



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:24 AM UTC

PDB ID : 8A4D / pdb_00008a4d
Title : 1-deoxy-D-xylulose 5-phosphate synthase from *Pseudomonas aeruginosa* with a thiamine analog inhibitor
Authors : Hamid, R.; Hirsch, A.
Deposited on : 2022-06-10
Resolution : 2.20 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 ⓘ 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

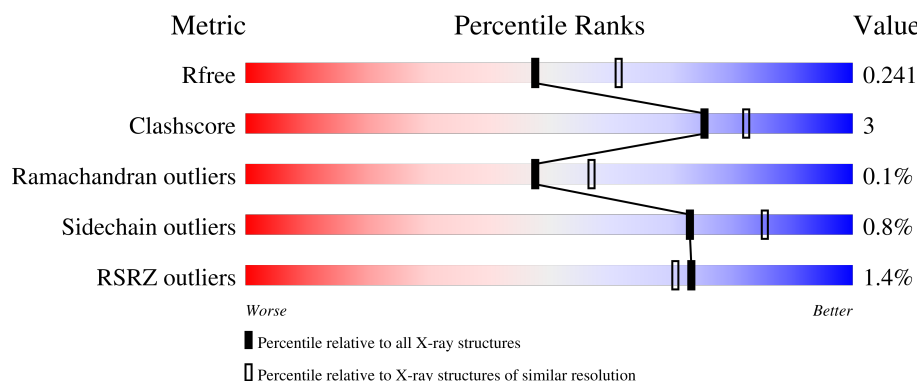
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	622	
1	B	622	
1	C	622	
1	D	622	
1	E	622	

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Mol	Chain	Length	Quality of chain
1	F	622	<div><div><div>%</div><div><div></div></div><div>82%</div><div>8%</div><div>10%</div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53294 atoms, of which 25374 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 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	564	Total	C	H	N	O	S	0	0	0
			8533	2717	4235	746	814	21			
1	B	558	Total	C	H	N	O	S	0	3	0
			8476	2695	4209	743	808	21			
1	C	563	Total	C	H	N	O	S	0	0	0
			8511	2710	4222	745	813	21			
1	D	560	Total	C	H	N	O	S	0	0	0
			8468	2696	4203	742	806	21			
1	E	563	Total	C	H	N	O	S	0	0	0
			8459	2708	4177	742	811	21			
1	F	562	Total	C	H	N	O	S	0	0	0
			8502	2707	4218	744	812	21			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B7V7R4
A	2	GLY	-	expression tag	UNP B7V7R4
A	3	SER	-	expression tag	UNP B7V7R4
A	4	SER	-	expression tag	UNP B7V7R4
A	5	HIS	-	expression tag	UNP B7V7R4
A	6	HIS	-	expression tag	UNP B7V7R4
A	7	HIS	-	expression tag	UNP B7V7R4
A	8	HIS	-	expression tag	UNP B7V7R4
A	9	HIS	-	expression tag	UNP B7V7R4
A	10	HIS	-	expression tag	UNP B7V7R4
A	11	SER	-	expression tag	UNP B7V7R4
A	12	SER	-	expression tag	UNP B7V7R4
A	13	GLY	-	expression tag	UNP B7V7R4
A	14	LEU	-	expression tag	UNP B7V7R4
A	15	VAL	-	expression tag	UNP B7V7R4
A	16	PRO	-	expression tag	UNP B7V7R4
A	17	ARG	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP B7V7R4
A	19	SER	-	expression tag	UNP B7V7R4
A	20	MET	-	expression tag	UNP B7V7R4
A	21	GLU	-	expression tag	UNP B7V7R4
A	22	ASN	-	expression tag	UNP B7V7R4
A	23	LEU	-	expression tag	UNP B7V7R4
A	24	TYR	-	expression tag	UNP B7V7R4
A	25	PHE	-	expression tag	UNP B7V7R4
A	26	GLN	-	expression tag	UNP B7V7R4
A	27	SER	-	expression tag	UNP B7V7R4
A	28	HIS	-	expression tag	UNP B7V7R4
A	235	GLY	-	linker	UNP B7V7R4
A	236	GLY	-	linker	UNP B7V7R4
A	237	GLY	-	linker	UNP B7V7R4
A	238	GLY	-	linker	UNP B7V7R4
A	239	GLY	-	linker	UNP B7V7R4
A	240	GLY	-	linker	UNP B7V7R4
B	1	MET	-	initiating methionine	UNP B7V7R4
B	2	GLY	-	expression tag	UNP B7V7R4
B	3	SER	-	expression tag	UNP B7V7R4
B	4	SER	-	expression tag	UNP B7V7R4
B	5	HIS	-	expression tag	UNP B7V7R4
B	6	HIS	-	expression tag	UNP B7V7R4
B	7	HIS	-	expression tag	UNP B7V7R4
B	8	HIS	-	expression tag	UNP B7V7R4
B	9	HIS	-	expression tag	UNP B7V7R4
B	10	HIS	-	expression tag	UNP B7V7R4
B	11	SER	-	expression tag	UNP B7V7R4
B	12	SER	-	expression tag	UNP B7V7R4
B	13	GLY	-	expression tag	UNP B7V7R4
B	14	LEU	-	expression tag	UNP B7V7R4
B	15	VAL	-	expression tag	UNP B7V7R4
B	16	PRO	-	expression tag	UNP B7V7R4
B	17	ARG	-	expression tag	UNP B7V7R4
B	18	GLY	-	expression tag	UNP B7V7R4
B	19	SER	-	expression tag	UNP B7V7R4
B	20	MET	-	expression tag	UNP B7V7R4
B	21	GLU	-	expression tag	UNP B7V7R4
B	22	ASN	-	expression tag	UNP B7V7R4
B	23	LEU	-	expression tag	UNP B7V7R4
B	24	TYR	-	expression tag	UNP B7V7R4
B	25	PHE	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLN	-	expression tag	UNP B7V7R4
B	27	SER	-	expression tag	UNP B7V7R4
B	28	HIS	-	expression tag	UNP B7V7R4
B	235	GLY	-	linker	UNP B7V7R4
B	236	GLY	-	linker	UNP B7V7R4
B	237	GLY	-	linker	UNP B7V7R4
B	238	GLY	-	linker	UNP B7V7R4
B	239	GLY	-	linker	UNP B7V7R4
B	240	GLY	-	linker	UNP B7V7R4
C	1	MET	-	initiating methionine	UNP B7V7R4
C	2	GLY	-	expression tag	UNP B7V7R4
C	3	SER	-	expression tag	UNP B7V7R4
C	4	SER	-	expression tag	UNP B7V7R4
C	5	HIS	-	expression tag	UNP B7V7R4
C	6	HIS	-	expression tag	UNP B7V7R4
C	7	HIS	-	expression tag	UNP B7V7R4
C	8	HIS	-	expression tag	UNP B7V7R4
C	9	HIS	-	expression tag	UNP B7V7R4
C	10	HIS	-	expression tag	UNP B7V7R4
C	11	SER	-	expression tag	UNP B7V7R4
C	12	SER	-	expression tag	UNP B7V7R4
C	13	GLY	-	expression tag	UNP B7V7R4
C	14	LEU	-	expression tag	UNP B7V7R4
C	15	VAL	-	expression tag	UNP B7V7R4
C	16	PRO	-	expression tag	UNP B7V7R4
C	17	ARG	-	expression tag	UNP B7V7R4
C	18	GLY	-	expression tag	UNP B7V7R4
C	19	SER	-	expression tag	UNP B7V7R4
C	20	MET	-	expression tag	UNP B7V7R4
C	21	GLU	-	expression tag	UNP B7V7R4
C	22	ASN	-	expression tag	UNP B7V7R4
C	23	LEU	-	expression tag	UNP B7V7R4
C	24	TYR	-	expression tag	UNP B7V7R4
C	25	PHE	-	expression tag	UNP B7V7R4
C	26	GLN	-	expression tag	UNP B7V7R4
C	27	SER	-	expression tag	UNP B7V7R4
C	28	HIS	-	expression tag	UNP B7V7R4
C	235	GLY	-	linker	UNP B7V7R4
C	236	GLY	-	linker	UNP B7V7R4
C	237	GLY	-	linker	UNP B7V7R4
C	238	GLY	-	linker	UNP B7V7R4
C	239	GLY	-	linker	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	240	GLY	-	linker	UNP B7V7R4
D	1	MET	-	initiating methionine	UNP B7V7R4
D	2	GLY	-	expression tag	UNP B7V7R4
D	3	SER	-	expression tag	UNP B7V7R4
D	4	SER	-	expression tag	UNP B7V7R4
D	5	HIS	-	expression tag	UNP B7V7R4
D	6	HIS	-	expression tag	UNP B7V7R4
D	7	HIS	-	expression tag	UNP B7V7R4
D	8	HIS	-	expression tag	UNP B7V7R4
D	9	HIS	-	expression tag	UNP B7V7R4
D	10	HIS	-	expression tag	UNP B7V7R4
D	11	SER	-	expression tag	UNP B7V7R4
D	12	SER	-	expression tag	UNP B7V7R4
D	13	GLY	-	expression tag	UNP B7V7R4
D	14	LEU	-	expression tag	UNP B7V7R4
D	15	VAL	-	expression tag	UNP B7V7R4
D	16	PRO	-	expression tag	UNP B7V7R4
D	17	ARG	-	expression tag	UNP B7V7R4
D	18	GLY	-	expression tag	UNP B7V7R4
D	19	SER	-	expression tag	UNP B7V7R4
D	20	MET	-	expression tag	UNP B7V7R4
D	21	GLU	-	expression tag	UNP B7V7R4
D	22	ASN	-	expression tag	UNP B7V7R4
D	23	LEU	-	expression tag	UNP B7V7R4
D	24	TYR	-	expression tag	UNP B7V7R4
D	25	PHE	-	expression tag	UNP B7V7R4
D	26	GLN	-	expression tag	UNP B7V7R4
D	27	SER	-	expression tag	UNP B7V7R4
D	28	HIS	-	expression tag	UNP B7V7R4
D	235	GLY	-	linker	UNP B7V7R4
D	236	GLY	-	linker	UNP B7V7R4
D	237	GLY	-	linker	UNP B7V7R4
D	238	GLY	-	linker	UNP B7V7R4
D	239	GLY	-	linker	UNP B7V7R4
D	240	GLY	-	linker	UNP B7V7R4
E	1	MET	-	initiating methionine	UNP B7V7R4
E	2	GLY	-	expression tag	UNP B7V7R4
E	3	SER	-	expression tag	UNP B7V7R4
E	4	SER	-	expression tag	UNP B7V7R4
E	5	HIS	-	expression tag	UNP B7V7R4
E	6	HIS	-	expression tag	UNP B7V7R4
E	7	HIS	-	expression tag	UNP B7V7R4

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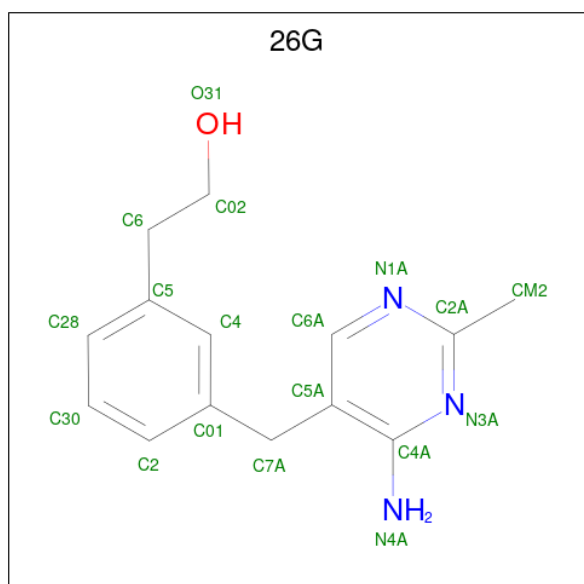
Chain	Residue	Modelled	Actual	Comment	Reference
E	8	HIS	-	expression tag	UNP B7V7R4
E	9	HIS	-	expression tag	UNP B7V7R4
E	10	HIS	-	expression tag	UNP B7V7R4
E	11	SER	-	expression tag	UNP B7V7R4
E	12	SER	-	expression tag	UNP B7V7R4
E	13	GLY	-	expression tag	UNP B7V7R4
E	14	LEU	-	expression tag	UNP B7V7R4
E	15	VAL	-	expression tag	UNP B7V7R4
E	16	PRO	-	expression tag	UNP B7V7R4
E	17	ARG	-	expression tag	UNP B7V7R4
E	18	GLY	-	expression tag	UNP B7V7R4
E	19	SER	-	expression tag	UNP B7V7R4
E	20	MET	-	expression tag	UNP B7V7R4
E	21	GLU	-	expression tag	UNP B7V7R4
E	22	ASN	-	expression tag	UNP B7V7R4
E	23	LEU	-	expression tag	UNP B7V7R4
E	24	TYR	-	expression tag	UNP B7V7R4
E	25	PHE	-	expression tag	UNP B7V7R4
E	26	GLN	-	expression tag	UNP B7V7R4
E	27	SER	-	expression tag	UNP B7V7R4
E	28	HIS	-	expression tag	UNP B7V7R4
E	235	GLY	-	linker	UNP B7V7R4
E	236	GLY	-	linker	UNP B7V7R4
E	237	GLY	-	linker	UNP B7V7R4
E	238	GLY	-	linker	UNP B7V7R4
E	239	GLY	-	linker	UNP B7V7R4
E	240	GLY	-	linker	UNP B7V7R4
F	1	MET	-	initiating methionine	UNP B7V7R4
F	2	GLY	-	expression tag	UNP B7V7R4
F	3	SER	-	expression tag	UNP B7V7R4
F	4	SER	-	expression tag	UNP B7V7R4
F	5	HIS	-	expression tag	UNP B7V7R4
F	6	HIS	-	expression tag	UNP B7V7R4
F	7	HIS	-	expression tag	UNP B7V7R4
F	8	HIS	-	expression tag	UNP B7V7R4
F	9	HIS	-	expression tag	UNP B7V7R4
F	10	HIS	-	expression tag	UNP B7V7R4
F	11	SER	-	expression tag	UNP B7V7R4
F	12	SER	-	expression tag	UNP B7V7R4
F	13	GLY	-	expression tag	UNP B7V7R4
F	14	LEU	-	expression tag	UNP B7V7R4
F	15	VAL	-	expression tag	UNP B7V7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	PRO	-	expression tag	UNP B7V7R4
F	17	ARG	-	expression tag	UNP B7V7R4
F	18	GLY	-	expression tag	UNP B7V7R4
F	19	SER	-	expression tag	UNP B7V7R4
F	20	MET	-	expression tag	UNP B7V7R4
F	21	GLU	-	expression tag	UNP B7V7R4
F	22	ASN	-	expression tag	UNP B7V7R4
F	23	LEU	-	expression tag	UNP B7V7R4
F	24	TYR	-	expression tag	UNP B7V7R4
F	25	PHE	-	expression tag	UNP B7V7R4
F	26	GLN	-	expression tag	UNP B7V7R4
F	27	SER	-	expression tag	UNP B7V7R4
F	28	HIS	-	expression tag	UNP B7V7R4
F	235	GLY	-	linker	UNP B7V7R4
F	236	GLY	-	linker	UNP B7V7R4
F	237	GLY	-	linker	UNP B7V7R4
F	238	GLY	-	linker	UNP B7V7R4
F	239	GLY	-	linker	UNP B7V7R4
F	240	GLY	-	linker	UNP B7V7R4

- Molecule 2 is 2-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]phenyl}ethanol (CCD ID: 26G) (formula: C₁₄H₁₇N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0
			35	14	17	3	1	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			35	14	17	3	1		
2	C	1	Total	C	H	N	O	0	0
			35	14	17	3	1		
2	D	1	Total	C	H	N	O	0	0
			35	14	17	3	1		
2	E	1	Total	C	H	N	O	0	0
			35	14	17	3	1		
2	F	1	Total	C	H	N	O	0	0
			35	14	17	3	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		
3	E	2	Total	Mg	0	0
			2	2		
3	F	3	Total	Mg	0	0
			3	3		

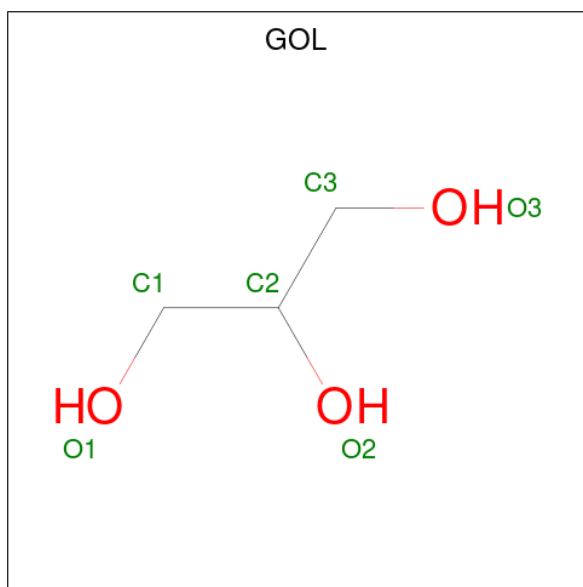
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	C	2	Total	Na	0	0
			2	2		
4	D	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C H O 14 3 8 3	0	0

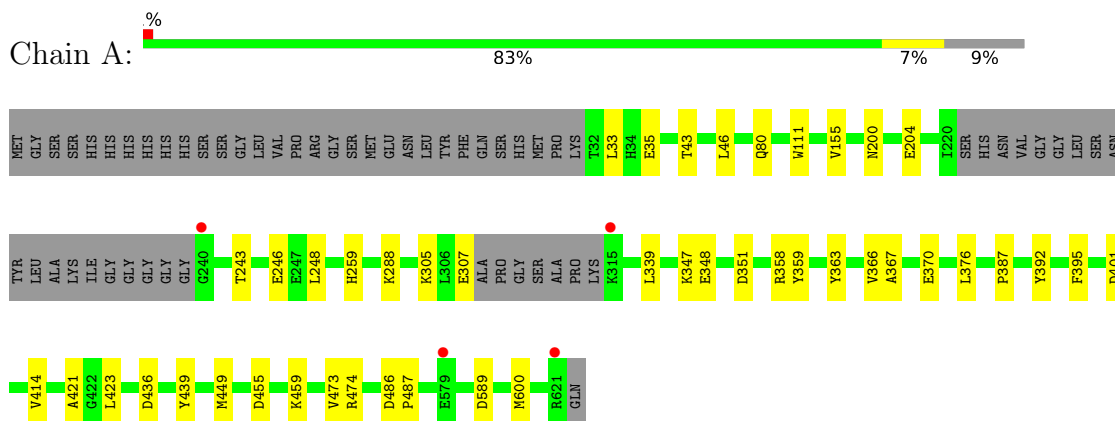
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	392	Total O 392 392	0	0
7	B	329	Total O 329 329	0	0
7	C	328	Total O 328 328	0	0
7	D	333	Total O 333 333	0	0
7	E	350	Total O 350 350	0	0
7	F	371	Total O 371 371	0	0

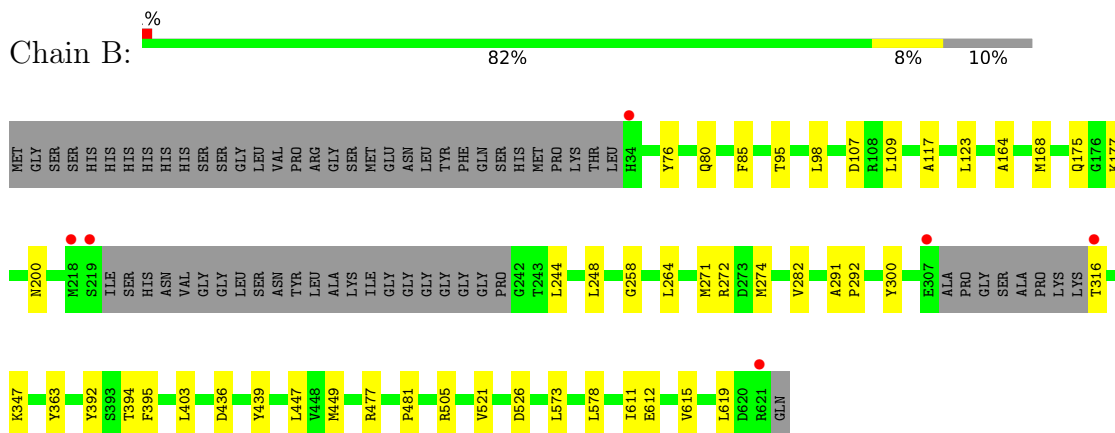
3 Residue-property plots [i](#)

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.

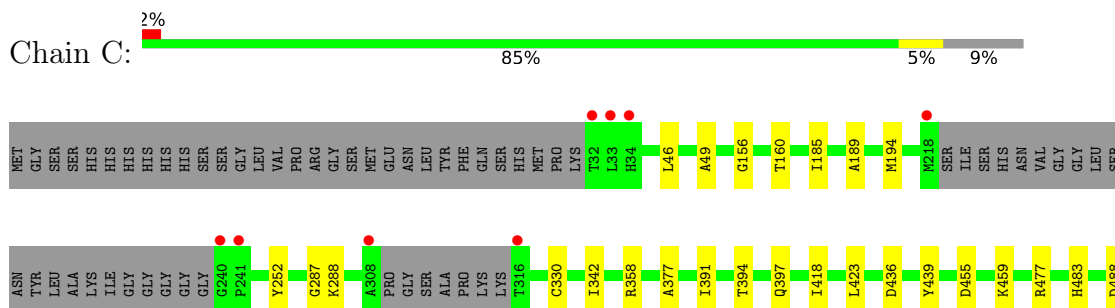
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

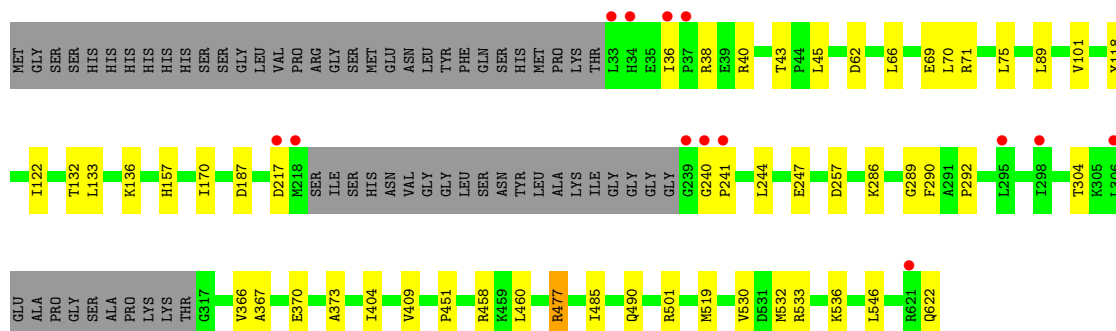
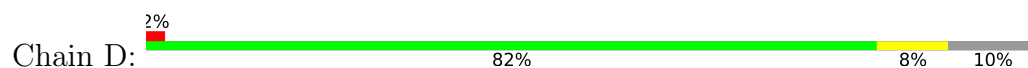


- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

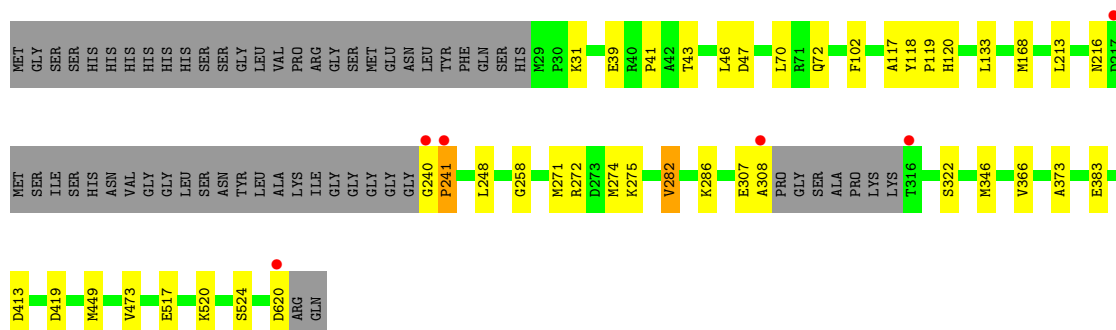
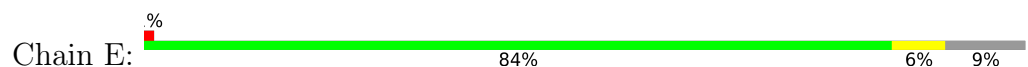




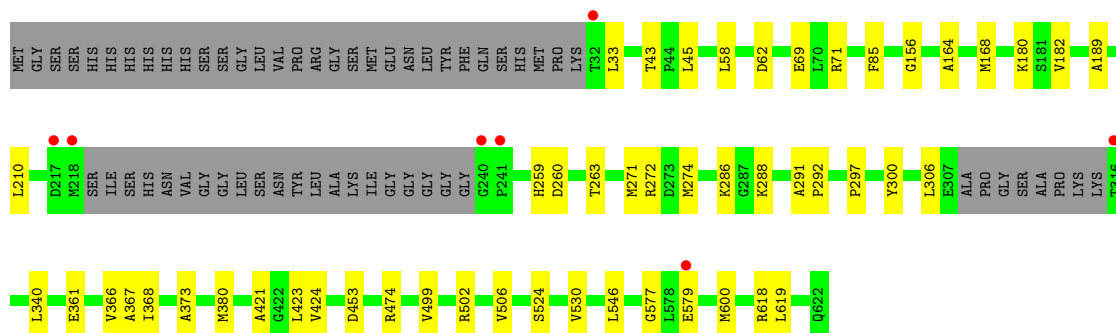
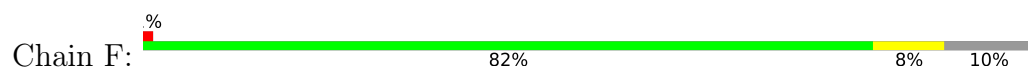
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.62Å 137.62Å 231.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.20 48.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.54-2.20) 99.6 (48.54-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.176 , 0.241 0.175 , 0.241	Depositor DCC
R_{free} test set	9360 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53294	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 26G, GOL, NA, MG

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	0.53	0/4383	0.64	0/5942
1	B	0.52	0/4358	0.64	1/5907 (0.0%)
1	C	0.52	0/4374	0.65	0/5931
1	D	0.51	0/4350	0.62	0/5897
1	E	0.51	0/4368	0.63	0/5923
1	F	0.53	0/4369	0.62	0/5924
All	All	0.52	0/26202	0.63	1/35524 (0.0%)

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
1	B	1	0
1	F	0	1
All	All	1	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	316	THR	N-CA-C	7.20	131.16	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	316	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	618	ARG	Sidechain

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	4298	4235	4271	26	0
1	B	4267	4209	4232	28	0
1	C	4289	4222	4255	17	0
1	D	4265	4203	4233	35	2
1	E	4282	4177	4248	26	2
1	F	4284	4218	4250	28	1
2	A	18	17	17	1	0
2	B	18	17	17	0	0
2	C	18	17	17	0	0
2	D	18	17	17	1	0
2	E	18	17	17	1	0
2	F	18	17	17	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
6	F	6	8	8	1	0
7	A	392	0	0	1	0
7	B	329	0	0	5	0
7	C	328	0	0	3	1
7	D	333	0	0	2	1
7	E	350	0	0	2	0
7	F	371	0	0	4	1
All	All	27920	25374	25599	155	4

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

The worst 5 of 155 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:F:286:LYS:HD3	7:F:1089:HOH:O	1.61	0.99
1:F:260:ASP:OD2	1:F:263:THR:OG1	1.95	0.85
1:E:517:GLU:OE2	1:E:520:LYS:NZ	2.28	0.66
1:F:423:LEU:HD13	1:F:600:MET:HB3	1.80	0.64
1:C:613:LYS:O	1:C:617:GLN:HG3	1.98	0.63

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:579:GLU:OE1	7:C:1078:HOH:O[4_455]	1.87	0.33
1:D:490:GLN:NE2	1:E:620:ASP:OD2[1_455]	1.96	0.24
7:D:981:HOH:O	7:F:805:HOH:O[4_455]	2.13	0.07
1:D:490:GLN:HE21	1:E:620:ASP:OD2[1_455]	1.56	0.04

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	558/622 (90%)	538 (96%)	19 (3%)	1 (0%)	43	51
1	B	555/622 (89%)	528 (95%)	26 (5%)	1 (0%)	43	51
1	C	557/622 (90%)	533 (96%)	23 (4%)	1 (0%)	43	51
1	D	554/622 (89%)	530 (96%)	24 (4%)	0	100	100
1	E	557/622 (90%)	534 (96%)	22 (4%)	1 (0%)	43	51
1	F	556/622 (89%)	533 (96%)	22 (4%)	1 (0%)	43	51
All	All	3337/3732 (89%)	3196 (96%)	136 (4%)	5 (0%)	48	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	241	PRO
1	A	351	ASP
1	B	526	ASP
1	F	156	GLY
1	C	156	GLY

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	446/490 (91%)	443 (99%)	3 (1%)	76	87
1	B	442/490 (90%)	440 (100%)	2 (0%)	81	90
1	C	444/490 (91%)	441 (99%)	3 (1%)	76	87
1	D	441/490 (90%)	435 (99%)	6 (1%)	59	75
1	E	443/490 (90%)	439 (99%)	4 (1%)	70	84
1	F	444/490 (91%)	440 (99%)	4 (1%)	70	84
All	All	2660/2940 (90%)	2638 (99%)	22 (1%)	73	85

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	31	LYS
1	E	524	SER
1	E	282	VAL
1	F	33	LEU
1	C	488	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	617	GLN
1	F	584	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	301	HIS
1	F	372	HIS
1	E	216	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 18 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	F	702	-	5,5,5	1.85	2 (40%)	5,5,5	1.08	0
2	26G	C	701	-	19,19,19	1.32	1 (5%)	25,25,25	1.63	5 (20%)
2	26G	E	701	-	19,19,19	1.35	2 (10%)	25,25,25	1.61	6 (24%)
2	26G	D	701	-	19,19,19	1.31	2 (10%)	25,25,25	1.43	3 (12%)
2	26G	F	701	-	19,19,19	1.45	1 (5%)	25,25,25	1.52	4 (16%)
2	26G	B	701	-	19,19,19	1.40	2 (10%)	25,25,25	1.84	6 (24%)
2	26G	A	701	-	19,19,19	1.24	1 (5%)	25,25,25	1.39	3 (12%)

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
6	GOL	F	702	-	-	2/4/4/4	-
2	26G	C	701	-	-	1/7/7/7	0/2/2/2
2	26G	E	701	-	-	1/7/7/7	0/2/2/2
2	26G	D	701	-	-	1/7/7/7	0/2/2/2
2	26G	F	701	-	-	1/7/7/7	0/2/2/2
2	26G	B	701	-	-	1/7/7/7	0/2/2/2
2	26G	A	701	-	-	1/7/7/7	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	26G	C4A-N4A	4.84	1.46	1.34
2	C	701	26G	C4A-N4A	4.45	1.45	1.34
2	E	701	26G	C4A-N4A	4.45	1.45	1.34
2	D	701	26G	C4A-N4A	4.40	1.45	1.34
2	B	701	26G	C4A-N4A	4.37	1.45	1.34

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	26G	N4A-C4A-N3A	3.85	122.22	117.03
2	B	701	26G	C5A-C4A-N4A	-3.85	116.96	122.14
2	B	701	26G	C5A-C7A-C01	-3.58	106.32	114.21
2	A	701	26G	CM2-C2A-N1A	3.45	120.88	117.20
2	F	701	26G	C5A-C7A-C01	-3.36	106.81	114.21

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

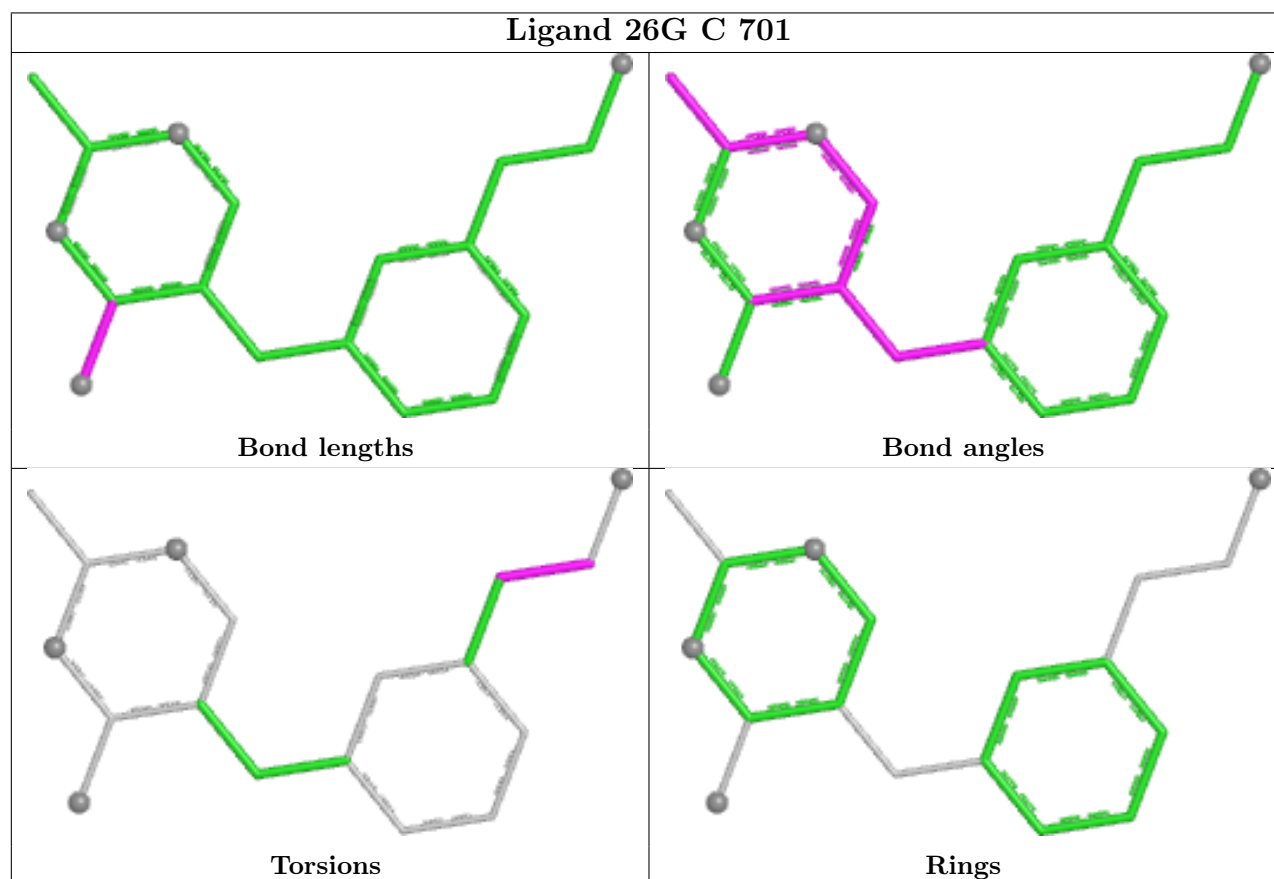
Mol	Chain	Res	Type	Atoms
6	F	702	GOL	O1-C1-C2-O2
6	F	702	GOL	O1-C1-C2-C3
2	A	701	26G	O31-C02-C6-C5
2	B	701	26G	O31-C02-C6-C5
2	C	701	26G	O31-C02-C6-C5

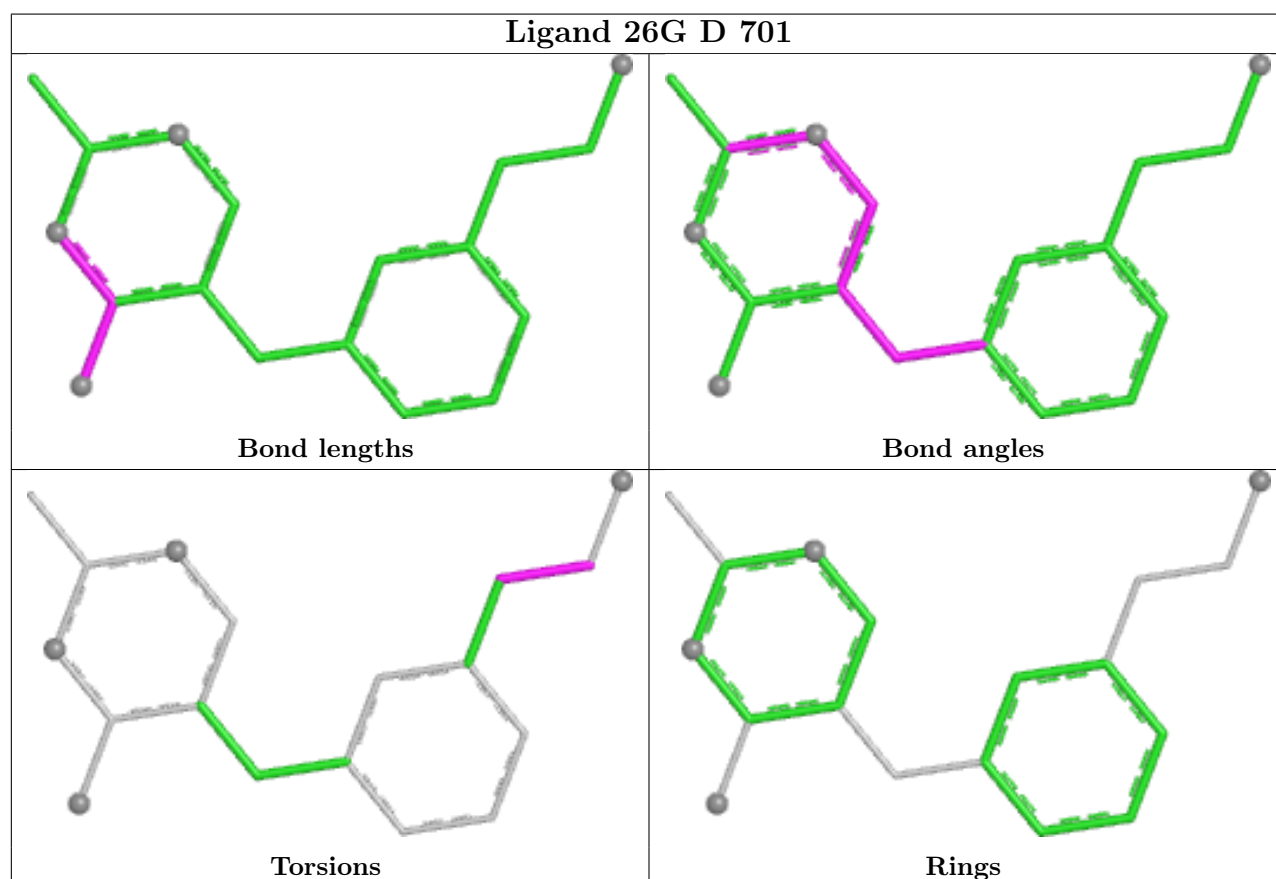
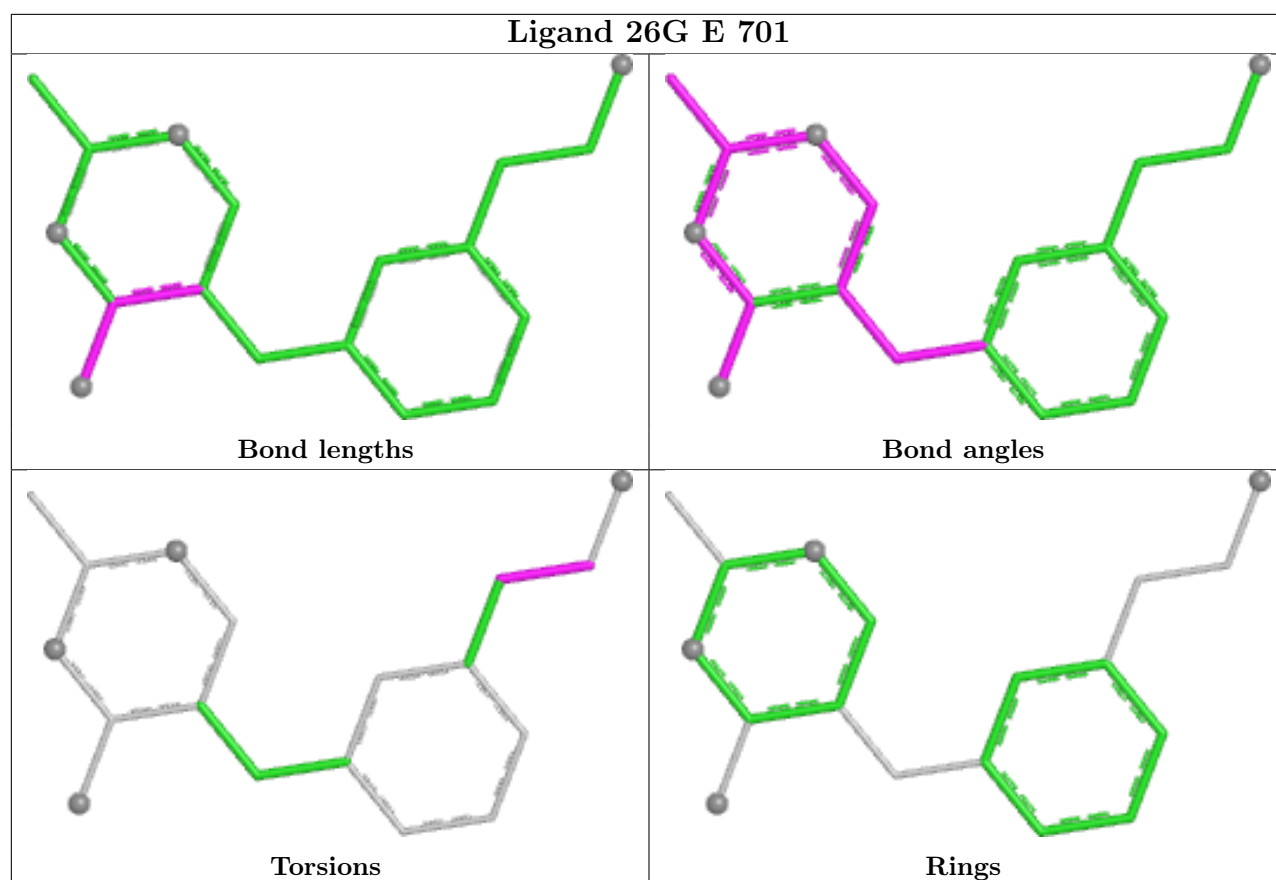
There are no ring outliers.

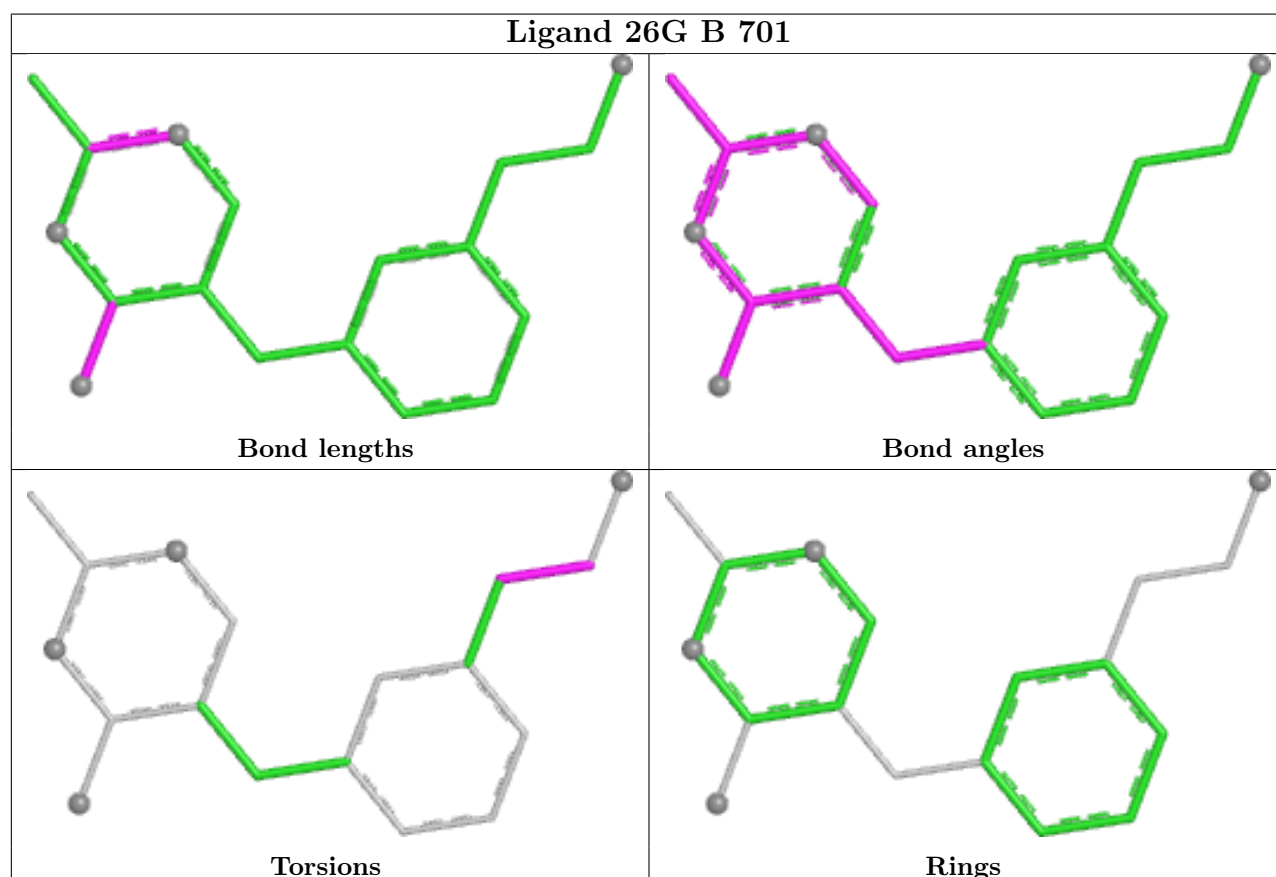
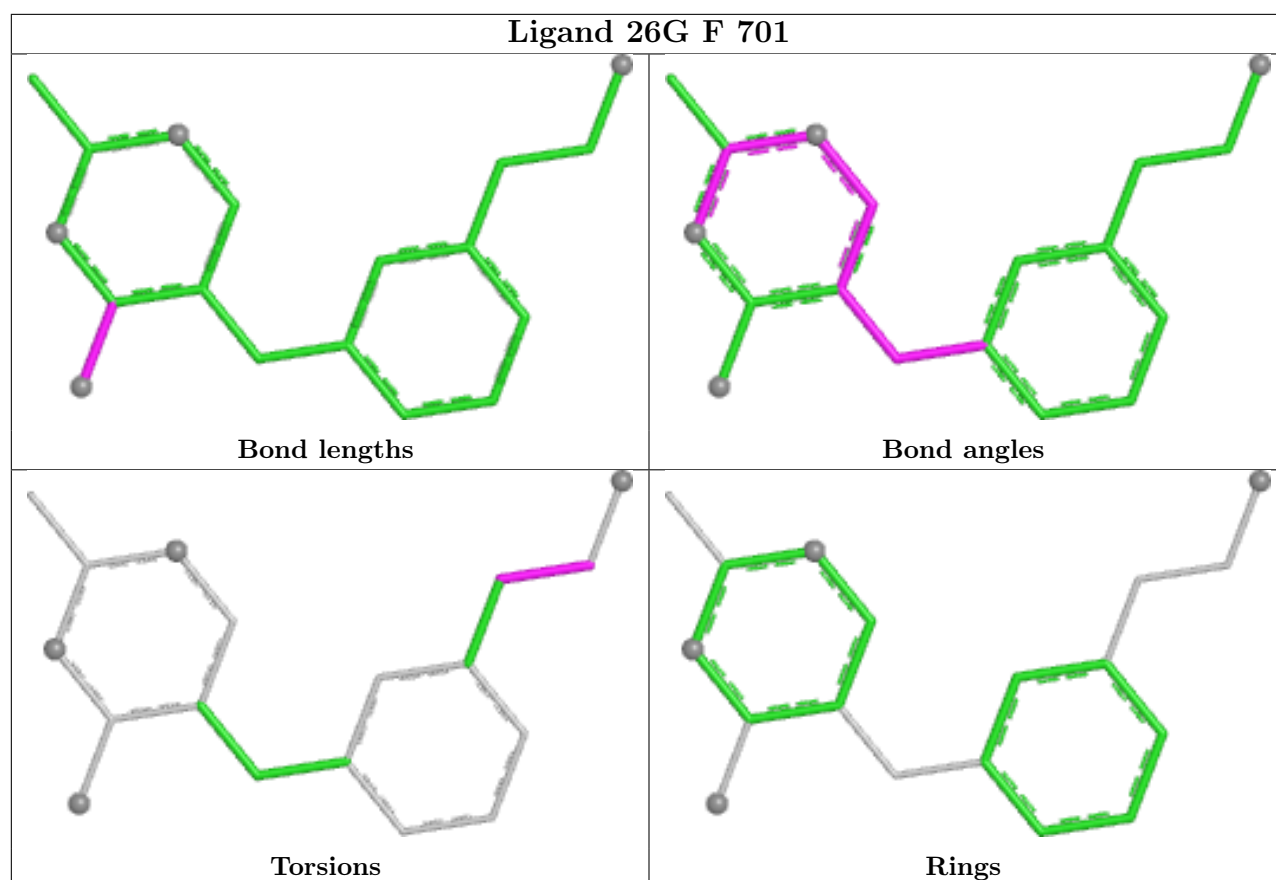
4 monomers are involved in 4 short contacts:

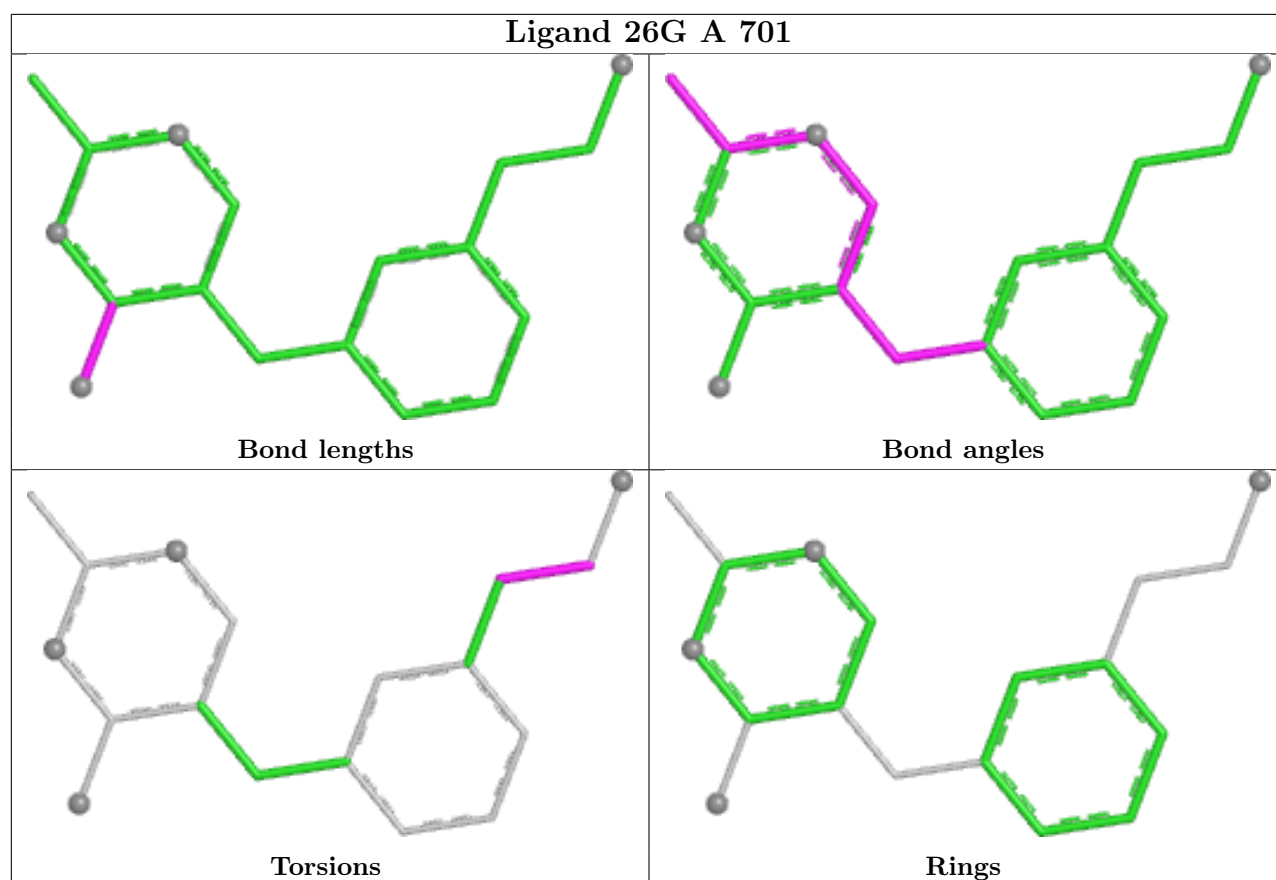
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	702	GOL	1	0
2	E	701	26G	1	0
2	D	701	26G	1	0
2	A	701	26G	1	0

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.









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	564/622 (90%)	-0.47	4 (0%) 84 82	17, 28, 47, 78	0
1	B	558/622 (89%)	-0.38	6 (1%) 78 76	19, 30, 52, 79	2 (0%)
1	C	563/622 (90%)	-0.37	11 (1%) 65 62	18, 30, 52, 95	0
1	D	560/622 (90%)	-0.33	13 (2%) 61 58	17, 30, 58, 95	0
1	E	563/622 (90%)	-0.43	6 (1%) 78 76	19, 29, 48, 88	0
1	F	562/622 (90%)	-0.48	7 (1%) 76 74	18, 28, 49, 97	0
All	All	3370/3732 (90%)	-0.41	47 (1%) 73 71	17, 29, 52, 97	2 (0%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	239	GLY	6.9
1	E	240	GLY	6.1
1	E	308	ALA	5.4
1	F	218	MET	4.2
1	F	32	THR	4.2

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 ⓘ

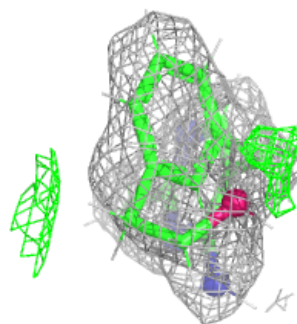
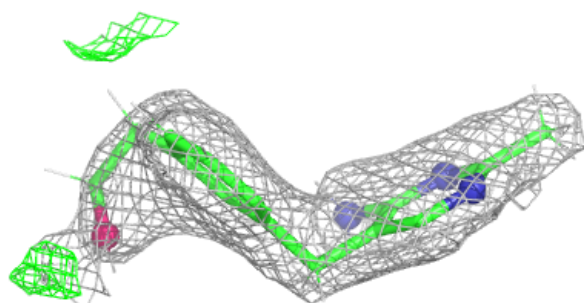
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	702	1/1	0.75	0.25	37,37,37,37	0
5	CA	B	703	1/1	0.75	0.19	72,72,72,72	0
3	MG	D	702	1/1	0.76	0.12	49,49,49,49	0
3	MG	B	702	1/1	0.85	0.19	39,39,39,39	0
4	NA	F	707	1/1	0.86	0.10	42,42,42,42	0
6	GOL	F	702	6/6	0.89	0.12	31,39,52,52	0
2	26G	C	701	18/18	0.90	0.10	26,42,61,70	0
2	26G	E	701	18/18	0.90	0.12	22,37,59,61	0
2	26G	F	701	18/18	0.90	0.12	26,42,57,65	0
3	MG	C	702	1/1	0.91	0.15	44,44,44,44	0
2	26G	B	701	18/18	0.91	0.11	17,33,51,58	0
3	MG	F	704	1/1	0.91	0.14	46,46,46,46	0
4	NA	C	704	1/1	0.92	0.08	32,32,32,32	0
3	MG	C	703	1/1	0.92	0.11	37,37,37,37	0
2	26G	D	701	18/18	0.92	0.10	25,42,57,61	0
2	26G	A	701	18/18	0.92	0.09	21,34,53,59	0
3	MG	E	702	1/1	0.93	0.12	42,42,42,42	0
4	NA	A	704	1/1	0.93	0.11	40,40,40,40	0
3	MG	F	705	1/1	0.94	0.06	30,30,30,30	0
3	MG	A	703	1/1	0.95	0.12	32,32,32,32	0
5	CA	F	706	1/1	0.96	0.14	47,47,47,47	0
3	MG	E	703	1/1	0.96	0.08	26,26,26,26	0
4	NA	D	703	1/1	0.97	0.05	26,26,26,26	0
4	NA	C	705	1/1	0.98	0.04	26,26,26,26	0
3	MG	F	703	1/1	0.99	0.03	22,22,22,22	0

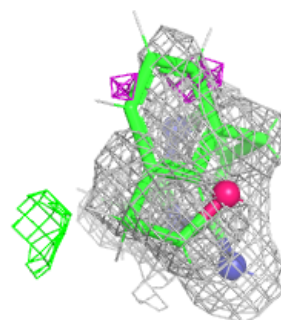
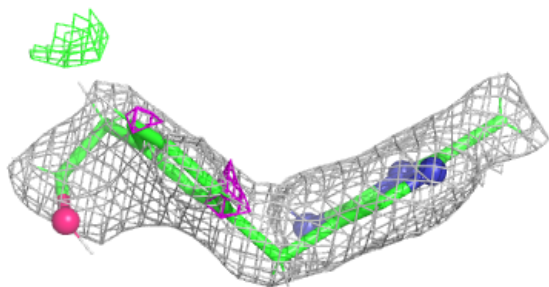
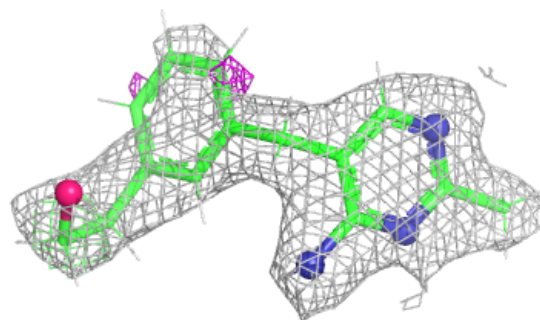
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 26G C 701:

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

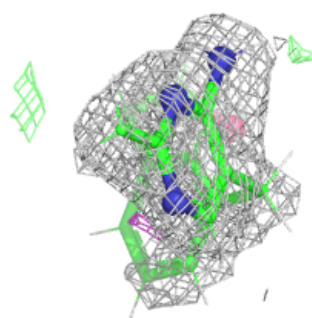
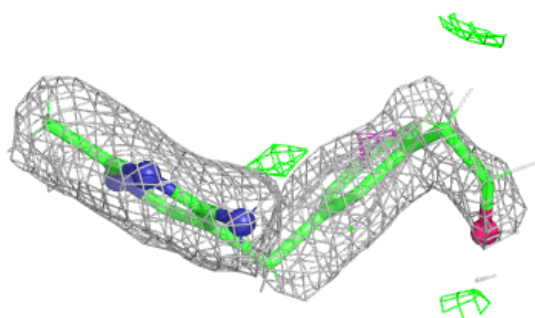
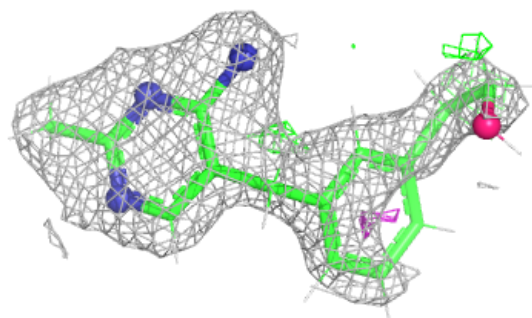
**Electron density around 26G E 701:**

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

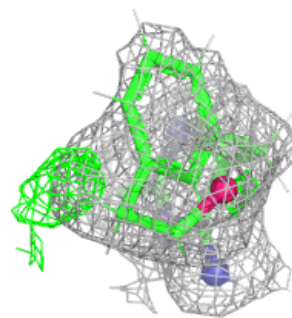
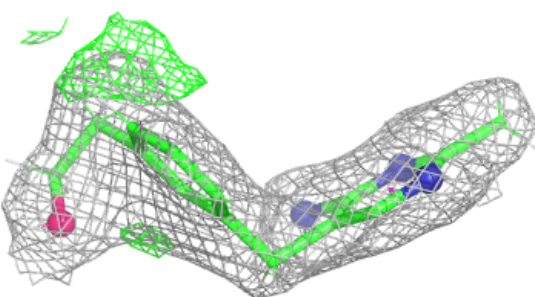
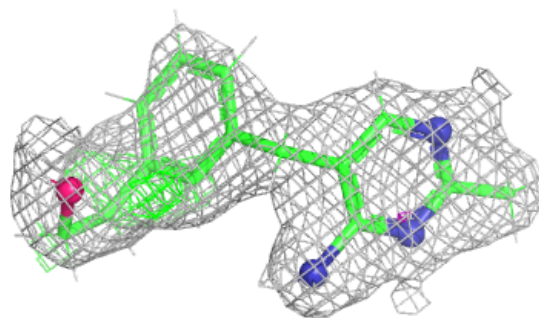


Electron density around 26G F 701:

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

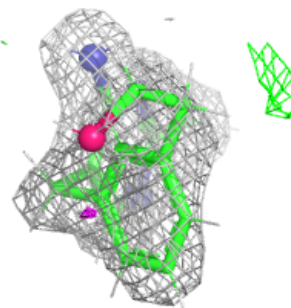
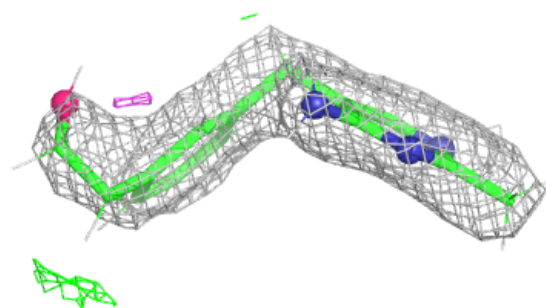
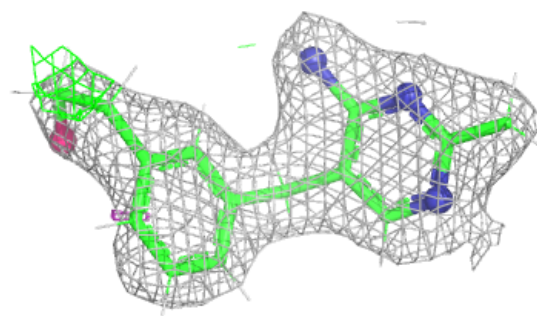
**Electron density around 26G B 701:**

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

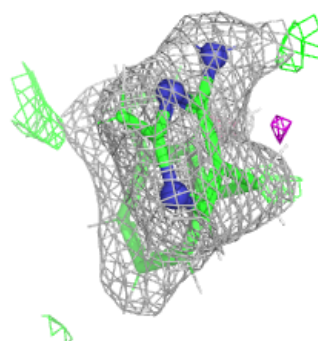
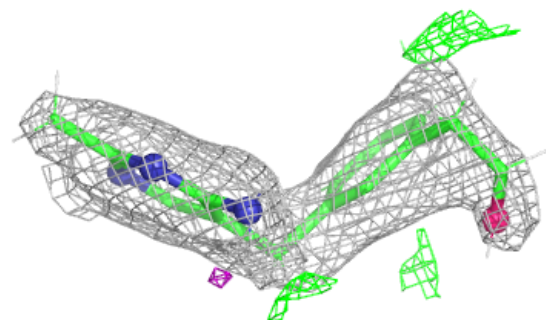
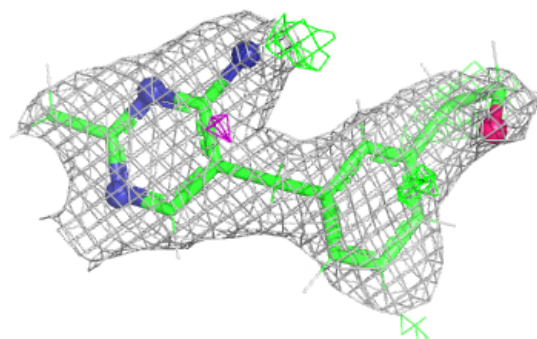


Electron density around 26G D 701:

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

**Electron density around 26G A 701:**

$2mF_o-DF_c$ (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.