



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:18 PM UTC

PDB ID : 5ENZ / pdb_00005enz
Title : S. aureus MnaA-UDP co-structure
Authors : Fischmann, T.O.
Deposited on : 2015-11-09
Resolution : 1.91 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

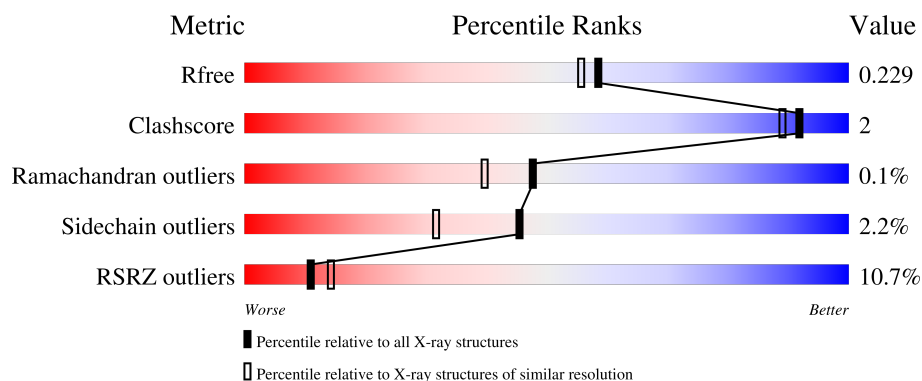
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	385	10% 90% 5% 5%
1	B	385	11% 90% 6% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6129 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

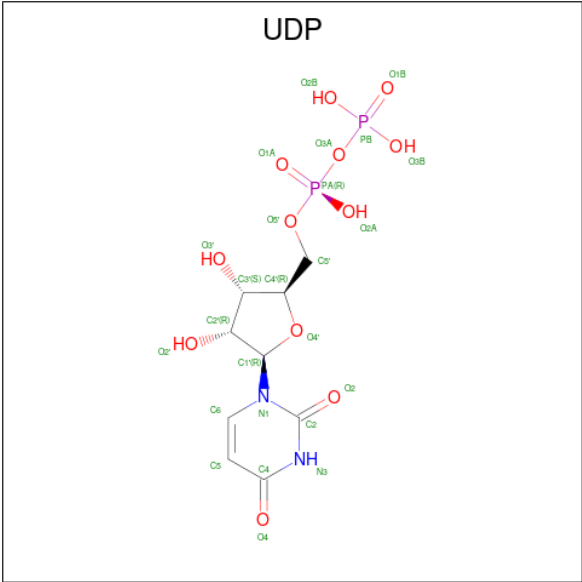
- Molecule 1 is a protein called UDP-GlcNAc 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	3
			2884	1842	483	547	12			
1	B	373	Total	C	N	O	S	0	0	2
			2959	1886	499	561	13			

There are 20 discrepancies between the modelled and reference sequences:

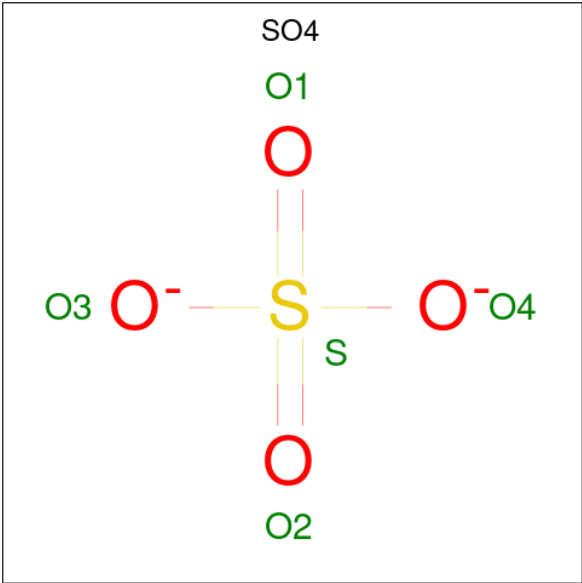
Chain	Residue	Modelled	Actual	Comment	Reference
A	376	GLY	-	expression tag	UNP Q9REV4
A	377	GLY	-	expression tag	UNP Q9REV4
A	378	HIS	-	expression tag	UNP Q9REV4
A	379	HIS	-	expression tag	UNP Q9REV4
A	380	HIS	-	expression tag	UNP Q9REV4
A	381	HIS	-	expression tag	UNP Q9REV4
A	382	HIS	-	expression tag	UNP Q9REV4
A	383	HIS	-	expression tag	UNP Q9REV4
A	384	HIS	-	expression tag	UNP Q9REV4
A	385	HIS	-	expression tag	UNP Q9REV4
B	376	GLY	-	expression tag	UNP Q9REV4
B	377	GLY	-	expression tag	UNP Q9REV4
B	378	HIS	-	expression tag	UNP Q9REV4
B	379	HIS	-	expression tag	UNP Q9REV4
B	380	HIS	-	expression tag	UNP Q9REV4
B	381	HIS	-	expression tag	UNP Q9REV4
B	382	HIS	-	expression tag	UNP Q9REV4
B	383	HIS	-	expression tag	UNP Q9REV4
B	384	HIS	-	expression tag	UNP Q9REV4
B	385	HIS	-	expression tag	UNP Q9REV4

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



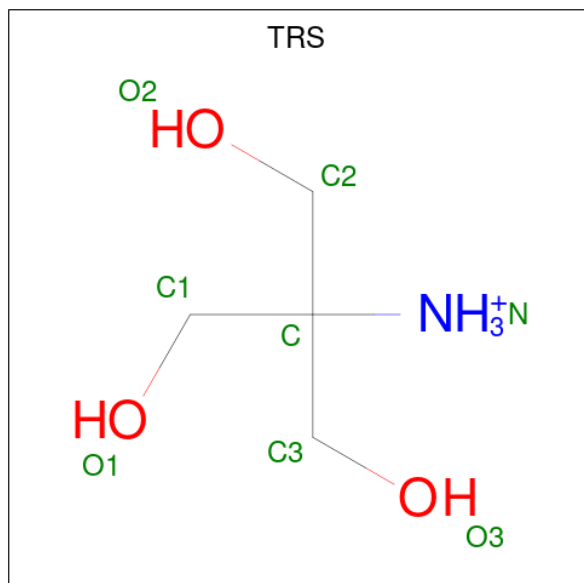
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

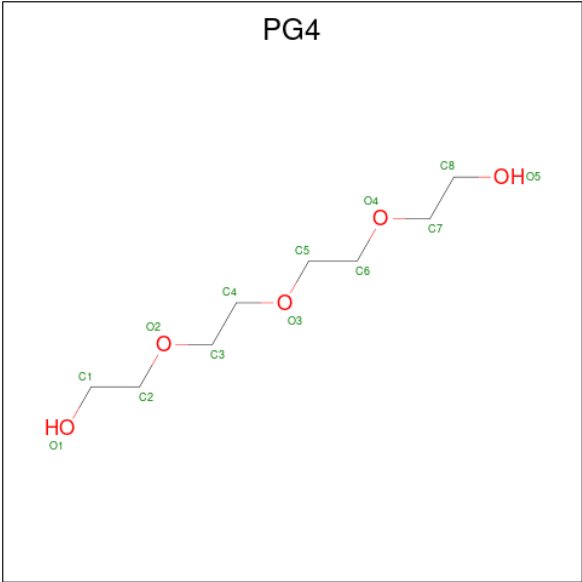
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

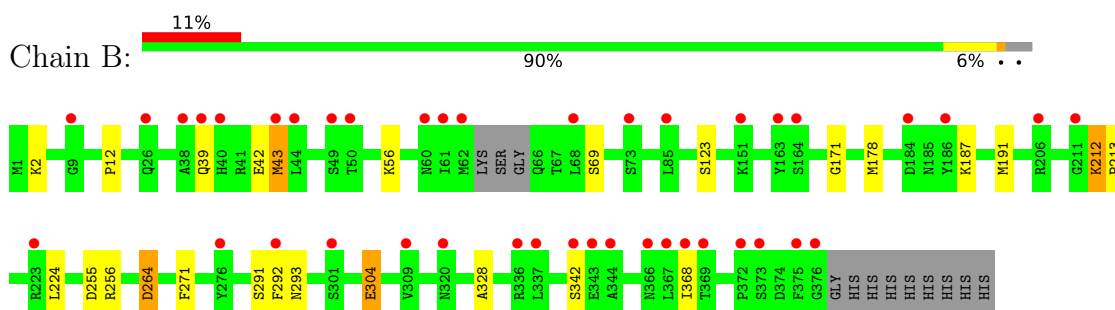


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		
6	B	96	Total	O	0	0
			96	96		

- Molecule 1: UDP-GlcNAc 2-epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.19Å 82.78Å 170.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.50 – 1.91 74.50 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.50-1.91) 99.9 (74.50-1.91)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.204 , 0.227 0.205 , 0.229	Depositor DCC
R_{free} test set	3062 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6129	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: UDP, SO4, PG4, TRS

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	0.87	0/2940	1.04	3/3975 (0.1%)
1	B	0.87	0/3017	1.06	6/4079 (0.1%)
All	All	0.87	0/5957	1.05	9/8054 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	GLN	N-CA-C	-8.09	102.40	111.14
1	B	342	SER	N-CA-C	6.37	118.02	111.14
1	B	123	SER	N-CA-C	-6.04	106.07	113.50
1	B	171	GLY	N-CA-C	-5.76	104.29	112.81
1	B	304	GLU	N-CA-C	-5.52	105.75	112.88
1	A	171	GLY	N-CA-C	-5.51	104.65	112.81
1	B	264	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	123	SER	N-CA-C	-5.27	107.02	113.50
1	A	264	ASP	CA-CB-CG	5.03	117.63	112.60

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	2884	0	2908	8	0
1	B	2959	0	2981	12	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
3	A	5	0	0	0	0
3	B	15	0	0	0	0
4	A	8	0	12	0	0
4	B	8	0	12	1	0
5	A	13	0	18	0	0
6	A	91	0	0	1	0
6	B	96	0	0	0	0
All	All	6129	0	5953	19	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 2.

All (19) 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:B:191:MET:HE1	1:B:271:PHE:HA	1.89	0.53
1:B:178:MET:HE3	1:B:292:PHE:CE1	2.44	0.52
1:A:178:MET:HE3	1:A:292:PHE:CE1	2.45	0.52
1:B:191:MET:CE	1:B:271:PHE:HA	2.41	0.50
1:B:178:MET:HE1	1:B:291:SER:HB2	1.94	0.48
1:A:191:MET:HE3	1:A:271:PHE:CE1	2.49	0.47
1:A:178:MET:HE1	1:A:291:SER:HB2	1.97	0.45
1:B:178:MET:HE1	1:B:291:SER:CB	2.47	0.45
1:A:178:MET:HE1	1:A:291:SER:CB	2.48	0.44
1:B:224:LEU:HD11	1:B:328:ALA:HB3	1.99	0.43
1:A:290:PRO:HB3	1:A:313:THR:HG21	2.00	0.43
1:B:255:ASP:OD2	1:B:256:ARG:HD3	2.18	0.43
1:A:191:MET:HE2	1:A:191:MET:HA	2.01	0.43
1:A:313:THR:HB	6:A:529:HOH:O	2.18	0.43
1:B:43:MET:HE1	1:B:264:ASP:HA	2.01	0.43
1:B:12:PRO:HB2	4:B:405:TRS:H12	2.01	0.42
1:B:212:LYS:N	1:B:213:PRO:CD	2.83	0.41
1:B:293:ASN:HD22	1:B:293:ASN:HA	1.73	0.41
1:A:76:ILE:HG22	1:B:69:SER:HB3	2.02	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	359/385 (93%)	354 (99%)	5 (1%)	0	100	100
1	B	369/385 (96%)	360 (98%)	8 (2%)	1 (0%)	36	26
All	All	728/770 (94%)	714 (98%)	13 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	LYS

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	320/339 (94%)	313 (98%)	7 (2%)	45	32
1	B	328/339 (97%)	321 (98%)	7 (2%)	47	33
All	All	648/678 (96%)	634 (98%)	14 (2%)	45	32

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	206	ARG
1	A	214	MET
1	A	273	LYS
1	A	279	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	314	LEU
1	A	368	ILE
1	B	2	LYS
1	B	42	GLU
1	B	43	MET
1	B	56	LYS
1	B	187	LYS
1	B	304	GLU
1	B	368	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	B	152	ASN
1	B	293	ASN
1	B	322	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](#)

9 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	$\# Z > 2$
5	PG4	A	404	-	12,12,12	0.18	0	11,11,11	0.15	0
3	SO4	B	404	-	4,4,4	0.74	0	6,6,6	0.30	0
3	SO4	B	402	-	4,4,4	0.40	0	6,6,6	0.46	0
4	TRS	A	403	-	7,7,7	0.20	0	9,9,9	0.23	0
3	SO4	A	402	-	4,4,4	0.26	0	6,6,6	0.20	0
4	TRS	B	405	-	7,7,7	0.18	0	9,9,9	0.41	0
2	UDP	A	401	-	25,26,26	0.63	1 (4%)	38,40,40	0.57	0
3	SO4	B	403	-	4,4,4	0.35	0	6,6,6	0.31	0
2	UDP	B	401	-	25,26,26	0.69	1 (4%)	38,40,40	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	A	404	-	-	4/10/10/10	-
4	TRS	A	403	-	-	3/9/9/9	-
4	TRS	B	405	-	-	7/9/9/9	-
2	UDP	A	401	-	-	0/16/32/32	0/2/2/2
2	UDP	B	401	-	-	1/16/32/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	UDP	PB-O1B	-2.19	1.43	1.50
2	A	401	UDP	PB-O1B	-2.00	1.44	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	405	TRS	N-C-C1-O1
4	B	405	TRS	N-C-C3-O3
5	A	404	PG4	C6-C5-O3-C4
5	A	404	PG4	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

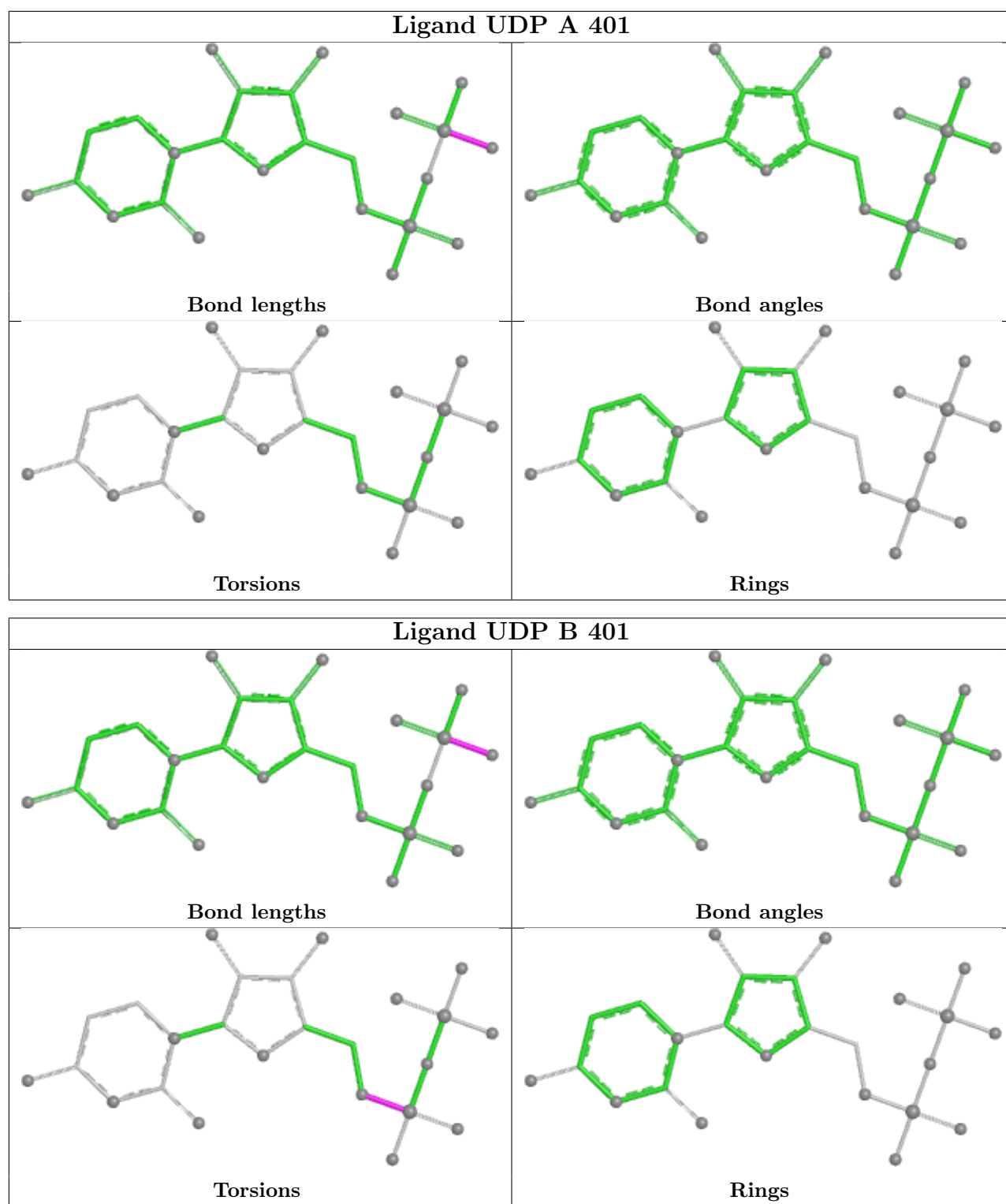
Mol	Chain	Res	Type	Atoms
4	B	405	TRS	C1-C-C3-O3
4	B	405	TRS	C2-C-C3-O3
2	B	401	UDP	C5'-O5'-PA-O3A
5	A	404	PG4	C8-C7-O4-C6
4	A	403	TRS	C1-C-C3-O3
4	B	405	TRS	C3-C-C1-O1
4	B	405	TRS	C3-C-C2-O2
5	A	404	PG4	O3-C5-C6-O4
4	A	403	TRS	C2-C-C3-O3
4	A	403	TRS	N-C-C3-O3
4	B	405	TRS	N-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	405	TRS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	365/385 (94%)	0.75	38 (10%)	11 15	24, 37, 64, 87	0
1	B	373/385 (96%)	0.74	41 (10%)	10 14	24, 38, 67, 87	0
All	All	738/770 (95%)	0.75	79 (10%)	11 14	24, 37, 65, 87	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	8.6
1	A	376	GLY	8.6
1	B	62	MET	7.6
1	B	376	GLY	7.4
1	A	60	ASN	5.8
1	B	39	GLN	5.6
1	B	43	MET	4.8
1	B	368	ILE	4.6
1	B	38	ALA	4.4
1	A	368	ILE	4.3
1	B	40	HIS	4.3
1	A	85	LEU	4.2
1	B	369	THR	3.9
1	A	302	VAL	3.7
1	A	44	LEU	3.6
1	B	344	ALA	3.6
1	B	372	PRO	3.6
1	B	292	PHE	3.5
1	A	210	ILE	3.5
1	B	9	GLY	3.4
1	B	163	TYR	3.4
1	B	60	ASN	3.3
1	A	303	THR	3.2
1	A	164	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	151	LYS	3.1
1	B	343	GLU	3.0
1	B	276	TYR	2.9
1	A	151	LYS	2.9
1	B	85	LEU	2.9
1	A	3	LYS	2.8
1	B	375	PHE	2.8
1	A	370	GLU	2.8
1	A	367	LEU	2.8
1	B	337	LEU	2.8
1	A	238	HIS	2.8
1	B	336	ARG	2.7
1	B	367	LEU	2.7
1	A	163	TYR	2.7
1	A	375	PHE	2.7
1	A	206	ARG	2.6
1	A	212	LYS	2.6
1	A	231	LEU	2.6
1	A	372	PRO	2.5
1	A	208	GLU	2.5
1	A	195	HIS	2.5
1	A	184	ASP	2.5
1	A	301	SER	2.4
1	A	318	GLY	2.4
1	A	1	MET	2.4
1	B	320	ASN	2.4
1	B	44	LEU	2.3
1	A	159	SER	2.3
1	A	363	TYR	2.3
1	B	186	TYR	2.3
1	A	155	SER	2.3
1	B	164	SER	2.3
1	B	342	SER	2.3
1	B	223	ARG	2.3
1	B	211	GLY	2.2
1	A	78	GLN	2.2
1	B	366	ASN	2.2
1	B	206	ARG	2.2
1	B	301	SER	2.2
1	B	373	SER	2.2
1	B	68	LEU	2.2
1	B	184	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	26	GLN	2.2
1	B	73	SER	2.2
1	A	67	THR	2.1
1	B	61	ILE	2.1
1	A	323	ASN	2.1
1	A	369	THR	2.1
1	A	229	THR	2.0
1	B	50	THR	2.0
1	A	81	GLN	2.0
1	A	74	LYS	2.0
1	B	49	SER	2.0
1	A	57	TYR	2.0
1	B	309	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](#)

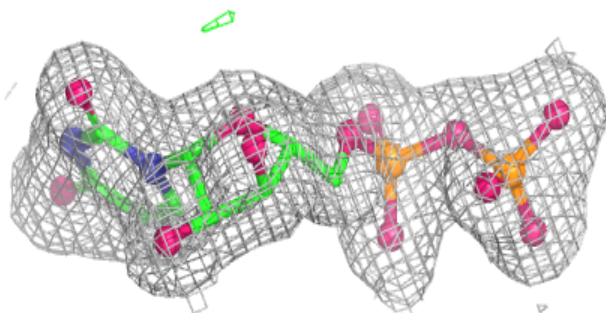
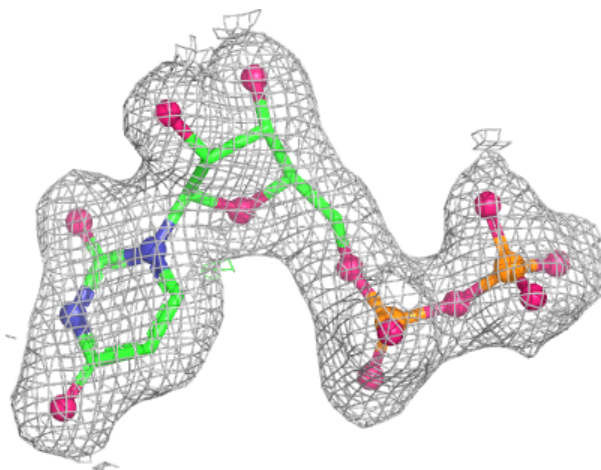
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

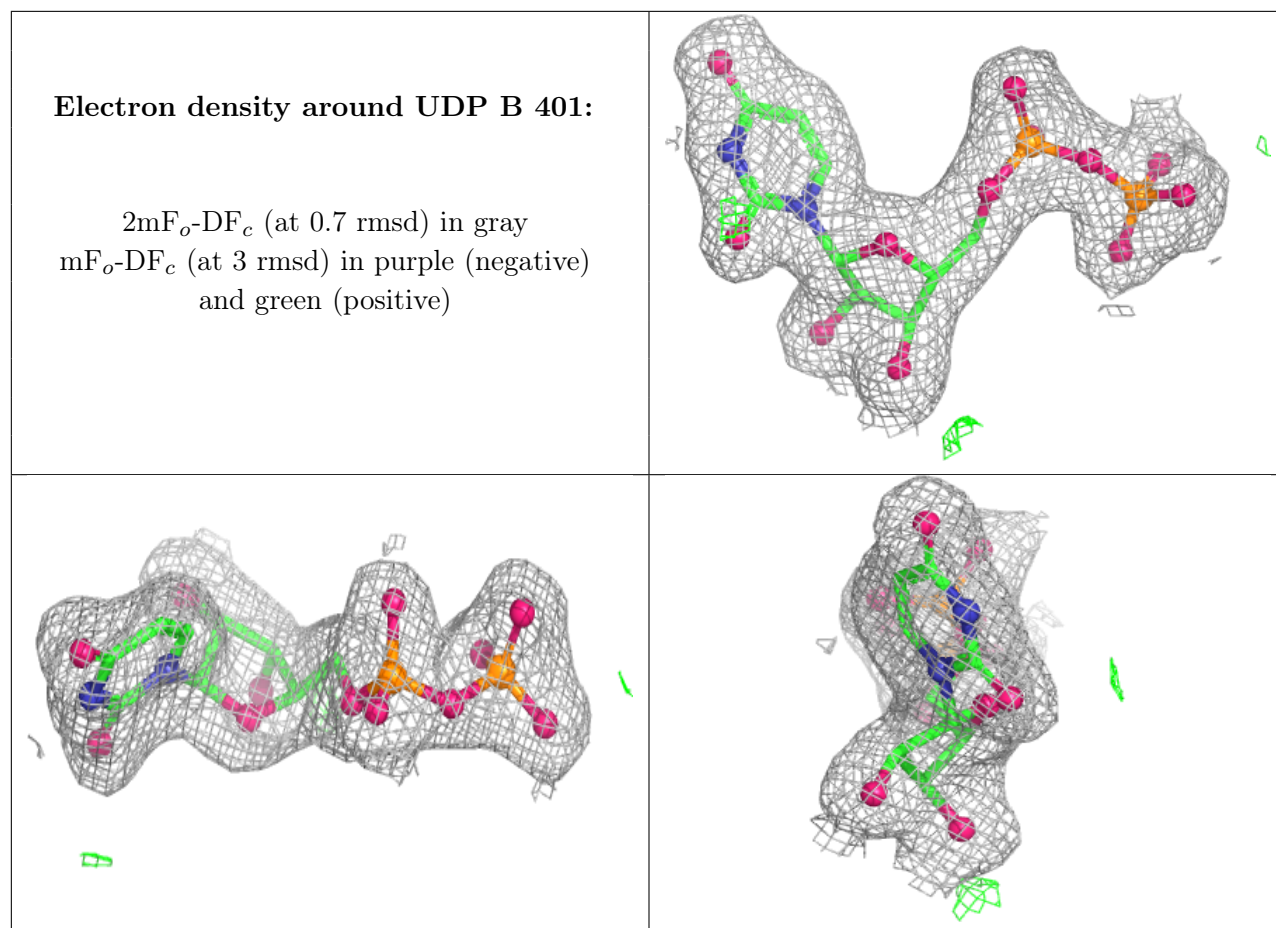
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PG4	A	404	13/13	0.77	0.23	75,76,79,79	0
4	TRS	A	403	8/8	0.87	0.12	43,48,51,52	0
4	TRS	B	405	8/8	0.93	0.08	30,33,35,35	0
3	SO4	B	403	5/5	0.96	0.10	39,39,45,45	0
3	SO4	A	402	5/5	0.96	0.07	35,35,40,40	0
3	SO4	B	404	5/5	0.97	0.08	26,27,29,30	5
2	UDP	A	401	25/25	0.98	0.05	24,27,31,32	0
2	UDP	B	401	25/25	0.98	0.04	24,26,29,30	0
3	SO4	B	402	5/5	0.99	0.07	32,34,36,39	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 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.