Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:33 PM JST

PDB ID	:	7YP6
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:

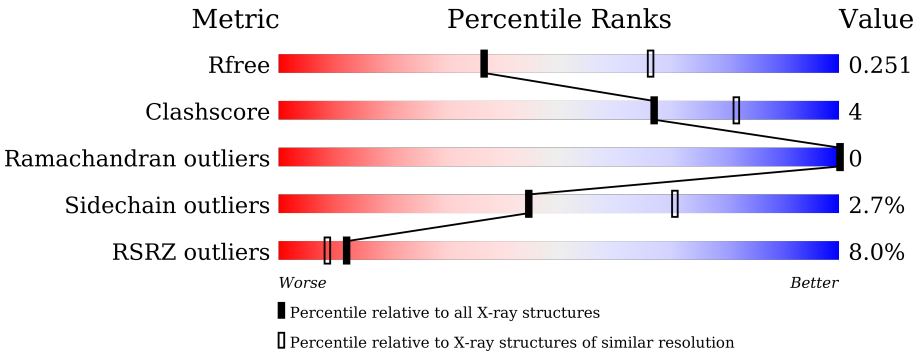
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	82% 12% • 5%
1	B	437	% 83% 11% • 5%
1	C	437	21% 73% 12% • 15%

2 Entry composition (i)

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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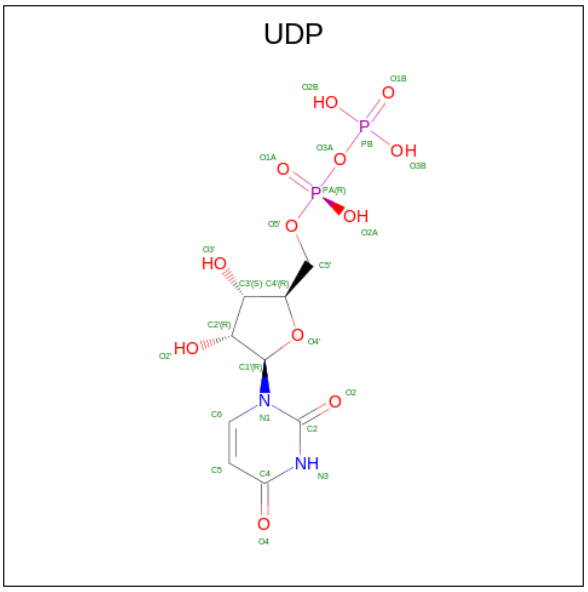
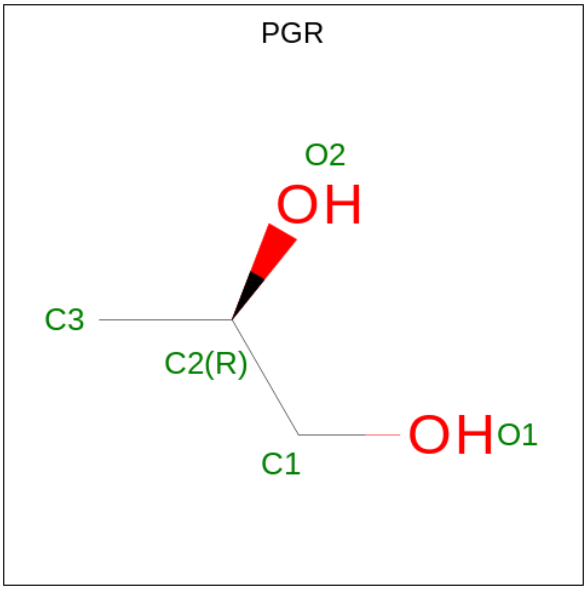
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP E5L4T5
B	-15	HIS	-	expression tag	UNP E5L4T5
B	-14	HIS	-	expression tag	UNP E5L4T5
B	-13	HIS	-	expression tag	UNP E5L4T5
B	-12	HIS	-	expression tag	UNP E5L4T5
B	-11	HIS	-	expression tag	UNP E5L4T5
B	-10	HIS	-	expression tag	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 (three-letter code: 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 (three-letter code: PGR) (formula: $C_3H_8O_2$).



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.

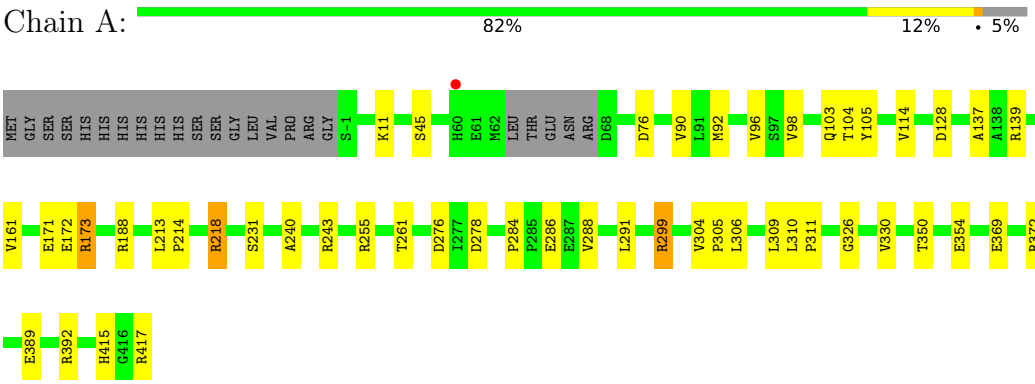
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	88	Total O 88 88	0	0
4	B	60	Total O 60 60	0	0
4	C	4	Total O 4 4	0	0

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.

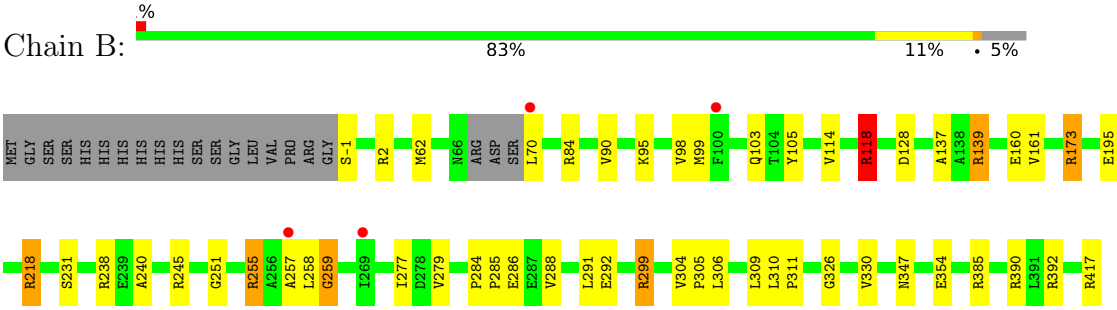
• Molecule 1: Glycosyltransferase

Chain A:



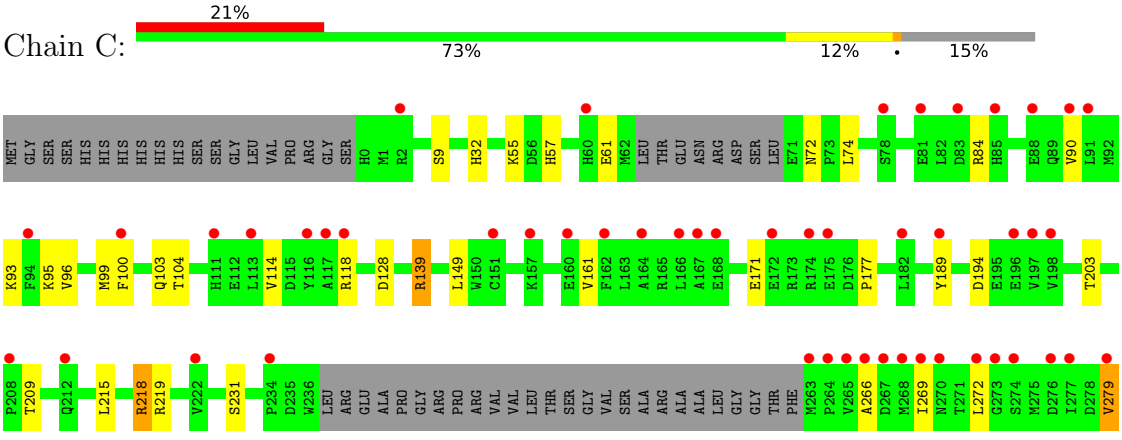
• Molecule 1: Glycosyltransferase

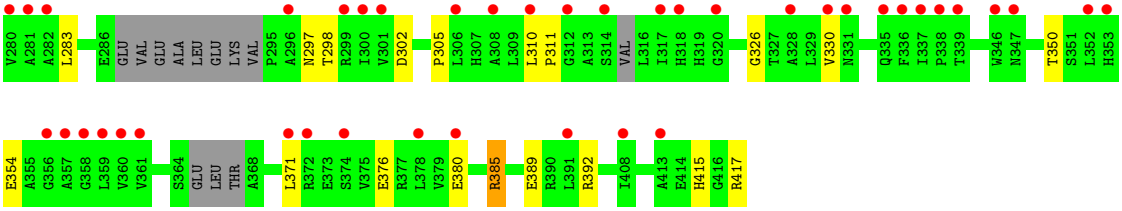
Chain B:



• Molecule 1: Glycosyltransferase

Chain C:




V280 A281 A282 L283 E286 GLU VAL GLU ALA LEU GLU LYS VAL P295 A296 N297 T298 R299 I300 V301 D302 P305 L306 H307 A308 L309 L310 P311 G312 A313 S314 VAL L316 I317 H318 H319 G320 G326 T327 A328 L329 V330 N331 Q335 F336 I337 P338 T339 W346 N347 T350 S351 L352 H353
E354 A355 G356 A357 G358 L359 V360 V361 S364 GLU LEU THR A368 L371 R372 E373 S374 V375 E376 R377 L378 V379 E380 R385 E389 H390 L391 R392 I408 A413 E414 H415 G416 R417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 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 64.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.12-2.60) 99.8 (64.04-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	3105 reflections (5.00%)	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)	0.33 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.57	3/3330 (0.1%)	0.81	4/4552 (0.1%)
1	B	0.53	3/3348 (0.1%)	0.82	4/4577 (0.1%)
1	C	0.41	0/3016	0.72	0/4118
All	All	0.51	6/9694 (0.1%)	0.79	8/13247 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	GLU	CD-OE1	6.45	1.32	1.25
1	A	389	GLU	CD-OE1	6.23	1.32	1.25
1	A	160	GLU	CD-OE2	5.71	1.31	1.25
1	B	195	GLU	CD-OE1	5.45	1.31	1.25
1	B	160	GLU	CD-OE1	5.35	1.31	1.25
1	B	195	GLU	CD-OE2	5.24	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	ARG	NE-CZ-NH2	-6.80	116.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	118	ARG	CB-CA-C	-5.55	99.29	110.40
1	A	11	LYS	CB-CA-C	5.46	121.32	110.40
1	B	139	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	299	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	76	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	372	ARG	NE-CZ-NH1	5.01	122.81	120.30

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
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

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Mol	Chain	Res	Type	Group
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 (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	3241	0	3180	22	0
1	B	3259	0	3201	22	0
1	C	2934	0	2857	30	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	74	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 4.

All (74) 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	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:HA	1:C:103:GLN:NE2	2.26	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
1:C:149:LEU:HD13	1:C:203:THR:HG23	1.94	0.49
1:B:347:ASN:HD22	3:B:507:PGR:H33	1.78	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: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:99:MET:HE3	1:C:100:PHE:CE2	2.51	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:371:LEU:C	1:C:371:LEU:CD2	2.86	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: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: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: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:A:173:ARG:NH1	1:C:55:LYS:HZ3	2.19	0.41
1:C:99:MET:CE	1:C:100:PHE:CE2	3.04	0.41
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 (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	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 (i)

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%)	336 (97%)	10 (3%)	42	68
1	B	348/366 (95%)	341 (98%)	7 (2%)	55	78
1	C	313/366 (86%)	303 (97%)	10 (3%)	39	65
All	All	1007/1098 (92%)	980 (97%)	27 (3%)	44	71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	THR
1	A	105	TYR
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	369	GLU
1	B	-1	SER
1	B	62	MET
1	B	105	TYR

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Mol	Chain	Res	Type
1	B	128	ASP
1	B	218	ARG
1	B	292	GLU
1	B	354	GLU
1	C	32	HIS
1	C	61	GLU
1	C	104	THR
1	C	128	ASP
1	C	171	GLU
1	C	215	LEU
1	C	272	LEU
1	C	279	VAL
1	C	283	LEU
1	C	302	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	145	HIS
1	A	402	HIS
1	A	415	HIS
1	B	66	ASN
1	B	103	GLN
1	B	307	HIS
1	C	57	HIS
1	C	72	ASN
1	C	103	GLN
1	C	121	GLN
1	C	307	HIS
1	C	331	ASN
1	C	415	HIS

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 monosaccharides 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	A	500	-	24,26,26	0.55	0	37,40,40	1.07	4 (10%)
3	PGR	B	508	-	3,4,4	0.12	0	1,4,4	0.23	0
3	PGR	A	504	-	3,4,4	0.44	0	1,4,4	0.21	0
3	PGR	A	508	-	3,4,4	0.11	0	1,4,4	0.59	0
3	PGR	A	502	-	3,4,4	0.44	0	1,4,4	0.40	0
2	UDP	B	500	-	24,26,26	0.62	0	37,40,40	1.08	3 (8%)
3	PGR	B	504	-	3,4,4	0.57	0	1,4,4	0.36	0
3	PGR	B	502	-	3,4,4	0.78	0	1,4,4	1.97	0
3	PGR	A	507	-	3,4,4	0.44	0	1,4,4	1.24	0
3	PGR	B	503	-	3,4,4	0.18	0	1,4,4	0.26	0
3	PGR	A	506	-	3,4,4	0.38	0	1,4,4	0.31	0
3	PGR	B	501	-	3,4,4	0.51	0	1,4,4	0.33	0
3	PGR	A	503	-	3,4,4	0.63	0	1,4,4	0.81	0
3	PGR	A	505	-	3,4,4	0.40	0	1,4,4	0.70	0
3	PGR	B	506	-	3,4,4	0.21	0	1,4,4	0.03	0
3	PGR	B	505	-	3,4,4	0.29	0	1,4,4	0.03	0
3	PGR	B	507	-	3,4,4	0.33	0	1,4,4	0.32	0
3	PGR	A	501	-	3,4,4	0.44	0	1,4,4	0.06	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	A	500	-	-	6/16/32/32	0/2/2/2

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	UDP	O2'-C2'-C1'	3.08	120.32	110.02
2	A	500	UDP	O2'-C2'-C1'	2.47	118.30	110.02
2	B	500	UDP	C3'-C2'-C1'	-2.27	97.11	101.43
2	A	500	UDP	C3'-C2'-C1'	-2.18	97.29	101.43
2	A	500	UDP	C2'-C3'-C4'	-2.06	98.64	102.64
2	A	500	UDP	O2A-PA-O1A	2.03	122.30	112.24
2	B	500	UDP	C2'-C1'-N1	2.03	118.96	113.22

There are no chirality outliers.

All (30) 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

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Mol	Chain	Res	Type	Atoms
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
2	B	500	UDP	PB-O3A-PA-O5'
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	502	PGR	O1-C1-C2-C3
3	B	508	PGR	O1-C1-C2-C3
2	A	500	UDP	C5'-O5'-PA-O1A
3	A	504	PGR	O1-C1-C2-O2
3	B	508	PGR	O1-C1-C2-O2

There are no ring outliers.

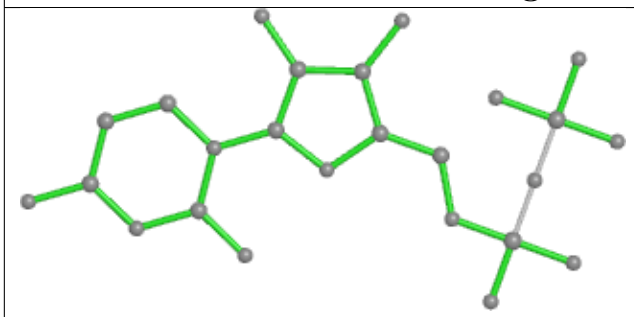
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	UDP	2	0
2	B	500	UDP	1	0
3	A	503	PGR	1	0
3	B	507	PGR	1	0

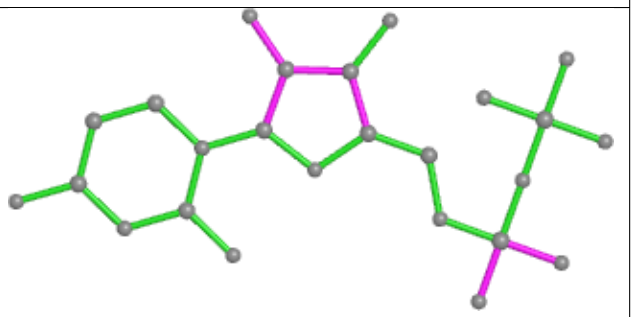
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

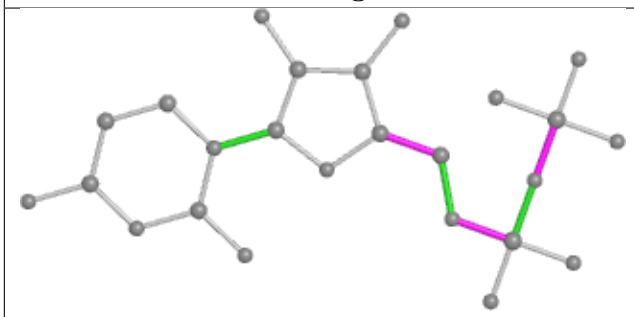
Ligand UDP A 500



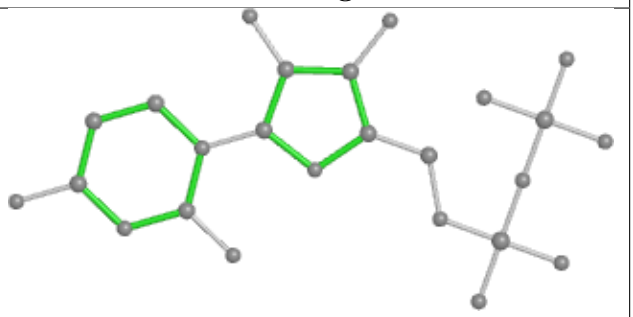
Bond lengths



Bond angles

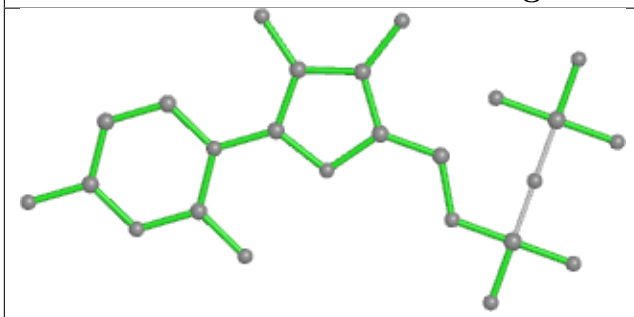


Torsions

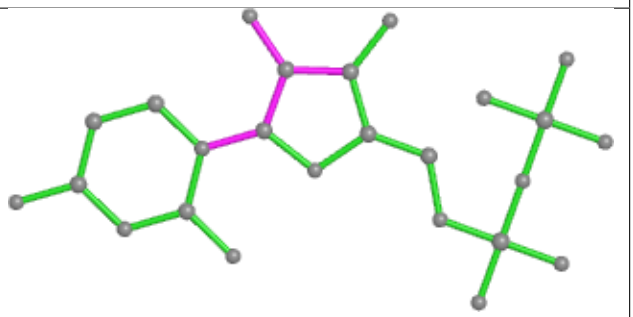


Rings

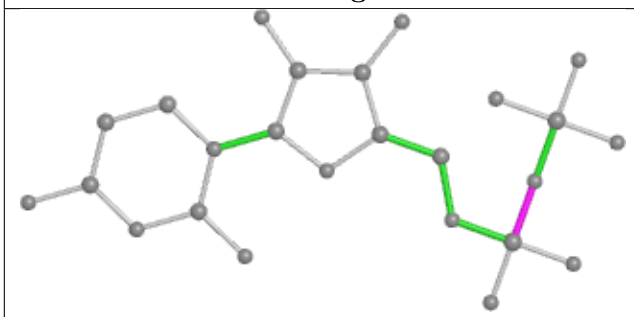
Ligand UDP B 500



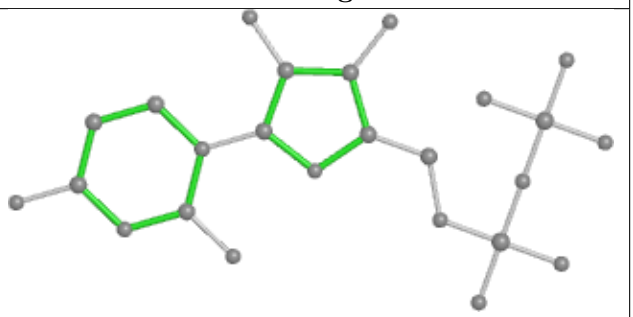
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.02	1 (0%)	95	95	34, 51, 100, 147	0
1	B	416/437 (95%)	0.03	4 (0%)	82	80	36, 57, 106, 134	0
1	C	372/437 (85%)	1.25	91 (24%)	0	0	66, 119, 167, 207	0
All	All	1202/1311 (91%)	0.41	96 (7%)	12	9	34, 66, 150, 207	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	ILE	11.7
1	C	301	VAL	8.0
1	C	272	LEU	7.4
1	C	265	VAL	6.7
1	C	268	MET	6.5
1	C	85	HIS	6.1
1	C	300	ILE	5.6
1	C	164	ALA	5.5
1	C	189	TYR	5.1
1	C	90	VAL	5.0
1	C	276	ASP	4.7
1	C	296	ALA	4.7
1	C	374	SER	4.6
1	C	378	LEU	4.5
1	C	282	ALA	4.5
1	C	212	GLN	4.4
1	C	280	VAL	4.4
1	C	273	GLY	4.3
1	C	317	ILE	4.2
1	C	358	GLY	4.1
1	C	336	PHE	4.0
1	C	359	LEU	3.9
1	C	338	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	279	VAL	3.8
1	C	162	PHE	3.8
1	C	274	SER	3.7
1	C	151	CYS	3.6
1	C	277	ILE	3.6
1	C	208	PRO	3.6
1	C	267	ASP	3.5
1	C	357	ALA	3.4
1	C	408	ILE	3.4
1	C	174	ARG	3.4
1	C	270	ASN	3.3
1	C	263	MET	3.3
1	C	320	GLY	3.3
1	C	281	ALA	3.3
1	C	198	VAL	3.3
1	C	118	ARG	3.2
1	C	166	LEU	3.2
1	C	175	GLU	3.1
1	C	182	LEU	3.1
1	C	168	GLU	3.1
1	C	172	GLU	3.1
1	C	318	HIS	3.1
1	C	266	ALA	3.1
1	C	347	ASN	3.0
1	C	352	LEU	3.0
1	C	353	HIS	3.0
1	C	81	GLU	3.0
1	C	113	LEU	2.9
1	C	328	ALA	2.9
1	C	60	HIS	2.8
1	C	88	GLU	2.8
1	C	331	ASN	2.7
1	B	269	ILE	2.7
1	C	337	ILE	2.7
1	C	299	ARG	2.7
1	B	257	ALA	2.7
1	C	160	GLU	2.7
1	C	312	GLY	2.7
1	C	339	THR	2.6
1	C	167	ALA	2.6
1	C	83	ASP	2.6
1	C	100	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	310	LEU	2.5
1	C	116	TYR	2.5
1	C	234	PRO	2.5
1	B	70	LEU	2.5
1	A	60	HIS	2.5
1	C	380	GLU	2.4
1	C	111	HIS	2.4
1	C	264	PRO	2.4
1	C	308	ALA	2.4
1	C	314	SER	2.4
1	C	360	VAL	2.4
1	C	196	GLU	2.3
1	C	413	ALA	2.3
1	C	78	SER	2.3
1	C	157	LYS	2.2
1	C	94	PHE	2.2
1	C	361	VAL	2.2
1	B	100	PHE	2.2
1	C	222	VAL	2.2
1	C	91	LEU	2.2
1	C	335	GLN	2.2
1	C	356	GLY	2.2
1	C	117	ALA	2.1
1	C	371	LEU	2.1
1	C	391	LEU	2.1
1	C	346	TRP	2.1
1	C	2	ARG	2.0
1	C	197	VAL	2.0
1	C	372	ARG	2.0
1	C	306	LEU	2.0
1	C	330	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 monosaccharides in this entry.

6.4 Ligands (i)

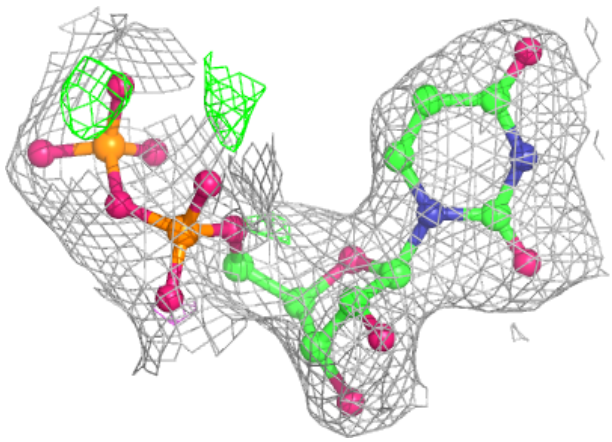
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

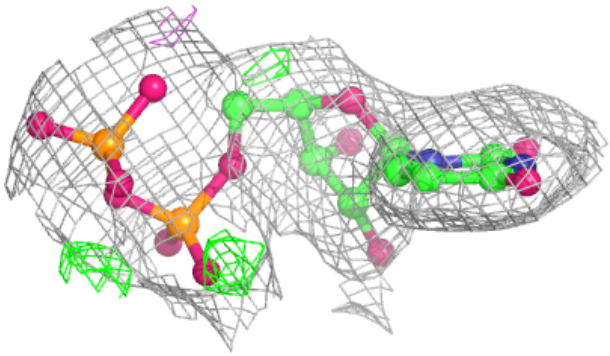
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGR	B	507	5/5	0.79	0.33	78,84,103,109	0
3	PGR	A	506	5/5	0.81	0.37	66,67,81,88	0
3	PGR	A	508	5/5	0.85	0.27	100,103,113,115	0
3	PGR	B	502	5/5	0.88	0.19	62,66,72,77	0
3	PGR	B	501	5/5	0.90	0.20	58,59,64,74	0
3	PGR	B	508	5/5	0.90	0.31	81,86,101,112	0
3	PGR	A	507	5/5	0.92	0.21	66,72,80,83	0
3	PGR	A	502	5/5	0.94	0.28	55,57,74,79	0
2	UDP	B	500	25/25	0.94	0.17	52,77,106,116	0
3	PGR	B	503	5/5	0.96	0.50	88,88,90,101	0
3	PGR	B	505	5/5	0.96	0.25	58,61,66,67	0
3	PGR	B	506	5/5	0.96	0.43	69,77,83,88	0
3	PGR	A	503	5/5	0.96	0.22	59,59,65,69	0
2	UDP	A	500	25/25	0.96	0.17	50,82,95,102	0
3	PGR	A	504	5/5	0.97	0.22	46,59,63,67	0
3	PGR	A	505	5/5	0.97	0.23	46,46,48,50	0
3	PGR	A	501	5/5	0.97	0.20	39,40,43,52	0
3	PGR	B	504	5/5	0.98	0.22	43,44,51,51	0

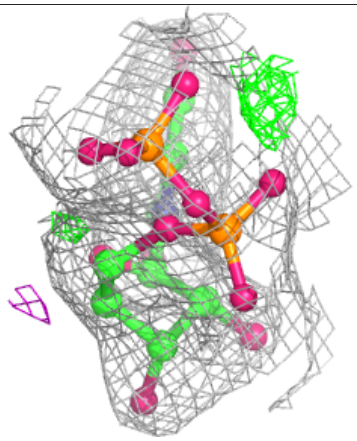
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

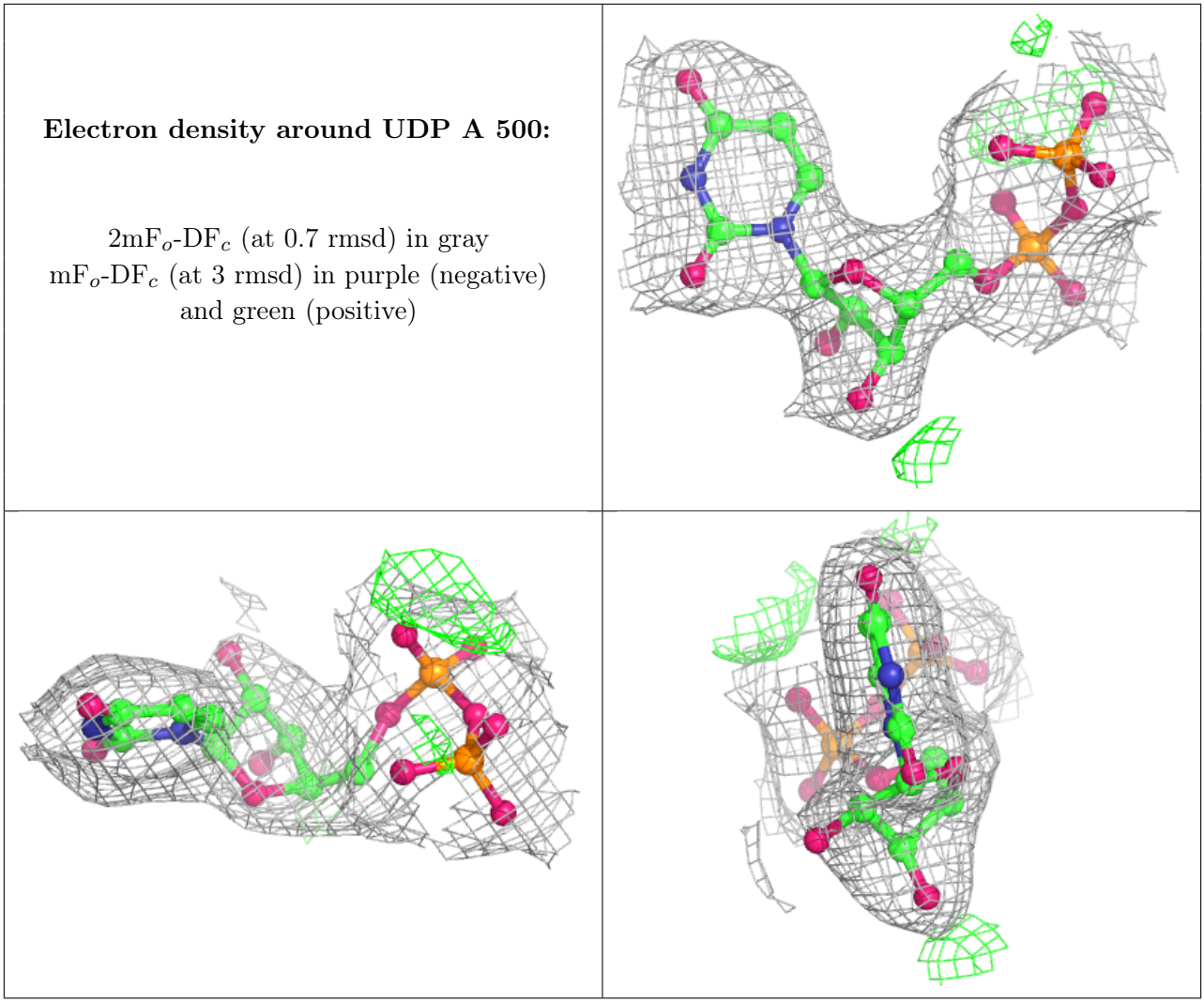






Electron density around UDP A 500:

$2mF_o$-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.