



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:28 PM UTC

PDB ID : 4X7M / pdb_00004x7m
Title : Crystal structure of S. aureus TarM G117R mutant in complex with UDP and UDP-GlcNAc
Authors : Worrall, L.J.; Sobhanifar, S.; Strynadka, N.C.
Deposited on : 2014-12-09
Resolution : 2.40 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

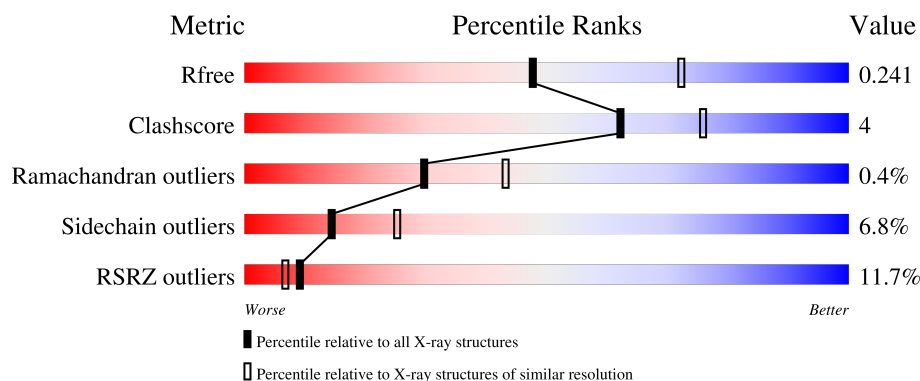
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	493	3% 82% 16% .
1	B	493	20% 82% 16% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8181 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.

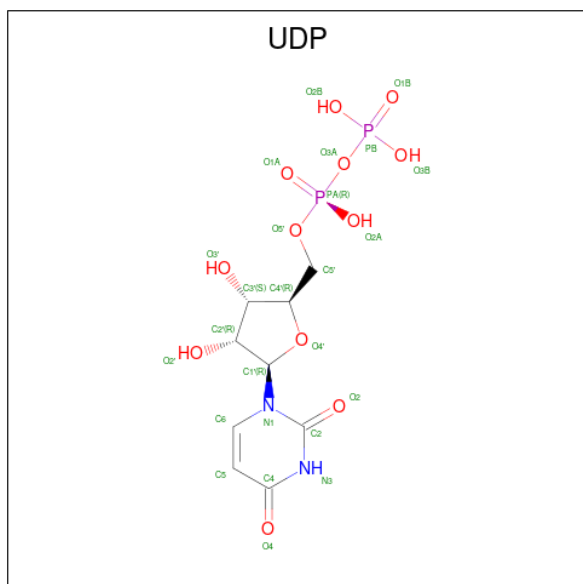
- Molecule 1 is a protein called TarM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			4024	2573	680	752	19			
1	B	493	Total	C	N	O	S	0	0	0
			4034	2582	681	752	19			

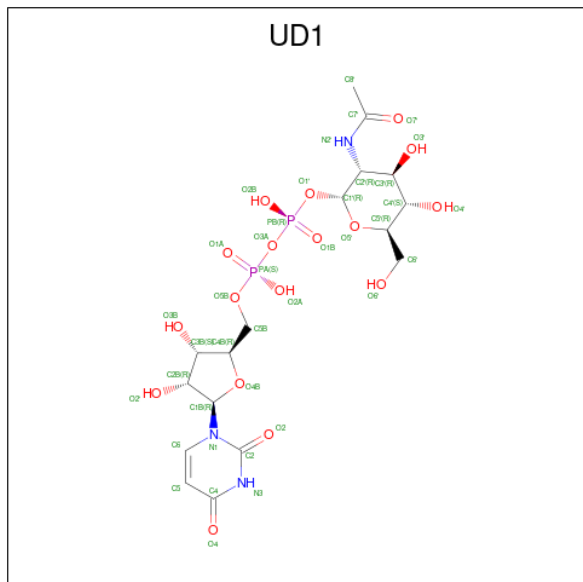
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	engineered mutation	UNP H0AM96
B	117	ARG	GLY	engineered mutation	UNP H0AM96

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

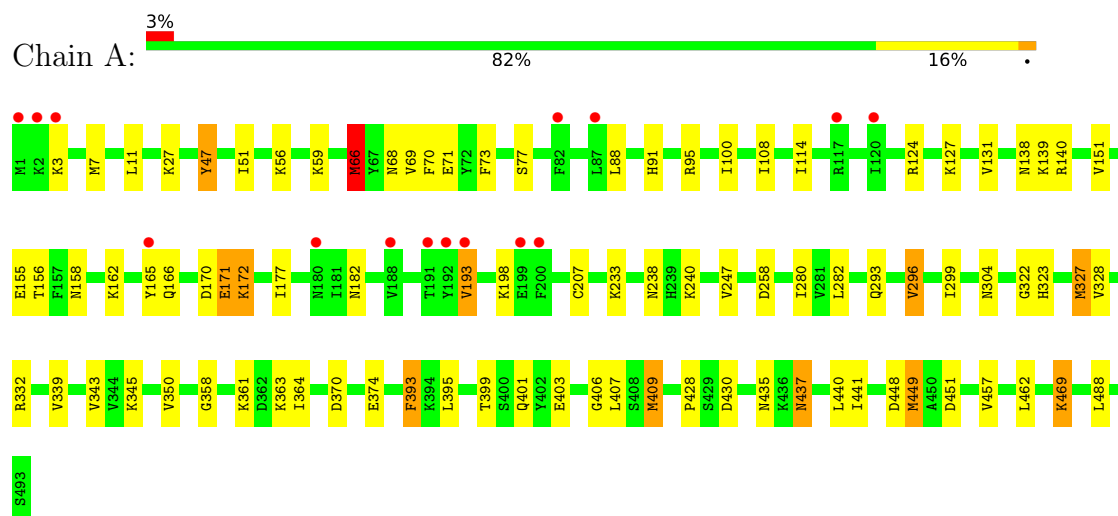
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	22	Total	O	0	0
			22	22		

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: TarM



• Molecule 1: TarM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.07Å 90.94Å 94.44Å 109.27° 99.03° 101.53°	Depositor
Resolution (Å)	46.04 – 2.40 46.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.04-2.40) 95.3 (46.04-2.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.39Å)	Xtriage
Refinement program	BUSTER, REFMAC	Depositor
R, R_{free}	0.233 , 0.274 (Not available) , 0.241	Depositor DCC
R_{free} test set	2505 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8181	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UD1, 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	0.88	3/4100 (0.1%)	1.40	20/5505 (0.4%)
1	B	0.86	3/4111 (0.1%)	1.42	23/5518 (0.4%)
All	All	0.87	6/8211 (0.1%)	1.41	43/11023 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	MET	SD-CE	-9.16	1.56	1.79
1	B	66	MET	SD-CE	-8.83	1.57	1.79
1	A	449	MET	SD-CE	-8.74	1.57	1.79
1	A	66	MET	SD-CE	-7.80	1.60	1.79
1	B	409	MET	SD-CE	-7.19	1.61	1.79
1	B	449	MET	SD-CE	-5.92	1.64	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	LEU	N-CA-C	6.98	119.91	111.82
1	B	304	ASN	CA-CB-CG	6.84	119.44	112.60
1	A	407	LEU	N-CA-C	6.48	118.34	111.28
1	B	193	VAL	N-CA-CB	6.47	118.34	112.06
1	B	430	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	282	LEU	N-CA-C	5.95	118.72	111.82
1	A	328	VAL	N-CA-C	5.77	114.25	107.84
1	A	393	PHE	CA-CB-CG	5.75	119.56	113.80
1	A	304	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	451	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	437	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	193	VAL	N-CA-CB	5.68	118.30	111.31
1	B	437	ASN	CA-CB-CG	5.65	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	370	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	448	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	451	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	393	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	170	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	220	ASP	CA-C-N	5.37	129.86	121.76
1	B	220	ASP	C-N-CA	5.37	129.86	121.76
1	B	16	GLY	CA-C-N	5.36	126.84	120.14
1	B	16	GLY	C-N-CA	5.36	126.84	120.14
1	B	370	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	104	GLU	N-CA-C	-5.33	106.09	113.18
1	A	358	GLY	CA-C-N	5.31	127.65	120.38
1	A	358	GLY	C-N-CA	5.31	127.65	120.38
1	B	251	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	70	PHE	CA-C-N	5.27	127.60	120.38
1	A	70	PHE	C-N-CA	5.27	127.60	120.38
1	B	19	THR	CA-C-N	5.24	127.62	120.54
1	B	19	THR	C-N-CA	5.24	127.62	120.54
1	B	358	GLY	CA-C-N	5.20	131.47	121.54
1	B	358	GLY	C-N-CA	5.20	131.47	121.54
1	A	448	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	56	LYS	CA-C-N	5.18	127.75	120.28
1	A	56	LYS	C-N-CA	5.18	127.75	120.28
1	B	56	LYS	CA-C-N	5.10	127.62	120.28
1	B	56	LYS	C-N-CA	5.10	127.62	120.28
1	A	406	GLY	CA-C-N	5.05	127.05	120.28
1	A	406	GLY	C-N-CA	5.05	127.05	120.28
1	B	20	SER	CA-C-N	5.00	127.25	120.65
1	B	20	SER	C-N-CA	5.00	127.25	120.65

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	4024	0	4038	32	0
1	B	4034	0	4056	35	0
2	A	25	0	11	0	0
3	B	39	0	25	4	0
4	A	37	0	0	3	0
4	B	22	0	0	1	0
All	All	8181	0	8130	67	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 4.

All (67) 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:47:TYR:CE1	1:A:66:MET:HE1	2.16	0.79
1:B:47:TYR:CE1	1:B:66:MET:HE1	2.17	0.79
1:B:88:LEU:CD2	1:B:151:VAL:HG11	2.16	0.74
1:B:250:VAL:HG12	3:B:501:UD1:H8'3	1.67	0.74
1:B:88:LEU:HD23	1:B:151:VAL:HG11	1.69	0.73
1:A:343:VAL:HG12	1:A:350:VAL:HG11	1.70	0.73
1:B:64:THR:HG21	4:B:608:HOH:O	1.90	0.71
1:B:343:VAL:HG12	1:B:350:VAL:HG11	1.71	0.71
1:A:339:VAL:HG21	1:A:449:MET:HE2	1.75	0.68
1:B:339:VAL:HG21	1:B:449:MET:HE2	1.74	0.68
1:A:332:ARG:HG3	1:A:401:GLN:HG2	1.79	0.64
1:B:332:ARG:HG3	1:B:401:GLN:HG2	1.80	0.63
1:B:399:THR:HG23	1:B:449:MET:HE1	1.82	0.62
1:B:403:GLU:HG3	3:B:501:UD1:O3'	2.01	0.60
1:A:156:THR:HB	1:A:165:TYR:HB3	1.84	0.59
1:B:156:THR:HB	1:B:165:TYR:HB3	1.85	0.58
1:A:296:VAL:HG12	1:A:299:ILE:HD11	1.87	0.57
1:B:177:ILE:HG12	1:B:193:VAL:HG12	1.87	0.56
1:A:399:THR:HG23	1:A:449:MET:HE1	1.87	0.55
1:B:7:MET:HG2	1:B:41:PHE:HZ	1.72	0.54
1:B:399:THR:CG2	1:B:449:MET:HE1	2.38	0.54
1:A:403:GLU:HG3	4:A:637:HOH:O	2.08	0.53
1:A:68:ASN:HB3	1:A:71:GLU:HB2	1.89	0.53
1:A:108:ILE:HG12	1:A:124:ARG:HG3	1.90	0.53
1:A:177:ILE:HG12	1:A:193:VAL:HG12	1.91	0.53
1:B:108:ILE:HG12	1:B:124:ARG:HG3	1.90	0.53
1:B:403:GLU:HG3	3:B:501:UD1:HO3'	1.74	0.53
1:B:51:ILE:HD11	1:B:66:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MET:HE2	1:A:361:LYS:HG3	1.91	0.52
1:B:140:ARG:HD2	1:B:161:ASN:OD1	2.10	0.52
1:A:399:THR:CG2	1:A:449:MET:HE1	2.40	0.51
1:A:409:MET:HE1	1:A:428:PRO:HG3	1.92	0.51
1:A:11:LEU:HB2	1:A:66:MET:HE2	1.92	0.51
1:B:306:VAL:HG11	1:B:410:ILE:HG21	1.94	0.50
1:A:51:ILE:HD11	1:A:66:MET:HE3	1.93	0.50
1:A:207:CYS:HB2	1:A:233:LYS:HG2	1.93	0.49
1:A:171:GLU:HG3	1:A:172:LYS:HD2	1.95	0.49
1:A:323:HIS:HE1	4:A:609:HOH:O	1.96	0.48
1:B:403:GLU:HA	3:B:501:UD1:H8'2	1.94	0.48
1:B:7:MET:HG2	1:B:41:PHE:CZ	2.48	0.48
1:B:247:VAL:HG13	1:B:280:ILE:HG22	1.96	0.48
1:B:68:ASN:HB3	1:B:71:GLU:HB2	1.95	0.47
1:A:158:ASN:HD21	1:A:162:LYS:HB2	1.78	0.47
1:A:293:GLN:HG2	4:A:606:HOH:O	2.13	0.47
1:B:78:ASN:OD1	1:B:170:ASP:HB2	2.14	0.47
1:B:155:GLU:HG2	1:B:166:GLN:HG2	1.97	0.47
1:A:88:LEU:HD23	1:A:151:VAL:HG11	1.95	0.47
1:B:437:ASN:HB3	1:B:469:LYS:HB3	1.97	0.47
1:B:11:LEU:HD12	1:B:66:MET:HE2	1.97	0.46
1:B:409:MET:HE1	1:B:428:PRO:HG3	1.98	0.46
1:B:158:ASN:HD21	1:B:162:LYS:HB2	1.81	0.45
1:A:91:HIS:O	1:A:95:ARG:HG2	2.17	0.45
1:B:26:SER:OG	1:B:64:THR:HB	2.16	0.45
1:A:437:ASN:HB3	1:A:469:LYS:HB3	1.99	0.45
1:A:155:GLU:HG2	1:A:166:GLN:HG2	2.00	0.44
1:A:322:GLY:HA3	1:A:393:PHE:CD2	2.52	0.44
1:A:247:VAL:HG13	1:A:280:ILE:HG22	2.00	0.44
1:B:322:GLY:HA3	1:B:393:PHE:CD2	2.53	0.44
1:A:11:LEU:HD12	1:A:66:MET:HE2	2.00	0.43
1:A:88:LEU:CD2	1:A:151:VAL:HG11	2.49	0.43
1:B:91:HIS:O	1:B:95:ARG:HG2	2.19	0.43
1:B:11:LEU:HB2	1:B:66:MET:HE2	2.00	0.43
1:B:332:ARG:CG	1:B:401:GLN:HG2	2.47	0.42
1:A:69:VAL:O	1:A:73:PHE:HD2	2.03	0.41
1:A:441:ILE:HG21	1:A:449:MET:HB2	2.04	0.40
1:A:47:TYR:CD1	1:A:66:MET:HE1	2.57	0.40
1:B:116:THR:O	1:B:117:ARG:CB	2.69	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	491/493 (100%)	465 (95%)	25 (5%)	1 (0%)	43	58
1	B	491/493 (100%)	470 (96%)	18 (4%)	3 (1%)	21	32
All	All	982/986 (100%)	935 (95%)	43 (4%)	4 (0%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	LEU
1	A	127	LYS
1	B	127	LYS
1	B	359	SER

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	447/450 (99%)	414 (93%)	33 (7%)	13	22
1	B	449/450 (100%)	421 (94%)	28 (6%)	16	29
All	All	896/900 (100%)	835 (93%)	61 (7%)	14	25

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	7	MET

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Mol	Chain	Res	Type
1	A	27	LYS
1	A	47	TYR
1	A	59	LYS
1	A	66	MET
1	A	77	SER
1	A	100	ILE
1	A	114	ILE
1	A	131	VAL
1	A	138	ASN
1	A	139	LYS
1	A	140	ARG
1	A	171	GLU
1	A	172	LYS
1	A	182	ASN
1	A	198	LYS
1	A	240	LYS
1	A	258	ASP
1	A	296	VAL
1	A	327	MET
1	A	345	LYS
1	A	363	LYS
1	A	364	ILE
1	A	374	GLU
1	A	395	LEU
1	A	430	ASP
1	A	435	ASN
1	A	440	LEU
1	A	457	VAL
1	A	462	LEU
1	A	469	LYS
1	A	488	LEU
1	B	3	LYS
1	B	7	MET
1	B	27	LYS
1	B	47	TYR
1	B	59	LYS
1	B	66	MET
1	B	82	PHE
1	B	100	ILE
1	B	131	VAL
1	B	138	ASN
1	B	139	LYS

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Mol	Chain	Res	Type
1	B	140	ARG
1	B	195	VAL
1	B	222	ILE
1	B	258	ASP
1	B	296	VAL
1	B	297	GLU
1	B	345	LYS
1	B	363	LYS
1	B	364	ILE
1	B	374	GLU
1	B	395	LEU
1	B	430	ASP
1	B	435	ASN
1	B	440	LEU
1	B	457	VAL
1	B	462	LEU
1	B	469	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	57	GLN
1	A	196	ASN
1	A	323	HIS
1	A	348	ASN
1	A	444	HIS
1	A	459	ASN
1	B	57	GLN
1	B	75	GLN
1	B	372	ASN
1	B	444	HIS
1	B	459	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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$
2	UDP	A	500	-	25,26,26	0.78	2 (8%)	38,40,40	0.69	0
3	UD1	B	501	-	40,41,41	2.40	9 (22%)	59,62,62	1.58	11 (18%)

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	500	-	-	2/16/32/32	0/2/2/2
3	UD1	B	501	-	-	11/26/63/63	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	UD1	PA-O3A	10.88	1.71	1.59
3	B	501	UD1	PB-O3A	5.80	1.65	1.59
3	B	501	UD1	C3'-C2'	3.22	1.59	1.53
2	A	500	UDP	PA-O3A	-2.76	1.56	1.59
3	B	501	UD1	O5'-C1'	2.67	1.48	1.41
3	B	501	UD1	C1'-C2'	2.62	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	UD1	C6-N1	2.35	1.43	1.38
3	B	501	UD1	C6-C5	2.18	1.40	1.35
3	B	501	UD1	PB-O1'	2.16	1.65	1.59
3	B	501	UD1	C2'-N2'	2.12	1.49	1.45
2	A	500	UDP	PB-O3B	-2.01	1.47	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	UD1	C4-N3-C2	-4.88	120.55	126.61
3	B	501	UD1	C5-C4-N3	3.82	120.15	114.80
3	B	501	UD1	N3-C2-N1	3.79	119.82	114.89
3	B	501	UD1	O4B-C4B-C5B	-3.43	98.36	109.33
3	B	501	UD1	O4-C4-C5	-2.82	120.30	125.16
3	B	501	UD1	O5'-C1'-O1'	-2.82	107.69	111.36
3	B	501	UD1	O1'-C1'-C2'	2.50	112.93	108.40
3	B	501	UD1	O3A-PA-O1A	2.26	117.51	110.70
3	B	501	UD1	C2'-N2'-C7'	2.24	128.34	123.11
3	B	501	UD1	PB-O1'-C1'	2.06	129.61	121.21
3	B	501	UD1	C1'-O5'-C5'	2.06	117.74	113.72

There are no chirality outliers.

All (13) torsion outliers are listed below:

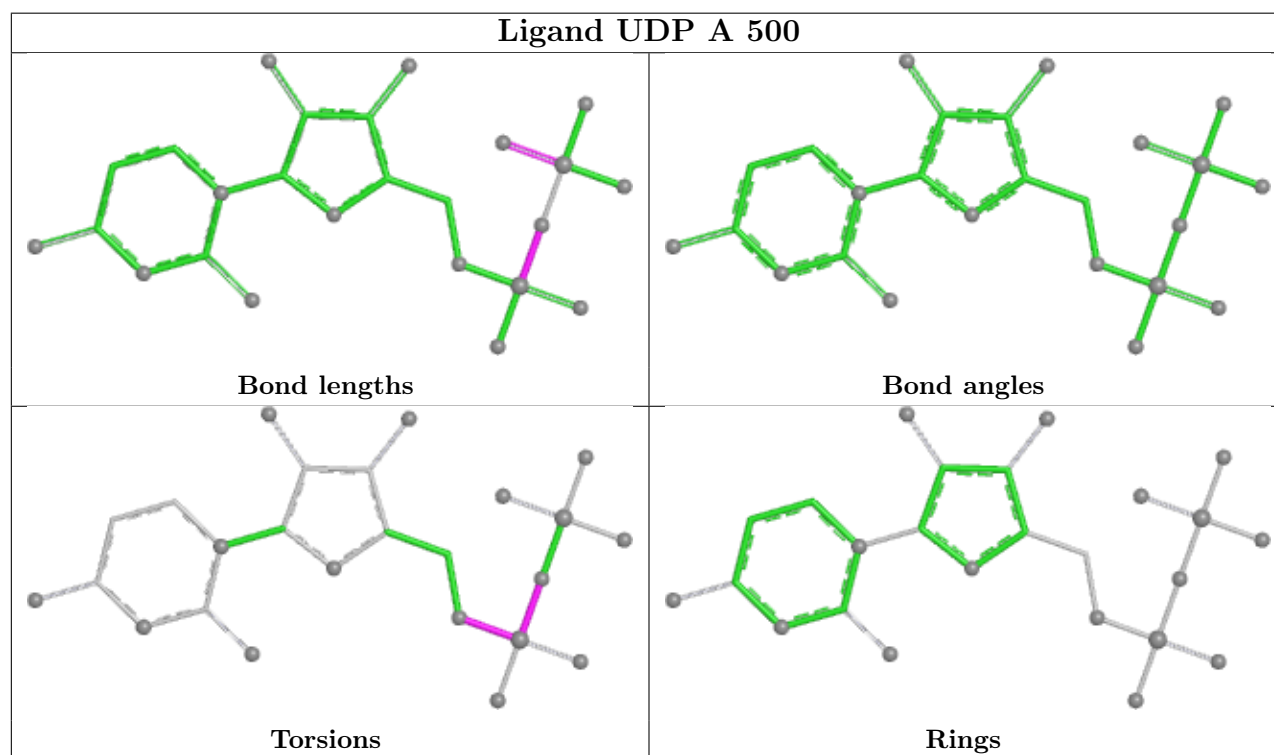
Mol	Chain	Res	Type	Atoms
2	A	500	UDP	C5'-O5'-PA-O1A
3	B	501	UD1	O5'-C1'-O1'-PB
3	B	501	UD1	C1'-O1'-PB-O3A
3	B	501	UD1	O5'-C5'-C6'-O6'
3	B	501	UD1	C4'-C5'-C6'-O6'
3	B	501	UD1	C8'-C7'-N2'-C2'
3	B	501	UD1	O7'-C7'-N2'-C2'
2	A	500	UDP	PB-O3A-PA-O5'
3	B	501	UD1	PA-O3A-PB-O1'
3	B	501	UD1	C5B-O5B-PA-O3A
3	B	501	UD1	C1'-O1'-PB-O2B
3	B	501	UD1	PA-O3A-PB-O1B
3	B	501	UD1	O4B-C4B-C5B-O5B

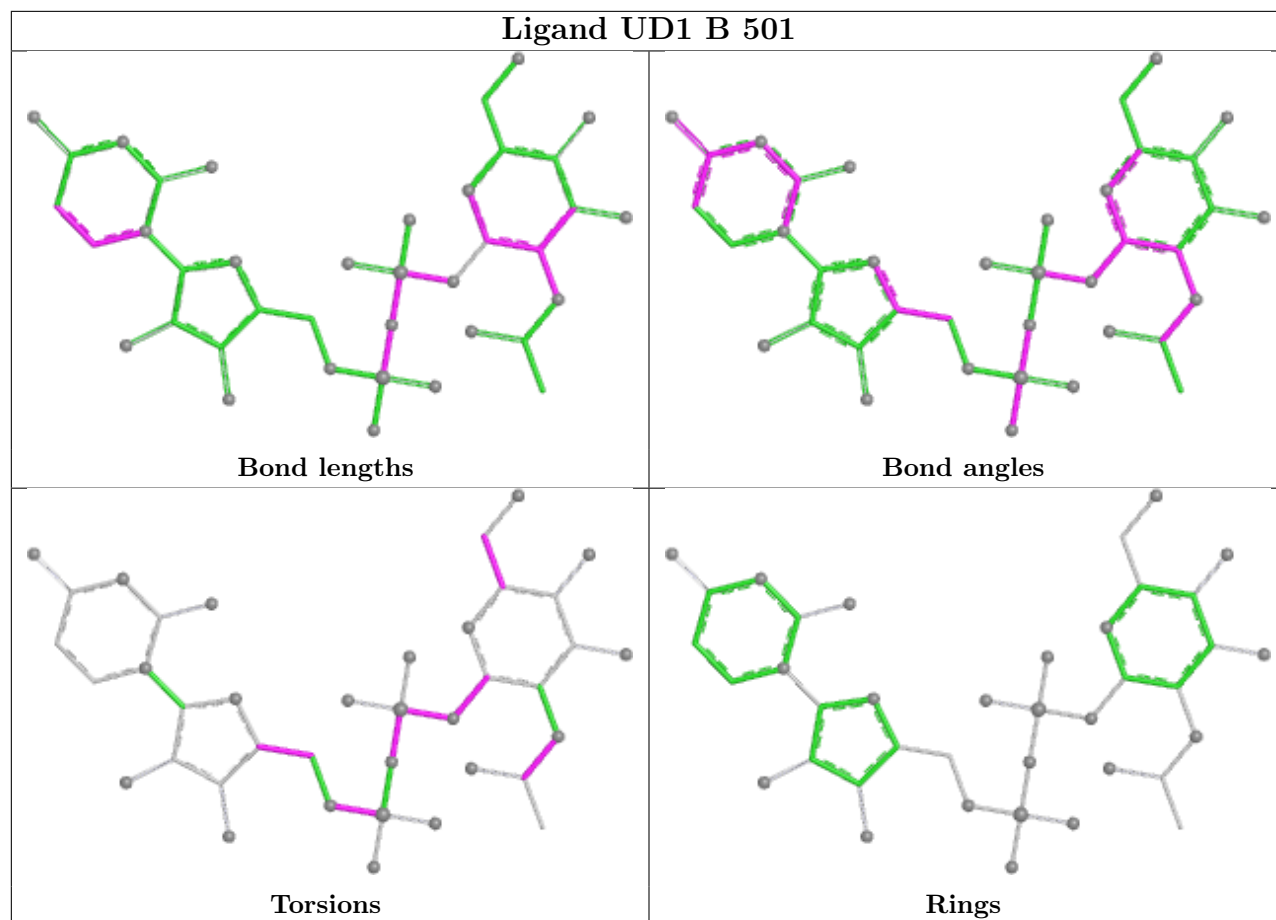
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	UD1	4	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	493/493 (100%)	0.46	15 (3%)	52	48	33, 78, 131, 154	0
1	B	493/493 (100%)	1.10	100 (20%)	3	2	34, 94, 161, 193	0
All	All	986/986 (100%)	0.78	115 (11%)	9	7	33, 85, 147, 193	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	THR	5.1
1	B	444	HIS	5.1
1	B	368	ILE	5.0
1	B	443	ASN	4.9
1	B	336	LEU	4.9
1	B	397	VAL	4.7
1	B	270	ILE	4.2
1	B	159	VAL	4.0
1	B	256	PHE	4.0
1	B	329	PRO	3.9
1	B	447	ASN	3.8
1	B	262	PHE	3.6
1	B	377	VAL	3.6
1	B	251	ASN	3.6
1	B	401	GLN	3.6
1	B	331	LYS	3.4
1	B	420	VAL	3.4
1	A	82	PHE	3.4
1	B	320	ILE	3.4
1	B	364	ILE	3.4
1	A	192	TYR	3.3
1	B	439	TYR	3.3
1	B	422	PHE	3.3
1	B	400	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	294	PHE	3.2
1	B	396	VAL	3.2
1	B	290	ILE	3.2
1	B	238	ASN	3.2
1	B	288	LEU	3.2
1	B	1	MET	3.1
1	B	261	ALA	3.1
1	B	398	SER	3.1
1	B	438	GLY	3.1
1	B	333	ILE	3.1
1	B	114	ILE	3.0
1	B	419	VAL	3.0
1	B	257	ASP	3.0
1	A	2	LYS	3.0
1	B	343	VAL	2.9
1	B	112	PHE	2.9
1	B	442	GLU	2.9
1	B	429	SER	2.9
1	B	250	VAL	2.9
1	B	402	TYR	2.9
1	B	489	ASN	2.9
1	B	263	LYS	2.8
1	B	441	ILE	2.8
1	B	246	GLY	2.8
1	B	426	TYR	2.8
1	B	399	THR	2.8
1	B	115	THR	2.7
1	B	446	ILE	2.7
1	B	421	ALA	2.7
1	B	352	PHE	2.6
1	B	325	SER	2.6
1	B	340	ALA	2.6
1	B	328	VAL	2.6
1	B	453	ILE	2.6
1	B	100	ILE	2.6
1	A	117	ARG	2.5
1	B	454	LEU	2.5
1	B	252	HIS	2.5
1	B	342	LEU	2.5
1	B	379	LEU	2.5
1	B	378	PHE	2.5
1	B	160	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.4
1	B	259	THR	2.4
1	B	359	SER	2.4
1	B	347	ASP	2.4
1	B	260	GLY	2.3
1	B	482	SER	2.3
1	B	370	ASP	2.3
1	A	200	PHE	2.3
1	B	116	THR	2.3
1	B	409	MET	2.3
1	A	180	ASN	2.3
1	B	255	ASN	2.3
1	A	191	THR	2.3
1	A	199	GLU	2.3
1	B	394	LYS	2.2
1	A	188	VAL	2.2
1	B	425	LYS	2.2
1	B	285	ALA	2.2
1	B	478	TYR	2.2
1	B	354	ILE	2.2
1	B	430	ASP	2.2
1	B	296	VAL	2.2
1	B	306	VAL	2.2
1	B	344	VAL	2.2
1	B	268	TYR	2.2
1	B	440	LEU	2.2
1	B	456	LEU	2.2
1	B	337	ILE	2.2
1	B	253	HIS	2.1
1	B	291	LEU	2.1
1	B	321	VAL	2.1
1	B	32	ALA	2.1
1	B	82	PHE	2.1
1	A	193	VAL	2.1
1	B	298	ASN	2.1
1	A	3	LYS	2.1
1	B	431	PHE	2.1
1	B	349	ALA	2.1
1	B	374	GLU	2.1
1	B	324	ILE	2.1
1	A	165	TYR	2.1
1	B	367	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	2.0
1	B	322	GLY	2.0
1	B	338	GLU	2.0
1	A	120	ILE	2.0
1	B	301	THR	2.0
1	B	449	MET	2.0
1	B	323	HIS	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](#)

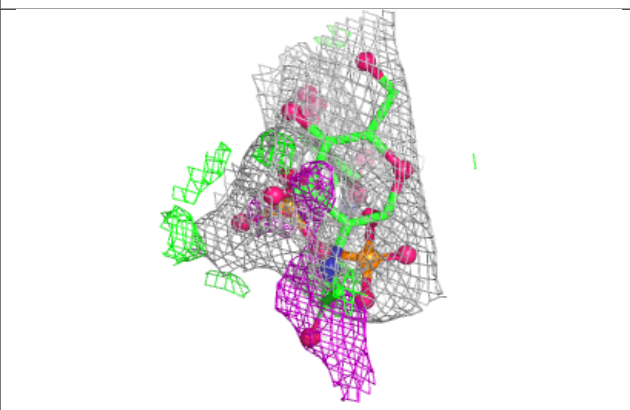
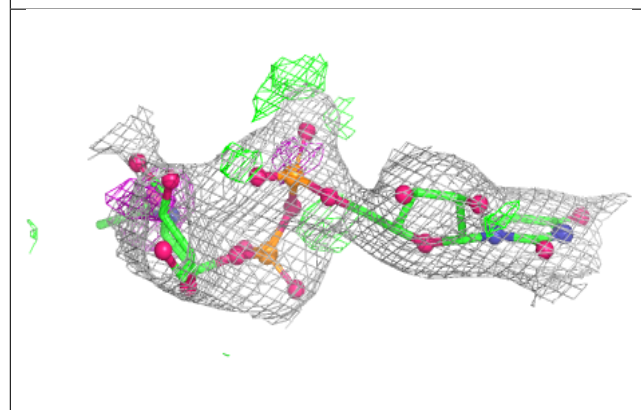
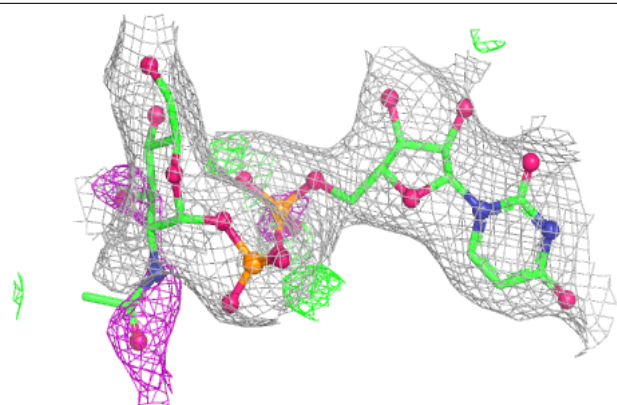
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UD1	B	501	39/39	0.86	0.13	61,70,91,94	0
2	UDP	A	500	25/25	0.91	0.10	52,62,71,73	0

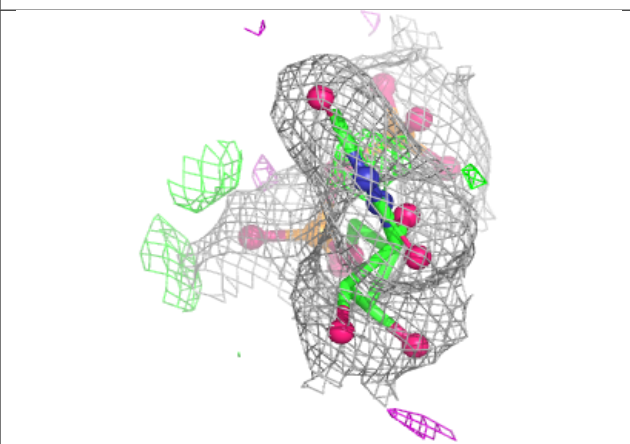
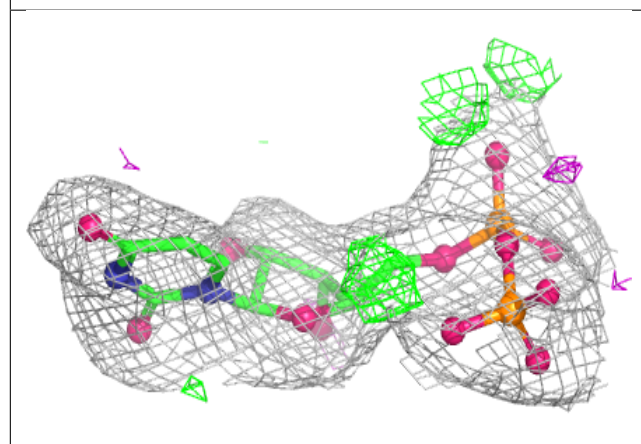
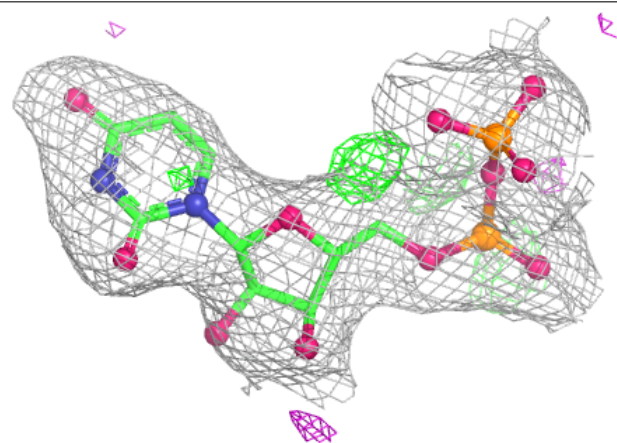
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UD1 B 501:

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

**Electron density around UDP A 500:**

$2mF_o-DF_c$ (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.