



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2021 – 08:01 PM EDT

PDB ID : 1RYW
Title : C115S MurA liganded with reaction products
Authors : Eschenburg, S.; Schonbrunn, E.
Deposited on : 2003-12-22
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

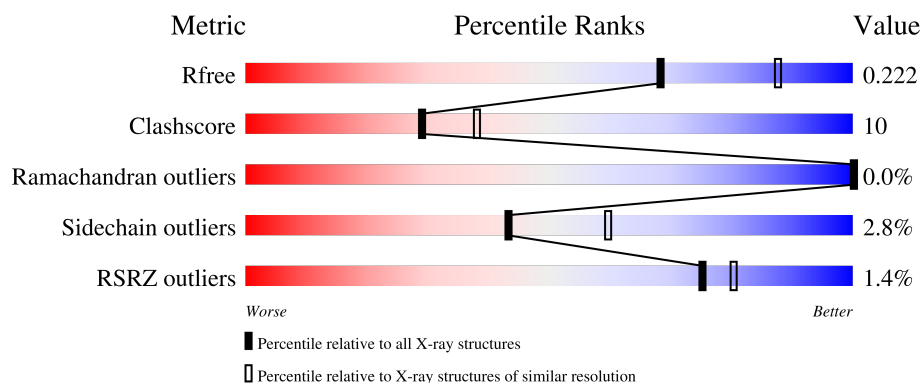
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	419	<div> <div>80%</div> <div>20%</div> </div>
1	B	419	<div> <div>82%</div> <div>18%</div> </div>
1	C	419	<div> <div>82%</div> <div>18%</div> </div>
1	D	419	<div> <div>79%</div> <div>21%</div> </div>
1	E	419	<div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	419	<div><div></div><div>4%</div><div>76%</div><div>23%</div><div></div></div>
1	G	419	<div><div></div><div>%</div><div>80%</div><div>20%</div><div></div></div>
1	H	419	<div><div></div><div>%</div><div>82%</div><div>17%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27527 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	6	0
			3173	1996	560	603	14			
1	B	419	Total	C	N	O	S	0	0	0
			3143	1976	554	600	13			
1	C	419	Total	C	N	O	S	0	0	0
			3143	1976	554	600	13			
1	D	419	Total	C	N	O	S	0	1	0
			3145	1977	554	601	13			
1	E	419	Total	C	N	O	S	0	2	0
			3149	1979	555	602	13			
1	F	419	Total	C	N	O	S	0	1	0
			3150	1980	557	600	13			
1	G	419	Total	C	N	O	S	0	2	0
			3155	1983	557	602	13			
1	H	419	Total	C	N	O	S	0	2	0
			3154	1983	557	600	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	engineered mutation	UNP P33038
A	115	SER	CYS	engineered mutation	UNP P33038
B	67	IAS	ASN	engineered mutation	UNP P33038
B	115	SER	CYS	engineered mutation	UNP P33038
C	67	IAS	ASN	engineered mutation	UNP P33038
C	115	SER	CYS	engineered mutation	UNP P33038
D	67	IAS	ASN	engineered mutation	UNP P33038
D	115	SER	CYS	engineered mutation	UNP P33038
E	67	IAS	ASN	engineered mutation	UNP P33038
E	115	SER	CYS	engineered mutation	UNP P33038
F	67	IAS	ASN	engineered mutation	UNP P33038
F	115	SER	CYS	engineered mutation	UNP P33038
G	67	IAS	ASN	engineered mutation	UNP P33038

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Chain	Residue	Modelled	Actual	Comment	Reference
G	115	SER	CYS	engineered mutation	UNP P33038
H	67	IAS	ASN	engineered mutation	UNP P33038
H	115	SER	CYS	engineered mutation	UNP P33038

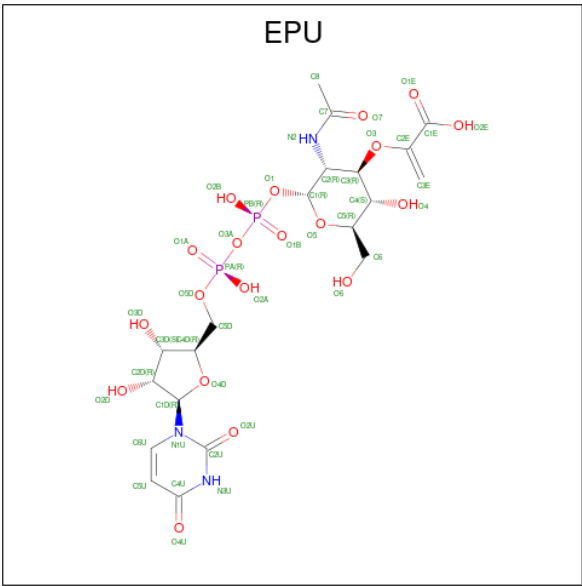
- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is URIDINE-DIPHOSPHATE-2(N-ACETYLGUCOSAMINYL) BUTYRIC

ACID (three-letter code: EPU) (formula: C₂₀H₂₉N₃O₁₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	E	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	F	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	G	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	H	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

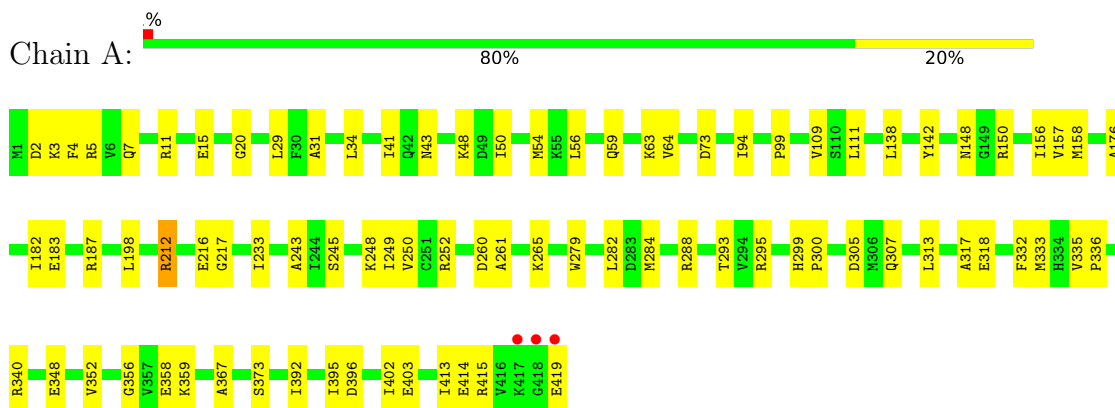
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	284	Total	O	0	0
			284	284		
5	B	253	Total	O	0	0
			253	253		
5	C	272	Total	O	0	0
			272	272		
5	D	208	Total	O	0	0
			208	208		
5	E	214	Total	O	0	0
			214	214		
5	F	136	Total	O	0	0
			136	136		
5	G	237	Total	O	0	0
			237	237		
5	H	212	Total	O	0	0
			212	212		

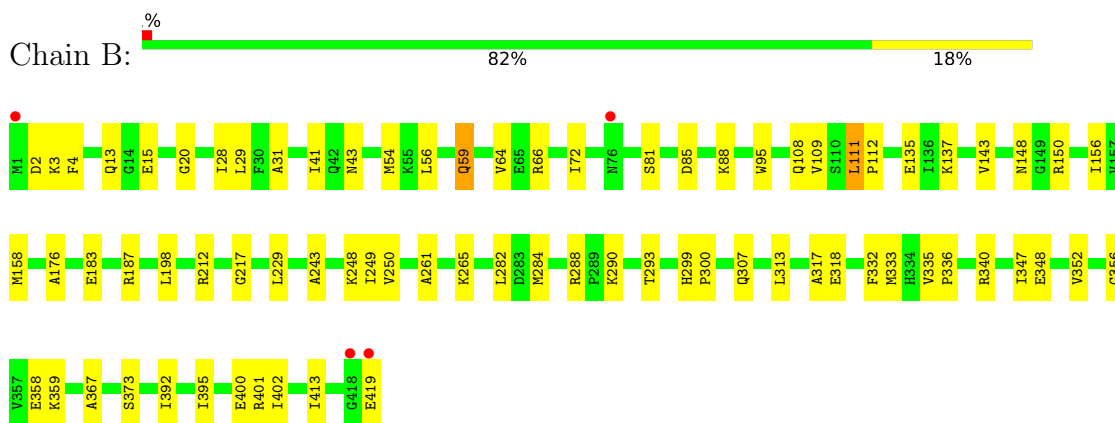
3 Residue-property plots

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.

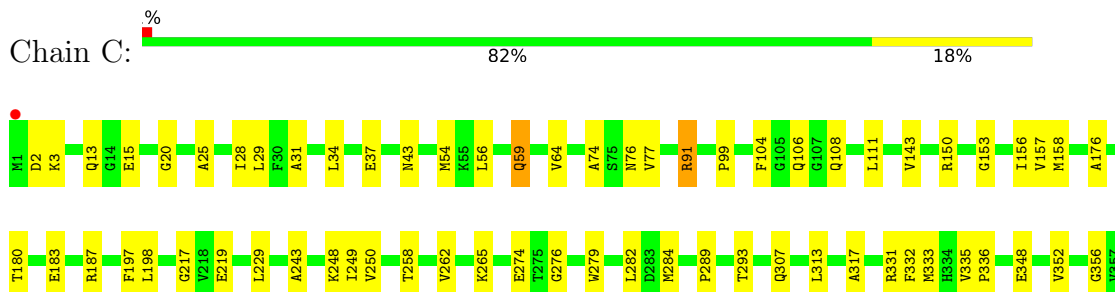
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

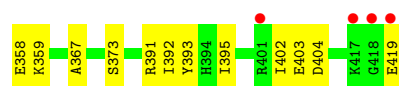


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

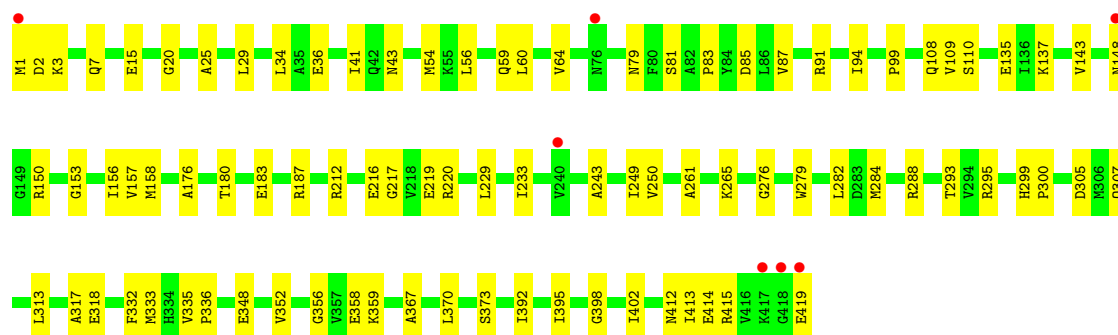
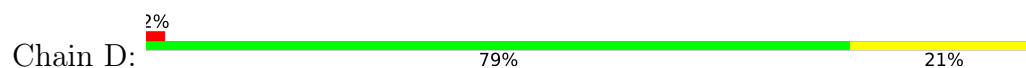


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

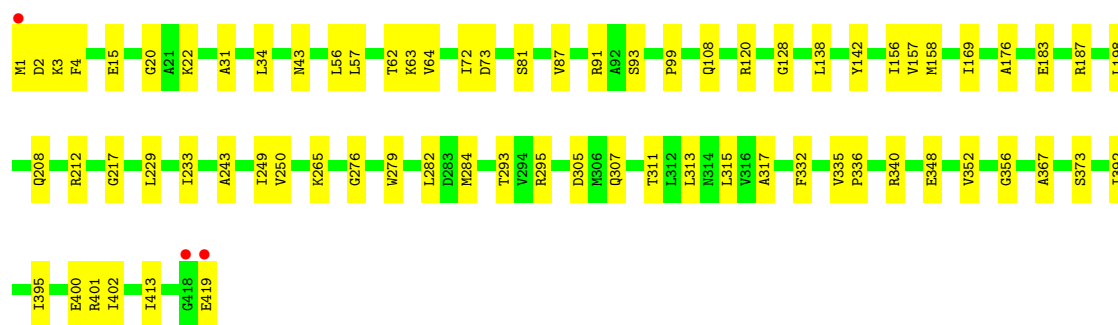
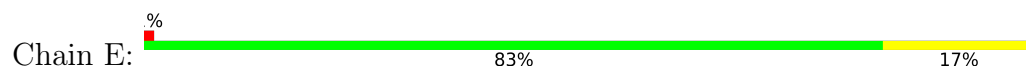




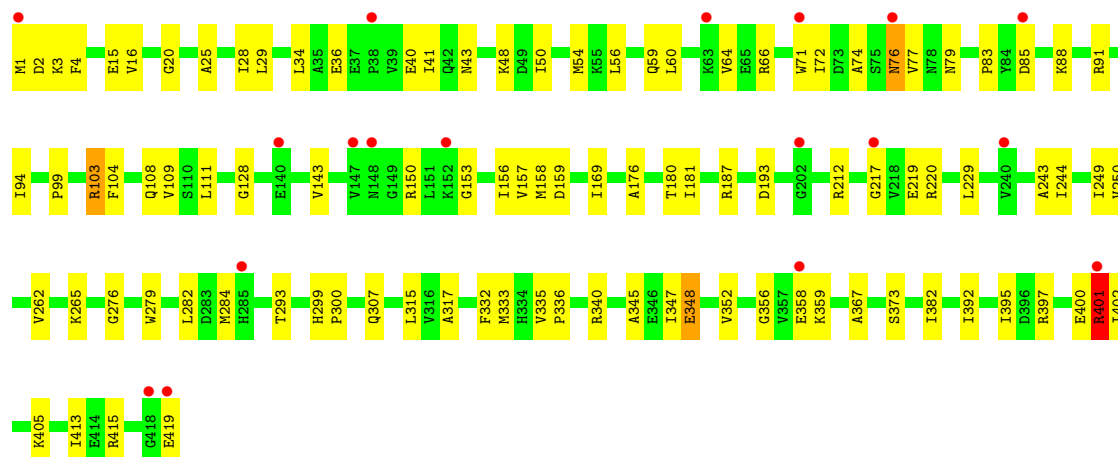
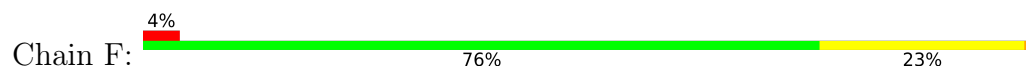
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



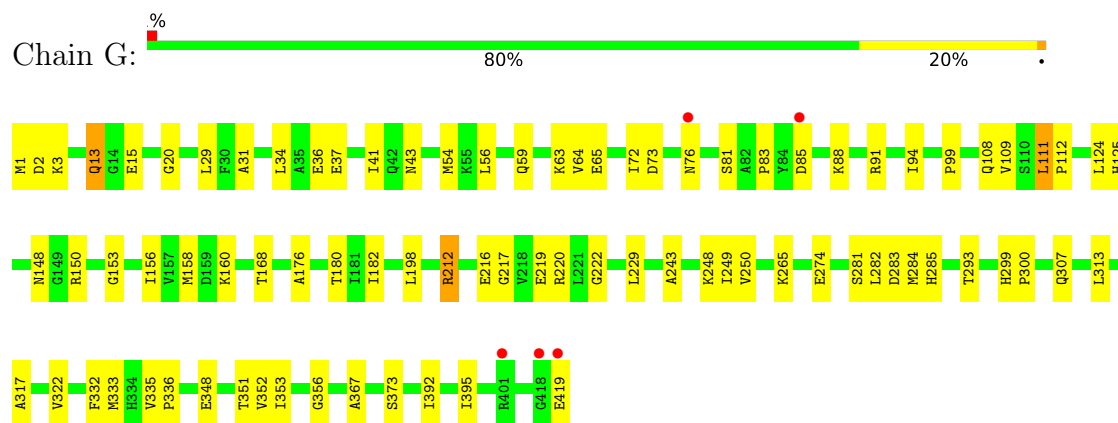
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



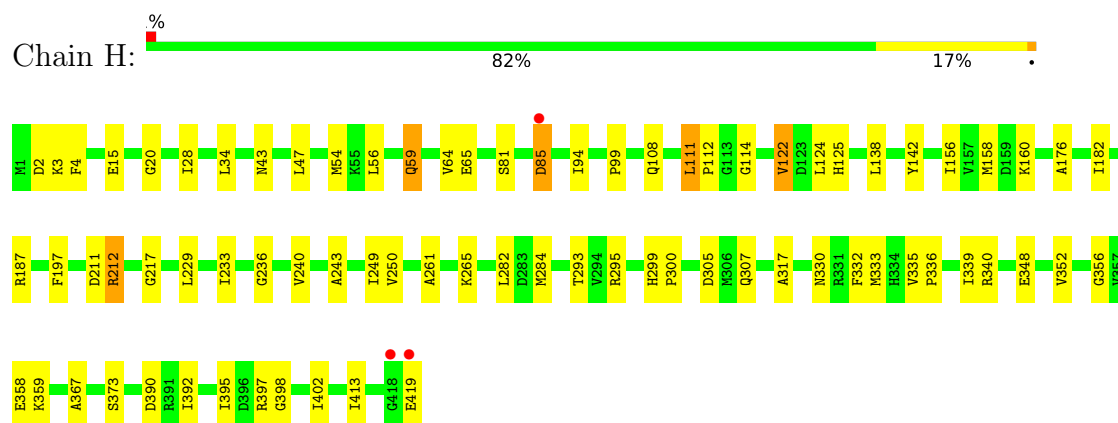
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



● Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



● Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.87Å 153.73Å 135.09Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 29.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.30) 98.9 (29.92-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.178 , 0.225 0.177 , 0.222	Depositor DCC
R_{free} test set	2801 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27527	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7730e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PO4, GOL, IAS, EPU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/3233	0.62	0/4376
1	B	0.36	0/3179	0.61	0/4305
1	C	0.36	0/3179	0.61	0/4305
1	D	0.35	0/3185	0.59	0/4313
1	E	0.36	0/3193	0.61	0/4324
1	F	0.34	0/3190	0.60	0/4319
1	G	0.36	0/3199	0.61	0/4332
1	H	0.35	0/3198	0.62	0/4329
All	All	0.36	0/25556	0.61	0/34603

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3173	0	3253	70	0
1	B	3143	0	3216	56	0
1	C	3143	0	3216	58	0
1	D	3145	0	3217	61	0
1	E	3149	0	3219	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3150	0	3225	75	0
1	G	3155	0	3227	67	0
1	H	3154	0	3230	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	H	5	0	0	1	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	2	0
3	D	44	0	26	1	0
3	E	44	0	26	3	0
3	F	44	0	26	1	0
3	G	44	0	26	1	0
3	H	44	0	26	3	0
4	A	12	0	16	5	0
4	B	12	0	16	3	0
4	C	30	0	40	7	0
4	D	12	0	16	1	0
4	E	12	0	16	2	0
4	F	6	0	8	1	0
4	G	6	0	8	2	0
4	H	12	0	16	3	0
5	A	284	0	0	7	0
5	B	253	0	0	3	0
5	C	272	0	0	4	0
5	D	208	0	0	3	0
5	E	214	0	0	2	0
5	F	136	0	0	1	0
5	G	237	0	0	7	0
5	H	212	0	0	3	0
All	All	27527	0	26147	498	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 10.

The worst 5 of 498 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:G:81:SER:HB2	1:G:108:GLN:HE21	1.40	0.86
1:B:54:MET:HE3	1:B:66:ARG:HB3	1.57	0.85
1:G:13:GLN:HG2	1:G:248:LYS:H	1.41	0.84
1:A:150:ARG:HD3	5:A:1069:HOH:O	1.78	0.83
1:C:54:MET:HG2	1:C:64:VAL:HG11	1.60	0.83

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	421/419 (100%)	413 (98%)	8 (2%)	0	100	100
1	B	415/419 (99%)	404 (97%)	11 (3%)	0	100	100
1	C	415/419 (99%)	407 (98%)	8 (2%)	0	100	100
1	D	416/419 (99%)	405 (97%)	11 (3%)	0	100	100
1	E	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
1	F	416/419 (99%)	399 (96%)	16 (4%)	1 (0%)	47	58
1	G	417/419 (100%)	409 (98%)	8 (2%)	0	100	100
1	H	417/419 (100%)	408 (98%)	9 (2%)	0	100	100
All	All	3334/3352 (100%)	3253 (98%)	80 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	401	ARG

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	335/329 (102%)	325 (97%)	10 (3%)	41	57
1	B	329/329 (100%)	322 (98%)	7 (2%)	53	70
1	C	329/329 (100%)	317 (96%)	12 (4%)	35	49
1	D	330/329 (100%)	321 (97%)	9 (3%)	44	61
1	E	331/329 (101%)	326 (98%)	5 (2%)	65	79
1	F	330/329 (100%)	318 (96%)	12 (4%)	35	49
1	G	331/329 (101%)	321 (97%)	10 (3%)	41	57
1	H	331/329 (101%)	320 (97%)	11 (3%)	38	53
All	All	2646/2632 (100%)	2570 (97%)	76 (3%)	43	58

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	76	ASN
1	H	211	ASP
1	G	148	ASN
1	H	59	GLN
1	H	348	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	148	ASN
1	H	108	GLN
1	E	330	ASN
1	H	330	ASN
1	G	148	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	IAS	F	67	1	4,7,8	0.74	0	2,8,10	1.32	0
1	IAS	A	67	1	4,7,8	0.69	0	2,8,10	1.24	0
1	IAS	C	67	1	4,7,8	0.71	0	2,8,10	1.29	0
1	IAS	B	67	1	4,7,8	0.68	0	2,8,10	1.23	0
1	IAS	H	67	1	4,7,8	0.64	0	2,8,10	1.31	0
1	IAS	E	67	1	4,7,8	0.52	0	2,8,10	1.39	0
1	IAS	G	67	1	4,7,8	0.52	0	2,8,10	1.35	0
1	IAS	D	67	1	4,7,8	0.46	0	2,8,10	1.40	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
1	IAS	F	67	1	-	0/3/7/8	-
1	IAS	A	67	1	-	0/3/7/8	-
1	IAS	C	67	1	-	0/3/7/8	-
1	IAS	B	67	1	-	0/3/7/8	-
1	IAS	H	67	1	-	0/3/7/8	-
1	IAS	E	67	1	-	0/3/7/8	-
1	IAS	G	67	1	-	0/3/7/8	-
1	IAS	D	67	1	-	0/3/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	GOL	A	2471	-	5,5,5	0.52	0	5,5,5	0.36	0
2	PO4	B	3461	-	4,4,4	1.73	0	6,6,6	0.43	0
4	GOL	H	9471	-	5,5,5	0.44	0	5,5,5	0.43	0
3	EPU	A	2450	-	36,46,46	2.27	15 (41%)	45,69,69	1.55	7 (15%)
4	GOL	C	4471	-	5,5,5	0.38	0	5,5,5	0.35	0
4	GOL	C	3473	-	5,5,5	0.47	0	5,5,5	0.50	0
4	GOL	D	5472	-	5,5,5	0.47	0	5,5,5	0.58	0
4	GOL	D	5471	-	5,5,5	0.47	0	5,5,5	0.39	0
3	EPU	D	5450	-	36,46,46	2.25	16 (44%)	45,69,69	1.52	7 (15%)
4	GOL	B	3472	-	5,5,5	0.51	0	5,5,5	0.49	0
2	PO4	C	4461	-	4,4,4	1.66	0	6,6,6	0.44	0
2	PO4	G	8461	-	4,4,4	1.68	0	6,6,6	0.46	0
4	GOL	C	4474	-	5,5,5	0.44	0	5,5,5	0.45	0
2	PO4	D	5461	-	4,4,4	1.68	0	6,6,6	0.43	0
2	PO4	F	7461	-	4,4,4	1.71	0	6,6,6	0.45	0
4	GOL	A	2472	-	5,5,5	0.68	0	5,5,5	0.51	0
4	GOL	F	7471	-	5,5,5	0.46	0	5,5,5	0.39	0
4	GOL	C	4472	-	5,5,5	0.51	0	5,5,5	0.49	0
4	GOL	G	8471	-	5,5,5	0.41	0	5,5,5	0.32	0
3	EPU	F	7450	-	36,46,46	2.33	15 (41%)	45,69,69	1.55	5 (11%)
4	GOL	H	9472	-	5,5,5	0.44	0	5,5,5	0.53	0
3	EPU	H	9450	-	36,46,46	2.26	13 (36%)	45,69,69	1.52	5 (11%)
3	EPU	B	3450	-	36,46,46	2.38	15 (41%)	45,69,69	1.56	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPU	E	6450	-	36,46,46	2.42	17 (47%)	45,69,69	1.62	6 (13%)
4	GOL	B	3471	-	5,5,5	0.38	0	5,5,5	0.35	0
3	EPU	G	8450	-	36,46,46	2.37	13 (36%)	45,69,69	1.55	5 (11%)
2	PO4	G	8462	-	4,4,4	1.58	0	6,6,6	0.45	0
4	GOL	E	6471	-	5,5,5	0.48	0	5,5,5	0.38	0
4	GOL	E	8472	-	5,5,5	0.46	0	5,5,5	0.54	0
2	PO4	E	6461	-	4,4,4	1.64	0	6,6,6	0.45	0
2	PO4	H	9461	-	4,4,4	1.73	1 (25%)	6,6,6	0.45	0
4	GOL	C	2473	-	5,5,5	0.40	0	5,5,5	0.54	0
2	PO4	A	2461	-	4,4,4	1.71	1 (25%)	6,6,6	0.40	0
3	EPU	C	4450	-	36,46,46	2.35	15 (41%)	45,69,69	1.51	6 (13%)

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	GOL	A	2471	-	-	0/4/4/4	-
4	GOL	H	9471	-	-	0/4/4/4	-
3	EPU	A	2450	-	-	7/26/71/71	0/3/3/3
4	GOL	C	4471	-	-	0/4/4/4	-
4	GOL	C	3473	-	-	0/4/4/4	-
4	GOL	D	5472	-	-	0/4/4/4	-
4	GOL	D	5471	-	-	0/4/4/4	-
3	EPU	D	5450	-	-	6/26/71/71	0/3/3/3
4	GOL	B	3472	-	-	0/4/4/4	-
4	GOL	C	4474	-	-	0/4/4/4	-
4	GOL	A	2472	-	-	0/4/4/4	-
4	GOL	F	7471	-	-	0/4/4/4	-
4	GOL	C	4472	-	-	0/4/4/4	-
4	GOL	G	8471	-	-	0/4/4/4	-
3	EPU	F	7450	-	-	7/26/71/71	0/3/3/3
4	GOL	H	9472	-	-	0/4/4/4	-
3	EPU	H	9450	-	-	8/26/71/71	0/3/3/3
3	EPU	B	3450	-	-	8/26/71/71	0/3/3/3
3	EPU	E	6450	-	-	7/26/71/71	0/3/3/3
4	GOL	B	3471	-	-	0/4/4/4	-
3	EPU	G	8450	-	-	6/26/71/71	0/3/3/3
4	GOL	E	6471	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	8472	-	-	0/4/4/4	-
4	GOL	C	2473	-	-	0/4/4/4	-
3	EPU	C	4450	-	-	6/26/71/71	0/3/3/3

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	8450	EPU	C6U-N1U	7.72	1.45	1.35
3	B	3450	EPU	C6U-N1U	7.62	1.45	1.35
3	E	6450	EPU	C6U-N1U	7.56	1.45	1.35
3	C	4450	EPU	C6U-N1U	7.43	1.45	1.35
3	F	7450	EPU	C6U-N1U	7.40	1.45	1.35

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6450	EPU	C5U-C4U-N3U	-3.87	114.79	123.31
3	F	7450	EPU	C5U-C4U-N3U	-3.84	114.86	123.31
3	A	2450	EPU	C5U-C4U-N3U	-3.81	114.93	123.31
3	D	5450	EPU	C5U-C4U-N3U	-3.71	115.14	123.31
3	B	3450	EPU	C5U-C4U-N3U	-3.70	115.18	123.31

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2450	EPU	C2D-C1D-N1U-C6U
3	A	2450	EPU	O4D-C1D-N1U-C6U
3	A	2450	EPU	C5D-O5D-PA-O1A
3	A	2450	EPU	C5D-O5D-PA-O2A
3	B	3450	EPU	C2D-C1D-N1U-C6U

There are no ring outliers.

22 monomers are involved in 27 short contacts:

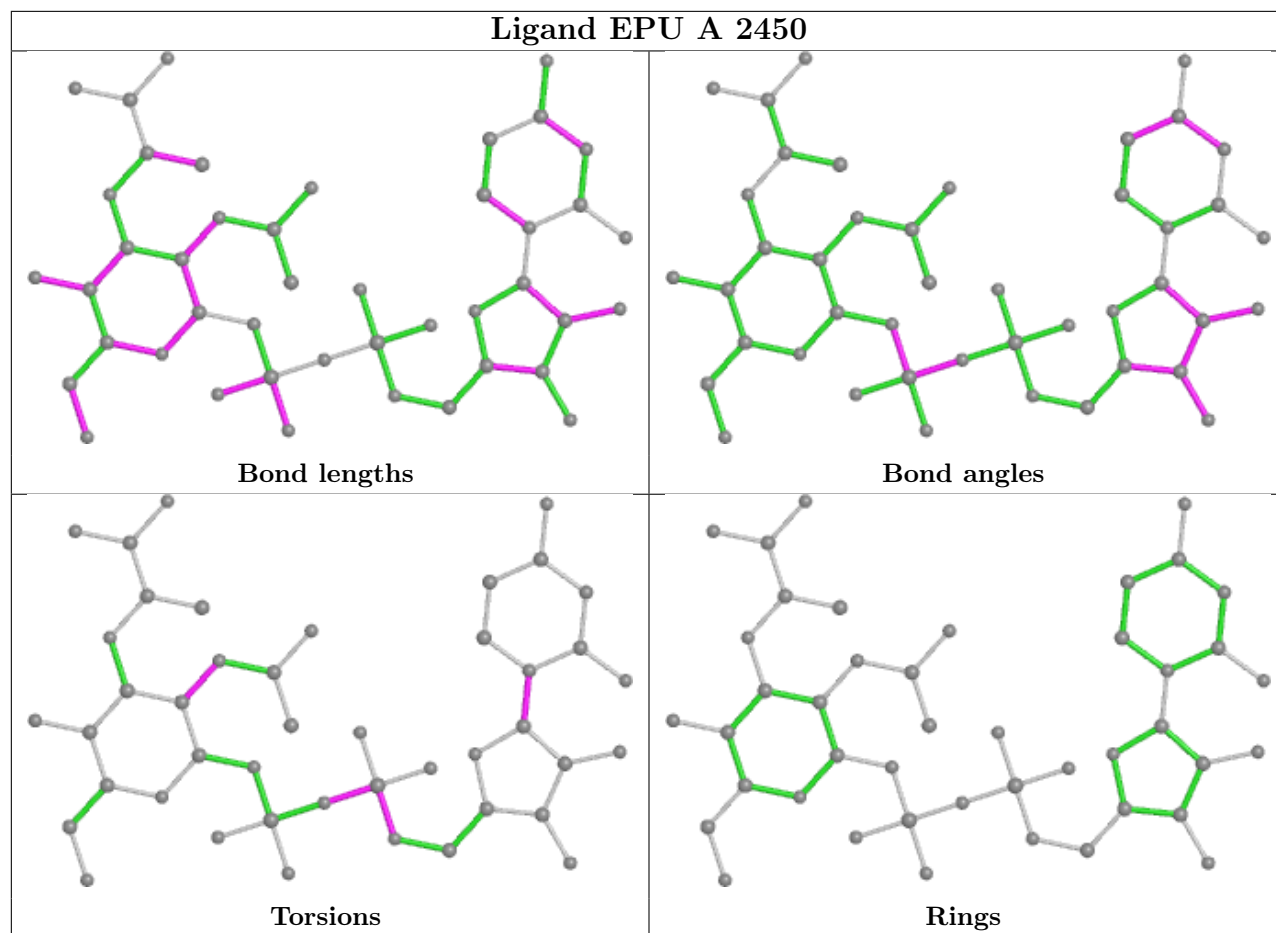
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2471	GOL	2	0
4	H	9471	GOL	3	0
3	A	2450	EPU	2	0
4	C	4471	GOL	3	0
4	C	3473	GOL	1	0

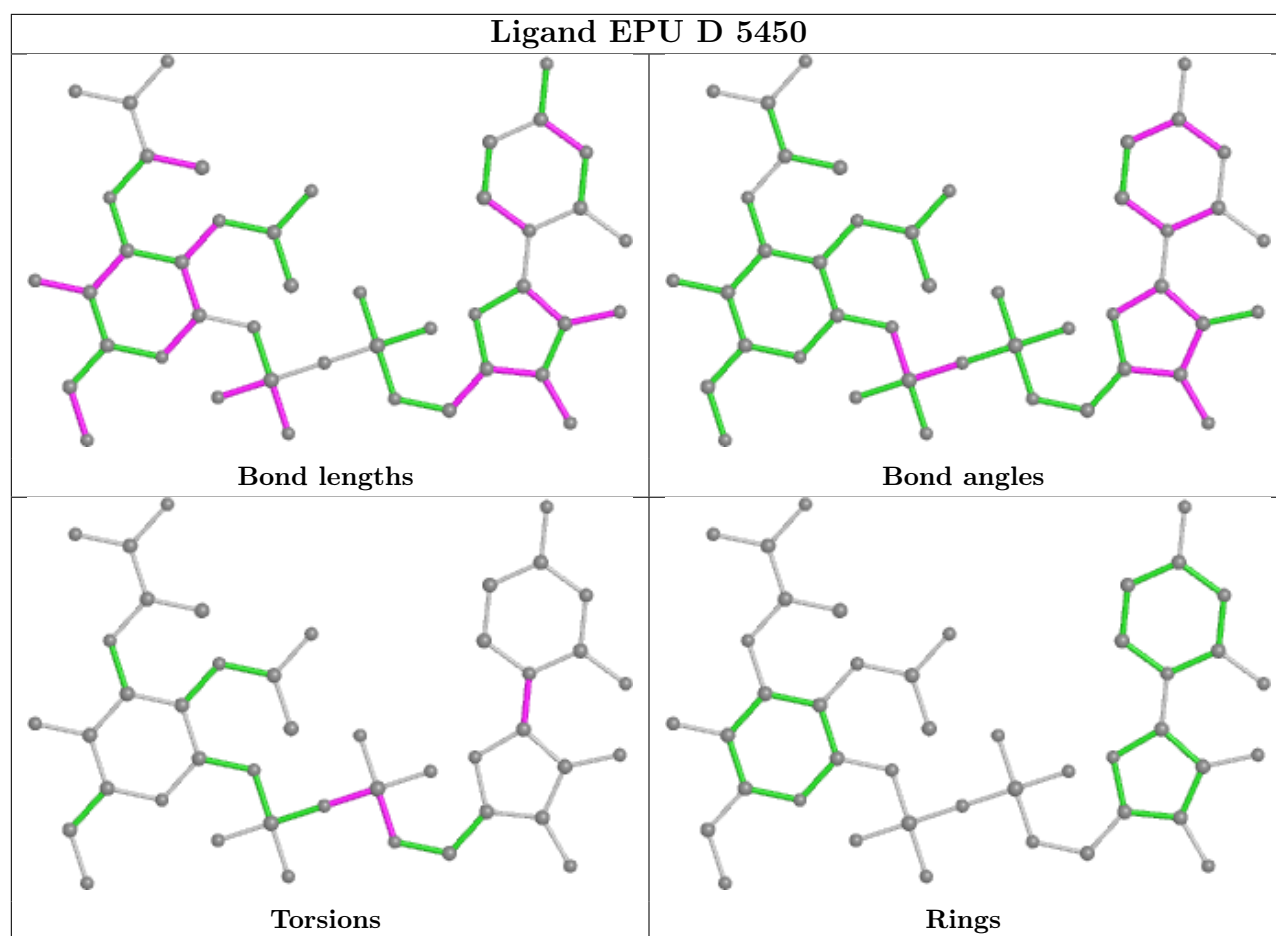
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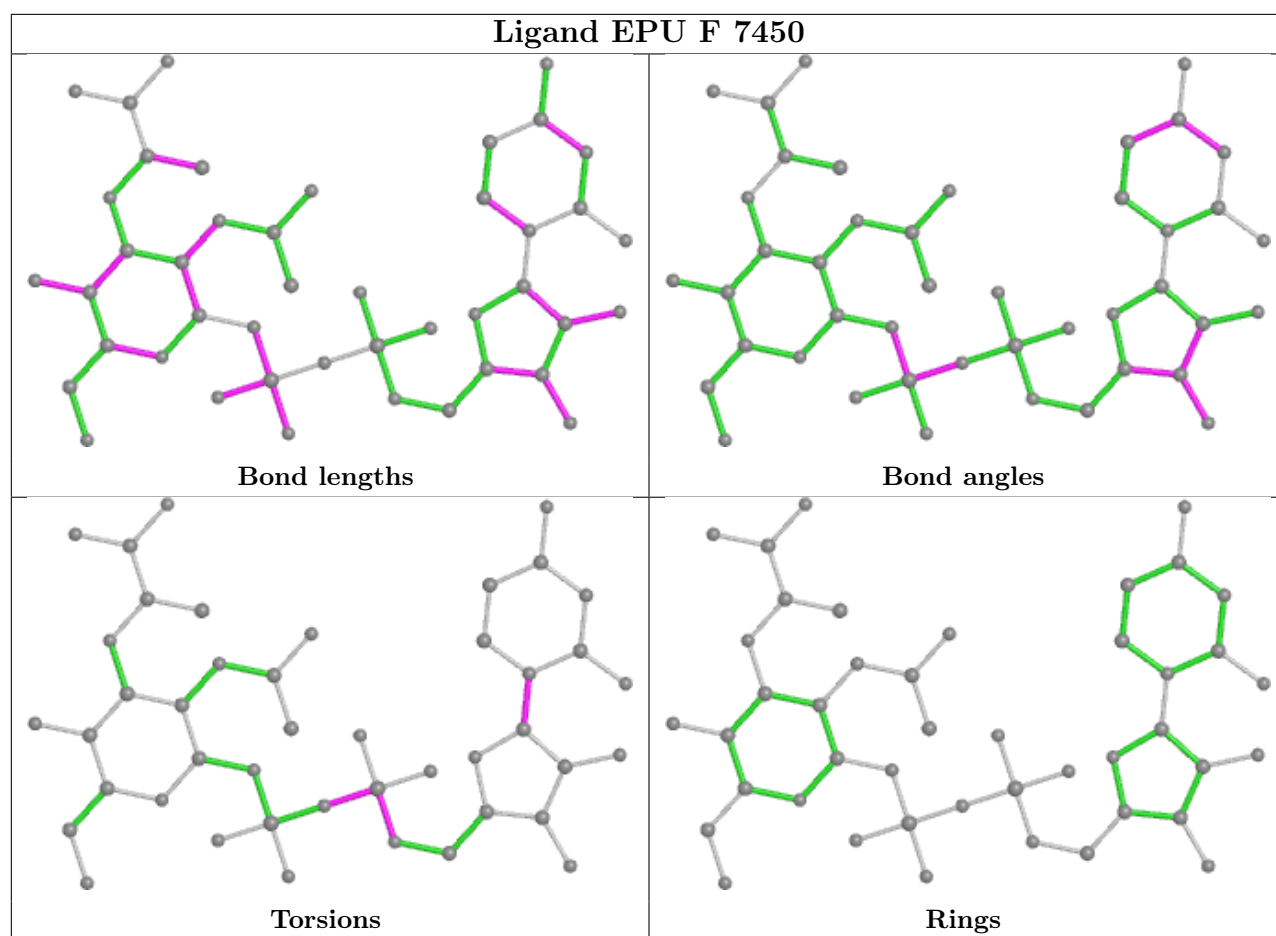
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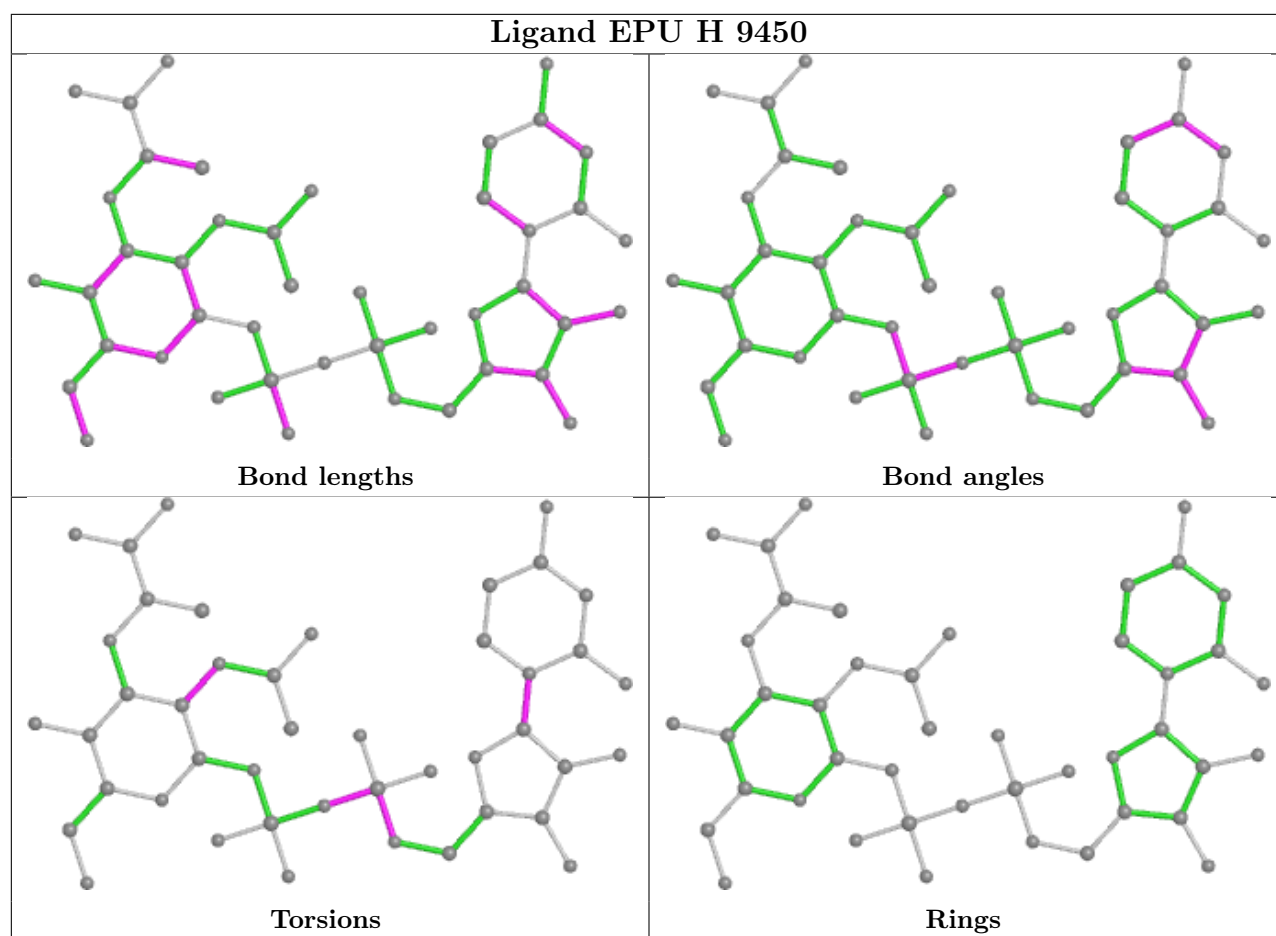
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5471	GOL	1	0
3	D	5450	EPU	1	0
4	C	4474	GOL	2	0
4	A	2472	GOL	3	0
4	F	7471	GOL	1	0
4	G	8471	GOL	2	0
3	F	7450	EPU	1	0
3	H	9450	EPU	3	0
3	B	3450	EPU	2	0
3	E	6450	EPU	3	0
4	B	3471	GOL	3	0
3	G	8450	EPU	1	0
4	E	6471	GOL	2	0
2	E	6461	PO4	1	0
2	H	9461	PO4	1	0
4	C	2473	GOL	1	0
3	C	4450	EPU	2	0

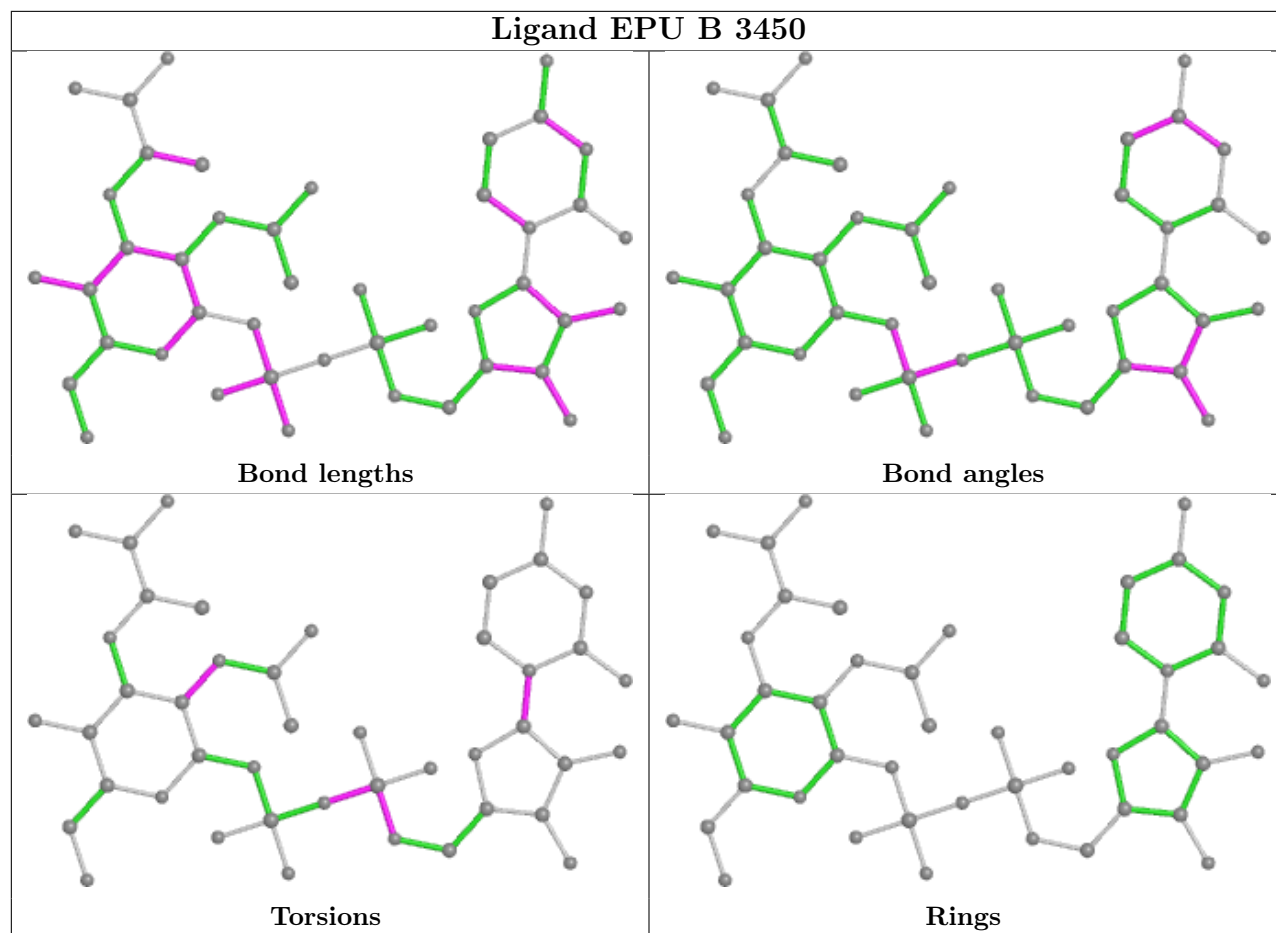
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

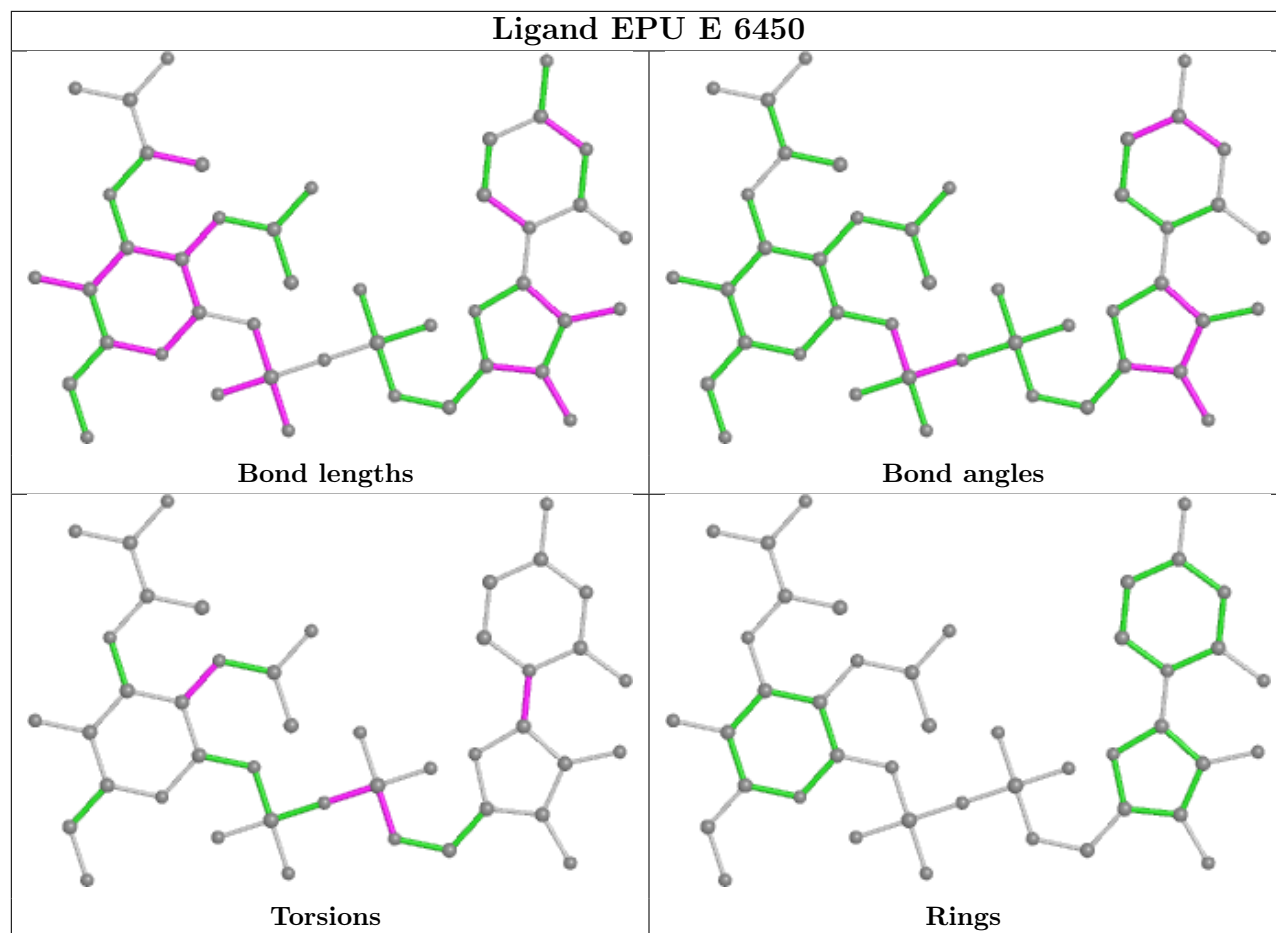


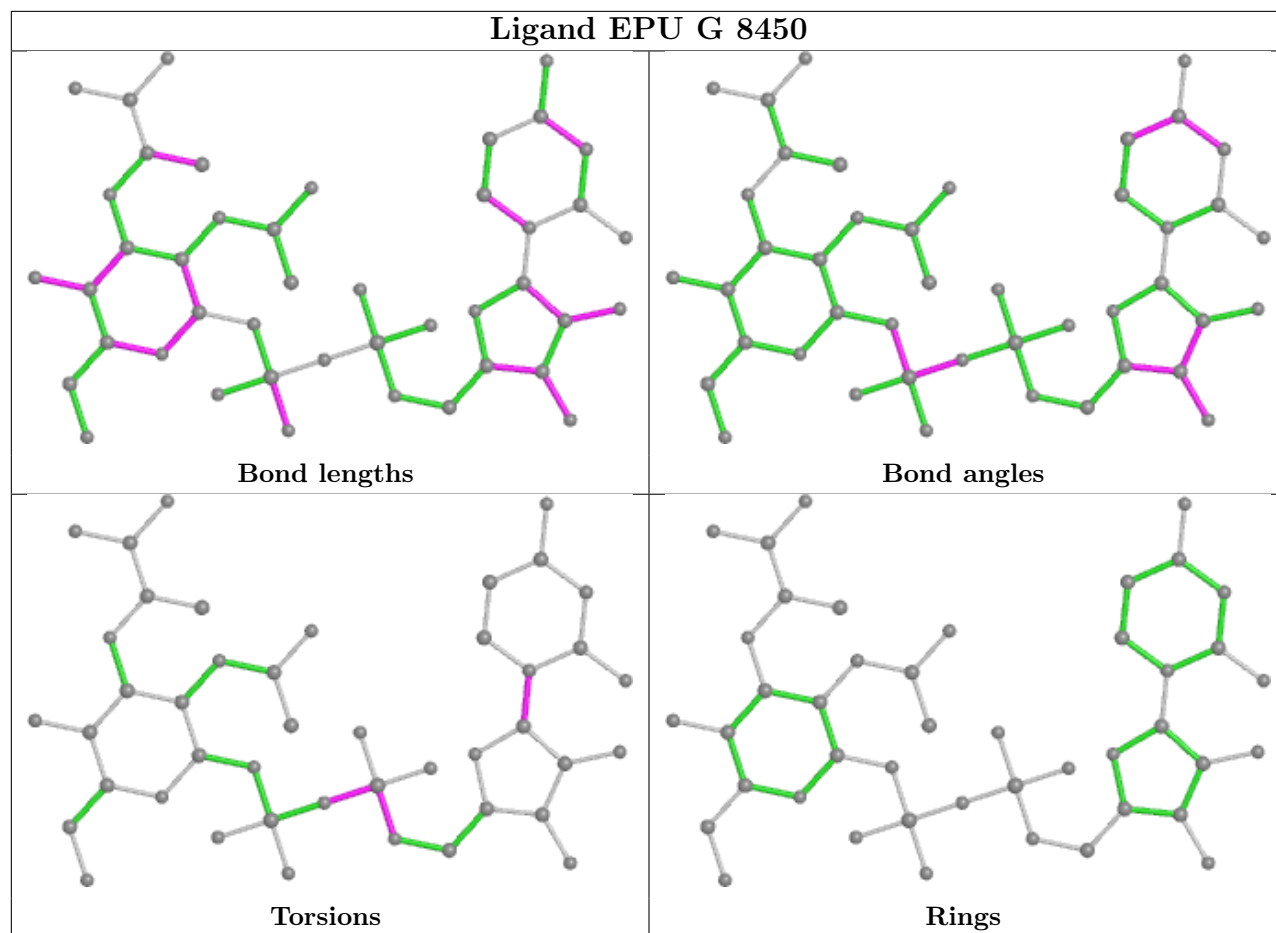


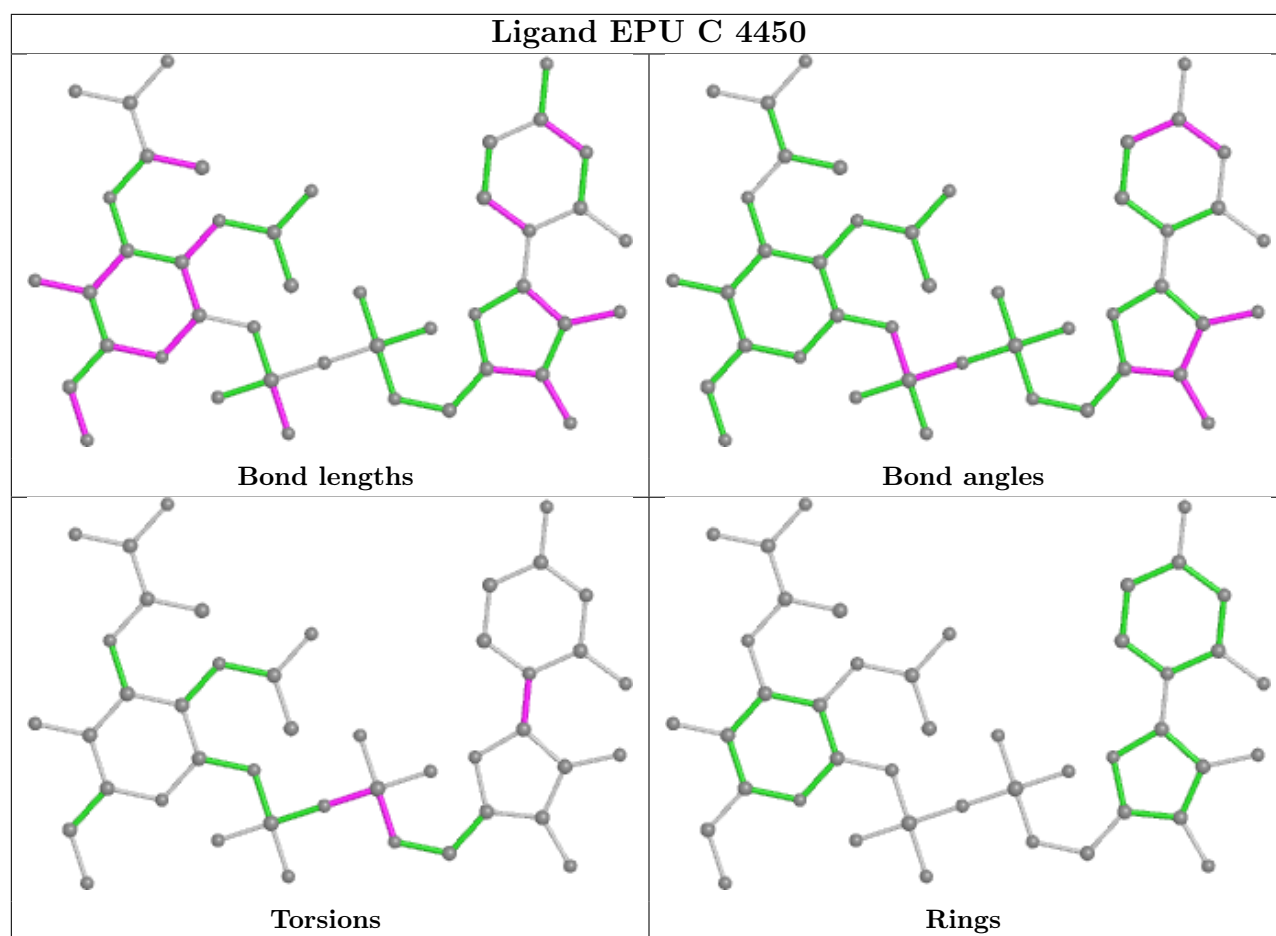












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	418/419 (99%)	-0.42	3 (0%) 87 91	7, 18, 33, 94	0
1	B	418/419 (99%)	-0.16	4 (0%) 82 86	10, 21, 38, 93	0
1	C	418/419 (99%)	-0.35	5 (1%) 79 83	9, 20, 35, 91	0
1	D	418/419 (99%)	-0.15	7 (1%) 70 76	10, 23, 40, 93	0
1	E	418/419 (99%)	-0.20	3 (0%) 87 91	12, 22, 36, 92	0
1	F	418/419 (99%)	0.26	18 (4%) 35 42	14, 29, 47, 95	0
1	G	418/419 (99%)	-0.19	5 (1%) 79 83	10, 22, 39, 94	0
1	H	418/419 (99%)	-0.27	3 (0%) 87 91	10, 21, 37, 92	0
All	All	3344/3352 (99%)	-0.19	48 (1%) 75 80	7, 22, 39, 95	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	418	GLY	9.2
1	F	419	GLU	8.8
1	A	419	GLU	7.5
1	H	419	GLU	7.0
1	B	419	GLU	6.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	IAS	F	67	8/9	0.81	0.30	34,36,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	IAS	B	67	8/9	0.93	0.15	23,26,29,35	0
1	IAS	D	67	8/9	0.95	0.17	24,27,29,31	0
1	IAS	E	67	8/9	0.96	0.19	22,26,28,34	0
1	IAS	C	67	8/9	0.96	0.14	20,21,28,28	0
1	IAS	H	67	8/9	0.96	0.13	18,22,24,24	0
1	IAS	G	67	8/9	0.97	0.14	21,23,25,28	0
1	IAS	A	67	8/9	0.97	0.09	13,16,17,18	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

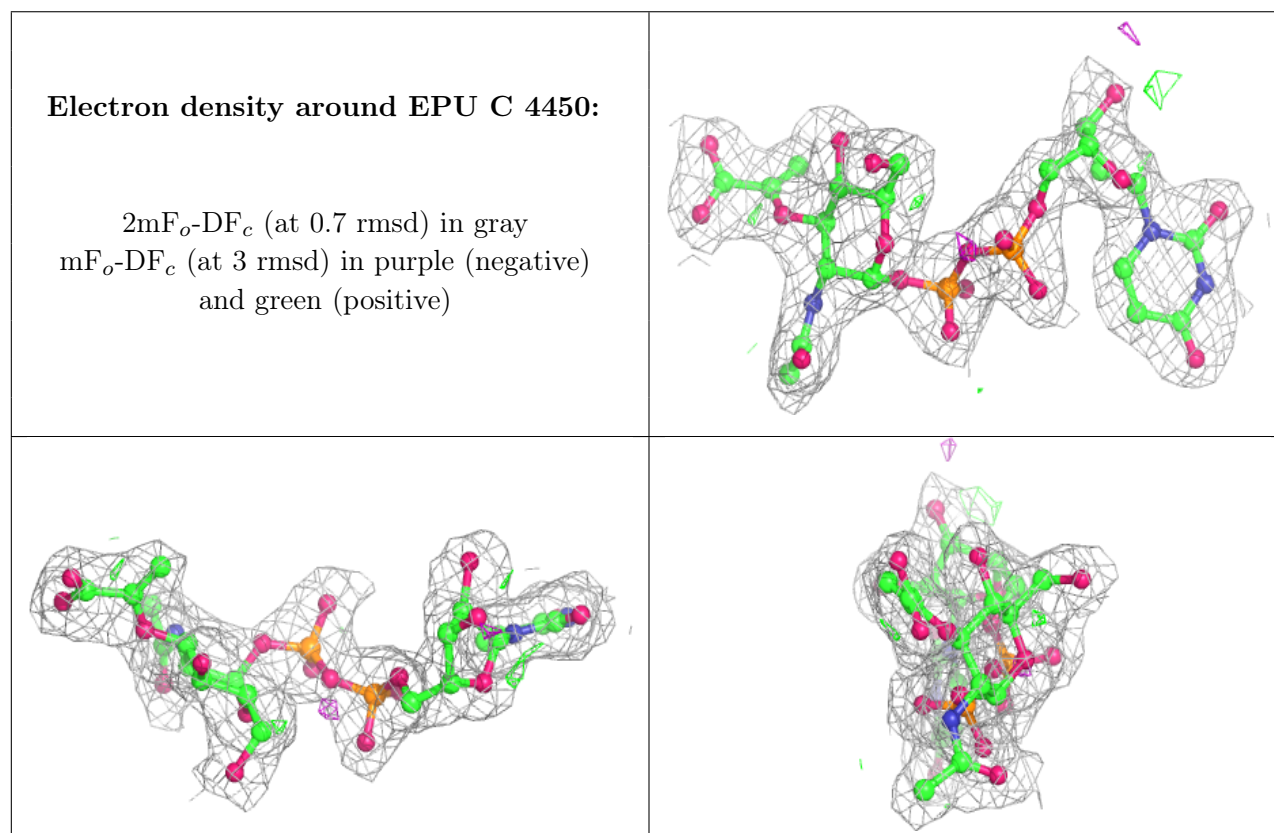
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	G	8462	5/5	0.74	0.22	91,92,93,93	0
4	GOL	C	4472	6/6	0.79	0.34	47,52,56,57	0
4	GOL	A	2472	6/6	0.81	0.25	43,46,46,50	0
4	GOL	C	3473	6/6	0.82	0.22	54,56,60,66	0
4	GOL	E	8472	6/6	0.82	0.34	51,56,59,61	0
4	GOL	C	2473	6/6	0.83	0.18	45,48,49,51	0
4	GOL	B	3472	6/6	0.85	0.27	53,55,55,58	0
4	GOL	F	7471	6/6	0.86	0.26	38,40,41,44	0
4	GOL	H	9472	6/6	0.86	0.29	40,47,50,52	0
4	GOL	D	5472	6/6	0.88	0.30	44,46,47,47	0
4	GOL	E	6471	6/6	0.89	0.23	23,27,30,33	0
4	GOL	A	2471	6/6	0.89	0.24	21,25,26,32	0
4	GOL	D	5471	6/6	0.90	0.26	24,29,34,38	0
4	GOL	C	4474	6/6	0.90	0.21	32,39,41,43	0
2	PO4	F	7461	5/5	0.91	0.21	64,65,66,70	0
4	GOL	G	8471	6/6	0.92	0.25	26,28,28,38	0
2	PO4	G	8461	5/5	0.92	0.19	50,52,55,58	0
2	PO4	B	3461	5/5	0.94	0.18	46,48,51,52	0
4	GOL	B	3471	6/6	0.94	0.22	23,25,27,32	0
4	GOL	C	4471	6/6	0.94	0.20	16,21,25,28	0
4	GOL	H	9471	6/6	0.94	0.22	24,28,30,36	0

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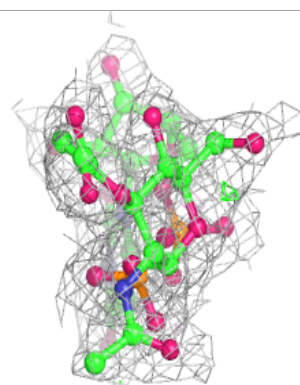
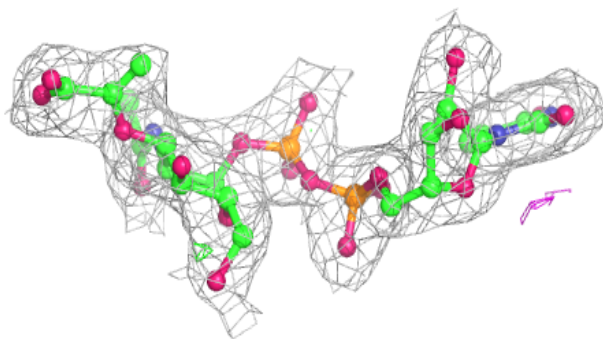
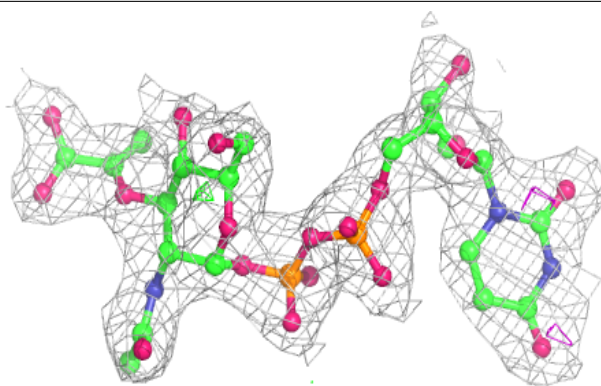
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	D	5461	5/5	0.94	0.17	54,55,58,61	0
2	PO4	A	2461	5/5	0.96	0.18	34,35,41,46	0
2	PO4	E	6461	5/5	0.96	0.15	47,50,50,52	0
2	PO4	H	9461	5/5	0.96	0.13	42,44,47,50	0
2	PO4	C	4461	5/5	0.96	0.15	42,45,48,50	0
3	EPU	C	4450	44/44	0.97	0.12	7,14,21,28	0
3	EPU	F	7450	44/44	0.97	0.13	14,21,27,29	0
3	EPU	G	8450	44/44	0.97	0.12	6,16,23,26	0
3	EPU	B	3450	44/44	0.97	0.11	8,16,20,24	0
3	EPU	A	2450	44/44	0.98	0.12	9,14,18,26	0
3	EPU	D	5450	44/44	0.98	0.10	10,17,27,31	0
3	EPU	H	9450	44/44	0.98	0.11	1,15,22,24	0
3	EPU	E	6450	44/44	0.98	0.11	8,15,21,22	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.

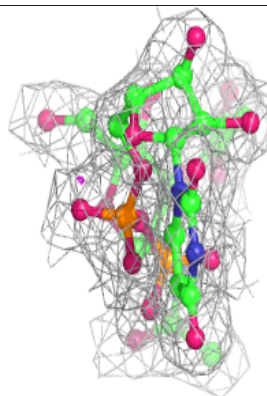
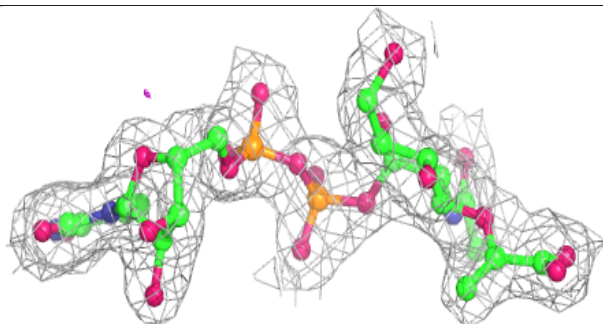
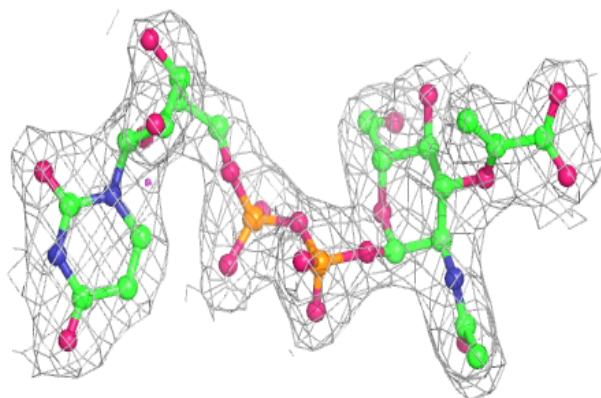


Electron density around EPU F 7450:

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

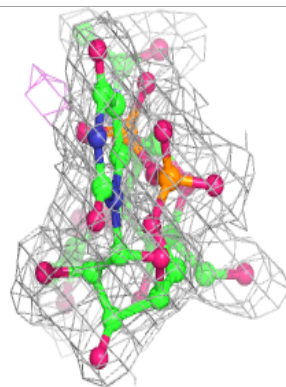
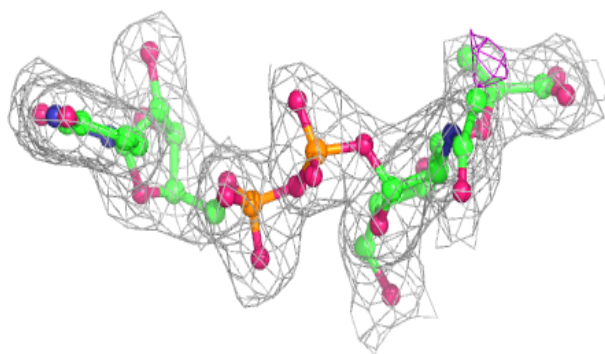
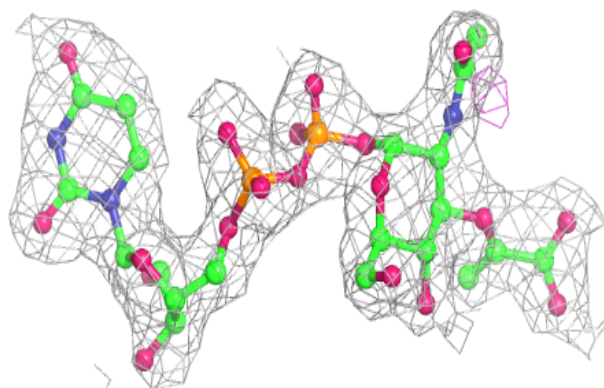
**Electron density around EPU G 8450:**

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

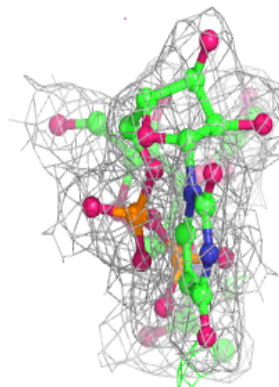
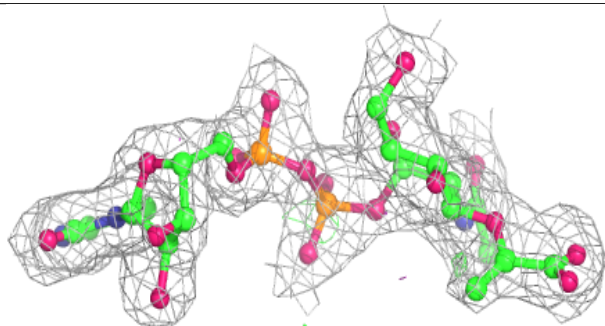
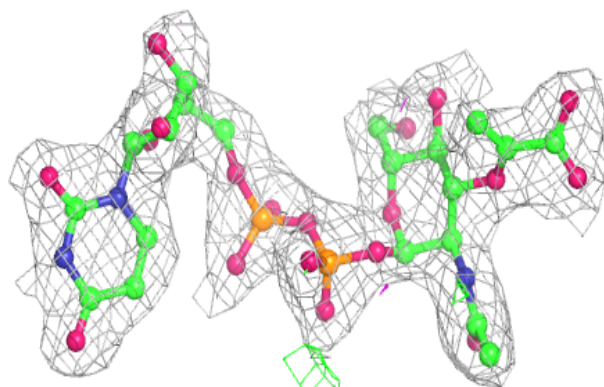


Electron density around EPU B 3450:

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

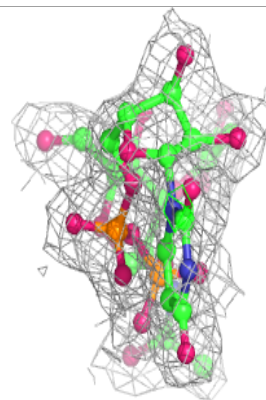
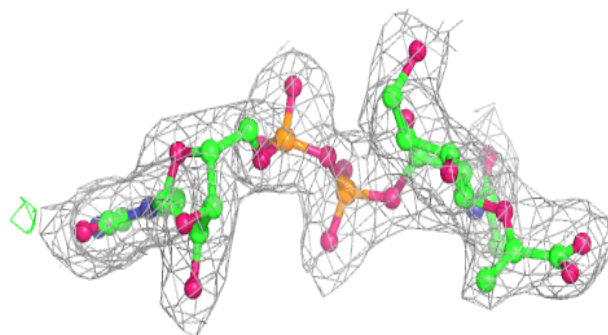
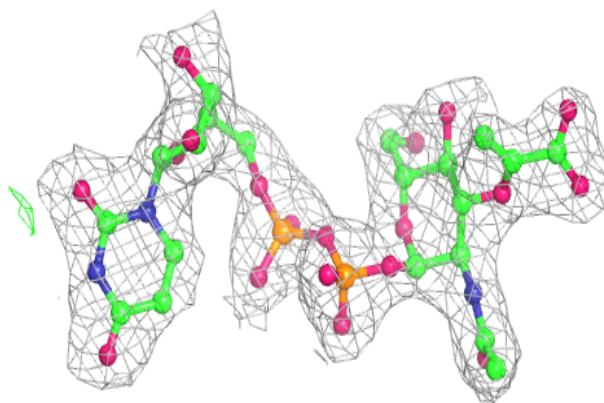
**Electron density around EPU A 2450:**

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

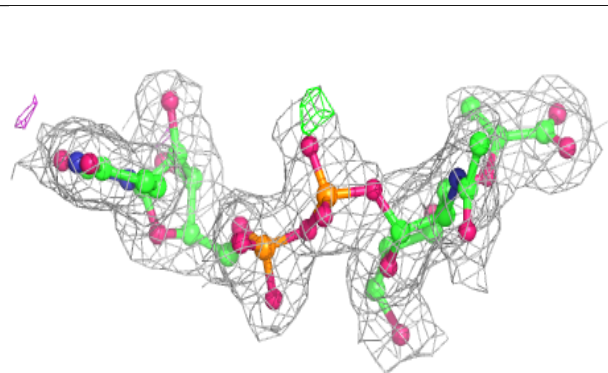
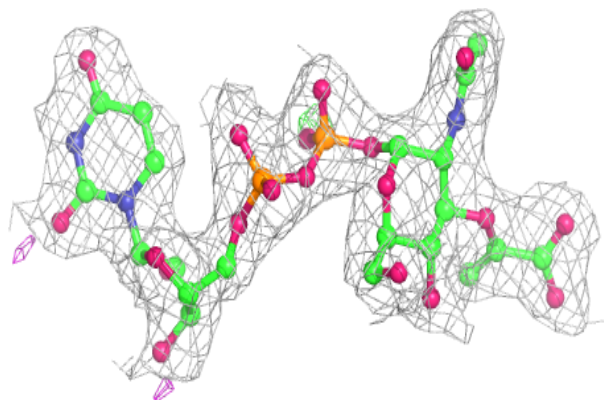


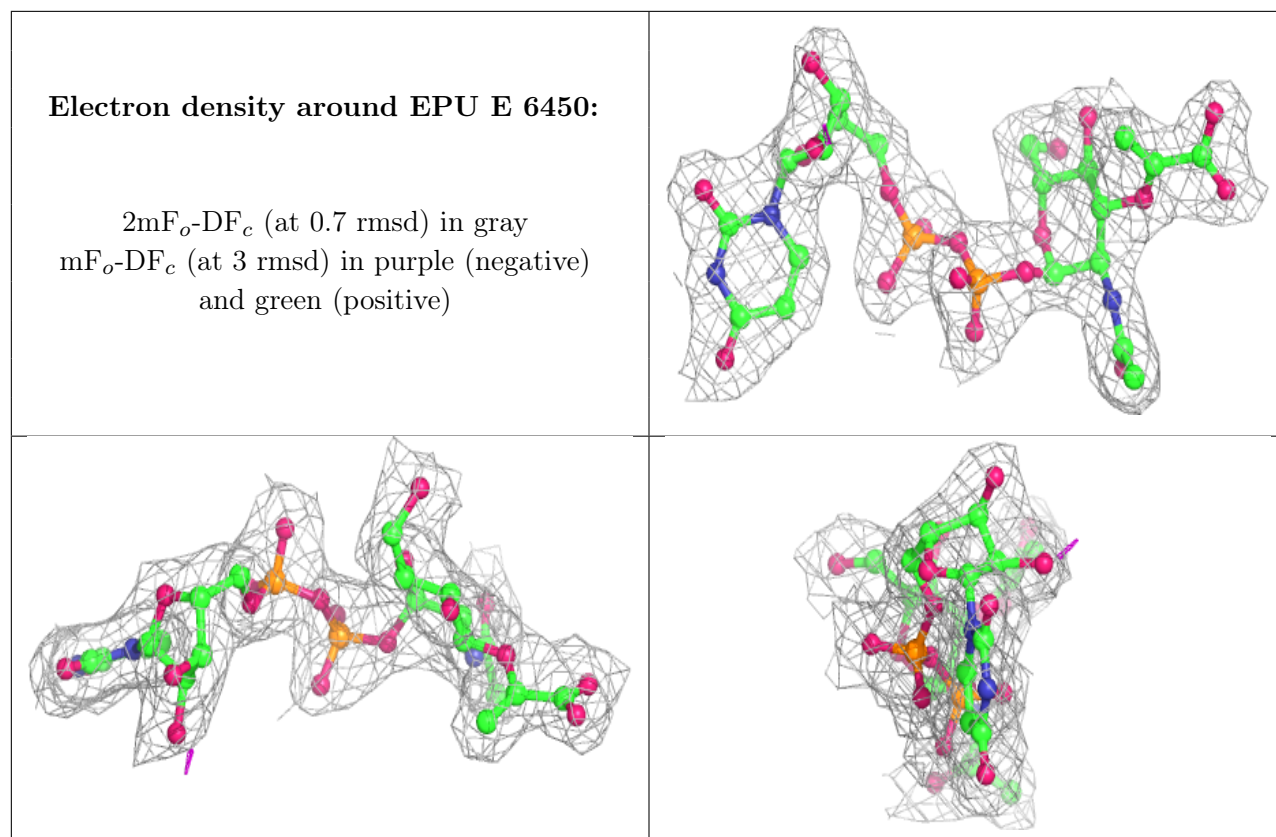
Electron density around EPU D 5450:

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

**Electron density around EPU H 9450:**

$2mF_o-DF_c$ (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.