



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:57 PM UTC

PDB ID : 9JF5 / pdb_00009jf5
Title : Arginine decarboxylase in *Aspergillus oryzae* complexed with arginine
Authors : Mikami, B.; Yasukawa, K.; Fujiwara, S.; Takita, T.; Mizutani, K.; Odagaki, Y.; Murakami, Y.
Deposited on : 2024-09-04
Resolution : 1.90 Å(reported)

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

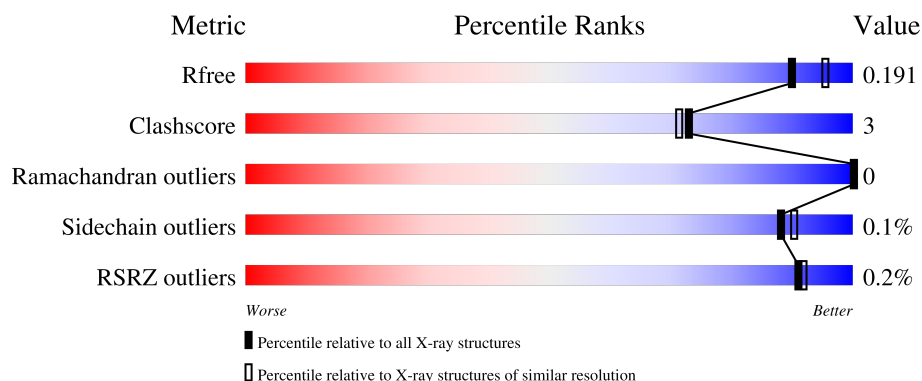
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



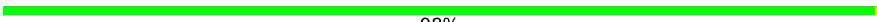
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	462	
1	C	462	
1	D	462	
2	E	42	

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Mol	Chain	Length	Quality of chain
2	F	42	 98% .
2	G	42	 98% .
2	H	42	 98% .

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	D	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15948 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	17	0
			3085	1960	524	590	11			
1	B	381	Total	C	N	O	S	0	10	0
			3033	1930	512	580	11			
1	C	382	Total	C	N	O	S	0	16	0
			3086	1964	523	588	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	41	Total	C	N	O	S	0	2	0
			335	217	57	60	1			
2	F	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			
2	G	41	Total	C	N	O	S	0	0	0
			321	208	54	58	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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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		

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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	E	1	Total	C	O	0	0
			4	2	2		

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

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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	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	F	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	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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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	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
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

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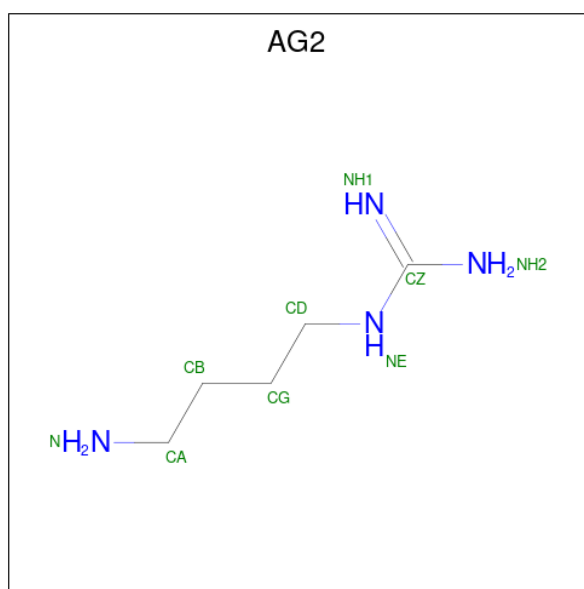
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total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

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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	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
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is AGMATINE (CCD ID: 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

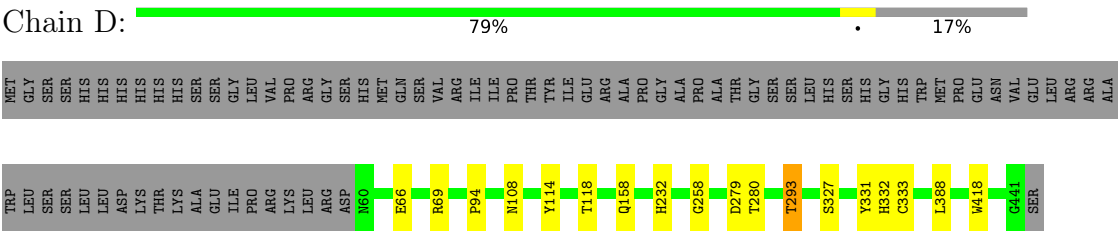
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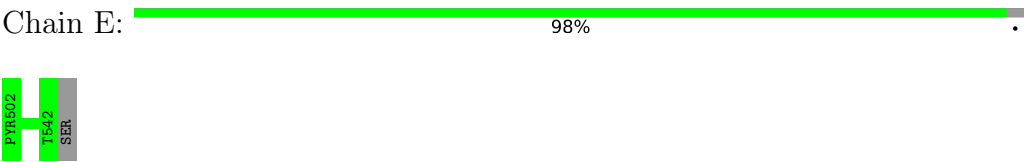
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	N	0	0
			9	5	4		

- Molecule 6 is water.

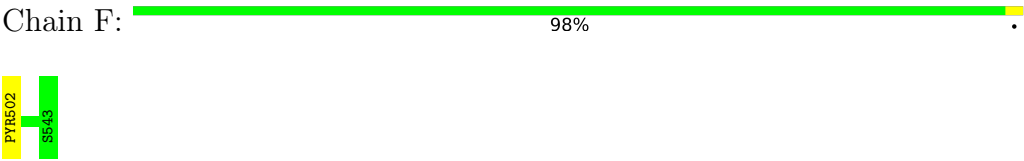
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	390	Total	O	0	0
			390	390		
6	E	34	Total	O	0	1
			35	35		
6	B	394	Total	O	0	1
			395	395		
6	F	29	Total	O	0	0
			29	29		
6	C	373	Total	O	0	1
			374	374		
6	G	32	Total	O	0	0
			32	32		
6	D	407	Total	O	0	1
			408	408		
6	H	30	Total	O	0	0
			30	30		



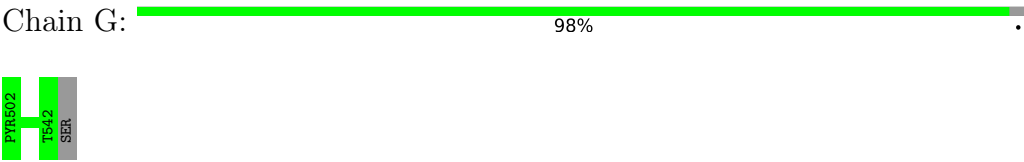
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein



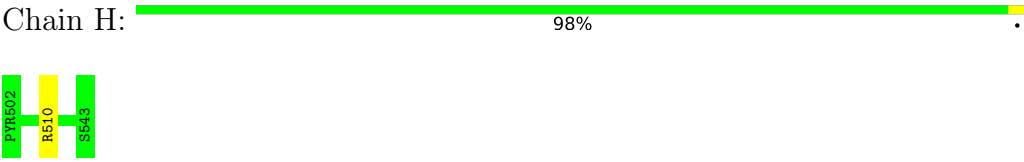
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.02Å 195.57Å 196.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 1.90 47.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.44-1.90) 99.8 (47.44-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.160 , 0.189 0.163 , 0.191	Depositor DCC
R_{free} test set	10045 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15948	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.27	0/3206	0.46	0/4356
1	B	0.28	0/3141	0.47	0/4266
1	C	0.27	0/3207	0.45	0/4353
1	D	0.28	0/3141	0.47	0/4270
2	E	0.24	0/342	0.47	0/462
2	F	0.27	0/337	0.46	0/456
2	G	0.24	0/322	0.46	0/436
2	H	0.25	0/337	0.48	0/456
All	All	0.27	0/14033	0.46	0/19055

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	502	PYR	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3085	0	2982	18	0
1	B	3033	0	2932	33	0
1	C	3086	0	2991	17	0
1	D	3038	0	2922	19	0
2	E	335	0	353	0	0
2	F	333	0	345	0	0
2	G	321	0	334	0	0
2	H	333	0	345	1	0
3	A	14	0	20	2	0
3	B	21	0	30	1	0
3	C	21	0	30	2	0
3	D	7	0	10	4	0
4	A	136	0	204	11	0
4	B	152	0	228	18	0
4	C	136	0	204	7	0
4	D	136	0	204	9	0
4	E	12	0	18	0	0
4	F	4	0	6	0	0
4	G	8	0	12	1	0
4	H	8	0	12	1	0
5	E	9	0	12	0	0
5	F	9	0	12	0	0
5	G	9	0	11	1	0
5	H	9	0	12	0	0
6	A	390	0	0	1	0
6	B	395	0	0	2	0
6	C	374	0	0	1	0
6	D	408	0	0	3	0
6	E	35	0	0	0	0
6	F	29	0	0	0	0
6	G	32	0	0	1	0
6	H	30	0	0	0	0
All	All	15948	0	14229	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (92) 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:C:142:PRO:HB3	3:C:502:PEG:H31	1.37	1.04
1:D:158:GLN:HE21	4:D:535:EDO:H12	1.43	0.83
1:C:162:ASP:HB2	4:C:510:EDO:H11	1.63	0.79
1:B:285:ARG:HH11	4:B:509:EDO:H21	1.49	0.77
1:D:258:GLY:H	4:D:524:EDO:H12	1.56	0.70
1:A:307:GLU:HG3	4:A:525:EDO:H12	1.72	0.70
1:D:280:THR:H	3:D:501:PEG:H22	1.57	0.69
1:B:61:VAL:HG13	1:B:62:GLU:H	1.57	0.69
1:B:345:ARG:HE	4:B:539:EDO:H11	1.57	0.69
1:D:279:ASP:HA	3:D:501:PEG:H11	1.75	0.68
1:D:94:PRO:HD3	4:D:515:EDO:H21	1.77	0.66
1:D:158:GLN:HE21	4:D:535:EDO:C1	2.08	0.64
1:B:115:LEU:HD22	3:B:501:PEG:H31	1.81	0.62
1:B:284:ARG:HH22	4:B:509:EDO:H22	1.66	0.61
1:A:108:ASN:HB2	4:A:513:EDO:H12	1.83	0.60
1:A:308:ARG:HE	4:A:536:EDO:H21	1.66	0.60
1:B:305[A]:GLN:NE2	6:B:602:HOH:O	2.35	0.58
1:A:292:GLY:H	3:A:501:PEG:H41	1.68	0.58
1:A:308:ARG:HE	4:A:536:EDO:C2	2.17	0.57
1:C:331:TYR:CZ	1:C:333:CYS:HB2	2.40	0.56
1:B:345:ARG:HE	4:B:539:EDO:C1	2.18	0.56
1:C:114:TYR:O	1:C:118:THR:HG23	2.06	0.56
1:A:256:LYS:HD3	4:A:530:EDO:H21	1.89	0.55
1:B:421:ASN:HA	4:B:531:EDO:H12	1.88	0.55
1:A:308:ARG:HH21	4:A:536:EDO:H21	1.70	0.55
1:C:258:GLY:H	4:C:521:EDO:H12	1.73	0.54
4:C:535:EDO:H21	6:C:913:HOH:O	2.07	0.54
1:B:125:GLU:HB2	4:B:534:EDO:H11	1.90	0.54
1:D:114:TYR:O	1:D:118[B]:THR:HG23	2.08	0.54
1:B:325:PHE:CD2	4:B:540:EDO:H21	2.42	0.53
1:D:118[B]:THR:HG22	6:D:830:HOH:O	2.09	0.53
1:D:158:GLN:NE2	4:D:535:EDO:H12	2.17	0.53
1:A:115:LEU:O	1:A:118[B]:THR:HG22	2.07	0.53
1:C:106[B]:VAL:HG21	1:C:146:ILE:HG23	1.90	0.53
1:D:331:TYR:CZ	1:D:333:CYS:HB2	2.44	0.52
1:D:108:ASN:HB2	4:D:517:EDO:H12	1.92	0.51
1:B:66:GLU:OE2	1:B:69[B]:ARG:NH2	2.36	0.50
1:D:69[A]:ARG:HH21	4:D:531:EDO:H12	1.76	0.50
1:B:69[B]:ARG:NH1	1:B:73:GLU:OE1	2.45	0.50
1:D:293[A]:THR:HG21	6:D:892:HOH:O	2.11	0.49
1:B:331:TYR:CZ	1:B:333:CYS:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:LYS:HE2	4:C:531:EDO:H21	1.95	0.49
1:D:293[A]:THR:HG22	4:D:506:EDO:O2	2.13	0.49
1:C:158:GLN:HG2	4:C:510:EDO:H12	1.94	0.48
1:B:104[B]:LYS:HG2	4:B:512:EDO:H22	1.96	0.48
1:B:139:ILE:HB	4:B:530:EDO:H12	1.96	0.47
1:A:103:LYS:HE3	3:A:502:PEG:H41	1.97	0.47
1:B:214:LYS:O	1:B:217:GLU:HG2	2.15	0.47
1:C:69[B]:ARG:NH1	1:C:73:GLU:OE1	2.48	0.46
1:B:238:GLN:HG2	4:B:523:EDO:H11	1.97	0.46
1:A:331:TYR:CZ	1:A:333:CYS:HB2	2.50	0.46
1:D:280:THR:H	3:D:501:PEG:C2	2.25	0.46
1:B:104[A]:LYS:HG2	4:B:512:EDO:H22	1.97	0.46
1:B:227:SER:O	1:B:256:LYS:HD2	2.16	0.46
1:B:66:GLU:CD	1:B:69[B]:ARG:HE	2.24	0.45
1:A:139:ILE:HB	4:A:528:EDO:H12	1.99	0.45
1:B:239:GLU:HA	4:B:523:EDO:H12	1.97	0.45
1:B:108:ASN:HB2	4:B:506:EDO:H11	1.98	0.45
1:C:388:LEU:HB2	1:C:418:TRP:CH2	2.52	0.45
1:C:214:LYS:O	1:C:217:GLU:HG2	2.17	0.45
1:B:232:HIS:CG	1:B:242:PHE:HB3	2.51	0.44
1:A:242:PHE:CE1	4:A:519:EDO:H22	2.52	0.44
1:B:208:VAL:HG21	1:B:238:GLN:HG3	1.98	0.44
3:D:501:PEG:H42	6:D:895:HOH:O	2.18	0.44
1:B:376:GLN:NE2	4:B:540:EDO:H22	2.33	0.43
1:C:356:THR:HG22	3:C:501:PEG:H41	2.00	0.43
1:C:174:ASN:O	1:C:178[A]:GLU:HG3	2.18	0.43
1:D:232:HIS:NE2	4:D:525:EDO:H22	2.32	0.43
1:A:69[B]:ARG:NH1	1:A:73:GLU:OE1	2.52	0.43
1:B:345:ARG:NE	4:B:539:EDO:H11	2.29	0.43
1:C:325:PHE:CE2	4:C:506:EDO:H22	2.54	0.43
1:B:114:TYR:O	1:B:118[A]:THR:HG23	2.19	0.42
1:D:66:GLU:OE2	1:D:69[B]:ARG:NH2	2.45	0.42
1:A:95:TYR:HE2	4:A:512:EDO:H22	1.85	0.42
1:A:242:PHE:HE1	4:A:519:EDO:H22	1.83	0.42
1:B:306:ASP:O	1:B:309:VAL:HG12	2.20	0.41
1:B:426:LYS:NZ	4:B:531:EDO:H11	2.35	0.41
1:A:232:HIS:CG	1:A:242:PHE:HB3	2.54	0.41
2:H:510:ARG:HB3	4:H:603:EDO:H22	2.01	0.41
1:A:95:TYR:O	1:A:107[B]:ARG:NH2	2.54	0.41
1:C:332[B]:HIS:HE1	5:G:601:AG2:HA2	1.86	0.41
1:D:327:SER:O	1:D:332[B]:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167[B]:LYS:NZ	6:B:607:HOH:O	2.47	0.41
1:C:91[B]:GLU:H	1:C:91[B]:GLU:HG2	1.65	0.41
1:B:200:ALA:HA	4:B:534:EDO:H21	2.03	0.41
1:C:256:LYS:HD2	4:C:519:EDO:H12	2.03	0.40
4:G:603:EDO:H22	6:G:701:HOH:O	2.21	0.40
1:B:95:TYR:O	1:B:107[B]:ARG:NH2	2.54	0.40
1:D:388:LEU:HB2	1:D:418:TRP:CH2	2.56	0.40
1:A:332[B]:HIS:HD2	1:A:437:PHE:HB2	1.85	0.40
4:A:522:EDO:H22	6:A:755:HOH:O	2.22	0.40
1:B:374:VAL:HG12	4:B:526:EDO:H22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	396/462 (86%)	386 (98%)	10 (2%)	0	100	100
1	B	389/462 (84%)	382 (98%)	7 (2%)	0	100	100
1	C	396/462 (86%)	388 (98%)	8 (2%)	0	100	100
1	D	389/462 (84%)	380 (98%)	9 (2%)	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	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
2	H	41/42 (98%)	40 (98%)	1 (2%)	0	100	100
All	All	1732/2016 (86%)	1694 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	336/389 (86%)	336 (100%)	0	100	100
1	B	329/389 (85%)	329 (100%)	0	100	100
1	C	336/389 (86%)	336 (100%)	0	100	100
1	D	329/389 (85%)	327 (99%)	2 (1%)	78	81
2	E	37/36 (103%)	37 (100%)	0	100	100
2	F	37/36 (103%)	37 (100%)	0	100	100
2	G	35/36 (97%)	35 (100%)	0	100	100
2	H	37/36 (103%)	37 (100%)	0	100	100
All	All	1476/1700 (87%)	1474 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	293[A]	THR
1	D	293[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	194	ASN
1	B	194	ASN
2	F	531	ASN
1	C	194	ASN
2	G	517	GLN
1	D	158	GLN
1	D	177	ASN

5.3.3 RNA ⓘ

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](#)

161 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	D	517	-	3,3,3	0.23	0	2,2,2	0.46	0
4	EDO	C	520	-	3,3,3	0.27	0	2,2,2	0.18	0
3	PEG	C	503	-	6,6,6	0.23	0	5,5,5	0.41	0
4	EDO	A	504	-	3,3,3	0.25	0	2,2,2	0.20	0
4	EDO	C	530	-	3,3,3	0.25	0	2,2,2	0.30	0
4	EDO	D	507	-	3,3,3	0.27	0	2,2,2	0.22	0
4	EDO	B	519	-	3,3,3	0.25	0	2,2,2	0.28	0
4	EDO	D	515	-	3,3,3	0.26	0	2,2,2	0.20	0
4	EDO	A	533	-	3,3,3	0.23	0	2,2,2	0.35	0
4	EDO	C	521	-	3,3,3	0.28	0	2,2,2	0.29	0
4	EDO	G	602	-	3,3,3	0.24	0	2,2,2	0.53	0
4	EDO	D	511	-	3,3,3	0.23	0	2,2,2	0.47	0
3	PEG	A	502	-	6,6,6	0.23	0	5,5,5	0.32	0
4	EDO	C	529	-	3,3,3	0.24	0	2,2,2	0.40	0
4	EDO	D	531	-	3,3,3	0.25	0	2,2,2	0.14	0
4	EDO	D	506	-	3,3,3	0.26	0	2,2,2	0.22	0
4	EDO	B	531	-	3,3,3	0.26	0	2,2,2	0.06	0
4	EDO	A	511	-	3,3,3	0.26	0	2,2,2	0.32	0
4	EDO	A	513	-	3,3,3	0.25	0	2,2,2	0.45	0
4	EDO	B	504	-	3,3,3	0.27	0	2,2,2	0.42	0
4	EDO	D	508	-	3,3,3	0.30	0	2,2,2	0.13	0
4	EDO	D	535	-	3,3,3	0.37	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	518	-	3,3,3	0.25	0	2,2,2	0.28	0
4	EDO	A	514	-	3,3,3	0.26	0	2,2,2	0.29	0
4	EDO	B	537	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	C	527	-	3,3,3	0.24	0	2,2,2	0.31	0
4	EDO	F	602	-	3,3,3	0.24	0	2,2,2	0.43	0
4	EDO	C	506	-	3,3,3	0.25	0	2,2,2	0.18	0
4	EDO	C	532	-	3,3,3	0.28	0	2,2,2	0.15	0
4	EDO	C	505	-	3,3,3	0.24	0	2,2,2	0.36	0
4	EDO	C	507	-	3,3,3	0.26	0	2,2,2	0.05	0
4	EDO	B	525	-	3,3,3	0.27	0	2,2,2	0.28	0
4	EDO	B	506	-	3,3,3	0.21	0	2,2,2	0.58	0
4	EDO	B	511	-	3,3,3	0.26	0	2,2,2	0.25	0
4	EDO	B	512	-	3,3,3	0.24	0	2,2,2	0.28	0
4	EDO	D	529	-	3,3,3	0.28	0	2,2,2	0.25	0
4	EDO	B	541	-	3,3,3	0.14	0	2,2,2	0.39	0
4	EDO	C	514	-	3,3,3	0.23	0	2,2,2	0.59	0
4	EDO	A	532	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	D	510	-	3,3,3	0.22	0	2,2,2	0.64	0
4	EDO	D	525	-	3,3,3	0.24	0	2,2,2	0.29	0
4	EDO	D	526	-	3,3,3	0.24	0	2,2,2	0.37	0
4	EDO	D	534	-	3,3,3	0.24	0	2,2,2	0.38	0
4	EDO	A	503	-	3,3,3	0.28	0	2,2,2	0.39	0
4	EDO	B	516	-	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	D	522	-	3,3,3	0.26	0	2,2,2	0.35	0
4	EDO	B	515	-	3,3,3	0.22	0	2,2,2	0.55	0
3	PEG	B	501	-	6,6,6	0.24	0	5,5,5	0.62	0
4	EDO	D	519	-	3,3,3	0.24	0	2,2,2	0.33	0
4	EDO	A	516	-	3,3,3	0.22	0	2,2,2	0.66	0
4	EDO	D	530	-	3,3,3	0.26	0	2,2,2	0.34	0
4	EDO	A	527	-	3,3,3	0.23	0	2,2,2	0.47	0
4	EDO	C	515	-	3,3,3	0.26	0	2,2,2	0.17	0
4	EDO	A	526	-	3,3,3	0.26	0	2,2,2	0.56	0
4	EDO	D	521	-	3,3,3	0.21	0	2,2,2	0.49	0
4	EDO	B	510	-	3,3,3	0.26	0	2,2,2	0.31	0
4	EDO	B	534	-	3,3,3	0.25	0	2,2,2	0.10	0
4	EDO	B	517	-	3,3,3	0.27	0	2,2,2	0.37	0
4	EDO	A	517	-	3,3,3	0.24	0	2,2,2	0.35	0
4	EDO	C	531	-	3,3,3	0.27	0	2,2,2	0.31	0
4	EDO	B	518	-	3,3,3	0.24	0	2,2,2	0.39	0
4	EDO	C	528	-	3,3,3	0.23	0	2,2,2	0.41	0
4	EDO	B	522	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	A	507	-	3,3,3	0.30	0	2,2,2	0.24	0
4	EDO	B	540	-	3,3,3	0.07	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	523	-	3,3,3	0.26	0	2,2,2	0.38	0
4	EDO	C	510	-	3,3,3	0.25	0	2,2,2	0.41	0
4	EDO	C	513	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	C	508	-	3,3,3	0.26	0	2,2,2	0.20	0
4	EDO	C	525	-	3,3,3	0.25	0	2,2,2	0.33	0
4	EDO	C	535	-	3,3,3	0.28	0	2,2,2	0.18	0
5	AG2	F	601	2	8,8,8	0.63	0	7,8,8	0.47	0
4	EDO	B	528	-	3,3,3	0.24	0	2,2,2	0.33	0
4	EDO	A	531	-	3,3,3	0.24	0	2,2,2	0.33	0
4	EDO	C	526	-	3,3,3	0.26	0	2,2,2	0.19	0
3	PEG	B	502	-	6,6,6	0.25	0	5,5,5	0.39	0
4	EDO	A	506	-	3,3,3	0.25	0	2,2,2	0.11	0
4	EDO	D	513	-	3,3,3	0.25	0	2,2,2	0.14	0
4	EDO	C	524	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	B	520	-	3,3,3	0.25	0	2,2,2	0.36	0
4	EDO	E	602	-	3,3,3	0.24	0	2,2,2	0.17	0
4	EDO	A	529	-	3,3,3	0.26	0	2,2,2	0.34	0
4	EDO	H	603	-	3,3,3	0.25	0	2,2,2	0.42	0
4	EDO	C	534	-	3,3,3	0.26	0	2,2,2	0.26	0
4	EDO	A	523	-	3,3,3	0.26	0	2,2,2	0.27	0
4	EDO	D	524	-	3,3,3	0.28	0	2,2,2	0.43	0
4	EDO	D	532	-	3,3,3	0.28	0	2,2,2	0.40	0
4	EDO	B	524	-	3,3,3	0.25	0	2,2,2	0.41	0
4	EDO	D	503	-	3,3,3	0.27	0	2,2,2	0.11	0
4	EDO	C	511	-	3,3,3	0.24	0	2,2,2	0.28	0
4	EDO	D	502	-	3,3,3	0.27	0	2,2,2	0.19	0
4	EDO	H	602	-	3,3,3	0.23	0	2,2,2	0.46	0
5	AG2	E	601	2	8,8,8	0.55	0	7,8,8	0.43	0
4	EDO	D	528	-	3,3,3	0.24	0	2,2,2	0.46	0
4	EDO	C	522	-	3,3,3	0.27	0	2,2,2	0.36	0
4	EDO	E	603	-	3,3,3	0.26	0	2,2,2	0.20	0
4	EDO	C	519	-	3,3,3	0.23	0	2,2,2	0.32	0
4	EDO	B	538	-	3,3,3	0.23	0	2,2,2	0.36	0
4	EDO	D	527	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	A	525	-	3,3,3	0.25	0	2,2,2	0.29	0
4	EDO	A	510	-	3,3,3	0.20	0	2,2,2	0.34	0
4	EDO	B	532	-	3,3,3	0.28	0	2,2,2	0.37	0
4	EDO	D	516	-	3,3,3	0.29	0	2,2,2	0.19	0
3	PEG	A	501	-	6,6,6	0.28	0	5,5,5	0.30	0
4	EDO	C	537	-	3,3,3	0.22	0	2,2,2	0.50	0
4	EDO	A	519	-	3,3,3	0.31	0	2,2,2	0.20	0
4	EDO	C	533	-	3,3,3	0.26	0	2,2,2	0.52	0
4	EDO	B	507	-	3,3,3	0.27	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	534	-	3,3,3	0.26	0	2,2,2	0.15	0
4	EDO	A	530	-	3,3,3	0.24	0	2,2,2	0.26	0
4	EDO	A	515	-	3,3,3	0.25	0	2,2,2	0.38	0
4	EDO	C	523	-	3,3,3	0.26	0	2,2,2	0.28	0
4	EDO	D	520	-	3,3,3	0.25	0	2,2,2	0.24	0
4	EDO	C	517	-	3,3,3	0.24	0	2,2,2	0.38	0
4	EDO	B	521	-	3,3,3	0.22	0	2,2,2	0.44	0
4	EDO	B	529	-	3,3,3	0.24	0	2,2,2	0.52	0
4	EDO	B	523	-	3,3,3	0.22	0	2,2,2	0.29	0
4	EDO	A	522	-	3,3,3	0.28	0	2,2,2	0.25	0
5	AG2	H	601	2	8,8,8	0.59	0	7,8,8	0.49	0
4	EDO	C	536	-	3,3,3	0.23	0	2,2,2	0.60	0
4	EDO	D	518	-	3,3,3	0.26	0	2,2,2	0.28	0
4	EDO	D	533	-	3,3,3	0.20	0	2,2,2	0.71	0
4	EDO	B	539	-	3,3,3	0.76	0	2,2,2	0.68	0
4	EDO	D	514	-	3,3,3	0.24	0	2,2,2	0.20	0
4	EDO	A	535	-	3,3,3	0.24	0	2,2,2	0.47	0
4	EDO	B	514	-	3,3,3	0.27	0	2,2,2	0.21	0
4	EDO	D	504	-	3,3,3	0.24	0	2,2,2	0.36	0
3	PEG	C	502	-	6,6,6	0.29	0	5,5,5	0.93	0
4	EDO	A	528	-	3,3,3	0.20	0	2,2,2	0.49	0
4	EDO	C	509	-	3,3,3	0.24	0	2,2,2	0.26	0
4	EDO	C	512	-	3,3,3	0.25	0	2,2,2	0.58	0
4	EDO	B	527	-	3,3,3	0.22	0	2,2,2	0.69	0
4	EDO	B	536	-	3,3,3	0.28	0	2,2,2	0.10	0
4	EDO	B	533	-	3,3,3	0.26	0	2,2,2	0.24	0
3	PEG	C	501	-	6,6,6	0.29	0	5,5,5	0.19	0
5	AG2	G	601	2	8,8,8	0.64	0	7,8,8	0.40	0
4	EDO	D	509	-	3,3,3	0.26	0	2,2,2	0.40	0
4	EDO	C	504	-	3,3,3	0.28	0	2,2,2	0.34	0
4	EDO	B	509	-	3,3,3	0.31	0	2,2,2	0.30	0
4	EDO	B	505	-	3,3,3	0.25	0	2,2,2	0.27	0
4	EDO	A	505	-	3,3,3	0.26	0	2,2,2	0.19	0
4	EDO	A	524	-	3,3,3	0.25	0	2,2,2	0.39	0
4	EDO	A	509	-	3,3,3	0.24	0	2,2,2	0.38	0
4	EDO	A	508	-	3,3,3	0.24	0	2,2,2	0.29	0
4	EDO	B	513	-	3,3,3	0.26	0	2,2,2	0.19	0
4	EDO	B	526	-	3,3,3	0.22	0	2,2,2	0.38	0
4	EDO	B	535	-	3,3,3	0.27	0	2,2,2	0.13	0
4	EDO	A	520	-	3,3,3	0.27	0	2,2,2	0.35	0
4	EDO	C	516	-	3,3,3	0.24	0	2,2,2	0.26	0
4	EDO	E	604	-	3,3,3	0.26	0	2,2,2	0.51	0
4	EDO	A	521	-	3,3,3	0.27	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	505	-	3,3,3	0.25	0	2,2,2	0.28	0
3	PEG	B	503	-	6,6,6	0.27	0	5,5,5	0.21	0
4	EDO	G	603	-	3,3,3	0.23	0	2,2,2	0.29	0
4	EDO	B	530	-	3,3,3	0.22	0	2,2,2	0.35	0
4	EDO	A	536	-	3,3,3	0.52	0	2,2,2	1.01	0
4	EDO	C	518	-	3,3,3	0.26	0	2,2,2	0.21	0
4	EDO	B	508	-	3,3,3	0.24	0	2,2,2	0.40	0
4	EDO	D	512	-	3,3,3	0.26	0	2,2,2	0.30	0
3	PEG	D	501	-	6,6,6	0.24	0	5,5,5	0.32	0
4	EDO	A	512	-	3,3,3	0.22	0	2,2,2	0.40	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	D	517	-	-	1/1/1/1	-
4	EDO	C	520	-	-	1/1/1/1	-
3	PEG	C	503	-	-	3/4/4/4	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	C	530	-	-	0/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	A	533	-	-	1/1/1/1	-
4	EDO	C	521	-	-	1/1/1/1	-
4	EDO	G	602	-	-	0/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
3	PEG	A	502	-	-	3/4/4/4	-
4	EDO	C	529	-	-	1/1/1/1	-
4	EDO	D	531	-	-	0/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	B	531	-	-	1/1/1/1	-
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	A	513	-	-	1/1/1/1	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	D	535	-	-	0/1/1/1	-
4	EDO	A	518	-	-	0/1/1/1	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	B	537	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	527	-	-	0/1/1/1	-
4	EDO	F	602	-	-	1/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
4	EDO	C	532	-	-	1/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
4	EDO	B	525	-	-	0/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	D	529	-	-	0/1/1/1	-
4	EDO	B	541	-	-	0/1/1/1	-
4	EDO	C	514	-	-	0/1/1/1	-
4	EDO	A	532	-	-	0/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	D	525	-	-	1/1/1/1	-
4	EDO	D	526	-	-	1/1/1/1	-
4	EDO	D	534	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	D	522	-	-	0/1/1/1	-
4	EDO	B	515	-	-	1/1/1/1	-
3	PEG	B	501	-	-	3/4/4/4	-
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	A	516	-	-	1/1/1/1	-
4	EDO	D	530	-	-	0/1/1/1	-
4	EDO	A	527	-	-	0/1/1/1	-
4	EDO	C	515	-	-	1/1/1/1	-
4	EDO	A	526	-	-	1/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	B	534	-	-	0/1/1/1	-
4	EDO	B	517	-	-	0/1/1/1	-
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	C	531	-	-	0/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
4	EDO	C	528	-	-	0/1/1/1	-
4	EDO	B	522	-	-	1/1/1/1	-
4	EDO	A	507	-	-	0/1/1/1	-
4	EDO	B	540	-	-	0/1/1/1	-
4	EDO	D	523	-	-	0/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	C	508	-	-	0/1/1/1	-
4	EDO	C	525	-	-	0/1/1/1	-
4	EDO	C	535	-	-	1/1/1/1	-
5	AG2	F	601	2	-	0/6/6/6	-
4	EDO	B	528	-	-	0/1/1/1	-
4	EDO	A	531	-	-	1/1/1/1	-
4	EDO	C	526	-	-	1/1/1/1	-
3	PEG	B	502	-	-	2/4/4/4	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
4	EDO	C	524	-	-	0/1/1/1	-
4	EDO	B	520	-	-	1/1/1/1	-
4	EDO	E	602	-	-	1/1/1/1	-
4	EDO	A	529	-	-	1/1/1/1	-
4	EDO	H	603	-	-	0/1/1/1	-
4	EDO	C	534	-	-	0/1/1/1	-
4	EDO	A	523	-	-	0/1/1/1	-
4	EDO	D	524	-	-	1/1/1/1	-
4	EDO	D	532	-	-	1/1/1/1	-
4	EDO	B	524	-	-	1/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	C	511	-	-	0/1/1/1	-
4	EDO	D	502	-	-	0/1/1/1	-
4	EDO	H	602	-	-	0/1/1/1	-
5	AG2	E	601	2	-	0/6/6/6	-
4	EDO	D	528	-	-	1/1/1/1	-
4	EDO	C	522	-	-	0/1/1/1	-
4	EDO	E	603	-	-	0/1/1/1	-
4	EDO	C	519	-	-	1/1/1/1	-
4	EDO	B	538	-	-	0/1/1/1	-
4	EDO	D	527	-	-	1/1/1/1	-
4	EDO	A	525	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	B	532	-	-	1/1/1/1	-
4	EDO	D	516	-	-	1/1/1/1	-
3	PEG	A	501	-	-	2/4/4/4	-
4	EDO	C	537	-	-	0/1/1/1	-
4	EDO	A	519	-	-	0/1/1/1	-
4	EDO	C	533	-	-	1/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	534	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
4	EDO	C	523	-	-	1/1/1/1	-
4	EDO	D	520	-	-	0/1/1/1	-
4	EDO	C	517	-	-	0/1/1/1	-
4	EDO	B	521	-	-	0/1/1/1	-
4	EDO	B	529	-	-	1/1/1/1	-
4	EDO	B	523	-	-	1/1/1/1	-
4	EDO	A	522	-	-	0/1/1/1	-
5	AG2	H	601	2	-	0/6/6/6	-
4	EDO	C	536	-	-	1/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	D	533	-	-	1/1/1/1	-
4	EDO	B	539	-	-	1/1/1/1	-
4	EDO	D	514	-	-	1/1/1/1	-
4	EDO	A	535	-	-	1/1/1/1	-
4	EDO	B	514	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
3	PEG	C	502	-	-	3/4/4/4	-
4	EDO	A	528	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	C	512	-	-	0/1/1/1	-
4	EDO	B	527	-	-	1/1/1/1	-
4	EDO	B	536	-	-	1/1/1/1	-
4	EDO	B	533	-	-	1/1/1/1	-
3	PEG	C	501	-	-	4/4/4/4	-
5	AG2	G	601	2	-	0/6/6/6	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	A	524	-	-	1/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	B	526	-	-	1/1/1/1	-
4	EDO	B	535	-	-	1/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	E	604	-	-	0/1/1/1	-
4	EDO	A	521	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	505	-	-	0/1/1/1	-
3	PEG	B	503	-	-	3/4/4/4	-
4	EDO	G	603	-	-	1/1/1/1	-
4	EDO	B	530	-	-	1/1/1/1	-
4	EDO	A	536	-	-	1/1/1/1	-
4	EDO	C	518	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	D	512	-	-	0/1/1/1	-
3	PEG	D	501	-	-	1/4/4/4	-
4	EDO	A	512	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	PEG	O2-C3-C4-O4
3	A	501	PEG	O2-C3-C4-O4
3	A	501	PEG	O1-C1-C2-O2
3	B	501	PEG	O1-C1-C2-O2
3	C	501	PEG	O2-C3-C4-O4
3	C	503	PEG	O1-C1-C2-O2
3	C	502	PEG	O2-C3-C4-O4
4	A	529	EDO	O1-C1-C2-O2
4	A	535	EDO	O1-C1-C2-O2
4	B	520	EDO	O1-C1-C2-O2
4	B	524	EDO	O1-C1-C2-O2
4	C	532	EDO	O1-C1-C2-O2
4	G	603	EDO	O1-C1-C2-O2
4	D	514	EDO	O1-C1-C2-O2
3	B	502	PEG	O1-C1-C2-O2
3	A	502	PEG	O2-C3-C4-O4
4	B	509	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
4	C	510	EDO	O1-C1-C2-O2
4	C	521	EDO	O1-C1-C2-O2
4	C	536	EDO	O1-C1-C2-O2
4	D	526	EDO	O1-C1-C2-O2
4	A	530	EDO	O1-C1-C2-O2
4	E	602	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	529	EDO	O1-C1-C2-O2
3	B	501	PEG	O2-C3-C4-O4
3	A	502	PEG	C1-C2-O2-C3
3	C	502	PEG	O1-C1-C2-O2
3	B	503	PEG	C1-C2-O2-C3
3	B	502	PEG	C4-C3-O2-C2
4	A	511	EDO	O1-C1-C2-O2
4	B	519	EDO	O1-C1-C2-O2
4	B	531	EDO	O1-C1-C2-O2
3	B	503	PEG	C4-C3-O2-C2
3	A	502	PEG	O1-C1-C2-O2
4	A	505	EDO	O1-C1-C2-O2
4	A	536	EDO	O1-C1-C2-O2
4	B	512	EDO	O1-C1-C2-O2
4	C	526	EDO	O1-C1-C2-O2
4	D	528	EDO	O1-C1-C2-O2
3	C	501	PEG	C4-C3-O2-C2
3	B	503	PEG	O1-C1-C2-O2
3	C	501	PEG	O1-C1-C2-O2
3	C	503	PEG	O2-C3-C4-O4
3	B	501	PEG	C1-C2-O2-C3
4	A	513	EDO	O1-C1-C2-O2
4	B	523	EDO	O1-C1-C2-O2
4	B	529	EDO	O1-C1-C2-O2
4	B	532	EDO	O1-C1-C2-O2
4	B	537	EDO	O1-C1-C2-O2
4	C	519	EDO	O1-C1-C2-O2
4	C	520	EDO	O1-C1-C2-O2
4	C	533	EDO	O1-C1-C2-O2
4	D	525	EDO	O1-C1-C2-O2
4	D	532	EDO	O1-C1-C2-O2
4	D	533	EDO	O1-C1-C2-O2
4	B	522	EDO	O1-C1-C2-O2
4	B	539	EDO	O1-C1-C2-O2
4	C	523	EDO	O1-C1-C2-O2
4	C	535	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
4	D	527	EDO	O1-C1-C2-O2
3	C	503	PEG	C4-C3-O2-C2
4	A	517	EDO	O1-C1-C2-O2
4	A	524	EDO	O1-C1-C2-O2
4	A	533	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	526	EDO	O1-C1-C2-O2
4	B	527	EDO	O1-C1-C2-O2
4	F	602	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
4	C	515	EDO	O1-C1-C2-O2
4	D	516	EDO	O1-C1-C2-O2
4	D	517	EDO	O1-C1-C2-O2
4	D	521	EDO	O1-C1-C2-O2
4	D	524	EDO	O1-C1-C2-O2
3	C	501	PEG	C1-C2-O2-C3
4	A	508	EDO	O1-C1-C2-O2
4	A	516	EDO	O1-C1-C2-O2
4	A	531	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	B	535	EDO	O1-C1-C2-O2
4	B	536	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
3	C	502	PEG	C1-C2-O2-C3
4	A	526	EDO	O1-C1-C2-O2
4	B	530	EDO	O1-C1-C2-O2
4	B	533	EDO	O1-C1-C2-O2
4	A	528	EDO	O1-C1-C2-O2

There are no ring outliers.

40 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	517	EDO	1	0
4	D	515	EDO	1	0
4	C	521	EDO	1	0
3	A	502	PEG	1	0
4	D	531	EDO	1	0
4	D	506	EDO	1	0
4	B	531	EDO	2	0
4	A	513	EDO	1	0
4	D	535	EDO	3	0
4	C	506	EDO	1	0
4	B	506	EDO	1	0
4	B	512	EDO	2	0
4	D	525	EDO	1	0
3	B	501	PEG	1	0
4	B	534	EDO	2	0

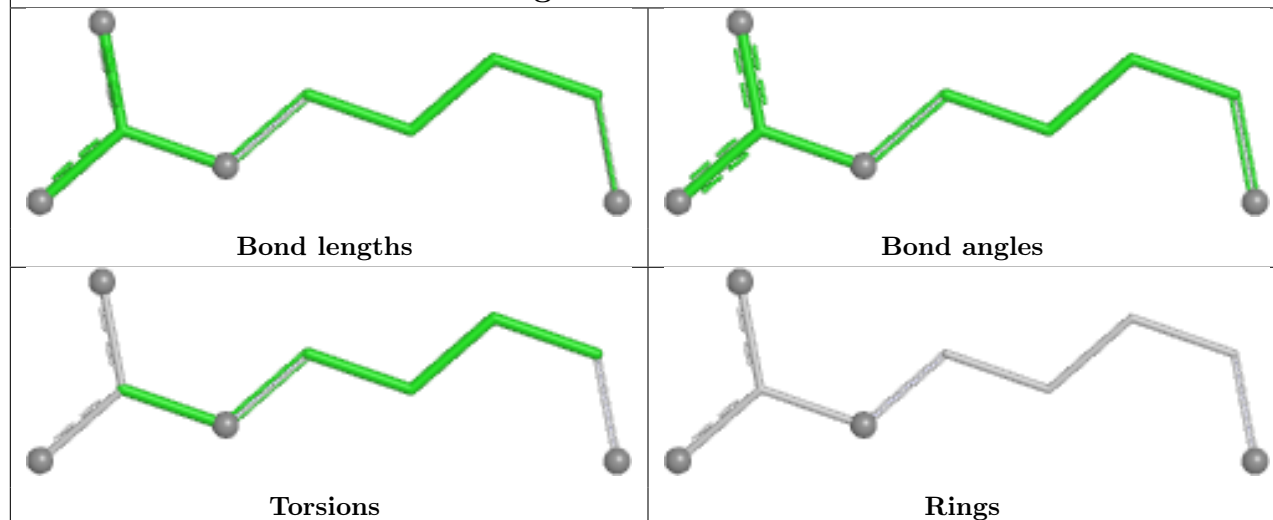
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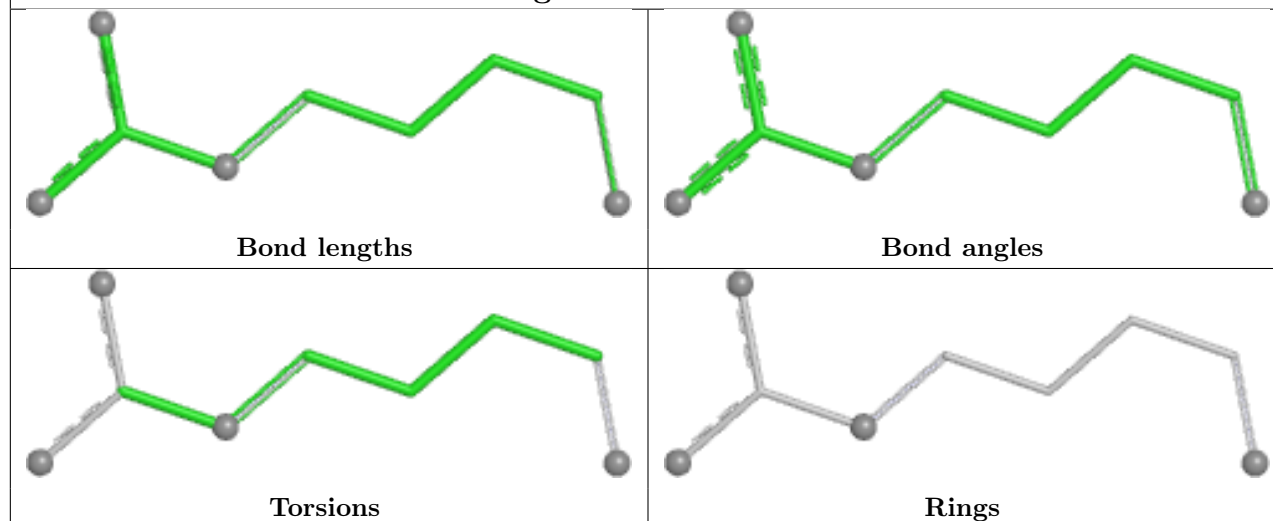
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	531	EDO	1	0
4	B	540	EDO	2	0
4	C	510	EDO	2	0
4	C	535	EDO	1	0
4	H	603	EDO	1	0
4	D	524	EDO	1	0
4	C	519	EDO	1	0
4	A	525	EDO	1	0
3	A	501	PEG	1	0
4	A	519	EDO	2	0
4	A	530	EDO	1	0
4	B	523	EDO	2	0
4	A	522	EDO	1	0
4	B	539	EDO	3	0
3	C	502	PEG	1	0
4	A	528	EDO	1	0
3	C	501	PEG	1	0
5	G	601	AG2	1	0
4	B	509	EDO	2	0
4	B	526	EDO	1	0
4	G	603	EDO	1	0
4	B	530	EDO	1	0
4	A	536	EDO	3	0
3	D	501	PEG	4	0
4	A	512	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 than 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.

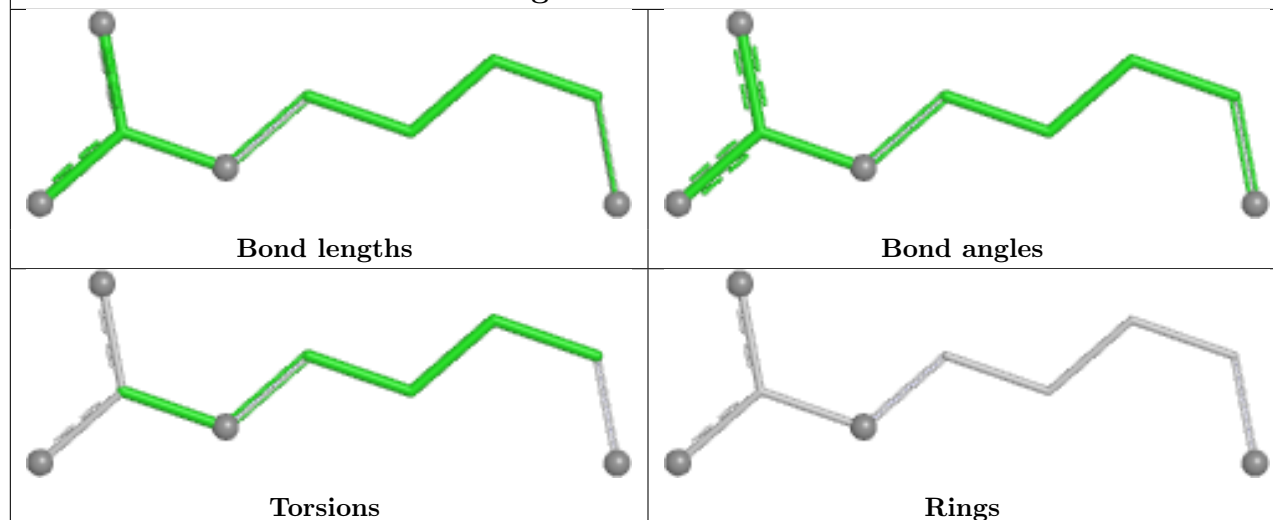
Ligand AG2 F 601

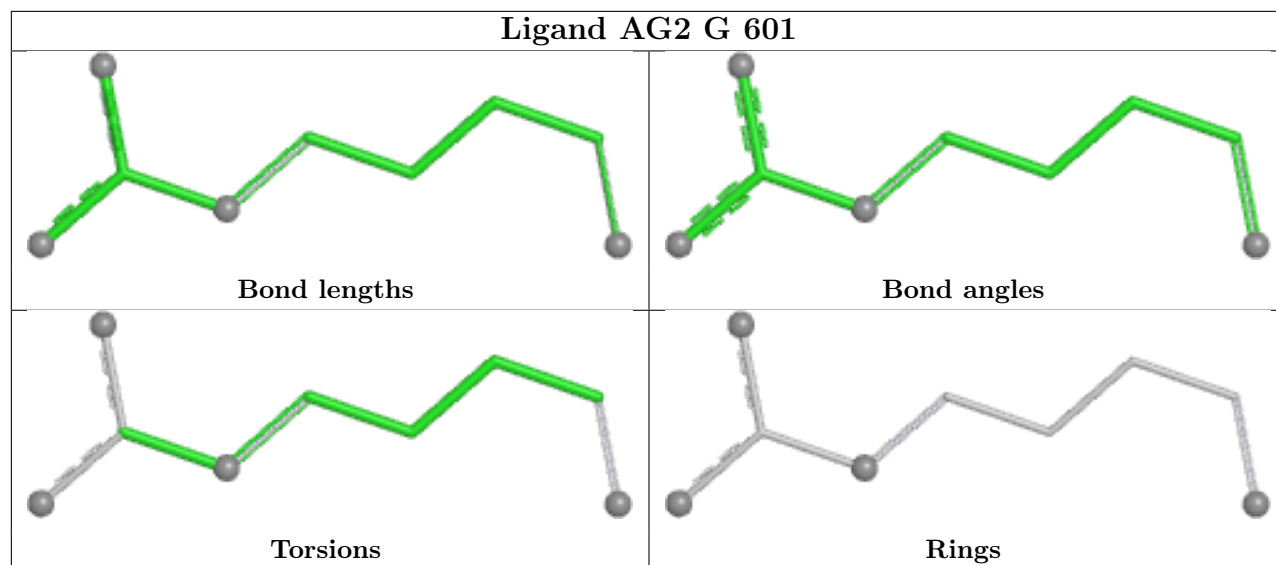


Ligand AG2 E 601



Ligand AG2 H 601





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.48	1 (0%) 90 91	14, 27, 38, 74	17 (4%)
1	B	381/462 (82%)	-0.44	1 (0%) 90 91	14, 26, 38, 71	10 (2%)
1	C	382/462 (82%)	-0.36	1 (0%) 90 91	14, 28, 41, 84	16 (4%)
1	D	382/462 (82%)	-0.43	0 100 100	14, 28, 40, 84	9 (2%)
2	E	40/42 (95%)	-0.44	0 100 100	15, 27, 48, 49	2 (5%)
2	F	41/42 (97%)	-0.29	0 100 100	15, 28, 45, 68	1 (2%)
2	G	40/42 (95%)	-0.32	0 100 100	23, 29, 50, 51	0
2	H	41/42 (97%)	-0.29	0 100 100	15, 29, 44, 69	1 (2%)
All	All	1688/2016 (83%)	-0.42	3 (0%) 91 92	14, 27, 41, 84	56 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	VAL	5.7
1	A	61	VAL	4.6
1	C	61	VAL	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	511	4/4	0.65	0.18	58,60,62,63	0
4	EDO	D	535	4/4	0.70	0.27	35,41,44,49	0
4	EDO	A	531	4/4	0.71	0.18	51,54,56,60	0
4	EDO	D	531	4/4	0.71	0.21	43,51,55,56	0
3	PEG	B	503	7/7	0.71	0.18	46,48,54,57	0
4	EDO	C	535	4/4	0.72	0.22	49,51,52,53	0
4	EDO	A	536	4/4	0.72	0.17	40,44,45,47	0
4	EDO	B	539	4/4	0.72	0.20	35,39,40,41	0
4	EDO	D	512	4/4	0.73	0.16	49,57,57,62	0
4	EDO	A	529	4/4	0.74	0.19	44,45,56,60	0
4	EDO	C	510	4/4	0.74	0.24	36,44,49,49	0
3	PEG	A	502	7/7	0.75	0.21	40,44,53,56	0
4	EDO	B	517	4/4	0.75	0.18	49,54,58,58	0
3	PEG	B	501	7/7	0.76	0.23	35,47,55,61	0
4	EDO	D	518	4/4	0.76	0.16	54,59,61,66	0
4	EDO	B	523	4/4	0.77	0.24	45,52,54,54	0
3	PEG	A	501	7/7	0.77	0.19	29,42,52,53	0
4	EDO	C	523	4/4	0.78	0.18	45,52,55,61	0
4	EDO	E	603	4/4	0.78	0.15	56,58,61,67	0
4	EDO	B	525	4/4	0.79	0.15	52,58,59,65	0
4	EDO	B	531	4/4	0.79	0.19	40,52,53,53	0
4	EDO	A	512	4/4	0.80	0.17	41,48,50,53	0
4	EDO	C	526	4/4	0.80	0.17	43,57,60,61	0
4	EDO	B	524	4/4	0.80	0.21	43,53,57,71	0
3	PEG	C	503	7/7	0.80	0.18	40,43,54,58	0
4	EDO	D	514	4/4	0.80	0.16	43,52,64,66	0
4	EDO	C	516	4/4	0.80	0.16	45,48,54,65	0
4	EDO	C	518	4/4	0.80	0.16	54,58,60,66	0
4	EDO	C	520	4/4	0.80	0.17	36,44,52,58	0
4	EDO	A	534	4/4	0.81	0.17	40,48,53,60	0
4	EDO	C	525	4/4	0.81	0.17	54,56,59,63	0
4	EDO	B	513	4/4	0.81	0.22	38,55,56,57	0
4	EDO	D	527	4/4	0.81	0.15	54,55,55,60	0
4	EDO	C	531	4/4	0.81	0.20	42,52,53,54	0
4	EDO	A	518	4/4	0.81	0.19	58,60,61,67	0
4	EDO	B	522	4/4	0.82	0.14	54,64,66,70	0
4	EDO	C	515	4/4	0.82	0.16	45,49,55,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	515	4/4	0.82	0.13	51,52,59,62	0
4	EDO	A	533	4/4	0.82	0.21	41,42,45,51	0
4	EDO	C	527	4/4	0.82	0.15	52,55,56,58	0
4	EDO	B	538	4/4	0.82	0.25	37,48,49,53	0
4	EDO	B	510	4/4	0.82	0.12	49,50,54,65	0
4	EDO	H	603	4/4	0.82	0.15	40,41,48,64	0
4	EDO	B	509	4/4	0.83	0.16	42,45,52,59	0
4	EDO	C	505	4/4	0.83	0.25	46,46,49,60	0
4	EDO	B	526	4/4	0.83	0.17	42,48,51,56	0
4	EDO	A	505	4/4	0.84	0.20	45,47,51,52	0
4	EDO	D	513	4/4	0.84	0.23	46,50,51,55	0
4	EDO	B	521	4/4	0.84	0.13	45,47,55,65	0
4	EDO	B	529	4/4	0.84	0.16	46,52,52,60	0
3	PEG	D	501	7/7	0.84	0.15	42,45,56,57	0
4	EDO	D	520	4/4	0.84	0.15	51,54,58,61	0
4	EDO	D	523	4/4	0.84	0.15	48,50,52,56	0
4	EDO	D	524	4/4	0.84	0.15	36,42,45,51	0
4	EDO	A	535	4/4	0.84	0.18	40,44,47,54	0
4	EDO	C	533	4/4	0.84	0.23	32,45,46,50	0
4	EDO	A	532	4/4	0.84	0.14	51,53,57,65	0
4	EDO	C	537	4/4	0.84	0.20	38,42,43,44	0
4	EDO	D	525	4/4	0.85	0.14	45,47,47,53	0
4	EDO	B	512	4/4	0.85	0.22	49,50,50,54	0
4	EDO	D	530	4/4	0.85	0.20	45,48,51,61	0
4	EDO	A	524	4/4	0.85	0.15	43,48,53,64	0
4	EDO	D	532	4/4	0.85	0.19	29,40,50,54	0
4	EDO	C	519	4/4	0.85	0.18	42,43,52,56	0
4	EDO	D	511	4/4	0.85	0.19	38,42,45,52	0
4	EDO	C	512	4/4	0.86	0.18	37,49,53,53	0
4	EDO	C	528	4/4	0.86	0.15	42,47,52,55	0
4	EDO	D	519	4/4	0.86	0.13	47,60,62,62	0
4	EDO	C	530	4/4	0.86	0.13	53,53,62,63	0
4	EDO	D	522	4/4	0.86	0.15	42,46,53,59	0
4	EDO	A	520	4/4	0.86	0.14	38,44,48,51	0
4	EDO	B	530	4/4	0.86	0.16	44,48,49,52	0
4	EDO	C	534	4/4	0.86	0.15	36,54,58,59	0
4	EDO	D	526	4/4	0.86	0.13	35,43,56,61	0
4	EDO	B	511	4/4	0.86	0.12	51,51,55,58	0
4	EDO	B	537	4/4	0.86	0.22	35,43,47,47	0
4	EDO	E	602	4/4	0.86	0.13	45,47,55,65	0
4	EDO	A	522	4/4	0.86	0.17	34,43,46,47	0
4	EDO	B	514	4/4	0.86	0.17	46,49,51,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	513	4/4	0.86	0.17	35,42,46,64	0
4	EDO	B	516	4/4	0.87	0.18	31,43,48,52	0
4	EDO	C	529	4/4	0.87	0.12	48,51,54,66	0
4	EDO	G	603	4/4	0.87	0.18	33,51,53,58	0
4	EDO	A	517	4/4	0.87	0.14	44,46,54,60	0
4	EDO	D	521	4/4	0.87	0.15	37,42,45,55	0
4	EDO	B	520	4/4	0.87	0.13	54,55,60,61	0
4	EDO	D	534	4/4	0.87	0.14	41,46,49,51	0
4	EDO	A	519	4/4	0.87	0.16	41,42,43,46	0
4	EDO	B	534	4/4	0.87	0.21	42,43,48,55	0
3	PEG	B	502	7/7	0.88	0.14	40,47,56,58	0
4	EDO	B	518	4/4	0.88	0.16	35,45,57,58	0
4	EDO	B	519	4/4	0.88	0.13	39,49,49,58	0
4	EDO	D	516	4/4	0.88	0.22	39,43,45,47	0
4	EDO	A	514	4/4	0.88	0.13	40,42,48,60	0
4	EDO	B	535	4/4	0.88	0.14	41,45,49,54	0
4	EDO	D	506	4/4	0.88	0.17	42,43,46,49	0
4	EDO	D	510	4/4	0.88	0.14	30,48,52,54	0
4	EDO	A	506	4/4	0.88	0.14	30,34,43,52	0
4	EDO	C	532	4/4	0.88	0.14	44,47,54,60	0
4	EDO	F	602	4/4	0.89	0.12	33,35,40,41	0
4	EDO	A	507	4/4	0.89	0.18	39,40,42,46	0
4	EDO	D	504	4/4	0.89	0.15	42,45,46,56	0
4	EDO	C	509	4/4	0.89	0.12	38,40,42,47	0
4	EDO	C	522	4/4	0.89	0.17	40,41,45,45	0
4	EDO	B	536	4/4	0.89	0.16	41,41,50,55	0
4	EDO	A	525	4/4	0.89	0.11	55,56,62,66	0
4	EDO	B	506	4/4	0.89	0.16	39,45,51,52	0
3	PEG	C	501	7/7	0.89	0.14	32,41,46,47	0
4	EDO	D	528	4/4	0.90	0.16	39,39,46,49	0
3	PEG	C	502	7/7	0.90	0.13	27,32,47,54	0
4	EDO	D	517	4/4	0.90	0.13	40,41,44,61	0
4	EDO	A	526	4/4	0.90	0.12	36,39,44,46	0
4	EDO	B	528	4/4	0.90	0.13	36,38,42,51	0
4	EDO	A	521	4/4	0.90	0.12	49,52,52,53	0
4	EDO	A	530	4/4	0.90	0.20	42,43,49,50	0
4	EDO	B	541	4/4	0.91	0.14	34,40,40,41	0
4	EDO	A	527	4/4	0.91	0.17	37,39,44,47	0
4	EDO	A	515	4/4	0.91	0.12	34,46,46,56	0
4	EDO	B	515	4/4	0.91	0.12	37,40,40,43	0
4	EDO	D	507	4/4	0.91	0.11	44,48,50,51	0
4	EDO	C	536	4/4	0.91	0.16	40,44,47,55	0

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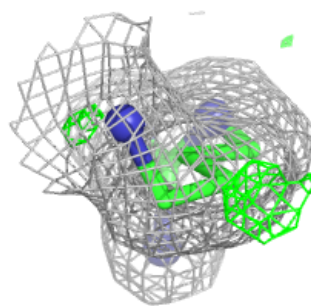
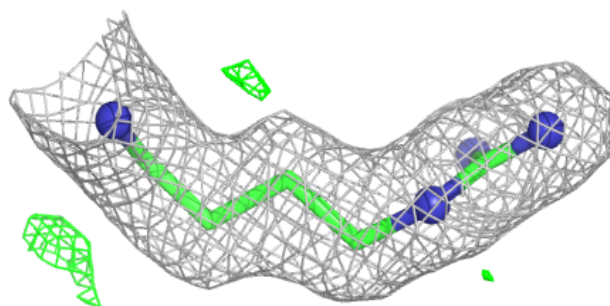
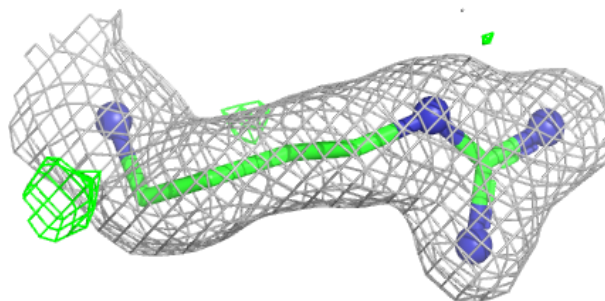
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	514	4/4	0.92	0.12	37,37,40,46	0
4	EDO	D	529	4/4	0.92	0.13	41,43,43,44	0
4	EDO	B	533	4/4	0.92	0.17	38,41,43,47	0
4	EDO	D	509	4/4	0.92	0.12	31,32,39,46	0
4	EDO	B	540	4/4	0.92	0.11	39,40,42,53	0
4	EDO	C	517	4/4	0.92	0.11	48,49,51,52	0
4	EDO	A	528	4/4	0.92	0.13	41,46,49,50	0
4	EDO	B	532	4/4	0.92	0.19	29,38,45,48	0
4	EDO	D	505	4/4	0.93	0.09	37,39,44,60	0
4	EDO	C	524	4/4	0.93	0.11	40,43,45,57	0
4	EDO	D	533	4/4	0.93	0.11	44,44,46,48	0
4	EDO	A	510	4/4	0.93	0.11	39,41,46,49	0
4	EDO	A	508	4/4	0.93	0.11	30,39,39,43	0
4	EDO	C	506	4/4	0.93	0.10	38,41,41,52	0
4	EDO	C	513	4/4	0.94	0.15	38,40,46,48	0
4	EDO	C	521	4/4	0.94	0.11	34,44,51,57	0
4	EDO	E	604	4/4	0.94	0.09	28,29,39,41	0
4	EDO	C	507	4/4	0.94	0.10	35,42,44,44	0
4	EDO	C	508	4/4	0.94	0.10	38,39,45,47	0
4	EDO	A	509	4/4	0.94	0.11	36,36,40,50	0
4	EDO	A	516	4/4	0.94	0.11	36,41,43,50	0
4	EDO	D	508	4/4	0.94	0.10	37,38,40,42	0
4	EDO	H	602	4/4	0.94	0.09	30,31,40,41	0
4	EDO	A	523	4/4	0.94	0.09	34,39,44,47	0
4	EDO	B	527	4/4	0.95	0.11	34,38,45,51	0
5	AG2	E	601	9/9	0.95	0.07	21,25,27,29	0
4	EDO	C	511	4/4	0.96	0.09	31,32,35,42	0
4	EDO	B	507	4/4	0.96	0.08	29,32,34,37	0
4	EDO	B	508	4/4	0.96	0.08	30,33,33,42	0
4	EDO	G	602	4/4	0.96	0.10	31,33,40,41	0
4	EDO	A	503	4/4	0.96	0.06	25,27,27,28	0
5	AG2	F	601	9/9	0.96	0.06	23,25,26,28	0
5	AG2	H	601	9/9	0.96	0.07	26,29,32,32	0
5	AG2	G	601	9/9	0.97	0.06	25,28,29,32	0
4	EDO	D	502	4/4	0.98	0.05	27,27,29,29	0
4	EDO	D	503	4/4	0.98	0.07	28,29,32,34	0
4	EDO	A	504	4/4	0.98	0.05	25,27,32,35	0
4	EDO	B	504	4/4	0.98	0.06	25,26,27,30	0
4	EDO	B	505	4/4	0.98	0.04	27,27,29,30	0
4	EDO	C	504	4/4	0.99	0.04	25,27,27,28	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.

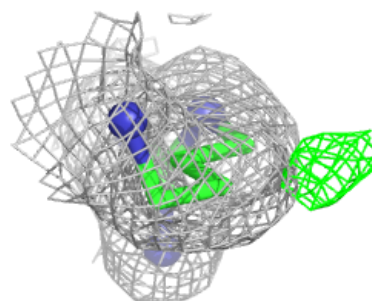
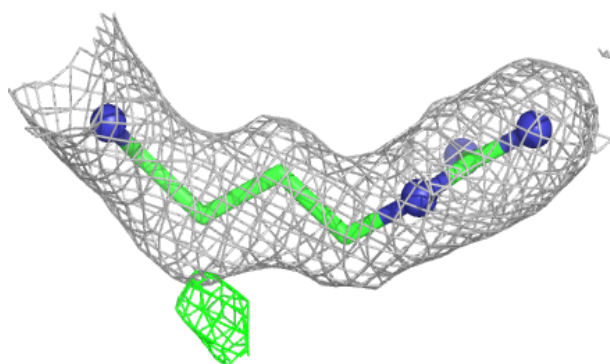
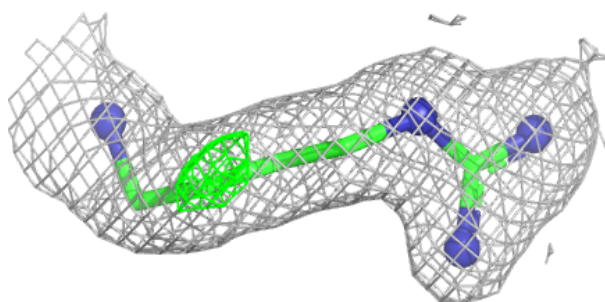
Electron density around AG2 E 601:

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



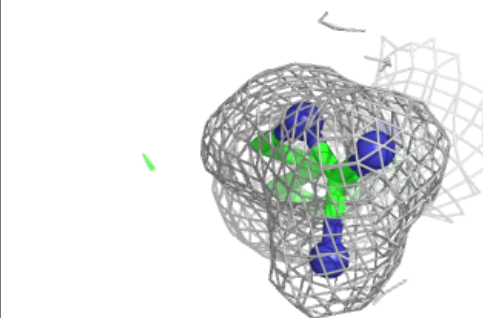
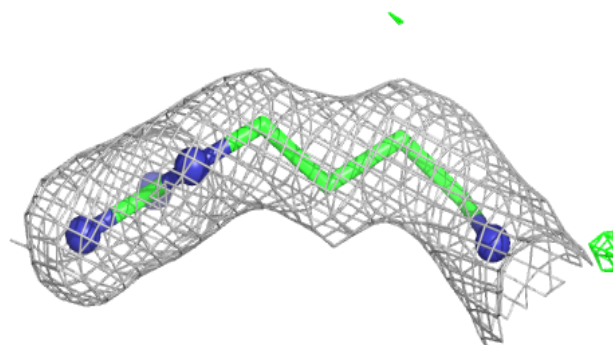
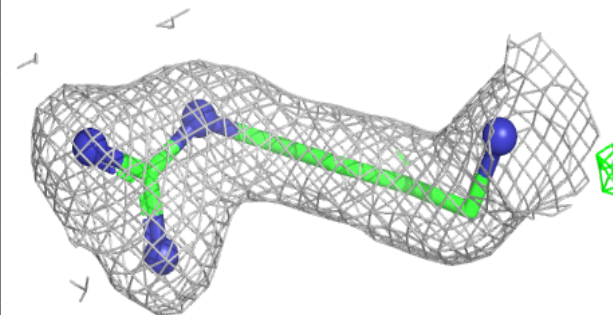
Electron density around AG2 F 601:

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

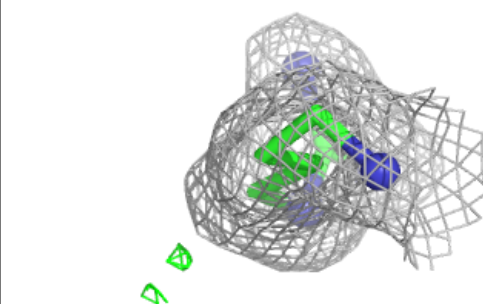
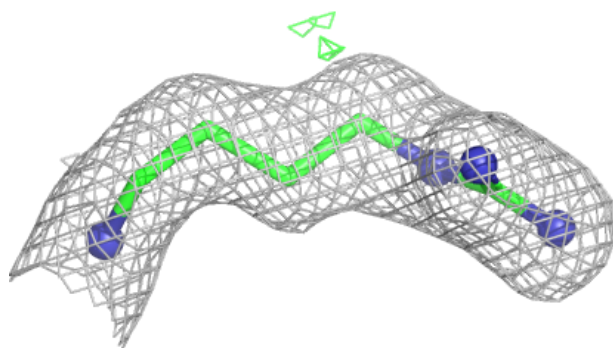
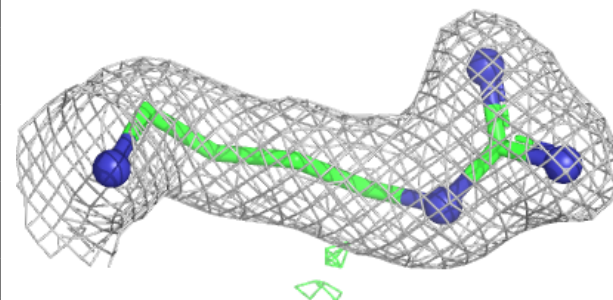


Electron density around AG2 H 601:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.