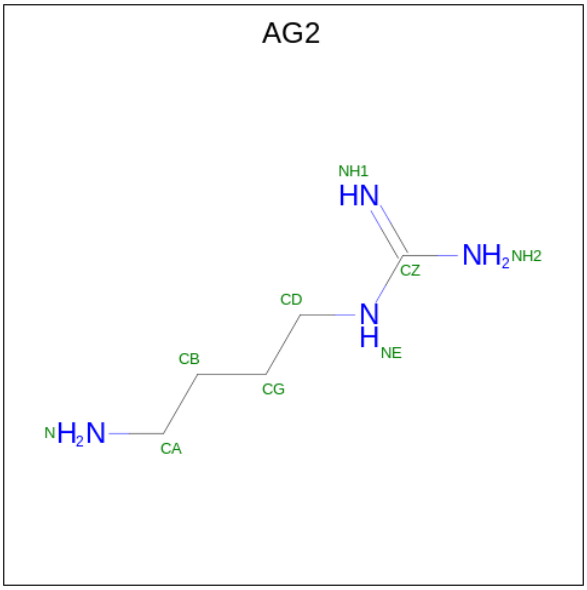
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is AGMATINE (three-letter code: AG2) (formula: $C_5H_{14}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C N 9 5 4	0	0
5	F	1	Total C N 9 5 4	0	0
5	G	1	Total C N 9 5 4	0	0
5	H	1	Total C N 9 5 4	0	0

- Molecule 6 is water.

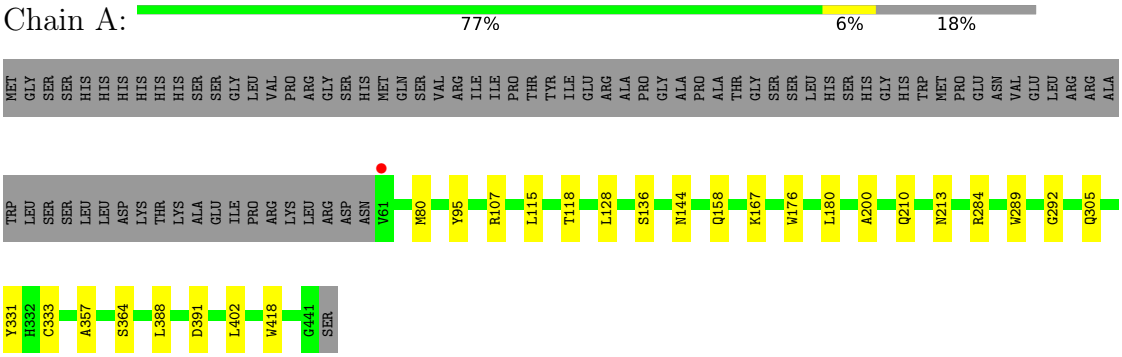
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	336	Total O 336 336	0	0
6	E	30	Total O 30 30	0	0
6	B	311	Total O 311 311	0	0
6	F	30	Total O 30 30	0	0
6	C	302	Total O 302 302	0	0
6	G	19	Total O 19 19	0	0
6	D	267	Total O 267 267	0	0
6	H	22	Total O 22 22	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

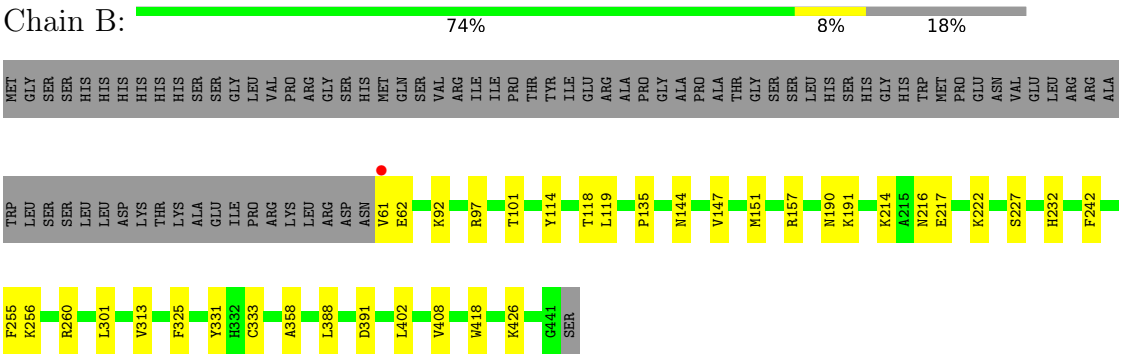
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain A:



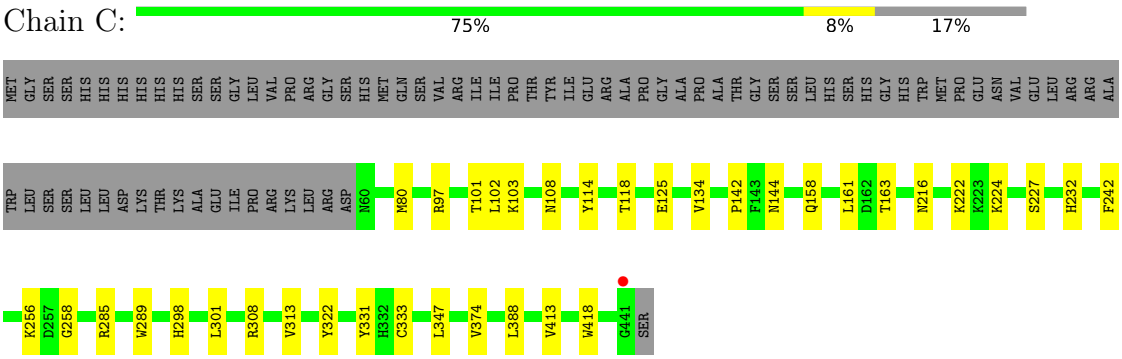
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain B:



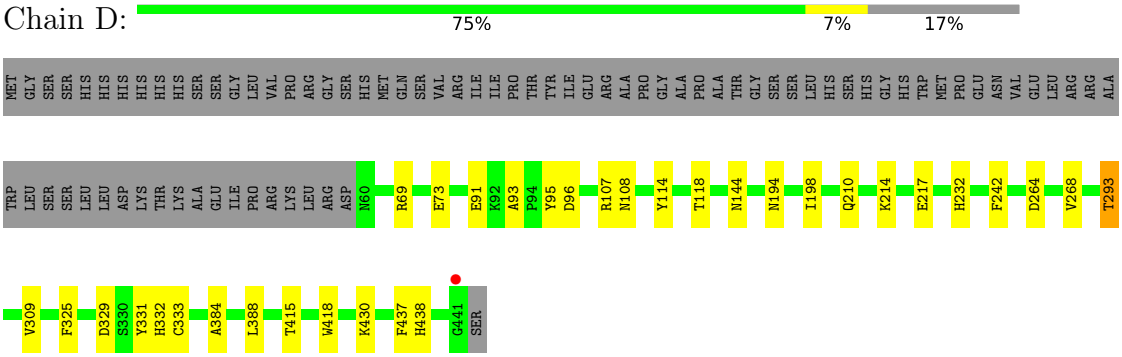
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain C:



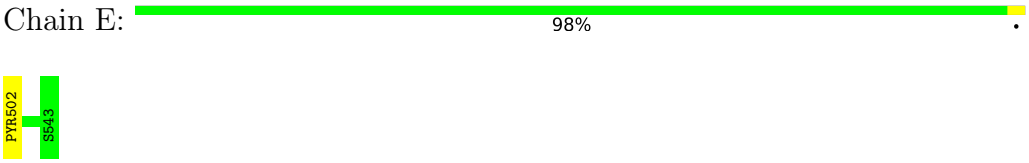
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain D:



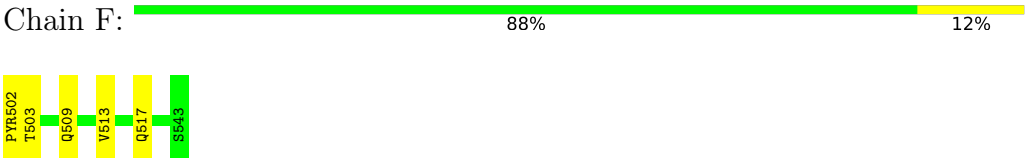
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain E:



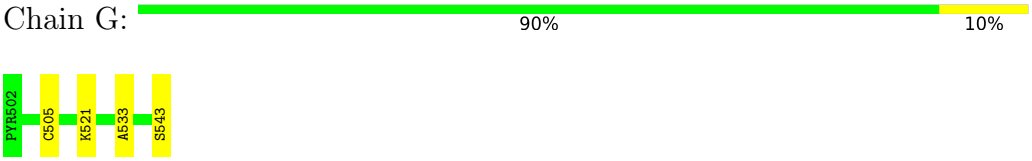
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain F:



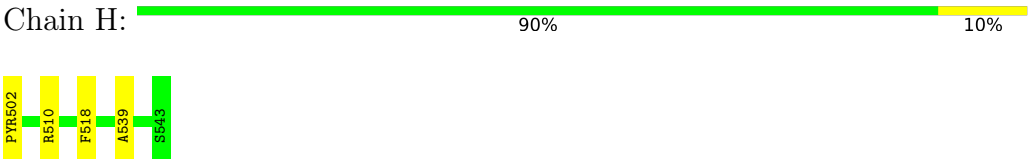
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain G:



• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	133.75Å 197.29Å 196.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.49 – 2.15 43.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.49-2.15) 99.7 (43.49-2.15)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.176 , 0.213 0.176 , 0.214	Depositor DCC
R_{free} test set	7001 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15402	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: PEG, AG2, EDO, PYR

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	A	0.37	0/3152	0.57	0/4282
1	B	0.36	0/3139	0.56	0/4264
1	C	0.37	0/3177	0.56	0/4314
1	D	0.36	0/3141	0.55	0/4270
2	E	0.35	0/337	0.55	0/456
2	F	0.33	0/337	0.54	0/456
2	G	0.34	0/328	0.57	0/444
2	H	0.32	0/337	0.54	0/456
All	All	0.36	0/13948	0.56	0/18942

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	502	PYR	Mainchain
2	F	502	PYR	Mainchain

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Mol	Chain	Res	Type	Group
2	H	502	PYR	Mainchain

5.2 Too-close contacts (i)

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	A	3040	0	2938	23	0
1	B	3031	0	2925	25	0
1	C	3062	0	2962	30	0
1	D	3038	0	2922	24	0
2	E	333	0	345	0	0
2	F	333	0	345	2	0
2	G	327	0	339	3	0
2	H	333	0	345	2	0
3	A	7	0	10	1	0
3	B	35	0	50	5	0
3	C	14	0	20	7	0
4	A	148	0	222	13	0
4	B	96	0	144	6	0
4	C	124	0	186	9	0
4	D	108	0	162	11	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
4	G	8	0	12	2	0
4	H	4	0	6	1	0
5	E	9	0	12	0	0
5	F	9	0	12	0	0
5	G	9	0	12	0	0
5	H	9	0	12	0	0
6	A	336	0	0	1	0
6	B	311	0	0	3	0
6	C	302	0	0	0	0
6	D	267	0	0	2	0
6	E	30	0	0	0	0
6	F	30	0	0	0	0
6	G	19	0	0	0	0
6	H	22	0	0	0	0
All	All	15402	0	13993	110	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 4.

The worst 5 of 110 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:A:357:ALA:H	4:A:517:EDO:H11	1.52	0.75
1:D:264:ASP:HA	4:D:522:EDO:H11	1.69	0.73
1:C:125:GLU:HB3	3:C:501:PEG:H31	1.71	0.71
1:D:384:ALA:HB1	4:D:525:EDO:H12	1.72	0.70
1:C:308:ARG:HH21	4:C:532:EDO:H22	1.57	0.70

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	A	390/462 (84%)	382 (98%)	8 (2%)	0	100	100
1	B	389/462 (84%)	382 (98%)	7 (2%)	0	100	100
1	C	393/462 (85%)	378 (96%)	15 (4%)	0	100	100
1	D	389/462 (84%)	378 (97%)	11 (3%)	0	100	100
2	E	41/42 (98%)	40 (98%)	1 (2%)	0	100	100
2	F	41/42 (98%)	40 (98%)	1 (2%)	0	100	100
2	G	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
2	H	41/42 (98%)	41 (100%)	0	0	100	100
All	All	1724/2016 (86%)	1679 (97%)	45 (3%)	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	A	330/389 (85%)	329 (100%)	1 (0%)	91 94
1	B	329/389 (85%)	328 (100%)	1 (0%)	91 94
1	C	333/389 (86%)	332 (100%)	1 (0%)	91 94
1	D	329/389 (85%)	324 (98%)	5 (2%)	60 66
2	E	37/36 (103%)	37 (100%)	0	100 100
2	F	37/36 (103%)	36 (97%)	1 (3%)	40 42
2	G	36/36 (100%)	35 (97%)	1 (3%)	38 40
2	H	37/36 (103%)	37 (100%)	0	100 100
All	All	1468/1700 (86%)	1458 (99%)	10 (1%)	84 86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	293[A]	THR
1	D	293[B]	THR
1	D	309	VAL
1	C	144	ASN
2	G	543	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
2	F	523	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

136 ligands 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	$\#\|Z\| > 2$
4	EDO	C	519	-	3,3,3	0.32	0	2,2,2	0.41	0
4	EDO	D	506	-	3,3,3	0.31	0	2,2,2	0.15	0
4	EDO	B	524	-	3,3,3	0.34	0	2,2,2	0.17	0
4	EDO	A	505	-	3,3,3	0.26	0	2,2,2	0.39	0
4	EDO	A	528	-	3,3,3	0.20	0	2,2,2	0.54	0
4	EDO	D	504	-	3,3,3	0.28	0	2,2,2	0.14	0
4	EDO	A	506	-	3,3,3	0.26	0	2,2,2	0.29	0
4	EDO	A	523	-	3,3,3	0.30	0	2,2,2	0.55	0
4	EDO	D	518	-	3,3,3	0.24	0	2,2,2	0.38	0
4	EDO	C	525	-	3,3,3	0.30	0	2,2,2	0.30	0
4	EDO	B	526	-	3,3,3	0.24	0	2,2,2	0.80	0
4	EDO	A	534	-	3,3,3	0.26	0	2,2,2	0.30	0
3	PEG	B	505	-	6,6,6	0.25	0	5,5,5	0.24	0
4	EDO	A	504	-	3,3,3	0.26	0	2,2,2	0.29	0
4	EDO	A	508	-	3,3,3	0.31	0	2,2,2	0.24	0
4	EDO	C	507	-	3,3,3	0.30	0	2,2,2	0.12	0
4	EDO	B	513	-	3,3,3	0.31	0	2,2,2	0.16	0
4	EDO	D	523	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	D	515	-	3,3,3	0.28	0	2,2,2	0.29	0
4	EDO	C	530	-	3,3,3	0.28	0	2,2,2	0.16	0
4	EDO	E	602	-	3,3,3	0.29	0	2,2,2	0.06	0
4	EDO	A	527	-	3,3,3	0.27	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	B	510	-	3,3,3	0.26	0	2,2,2	0.36	0
4	EDO	D	522	-	3,3,3	0.27	0	2,2,2	0.24	0
4	EDO	C	511	-	3,3,3	0.26	0	2,2,2	0.40	0
4	EDO	C	517	-	3,3,3	0.26	0	2,2,2	0.42	0
4	EDO	A	517	-	3,3,3	0.27	0	2,2,2	0.57	0
4	EDO	D	502	-	3,3,3	0.26	0	2,2,2	0.41	0
4	EDO	A	515	-	3,3,3	0.28	0	2,2,2	0.31	0
4	EDO	C	504	-	3,3,3	0.28	0	2,2,2	0.05	0
4	EDO	A	536	-	3,3,3	0.28	0	2,2,2	0.29	0
4	EDO	A	532	-	3,3,3	0.28	0	2,2,2	0.20	0
4	EDO	A	538	-	3,3,3	0.29	0	2,2,2	0.32	0
4	EDO	C	527	-	3,3,3	0.34	0	2,2,2	0.15	0
4	EDO	A	524	-	3,3,3	0.31	0	2,2,2	0.18	0
4	EDO	A	525	-	3,3,3	0.35	0	2,2,2	0.22	0
4	EDO	A	522	-	3,3,3	0.33	0	2,2,2	0.13	0
4	EDO	D	509	-	3,3,3	0.30	0	2,2,2	0.18	0
4	EDO	A	511	-	3,3,3	0.36	0	2,2,2	0.24	0
4	EDO	C	515	-	3,3,3	0.30	0	2,2,2	0.18	0
4	EDO	D	516	-	3,3,3	0.27	0	2,2,2	0.26	0
4	EDO	D	507	-	3,3,3	0.30	0	2,2,2	0.16	0
4	EDO	D	501	-	3,3,3	0.28	0	2,2,2	0.21	0
4	EDO	B	508	-	3,3,3	0.22	0	2,2,2	0.54	0
4	EDO	B	528	-	3,3,3	0.30	0	2,2,2	0.18	0
4	EDO	A	513	-	3,3,3	0.24	0	2,2,2	0.39	0
4	EDO	D	511	-	3,3,3	0.29	0	2,2,2	0.24	0
4	EDO	C	512	-	3,3,3	0.28	0	2,2,2	0.48	0
4	EDO	A	509	-	3,3,3	0.26	0	2,2,2	0.45	0
4	EDO	A	529	-	3,3,3	0.27	0	2,2,2	0.31	0
4	EDO	C	514	-	3,3,3	0.32	0	2,2,2	0.06	0
4	EDO	C	522	-	3,3,3	0.29	0	2,2,2	0.09	0
4	EDO	A	507	-	3,3,3	0.38	0	2,2,2	0.16	0
4	EDO	C	518	-	3,3,3	0.34	0	2,2,2	0.17	0
4	EDO	G	603	-	3,3,3	0.33	0	2,2,2	0.27	0
4	EDO	B	515	-	3,3,3	0.30	0	2,2,2	0.06	0
4	EDO	A	530	-	3,3,3	0.37	0	2,2,2	0.16	0
4	EDO	C	516	-	3,3,3	0.27	0	2,2,2	0.30	0
4	EDO	C	532	-	3,3,3	0.24	0	2,2,2	0.32	0
4	EDO	A	518	-	3,3,3	0.30	0	2,2,2	0.28	0
4	EDO	A	519	-	3,3,3	0.32	0	2,2,2	0.24	0
4	EDO	C	509	-	3,3,3	0.32	0	2,2,2	0.10	0
5	AG2	G	601	2	8,8,8	0.55	0	7,8,8	0.50	0
4	EDO	B	519	-	3,3,3	0.26	0	2,2,2	0.43	0
4	EDO	D	526	-	3,3,3	0.25	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	512	-	3,3,3	0.26	0	2,2,2	0.23	0
3	PEG	C	502	-	6,6,6	0.27	0	5,5,5	0.52	0
4	EDO	A	526	-	3,3,3	0.28	0	2,2,2	0.25	0
4	EDO	A	520	-	3,3,3	0.27	0	2,2,2	0.34	0
4	EDO	C	508	-	3,3,3	0.26	0	2,2,2	0.27	0
4	EDO	B	525	-	3,3,3	0.33	0	2,2,2	0.44	0
4	EDO	C	510	-	3,3,3	0.25	0	2,2,2	0.10	0
4	EDO	C	506	-	3,3,3	0.31	0	2,2,2	0.07	0
4	EDO	G	602	-	3,3,3	0.36	0	2,2,2	0.29	0
5	AG2	F	601	2	8,8,8	0.60	0	7,8,8	0.51	0
4	EDO	F	602	-	3,3,3	0.33	0	2,2,2	0.21	0
4	EDO	D	521	-	3,3,3	0.28	0	2,2,2	0.23	0
4	EDO	B	511	-	3,3,3	0.29	0	2,2,2	0.24	0
4	EDO	A	514	-	3,3,3	0.28	0	2,2,2	0.16	0
4	EDO	D	512	-	3,3,3	0.28	0	2,2,2	0.06	0
4	EDO	B	516	-	3,3,3	0.32	0	2,2,2	0.19	0
4	EDO	D	510	-	3,3,3	0.22	0	2,2,2	0.37	0
3	PEG	C	501	-	6,6,6	0.30	0	5,5,5	0.46	0
4	EDO	C	524	-	3,3,3	0.29	0	2,2,2	0.08	0
4	EDO	A	537	-	3,3,3	0.30	0	2,2,2	0.22	0
4	EDO	C	531	-	3,3,3	0.30	0	2,2,2	0.20	0
4	EDO	H	602	-	3,3,3	0.28	0	2,2,2	0.22	0
4	EDO	B	521	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	B	514	-	3,3,3	0.21	0	2,2,2	0.50	0
5	AG2	E	601	2	8,8,8	0.56	0	7,8,8	0.48	0
4	EDO	B	506	-	3,3,3	0.29	0	2,2,2	0.10	0
4	EDO	B	523	-	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	C	526	-	3,3,3	0.29	0	2,2,2	0.23	0
3	PEG	B	504	-	6,6,6	0.27	0	5,5,5	0.50	0
4	EDO	D	508	-	3,3,3	0.27	0	2,2,2	0.44	0
4	EDO	D	527	-	3,3,3	0.29	0	2,2,2	0.32	0
3	PEG	A	501	-	6,6,6	0.31	0	5,5,5	0.28	0
4	EDO	A	516	-	3,3,3	0.29	0	2,2,2	0.24	0
4	EDO	C	513	-	3,3,3	0.28	0	2,2,2	0.10	0
4	EDO	B	518	-	3,3,3	0.29	0	2,2,2	0.27	0
3	PEG	B	503	-	6,6,6	0.25	0	5,5,5	0.25	0
4	EDO	B	527	-	3,3,3	0.28	0	2,2,2	0.26	0
4	EDO	B	512	-	3,3,3	0.31	0	2,2,2	0.06	0
4	EDO	D	505	-	3,3,3	0.32	0	2,2,2	0.29	0
4	EDO	B	522	-	3,3,3	0.26	0	2,2,2	0.21	0
4	EDO	B	509	-	3,3,3	0.28	0	2,2,2	0.22	0
4	EDO	C	520	-	3,3,3	0.28	0	2,2,2	0.30	0
4	EDO	A	531	-	3,3,3	0.32	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	C	529	-	3,3,3	0.30	0	2,2,2	0.49	0
4	EDO	B	520	-	3,3,3	0.26	0	2,2,2	0.42	0
4	EDO	D	525	-	3,3,3	0.22	0	2,2,2	0.28	0
4	EDO	D	519	-	3,3,3	0.30	0	2,2,2	0.23	0
4	EDO	A	533	-	3,3,3	0.31	0	2,2,2	0.14	0
3	PEG	B	501	-	6,6,6	0.21	0	5,5,5	0.26	0
4	EDO	B	517	-	3,3,3	0.21	0	2,2,2	0.91	0
4	EDO	A	521	-	3,3,3	0.29	0	2,2,2	0.17	0
4	EDO	D	503	-	3,3,3	0.26	0	2,2,2	0.26	0
4	EDO	D	517	-	3,3,3	0.30	0	2,2,2	0.17	0
4	EDO	A	510	-	3,3,3	0.26	0	2,2,2	0.18	0
4	EDO	D	513	-	3,3,3	0.27	0	2,2,2	0.32	0
4	EDO	C	528	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	C	503	-	3,3,3	0.36	0	2,2,2	0.14	0
5	AG2	H	601	2	8,8,8	0.51	0	7,8,8	0.38	0
4	EDO	B	529	-	3,3,3	0.30	0	2,2,2	0.22	0
3	PEG	B	502	-	6,6,6	0.19	0	5,5,5	0.43	0
4	EDO	C	533	-	3,3,3	0.27	0	2,2,2	0.39	0
4	EDO	D	524	-	3,3,3	0.30	0	2,2,2	0.21	0
4	EDO	A	503	-	3,3,3	0.30	0	2,2,2	0.26	0
4	EDO	C	505	-	3,3,3	0.28	0	2,2,2	0.10	0
4	EDO	C	523	-	3,3,3	0.35	0	2,2,2	0.15	0
4	EDO	B	507	-	3,3,3	0.28	0	2,2,2	0.19	0
4	EDO	A	535	-	3,3,3	0.33	0	2,2,2	0.27	0
4	EDO	D	520	-	3,3,3	0.29	0	2,2,2	0.21	0
4	EDO	A	502	-	3,3,3	0.19	0	2,2,2	0.25	0
4	EDO	C	521	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	D	514	-	3,3,3	0.24	0	2,2,2	0.35	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	C	519	-	-	1/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	B	524	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	A	528	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	C	525	-	-	0/1/1/1	-
4	EDO	B	526	-	-	1/1/1/1	-
4	EDO	A	534	-	-	0/1/1/1	-
3	PEG	B	505	-	-	1/4/4/4	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	D	523	-	-	1/1/1/1	-
4	EDO	D	515	-	-	0/1/1/1	-
4	EDO	C	530	-	-	1/1/1/1	-
4	EDO	E	602	-	-	1/1/1/1	-
4	EDO	A	527	-	-	0/1/1/1	-
4	EDO	B	510	-	-	1/1/1/1	-
4	EDO	D	522	-	-	1/1/1/1	-
4	EDO	C	511	-	-	0/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	A	517	-	-	0/1/1/1	-
4	EDO	D	502	-	-	1/1/1/1	-
4	EDO	A	515	-	-	1/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	A	536	-	-	0/1/1/1	-
4	EDO	A	532	-	-	0/1/1/1	-
4	EDO	A	538	-	-	0/1/1/1	-
4	EDO	C	527	-	-	0/1/1/1	-
4	EDO	A	524	-	-	0/1/1/1	-
4	EDO	A	525	-	-	1/1/1/1	-
4	EDO	A	522	-	-	0/1/1/1	-
4	EDO	D	509	-	-	1/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	D	501	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	B	528	-	-	1/1/1/1	-
4	EDO	A	513	-	-	1/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	C	512	-	-	0/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	529	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	514	-	-	1/1/1/1	-
4	EDO	C	522	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
4	EDO	G	603	-	-	0/1/1/1	-
4	EDO	B	515	-	-	0/1/1/1	-
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	C	532	-	-	0/1/1/1	-
4	EDO	A	518	-	-	1/1/1/1	-
4	EDO	A	519	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
5	AG2	G	601	2	-	0/6/6/6	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	D	526	-	-	0/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
3	PEG	C	502	-	-	2/4/4/4	-
4	EDO	A	526	-	-	0/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
4	EDO	C	508	-	-	0/1/1/1	-
4	EDO	B	525	-	-	1/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
4	EDO	G	602	-	-	1/1/1/1	-
5	AG2	F	601	2	-	0/6/6/6	-
4	EDO	F	602	-	-	1/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	D	512	-	-	0/1/1/1	-
4	EDO	B	516	-	-	1/1/1/1	-
4	EDO	D	510	-	-	0/1/1/1	-
3	PEG	C	501	-	-	2/4/4/4	-
4	EDO	C	524	-	-	0/1/1/1	-
4	EDO	A	537	-	-	0/1/1/1	-
4	EDO	C	531	-	-	1/1/1/1	-
4	EDO	H	602	-	-	0/1/1/1	-
4	EDO	B	521	-	-	1/1/1/1	-
4	EDO	B	514	-	-	0/1/1/1	-
5	AG2	E	601	2	-	0/6/6/6	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	B	523	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	526	-	-	0/1/1/1	-
3	PEG	B	504	-	-	2/4/4/4	-
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	D	527	-	-	1/1/1/1	-
3	PEG	A	501	-	-	2/4/4/4	-
4	EDO	A	516	-	-	0/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
3	PEG	B	503	-	-	1/4/4/4	-
4	EDO	B	527	-	-	0/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	B	522	-	-	0/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
4	EDO	C	520	-	-	0/1/1/1	-
4	EDO	A	531	-	-	1/1/1/1	-
4	EDO	C	529	-	-	0/1/1/1	-
4	EDO	B	520	-	-	0/1/1/1	-
4	EDO	D	525	-	-	0/1/1/1	-
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	A	533	-	-	1/1/1/1	-
3	PEG	B	501	-	-	1/4/4/4	-
4	EDO	B	517	-	-	1/1/1/1	-
4	EDO	A	521	-	-	0/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	D	517	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	C	528	-	-	1/1/1/1	-
4	EDO	C	503	-	-	1/1/1/1	-
5	AG2	H	601	2	-	0/6/6/6	-
4	EDO	B	529	-	-	0/1/1/1	-
3	PEG	B	502	-	-	2/4/4/4	-
4	EDO	C	533	-	-	0/1/1/1	-
4	EDO	D	524	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	C	505	-	-	0/1/1/1	-
4	EDO	C	523	-	-	1/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	535	-	-	0/1/1/1	-
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	A	502	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	521	-	-	0/1/1/1	-
4	EDO	D	514	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	PEG	O1-C1-C2-O2
3	C	501	PEG	O2-C3-C4-O4
4	A	518	EDO	O1-C1-C2-O2
4	B	526	EDO	O1-C1-C2-O2
3	A	501	PEG	O2-C3-C4-O4

There are no ring outliers.

39 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	EDO	1	0
4	C	525	EDO	2	0
4	A	534	EDO	1	0
4	C	530	EDO	2	0
4	D	522	EDO	3	0
4	A	517	EDO	1	0
4	A	515	EDO	1	0
4	C	527	EDO	1	0
4	C	512	EDO	1	0
4	C	518	EDO	1	0
4	G	603	EDO	1	0
4	A	530	EDO	2	0
4	C	532	EDO	2	0
4	A	518	EDO	2	0
4	A	512	EDO	1	0
3	C	502	PEG	4	0
4	A	526	EDO	1	0
4	B	525	EDO	1	0
4	G	602	EDO	1	0
4	A	514	EDO	1	0
3	C	501	PEG	4	0
4	C	524	EDO	1	0

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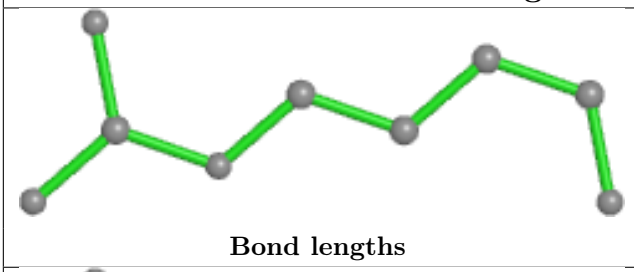
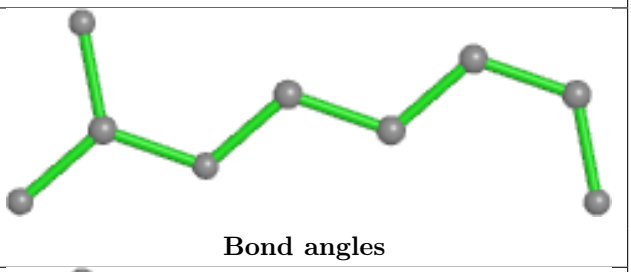
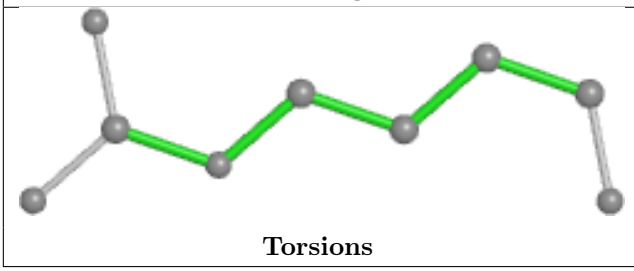
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	602	EDO	1	0
4	B	521	EDO	2	0
4	B	514	EDO	1	0
4	B	523	EDO	1	0
3	B	504	PEG	1	0
4	D	527	EDO	1	0
3	A	501	PEG	1	0
4	D	505	EDO	1	0
4	D	525	EDO	1	0
4	A	533	EDO	2	0
3	B	501	PEG	2	0
4	A	510	EDO	1	0
4	D	513	EDO	2	0
4	B	529	EDO	1	0
3	B	502	PEG	2	0
4	D	520	EDO	1	0
4	D	514	EDO	1	0

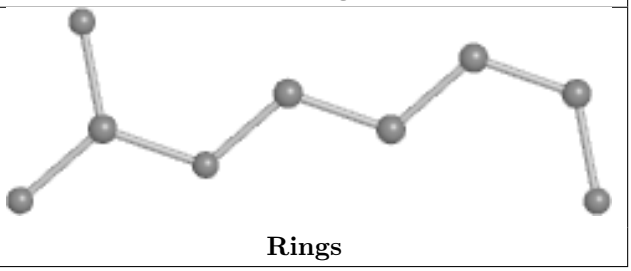
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 AG2 G 601

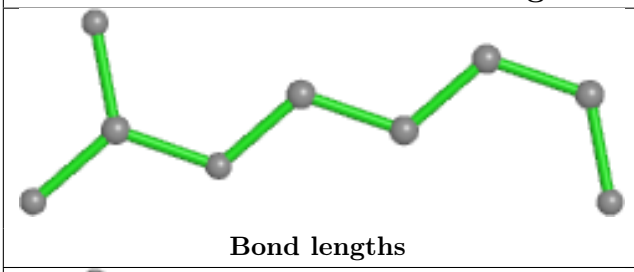

Bond lengths

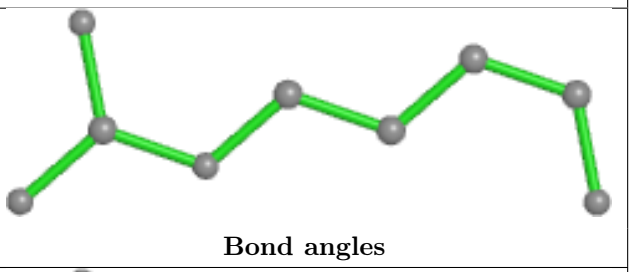

Bond angles

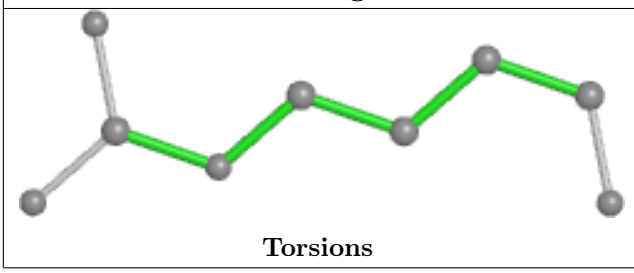

Torsions

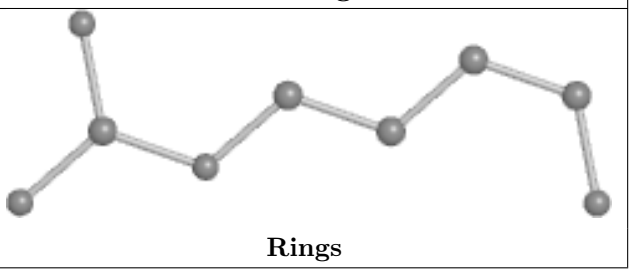

Rings

Ligand AG2 F 601

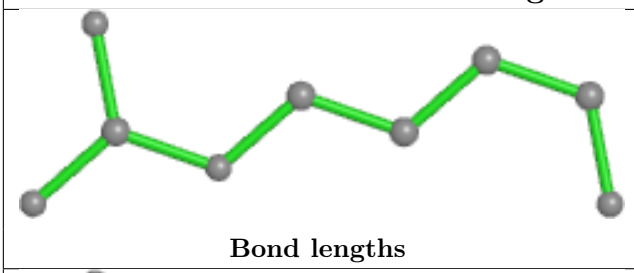

Bond lengths

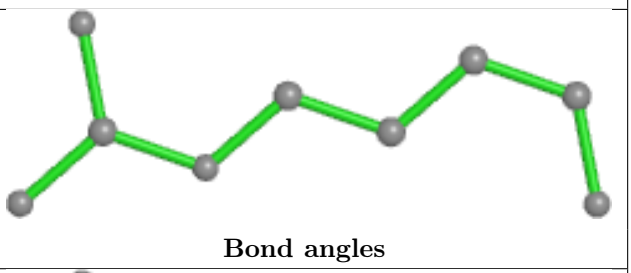

Bond angles

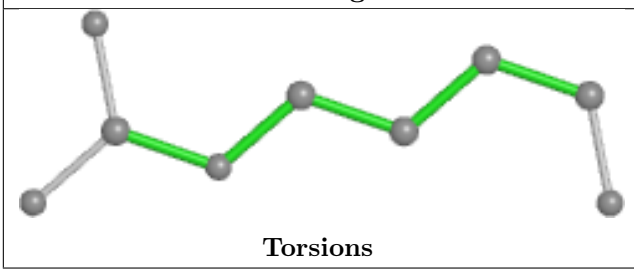

Torsions

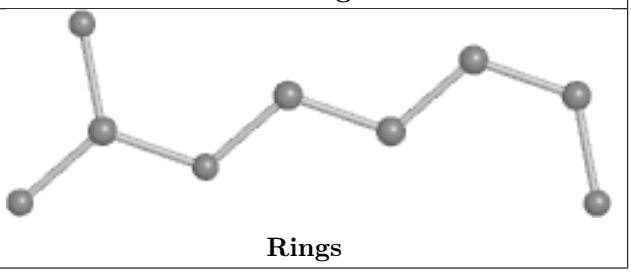

Rings

Ligand AG2 E 601

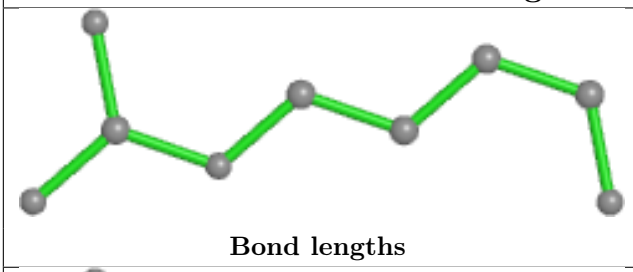

Bond lengths


Bond angles

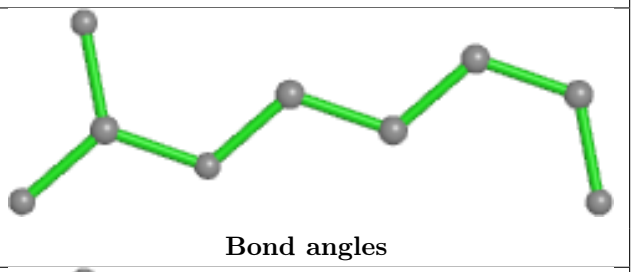

Torsions


Rings

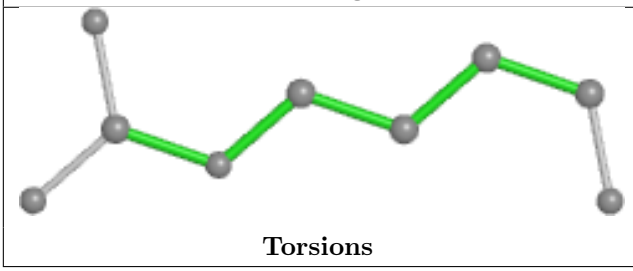
Ligand AG2 H 601



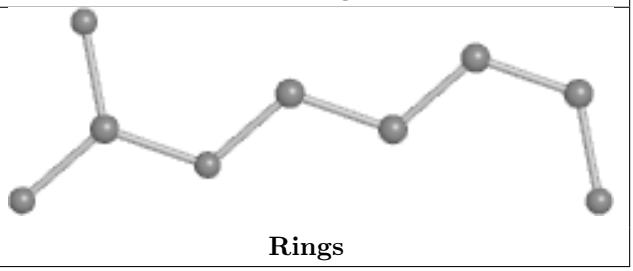
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	381/462 (82%)	-0.49	1 (0%)	90	92	18, 37, 49, 80	11 (2%)
1	B	381/462 (82%)	-0.39	1 (0%)	90	92	18, 37, 57, 77	10 (2%)
1	C	382/462 (82%)	-0.26	1 (0%)	90	92	18, 39, 54, 97	13 (3%)
1	D	382/462 (82%)	-0.19	1 (0%)	90	92	18, 41, 62, 105	9 (2%)
2	E	41/42 (97%)	-0.37	0	100	100	20, 37, 56, 81	1 (2%)
2	F	41/42 (97%)	-0.38	0	100	100	22, 41, 57, 80	1 (2%)
2	G	41/42 (97%)	-0.09	0	100	100	32, 40, 61, 77	0
2	H	41/42 (97%)	-0.16	0	100	100	22, 43, 55, 83	1 (2%)
All	All	1690/2016 (83%)	-0.32	4 (0%)	92	93	18, 39, 57, 105	46 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	VAL	3.2
1	B	61	VAL	2.7
1	D	441	GLY	2.4
1	C	441	GLY	2.4

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 (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	D	524	4/4	0.66	0.23	60,67,71,72	0
3	PEG	C	502	7/7	0.67	0.23	47,59,63,65	0
4	EDO	B	514	4/4	0.69	0.17	61,61,61,77	0
4	EDO	D	511	4/4	0.70	0.13	69,71,75,77	0
4	EDO	B	523	4/4	0.71	0.26	61,63,67,81	0
4	EDO	D	516	4/4	0.72	0.14	70,78,80,82	0
4	EDO	A	524	4/4	0.72	0.16	58,64,66,67	0
4	EDO	D	509	4/4	0.73	0.19	55,56,60,62	0
3	PEG	B	505	7/7	0.74	0.17	60,64,66,71	0
4	EDO	B	515	4/4	0.74	0.16	66,68,71,72	0
4	EDO	A	530	4/4	0.74	0.23	51,52,57,57	0
4	EDO	G	602	4/4	0.74	0.20	45,62,63,73	0
4	EDO	A	531	4/4	0.75	0.16	56,57,61,78	0
4	EDO	A	512	4/4	0.76	0.25	47,59,63,68	0
4	EDO	A	535	4/4	0.77	0.20	47,53,56,60	0
4	EDO	B	519	4/4	0.77	0.18	64,65,66,76	0
4	EDO	B	521	4/4	0.77	0.15	56,62,64,70	0
4	EDO	C	531	4/4	0.78	0.18	58,61,62,62	0
4	EDO	A	511	4/4	0.78	0.23	36,50,52,54	0
4	EDO	C	510	4/4	0.79	0.25	43,55,60,62	0
4	EDO	D	521	4/4	0.79	0.14	67,71,76,80	0
4	EDO	C	517	4/4	0.79	0.22	55,59,67,67	0
4	EDO	B	525	4/4	0.80	0.18	33,48,61,62	0
4	EDO	C	523	4/4	0.80	0.18	61,61,64,68	0
4	EDO	A	515	4/4	0.80	0.21	50,51,58,66	0
4	EDO	D	515	4/4	0.81	0.13	68,74,76,81	0
4	EDO	B	524	4/4	0.81	0.16	49,50,55,57	0
4	EDO	A	519	4/4	0.81	0.18	42,47,52,56	0
3	PEG	A	501	7/7	0.81	0.18	32,51,59,61	0
4	EDO	D	520	4/4	0.82	0.14	64,65,67,69	0
4	EDO	C	504	4/4	0.82	0.20	49,51,53,59	0
4	EDO	A	523	4/4	0.82	0.13	45,52,58,59	0
4	EDO	D	526	4/4	0.82	0.15	59,59,63,75	0
4	EDO	A	529	4/4	0.83	0.20	56,60,65,69	0
4	EDO	G	603	4/4	0.83	0.18	47,53,57,58	0
4	EDO	A	513	4/4	0.83	0.15	48,53,55,72	0
4	EDO	D	522	4/4	0.83	0.13	59,66,69,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	528	4/4	0.83	0.17	41,53,53,57	0
4	EDO	A	525	4/4	0.83	0.20	48,54,56,66	0
4	EDO	A	538	4/4	0.84	0.15	55,63,66,71	0
4	EDO	C	527	4/4	0.84	0.20	51,54,58,58	0
4	EDO	A	522	4/4	0.84	0.19	55,57,57,59	0
4	EDO	A	532	4/4	0.84	0.18	47,52,57,61	0
4	EDO	A	509	4/4	0.84	0.15	44,46,52,62	0
4	EDO	D	506	4/4	0.84	0.12	66,70,71,76	0
4	EDO	C	522	4/4	0.84	0.21	53,61,61,67	0
4	EDO	D	510	4/4	0.84	0.17	46,53,55,60	0
4	EDO	D	512	4/4	0.85	0.18	55,58,64,65	0
4	EDO	C	511	4/4	0.85	0.16	39,43,48,52	0
4	EDO	C	524	4/4	0.85	0.17	54,60,62,64	0
4	EDO	D	503	4/4	0.85	0.17	58,60,63,78	0
3	PEG	B	501	7/7	0.85	0.18	50,55,62,75	0
4	EDO	C	530	4/4	0.85	0.16	41,53,54,58	0
4	EDO	D	523	4/4	0.85	0.12	45,57,58,64	0
4	EDO	B	511	4/4	0.85	0.17	52,52,63,66	0
4	EDO	D	525	4/4	0.85	0.17	46,51,53,58	0
4	EDO	C	533	4/4	0.85	0.13	46,50,56,62	0
4	EDO	H	602	4/4	0.85	0.15	54,58,59,75	0
4	EDO	A	527	4/4	0.86	0.12	58,62,66,68	0
4	EDO	C	507	4/4	0.86	0.16	47,47,55,63	0
4	EDO	A	528	4/4	0.86	0.13	40,48,51,58	0
4	EDO	C	525	4/4	0.86	0.14	46,50,61,62	0
4	EDO	C	526	4/4	0.86	0.17	51,61,62,65	0
3	PEG	B	504	7/7	0.86	0.11	32,43,51,54	0
4	EDO	C	514	4/4	0.86	0.14	65,70,72,78	0
4	EDO	C	516	4/4	0.86	0.13	63,64,67,70	0
4	EDO	B	513	4/4	0.86	0.15	57,64,73,75	0
3	PEG	B	502	7/7	0.87	0.13	38,48,56,62	0
4	EDO	A	521	4/4	0.87	0.16	64,68,69,77	0
4	EDO	D	517	4/4	0.87	0.16	64,68,69,71	0
4	EDO	D	519	4/4	0.87	0.14	52,55,59,67	0
4	EDO	A	510	4/4	0.87	0.18	54,59,59,59	0
4	EDO	C	515	4/4	0.87	0.14	61,63,64,65	0
4	EDO	D	505	4/4	0.87	0.14	41,45,56,56	0
4	EDO	B	512	4/4	0.87	0.19	51,55,59,67	0
4	EDO	A	533	4/4	0.87	0.22	53,54,59,67	0
4	EDO	C	529	4/4	0.87	0.17	43,49,52,62	0
4	EDO	C	518	4/4	0.87	0.17	49,60,61,65	0
4	EDO	C	520	4/4	0.87	0.19	53,58,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	E	602	4/4	0.88	0.18	57,60,61,67	0
4	EDO	B	508	4/4	0.88	0.14	48,49,63,65	0
3	PEG	B	503	7/7	0.88	0.12	64,67,75,75	0
4	EDO	A	514	4/4	0.88	0.12	54,55,62,72	0
4	EDO	C	532	4/4	0.88	0.10	46,51,58,60	0
4	EDO	D	527	4/4	0.88	0.15	44,48,49,57	0
4	EDO	D	514	4/4	0.88	0.13	48,52,55,63	0
4	EDO	B	516	4/4	0.89	0.18	56,58,62,67	0
4	EDO	D	513	4/4	0.89	0.13	51,53,63,65	0
4	EDO	A	534	4/4	0.90	0.09	54,57,57,65	0
4	EDO	B	526	4/4	0.90	0.11	42,45,49,51	0
4	EDO	C	519	4/4	0.90	0.17	45,50,57,58	0
4	EDO	C	528	4/4	0.90	0.27	44,47,49,55	0
3	PEG	C	501	7/7	0.90	0.13	38,44,60,66	0
4	EDO	A	520	4/4	0.90	0.13	56,60,62,68	0
4	EDO	C	505	4/4	0.90	0.13	46,47,56,69	0
4	EDO	D	518	4/4	0.90	0.13	42,44,46,56	0
4	EDO	C	506	4/4	0.90	0.14	53,54,56,64	0
4	EDO	A	526	4/4	0.91	0.11	46,53,59,64	0
4	EDO	D	504	4/4	0.91	0.11	43,46,53,63	0
4	EDO	A	506	4/4	0.91	0.13	41,44,47,59	0
4	EDO	B	520	4/4	0.91	0.15	54,57,60,64	0
4	EDO	D	508	4/4	0.91	0.13	44,48,52,53	0
4	EDO	B	510	4/4	0.92	0.10	44,47,47,58	0
4	EDO	B	517	4/4	0.92	0.13	43,47,50,50	0
4	EDO	B	527	4/4	0.92	0.13	42,49,57,62	0
4	EDO	B	518	4/4	0.92	0.12	49,51,54,56	0
4	EDO	B	529	4/4	0.92	0.12	47,48,54,59	0
4	EDO	F	602	4/4	0.92	0.11	43,45,45,55	0
4	EDO	A	508	4/4	0.92	0.13	45,51,54,60	0
4	EDO	A	537	4/4	0.92	0.09	49,49,54,55	0
4	EDO	C	521	4/4	0.92	0.14	49,57,59,66	0
4	EDO	A	505	4/4	0.92	0.11	39,39,51,51	0
4	EDO	A	516	4/4	0.92	0.10	41,52,54,63	0
4	EDO	A	517	4/4	0.92	0.13	36,39,45,55	0
4	EDO	C	512	4/4	0.93	0.12	51,55,57,70	0
4	EDO	C	509	4/4	0.93	0.08	45,45,46,53	0
4	EDO	A	504	4/4	0.93	0.10	40,43,51,57	0
4	EDO	D	507	4/4	0.93	0.14	61,67,70,76	0
4	EDO	B	522	4/4	0.93	0.17	46,58,58,60	0
4	EDO	B	509	4/4	0.94	0.12	51,51,54,56	0
4	EDO	A	507	4/4	0.94	0.12	39,47,52,57	0

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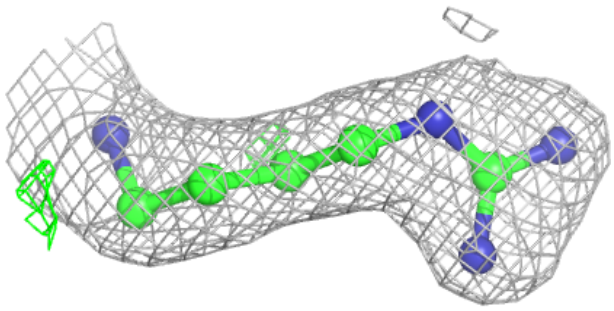
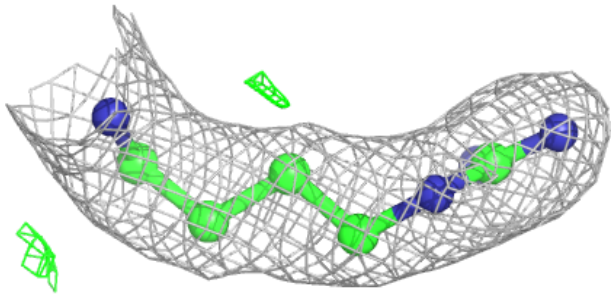
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	536	4/4	0.94	0.12	38,61,65,68	0
4	EDO	B	507	4/4	0.94	0.10	39,40,41,42	0
4	EDO	A	518	4/4	0.94	0.16	44,47,48,48	0
4	EDO	C	513	4/4	0.94	0.15	44,48,58,61	0
4	EDO	A	502	4/4	0.95	0.07	29,33,34,34	0
4	EDO	D	502	4/4	0.95	0.09	42,45,47,47	0
5	AG2	E	601	9/9	0.95	0.07	30,32,40,41	0
5	AG2	F	601	9/9	0.95	0.08	31,35,36,39	0
5	AG2	G	601	9/9	0.95	0.08	34,36,43,45	0
5	AG2	H	601	9/9	0.95	0.08	34,39,43,47	0
4	EDO	C	503	4/4	0.96	0.07	31,32,33,38	0
4	EDO	D	501	4/4	0.96	0.07	35,36,37,40	0
4	EDO	C	508	4/4	0.96	0.09	43,46,51,53	0
4	EDO	B	506	4/4	0.97	0.07	34,35,40,41	0
4	EDO	A	503	4/4	0.97	0.08	38,43,43,44	0

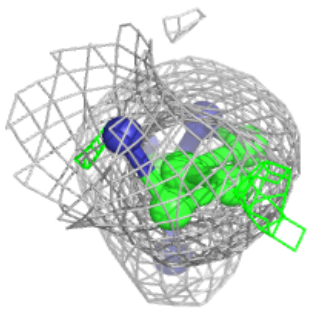
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AG2 E 601:

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

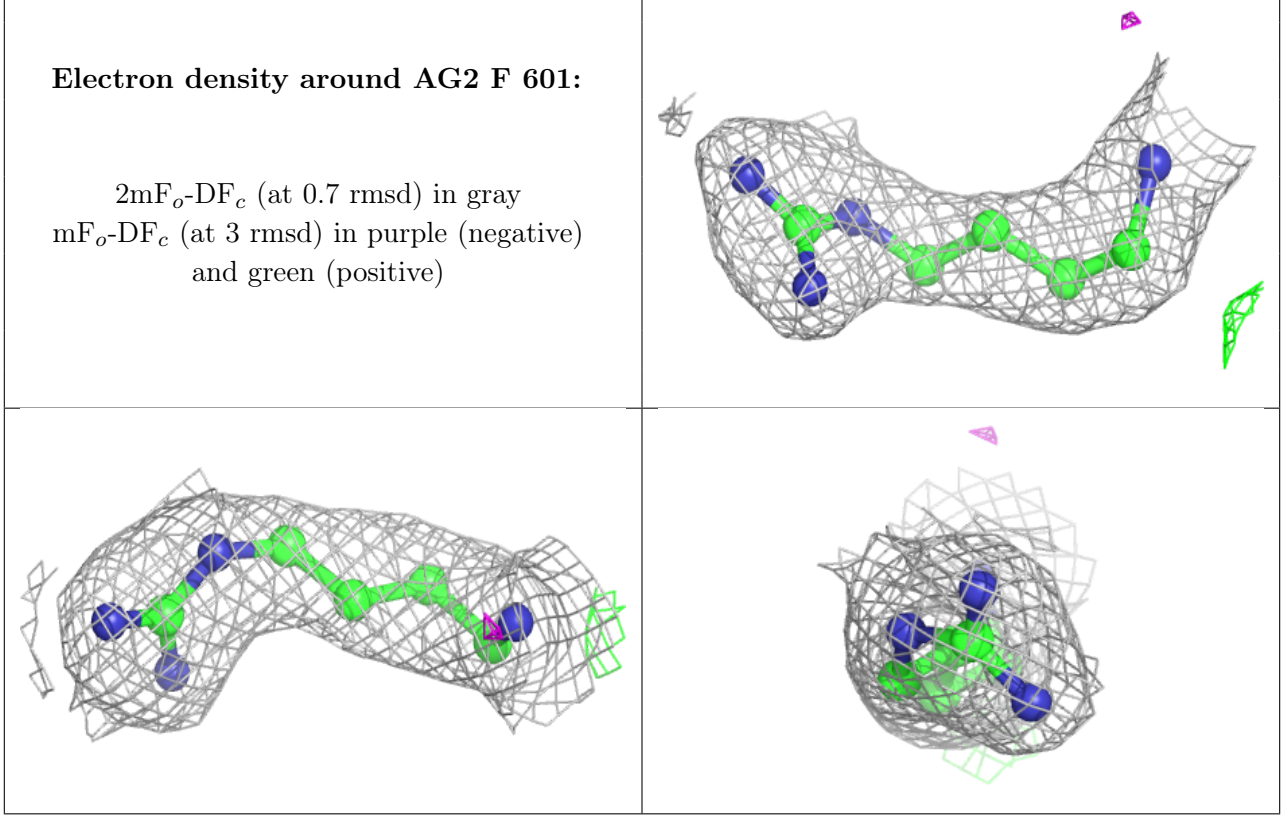






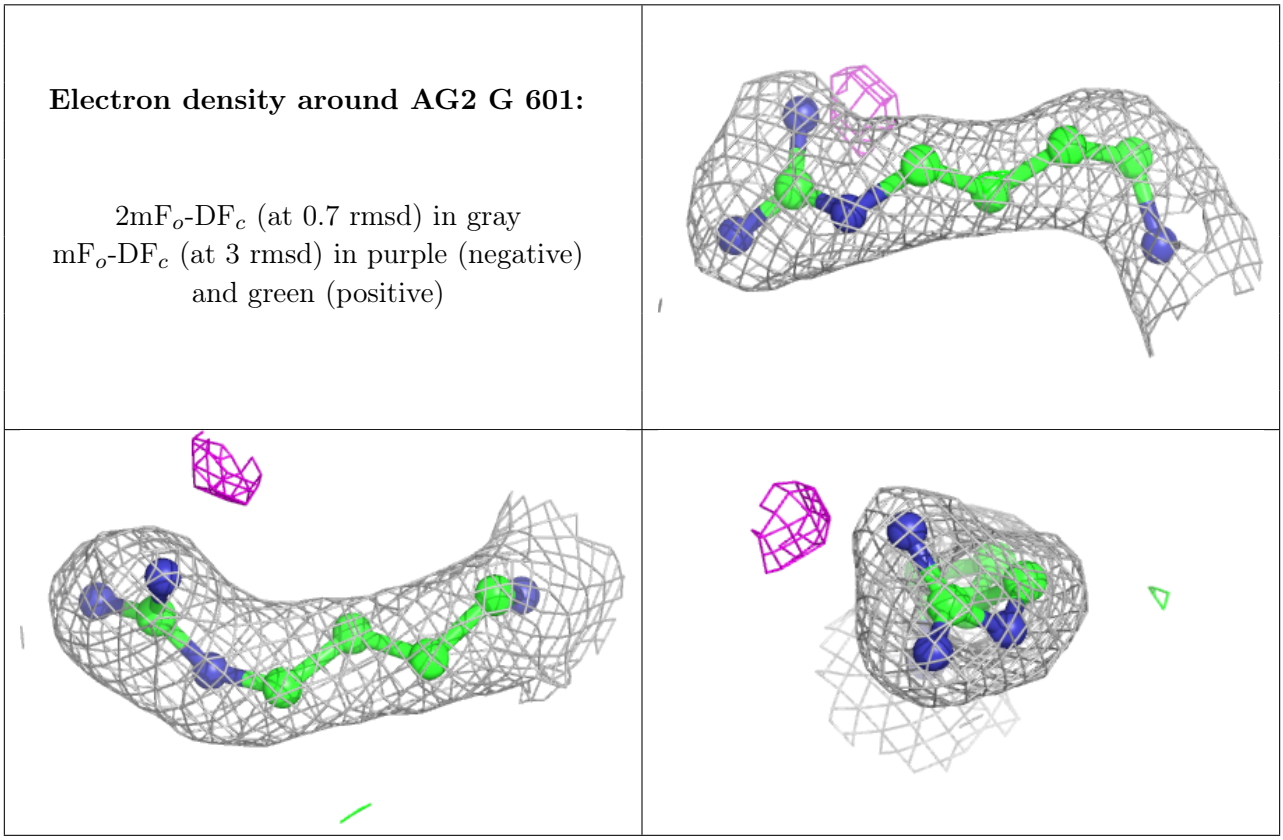
Electron density around AG2 F 601:

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



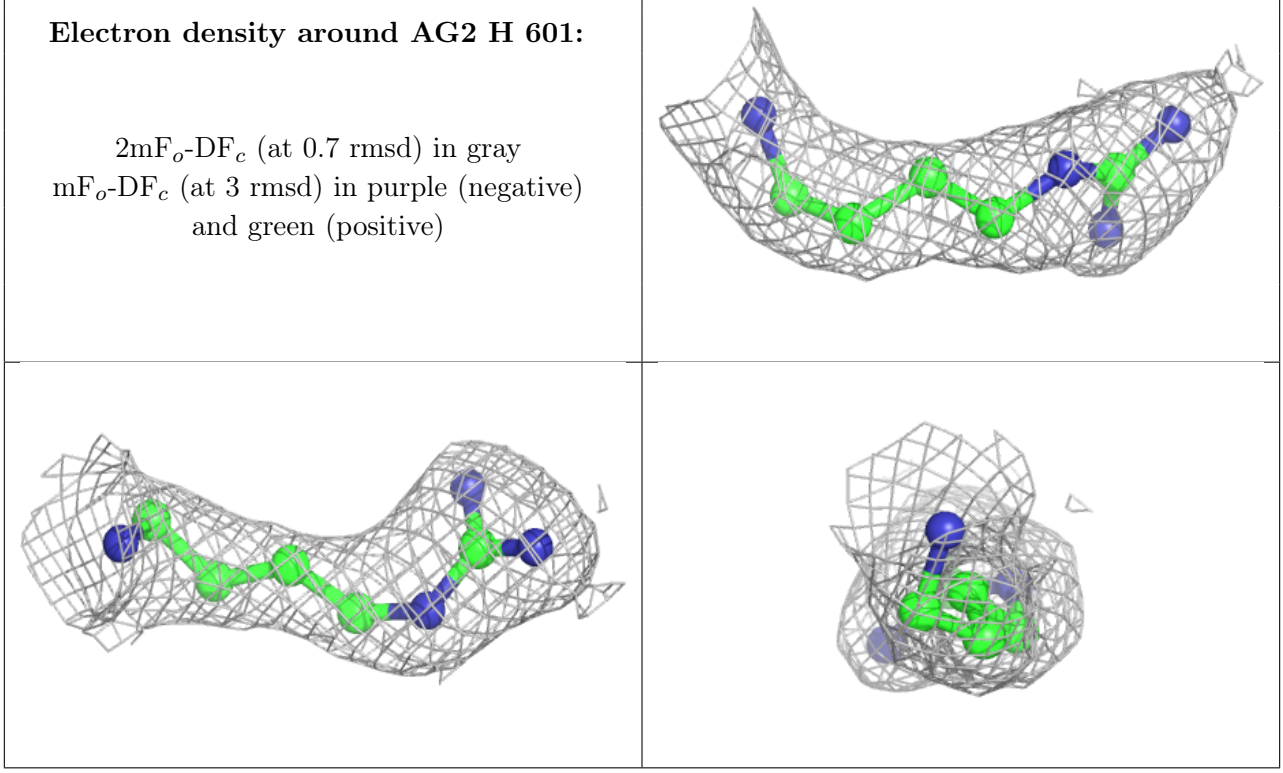
Electron density around AG2 G 601:

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



Electron density around AG2 H 601:

$2mF_o$-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.