



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:44 PM UTC

PDB ID : 8VH7 / pdb_00008vh7
Title : Crystal structure of heparosan synthase 2 from *Pasteurella multocida* at 1.98 Å
Authors : Pedersen, L.C.; Liu, J.; Stancanelli, E.; Krahn, J.M.
Deposited on : 2023-12-31
Resolution : 1.98 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

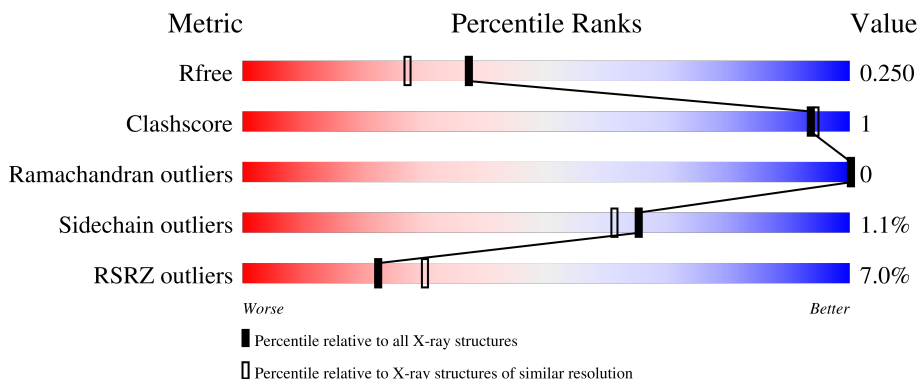
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	552	6% 89% 5% 5%
1	B	552	7% 92% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17480 atoms, of which 8173 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 Heparosan synthase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	522	Total	C	H	N	O	S	0	3	0
			8165	2655	4025	693	771	21			
1	B	522	Total	C	H	N	O	S	0	1	0
			8174	2654	4032	694	773	21			

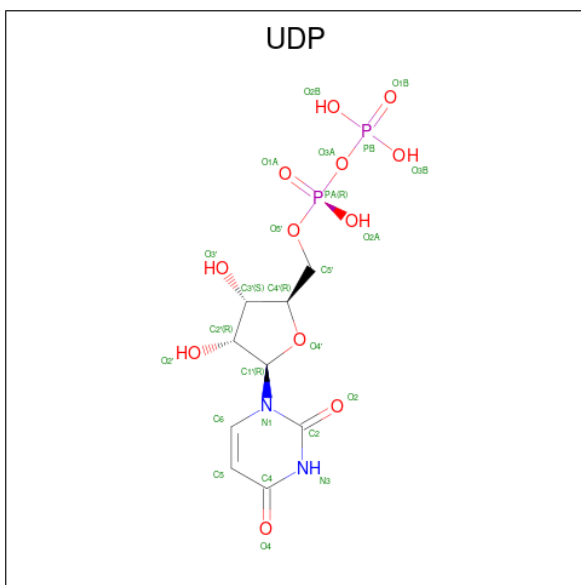
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	GLY	-	expression tag	UNP Q5SGE1
A	94	SER	-	expression tag	UNP Q5SGE1
A	95	ALA	-	expression tag	UNP Q5SGE1
A	96	ALA	-	expression tag	UNP Q5SGE1
A	97	ALA	-	expression tag	UNP Q5SGE1
B	93	GLY	-	expression tag	UNP Q5SGE1
B	94	SER	-	expression tag	UNP Q5SGE1
B	95	ALA	-	expression tag	UNP Q5SGE1
B	96	ALA	-	expression tag	UNP Q5SGE1
B	97	ALA	-	expression tag	UNP Q5SGE1

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

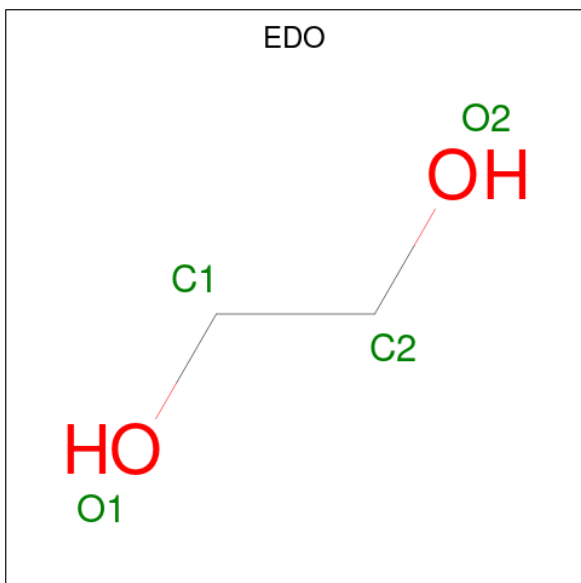
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
3	A	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
3	B	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0
3	B	1	Total 36	C 9	H 11	N 2	O 12	P 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Na 3 3	0	0
5	B	1	Total Na 1 1	0	0

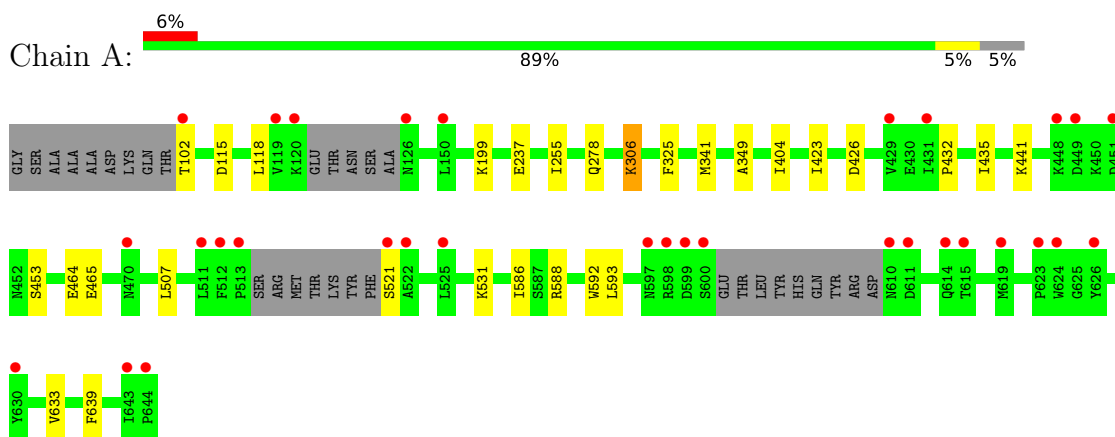
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	444	Total O 451 451	0	7
6	B	408	Total O 418 418	0	10

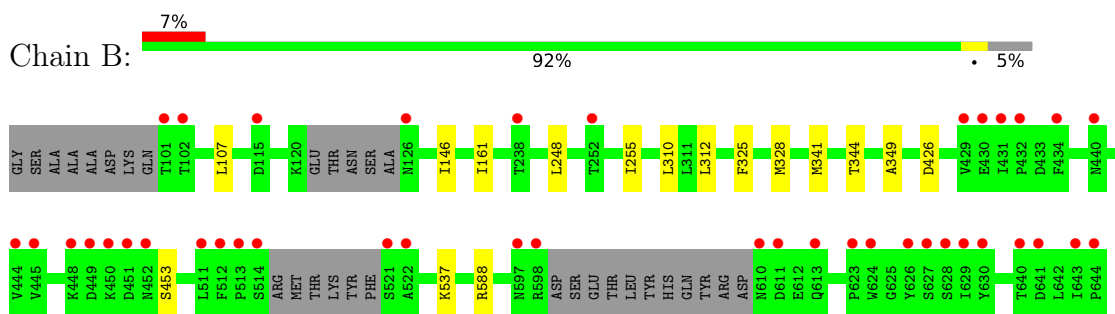
3 Residue-property plots [i](#)

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: Heparosan synthase B



• Molecule 1: Heparosan synthase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.18Å 163.18Å 84.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.70 – 1.98 45.70 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.70-1.98) 88.8 (45.70-1.98)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.249 0.208 , 0.250	Depositor DCC
R_{free} test set	2052 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17480	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 63.04 % 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 1.0271e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, EDO, NA, UDP

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	0.30	0/4237	0.51	0/5745
1	B	0.29	0/4230	0.49	0/5737
All	All	0.29	0/8467	0.50	0/11482

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4140	4025	4023	14	0
1	B	4142	4032	4031	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	50	22	22	0	0
3	B	50	22	22	0	0
4	A	20	30	30	1	0
4	B	28	42	42	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	451	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	418	0	0	1	0
All	All	9307	8173	8170	24	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 1.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LYS:NZ	6:A:802[A]:HOH:O	2.24	0.70
1:A:341:MET:HE1	1:A:349:ALA:HB2	1.75	0.68
1:A:102:THR:HG22	1:A:255:ILE:HD12	1.79	0.65
1:B:341:MET:HE1	1:B:349:ALA:HB2	1.83	0.61
1:B:310:LEU:HD21	1:B:312:LEU:HD12	1.83	0.60
1:A:464:GLU:OE2	6:A:801:HOH:O	2.17	0.58
1:B:426:ASP:OD2	1:B:453:SER:OG	2.24	0.55
1:A:426:ASP:OD2	1:A:453:SER:OG	2.26	0.54
1:A:441:LYS:NZ	6:A:804:HOH:O	2.26	0.48
1:B:107:LEU:HD11	1:B:255:ILE:CD1	2.43	0.48
1:A:278:GLN:NE2	6:A:1153[B]:HOH:O	2.48	0.47
1:A:592:TRP:HA	4:A:710:EDO:H21	1.97	0.47
1:B:248:LEU:CD2	1:B:255:ILE:HD13	2.46	0.45
1:A:507:LEU:HD13	1:A:593:LEU:HD22	1.97	0.45
1:A:115:ASP:HA	1:A:118:LEU:HD12	1.99	0.44
1:A:404:ILE:HD11	1:A:432:PRO:HG3	1.99	0.44
1:A:423:ILE:HD13	1:A:435:ILE:HD12	1.99	0.44
1:A:237:GLU:O	1:A:306:LYS:NZ	2.32	0.44
1:B:344:THR:HG23	6:B:1098:HOH:O	2.18	0.42
1:B:107:LEU:HD11	1:B:255:ILE:HD11	2.02	0.42
1:B:146:ILE:HD11	1:B:161:ILE:HD13	2.02	0.42
1:B:248:LEU:HD23	1:B:255:ILE:HD13	2.02	0.41
1:B:328:MET:HE3	1:B:341:MET:HA	2.03	0.40
1:A:633:VAL:HG13	1:A:639:PHE:O	2.20	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	517/552 (94%)	509 (98%)	8 (2%)	0	100	100
1	B	515/552 (93%)	507 (98%)	8 (2%)	0	100	100
All	All	1032/1104 (94%)	1016 (98%)	16 (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	451/504 (90%)	443 (98%)	8 (2%)	51	46
1	B	454/504 (90%)	451 (99%)	3 (1%)	76	73
All	All	905/1008 (90%)	894 (99%)	11 (1%)	65	58

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	LYS
1	A	306	LYS
1	A	325	PHE
1	A	465[A]	GLU
1	A	465[B]	GLU
1	A	521	SER
1	A	586	ILE
1	A	588	ARG

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Mol	Chain	Res	Type
1	B	325	PHE
1	B	537	LYS
1	B	588	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	339	GLN
1	A	369	GLN
1	A	497	ASN
1	B	339	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\# Z > 2$
3	UDP	B	702	2	25,26,26	0.67	1 (4%)	38,40,40	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	707	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	B	712	-	3,3,3	0.47	0	2,2,2	0.25	0
4	EDO	A	706	-	3,3,3	0.46	0	2,2,2	0.16	0
4	EDO	A	711	-	3,3,3	0.43	0	2,2,2	0.21	0
4	EDO	B	708	-	3,3,3	0.41	0	2,2,2	0.38	0
4	EDO	B	711	-	3,3,3	0.38	0	2,2,2	0.49	0
4	EDO	A	705	-	3,3,3	0.39	0	2,2,2	0.21	0
4	EDO	B	709	-	3,3,3	0.43	0	2,2,2	0.30	0
3	UDP	A	704	2	25,26,26	0.58	0	38,40,40	1.07	2 (5%)
4	EDO	A	712	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	B	710	-	3,3,3	0.42	0	2,2,2	0.40	0
3	UDP	A	702	2	25,26,26	0.59	0	38,40,40	0.68	0
4	EDO	B	706	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EDO	A	710	-	3,3,3	0.40	0	2,2,2	0.44	0
3	UDP	B	704	2	25,26,26	0.67	0	38,40,40	1.16	2 (5%)

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
3	UDP	B	702	2	-	0/16/32/32	0/2/2/2
4	EDO	B	707	-	-	1/1/1/1	-
4	EDO	B	712	-	-	1/1/1/1	-
4	EDO	A	706	-	-	1/1/1/1	-
4	EDO	A	711	-	-	1/1/1/1	-
4	EDO	B	708	-	-	0/1/1/1	-
4	EDO	B	711	-	-	1/1/1/1	-
4	EDO	A	705	-	-	0/1/1/1	-
4	EDO	B	709	-	-	1/1/1/1	-
3	UDP	A	704	2	-	0/16/32/32	0/2/2/2
4	EDO	A	712	-	-	1/1/1/1	-
4	EDO	B	710	-	-	0/1/1/1	-
3	UDP	A	702	2	-	0/16/32/32	0/2/2/2
4	EDO	B	706	-	-	1/1/1/1	-
4	EDO	A	710	-	-	0/1/1/1	-
3	UDP	B	704	2	-	0/16/32/32	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	UDP	PA-O3A	2.20	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	UDP	O2-C2-N1	3.65	127.55	122.80
3	A	704	UDP	O2-C2-N1	2.90	126.57	122.80
3	B	704	UDP	C4-N3-C2	2.76	130.05	126.61
3	A	704	UDP	C4-N3-C2	2.22	129.38	126.61

There are no chirality outliers.

All (8) torsion outliers are listed below:

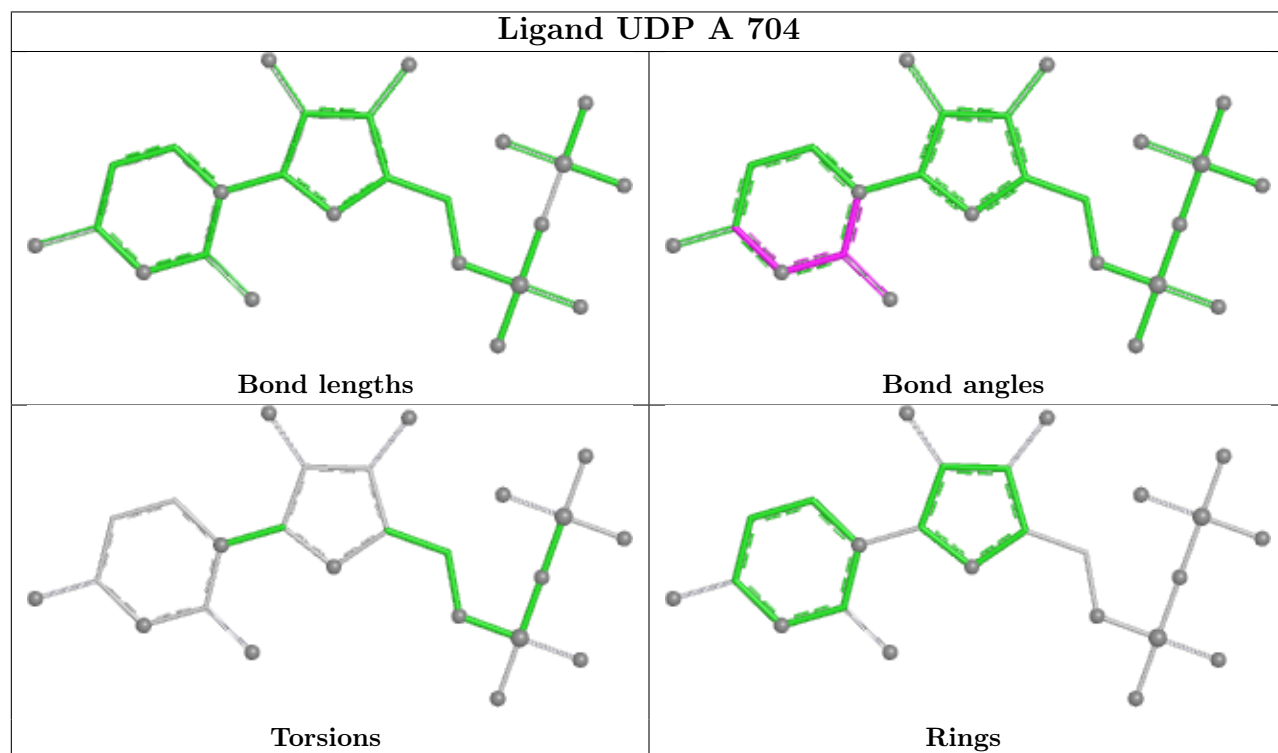
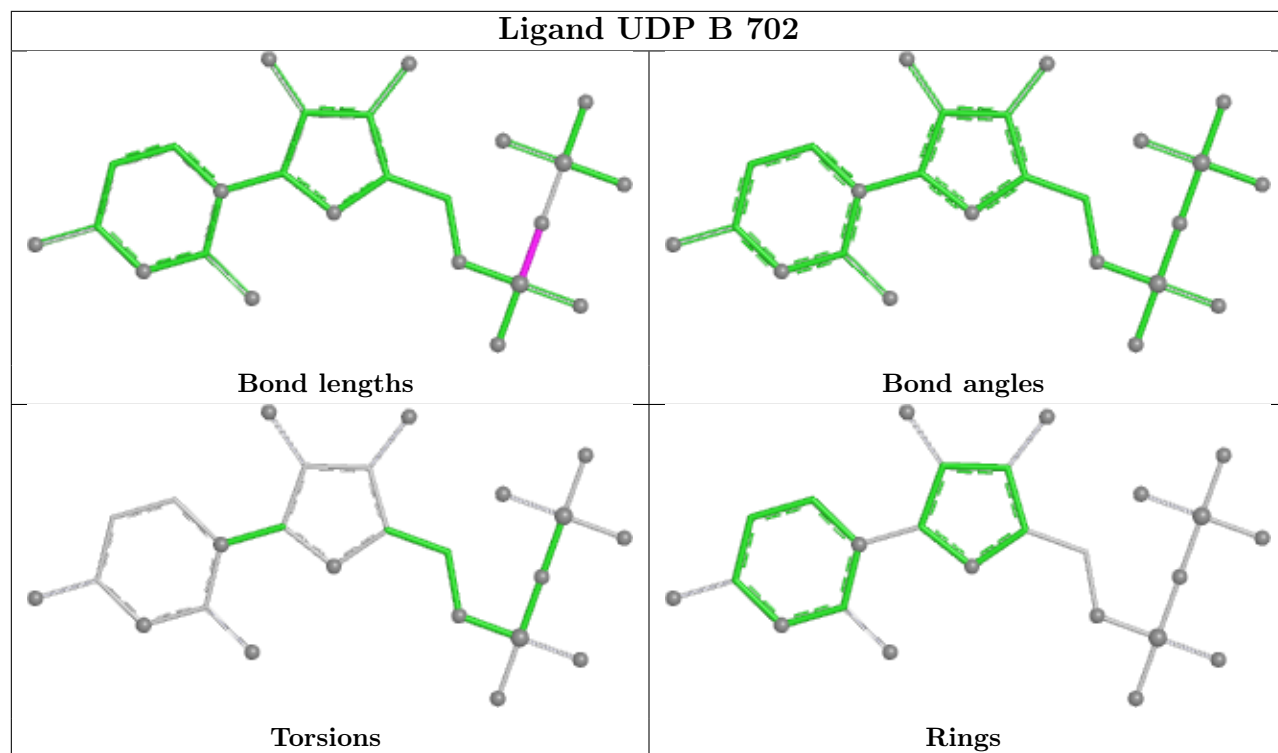
Mol	Chain	Res	Type	Atoms
4	A	711	EDO	O1-C1-C2-O2
4	B	706	EDO	O1-C1-C2-O2
4	B	709	EDO	O1-C1-C2-O2
4	B	711	EDO	O1-C1-C2-O2
4	A	706	EDO	O1-C1-C2-O2
4	A	712	EDO	O1-C1-C2-O2
4	B	712	EDO	O1-C1-C2-O2
4	B	707	EDO	O1-C1-C2-O2

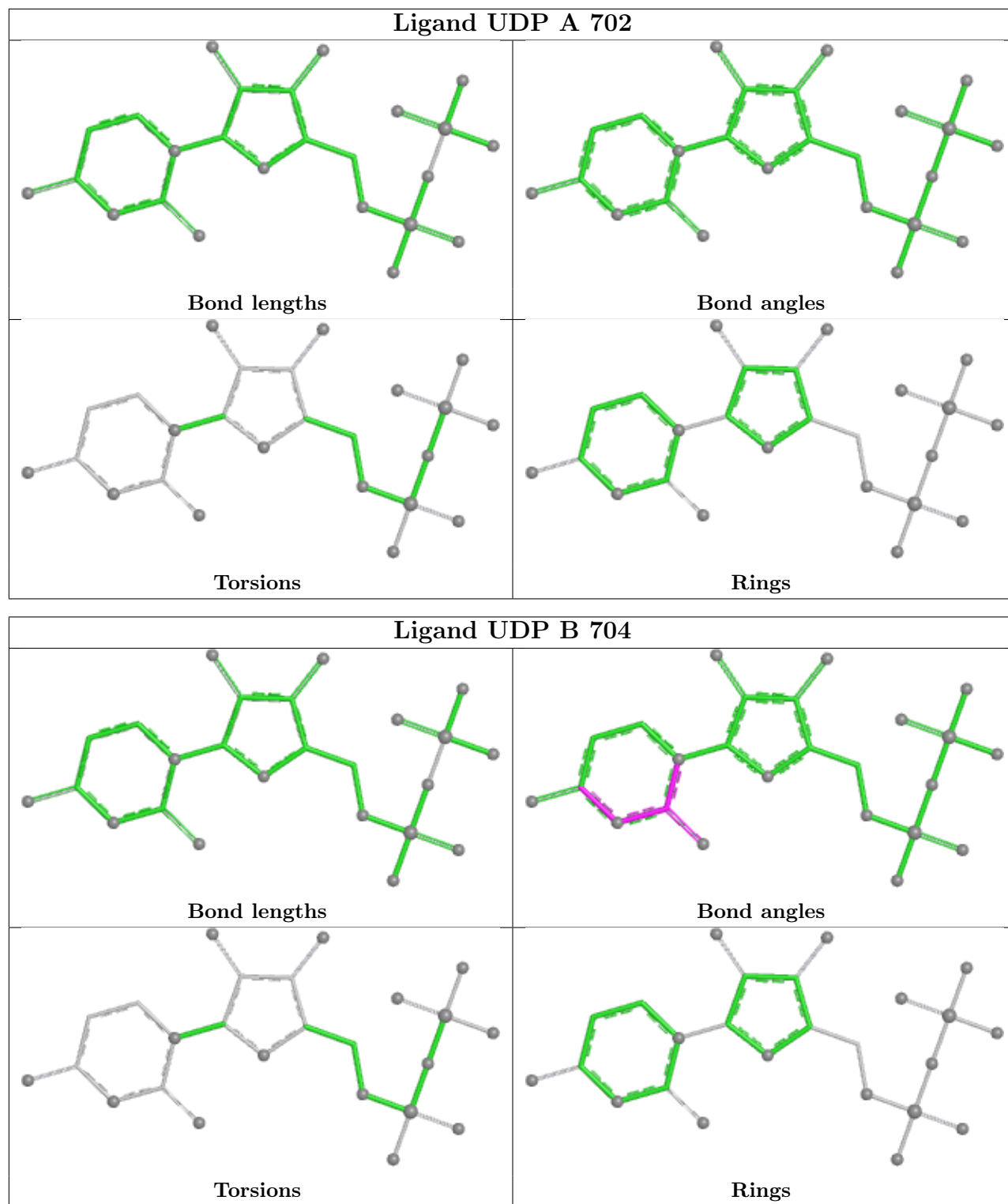
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	710	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	522/552 (94%)	0.43	32 (6%)	27 35	18, 29, 60, 95	3 (0%)
1	B	522/552 (94%)	0.52	41 (7%)	18 25	12, 29, 60, 90	1 (0%)
All	All	1044/1104 (94%)	0.47	73 (6%)	22 30	12, 29, 61, 95	4 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	THR	7.4
1	B	610	ASN	6.1
1	A	597	ASN	5.6
1	B	514	SER	5.6
1	B	521	SER	4.7
1	A	644	PRO	4.4
1	A	610	ASN	4.2
1	A	511	LEU	4.1
1	B	511	LEU	4.1
1	A	626	TYR	4.0
1	B	628	SER	3.9
1	A	431	ILE	3.9
1	A	513	PRO	3.7
1	A	623	PRO	3.7
1	B	623	PRO	3.7
1	B	522	ALA	3.7
1	B	630	TYR	3.7
1	A	600	SER	3.6
1	A	119	VAL	3.6
1	B	626	TYR	3.6
1	A	598	ARG	3.6
1	A	611	ASP	3.6
1	A	525	LEU	3.6
1	A	512	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	429	VAL	3.4
1	B	444	VAL	3.4
1	A	599	ASP	3.4
1	B	598	ARG	3.4
1	B	252	THR	3.3
1	B	449	ASP	3.1
1	A	522	ALA	3.1
1	A	630	TYR	2.8
1	B	431	ILE	2.8
1	A	643	ILE	2.8
1	B	597	ASN	2.7
1	B	430	GLU	2.7
1	B	434	PHE	2.7
1	B	613	GLN	2.6
1	B	627	SER	2.6
1	B	644	PRO	2.6
1	B	452	ASN	2.6
1	B	451	ASP	2.6
1	A	624	TRP	2.5
1	A	448	LYS	2.5
1	B	611	ASP	2.5
1	B	624	TRP	2.5
1	B	432	PRO	2.4
1	B	513	PRO	2.4
1	A	521	SER	2.4
1	A	150	LEU	2.4
1	B	643	ILE	2.4
1	B	512	PHE	2.3
1	A	615	THR	2.3
1	A	470	ASN	2.3
1	B	126	ASN	2.3
1	A	449	ASP	2.3
1	A	614	GLN	2.3
1	A	619	MET	2.3
1	A	120	LYS	2.3
1	B	115	ASP	2.3
1	B	445	VAL	2.2
1	B	448	LYS	2.2
1	B	102	THR	2.2
1	B	640	THR	2.2
1	A	126	ASN	2.1
1	B	629	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	238	THR	2.1
1	A	451	ASP	2.1
1	B	440	ASN	2.1
1	B	450	LYS	2.0
1	B	641	ASP	2.0
1	A	102	THR	2.0
1	B	429	VAL	2.0

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 [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(Å ²)	Q<0.9
4	EDO	B	707	4/4	0.59	0.23	54,64,68,70	0
4	EDO	A	711	4/4	0.63	0.22	41,59,71,71	0
5	NA	A	709	1/1	0.66	0.38	58,58,58,58	0
4	EDO	B	706	4/4	0.70	0.20	53,63,76,76	0
4	EDO	A	712	4/4	0.72	0.22	50,60,64,64	0
4	EDO	A	710	4/4	0.75	0.23	41,49,53,53	0
4	EDO	B	708	4/4	0.80	0.15	44,52,61,63	0
4	EDO	A	706	4/4	0.83	0.13	22,31,40,48	0
4	EDO	B	710	4/4	0.86	0.15	30,43,53,63	0
4	EDO	B	712	4/4	0.87	0.14	24,30,41,47	0
4	EDO	A	705	4/4	0.88	0.14	28,47,53,62	0
4	EDO	B	711	4/4	0.89	0.13	26,38,49,58	0
5	NA	A	708	1/1	0.93	0.10	44,44,44,44	0
4	EDO	B	709	4/4	0.93	0.11	19,26,31,35	0
3	UDP	B	702	25/25	0.95	0.07	26,35,48,57	0
3	UDP	A	702	25/25	0.96	0.07	28,34,47,52	0

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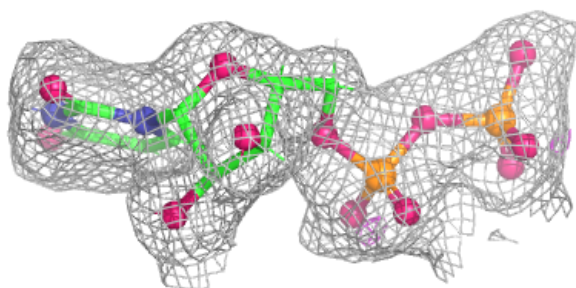
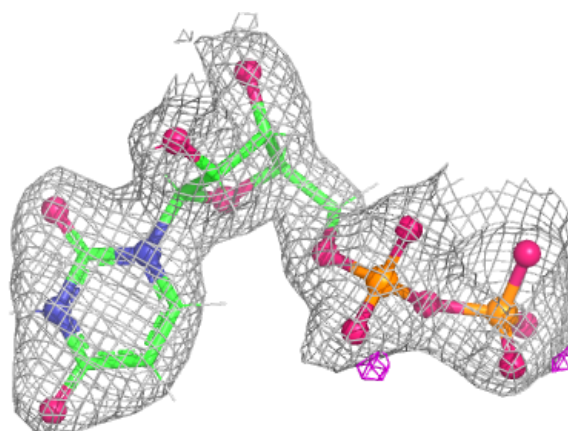
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	B	705	1/1	0.96	0.09	25,25,25,25	0
3	UDP	A	704	25/25	0.97	0.06	14,20,24,26	0
5	NA	A	707	1/1	0.98	0.04	27,27,27,27	0
3	UDP	B	704	25/25	0.98	0.04	15,20,24,24	0
2	MN	A	701	1/1	0.99	0.03	31,31,31,31	0
2	MN	B	703	1/1	1.00	0.02	22,22,22,22	0
2	MN	A	703	1/1	1.00	0.04	22,22,22,22	0
2	MN	B	701	1/1	1.00	0.02	31,31,31,31	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.

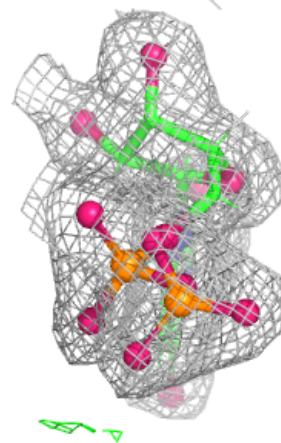
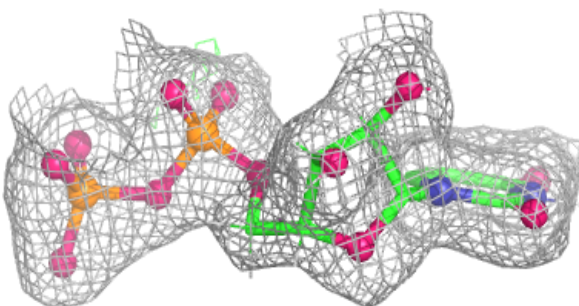
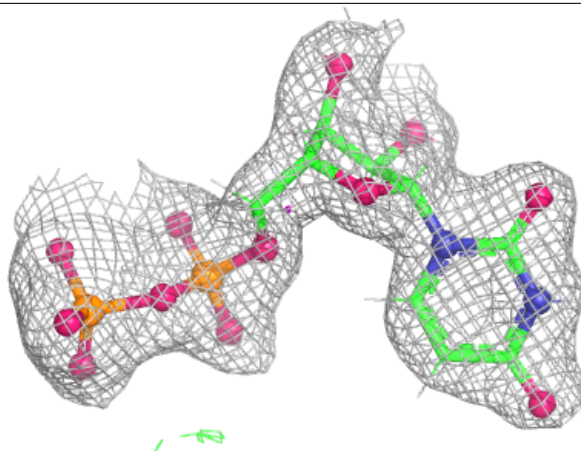
Electron density around UDP B 702:

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



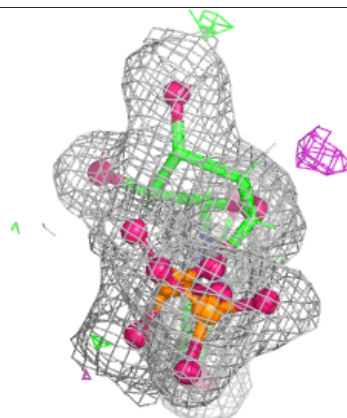
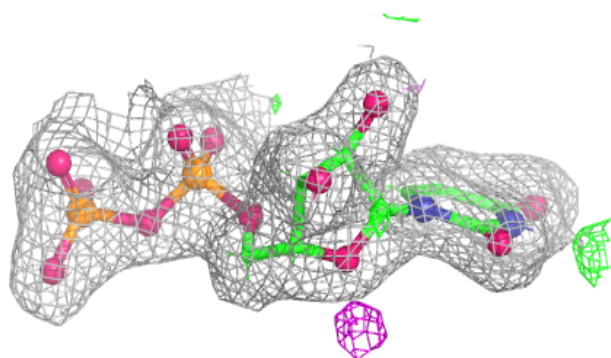
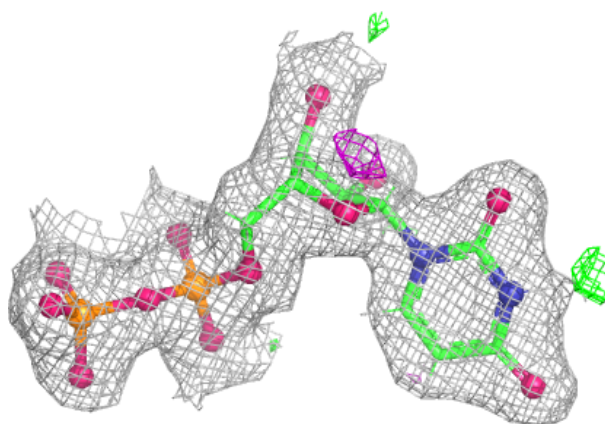
Electron density around UDP A 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



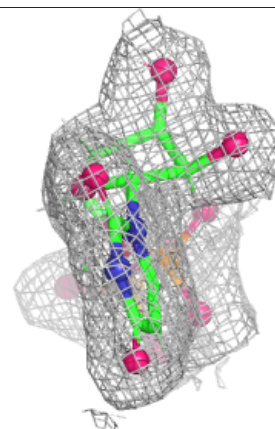
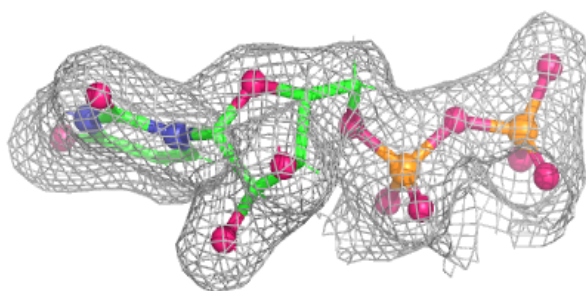
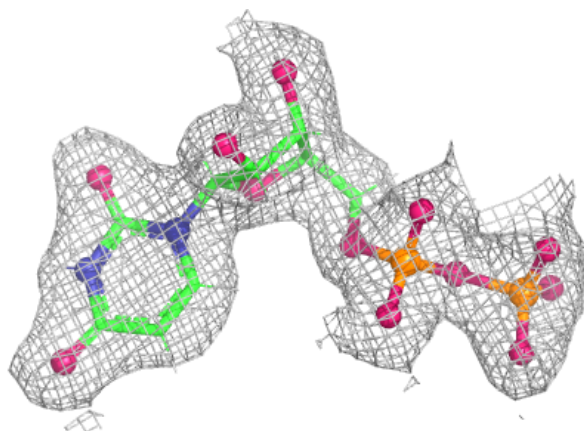
Electron density around UDP A 704:

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and green (positive)



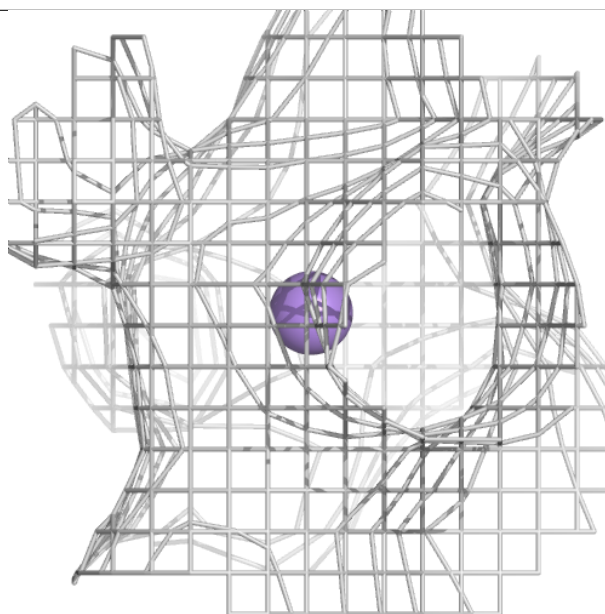
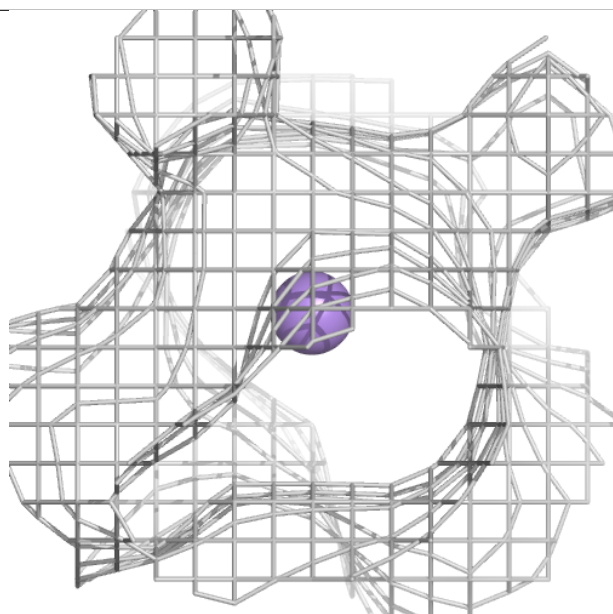
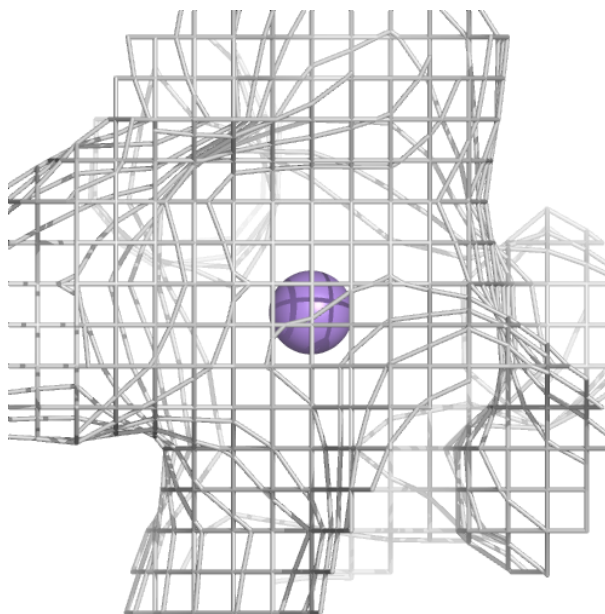
Electron density around UDP B 704:

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and green (positive)



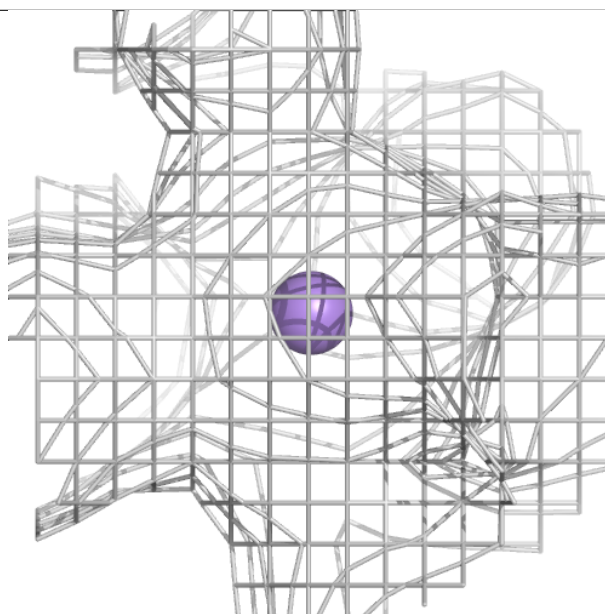
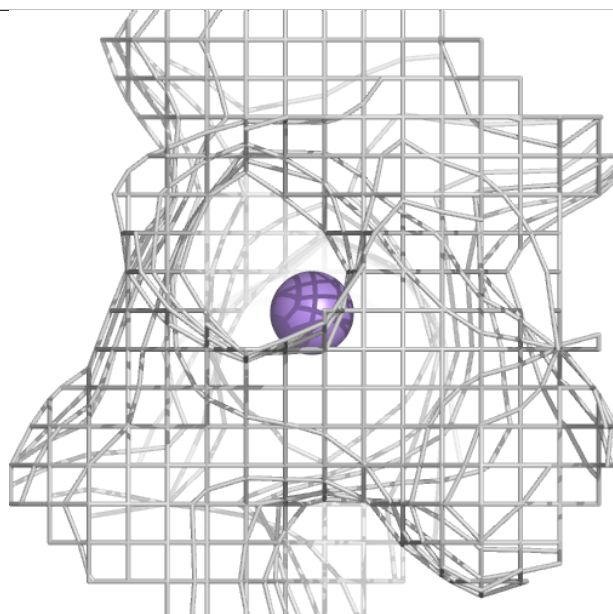
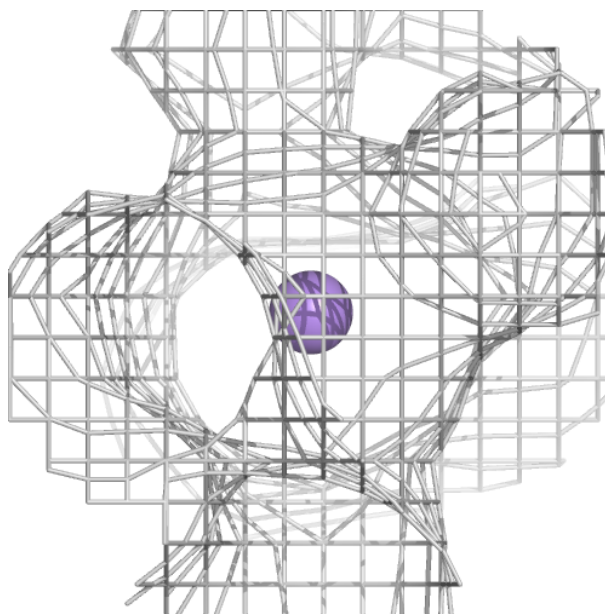
Electron density around MN A 701:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



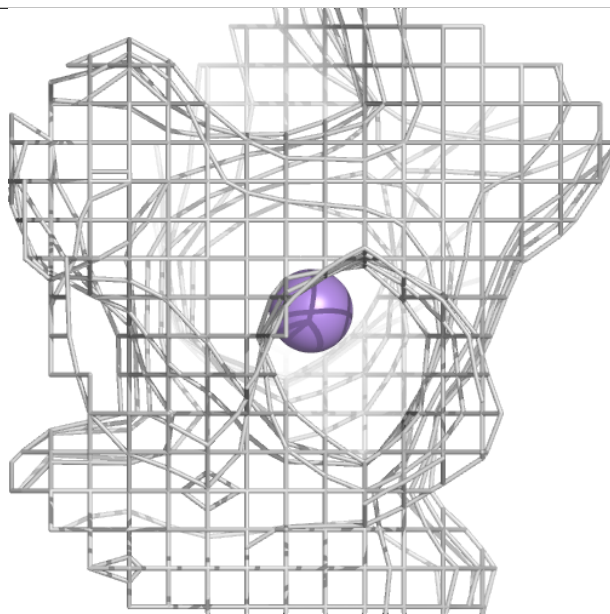
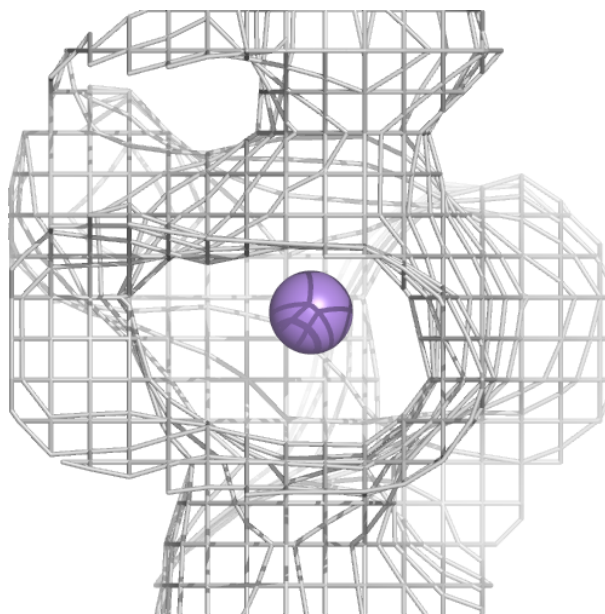
Electron density around MN B 703:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



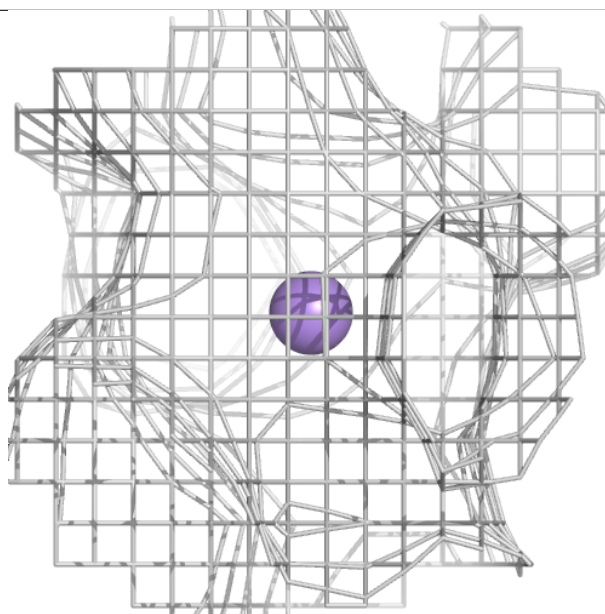
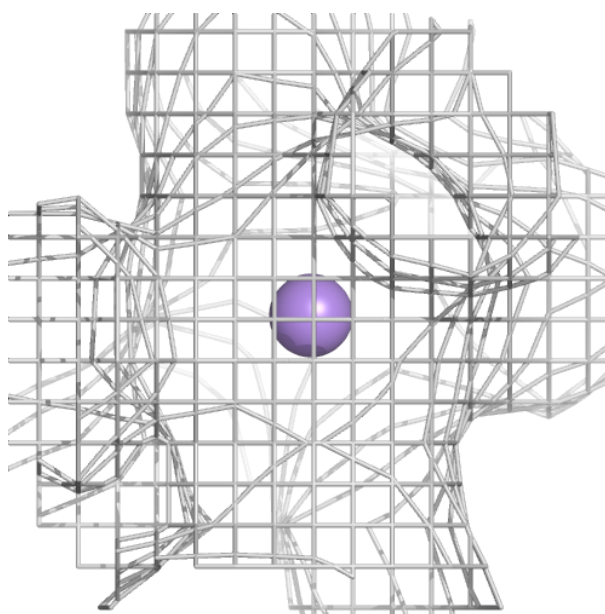
Electron density around MN A 703:

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



Electron density around MN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.