



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:22 PM UTC

PDB ID : 7YP6 / pdb_00007yp6
Title : Crystal structure of elaiophylin glycosyltransferase in complex with UDP
Authors : Xu, T.; Liu, Q.; Gan, Q.; Liu, J.
Deposited on : 2022-08-02
Resolution : 2.60 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

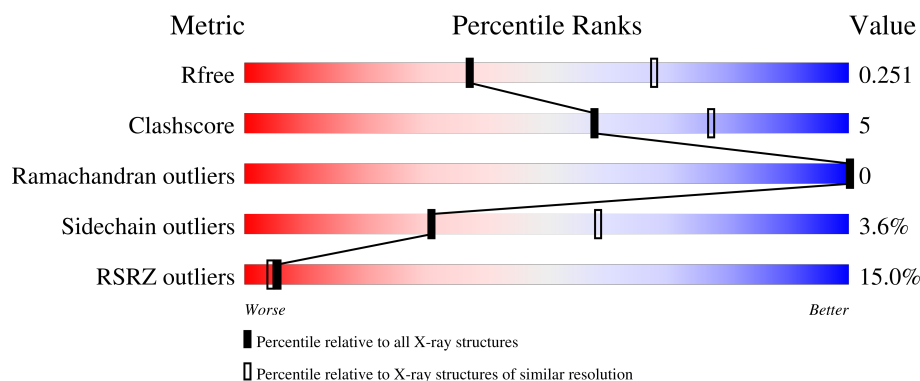
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	437	
1	B	437	
1	C	437	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9716 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3241	2062	569	597	13			
1	B	416	Total	C	N	O	S	0	0	0
			3259	2074	572	600	13			
1	C	372	Total	C	N	O	S	0	0	0
			2934	1871	514	536	13			

There are 60 discrepancies between the modelled and reference sequences:

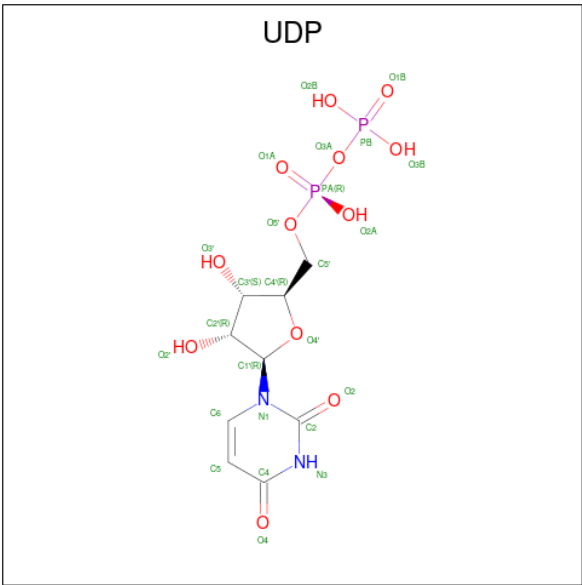
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E5L4T5
A	-18	GLY	-	expression tag	UNP E5L4T5
A	-17	SER	-	expression tag	UNP E5L4T5
A	-16	SER	-	expression tag	UNP E5L4T5
A	-15	HIS	-	expression tag	UNP E5L4T5
A	-14	HIS	-	expression tag	UNP E5L4T5
A	-13	HIS	-	expression tag	UNP E5L4T5
A	-12	HIS	-	expression tag	UNP E5L4T5
A	-11	HIS	-	expression tag	UNP E5L4T5
A	-10	HIS	-	expression tag	UNP E5L4T5
A	-9	SER	-	expression tag	UNP E5L4T5
A	-8	SER	-	expression tag	UNP E5L4T5
A	-7	GLY	-	expression tag	UNP E5L4T5
A	-6	LEU	-	expression tag	UNP E5L4T5
A	-5	VAL	-	expression tag	UNP E5L4T5
A	-4	PRO	-	expression tag	UNP E5L4T5
A	-3	ARG	-	expression tag	UNP E5L4T5
A	-2	GLY	-	expression tag	UNP E5L4T5
A	-1	SER	-	expression tag	UNP E5L4T5
A	0	HIS	-	expression tag	UNP E5L4T5
B	-19	MET	-	initiating methionine	UNP E5L4T5
B	-18	GLY	-	expression tag	UNP E5L4T5
B	-17	SER	-	expression tag	UNP E5L4T5

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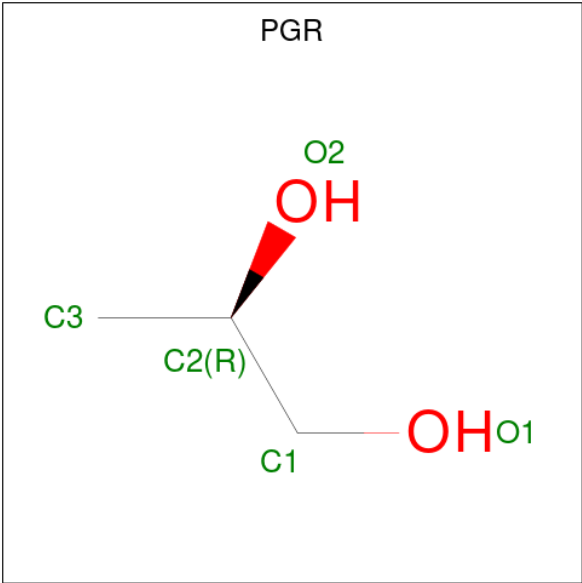
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP E5L4T5
B	-15	HIS	-	expression tag	UNP E5L4T5
B	-14	HIS	-	expression tag	UNP E5L4T5
B	-13	HIS	-	expression tag	UNP E5L4T5
B	-12	HIS	-	expression tag	UNP E5L4T5
B	-11	HIS	-	expression tag	UNP E5L4T5
B	-10	HIS	-	expression tag	UNP E5L4T5
B	-9	SER	-	expression tag	UNP E5L4T5
B	-8	SER	-	expression tag	UNP E5L4T5
B	-7	GLY	-	expression tag	UNP E5L4T5
B	-6	LEU	-	expression tag	UNP E5L4T5
B	-5	VAL	-	expression tag	UNP E5L4T5
B	-4	PRO	-	expression tag	UNP E5L4T5
B	-3	ARG	-	expression tag	UNP E5L4T5
B	-2	GLY	-	expression tag	UNP E5L4T5
B	-1	SER	-	expression tag	UNP E5L4T5
B	0	HIS	-	expression tag	UNP E5L4T5
C	-19	MET	-	initiating methionine	UNP E5L4T5
C	-18	GLY	-	expression tag	UNP E5L4T5
C	-17	SER	-	expression tag	UNP E5L4T5
C	-16	SER	-	expression tag	UNP E5L4T5
C	-15	HIS	-	expression tag	UNP E5L4T5
C	-14	HIS	-	expression tag	UNP E5L4T5
C	-13	HIS	-	expression tag	UNP E5L4T5
C	-12	HIS	-	expression tag	UNP E5L4T5
C	-11	HIS	-	expression tag	UNP E5L4T5
C	-10	HIS	-	expression tag	UNP E5L4T5
C	-9	SER	-	expression tag	UNP E5L4T5
C	-8	SER	-	expression tag	UNP E5L4T5
C	-7	GLY	-	expression tag	UNP E5L4T5
C	-6	LEU	-	expression tag	UNP E5L4T5
C	-5	VAL	-	expression tag	UNP E5L4T5
C	-4	PRO	-	expression tag	UNP E5L4T5
C	-3	ARG	-	expression tag	UNP E5L4T5
C	-2	GLY	-	expression tag	UNP E5L4T5
C	-1	SER	-	expression tag	UNP E5L4T5
C	0	HIS	-	expression tag	UNP E5L4T5

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



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 R-1,2-PROPANEDIOL (CCD ID: PGR) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	A	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0

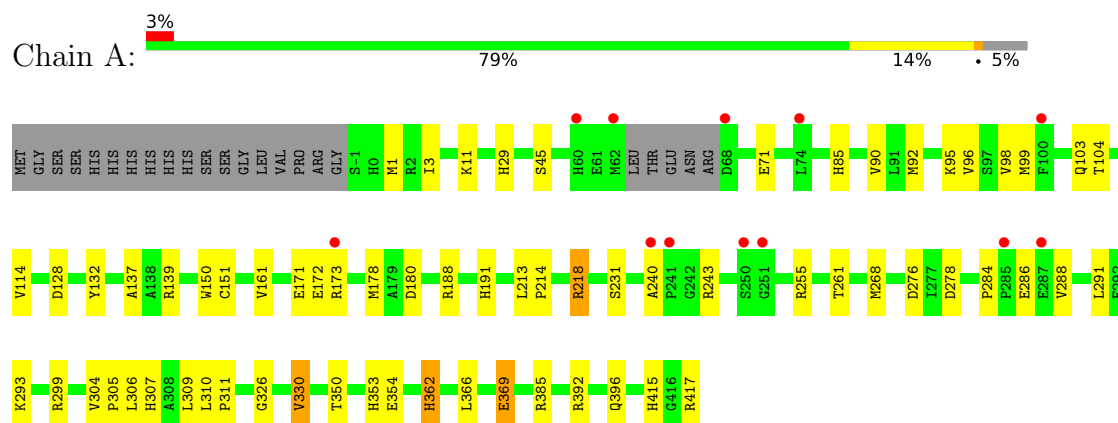
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	60	Total O 60 60	0	0
4	C	4	Total O 4 4	0	0

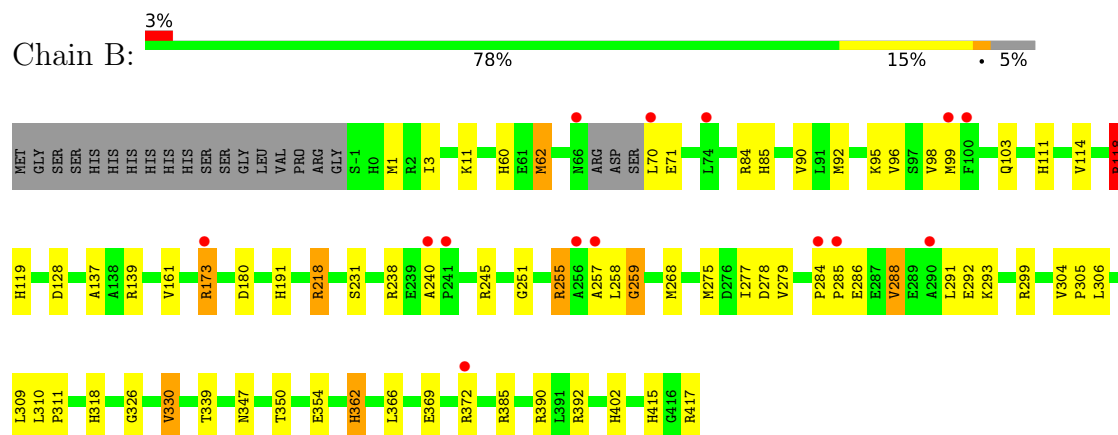
3 Residue-property plots [i](#)

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.

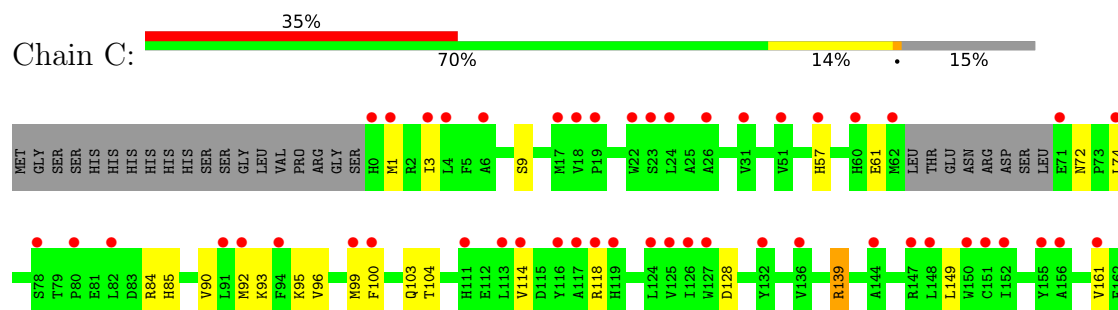
• Molecule 1: Glycosyltransferase

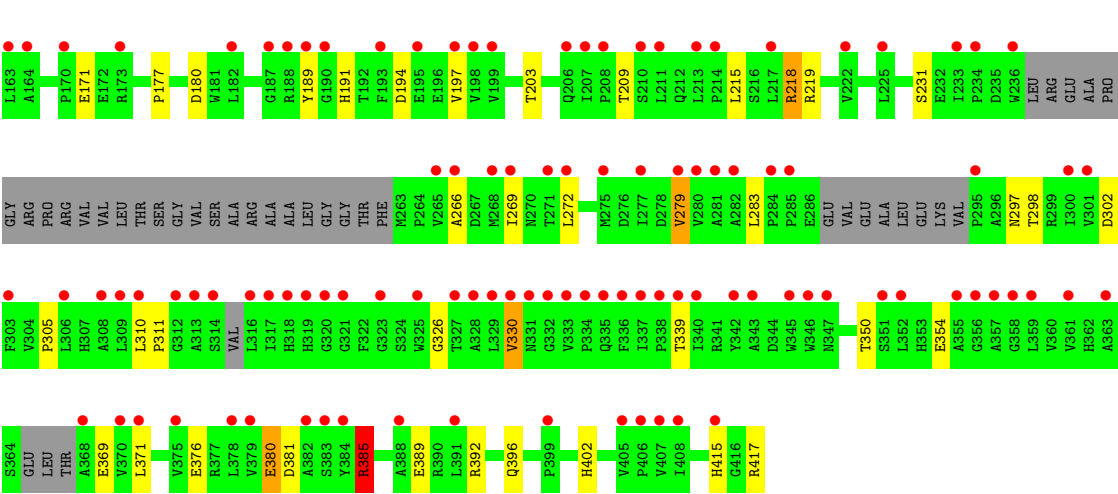


• Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	66.80Å 131.86Å 225.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.12 – 2.60 64.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.12-2.60) 99.8 (64.12-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.212 , 0.247 0.217 , 0.251	Depositor DCC
R_{free} test set	3106 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9716	wwPDB-VP
Average B, all atoms (Å ²)	78.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGR, 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	0.79	6/3330 (0.2%)	1.06	4/4552 (0.1%)
1	B	0.77	9/3348 (0.3%)	1.06	5/4577 (0.1%)
1	C	0.68	3/3016 (0.1%)	1.00	4/4118 (0.1%)
All	All	0.75	18/9694 (0.2%)	1.04	13/13247 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	16
1	C	0	7
All	All	0	34

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	HIS	CE1-NE2	9.87	1.42	1.32
1	A	191	HIS	CE1-NE2	9.28	1.41	1.32
1	B	318	HIS	CE1-NE2	7.36	1.40	1.32
1	A	85	HIS	CE1-NE2	6.84	1.39	1.32
1	B	362	HIS	CE1-NE2	6.04	1.38	1.32
1	A	307	HIS	CE1-NE2	6.00	1.38	1.32
1	B	111	HIS	CE1-NE2	5.66	1.38	1.32
1	B	402	HIS	CE1-NE2	5.63	1.38	1.32
1	A	353	HIS	CE1-NE2	5.54	1.38	1.32
1	B	119	HIS	CE1-NE2	5.54	1.38	1.32
1	A	362	HIS	CE1-NE2	5.47	1.38	1.32
1	C	191	HIS	CE1-NE2	5.41	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	HIS	CE1-NE2	5.38	1.38	1.32
1	C	85	HIS	CE1-NE2	5.32	1.37	1.32
1	B	415	HIS	CE1-NE2	5.29	1.37	1.32
1	B	85	HIS	CE1-NE2	5.28	1.37	1.32
1	C	402	HIS	CE1-NE2	5.13	1.37	1.32
1	B	60	HIS	CE1-NE2	5.06	1.37	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	CB-CA-C	-7.38	99.29	110.88
1	A	11	LYS	CB-CA-C	6.34	121.32	110.79
1	A	369	GLU	CB-CG-CD	6.14	123.04	112.60
1	C	369	GLU	CB-CA-C	-6.02	101.38	110.90
1	B	11	LYS	CB-CA-C	5.78	120.39	110.79
1	B	278	ASP	CB-CA-C	-5.59	100.63	109.80
1	C	381	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	180	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	293	LYS	CB-CA-C	5.39	119.40	109.71
1	A	180	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	180	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	380	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	293	LYS	CB-CA-C	5.02	118.55	109.37

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	173	ARG	Sidechain
1	A	188	ARG	Sidechain
1	A	218	ARG	Sidechain
1	A	240	ALA	Peptide
1	A	243	ARG	Sidechain
1	A	255	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	385	ARG	Sidechain
1	A	392	ARG	Sidechain
1	A	417	ARG	Sidechain
1	B	118	ARG	Sidechain
1	B	139	ARG	Sidechain
1	B	173	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	218	ARG	Sidechain
1	B	238	ARG	Sidechain
1	B	240	ALA	Peptide
1	B	245	ARG	Sidechain
1	B	255	ARG	Sidechain
1	B	258	LEU	Peptide
1	B	259	GLY	Peptide
1	B	299	ARG	Sidechain
1	B	385	ARG	Sidechain
1	B	390	ARG	Sidechain
1	B	392	ARG	Sidechain
1	B	417	ARG	Sidechain
1	B	84	ARG	Sidechain
1	C	118	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	218	ARG	Sidechain
1	C	385	ARG	Sidechain
1	C	392	ARG	Sidechain
1	C	417	ARG	Sidechain
1	C	84	ARG	Sidechain

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	3241	0	3180	27	0
1	B	3259	0	3201	28	0
1	C	2934	0	2857	32	0
2	A	25	0	11	2	0
2	B	25	0	11	1	0
3	A	40	0	64	1	0
3	B	40	0	64	1	0
4	A	88	0	0	3	2
4	B	60	0	0	1	1
4	C	4	0	0	0	0
All	All	9716	0	9388	86	3

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 5.

All (86) 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:173:ARG:HG2	1:B:173:ARG:HH11	1.46	0.79
1:A:98:VAL:HG12	1:A:103:GLN:HE21	1.53	0.73
1:A:218:ARG:HD2	4:A:664:HOH:O	1.92	0.70
1:A:45:SER:OG	4:A:601:HOH:O	2.10	0.68
1:C:371:LEU:C	1:C:371:LEU:HD23	2.18	0.68
1:A:276:ASP:O	3:A:503:PGR:H11	1.98	0.62
1:A:98:VAL:HG12	1:A:103:GLN:NE2	2.13	0.62
1:A:304:VAL:HG11	1:A:309:LEU:HD22	1.83	0.60
1:C:9:SER:OG	1:C:57:HIS:HE1	1.84	0.60
1:B:275:MET:HE1	1:B:372:ARG:HA	1.84	0.59
1:B:291:LEU:O	4:B:601:HOH:O	2.16	0.59
1:B:285:PRO:O	1:B:288:VAL:HG22	2.04	0.58
1:C:279:VAL:HG11	1:C:298:THR:HG22	1.86	0.58
1:C:326:GLY:O	1:C:330:VAL:HG13	2.04	0.57
1:A:326:GLY:O	1:A:330:VAL:HG13	2.04	0.57
1:C:279:VAL:CG1	1:C:298:THR:HG22	2.34	0.57
1:C:350:THR:O	1:C:354:GLU:HG2	2.04	0.57
1:B:98:VAL:HG12	1:B:103:GLN:NE2	2.19	0.57
1:A:218:ARG:NH1	1:A:415:HIS:HE1	2.04	0.56
1:B:326:GLY:O	1:B:330:VAL:HG13	2.06	0.56
1:A:92:MET:O	1:A:96:VAL:HG23	2.07	0.55
1:B:231:SER:HB2	1:B:305:PRO:HB3	1.87	0.55
1:A:218:ARG:CD	4:A:664:HOH:O	2.54	0.55
1:A:1:MET:HE3	1:A:3:ILE:HD11	1.89	0.54
1:B:118:ARG:HH11	1:B:118:ARG:HG3	1.72	0.54
1:A:231:SER:HB2	1:A:305:PRO:HB3	1.89	0.54
1:A:98:VAL:CG1	1:A:103:GLN:HE21	2.18	0.53
1:C:218:ARG:NH1	1:C:415:HIS:HE1	2.07	0.53
1:B:92:MET:HE3	1:B:96:VAL:HG23	1.91	0.53
1:A:99:MET:CG	1:C:92:MET:HE1	2.39	0.53
1:A:350:THR:O	1:A:354:GLU:HG2	2.09	0.51
1:B:255:ARG:O	1:B:259:GLY:CA	2.59	0.51
1:A:284:PRO:O	1:A:288:VAL:HG23	2.11	0.51
1:C:99:MET:HE3	1:C:100:PHE:CE2	2.46	0.51
1:C:99:MET:HA	1:C:103:GLN:NE2	2.26	0.50
1:C:1:MET:HE3	1:C:3:ILE:HD11	1.93	0.50
1:B:251:GLY:HA3	2:B:500:UDP:O2B	2.12	0.49
1:B:284:PRO:O	1:B:288:VAL:HG13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:HD13	1:C:203:THR:HG23	1.94	0.49
1:B:1:MET:HE3	1:B:3:ILE:HD11	1.95	0.49
1:B:347:ASN:HD22	3:B:507:PGR:H33	1.78	0.48
1:A:268:MET:HE3	1:A:366:LEU:HD21	1.95	0.48
1:B:310:LEU:N	1:B:311:PRO:CD	2.77	0.48
1:C:310:LEU:N	1:C:311:PRO:CD	2.77	0.48
1:A:306:LEU:HD12	2:A:500:UDP:O2'	2.14	0.47
1:C:371:LEU:C	1:C:371:LEU:CD2	2.86	0.47
1:B:70:LEU:HD22	1:B:257:ALA:HA	1.95	0.47
1:C:139:ARG:HH22	1:C:194:ASP:HB2	1.80	0.47
1:A:310:LEU:N	1:A:311:PRO:CD	2.78	0.47
1:B:304:VAL:HG11	1:B:309:LEU:HD22	1.97	0.47
1:A:304:VAL:CG1	1:A:309:LEU:HD22	2.45	0.47
1:C:376:GLU:O	1:C:380:GLU:HG2	2.15	0.47
1:C:93:LYS:O	1:C:96:VAL:HG12	2.16	0.46
1:C:385:ARG:O	1:C:389:GLU:HG2	2.16	0.46
1:B:90:VAL:HG21	1:B:161:VAL:HG12	1.98	0.45
1:B:173:ARG:HH11	1:B:173:ARG:CG	2.24	0.45
1:C:231:SER:HB2	1:C:305:PRO:HB3	1.99	0.45
1:A:90:VAL:HG21	1:A:161:VAL:HG12	1.99	0.45
2:A:500:UDP:O3B	2:A:500:UDP:H5'2	2.17	0.44
1:B:277:ILE:HG13	1:B:279:VAL:HG23	1.98	0.44
1:B:255:ARG:NH1	1:B:286:GLU:HB2	2.33	0.44
1:C:90:VAL:HG21	1:C:161:VAL:HG12	2.00	0.43
1:C:72:ASN:HD21	1:C:74:LEU:HB2	1.83	0.43
1:C:297:ASN:OD1	1:C:298:THR:HG23	2.18	0.43
1:A:99:MET:HG2	1:C:92:MET:HE1	2.01	0.42
1:B:62:MET:HE3	1:B:62:MET:HB3	1.96	0.42
1:C:139:ARG:NH2	1:C:194:ASP:HB2	2.35	0.42
1:B:114:VAL:HG22	1:B:137:ALA:HA	2.01	0.42
1:A:71:GLU:CD	1:A:362:HIS:HE2	2.27	0.41
1:C:266:ALA:O	1:C:269:ILE:HG13	2.20	0.41
1:B:95:LYS:O	1:B:99:MET:HG2	2.20	0.41
1:B:71:GLU:CD	1:B:362:HIS:HE2	2.28	0.41
1:C:218:ARG:HH11	1:C:415:HIS:CE1	2.37	0.41
1:A:114:VAL:HG22	1:A:137:ALA:HA	2.03	0.41
1:A:132:TYR:CZ	1:A:178:MET:HE1	2.56	0.41
1:B:268:MET:HE3	1:B:366:LEU:HD21	2.02	0.41
1:C:9:SER:OG	1:C:57:HIS:CE1	2.70	0.41
1:A:150:TRP:CZ3	1:A:151:CYS:HB3	2.56	0.41
1:C:99:MET:CE	1:C:100:PHE:CE2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:VAL:HG11	1:C:189:TYR:CE2	2.56	0.41
1:C:279:VAL:HG13	1:C:298:THR:HA	2.03	0.41
1:A:213:LEU:HA	1:A:214:PRO:HD3	1.96	0.40
1:C:95:LYS:HG2	1:C:177:PRO:HG3	2.02	0.40
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.94	0.40
1:B:98:VAL:CG1	1:B:103:GLN:HE21	2.35	0.40
1:C:209:THR:HG23	1:C:219:ARG:NH2	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:606:HOH:O	4:A:676:HOH:O[4_455]	1.98	0.22
4:A:682:HOH:O	4:A:682:HOH:O[4_455]	1.99	0.21
4:B:614:HOH:O	4:B:657:HOH:O[4_565]	2.05	0.15

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	410/437 (94%)	396 (97%)	14 (3%)	0	100	100
1	B	412/437 (94%)	399 (97%)	13 (3%)	0	100	100
1	C	360/437 (82%)	351 (98%)	9 (2%)	0	100	100
All	All	1182/1311 (90%)	1146 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/366 (94%)	334 (96%)	12 (4%)	32	59
1	B	348/366 (95%)	338 (97%)	10 (3%)	37	65
1	C	313/366 (86%)	299 (96%)	14 (4%)	24	50
All	All	1007/1098 (92%)	971 (96%)	36 (4%)	31	58

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	104	THR
1	A	128	ASP
1	A	171	GLU
1	A	172	GLU
1	A	261	THR
1	A	278	ASP
1	A	286	GLU
1	A	291	LEU
1	A	330	VAL
1	A	369	GLU
1	A	396	GLN
1	B	62	MET
1	B	128	ASP
1	B	218	ARG
1	B	288	VAL
1	B	292	GLU
1	B	330	VAL
1	B	339	THR
1	B	350	THR
1	B	354	GLU
1	B	369	GLU
1	C	61	GLU
1	C	104	THR
1	C	128	ASP
1	C	171	GLU
1	C	197	VAL
1	C	215	LEU
1	C	272	LEU
1	C	279	VAL

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Mol	Chain	Res	Type
1	C	283	LEU
1	C	302	ASP
1	C	330	VAL
1	C	339	THR
1	C	385	ARG
1	C	396	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	145	HIS
1	A	206	GLN
1	A	395	ASN
1	A	402	HIS
1	A	415	HIS
1	B	103	GLN
1	B	206	GLN
1	B	307	HIS
1	B	395	ASN
1	C	36	ASN
1	C	57	HIS
1	C	72	ASN
1	C	103	GLN
1	C	121	GLN
1	C	191	HIS
1	C	307	HIS
1	C	319	HIS
1	C	331	ASN
1	C	395	ASN
1	C	415	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	B	500	-	25,26,26	0.77	1 (4%)	38,40,40	1.07	3 (7%)
2	UDP	A	500	-	25,26,26	0.62	0	38,40,40	1.11	5 (13%)
3	PGR	A	502	-	4,4,4	0.69	0	4,4,4	0.46	0
3	PGR	A	505	-	4,4,4	0.72	0	4,4,4	0.72	0
3	PGR	A	508	-	4,4,4	0.51	0	4,4,4	0.87	0
3	PGR	B	501	-	4,4,4	0.77	0	4,4,4	0.58	0
3	PGR	A	503	-	4,4,4	0.80	0	4,4,4	0.74	0
3	PGR	B	506	-	4,4,4	0.54	0	4,4,4	0.62	0
3	PGR	B	503	-	4,4,4	0.56	0	4,4,4	0.55	0
3	PGR	A	504	-	4,4,4	0.70	0	4,4,4	0.40	0
3	PGR	B	504	-	4,4,4	0.74	0	4,4,4	0.34	0
3	PGR	A	501	-	4,4,4	0.59	0	4,4,4	0.38	0
3	PGR	B	505	-	4,4,4	0.60	0	4,4,4	0.49	0
3	PGR	B	508	-	4,4,4	0.53	0	4,4,4	0.79	0
3	PGR	A	507	-	4,4,4	0.61	0	4,4,4	1.86	1 (25%)
3	PGR	A	506	-	4,4,4	0.70	0	4,4,4	0.51	0
3	PGR	B	502	-	4,4,4	0.88	0	4,4,4	2.00	1 (25%)
3	PGR	B	507	-	4,4,4	0.64	0	4,4,4	0.82	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
2	UDP	B	500	-	-	1/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	500	-	-	6/16/32/32	0/2/2/2
3	PGR	A	502	-	-	2/2/2/2	-
3	PGR	A	505	-	-	2/2/2/2	-
3	PGR	A	508	-	-	0/2/2/2	-
3	PGR	B	501	-	-	2/2/2/2	-
3	PGR	A	503	-	-	2/2/2/2	-
3	PGR	B	506	-	-	2/2/2/2	-
3	PGR	B	503	-	-	2/2/2/2	-
3	PGR	A	504	-	-	1/2/2/2	-
3	PGR	B	504	-	-	1/2/2/2	-
3	PGR	A	501	-	-	0/2/2/2	-
3	PGR	B	505	-	-	0/2/2/2	-
3	PGR	B	508	-	-	1/2/2/2	-
3	PGR	A	507	-	-	2/2/2/2	-
3	PGR	A	506	-	-	2/2/2/2	-
3	PGR	B	502	-	-	2/2/2/2	-
3	PGR	B	507	-	-	0/2/2/2	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	UDP	PA-O3A	2.27	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	PGR	O2-C2-C1	-3.02	100.19	114.99
3	B	502	PGR	O2-C2-C1	-3.01	100.24	114.99
2	B	500	UDP	O2'-C2'-C1'	2.97	120.32	110.10
2	A	500	UDP	O2'-C2'-C1'	2.38	118.30	110.10
2	B	500	UDP	C3'-C2'-C1'	-2.30	97.11	101.46
2	A	500	UDP	C3'-C2'-C1'	-2.21	97.29	101.46
2	A	500	UDP	O3A-PA-O1A	-2.14	104.26	110.70
2	A	500	UDP	O2A-PA-O1A	2.12	122.30	112.44
2	A	500	UDP	C2'-C3'-C4'	-2.05	98.64	102.61
2	B	500	UDP	C2'-C1'-N1	2.05	118.96	113.25

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	UDP	O4'-C4'-C5'-O5'
2	A	500	UDP	C5'-O5'-PA-O3A
2	A	500	UDP	PA-O3A-PB-O2B
2	A	500	UDP	PA-O3A-PB-O3B
3	A	502	PGR	O1-C1-C2-C3
3	A	502	PGR	O1-C1-C2-O2
3	A	503	PGR	O1-C1-C2-O2
3	A	505	PGR	O1-C1-C2-O2
3	A	506	PGR	O1-C1-C2-C3
3	A	506	PGR	O1-C1-C2-O2
3	A	507	PGR	O1-C1-C2-O2
3	B	501	PGR	O1-C1-C2-C3
3	B	501	PGR	O1-C1-C2-O2
3	B	502	PGR	O1-C1-C2-O2
3	B	503	PGR	O1-C1-C2-C3
3	B	503	PGR	O1-C1-C2-O2
3	B	506	PGR	O1-C1-C2-C3
3	B	506	PGR	O1-C1-C2-O2
2	A	500	UDP	C3'-C4'-C5'-O5'
3	B	504	PGR	O1-C1-C2-O2
3	A	503	PGR	O1-C1-C2-C3
3	A	504	PGR	O1-C1-C2-C3
3	A	505	PGR	O1-C1-C2-C3
3	A	507	PGR	O1-C1-C2-C3
3	B	508	PGR	O1-C1-C2-C3
2	B	500	UDP	PB-O3A-PA-O5'
2	A	500	UDP	C5'-O5'-PA-O1A
3	B	502	PGR	O1-C1-C2-C3

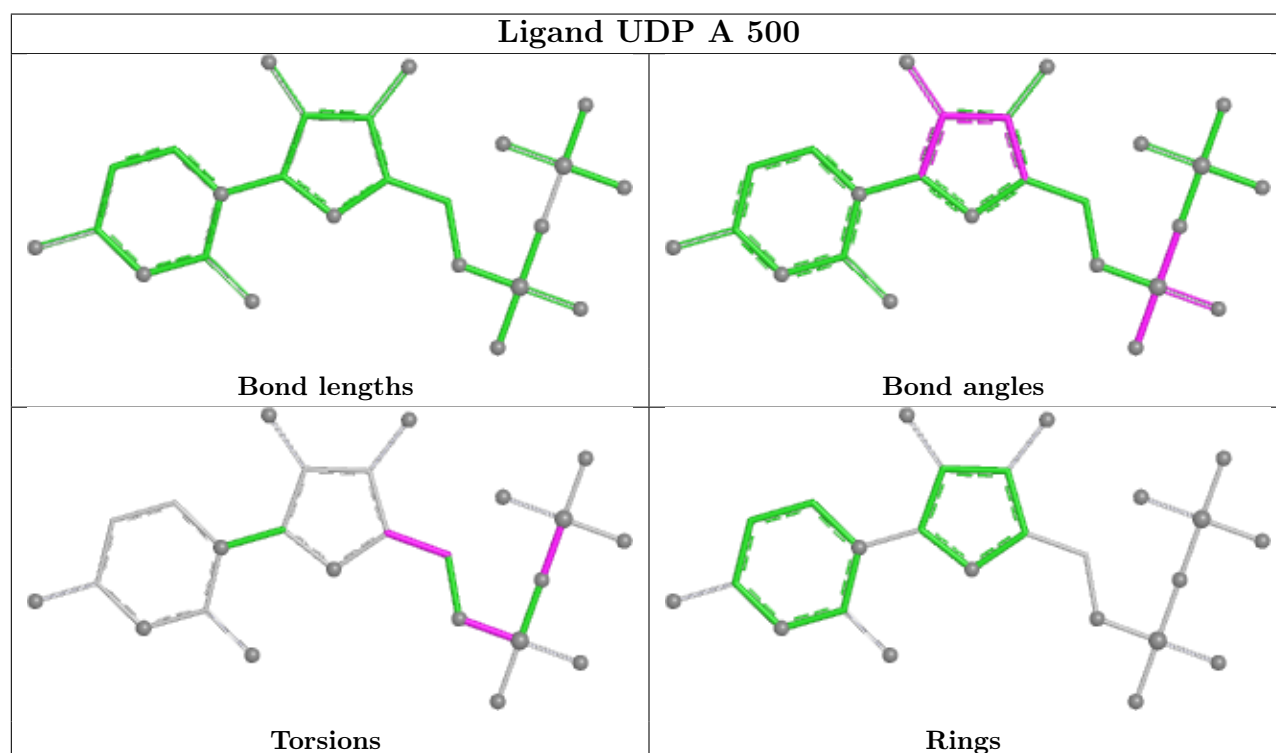
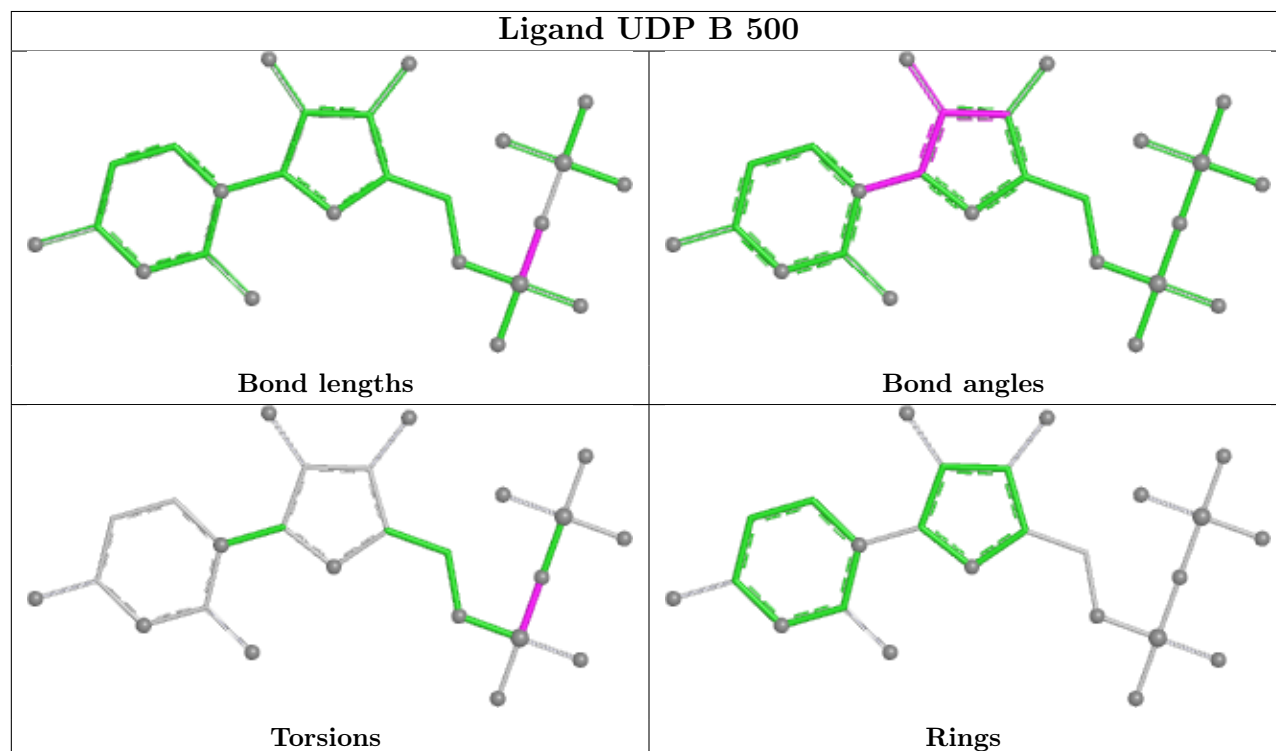
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	UDP	1	0
2	A	500	UDP	2	0
3	A	503	PGR	1	0
3	B	507	PGR	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 [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	414/437 (94%)	0.01	12 (2%) 53 48	34, 51, 100, 147	0
1	B	416/437 (95%)	0.08	14 (3%) 48 42	36, 57, 106, 134	0
1	C	372/437 (85%)	1.95	154 (41%) 0 0	66, 119, 167, 207	0
All	All	1202/1311 (91%)	0.64	180 (14%) 5 4	34, 66, 150, 207	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	ALA	5.8
1	C	116	TYR	5.0
1	C	269	ILE	4.8
1	C	280	VAL	4.8
1	C	338	PRO	4.7
1	C	371	LEU	4.7
1	C	155	TYR	4.7
1	C	317	ILE	4.6
1	C	151	CYS	4.6
1	C	211	LEU	4.5
1	C	303	PHE	4.4
1	C	272	LEU	4.4
1	C	266	ALA	4.3
1	C	320	GLY	4.3
1	C	82	LEU	4.2
1	C	308	ALA	4.2
1	C	189	TYR	4.2
1	C	336	PHE	4.1
1	C	357	ALA	4.1
1	C	233	ILE	4.0
1	B	70	LEU	4.0
1	C	265	VAL	4.0
1	C	310	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	222	VAL	3.9
1	C	268	MET	3.8
1	C	355	ALA	3.8
1	C	316	LEU	3.8
1	A	241	PRO	3.8
1	C	325	TRP	3.7
1	C	208	PRO	3.7
1	C	156	ALA	3.6
1	C	126	ILE	3.6
1	C	309	LEU	3.6
1	C	277	ILE	3.6
1	C	144	ALA	3.6
1	C	100	PHE	3.6
1	C	114	VAL	3.5
1	C	370	VAL	3.5
1	C	111	HIS	3.5
1	B	100	PHE	3.5
1	C	152	ILE	3.4
1	C	378	LEU	3.4
1	C	407	VAL	3.4
1	C	164	ALA	3.4
1	C	213	LEU	3.4
1	C	78	SER	3.3
1	C	94	PHE	3.3
1	C	306	LEU	3.3
1	C	199	VAL	3.3
1	A	62	MET	3.3
1	C	206	GLN	3.3
1	C	335	GLN	3.3
1	C	0	HIS	3.2
1	C	198	VAL	3.2
1	A	60	HIS	3.2
1	C	217	LEU	3.2
1	C	74	LEU	3.2
1	C	113	LEU	3.2
1	C	182	LEU	3.2
1	C	26	ALA	3.2
1	C	195	GLU	3.1
1	C	406	PRO	3.1
1	C	321	GLY	3.1
1	A	240	ALA	3.1
1	C	207	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	161	VAL	3.1
1	C	388	ALA	3.1
1	C	330	VAL	3.1
1	C	4	LEU	3.0
1	C	301	VAL	3.0
1	C	318	HIS	3.0
1	C	323	GLY	3.0
1	C	117	ALA	3.0
1	C	236	TRP	3.0
1	C	285	PRO	3.0
1	C	51	VAL	3.0
1	B	66	ASN	2.9
1	C	351	SER	2.9
1	B	99	MET	2.9
1	C	337	ILE	2.9
1	C	339	THR	2.9
1	C	197	VAL	2.9
1	C	379	VAL	2.9
1	C	332	GLY	2.9
1	C	136	VAL	2.9
1	B	173	ARG	2.8
1	C	408	ILE	2.8
1	C	359	LEU	2.8
1	C	314	SER	2.8
1	C	312	GLY	2.8
1	C	119	HIS	2.8
1	C	80	PRO	2.8
1	C	300	ILE	2.8
1	C	271	THR	2.8
1	C	275	MET	2.8
1	C	331	ASN	2.7
1	C	363	ALA	2.7
1	C	193	PHE	2.7
1	C	334	PRO	2.7
1	C	62	MET	2.7
1	C	358	GLY	2.7
1	C	118	ARG	2.7
1	C	173	ARG	2.7
1	C	333	VAL	2.7
1	B	241	PRO	2.7
1	B	285	PRO	2.7
1	C	163	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	18	VAL	2.7
1	C	125	VAL	2.7
1	C	391	LEU	2.6
1	C	356	GLY	2.6
1	C	127	TRP	2.6
1	C	345	TRP	2.6
1	C	214	PRO	2.6
1	B	257	ALA	2.6
1	C	383	SER	2.6
1	C	234	PRO	2.6
1	C	279	VAL	2.6
1	C	23	SER	2.6
1	C	384	TYR	2.6
1	B	240	ALA	2.6
1	C	361	VAL	2.6
1	C	405	VAL	2.6
1	C	150	TRP	2.5
1	C	329	LEU	2.5
1	C	22	TRP	2.5
1	C	352	LEU	2.5
1	C	319	HIS	2.5
1	A	100	PHE	2.5
1	C	99	MET	2.5
1	A	68	ASP	2.5
1	B	74	LEU	2.5
1	B	284	PRO	2.5
1	C	328	ALA	2.5
1	C	148	LEU	2.5
1	C	225	LEU	2.5
1	C	284	PRO	2.5
1	B	256	ALA	2.4
1	C	281	ALA	2.4
1	C	282	ALA	2.4
1	C	187	GLY	2.4
1	C	190	GLY	2.4
1	C	6	ALA	2.4
1	C	24	LEU	2.3
1	C	91	LEU	2.3
1	C	295	PRO	2.3
1	C	210	SER	2.3
1	C	313	ALA	2.2
1	C	327	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	132	TYR	2.2
1	C	124	LEU	2.2
1	B	290	ALA	2.2
1	C	382	ALA	2.2
1	C	188	ARG	2.2
1	A	285	PRO	2.2
1	C	170	PRO	2.2
1	A	250	SER	2.2
1	C	3	ILE	2.2
1	C	415	HIS	2.2
1	A	287	GLU	2.2
1	B	372	ARG	2.2
1	C	375	VAL	2.2
1	C	60	HIS	2.2
1	C	1	MET	2.2
1	C	92	MET	2.2
1	C	31	VAL	2.2
1	C	399	PRO	2.1
1	A	251	GLY	2.1
1	C	340	ILE	2.1
1	C	71	GLU	2.1
1	A	173	ARG	2.1
1	C	19	PRO	2.1
1	C	147	ARG	2.1
1	C	57	HIS	2.1
1	C	342	TYR	2.1
1	A	74	LEU	2.1
1	C	346	TRP	2.0
1	C	17	MET	2.0
1	C	347	ASN	2.0
1	C	343	ALA	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

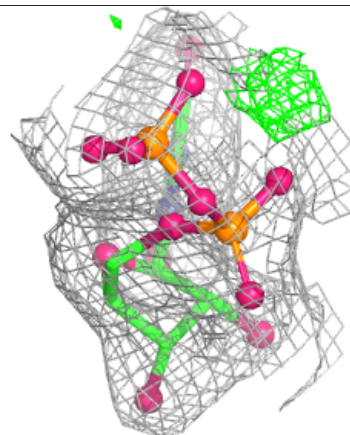
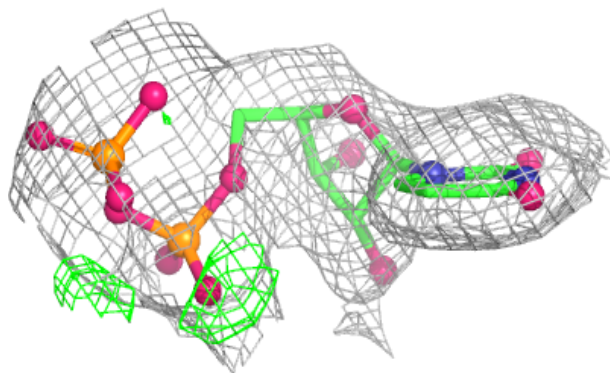
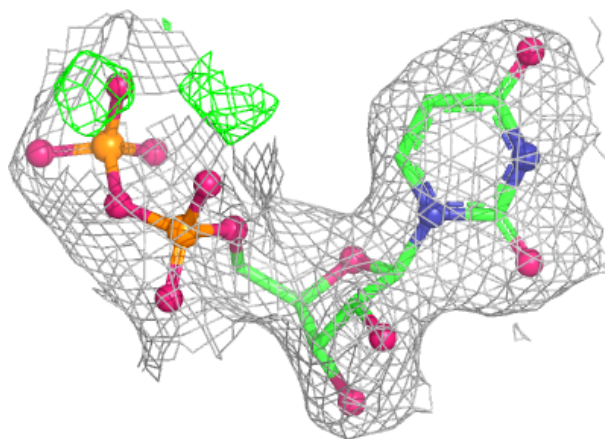
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PGR	B	507	5/5	0.72	0.30	78,84,103,109	0
3	PGR	A	507	5/5	0.79	0.22	66,72,80,83	0
3	PGR	B	502	5/5	0.80	0.20	62,66,72,77	0
3	PGR	A	506	5/5	0.83	0.27	66,67,81,88	0
3	PGR	A	508	5/5	0.87	0.25	100,103,113,115	0
3	PGR	B	501	5/5	0.89	0.15	58,59,64,74	0
2	UDP	B	500	25/25	0.90	0.12	52,77,106,116	0
3	PGR	B	508	5/5	0.90	0.23	81,86,101,112	0
3	PGR	A	502	5/5	0.92	0.16	55,57,74,79	0
3	PGR	B	503	5/5	0.94	0.15	88,88,90,101	0
2	UDP	A	500	25/25	0.95	0.09	50,82,95,102	0
3	PGR	B	505	5/5	0.96	0.15	58,61,66,67	0
3	PGR	A	503	5/5	0.96	0.11	59,59,65,69	0
3	PGR	A	504	5/5	0.96	0.10	46,59,63,67	0
3	PGR	A	501	5/5	0.97	0.08	39,40,43,52	0
3	PGR	B	506	5/5	0.97	0.11	69,77,83,88	0
3	PGR	A	505	5/5	0.97	0.09	46,46,48,50	0
3	PGR	B	504	5/5	0.97	0.08	43,44,51,51	0

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

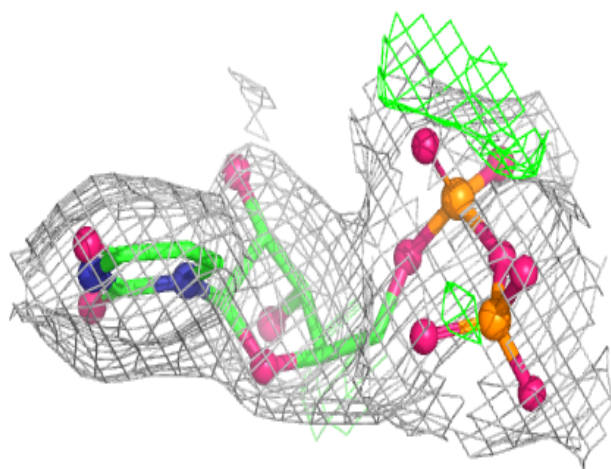
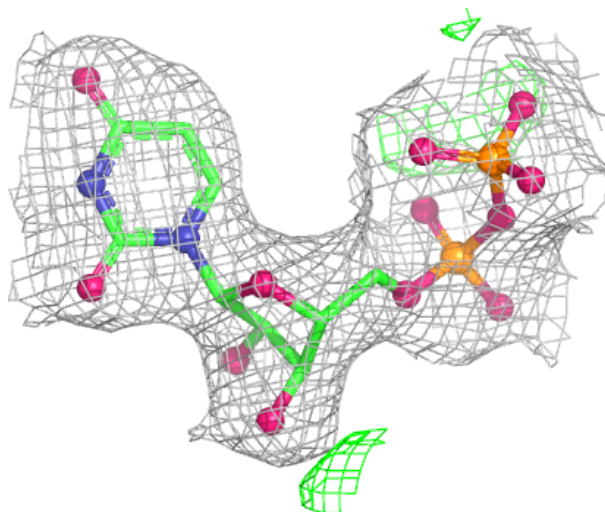
Electron density around UDP B 500:

$2mF_o-DF_c$ (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.