



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 08:32 PM JST

PDB ID : 7VZA
Title : The crystal structure of Non-hydrolyzing UDPGlcNAc 2-epimerase in complex with UDP
Authors : Li, T.L.; Rajesh, R.
Deposited on : 2021-11-15
Resolution : 2.58 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

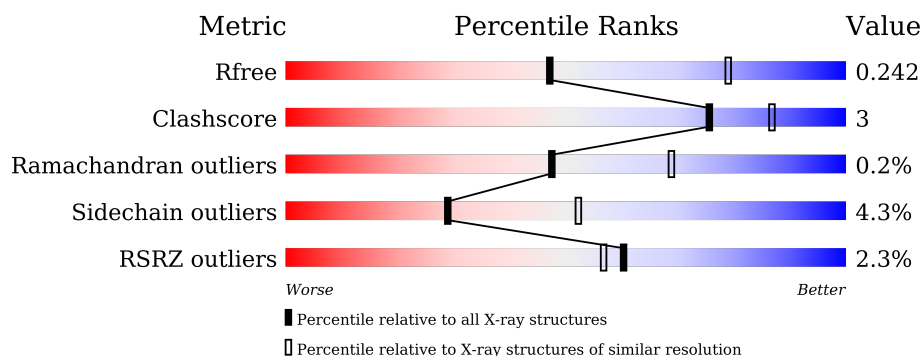
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	375	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>••</div> </div>
1	B	375	<div> <div>%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	C	375	<div> <div>2%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
1	D	375	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	E	375	<div> <div>%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
1	F	375	<div> <div>2%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	375	<div><div></div><div>3%</div><div>85%</div><div>10%</div><div></div><div></div></div>
1	H	375	<div><div></div><div>3%</div><div>87%</div><div>8%</div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22745 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.

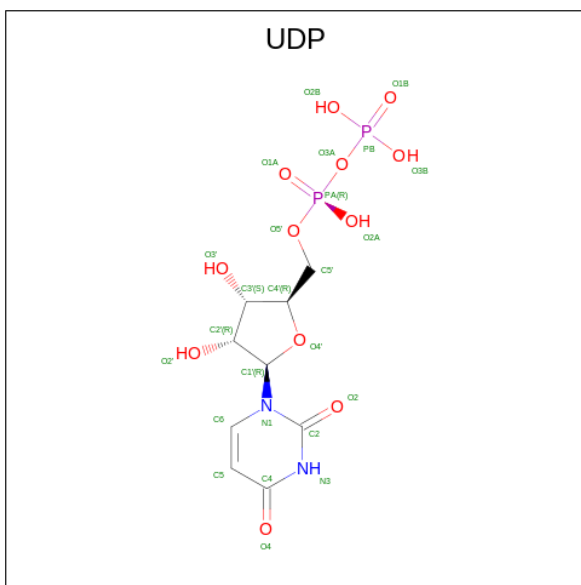
- Molecule 1 is a protein called Putative UDP-N-acetylglucosamine 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2831	1774	518	524	15			
1	B	362	Total	C	N	O	S	0	0	0
			2790	1752	509	515	14			
1	C	355	Total	C	N	O	S	0	0	0
			2737	1720	498	505	14			
1	D	359	Total	C	N	O	S	0	0	0
			2768	1738	506	510	14			
1	E	360	Total	C	N	O	S	0	0	0
			2774	1742	506	512	14			
1	F	360	Total	C	N	O	S	0	0	0
			2771	1740	504	513	14			
1	G	359	Total	C	N	O	S	0	0	0
			2764	1736	502	511	15			
1	H	359	Total	C	N	O	S	0	0	0
			2768	1739	503	512	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A0A0K1H2R6
B	0	HIS	-	expression tag	UNP A0A0K1H2R6
C	0	HIS	-	expression tag	UNP A0A0K1H2R6
D	0	HIS	-	expression tag	UNP A0A0K1H2R6
E	0	HIS	-	expression tag	UNP A0A0K1H2R6
F	0	HIS	-	expression tag	UNP A0A0K1H2R6
G	0	HIS	-	expression tag	UNP A0A0K1H2R6
H	0	HIS	-	expression tag	UNP A0A0K1H2R6

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	B	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	C	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	D	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	E	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	F	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	G	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	H	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0

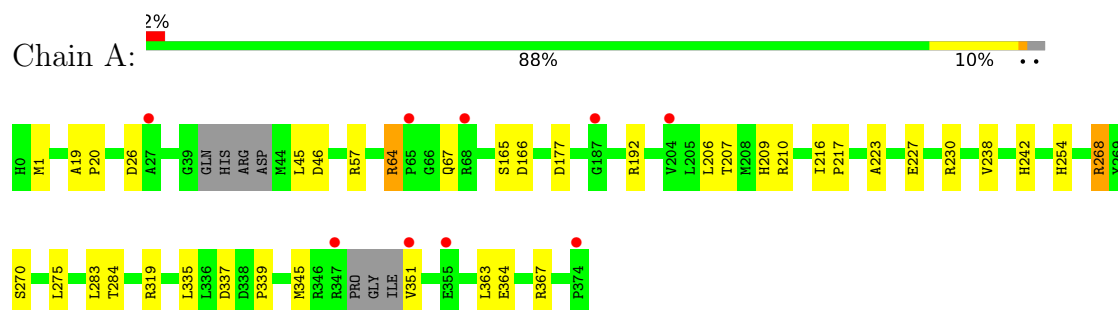
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	57	Total 57	O 57	0	0
4	C	39	Total 39	O 39	0	0
4	D	41	Total 41	O 41	0	0
4	E	66	Total 66	O 66	0	0
4	F	48	Total 48	O 48	0	0
4	G	40	Total 40	O 40	0	0
4	H	20	Total 20	O 20	0	0

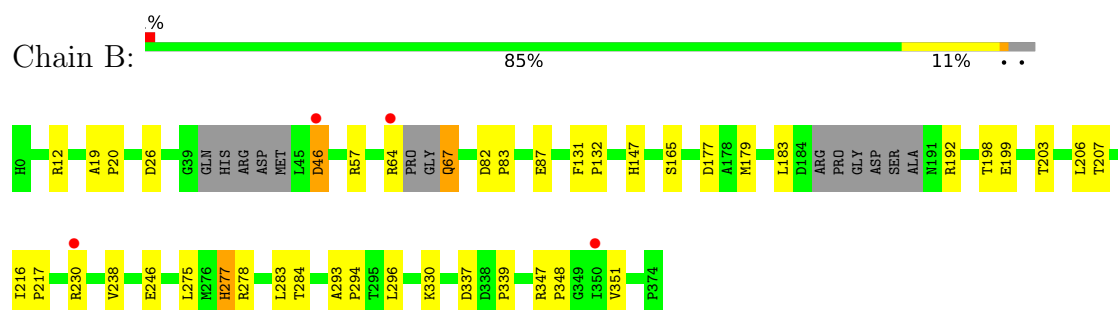
3 Residue-property plots [i](#)

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.

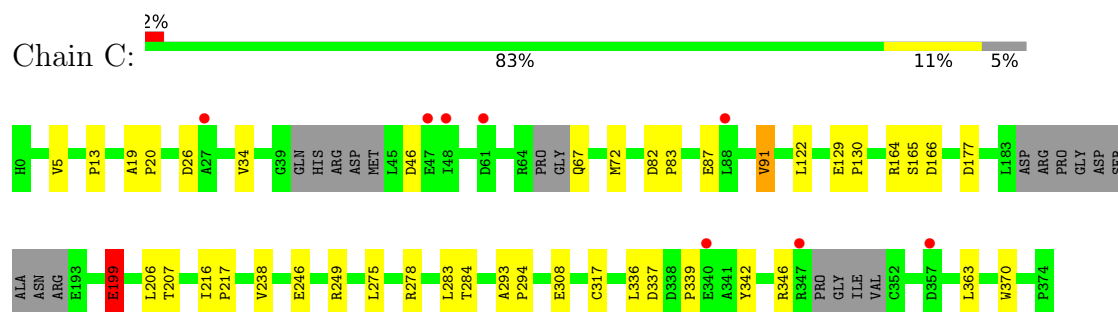
- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase



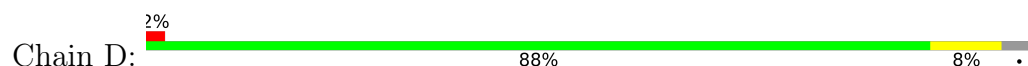
- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase

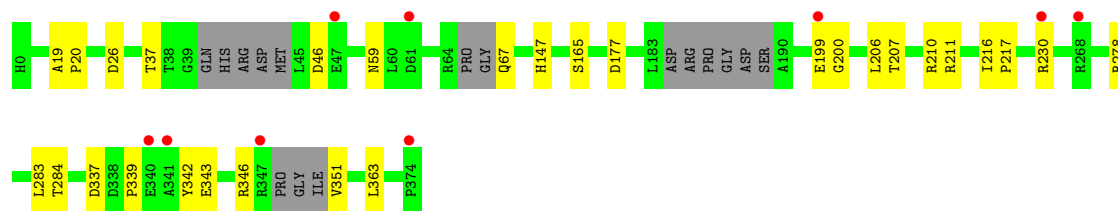


- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase

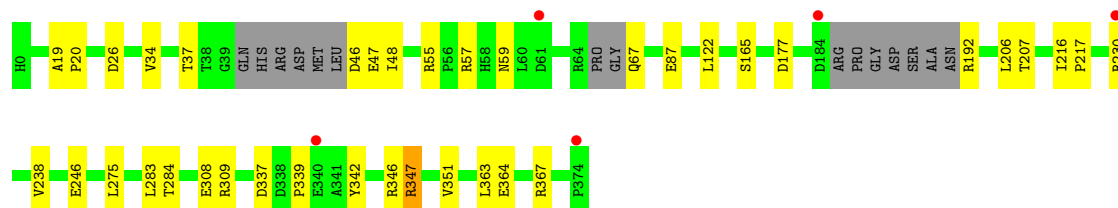
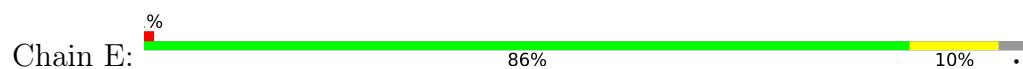


- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase

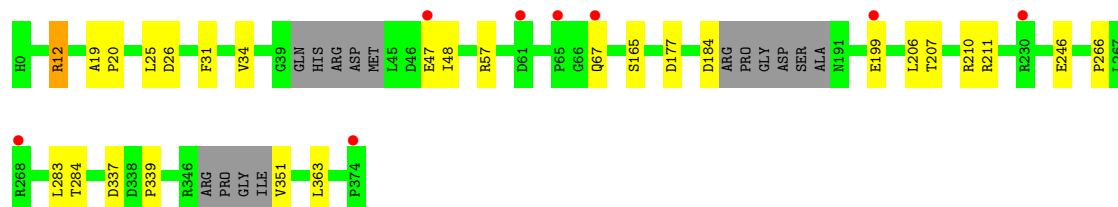
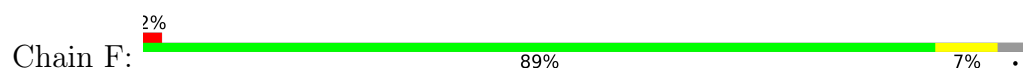




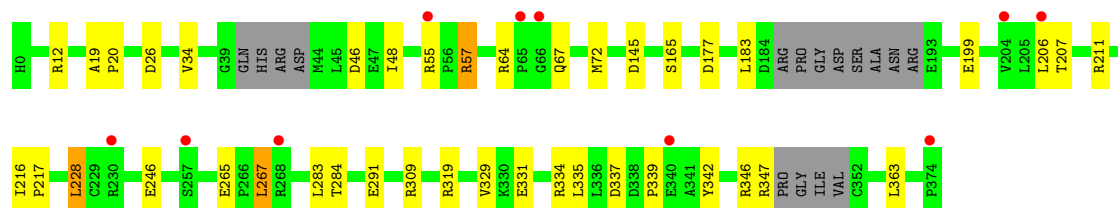
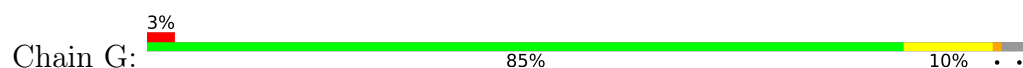
- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase



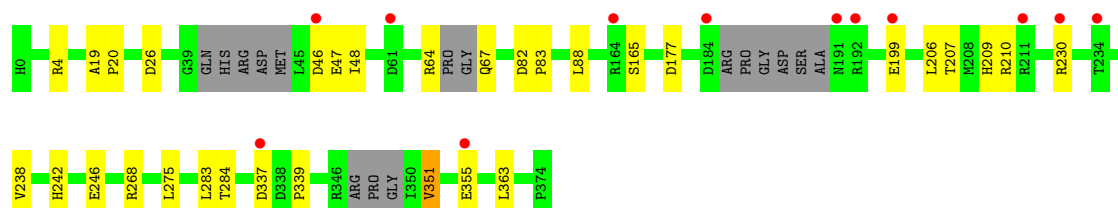
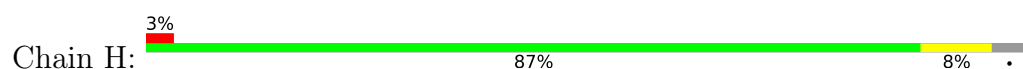
- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase



- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase



- Molecule 1: Putative UDP-N-acetylglucosamine 2-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.82Å 104.77Å 106.31Å 74.54° 73.05° 68.39°	Depositor
Resolution (Å)	19.89 – 2.58 19.89 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.89-2.58) 94.1 (19.89-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.59Å)	Xtriage
Refinement program	PHENIX v1.0	Depositor
R, R_{free}	0.210 , 0.249 0.211 , 0.242	Depositor DCC
R_{free} test set	4644 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22745	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: UDP, NA

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	0.66	0/2881	0.80	0/3913
1	B	0.66	0/2838	0.79	1/3854 (0.0%)
1	C	0.66	0/2783	0.80	0/3777
1	D	0.66	0/2814	0.79	0/3819
1	E	0.67	0/2822	0.80	0/3832
1	F	0.66	0/2819	0.78	0/3829
1	G	0.67	0/2812	0.80	0/3818
1	H	0.66	0/2814	0.78	0/3820
All	All	0.66	0/22583	0.79	1/30662 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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	2831	0	2857	19	0
1	B	2790	0	2821	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2737	0	2767	21	0
1	D	2768	0	2800	19	0
1	E	2774	0	2804	14	0
1	F	2771	0	2797	11	0
1	G	2764	0	2791	21	0
1	H	2768	0	2797	12	0
2	A	25	0	11	1	0
2	B	25	0	11	0	0
2	C	25	0	11	2	0
2	D	25	0	11	0	0
2	E	25	0	11	0	0
2	F	25	0	11	0	0
2	G	25	0	11	1	0
2	H	25	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	23	0	0	1	0
4	B	57	0	0	3	0
4	C	39	0	0	3	0
4	D	41	0	0	3	0
4	E	66	0	0	0	0
4	F	48	0	0	1	0
4	G	40	0	0	1	0
4	H	20	0	0	0	0
All	All	22745	0	22522	137	0

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

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:PRO:HG3	2:C:401:UDP:O1A	1.57	1.02
1:G:331:GLU:O	1:G:335:LEU:CD1	2.26	0.83
1:G:228:LEU:HD11	1:G:329:VAL:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:GLU:O	1:G:335:LEU:HD12	1.89	0.73
1:C:13:PRO:CG	2:C:401:UDP:O1A	2.35	0.73
1:H:88:LEU:O	1:H:88:LEU:HG	1.89	0.73
1:G:331:GLU:O	1:G:335:LEU:HD13	1.89	0.72
1:A:319:ARG:HD2	1:A:345:MET:HE2	1.74	0.70
1:G:228:LEU:HD13	1:G:329:VAL:HG22	1.74	0.70
1:A:319:ARG:HD3	1:A:345:MET:CE	2.22	0.69
1:A:319:ARG:HD3	1:A:345:MET:HE1	1.75	0.68
1:G:265:GLU:O	1:G:267:LEU:HD13	1.93	0.68
1:D:211:ARG:NH1	4:D:501:HOH:O	2.28	0.66
1:A:319:ARG:CD	1:A:345:MET:CE	2.76	0.63
1:B:277:HIS:NE2	1:B:296:LEU:HD22	2.14	0.62
1:A:319:ARG:CD	1:A:345:MET:HE2	2.29	0.62
1:B:277:HIS:CD2	1:D:339:PRO:HG2	2.36	0.61
1:H:209:HIS:HB2	1:H:242:HIS:CD2	2.38	0.59
1:A:335:LEU:HD21	1:A:345:MET:HE3	1.84	0.59
1:G:228:LEU:CD1	1:G:329:VAL:HG22	2.32	0.59
1:E:37:THR:OG1	1:E:59:ASN:ND2	2.36	0.57
1:C:317:CYS:SG	4:C:539:HOH:O	2.54	0.57
1:D:211:ARG:NH1	4:D:504:HOH:O	2.37	0.57
1:H:207:THR:O	1:H:284:THR:HA	2.05	0.57
1:A:207:THR:O	1:A:284:THR:HA	2.05	0.57
1:E:207:THR:O	1:E:284:THR:HA	2.05	0.57
1:F:207:THR:O	1:F:284:THR:HA	2.05	0.57
1:F:184:ASP:C	4:F:509:HOH:O	2.43	0.56
1:B:207:THR:O	1:B:284:THR:HA	2.05	0.56
1:C:207:THR:O	1:C:284:THR:HA	2.06	0.56
1:D:207:THR:O	1:D:284:THR:HA	2.05	0.56
1:G:207:THR:O	1:G:284:THR:HA	2.05	0.56
1:G:12:ARG:NH1	2:G:401:UDP:O2	2.39	0.56
1:E:122:LEU:HB3	1:E:308:GLU:HB2	1.88	0.55
1:G:291:GLU:OE1	1:G:309:ARG:NE	2.38	0.55
1:B:12:ARG:NH2	4:B:501:HOH:O	2.22	0.55
1:E:57:ARG:NH1	1:E:87:GLU:OE1	2.40	0.54
1:F:206:LEU:HA	1:F:283:LEU:O	2.08	0.54
1:D:206:LEU:HA	1:D:283:LEU:O	2.08	0.54
1:G:206:LEU:HA	1:G:283:LEU:O	2.08	0.53
1:A:206:LEU:HA	1:A:283:LEU:O	2.08	0.53
1:C:91:VAL:HG11	1:C:370:TRP:CE3	2.44	0.53
1:H:206:LEU:HA	1:H:283:LEU:O	2.08	0.53
1:B:277:HIS:NE2	1:D:339:PRO:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:THR:OG1	1:D:59:ASN:ND2	2.37	0.53
1:C:206:LEU:HA	1:C:283:LEU:O	2.08	0.53
1:B:206:LEU:HA	1:B:283:LEU:O	2.09	0.53
1:E:346:ARG:O	1:E:347:ARG:C	2.47	0.53
1:H:4:ARG:HD3	1:H:88:LEU:HG	1.90	0.53
1:E:206:LEU:HA	1:E:283:LEU:O	2.08	0.53
1:H:88:LEU:O	1:H:88:LEU:CG	2.55	0.52
1:D:147:HIS:HD2	4:D:511:HOH:O	1.92	0.52
1:B:347:ARG:HA	1:D:200:GLY:HA2	1.91	0.52
1:F:12:ARG:NH1	1:F:266:PRO:HB3	2.24	0.52
1:B:19:ALA:HB3	1:B:20:PRO:HD3	1.92	0.52
1:A:209:HIS:HB2	1:A:242:HIS:CD2	2.45	0.51
1:G:291:GLU:OE1	1:G:309:ARG:NH2	2.41	0.51
1:B:57:ARG:HD2	1:B:87:GLU:OE1	2.10	0.51
1:B:183:LEU:HB2	1:D:343:GLU:HG2	1.91	0.51
1:A:254:HIS:CE1	4:A:511:HOH:O	2.63	0.51
1:G:34:VAL:HG13	1:G:57:ARG:HD3	1.92	0.50
1:D:19:ALA:HB3	1:D:20:PRO:HD3	1.94	0.50
1:F:31:PHE:CE1	1:F:363:LEU:HD22	2.47	0.49
1:B:277:HIS:CE1	1:D:339:PRO:CB	2.96	0.49
1:A:223:ALA:O	1:A:227:GLU:HG3	2.12	0.49
1:A:19:ALA:HB3	1:A:20:PRO:HD3	1.94	0.49
1:C:19:ALA:HB3	1:C:20:PRO:HD3	1.95	0.49
1:F:19:ALA:HB3	1:F:20:PRO:HD3	1.95	0.49
1:E:364:GLU:OE1	1:E:367:ARG:NH1	2.46	0.48
1:B:277:HIS:CD2	1:D:339:PRO:CG	2.96	0.48
1:C:199:GLU:HA	1:C:278:ARG:HH12	1.79	0.48
1:G:19:ALA:HB3	1:G:20:PRO:HD3	1.94	0.48
1:A:64:ARG:HE	1:A:64:ARG:HB3	1.52	0.47
1:A:364:GLU:OE1	1:A:367:ARG:NH1	2.46	0.47
2:A:401:UDP:O2B	2:A:401:UDP:H5'2	2.15	0.47
1:F:25:LEU:HD23	1:F:363:LEU:HD21	1.97	0.47
1:G:267:LEU:HD13	1:G:267:LEU:N	2.30	0.47
1:H:19:ALA:HB3	1:H:20:PRO:HD3	1.97	0.47
1:A:268:ARG:HD2	1:A:270:SER:OG	2.14	0.47
1:B:277:HIS:CE1	1:D:339:PRO:HB2	2.50	0.46
1:G:319:ARG:CZ	1:G:334:ARG:HH12	2.29	0.46
1:C:5:VAL:HG22	1:C:91:VAL:HG23	1.98	0.46
1:E:19:ALA:HB3	1:E:20:PRO:HD3	1.98	0.45
1:E:238:VAL:HG11	1:E:275:LEU:HD21	1.98	0.45
1:B:238:VAL:HG11	1:B:275:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:VAL:HG13	1:F:57:ARG:HD3	1.98	0.45
1:G:216:ILE:HB	1:G:217:PRO:HD3	1.98	0.45
1:C:216:ILE:HB	1:C:217:PRO:HD3	1.98	0.45
1:G:12:ARG:CZ	1:G:48:ILE:HD11	2.47	0.45
1:G:211:ARG:HG2	4:G:537:HOH:O	2.17	0.45
1:B:277:HIS:NE2	1:D:339:PRO:CB	2.81	0.43
1:C:336:LEU:HA	4:C:505:HOH:O	2.18	0.43
1:B:198:THR:HG22	1:B:203:THR:HG21	2.00	0.43
1:B:216:ILE:HB	1:B:217:PRO:HD3	1.99	0.43
1:C:122:LEU:HB3	1:C:308:GLU:HB2	1.99	0.43
1:E:342:TYR:CE2	1:E:346:ARG:HD2	2.53	0.43
1:C:337:ASP:O	1:C:339:PRO:HD3	2.19	0.43
1:B:147:HIS:HE1	4:B:547:HOH:O	2.02	0.43
1:C:238:VAL:HG11	1:C:275:LEU:HD21	2.01	0.43
1:F:47:GLU:HG2	1:F:48:ILE:N	2.33	0.43
1:A:238:VAL:HG11	1:A:275:LEU:HD21	2.01	0.43
1:B:277:HIS:CG	1:D:339:PRO:HG2	2.54	0.43
1:E:216:ILE:HB	1:E:217:PRO:HD3	2.00	0.43
1:D:342:TYR:CE1	1:D:346:ARG:HD2	2.54	0.43
1:B:337:ASP:O	1:B:339:PRO:HD3	2.19	0.42
1:D:216:ILE:HB	1:D:217:PRO:HD3	2.02	0.42
1:D:337:ASP:O	1:D:339:PRO:HD3	2.18	0.42
1:F:12:ARG:HG3	1:F:48:ILE:HD11	2.01	0.42
1:H:337:ASP:O	1:H:339:PRO:HD3	2.20	0.42
1:C:82:ASP:HB2	1:C:83:PRO:CD	2.49	0.42
1:E:337:ASP:O	1:E:339:PRO:HD3	2.19	0.42
1:G:337:ASP:O	1:G:339:PRO:HD3	2.19	0.42
1:E:308:GLU:HG2	1:E:309:ARG:HD2	2.02	0.42
1:A:216:ILE:HB	1:A:217:PRO:HD3	2.01	0.42
1:B:347:ARG:N	1:B:348:PRO:CD	2.82	0.42
1:A:337:ASP:O	1:A:339:PRO:HD3	2.20	0.42
1:G:342:TYR:CE1	1:G:346:ARG:HD2	2.55	0.42
1:F:337:ASP:O	1:F:339:PRO:HD3	2.19	0.42
1:H:351:VAL:HG21	1:H:355:GLU:OE1	2.20	0.42
1:H:238:VAL:HG11	1:H:275:LEU:HD21	2.02	0.41
1:B:67:GLN:N	4:B:510:HOH:O	2.53	0.41
1:C:82:ASP:HB2	1:C:83:PRO:HD3	2.02	0.41
1:B:82:ASP:HB2	1:B:83:PRO:CD	2.50	0.41
1:B:277:HIS:CE1	1:B:296:LEU:HD22	2.55	0.41
1:C:34:VAL:HG11	1:C:87:GLU:HB3	2.02	0.41
1:B:238:VAL:CG1	1:B:275:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ARG:HG2	4:C:535:HOH:O	2.20	0.41
1:H:47:GLU:HG2	1:H:48:ILE:N	2.34	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.96	0.41
1:C:129:GLU:HA	1:C:130:PRO:HA	1.94	0.41
1:H:82:ASP:HB2	1:H:83:PRO:CD	2.50	0.41
1:B:46:ASP:OD1	1:B:46:ASP:N	2.54	0.41
1:C:342:TYR:CE2	1:C:346:ARG:HD2	2.56	0.41
1:B:131:PHE:HA	1:B:132:PRO:HA	1.89	0.40
1:C:293:ALA:HB3	1:C:294:PRO:HD3	2.03	0.40
1:B:293:ALA:HB3	1:B:294:PRO:HD3	2.03	0.40
1:E:34:VAL:HG11	1:E:87:GLU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/375 (96%)	352 (97%)	10 (3%)	0	100	100
1	B	354/375 (94%)	346 (98%)	7 (2%)	1 (0%)	41	62
1	C	345/375 (92%)	337 (98%)	7 (2%)	1 (0%)	41	62
1	D	349/375 (93%)	339 (97%)	9 (3%)	1 (0%)	41	62
1	E	352/375 (94%)	342 (97%)	9 (3%)	1 (0%)	41	62
1	F	352/375 (94%)	344 (98%)	7 (2%)	1 (0%)	41	62
1	G	351/375 (94%)	344 (98%)	6 (2%)	1 (0%)	41	62
1	H	349/375 (93%)	341 (98%)	7 (2%)	1 (0%)	41	62
All	All	2814/3000 (94%)	2745 (98%)	62 (2%)	7 (0%)	47	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	199	GLU
1	D	199	GLU
1	E	347	ARG
1	F	199	GLU
1	G	199	GLU
1	B	199	GLU
1	C	199	GLU

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	299/305 (98%)	284 (95%)	15 (5%)	24	45
1	B	295/305 (97%)	282 (96%)	13 (4%)	28	51
1	C	289/305 (95%)	277 (96%)	12 (4%)	30	53
1	D	292/305 (96%)	282 (97%)	10 (3%)	37	60
1	E	293/305 (96%)	280 (96%)	13 (4%)	28	51
1	F	293/305 (96%)	284 (97%)	9 (3%)	40	64
1	G	292/305 (96%)	276 (94%)	16 (6%)	21	41
1	H	293/305 (96%)	281 (96%)	12 (4%)	30	54
All	All	2346/2440 (96%)	2246 (96%)	100 (4%)	29	52

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	ASP
1	A	46	ASP
1	A	57	ARG
1	A	64	ARG
1	A	67	GLN
1	A	165	SER
1	A	166	ASP
1	A	177	ASP

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Mol	Chain	Res	Type
1	A	192	ARG
1	A	210	ARG
1	A	230	ARG
1	A	268	ARG
1	A	351	VAL
1	A	363	LEU
1	B	26	ASP
1	B	46	ASP
1	B	64	ARG
1	B	67	GLN
1	B	165	SER
1	B	177	ASP
1	B	179	MET
1	B	192	ARG
1	B	230	ARG
1	B	246	GLU
1	B	277	HIS
1	B	330	LYS
1	B	351	VAL
1	C	26	ASP
1	C	46	ASP
1	C	67	GLN
1	C	72	MET
1	C	91	VAL
1	C	164	ARG
1	C	165	SER
1	C	166	ASP
1	C	177	ASP
1	C	199	GLU
1	C	246	GLU
1	C	363	LEU
1	D	26	ASP
1	D	46	ASP
1	D	67	GLN
1	D	165	SER
1	D	177	ASP
1	D	210	ARG
1	D	230	ARG
1	D	278	ARG
1	D	351	VAL
1	D	363	LEU
1	E	26	ASP

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Mol	Chain	Res	Type
1	E	46	ASP
1	E	47	GLU
1	E	48	ILE
1	E	55	ARG
1	E	67	GLN
1	E	165	SER
1	E	177	ASP
1	E	192	ARG
1	E	230	ARG
1	E	246	GLU
1	E	351	VAL
1	E	363	LEU
1	F	12	ARG
1	F	26	ASP
1	F	67	GLN
1	F	165	SER
1	F	177	ASP
1	F	210	ARG
1	F	211	ARG
1	F	246	GLU
1	F	351	VAL
1	G	26	ASP
1	G	46	ASP
1	G	55	ARG
1	G	57	ARG
1	G	64	ARG
1	G	67	GLN
1	G	72	MET
1	G	145	ASP
1	G	165	SER
1	G	177	ASP
1	G	183	LEU
1	G	228	LEU
1	G	246	GLU
1	G	267	LEU
1	G	347	ARG
1	G	363	LEU
1	H	26	ASP
1	H	46	ASP
1	H	64	ARG
1	H	67	GLN
1	H	165	SER

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Mol	Chain	Res	Type
1	H	177	ASP
1	H	210	ARG
1	H	230	ARG
1	H	246	GLU
1	H	268	ARG
1	H	351	VAL
1	H	363	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	C	58	HIS
1	D	59	ASN
1	D	147	HIS
1	E	59	ASN
1	F	58	HIS
1	H	242	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
2	UDP	A	401	-	24,26,26	1.21	3 (12%)	37,40,40	1.84	5 (13%)
2	UDP	H	401	-	24,26,26	1.06	2 (8%)	37,40,40	1.71	6 (16%)
2	UDP	D	401	-	24,26,26	1.19	2 (8%)	37,40,40	1.71	6 (16%)
2	UDP	E	401	-	24,26,26	1.52	3 (12%)	37,40,40	1.83	10 (27%)
2	UDP	B	401	-	24,26,26	1.20	3 (12%)	37,40,40	1.48	7 (18%)
2	UDP	G	401	-	24,26,26	1.27	3 (12%)	37,40,40	1.95	8 (21%)
2	UDP	C	401	-	24,26,26	1.16	3 (12%)	37,40,40	1.88	9 (24%)
2	UDP	F	401	-	24,26,26	1.22	2 (8%)	37,40,40	1.71	9 (24%)

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
2	UDP	A	401	-	-	3/16/32/32	0/2/2/2
2	UDP	H	401	-	-	3/16/32/32	0/2/2/2
2	UDP	D	401	-	-	0/16/32/32	0/2/2/2
2	UDP	E	401	-	-	4/16/32/32	0/2/2/2
2	UDP	B	401	-	-	4/16/32/32	0/2/2/2
2	UDP	G	401	-	-	2/16/32/32	0/2/2/2
2	UDP	C	401	-	-	3/16/32/32	0/2/2/2
2	UDP	F	401	-	-	4/16/32/32	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	UDP	C4-N3	-3.64	1.32	1.38
2	E	401	UDP	C2-N3	-3.40	1.31	1.38
2	G	401	UDP	C2-N3	-3.27	1.32	1.38
2	F	401	UDP	C2-N1	3.16	1.43	1.38
2	E	401	UDP	C2-N1	2.98	1.43	1.38
2	D	401	UDP	C2-N1	2.98	1.43	1.38
2	A	401	UDP	C2-N1	2.88	1.43	1.38
2	B	401	UDP	C6-C5	2.79	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	UDP	C4-N3	-2.64	1.33	1.38
2	H	401	UDP	C2-N3	-2.52	1.33	1.38
2	D	401	UDP	C2-N3	-2.50	1.33	1.38
2	G	401	UDP	C4-N3	-2.50	1.34	1.38
2	A	401	UDP	C6-C5	2.40	1.40	1.35
2	C	401	UDP	C6-C5	2.32	1.40	1.35
2	H	401	UDP	C4-N3	-2.26	1.34	1.38
2	F	401	UDP	C2-N3	-2.21	1.34	1.38
2	C	401	UDP	C5-C4	-2.20	1.38	1.43
2	G	401	UDP	C2-N1	2.15	1.41	1.38
2	B	401	UDP	C5-C4	-2.02	1.39	1.43
2	A	401	UDP	C5-C4	-2.00	1.39	1.43
2	B	401	UDP	C4-N3	-2.00	1.35	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	UDP	N3-C2-N1	5.66	122.40	114.89
2	G	401	UDP	N3-C2-N1	5.31	121.94	114.89
2	E	401	UDP	C5-C4-N3	5.25	122.69	114.84
2	G	401	UDP	C4-N3-C2	-5.04	119.94	126.58
2	A	401	UDP	C4-N3-C2	-5.02	119.95	126.58
2	H	401	UDP	C4-N3-C2	-4.70	120.38	126.58
2	D	401	UDP	C4-N3-C2	-4.65	120.45	126.58
2	E	401	UDP	C4-N3-C2	-4.63	120.48	126.58
2	H	401	UDP	N3-C2-N1	4.62	121.02	114.89
2	F	401	UDP	C4-N3-C2	-4.52	120.61	126.58
2	D	401	UDP	N3-C2-N1	4.42	120.75	114.89
2	A	401	UDP	C5-C4-N3	4.40	121.42	114.84
2	C	401	UDP	C4-N3-C2	-4.26	120.96	126.58
2	A	401	UDP	O4-C4-C5	-4.09	117.97	125.16
2	A	401	UDP	N3-C2-N1	4.08	120.30	114.89
2	F	401	UDP	C5-C4-N3	3.94	120.74	114.84
2	H	401	UDP	C5-C4-N3	3.92	120.70	114.84
2	C	401	UDP	O2-C2-N1	-3.84	117.68	122.79
2	G	401	UDP	O3B-PB-O3A	-3.75	92.06	104.64
2	D	401	UDP	C5-C4-N3	3.74	120.44	114.84
2	E	401	UDP	N3-C2-N1	3.67	119.76	114.89
2	F	401	UDP	N3-C2-N1	3.61	119.68	114.89
2	B	401	UDP	N3-C2-N1	3.60	119.67	114.89
2	G	401	UDP	C5-C4-N3	3.48	120.05	114.84
2	G	401	UDP	O2-C2-N3	-3.21	115.53	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	UDP	O2B-PB-O3A	3.18	115.29	104.64
2	H	401	UDP	O2-C2-N1	-3.13	118.63	122.79
2	B	401	UDP	C4-N3-C2	-3.08	122.53	126.58
2	G	401	UDP	O3B-PB-O2B	2.93	118.83	107.64
2	F	401	UDP	O4-C4-C5	-2.92	120.03	125.16
2	H	401	UDP	O4-C4-C5	-2.91	120.05	125.16
2	E	401	UDP	O2-C2-N3	-2.88	116.13	121.50
2	B	401	UDP	C5-C4-N3	2.81	119.04	114.84
2	C	401	UDP	C6-N1-C2	-2.70	117.53	120.99
2	F	401	UDP	O4'-C1'-C2'	-2.63	100.90	106.64
2	C	401	UDP	O4-C4-C5	-2.63	120.53	125.16
2	C	401	UDP	PA-O3A-PB	-2.57	124.00	132.83
2	F	401	UDP	O2-C2-N3	-2.56	116.74	121.50
2	B	401	UDP	C2'-C1'-N1	2.48	120.25	113.22
2	C	401	UDP	C5-C4-N3	2.48	118.55	114.84
2	D	401	UDP	O2-C2-N3	-2.44	116.96	121.50
2	G	401	UDP	O2'-C2'-C3'	-2.42	104.00	111.82
2	E	401	UDP	C2'-C1'-N1	2.40	120.02	113.22
2	C	401	UDP	O5'-PA-O1A	-2.40	99.69	109.07
2	B	401	UDP	O3B-PB-O3A	2.40	112.69	104.64
2	E	401	UDP	O3A-PB-O1B	-2.37	98.04	111.19
2	F	401	UDP	C1'-N1-C2	2.37	121.86	117.57
2	F	401	UDP	O3B-PB-O2B	2.36	116.66	107.64
2	D	401	UDP	O5'-PA-O1A	-2.31	100.04	109.07
2	B	401	UDP	O4-C4-C5	-2.30	121.11	125.16
2	D	401	UDP	O4-C4-N3	-2.30	115.93	119.31
2	H	401	UDP	PA-O3A-PB	-2.30	124.95	132.83
2	G	401	UDP	O4-C4-C5	-2.24	121.22	125.16
2	E	401	UDP	O4-C4-C5	-2.23	121.23	125.16
2	E	401	UDP	O4-C4-N3	-2.21	116.06	119.31
2	A	401	UDP	PA-O3A-PB	-2.20	125.29	132.83
2	C	401	UDP	O2A-PA-O1A	2.08	122.54	112.24
2	B	401	UDP	O4'-C1'-N1	-2.05	103.69	108.36
2	E	401	UDP	O3B-PB-O2B	2.03	115.39	107.64
2	F	401	UDP	C2'-C1'-N1	2.01	118.90	113.22

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	UDP	C5'-O5'-PA-O1A
2	C	401	UDP	C3'-C4'-C5'-O5'

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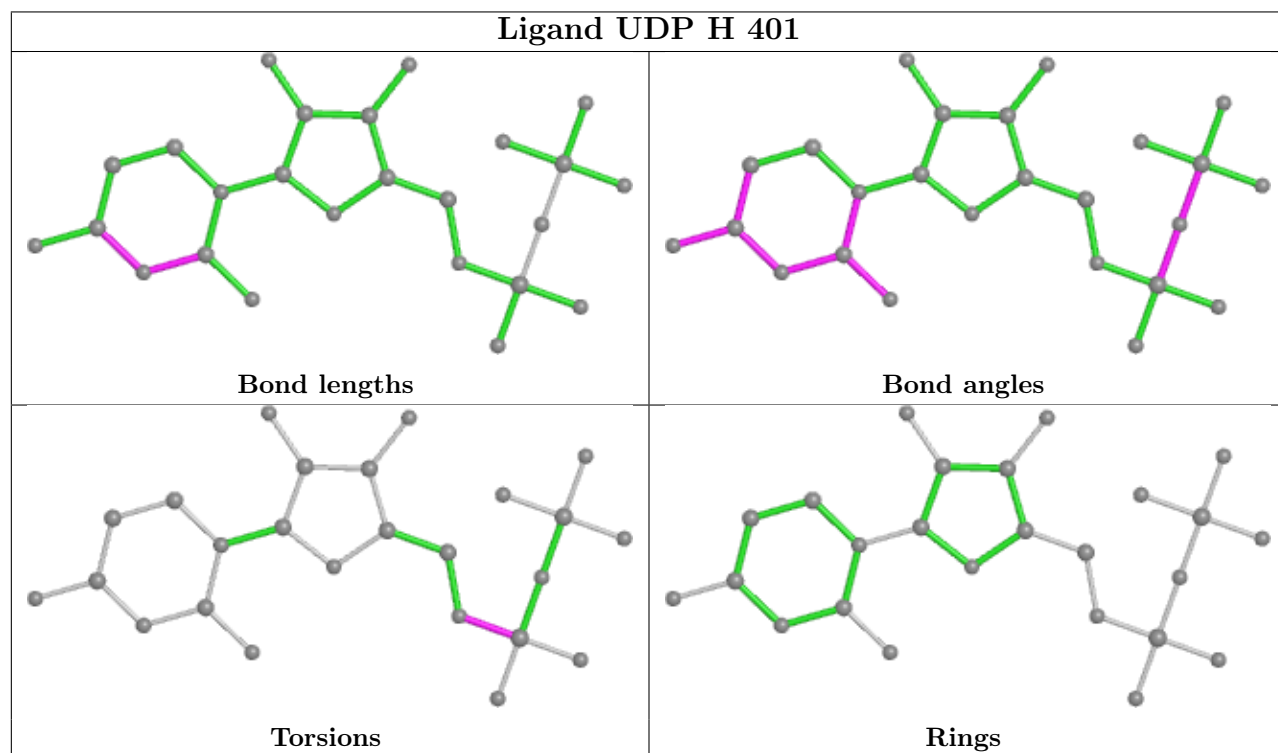
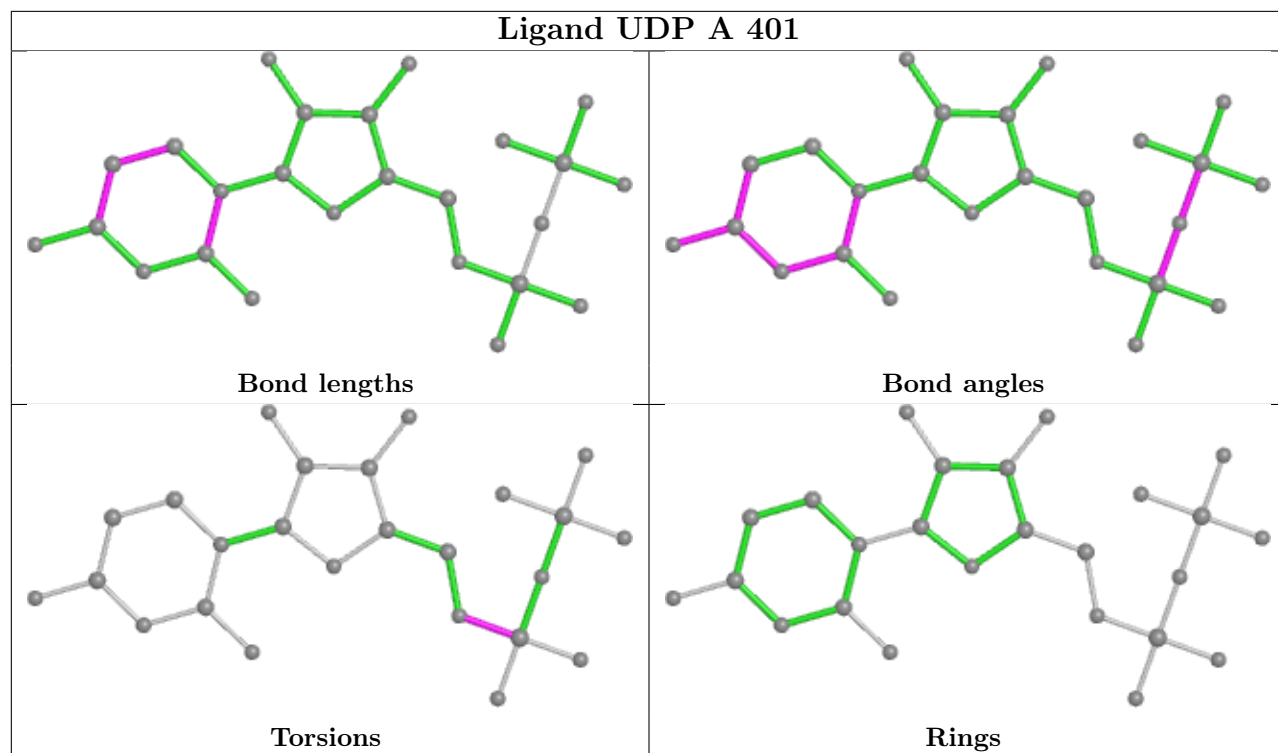
Mol	Chain	Res	Type	Atoms
2	C	401	UDP	O4'-C4'-C5'-O5'
2	F	401	UDP	C3'-C4'-C5'-O5'
2	F	401	UDP	O4'-C4'-C5'-O5'
2	H	401	UDP	C5'-O5'-PA-O1A
2	H	401	UDP	C5'-O5'-PA-O2A
2	E	401	UDP	C3'-C4'-C5'-O5'
2	F	401	UDP	PB-O3A-PA-O1A
2	E	401	UDP	O4'-C4'-C5'-O5'
2	A	401	UDP	C5'-O5'-PA-O3A
2	B	401	UDP	C3'-C4'-C5'-O5'
2	B	401	UDP	PB-O3A-PA-O1A
2	C	401	UDP	PB-O3A-PA-O1A
2	E	401	UDP	PB-O3A-PA-O2A
2	A	401	UDP	C5'-O5'-PA-O2A
2	G	401	UDP	C3'-C4'-C5'-O5'
2	G	401	UDP	O4'-C4'-C5'-O5'
2	F	401	UDP	PB-O3A-PA-O2A
2	B	401	UDP	O4'-C4'-C5'-O5'
2	H	401	UDP	C5'-O5'-PA-O3A
2	B	401	UDP	PB-O3A-PA-O2A
2	E	401	UDP	PB-O3A-PA-O1A

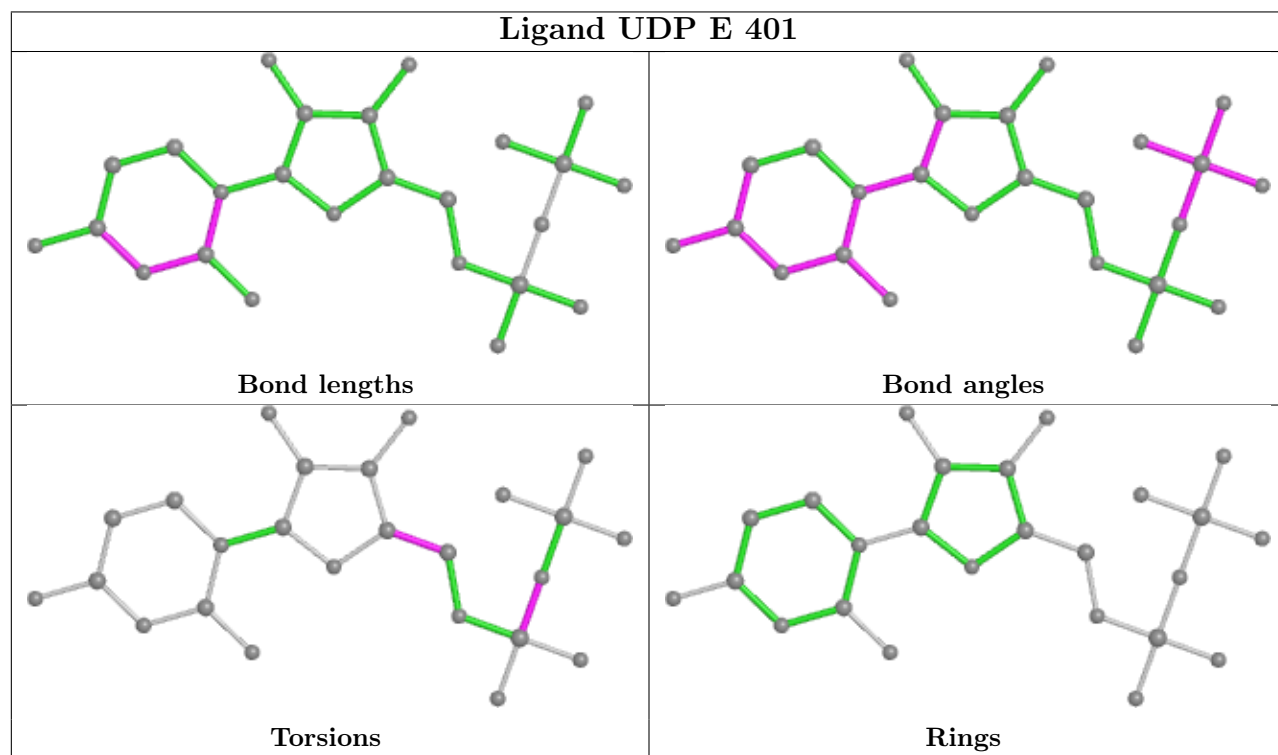
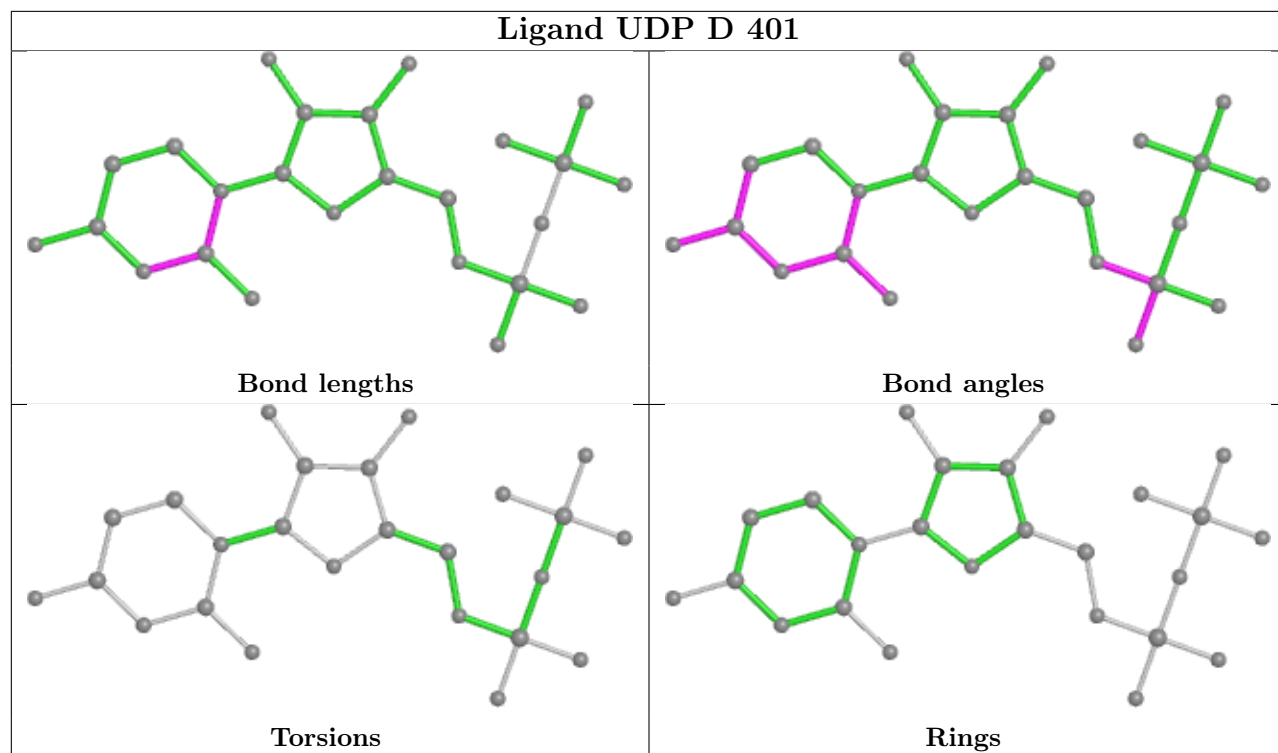
There are no ring outliers.

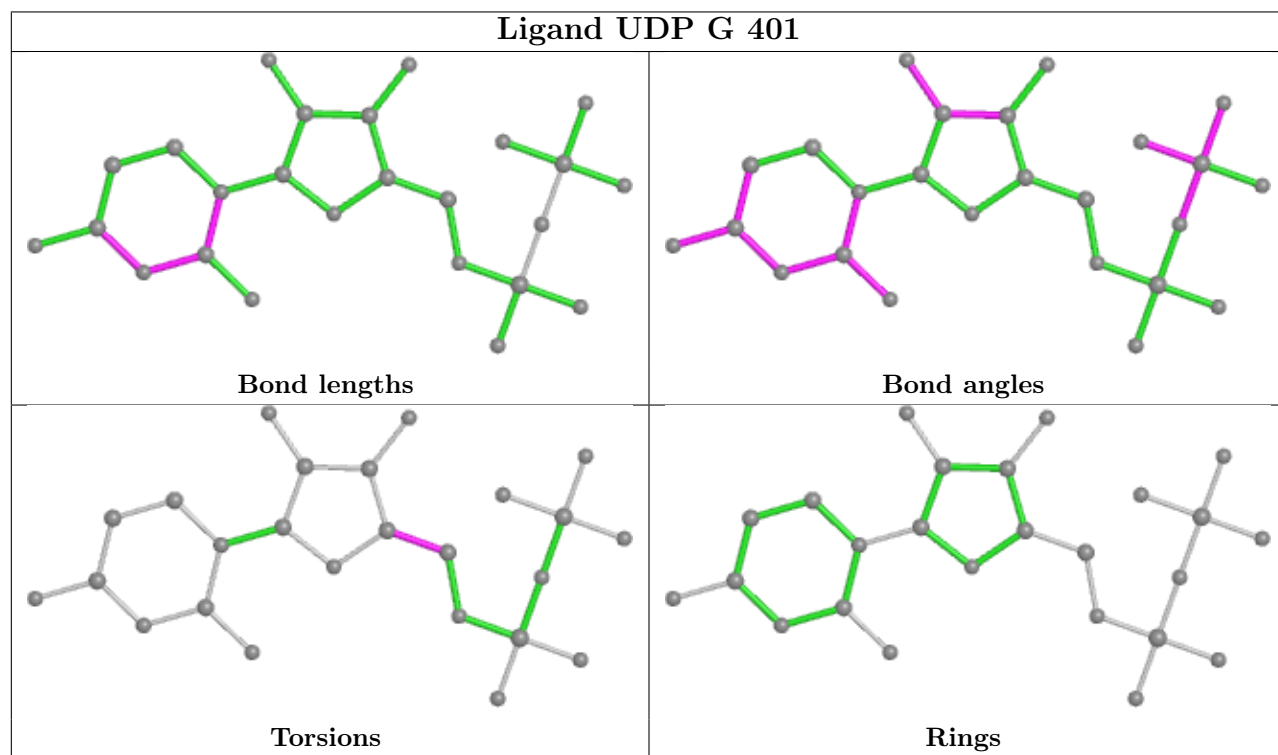
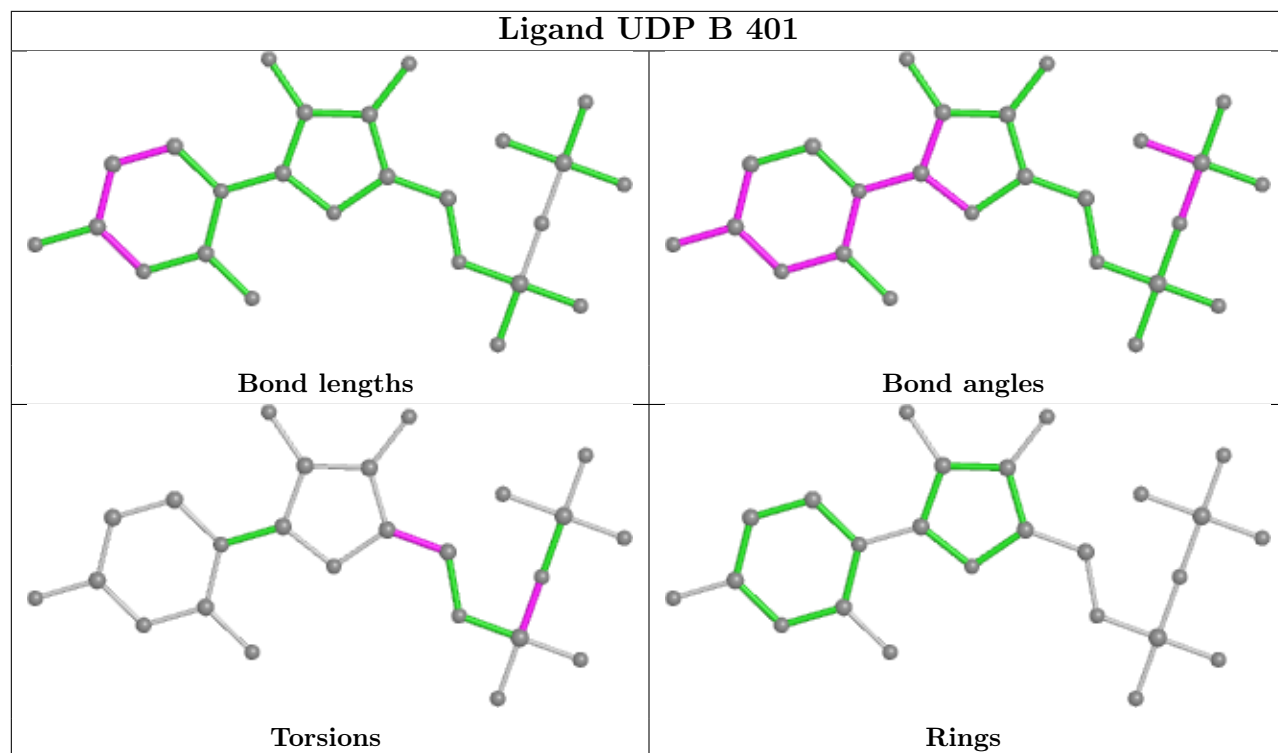
3 monomers are involved in 4 short contacts:

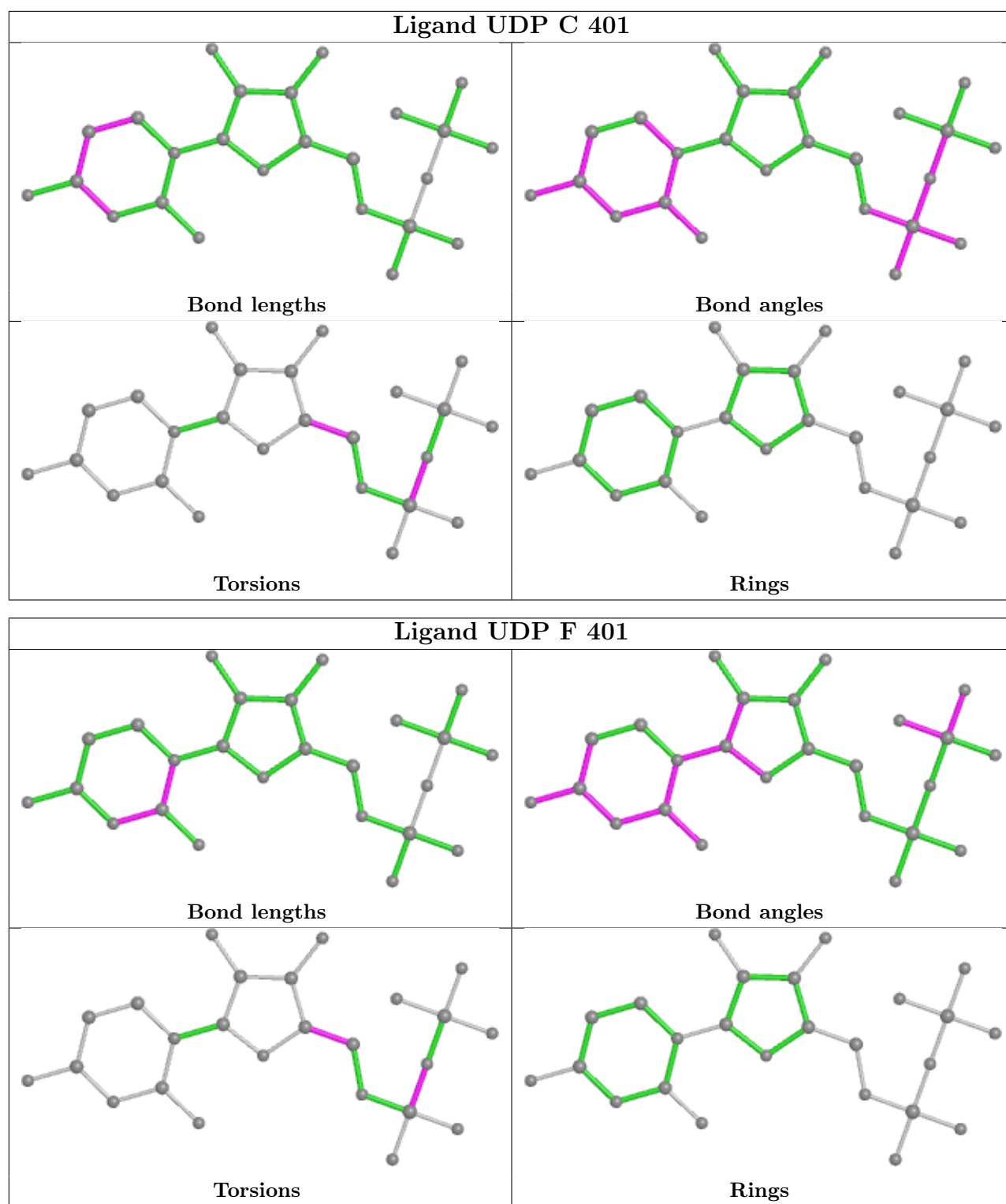
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	UDP	1	0
2	G	401	UDP	1	0
2	C	401	UDP	2	0

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 ⓘ

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	368/375 (98%)	-0.02	9 (2%) 59 55	24, 46, 71, 93	0
1	B	362/375 (96%)	-0.12	4 (1%) 80 79	16, 40, 69, 101	0
1	C	355/375 (94%)	0.08	8 (2%) 60 57	27, 48, 82, 115	0
1	D	359/375 (95%)	-0.11	9 (2%) 57 53	21, 42, 72, 98	0
1	E	360/375 (96%)	-0.10	5 (1%) 75 73	18, 40, 68, 98	0
1	F	360/375 (96%)	-0.04	8 (2%) 62 58	28, 45, 73, 99	0
1	G	359/375 (95%)	0.03	10 (2%) 53 49	23, 49, 74, 96	0
1	H	359/375 (95%)	0.17	12 (3%) 46 42	31, 55, 83, 112	0
All	All	2882/3000 (96%)	-0.01	65 (2%) 60 57	16, 45, 76, 115	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	355	GLU	5.0
1	C	47	GLU	5.0
1	H	230	ARG	4.4
1	D	374	PRO	4.3
1	A	351	VAL	3.9
1	A	65	PRO	3.9
1	F	374	PRO	3.7
1	B	230	ARG	3.5
1	C	357	ASP	3.3
1	H	234	THR	3.3
1	G	374	PRO	3.2
1	B	64	ARG	3.1
1	C	61	ASP	3.1
1	H	184	ASP	2.9
1	G	340	GLU	2.9
1	G	66	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	61	ASP	2.8
1	F	230	ARG	2.8
1	D	268	ARG	2.8
1	G	55	ARG	2.7
1	C	27	ALA	2.6
1	G	230	ARG	2.6
1	E	61	ASP	2.6
1	H	191	ASN	2.6
1	B	46	ASP	2.6
1	C	347	ARG	2.5
1	E	184	ASP	2.5
1	F	65	PRO	2.5
1	F	268	ARG	2.5
1	H	337	ASP	2.5
1	C	48	ILE	2.5
1	A	68	ARG	2.4
1	A	374	PRO	2.4
1	G	257	SER	2.4
1	A	355	GLU	2.4
1	A	347	ARG	2.3
1	F	61	ASP	2.3
1	E	230	ARG	2.3
1	A	187	GLY	2.3
1	C	88	LEU	2.3
1	A	204	VAL	2.2
1	D	199	GLU	2.2
1	H	46	ASP	2.2
1	D	341	ALA	2.2
1	E	374	PRO	2.2
1	D	47	GLU	2.2
1	D	230	ARG	2.2
1	G	204	VAL	2.2
1	D	61	ASP	2.2
1	G	206	LEU	2.2
1	A	27	ALA	2.1
1	H	164	ARG	2.1
1	D	347	ARG	2.1
1	B	350	ILE	2.1
1	C	340	GLU	2.1
1	F	199	GLU	2.1
1	G	65	PRO	2.0
1	D	340	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	199	GLU	2.0
1	E	340	GLU	2.0
1	F	67	GLN	2.0
1	G	268	ARG	2.0
1	H	192	ARG	2.0
1	F	47	GLU	2.0
1	H	211	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

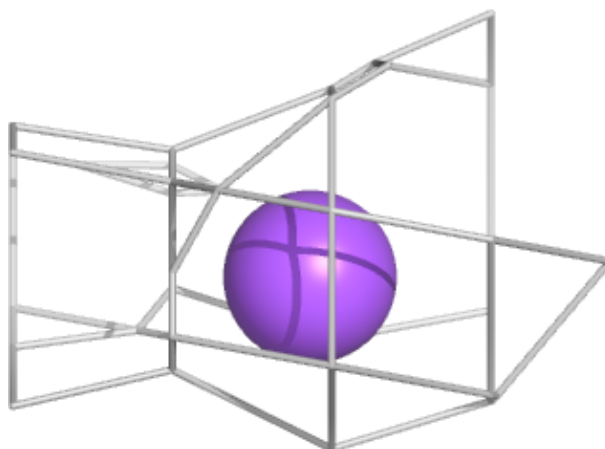
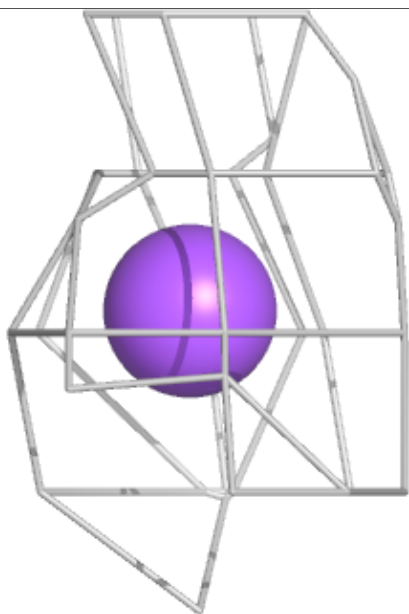
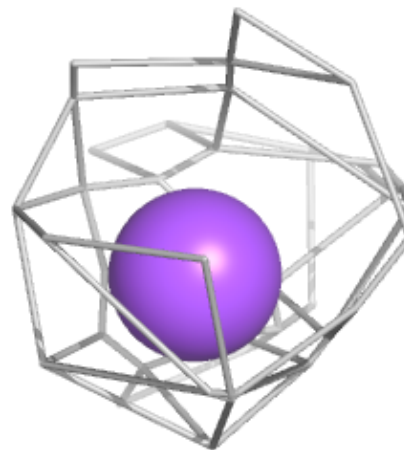
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	E	402	1/1	0.58	0.28	57,57,57,57	0
3	NA	C	402	1/1	0.76	0.14	72,72,72,72	0
3	NA	H	402	1/1	0.83	0.23	48,48,48,48	0
3	NA	F	402	1/1	0.86	0.18	50,50,50,50	0
3	NA	G	402	1/1	0.86	0.28	53,53,53,53	0
3	NA	A	402	1/1	0.86	0.18	46,46,46,46	0
3	NA	D	402	1/1	0.90	0.29	56,56,56,56	0
3	NA	B	402	1/1	0.92	0.30	59,59,59,59	0
2	UDP	C	401	25/25	0.97	0.11	32,39,46,47	0
2	UDP	D	401	25/25	0.97	0.09	27,30,33,35	0
2	UDP	E	401	25/25	0.98	0.08	20,24,30,32	0
2	UDP	F	401	25/25	0.98	0.09	27,31,36,43	0
2	UDP	G	401	25/25	0.98	0.07	35,39,43,44	0
2	UDP	H	401	25/25	0.98	0.08	30,37,42,43	0
2	UDP	A	401	25/25	0.98	0.08	27,30,33,34	0
2	UDP	B	401	25/25	0.98	0.08	21,24,26,27	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.

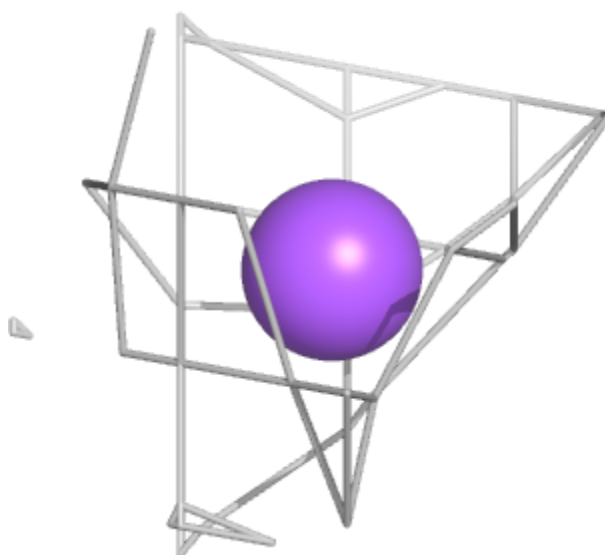
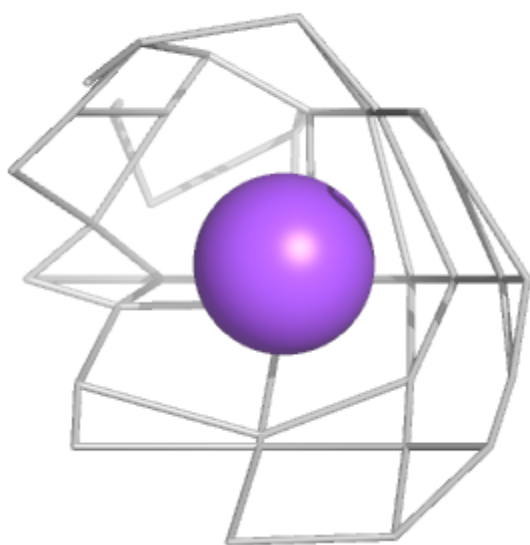
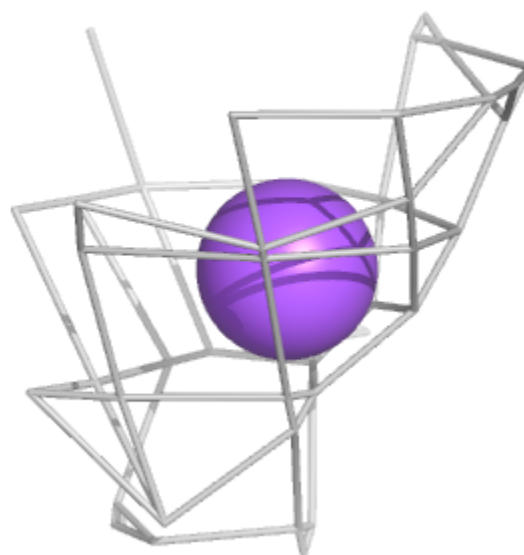
Electron density around NA E 402:

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



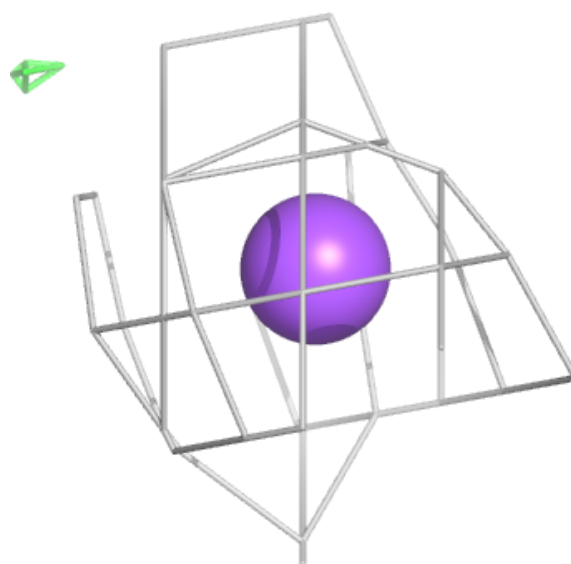
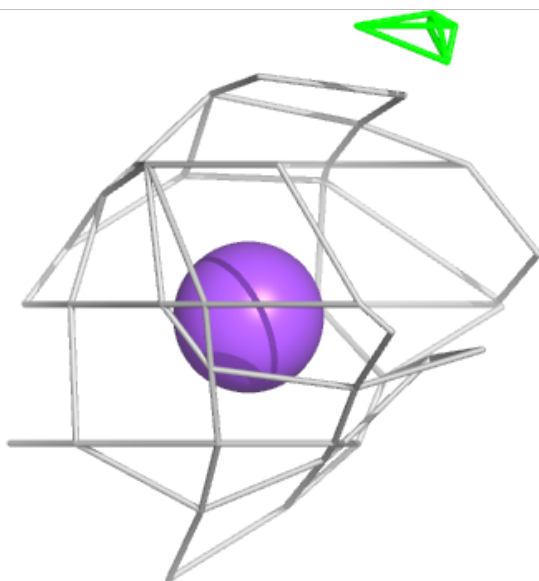
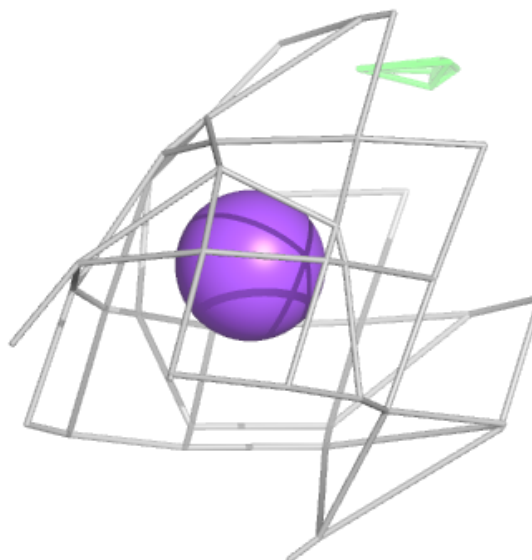
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and green (positive)



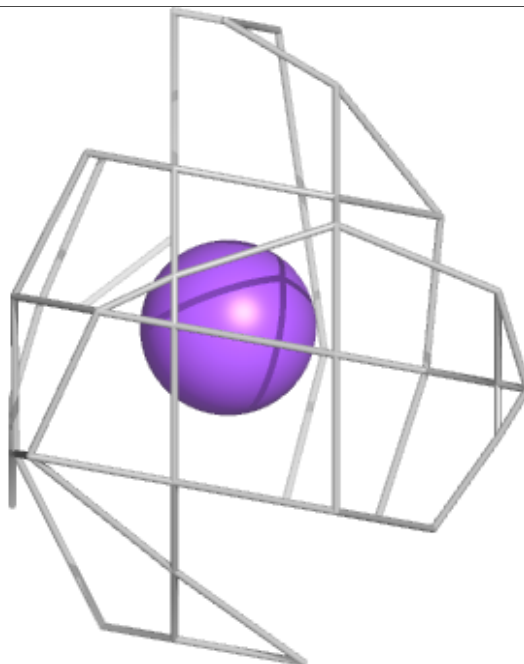
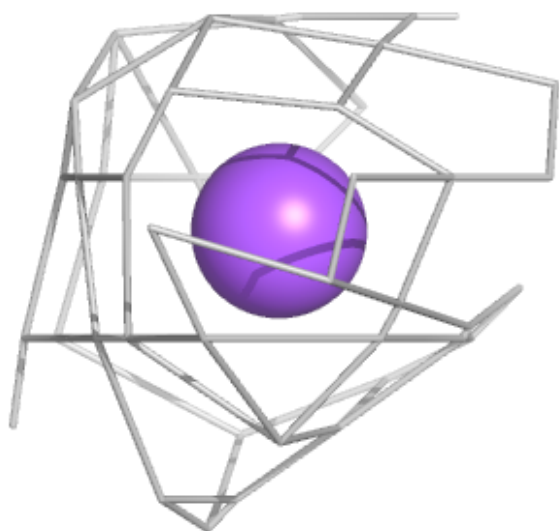
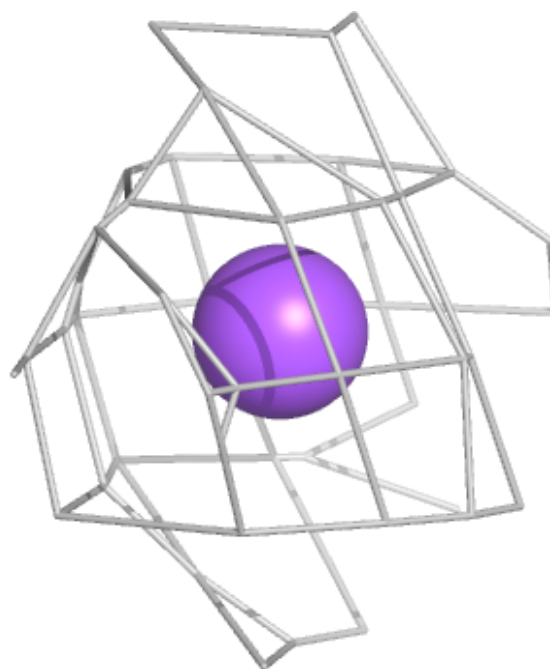
Electron density around NA H 402:

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and green (positive)



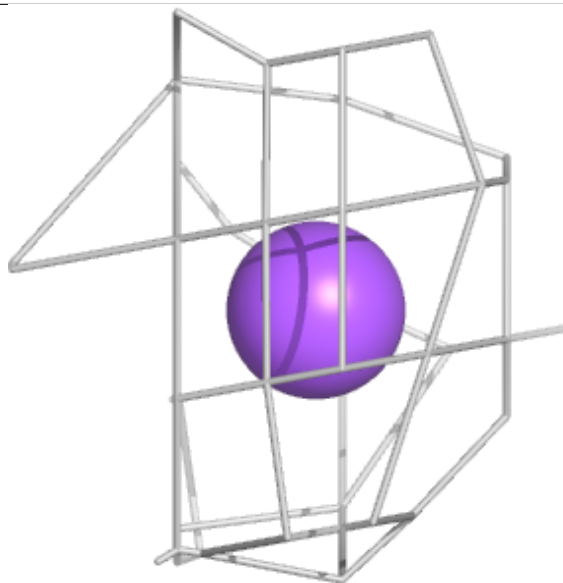
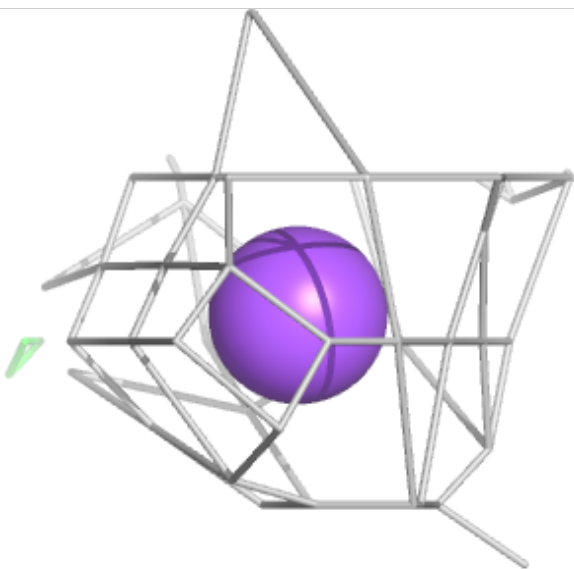
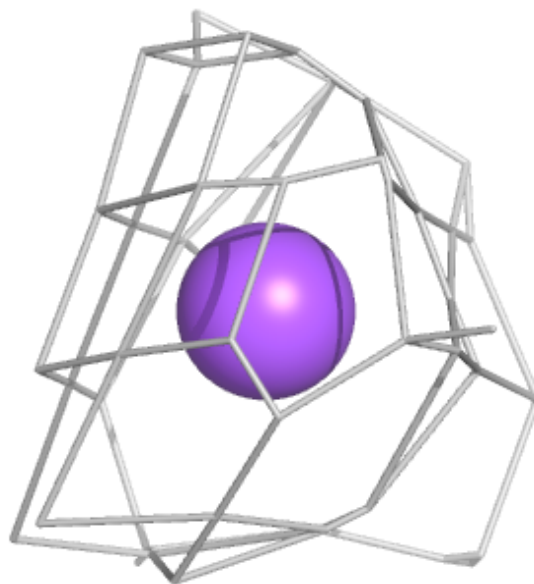
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and green (positive)



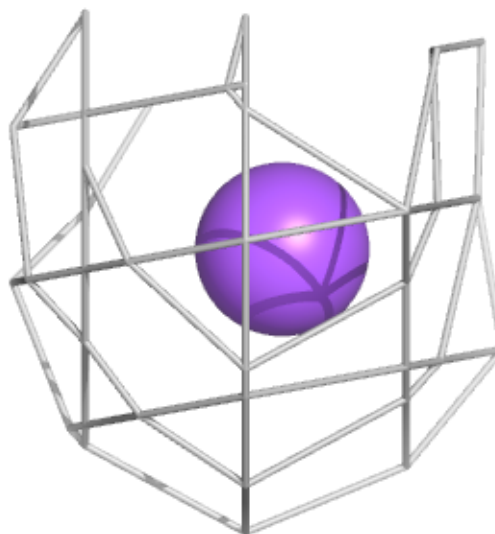
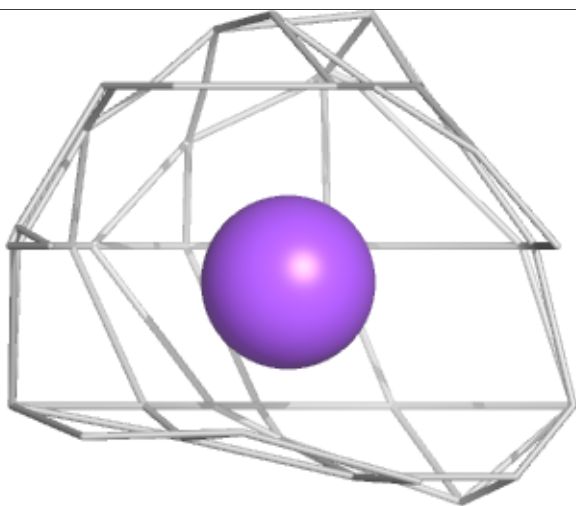
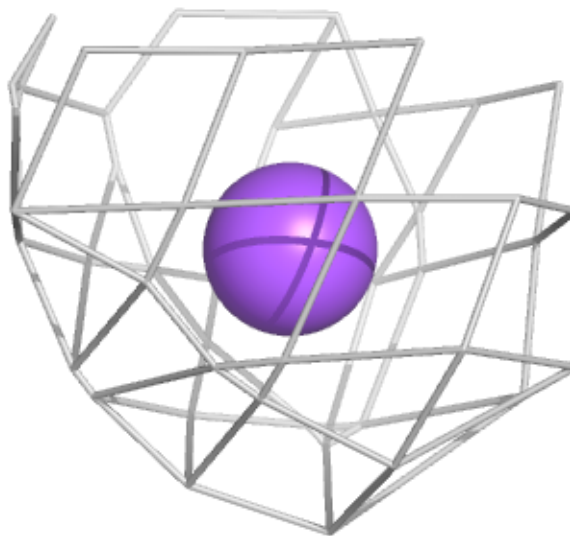
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and green (positive)



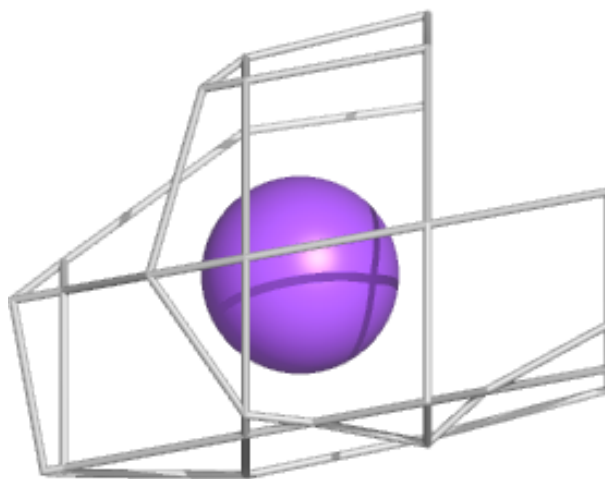
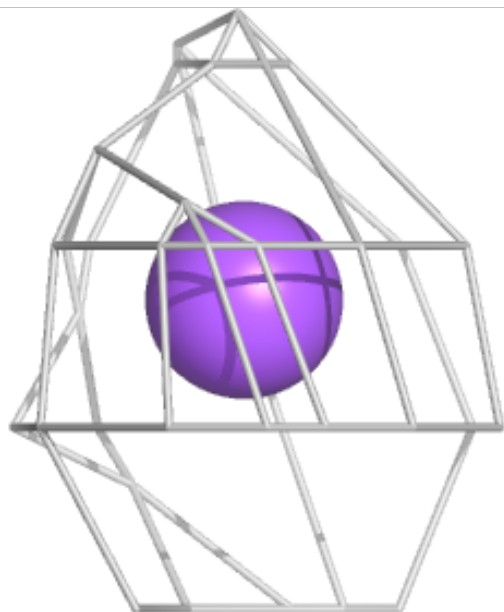
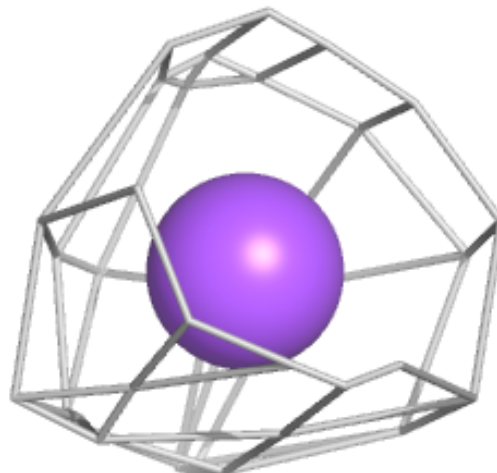
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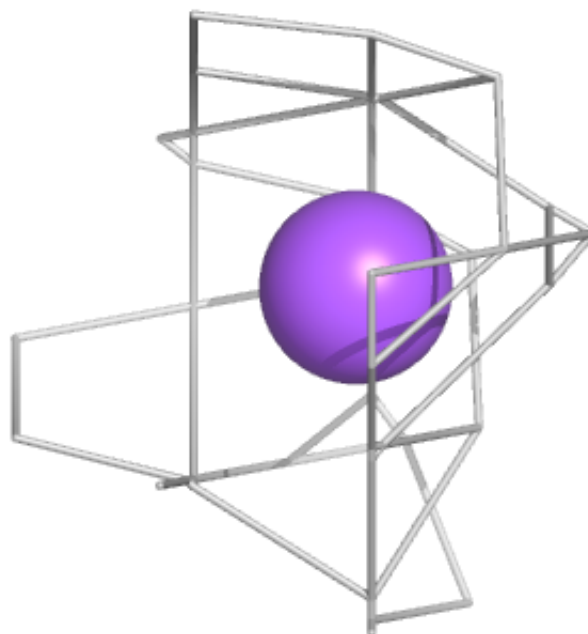
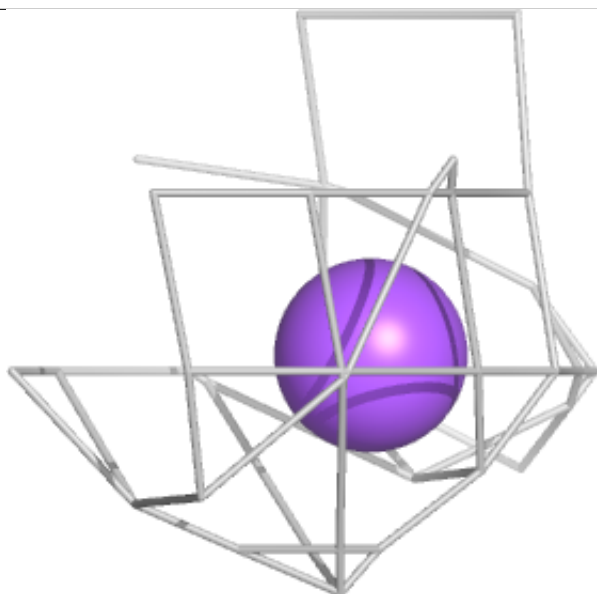
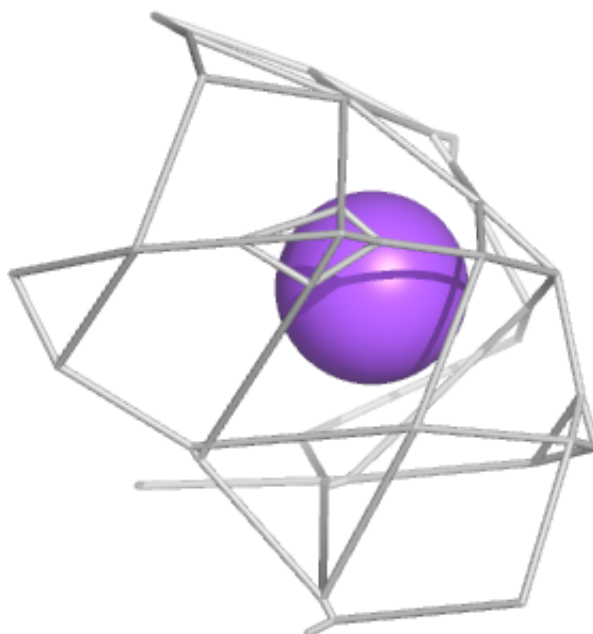
Electron density around NA D 402:

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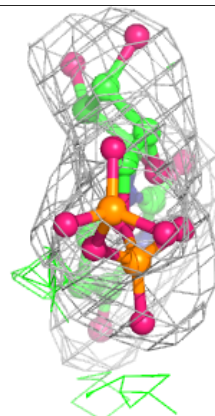
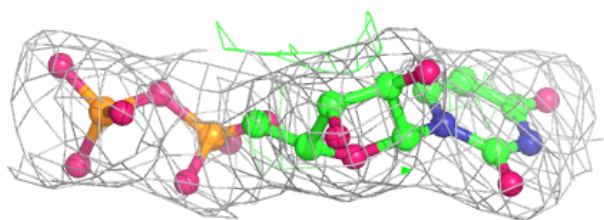
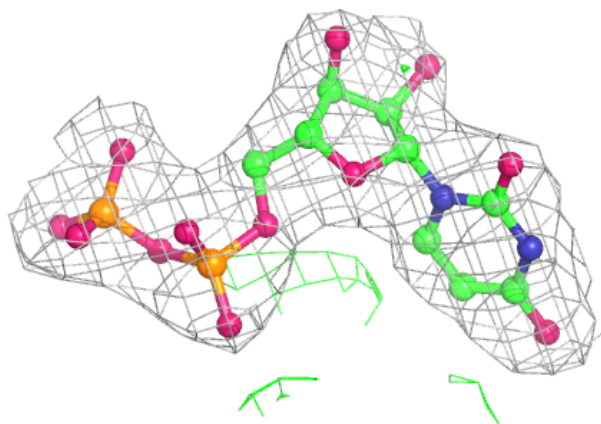
Electron density around NA B 402:

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and green (positive)

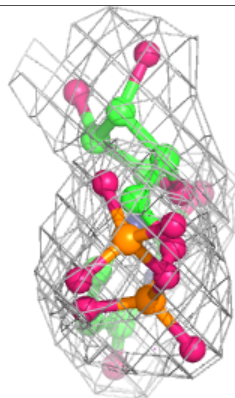
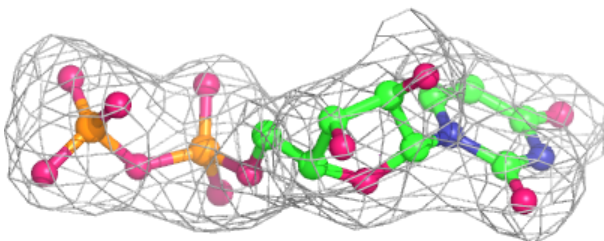
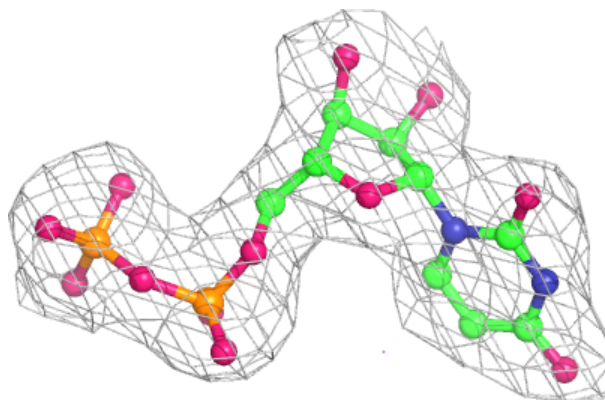


Electron density around UDP C 401:

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and green (positive)

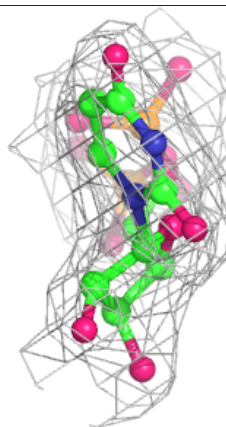
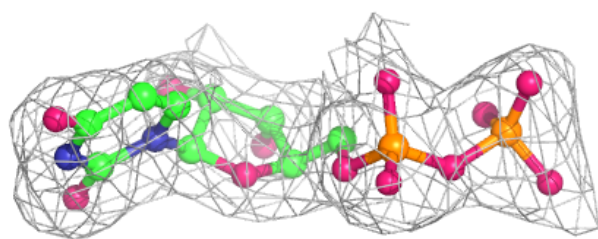
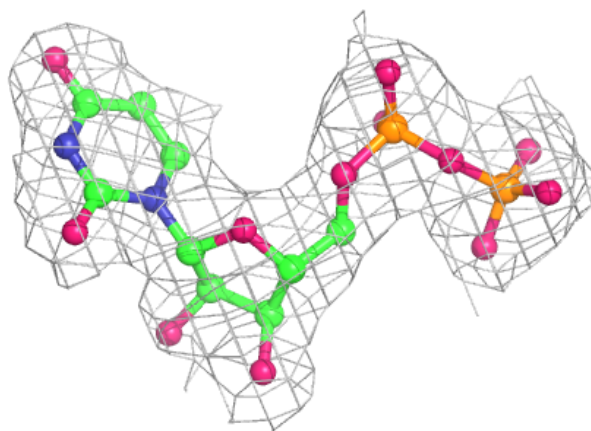
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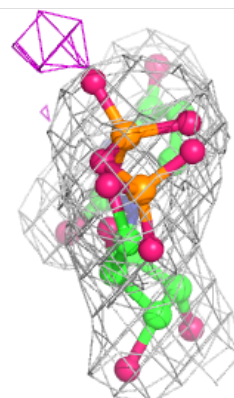
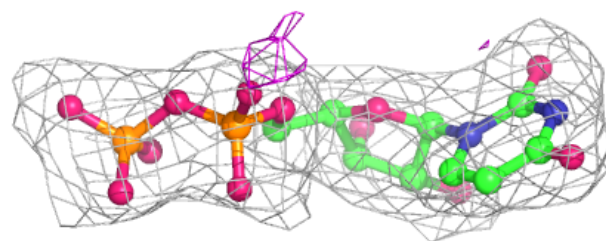
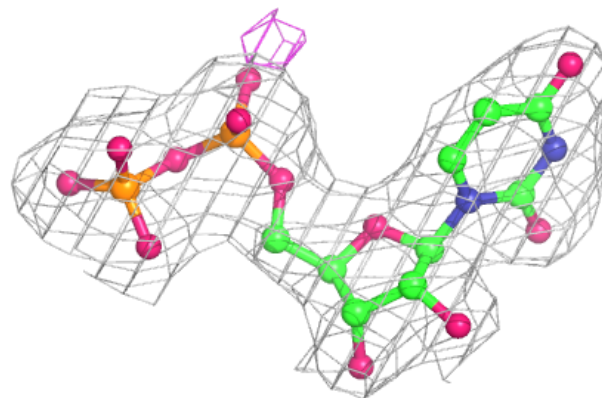


Electron density around UDP E 401:

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and green (positive)

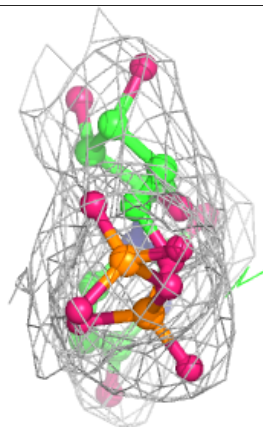
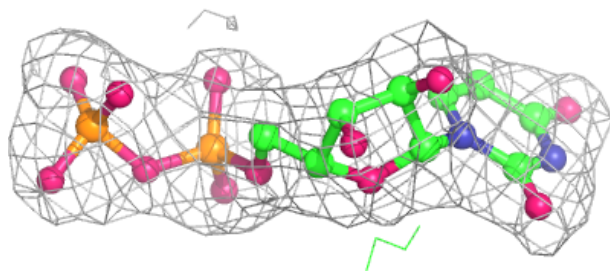
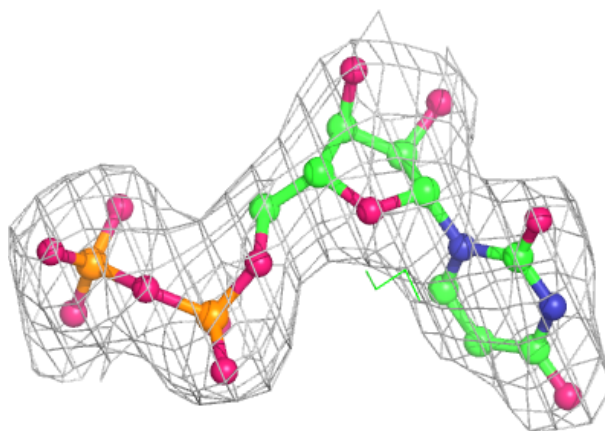
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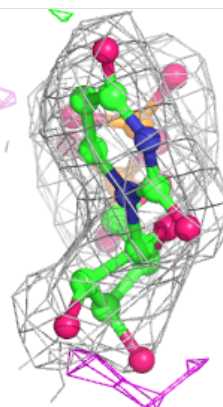
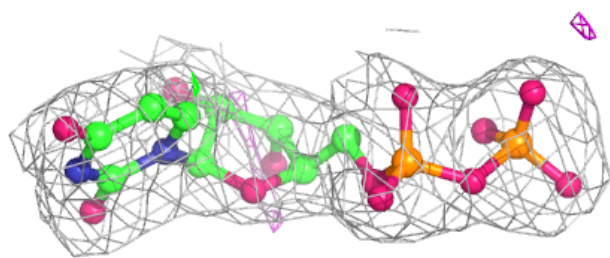
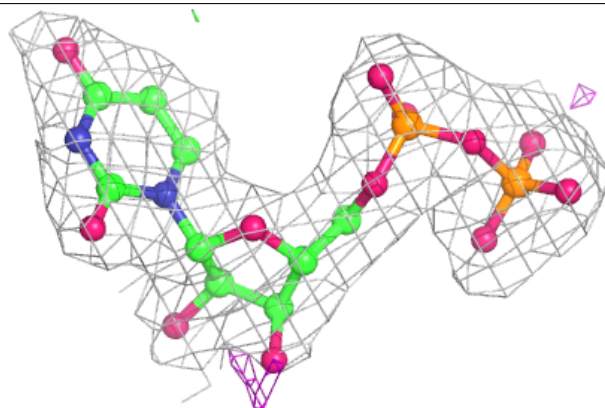


Electron density around UDP G 401:

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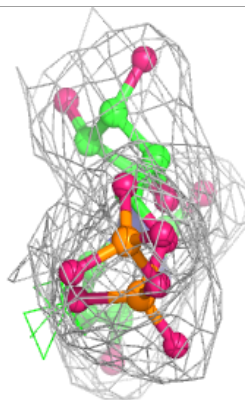
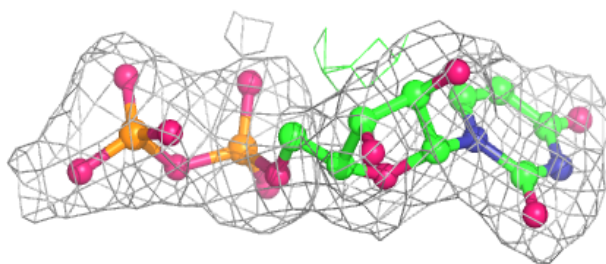
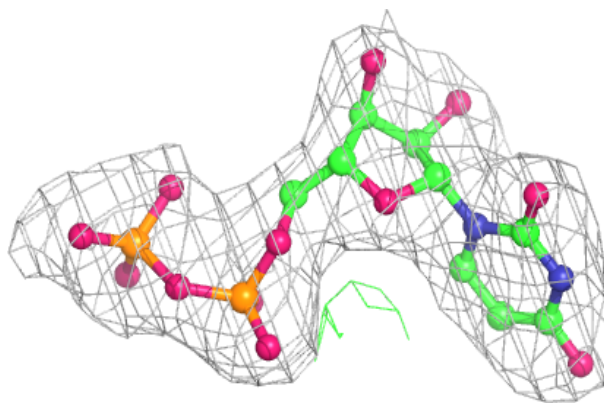
**Electron density around UDP H 401:**

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and green (positive)

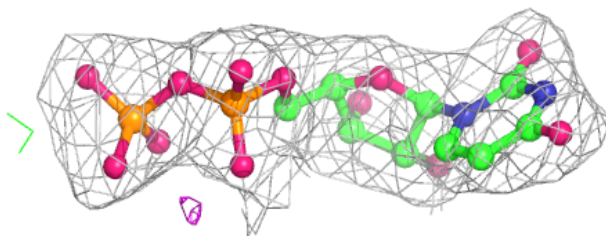
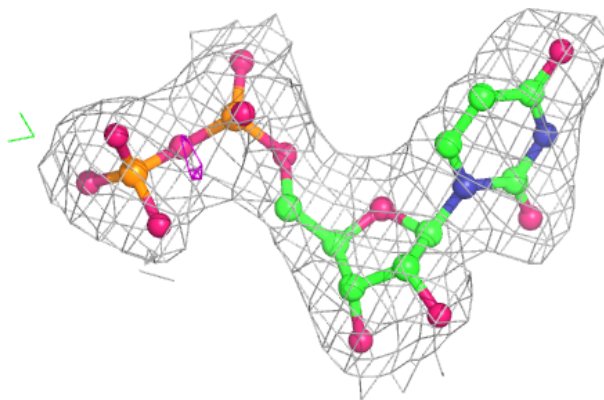


Electron density around UDP A 401:

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

**Electron density around UDP B 401:**

$2mF_o-DF_c$ (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.