Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 12:53 PM EST

PDB ID	:	5EKP
Title	:	Structure of the polyisoprenyl-phosphate glycosyltransferase GtrB (WT)
Authors	:	Ardiccioni, C.; Clarke, O.B.; Tomasek, D.; Banerjee, S.; Rajashankar, K.R.; Liu, Q.; Shapiro, L.; Mancia, F.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on	:	2015-11-03
Resolution	:	3.19 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 (i) 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 (i)) were used in the production of this report:

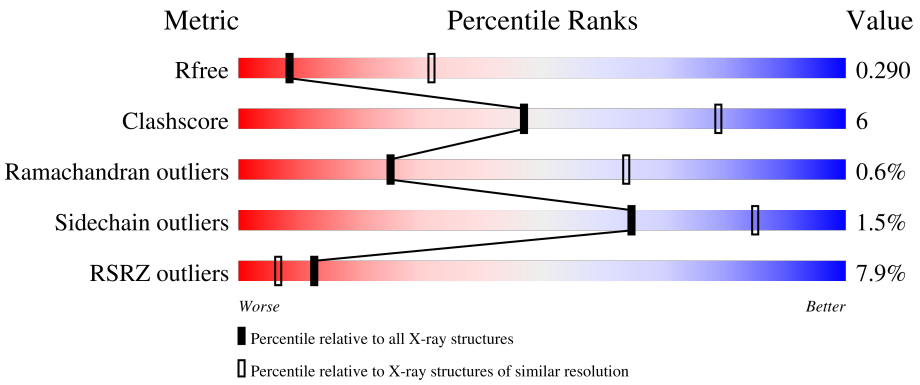
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	341	5% 68% 16% • 16%
1	B	341	6% 75% 12% • 12%
1	C	341	9% 78% 11% • 10%
1	D	341	8% 72% 14% • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9240 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 Uncharacterized glycosyltransferase sll0501.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	307	2354	1537	384	425	8	0	0	0
			Total	C	N	O	S			
1	A	288	2225	1455	357	407	6	0	0	0
			Total	C	N	O	S			
1	B	299	2280	1487	369	416	8	0	0	0
			Total	C	N	O	S			
1	D	296	2277	1490	367	412	8	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	initiating methionine	UNP Q55487
C	-21	HIS	-	expression tag	UNP Q55487
C	-20	HIS	-	expression tag	UNP Q55487
C	-19	HIS	-	expression tag	UNP Q55487
C	-18	HIS	-	expression tag	UNP Q55487
C	-17	HIS	-	expression tag	UNP Q55487
C	-16	HIS	-	expression tag	UNP Q55487
C	-15	SER	-	expression tag	UNP Q55487
C	-14	SER	-	expression tag	UNP Q55487
C	-13	GLY	-	expression tag	UNP Q55487
C	-12	VAL	-	expression tag	UNP Q55487
C	-11	ASP	-	expression tag	UNP Q55487
C	-10	LEU	-	expression tag	UNP Q55487
C	-9	GLY	-	expression tag	UNP Q55487
C	-8	THR	-	expression tag	UNP Q55487
C	-7	GLU	-	expression tag	UNP Q55487
C	-6	ASN	-	expression tag	UNP Q55487
C	-5	LEU	-	expression tag	UNP Q55487
C	-4	TYR	-	expression tag	UNP Q55487
C	-3	PHE	-	expression tag	UNP Q55487
C	-2	GLN	-	expression tag	UNP Q55487

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q55487
C	0	ASN	-	expression tag	UNP Q55487
C	1	ALA	-	expression tag	UNP Q55487
A	-22	MET	-	initiating methionine	UNP Q55487
A	-21	HIS	-	expression tag	UNP Q55487
A	-20	HIS	-	expression tag	UNP Q55487
A	-19	HIS	-	expression tag	UNP Q55487
A	-18	HIS	-	expression tag	UNP Q55487
A	-17	HIS	-	expression tag	UNP Q55487
A	-16	HIS	-	expression tag	UNP Q55487
A	-15	SER	-	expression tag	UNP Q55487
A	-14	SER	-	expression tag	UNP Q55487
A	-13	GLY	-	expression tag	UNP Q55487
A	-12	VAL	-	expression tag	UNP Q55487
A	-11	ASP	-	expression tag	UNP Q55487
A	-10	LEU	-	expression tag	UNP Q55487
A	-9	GLY	-	expression tag	UNP Q55487
A	-8	THR	-	expression tag	UNP Q55487
A	-7	GLU	-	expression tag	UNP Q55487
A	-6	ASN	-	expression tag	UNP Q55487
A	-5	LEU	-	expression tag	UNP Q55487
A	-4	TYR	-	expression tag	UNP Q55487
A	-3	PHE	-	expression tag	UNP Q55487
A	-2	GLN	-	expression tag	UNP Q55487
A	-1	SER	-	expression tag	UNP Q55487
A	0	ASN	-	expression tag	UNP Q55487
A	1	ALA	-	expression tag	UNP Q55487
B	-22	MET	-	initiating methionine	UNP Q55487
B	-21	HIS	-	expression tag	UNP Q55487
B	-20	HIS	-	expression tag	UNP Q55487
B	-19	HIS	-	expression tag	UNP Q55487
B	-18	HIS	-	expression tag	UNP Q55487
B	-17	HIS	-	expression tag	UNP Q55487
B	-16	HIS	-	expression tag	UNP Q55487
B	-15	SER	-	expression tag	UNP Q55487
B	-14	SER	-	expression tag	UNP Q55487
B	-13	GLY	-	expression tag	UNP Q55487
B	-12	VAL	-	expression tag	UNP Q55487
B	-11	ASP	-	expression tag	UNP Q55487
B	-10	LEU	-	expression tag	UNP Q55487
B	-9	GLY	-	expression tag	UNP Q55487
B	-8	THR	-	expression tag	UNP Q55487

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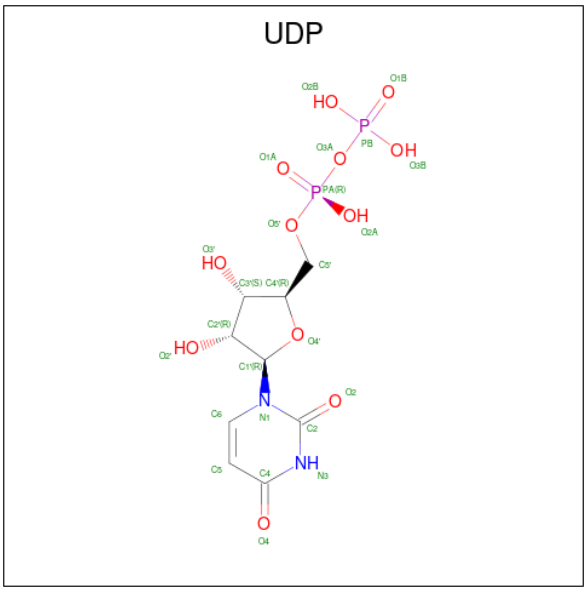
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLU	-	expression tag	UNP Q55487
B	-6	ASN	-	expression tag	UNP Q55487
B	-5	LEU	-	expression tag	UNP Q55487
B	-4	TYR	-	expression tag	UNP Q55487
B	-3	PHE	-	expression tag	UNP Q55487
B	-2	GLN	-	expression tag	UNP Q55487
B	-1	SER	-	expression tag	UNP Q55487
B	0	ASN	-	expression tag	UNP Q55487
B	1	ALA	-	expression tag	UNP Q55487
D	-22	MET	-	initiating methionine	UNP Q55487
D	-21	HIS	-	expression tag	UNP Q55487
D	-20	HIS	-	expression tag	UNP Q55487
D	-19	HIS	-	expression tag	UNP Q55487
D	-18	HIS	-	expression tag	UNP Q55487
D	-17	HIS	-	expression tag	UNP Q55487
D	-16	HIS	-	expression tag	UNP Q55487
D	-15	SER	-	expression tag	UNP Q55487
D	-14	SER	-	expression tag	UNP Q55487
D	-13	GLY	-	expression tag	UNP Q55487
D	-12	VAL	-	expression tag	UNP Q55487
D	-11	ASP	-	expression tag	UNP Q55487
D	-10	LEU	-	expression tag	UNP Q55487
D	-9	GLY	-	expression tag	UNP Q55487
D	-8	THR	-	expression tag	UNP Q55487
D	-7	GLU	-	expression tag	UNP Q55487
D	-6	ASN	-	expression tag	UNP Q55487
D	-5	LEU	-	expression tag	UNP Q55487
D	-4	TYR	-	expression tag	UNP Q55487
D	-3	PHE	-	expression tag	UNP Q55487
D	-2	GLN	-	expression tag	UNP Q55487
D	-1	SER	-	expression tag	UNP Q55487
D	0	ASN	-	expression tag	UNP Q55487
D	1	ALA	-	expression tag	UNP Q55487

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



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

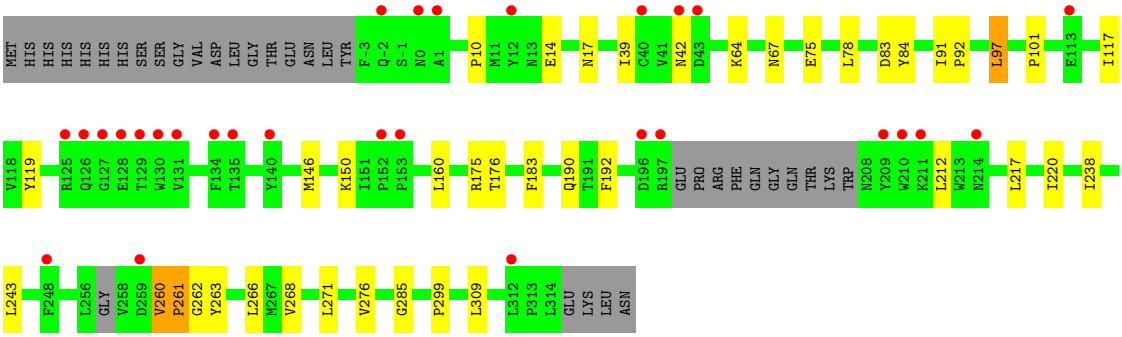
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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.

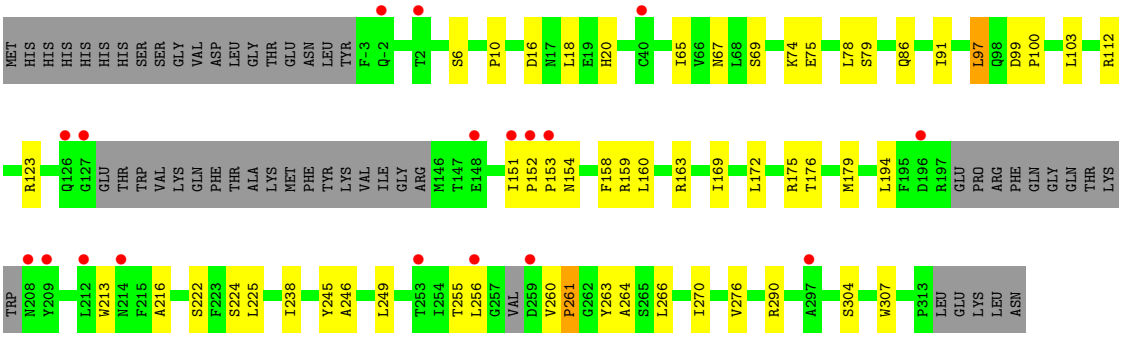
• Molecule 1: Uncharacterized glycosyltransferase sll0501

Chain C:



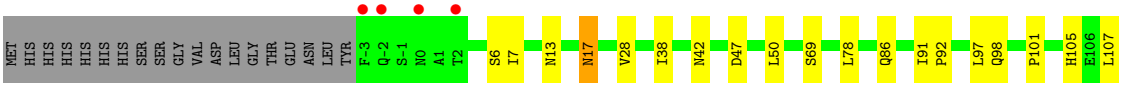
• Molecule 1: Uncharacterized glycosyltransferase sll0501

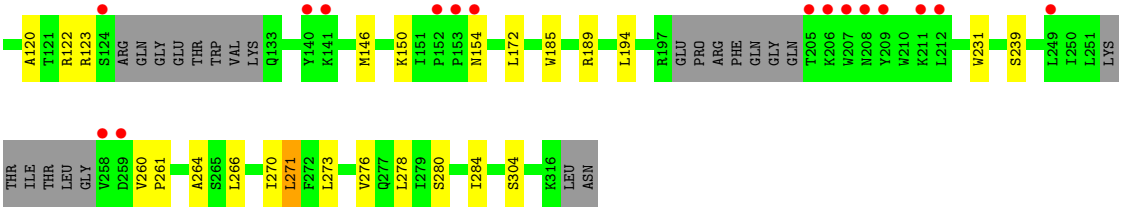
Chain A:



• Molecule 1: Uncharacterized glycosyltransferase sll0501

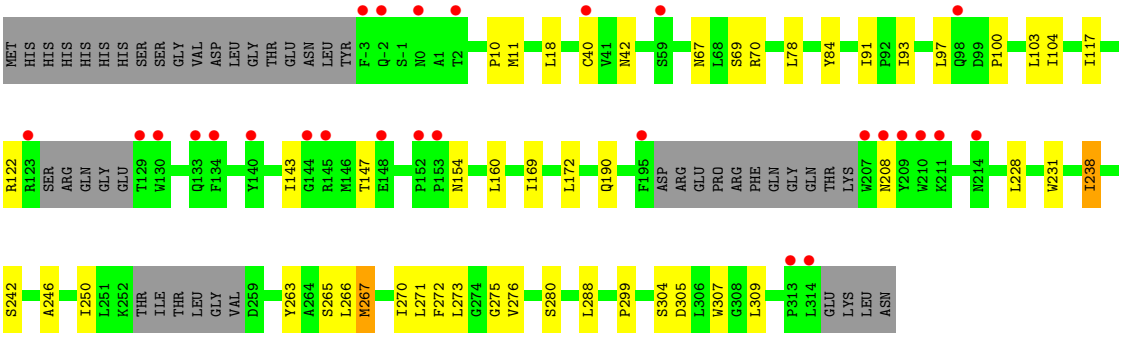
Chain B:





- Molecule 1: Uncharacterized glycosyltransferase sll0501

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.33Å 137.52Å 101.45Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	19.99 – 3.19 19.99 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.99-3.19) 98.8 (19.99-3.19)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.22Å)	Xtriage
Refinement program	PHENIX dev_2210	Depositor
R, R_{free}	0.248 , 0.291 0.249 , 0.290	Depositor DCC
R_{free} test set	1727 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	125.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 115.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9240	wwPDB-VP
Average B, all atoms (Å^2)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, MG

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	0.24	0/2271	0.41	0/3095
1	B	0.24	0/2328	0.40	0/3177
1	C	0.24	0/2406	0.42	0/3283
1	D	0.24	0/2325	0.39	0/3170
All	All	0.24	0/9330	0.41	0/12725

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2225	0	2192	31	0
1	B	2280	0	2185	33	0
1	C	2354	0	2270	33	0
1	D	2277	0	2220	40	0
2	A	25	0	11	1	0
2	B	25	0	11	1	0
2	C	25	0	11	0	0
2	D	25	0	11	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	9240	0	8911	112	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 6.

All (112) 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:152:PRO:O	1:A:154:ASN:N	2.13	0.81
1:C:263:TYR:HE1	1:D:266:LEU:HB2	1.53	0.73
1:C:260:VAL:HG22	1:C:261:PRO:HD2	1.71	0.72
1:A:74:LYS:HE2	2:A:401:UDP:H5'2	1.69	0.72
1:B:185:TRP:O	1:D:70:ARG:NH2	2.25	0.69
1:B:97:LEU:HD11	1:B:101:PRO:HG3	1.77	0.67
1:B:231:TRP:HE1	1:B:280:SER:HG	1.44	0.63
1:B:6:SER:OG	1:B:86:GLN:O	2.15	0.63
1:B:270:ILE:HB	1:D:270:ILE:HD13	1.80	0.62
1:D:231:TRP:HE1	1:D:280:SER:HG	1.47	0.61
1:A:270:ILE:HG22	1:B:270:ILE:HG12	1.83	0.61
1:D:91:ILE:HD11	1:D:160:LEU:HD12	1.83	0.60
1:A:123:ARG:HG2	1:A:194:LEU:HD23	1.83	0.60
1:C:263:TYR:OH	1:D:265:SER:OG	2.17	0.60
1:B:189:ARG:NH1	1:D:305:ASP:OD2	2.35	0.59
1:C:238:ILE:HD11	1:C:276:VAL:HG21	1.85	0.58
1:C:97:LEU:HD11	1:C:101:PRO:HD3	1.86	0.57
1:A:100:PRO:HG2	1:A:103:LEU:HD13	1.85	0.57
1:C:91:ILE:HD11	1:C:160:LEU:HD12	1.86	0.57
1:D:117:ILE:HB	1:D:190:GLN:HG2	1.86	0.56
1:B:78:LEU:HD11	1:B:92:PRO:HB3	1.87	0.56
1:B:239:SER:OG	1:D:275:GLY:O	2.21	0.55
1:B:266:LEU:HD21	1:D:266:LEU:HD23	1.88	0.55
1:C:117:ILE:HB	1:C:190:GLN:HG2	1.89	0.55
1:A:69:SER:HA	1:A:304:SER:HB2	1.88	0.55
1:A:238:ILE:HD11	1:A:276:VAL:HG21	1.89	0.55
1:D:100:PRO:HG2	1:D:103:LEU:HD13	1.88	0.54
1:D:169:ILE:HA	1:D:172:LEU:HD13	1.89	0.54
1:B:123:ARG:HD3	1:B:194:LEU:HB3	1.89	0.52
1:C:14:GLU:OE1	1:C:17:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ASN:ND2	1:D:67:ASN:OD1	2.42	0.52
1:A:6:SER:OG	1:A:86:GLN:O	2.28	0.51
1:A:260:VAL:HG12	1:A:261:PRO:HD2	1.91	0.51
1:B:69:SER:HA	1:B:304:SER:HB2	1.92	0.51
1:C:217:LEU:HD12	1:C:220:ILE:HD11	1.93	0.51
1:C:42:ASN:ND2	1:C:67:ASN:OD1	2.42	0.51
1:C:263:TYR:HH	1:D:265:SER:HG	1.43	0.50
1:A:91:ILE:HD11	1:A:160:LEU:HD12	1.93	0.50
1:C:266:LEU:HD21	1:A:266:LEU:HB3	1.94	0.50
1:C:271:LEU:HD11	1:D:242:SER:O	2.12	0.50
1:A:99:ASP:HB3	1:A:158:PHE:CD2	2.47	0.49
1:B:107:LEU:HD21	1:B:120:ALA:HB2	1.94	0.49
1:A:75:GLU:HB3	1:A:176:THR:HG23	1.95	0.49
1:B:172:LEU:HD11	1:D:299:PRO:HD3	1.94	0.49
1:C:268:VAL:HG21	1:D:250:ILE:HD13	1.95	0.49
1:A:159:ARG:HD3	1:A:179:MET:HE1	1.95	0.49
1:D:11:MET:HE1	1:D:40:CYS:HB3	1.95	0.48
1:A:10:PRO:HD3	1:A:78:LEU:HD13	1.94	0.48
1:B:270:ILE:HD13	1:D:270:ILE:HG12	1.94	0.48
1:D:93:ILE:HD11	1:D:104:ILE:HD11	1.96	0.48
1:C:119:TYR:HB2	1:C:192:PHE:HB3	1.96	0.48
1:B:7:ILE:HD11	1:B:38:ILE:HG12	1.96	0.48
1:C:83:ASP:OD1	1:C:175:ARG:NH2	2.47	0.47
1:D:143:ILE:HD12	1:D:147:THR:HG23	1.95	0.47
1:A:20:HIS:CD2	1:A:97:LEU:HD21	2.50	0.47
1:A:213:TRP:HA	1:A:216:ALA:HB3	1.97	0.47
1:C:263:TYR:CE1	1:D:266:LEU:HB2	2.42	0.47
1:C:260:VAL:HG12	1:A:263:TYR:CE2	2.49	0.47
1:A:276:VAL:HG13	1:B:278:LEU:HD21	1.97	0.47
1:C:10:PRO:HD3	1:C:78:LEU:HD13	1.97	0.46
1:D:272:PHE:HD2	1:D:273:LEU:HD22	1.80	0.46
1:A:245:TYR:O	1:A:249:LEU:HB3	2.15	0.46
1:A:261:PRO:HB2	1:A:264:ALA:HB3	1.98	0.46
1:C:268:VAL:HG22	1:D:246:ALA:HB1	1.97	0.46
1:D:122:ARG:N	1:D:154:ASN:OD1	2.49	0.46
1:C:84:TYR:HB3	1:C:309:LEU:HD13	1.97	0.45
1:D:11:MET:HA	2:D:401:UDP:O2'	2.17	0.45
1:A:16:ASP:OD2	1:A:16:ASP:N	2.44	0.45
1:A:67:ASN:HB2	1:A:307:TRP:HZ3	1.81	0.45
1:A:79:SER:HB3	1:A:175:ARG:NH2	2.31	0.45
1:A:169:ILE:HG22	1:A:172:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:PRO:HD3	1:D:172:LEU:HD11	1.99	0.44
1:C:78:LEU:HD11	1:C:92:PRO:HB3	1.99	0.44
1:C:271:LEU:HD11	1:D:242:SER:C	2.38	0.44
1:B:122:ARG:O	1:B:154:ASN:ND2	2.50	0.44
1:C:260:VAL:HG13	1:C:261:PRO:N	2.32	0.44
1:C:39:ILE:HD13	1:C:64:LYS:HB2	1.99	0.43
1:A:65:ILE:HB	1:A:307:TRP:HB2	2.01	0.43
1:B:266:LEU:HA	1:D:267:MET:HE3	1.99	0.43
1:C:150:LYS:HZ2	1:C:183:PHE:HE2	1.66	0.43
1:B:28:VAL:O	1:B:105:HIS:NE2	2.51	0.43
2:B:401:UDP:H6	2:B:401:UDP:H5'2	1.83	0.43
1:C:285:GLY:O	1:D:228:LEU:HD21	2.19	0.43
1:B:42:ASN:ND2	1:B:50:LEU:HB2	2.34	0.43
1:B:97:LEU:HD12	1:B:97:LEU:HA	1.85	0.43
1:D:10:PRO:HD3	1:D:78:LEU:HD13	2.01	0.43
1:C:266:LEU:HD12	1:C:266:LEU:HA	1.93	0.42
1:A:222:SER:OG	1:A:290:ARG:NH1	2.53	0.42
1:C:97:LEU:HD21	1:C:101:PRO:HG3	2.02	0.42
1:A:246:ALA:HB3	1:B:271:LEU:HD22	2.00	0.42
1:B:7:ILE:HG22	1:B:91:ILE:HG23	2.02	0.42
1:B:17:ASN:OD1	1:B:17:ASN:N	2.53	0.42
1:D:67:ASN:HB2	1:D:307:TRP:HZ3	1.85	0.42
1:D:84:TYR:HB3	1:D:309:LEU:HD13	2.01	0.42
1:C:271:LEU:HD12	1:D:246:ALA:HB3	2.02	0.42
1:D:18:LEU:HD23	1:D:18:LEU:HA	1.86	0.41
1:A:255:THR:HG23	1:A:256:LEU:HD12	2.01	0.41
1:D:238:ILE:HD11	1:D:276:VAL:HG21	2.02	0.41
1:B:266:LEU:HB2	1:D:263:TYR:HE1	1.85	0.41
1:D:69:SER:HA	1:D:304:SER:HB2	2.02	0.41
1:C:39:ILE:HD12	1:C:309:LEU:HD11	2.01	0.41
1:B:123:ARG:CG	1:B:194:LEU:HB3	2.51	0.41
1:B:146:MET:HB2	1:B:146:MET:HE3	1.90	0.41
1:B:273:LEU:HA	1:B:276:VAL:HG12	2.01	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.78	0.41
1:B:150:LYS:HD2	1:B:150:LYS:HA	1.96	0.41
1:D:267:MET:HG3	1:D:271:LEU:HD13	2.02	0.41
1:A:224:SER:O	1:A:225:LEU:HB2	2.20	0.41
1:B:261:PRO:HB2	1:B:264:ALA:HB3	2.02	0.40
1:C:75:GLU:HB3	1:C:176:THR:HB	2.03	0.40
1:B:284:ILE:HG23	1:D:288:LEU:HD22	2.04	0.40
1:B:13:ASN:HA	1:B:47:ASP:OD1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/341 (82%)	255 (91%)	22 (8%)	3 (1%)	14	51
1	B	291/341 (85%)	277 (95%)	14 (5%)	0	100	100
1	C	301/341 (88%)	286 (95%)	12 (4%)	3 (1%)	15	54
1	D	288/341 (84%)	275 (96%)	12 (4%)	1 (0%)	41	74
All	All	1160/1364 (85%)	1093 (94%)	60 (5%)	7 (1%)	25	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	260	VAL
1	A	153	PRO
1	C	261	PRO
1	A	151	ILE
1	D	208	ASN
1	C	262	GLY
1	A	261	PRO

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	231/301 (77%)	228 (99%)	3 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	228/301 (76%)	224 (98%)	4 (2%)	59	82
1	C	236/301 (78%)	232 (98%)	4 (2%)	60	83
1	D	232/301 (77%)	229 (99%)	3 (1%)	69	87
All	All	927/1204 (77%)	913 (98%)	14 (2%)	65	85

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

Mol	Chain	Res	Type
1	C	97	LEU
1	C	146	MET
1	C	212	LEU
1	C	243	LEU
1	A	97	LEU
1	A	112	ARG
1	A	163	ARG
1	B	17	ASN
1	B	98	GLN
1	B	260	VAL
1	B	271	LEU
1	D	97	LEU
1	D	238	ILE
1	D	267	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UDP	B	401	3	24,26,26	0.94	0	37,40,40	1.67	7 (18%)
2	UDP	D	401	3	24,26,26	0.95	0	37,40,40	1.68	7 (18%)
2	UDP	A	401	3	24,26,26	0.94	0	37,40,40	1.66	6 (16%)
2	UDP	C	401	3	24,26,26	0.95	0	37,40,40	1.69	7 (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	B	401	3	-	2/16/32/32	0/2/2/2
2	UDP	D	401	3	-	4/16/32/32	0/2/2/2
2	UDP	A	401	3	-	6/16/32/32	0/2/2/2
2	UDP	C	401	3	-	7/16/32/32	0/2/2/2

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	UDP	C4-N3-C2	-5.19	119.74	126.58
2	C	401	UDP	C4-N3-C2	-5.17	119.76	126.58
2	A	401	UDP	C4-N3-C2	-5.13	119.81	126.58
2	B	401	UDP	C4-N3-C2	-4.99	119.99	126.58
2	B	401	UDP	N3-C2-N1	3.95	120.14	114.89
2	D	401	UDP	PA-O3A-PB	-3.88	119.50	132.83
2	C	401	UDP	N3-C2-N1	3.87	120.02	114.89
2	A	401	UDP	PA-O3A-PB	-3.78	119.86	132.83
2	A	401	UDP	N3-C2-N1	3.78	119.90	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	UDP	N3-C2-N1	3.75	119.87	114.89
2	B	401	UDP	PA-O3A-PB	-3.67	120.22	132.83
2	C	401	UDP	PA-O3A-PB	-3.65	120.30	132.83
2	B	401	UDP	C5-C4-N3	3.22	119.66	114.84
2	C	401	UDP	C5-C4-N3	3.06	119.41	114.84
2	D	401	UDP	C5-C4-N3	3.06	119.41	114.84
2	A	401	UDP	C5-C4-N3	3.04	119.38	114.84
2	B	401	UDP	O4-C4-C5	-2.92	120.02	125.16
2	D	401	UDP	O4-C4-C5	-2.80	120.24	125.16
2	C	401	UDP	O4-C4-C5	-2.78	120.28	125.16
2	A	401	UDP	O4-C4-C5	-2.67	120.46	125.16
2	B	401	UDP	O2-C2-N1	-2.21	119.84	122.79
2	C	401	UDP	O2-C2-N1	-2.21	119.85	122.79
2	B	401	UDP	C3'-C2'-C1'	2.18	105.56	101.43
2	A	401	UDP	O2-C2-N1	-2.11	119.98	122.79
2	D	401	UDP	C5-C6-N1	-2.10	118.29	121.81
2	C	401	UDP	C3'-C2'-C1'	2.09	105.39	101.43
2	D	401	UDP	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	UDP	C5'-O5'-PA-O2A
2	C	401	UDP	C5'-O5'-PA-O3A
2	A	401	UDP	C5'-O5'-PA-O1A
2	A	401	UDP	C5'-O5'-PA-O2A
2	A	401	UDP	C5'-O5'-PA-O3A
2	B	401	UDP	PA-O3A-PB-O3B
2	C	401	UDP	O4'-C4'-C5'-O5'
2	D	401	UDP	O4'-C4'-C5'-O5'
2	C	401	UDP	C3'-C4'-C5'-O5'
2	A	401	UDP	C3'-C4'-C5'-O5'
2	A	401	UDP	O4'-C4'-C5'-O5'
2	D	401	UDP	C5'-O5'-PA-O3A
2	A	401	UDP	PB-O3A-PA-O1A
2	C	401	UDP	C5'-O5'-PA-O1A
2	D	401	UDP	C3'-C4'-C5'-O5'
2	C	401	UDP	PA-O3A-PB-O3B
2	D	401	UDP	PA-O3A-PB-O3B
2	C	401	UDP	PB-O3A-PA-O2A
2	B	401	UDP	O4'-C4'-C5'-O5'

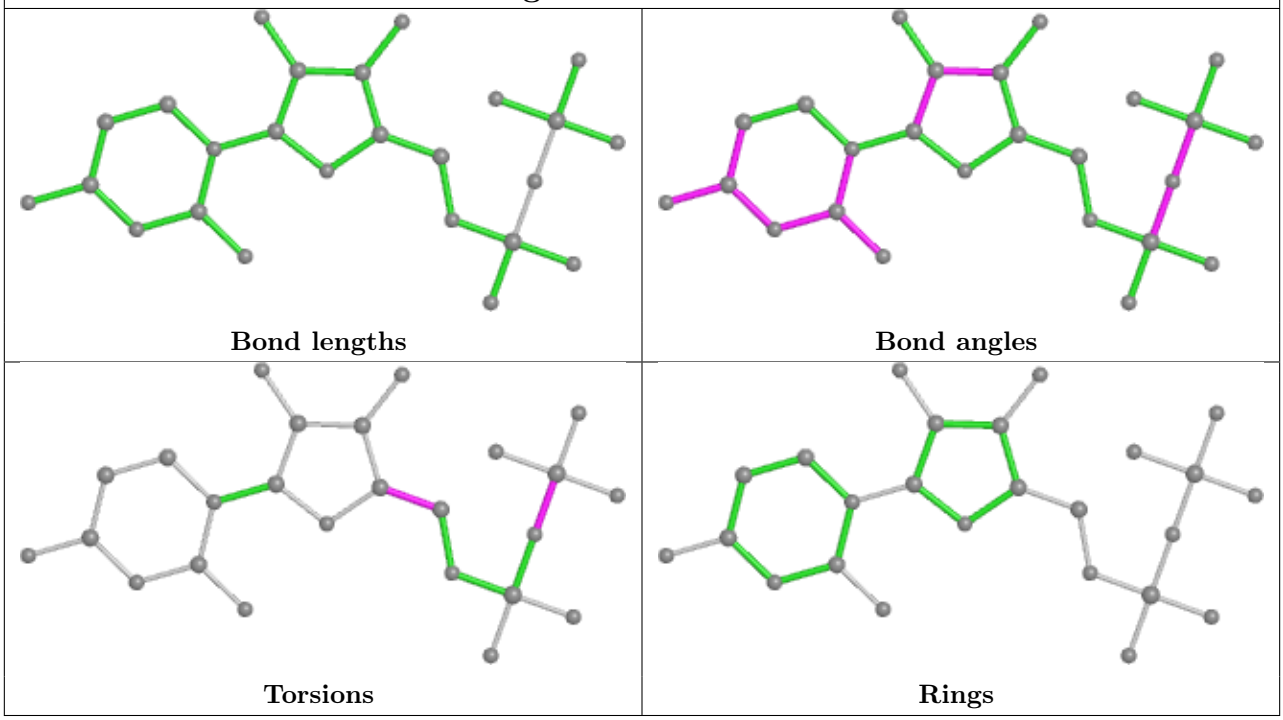
There are no ring outliers.

3 monomers are involved in 3 short contacts:

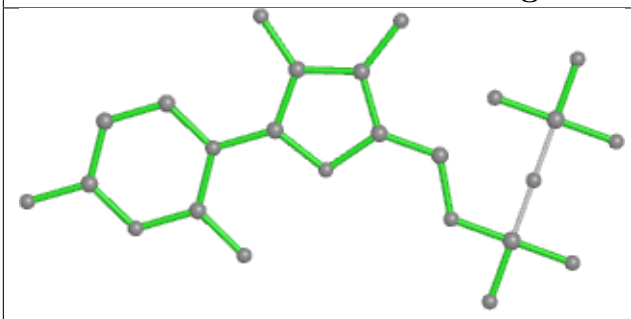
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	UDP	1	0
2	D	401	UDP	1	0
2	A	401	UDP	1	0

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.

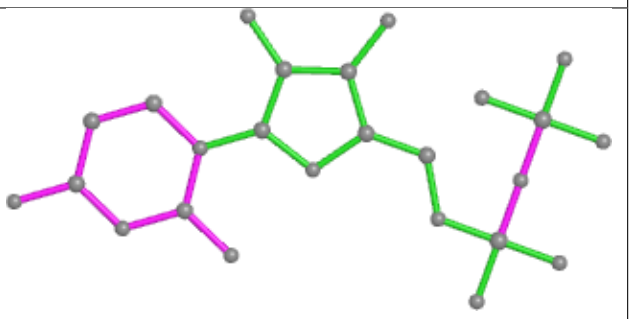
Ligand UDP B 401



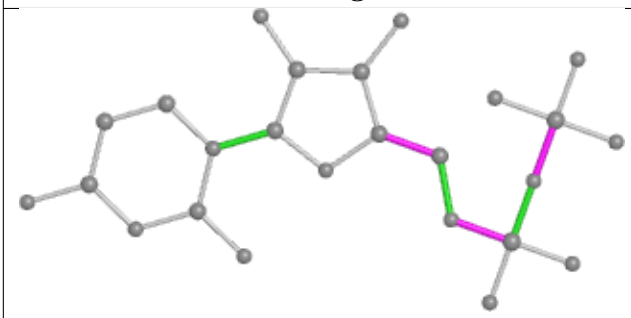
Ligand UDP D 401



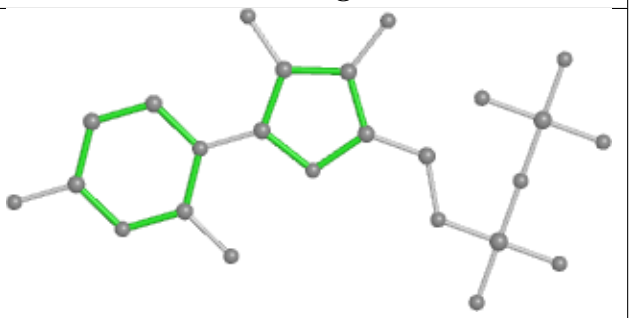
Bond lengths



Bond angles

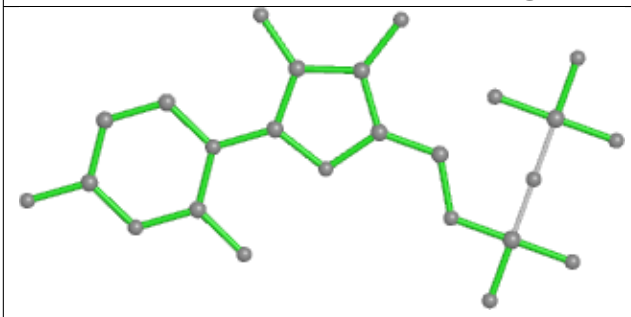


Torsions

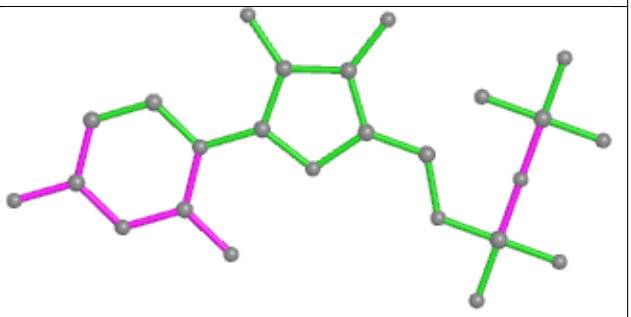


Rings

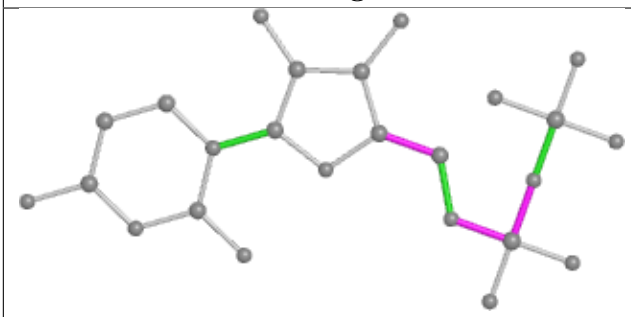
Ligand UDP A 401



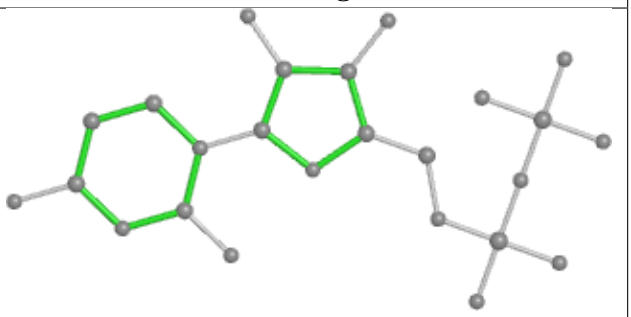
Bond lengths



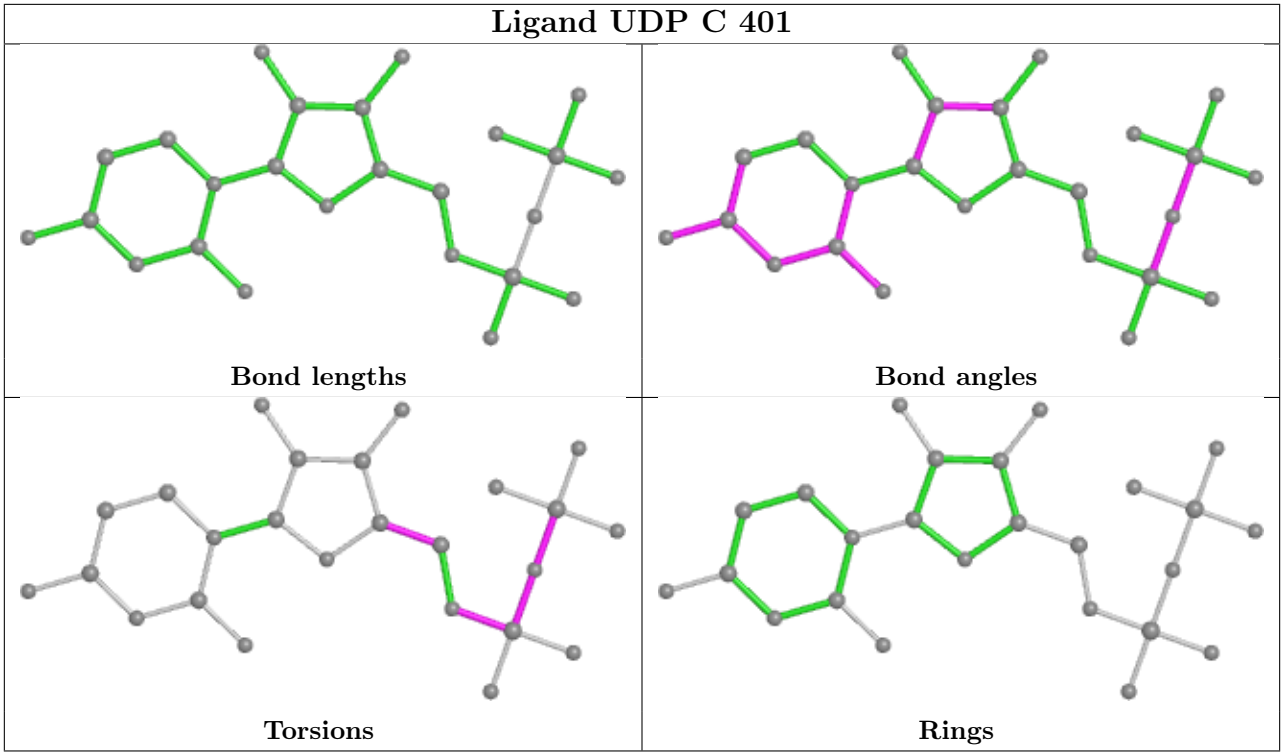
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	288/341 (84%)	0.11	18 (6%)	20	11	89, 145, 270, 355	0
1	B	299/341 (87%)	0.17	20 (6%)	17	10	79, 138, 305, 393	0
1	C	307/341 (90%)	0.25	29 (9%)	8	4	104, 162, 303, 391	0
1	D	296/341 (86%)	0.19	27 (9%)	9	5	92, 160, 307, 427	0
All	All	1190/1364 (87%)	0.18	94 (7%)	12	6	79, 152, 300, 427	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	THR	14.2
1	D	130	TRP	8.1
1	D	129	THR	7.6
1	C	128	GLU	7.3
1	C	129	THR	6.4
1	B	0	ASN	6.4
1	B	206	LYS	6.3
1	C	126	GLN	5.8
1	A	153	PRO	5.5
1	A	127	GLY	5.5
1	B	207	TRP	5.5
1	B	258	VAL	5.2
1	B	208	ASN	5.2
1	B	211	LYS	5.2
1	D	133	GLN	5.1
1	C	127	GLY	4.9
1	C	131	VAL	4.8
1	D	211	LYS	4.8
1	C	134	PHE	4.6
1	D	207	TRP	4.5
1	A	152	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	211	LYS	4.5
1	D	153	PRO	4.1
1	C	-2	GLN	4.1
1	C	40	CYS	4.1
1	B	-2	GLN	4.0
1	C	152	PRO	3.9
1	B	152	PRO	3.9
1	B	124	SER	3.8
1	A	148	GLU	3.8
1	D	208	ASN	3.8
1	D	-2	GLN	3.6
1	A	126	GLN	3.6
1	B	-3	PHE	3.5
1	B	209	TYR	3.5
1	B	212	LEU	3.5
1	C	130	TRP	3.4
1	A	151	ILE	3.4
1	B	2	THR	3.3
1	D	40	CYS	3.3
1	D	314	LEU	3.3
1	D	140	TYR	3.3
1	C	153	PRO	3.3
1	C	196	ASP	3.2
1	A	214	ASN	3.2
1	D	313	PRO	3.2
1	C	214	ASN	3.1
1	D	98	GLN	3.0
1	D	195	PHE	3.0
1	A	253	THR	2.9
1	C	259	ASP	2.9
1	A	208	ASN	2.8
1	B	141	LYS	2.8
1	A	40	CYS	2.8
1	D	145	ARG	2.8
1	A	2	THR	2.8
1	C	113	GLU	2.7
1	C	197	ARG	2.7
1	C	43	ASP	2.7
1	C	0	ASN	2.6
1	D	0	ASN	2.6
1	D	2	THR	2.6
1	A	212	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	-2	GLN	2.6
1	C	42	ASN	2.5
1	D	-3	PHE	2.5
1	D	210	TRP	2.5
1	B	153	PRO	2.5
1	D	214	ASN	2.4
1	C	248	PHE	2.4
1	B	259	ASP	2.4
1	C	210	TRP	2.4
1	B	140	TYR	2.3
1	A	259	ASP	2.3
1	A	209	TYR	2.3
1	C	312	LEU	2.3
1	A	256	LEU	2.3
1	C	135	THR	2.2
1	D	134	PHE	2.2
1	B	249	LEU	2.2
1	D	59	SER	2.2
1	D	148	GLU	2.2
1	C	209	TYR	2.2
1	D	144	GLY	2.2
1	D	209	TYR	2.2
1	A	196	ASP	2.2
1	C	125	ARG	2.1
1	C	1	ALA	2.1
1	D	152	PRO	2.1
1	A	297	ALA	2.1
1	C	140	TYR	2.1
1	D	123	ARG	2.1
1	B	154	ASN	2.0
1	C	12	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

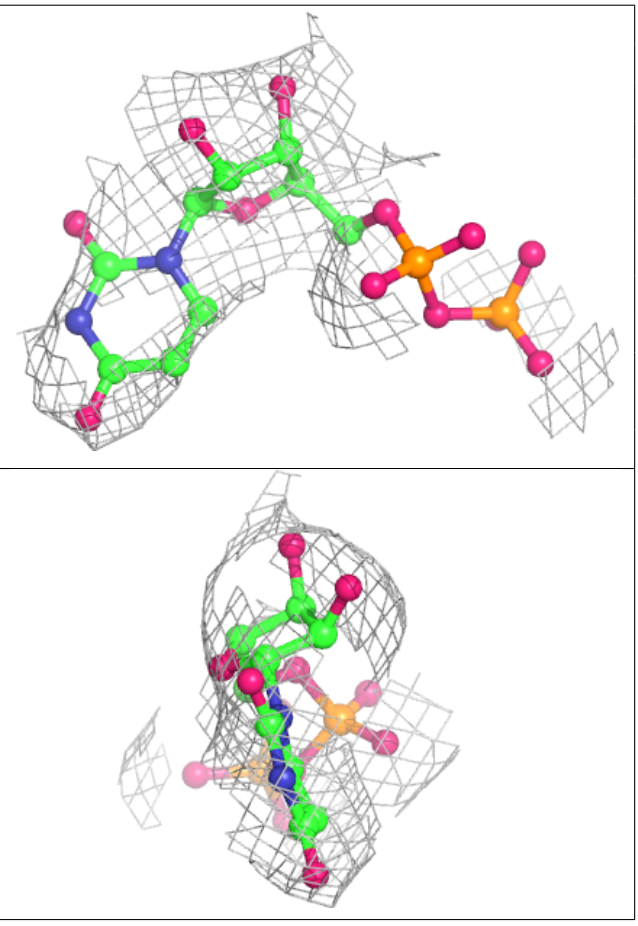
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	402	1/1	0.70	0.10	169,169,169,169	0
3	MG	B	402	1/1	0.84	0.08	149,149,149,149	0
2	UDP	D	401	25/25	0.87	0.18	119,161,249,252	0
2	UDP	B	401	25/25	0.90	0.18	104,131,226,228	0
2	UDP	C	401	25/25	0.91	0.18	111,157,212,219	0
3	MG	C	402	1/1	0.93	0.05	136,136,136,136	0
3	MG	D	402	1/1	0.93	0.24	153,153,153,153	0
2	UDP	A	401	25/25	0.94	0.14	99,125,220,230	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.

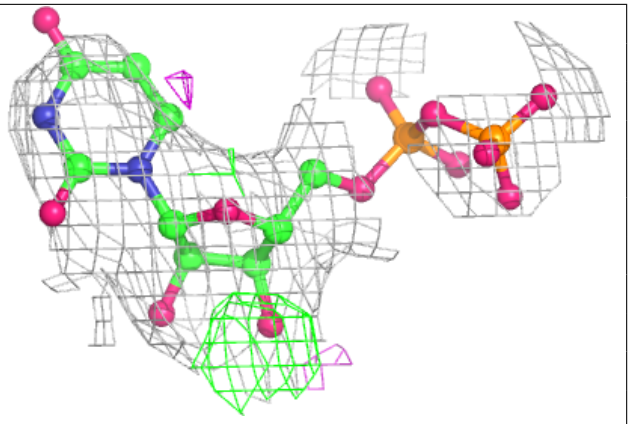
Electron density around UDP D 401:

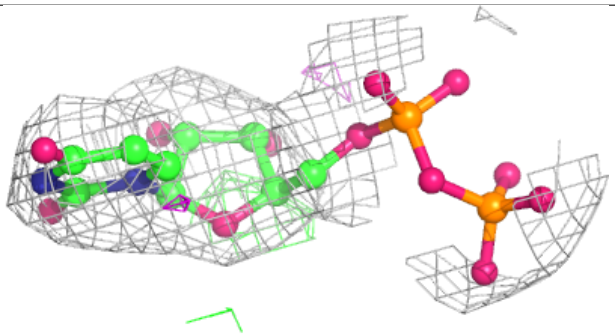
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

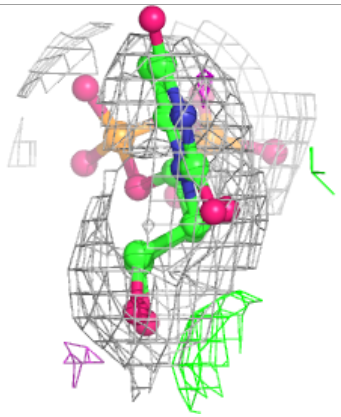


Electron density around UDP B 401:

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

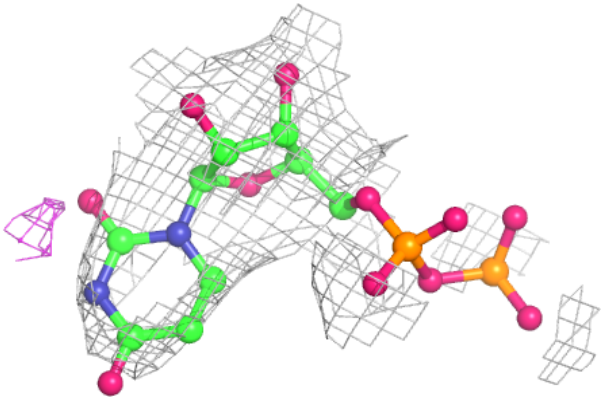


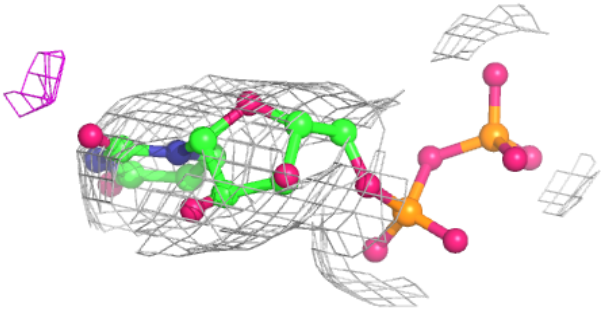


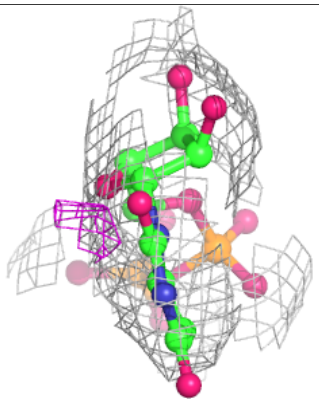


Electron density around UDP C 401:

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

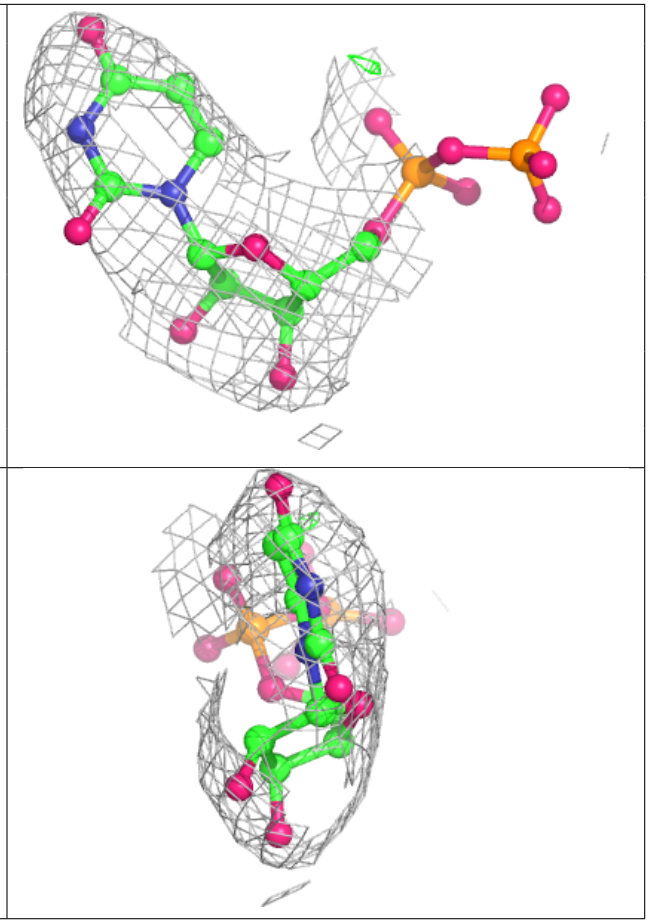






Electron density around UDP A 401:

$2mF_o$-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 (i)

There are no such residues in this entry.