



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 02:52 am BST

PDB ID : 3MJR
Title : Human dCK complex with Acyclic Nucleoside
Authors : Hazra, S.; Lavie, A.
Deposited on : 2010-04-13
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.11
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) : 2.11

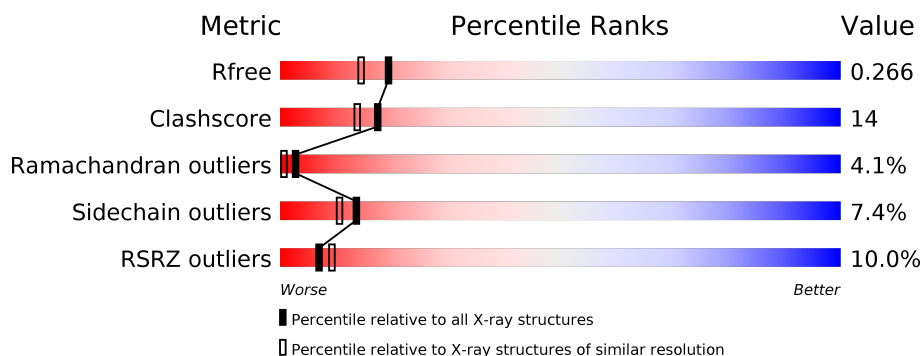
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	279	
1	B	279	
1	C	279	
1	D	279	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AC2	A	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7428 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1866	1196	310	354	6			
1	B	226	Total	C	N	O	S	0	0	0
			1815	1161	303	345	6			
1	C	222	Total	C	N	O	S	0	0	0
			1757	1119	295	338	5			
1	D	221	Total	C	N	O	S	0	0	0
			1777	1140	294	338	5			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP P27707
A	-17	GLY	-	EXPRESSION TAG	UNP P27707
A	-16	SER	-	EXPRESSION TAG	UNP P27707
A	-15	SER	-	EXPRESSION TAG	UNP P27707
A	-14	HIS	-	EXPRESSION TAG	UNP P27707
A	-13	HIS	-	EXPRESSION TAG	UNP P27707
A	-12	HIS	-	EXPRESSION TAG	UNP P27707
A	-11	HIS	-	EXPRESSION TAG	UNP P27707
A	-10	HIS	-	EXPRESSION TAG	UNP P27707
A	-9	HIS	-	EXPRESSION TAG	UNP P27707
A	-8	SER	-	EXPRESSION TAG	UNP P27707
A	-7	GLY	-	EXPRESSION TAG	UNP P27707
A	-6	LEU	-	EXPRESSION TAG	UNP P27707
A	-5	VAL	-	EXPRESSION TAG	UNP P27707
A	-4	PRO	-	EXPRESSION TAG	UNP P27707
A	-3	ARG	-	EXPRESSION TAG	UNP P27707
A	-2	GLY	-	EXPRESSION TAG	UNP P27707
A	-1	SER	-	EXPRESSION TAG	UNP P27707
A	0	HIS	-	EXPRESSION TAG	UNP P27707
A	9	SER	CYS	CONFLICT	UNP P27707
A	45	SER	CYS	CONFLICT	UNP P27707

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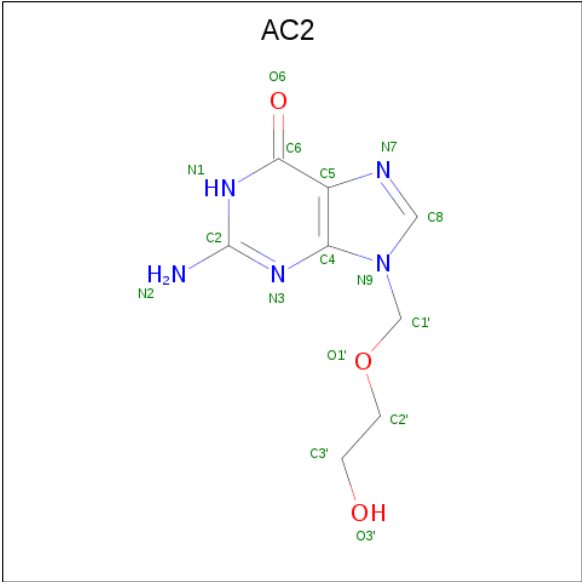
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	SER	CYS	CONFLICT	UNP P27707
A	146	SER	CYS	CONFLICT	UNP P27707
B	-18	MET	-	EXPRESSION TAG	UNP P27707
B	-17	GLY	-	EXPRESSION TAG	UNP P27707
B	-16	SER	-	EXPRESSION TAG	UNP P27707
B	-15	SER	-	EXPRESSION TAG	UNP P27707
B	-14	HIS	-	EXPRESSION TAG	UNP P27707
B	-13	HIS	-	EXPRESSION TAG	UNP P27707
B	-12	HIS	-	EXPRESSION TAG	UNP P27707
B	-11	HIS	-	EXPRESSION TAG	UNP P27707
B	-10	HIS	-	EXPRESSION TAG	UNP P27707
B	-9	HIS	-	EXPRESSION TAG	UNP P27707
B	-8	SER	-	EXPRESSION TAG	UNP P27707
B	-7	GLY	-	EXPRESSION TAG	UNP P27707
B	-6	LEU	-	EXPRESSION TAG	UNP P27707
B	-5	VAL	-	EXPRESSION TAG	UNP P27707
B	-4	PRO	-	EXPRESSION TAG	UNP P27707
B	-3	ARG	-	EXPRESSION TAG	UNP P27707
B	-2	GLY	-	EXPRESSION TAG	UNP P27707
B	-1	SER	-	EXPRESSION TAG	UNP P27707
B	0	HIS	-	EXPRESSION TAG	UNP P27707
B	9	SER	CYS	CONFLICT	UNP P27707
B	45	SER	CYS	CONFLICT	UNP P27707
B	59	SER	CYS	CONFLICT	UNP P27707
B	146	SER	CYS	CONFLICT	UNP P27707
C	-18	MET	-	EXPRESSION TAG	UNP P27707
C	-17	GLY	-	EXPRESSION TAG	UNP P27707
C	-16	SER	-	EXPRESSION TAG	UNP P27707
C	-15	SER	-	EXPRESSION TAG	UNP P27707
C	-14	HIS	-	EXPRESSION TAG	UNP P27707
C	-13	HIS	-	EXPRESSION TAG	UNP P27707
C	-12	HIS	-	EXPRESSION TAG	UNP P27707
C	-11	HIS	-	EXPRESSION TAG	UNP P27707
C	-10	HIS	-	EXPRESSION TAG	UNP P27707
C	-9	HIS	-	EXPRESSION TAG	UNP P27707
C	-8	SER	-	EXPRESSION TAG	UNP P27707
C	-7	GLY	-	EXPRESSION TAG	UNP P27707
C	-6	LEU	-	EXPRESSION TAG	UNP P27707
C	-5	VAL	-	EXPRESSION TAG	UNP P27707
C	-4	PRO	-	EXPRESSION TAG	UNP P27707
C	-3	ARG	-	EXPRESSION TAG	UNP P27707
C	-2	GLY	-	EXPRESSION TAG	UNP P27707

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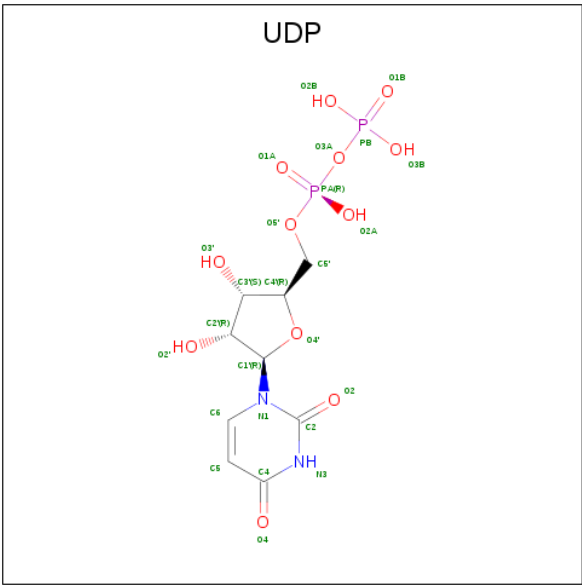
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP P27707
C	0	HIS	-	EXPRESSION TAG	UNP P27707
C	9	SER	CYS	CONFLICT	UNP P27707
C	45	SER	CYS	CONFLICT	UNP P27707
C	59	SER	CYS	CONFLICT	UNP P27707
C	146	SER	CYS	CONFLICT	UNP P27707
D	-18	MET	-	EXPRESSION TAG	UNP P27707
D	-17	GLY	-	EXPRESSION TAG	UNP P27707
D	-16	SER	-	EXPRESSION TAG	UNP P27707
D	-15	SER	-	EXPRESSION TAG	UNP P27707
D	-14	HIS	-	EXPRESSION TAG	UNP P27707
D	-13	HIS	-	EXPRESSION TAG	UNP P27707
D	-12	HIS	-	EXPRESSION TAG	UNP P27707
D	-11	HIS	-	EXPRESSION TAG	UNP P27707
D	-10	HIS	-	EXPRESSION TAG	UNP P27707
D	-9	HIS	-	EXPRESSION TAG	UNP P27707
D	-8	SER	-	EXPRESSION TAG	UNP P27707
D	-7	GLY	-	EXPRESSION TAG	UNP P27707
D	-6	LEU	-	EXPRESSION TAG	UNP P27707
D	-5	VAL	-	EXPRESSION TAG	UNP P27707
D	-4	PRO	-	EXPRESSION TAG	UNP P27707
D	-3	ARG	-	EXPRESSION TAG	UNP P27707
D	-2	GLY	-	EXPRESSION TAG	UNP P27707
D	-1	SER	-	EXPRESSION TAG	UNP P27707
D	0	HIS	-	EXPRESSION TAG	UNP P27707
D	9	SER	CYS	CONFLICT	UNP P27707
D	45	SER	CYS	CONFLICT	UNP P27707
D	59	SER	CYS	CONFLICT	UNP P27707
D	146	SER	CYS	CONFLICT	UNP P27707

- Molecule 2 is 9-HYROXYETHOXYMETHYLGUANINE (three-letter code: AC2) (formula: $C_8H_{11}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	8	5	3		
2	B	1	Total	C	N	O	0	0
			16	8	5	3		
2	D	1	Total	C	N	O	0	0
			16	8	5	3		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	32	Total	O	0	0
			32	32		
4	C	7	Total	O	0	0
			7	7		
4	D	4	Total	O	0	0
			4	4		

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

57% 22% 18%

MET GLY SER HIS HIS HIS HIS HIS SER GLY LEU VAL PRO ARG GLY SER HIS MET MET ALA THR PRO PRO LYS ARG SER SER PRO SER PHE SER SER ALA ALA SER SER GLY GLY THR R20 K23 I24 S25 I26 I30 A31 S35 V38 N39 V50 N60 VAL GLN SER THR

Chain B:

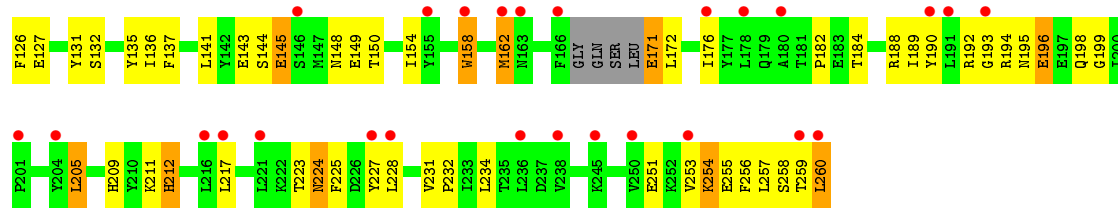
61% 18% 19%

Row 1	Row 2	Row 3
Met	Val	Met
Gly	Val	Gly
Ser	Gln	Ser
His	Ser	His
His	Thr	His
His	Gln	His
His	Asp	His
His	Phe	His
Gly	Glu	Gly
Ser	Glu	Ser
Leu	Leu	Leu
Val	Thr	Val
Pro	Met	Pro
Arg	Ser	Arg
Gly	Q75	Gly
Ser	K76	Ser
His	N77	His
Met		Met
Ala	V81	Ala
Thr	L82	Thr
Pro	Q83	Pro
Pro	M84	Pro
Lys		Lys
Arg	E87	Arg
Ser		Ser
Ser	W92	Ser
Pro		Pro
Ser	Q97	Ser
Phe		Phe
Ser	L102	Ser
Ala		Ala
Ser	R106	Ser
Ser	A107	Ser
Glu	Q108	Glu
Gly		Gly
Thr	L112	Thr
R20	N113	R20
	G114	
S25	K115	S25
I26	L116	I26
	K117	
A31	D118	A31
	A119	
K34		K34
V38	L124	V38
	F125	
L41	F126	L41
	E127	
W43	R128	W43
P43	S129	P43
V50	V130	V50
E53	D133	E53
P54	W158	P54
V55		V55
V58	M162	V58

Chain C:

17% 52% 24% 20%

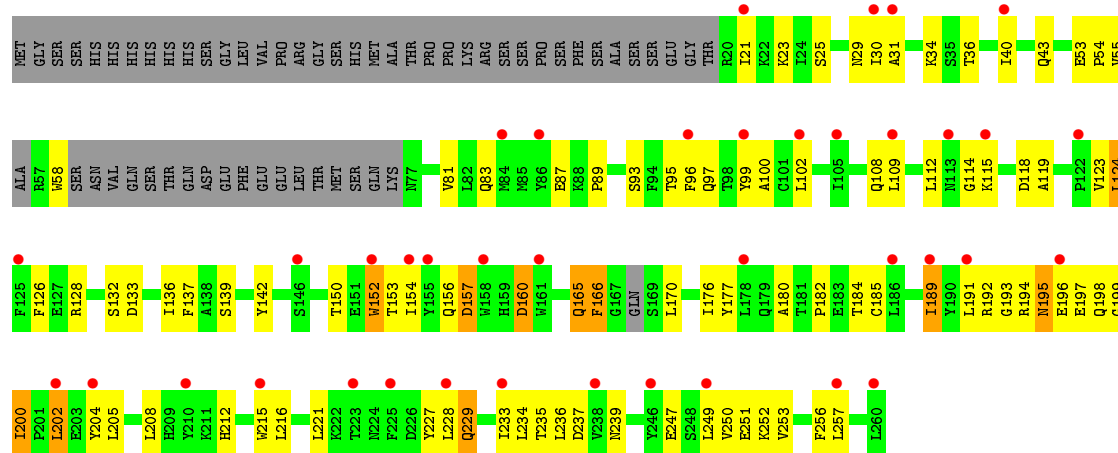
Amino Acid	Category
MET	Grey
GLY	Grey
SER	Grey
SER	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
HIS	Grey
ASN	Grey
HIS	Grey
GLN	Grey
SER	Grey
GLY	Grey
LEU	Grey
VAL	Grey
PRO	Grey
ARG	Grey
GLY	Grey
GLU	Grey
SER	Grey
HIS	Grey
LEU	Grey
MET	Grey
ALA	Grey
THR	Grey
PRO	Grey
PRO	Grey
LYS	Grey
ARG	Grey
SER	Grey
SER	Grey
PRO	Grey
GLN	Grey
SER	Grey
PHE	Grey
SER	Grey
SER	Grey
ALA	Grey
SER	Grey
SER	Grey
GLU	Grey
GLY	Grey
THR	Grey
R20	Green
K21	Yellow
K22	Yellow
K23	Green
I24	Green
S25	Yellow
I26	Green
E27	Green
G28	Green
A31	Yellow
A32	Green
G33	Green
T36	Yellow
F37	Yellow
N38	Yellow
V39	Yellow
I40	Yellow
I41	Yellow
L41	Yellow
L42	Yellow
L43	Yellow
D47	Green
V55	Green
A56	Green
R57	Green
W58	Yellow
S59	Yellow
ASN	Grey
VAL	Grey
GLN	Grey
SER	Grey
THR	Grey
GLN	Grey
ASP	Grey
GLU	Grey
PHE	Grey
GLU	Grey
GLU	Grey
LEU	Grey
THR	Grey
MET	Grey
S74	Green
G78	Green
G79	Green
L82	Green
GLN	Grey
M84	Green
M85	Green
Y86	Green
R91	Yellow
F96	Green
Q97	Yellow
T98	Yellow
Y99	Yellow
A100	Yellow
G101	Yellow
L102	Yellow
S103	Yellow
R104	Yellow
I105	Yellow
Q108	Yellow
L109	Yellow
G114	Green
K115	Green
D116	Green
A119	Green
K120	Green
K121	Green
P122	Green
V123	Green
L124	Green
L125	Green



● Molecule 1: Deoxycytidine kinase



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	97.31Å 97.31Å 121.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.8 (30.00-2.10) 97.6 (29.65-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.312 0.263 , 0.266	Depositor DCC
R_{free} test set	6565 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1139e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: AC2, 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	0.46	0/1910	0.62	0/2590
1	B	0.46	0/1857	0.63	0/2520
1	C	0.37	0/1796	0.56	1/2437 (0.0%)
1	D	0.38	0/1816	0.58	0/2462
All	All	0.42	0/7379	0.60	1/10009 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	LEU	CA-CB-CG	5.03	126.86	115.30

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	1866	0	1765	51	0
1	B	1815	0	1688	35	0
1	C	1757	0	1606	41	0
1	D	1777	0	1670	72	0
2	A	16	0	11	9	0
2	B	16	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	0	10	3	0
3	A	25	0	11	2	0
3	B	25	0	11	0	0
3	C	25	0	11	0	0
3	D	25	0	11	1	0
4	A	22	0	0	2	0
4	B	32	0	0	4	0
4	C	7	0	0	3	0
4	D	4	0	0	0	0
All	All	7428	0	6805	195	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 14.

The worst 5 of 195 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:93:SER:O	1:A:96:PHE:O	1.58	1.22
1:B:53:GLU:OE1	2:B:401:AC2:N2	1.71	1.21
1:A:200:ILE:HB	1:A:201:PRO:HD3	1.38	1.01
1:D:180:ALA:HA	1:D:239:ASN:HD21	1.27	0.95
1:A:38:VAL:HG22	1:A:50:VAL:HG22	1.51	0.93

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	224/279 (80%)	201 (90%)	11 (5%)	12 (5%)	<div>20</div>
1	B	220/279 (79%)	188 (86%)	24 (11%)	8 (4%)	<div>31</div>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	214/279 (77%)	173 (81%)	36 (17%)	5 (2%)	6	2
1	D	213/279 (76%)	179 (84%)	23 (11%)	11 (5%)	2	0
All	All	871/1116 (78%)	741 (85%)	94 (11%)	36 (4%)	3	1

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	119	ALA
1	A	200	ILE
1	B	115	LYS
1	B	117	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/255 (77%)	184 (93%)	13 (7%)	16	14
1	B	187/255 (73%)	180 (96%)	7 (4%)	34	35
1	C	177/255 (69%)	156 (88%)	21 (12%)	5	2
1	D	185/255 (72%)	171 (92%)	14 (8%)	13	10
All	All	746/1020 (73%)	691 (93%)	55 (7%)	13	10

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	101	CYS
1	C	150	THR
1	D	191	LEU
1	C	109	LEU
1	C	124	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	218	HIS
1	B	229	GLN
1	C	229	GLN
1	B	97	GLN
1	C	224	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	AC2	A	301	-	12,17,17	1.50	1 (8%)	11,23,23	2.40	5 (45%)
3	UDP	C	501	-	20,26,26	1.19	1 (5%)	25,40,40	1.15	2 (8%)
2	AC2	B	401	-	12,17,17	1.43	1 (8%)	11,23,23	2.38	5 (45%)
3	UDP	A	261	-	20,26,26	1.20	1 (5%)	25,40,40	1.07	2 (8%)
2	AC2	D	601	-	12,17,17	1.52	1 (8%)	11,23,23	2.38	4 (36%)
3	UDP	D	261	-	20,26,26	1.18	1 (5%)	25,40,40	1.21	1 (4%)
3	UDP	B	261	-	20,26,26	1.25	1 (5%)	25,40,40	0.83	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	AC2	A	301	-	-	1/3/5/5	0/2/2/2
3	UDP	C	501	-	-	4/14/32/32	0/2/2/2
2	AC2	B	401	-	-	1/3/5/5	0/2/2/2
3	UDP	A	261	-	-	0/14/32/32	0/2/2/2
2	AC2	D	601	-	-	1/3/5/5	0/2/2/2
3	UDP	D	261	-	-	6/14/32/32	0/2/2/2
3	UDP	B	261	-	-	3/14/32/32	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	AC2	O6-C6	4.79	1.36	1.24
2	D	601	AC2	O6-C6	4.63	1.36	1.24
2	B	401	AC2	O6-C6	4.56	1.36	1.24
3	A	261	UDP	C4-N3	3.56	1.39	1.33
3	C	501	UDP	C4-N3	3.36	1.38	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	AC2	N3-C2-N1	-4.54	121.17	127.22
2	A	301	AC2	N3-C2-N1	-4.34	121.43	127.22
2	B	401	AC2	C2-N3-C4	4.26	120.22	115.36
2	D	601	AC2	C2-N3-C4	4.22	120.17	115.36
2	B	401	AC2	N3-C2-N1	-4.03	121.84	127.22

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

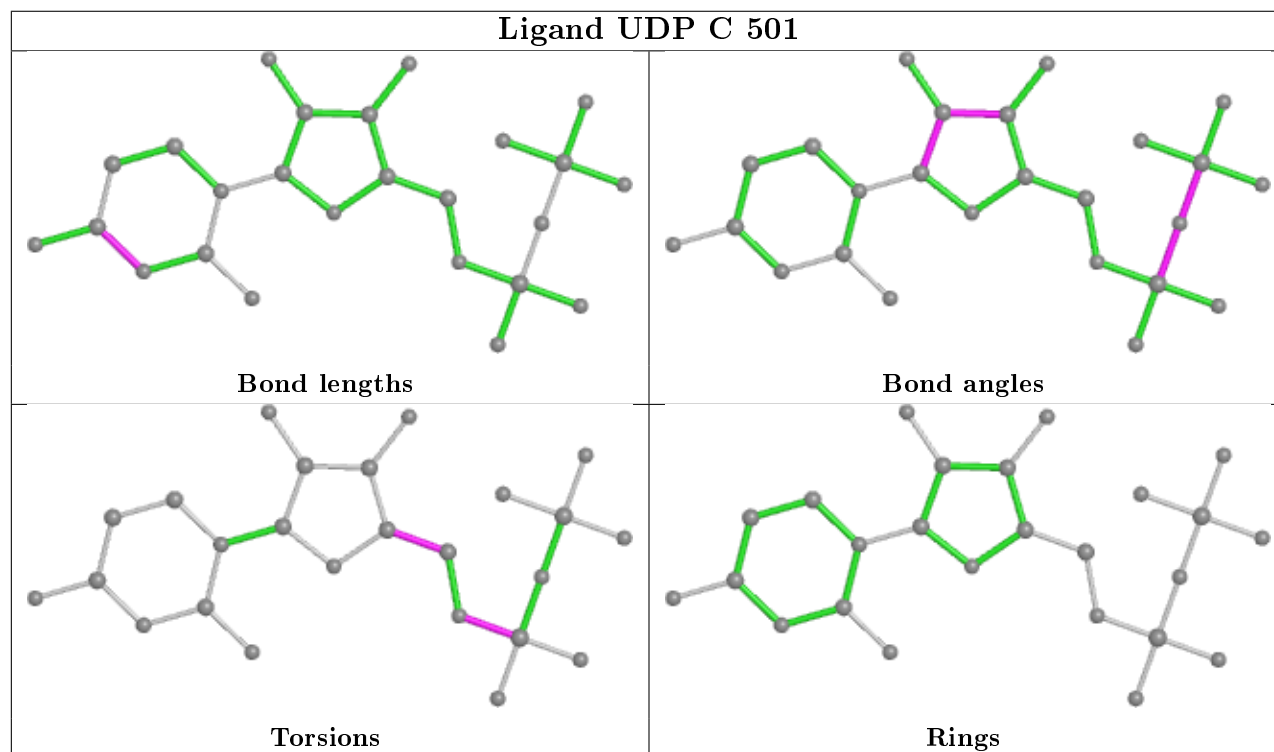
Mol	Chain	Res	Type	Atoms
3	C	501	UDP	C5'-O5'-PA-O1A
3	C	501	UDP	C5'-O5'-PA-O3A
3	D	261	UDP	C2'-C1'-N1-C6
3	D	261	UDP	O4'-C1'-N1-C6
3	D	261	UDP	C5'-O5'-PA-O1A

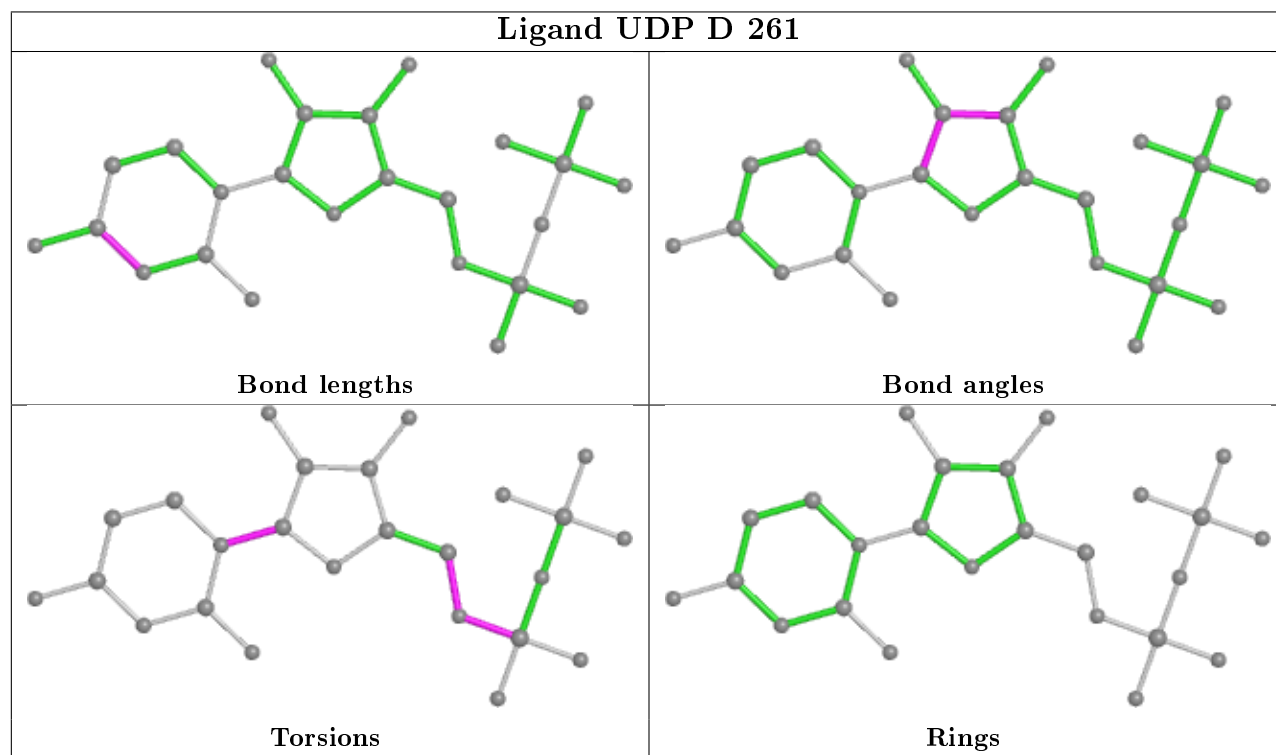
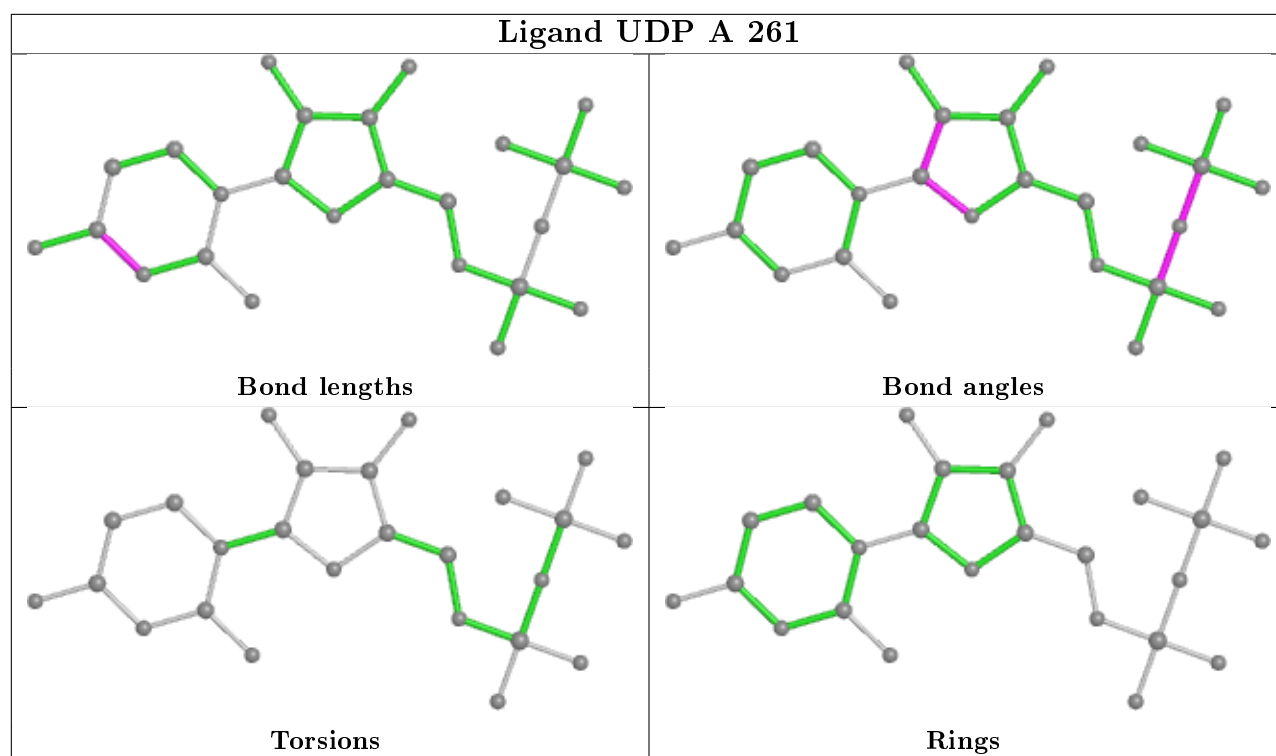
There are no ring outliers.

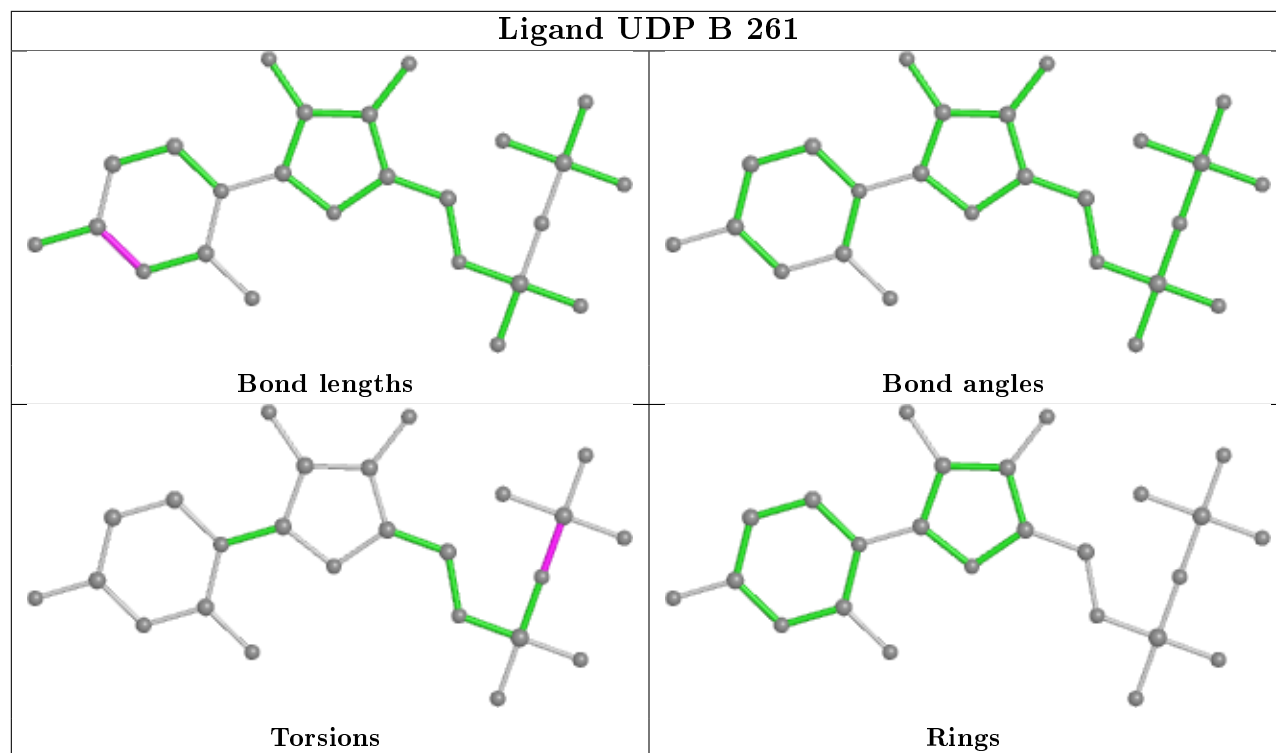
5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AC2	9	0
2	B	401	AC2	2	0
3	A	261	UDP	2	0
2	D	601	AC2	3	0
3	D	261	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 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 [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	230/279 (82%)	0.26	2 (0%) 84 86	21, 32, 43, 49	0
1	B	226/279 (81%)	0.25	1 (0%) 92 93	21, 32, 43, 47	0
1	C	222/279 (79%)	1.17	48 (21%) 0 0	44, 55, 63, 65	0
1	D	221/279 (79%)	1.03	39 (17%) 1 1	45, 54, 59, 62	0
All	All	899/1116 (80%)	0.67	90 (10%) 7 9	21, 45, 60, 65	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	LEU	8.1
1	C	96	PHE	6.9
1	D	158	TRP	6.2
1	C	238	VAL	6.0
1	C	180	ALA	5.4

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](#)

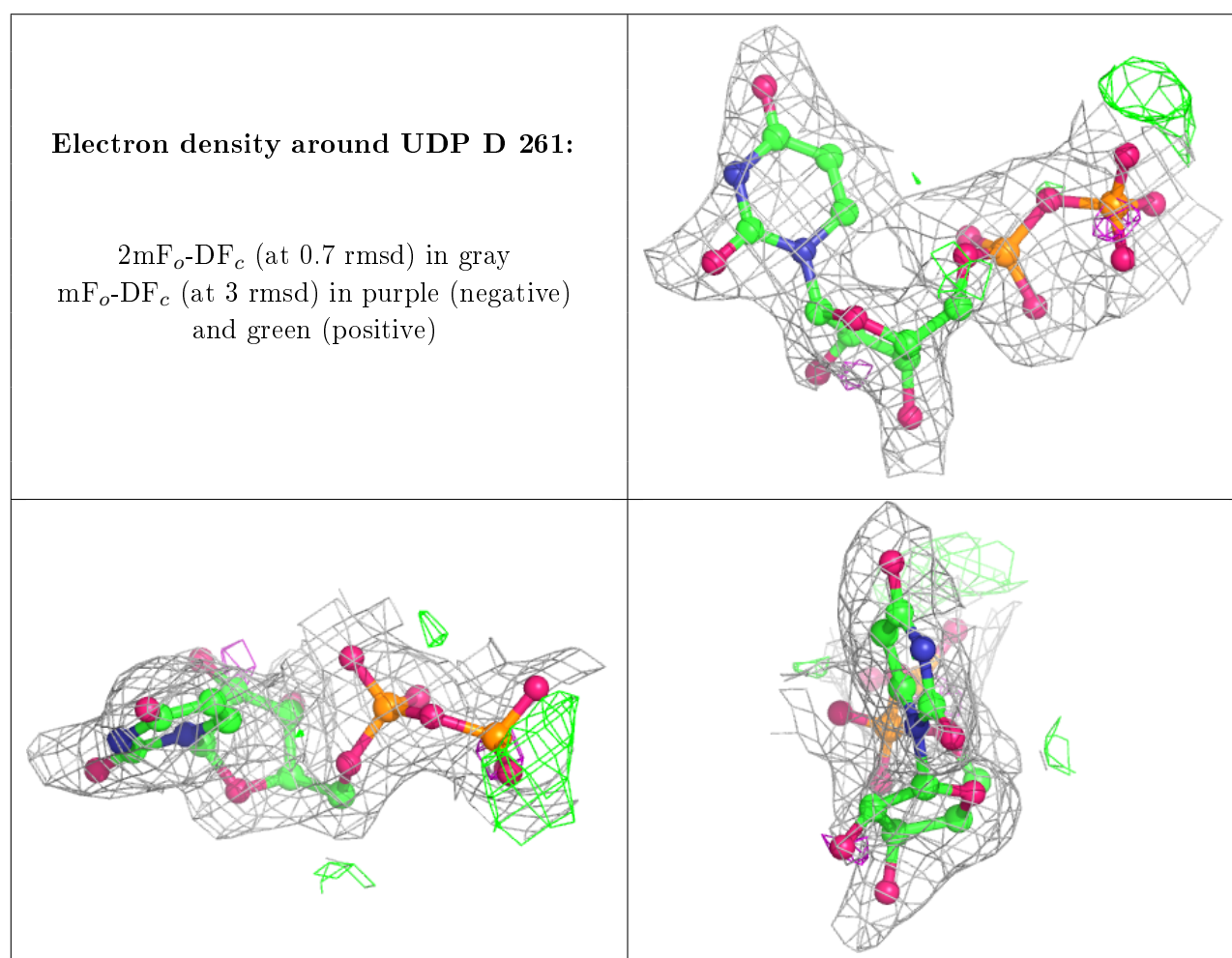
There are no carbohydrates in this entry.

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.

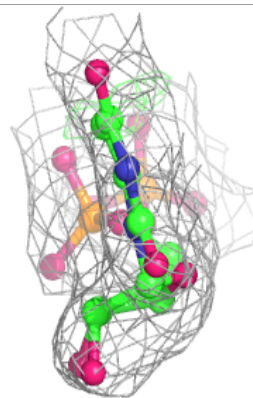
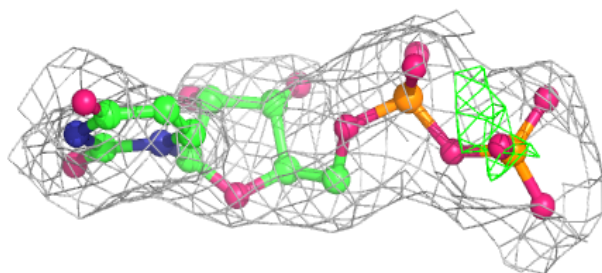
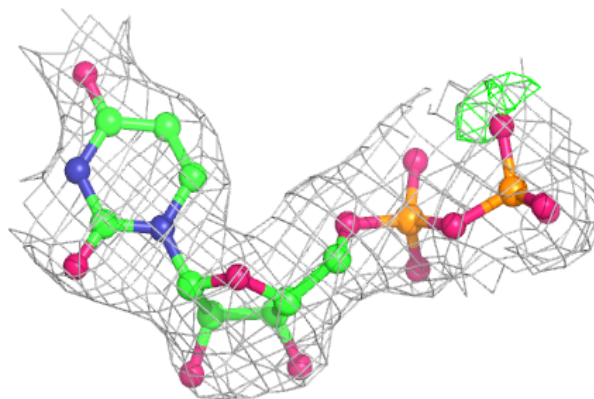
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AC2	D	601	16/16	0.78	0.18	53,54,56,56	0
2	AC2	A	301	16/16	0.81	0.19	61,62,65,65	0
3	UDP	D	261	25/25	0.86	0.13	45,51,59,59	0
3	UDP	C	501	25/25	0.87	0.15	53,59,61,61	0
2	AC2	B	401	16/16	0.92	0.13	41,44,46,46	0
3	UDP	A	261	25/25	0.96	0.12	29,37,38,39	0
3	UDP	B	261	25/25	0.97	0.13	21,31,33,34	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.

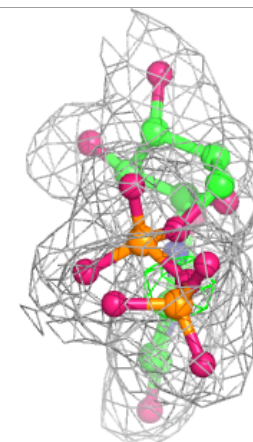
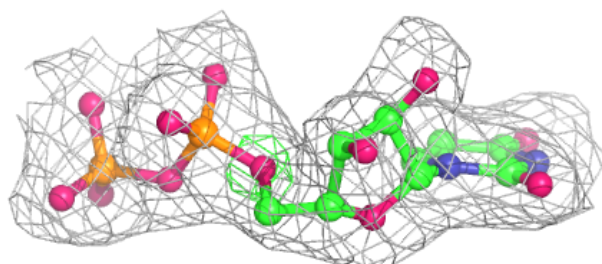
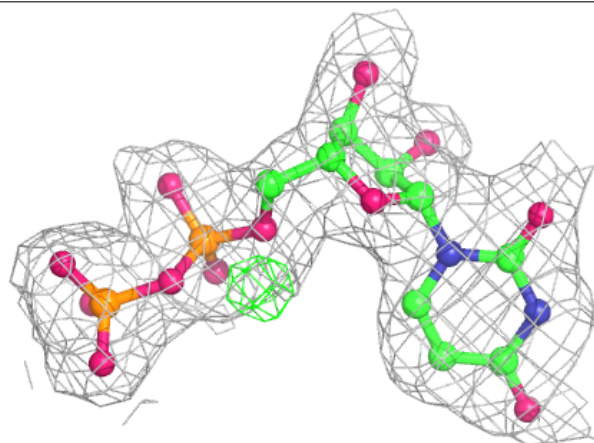


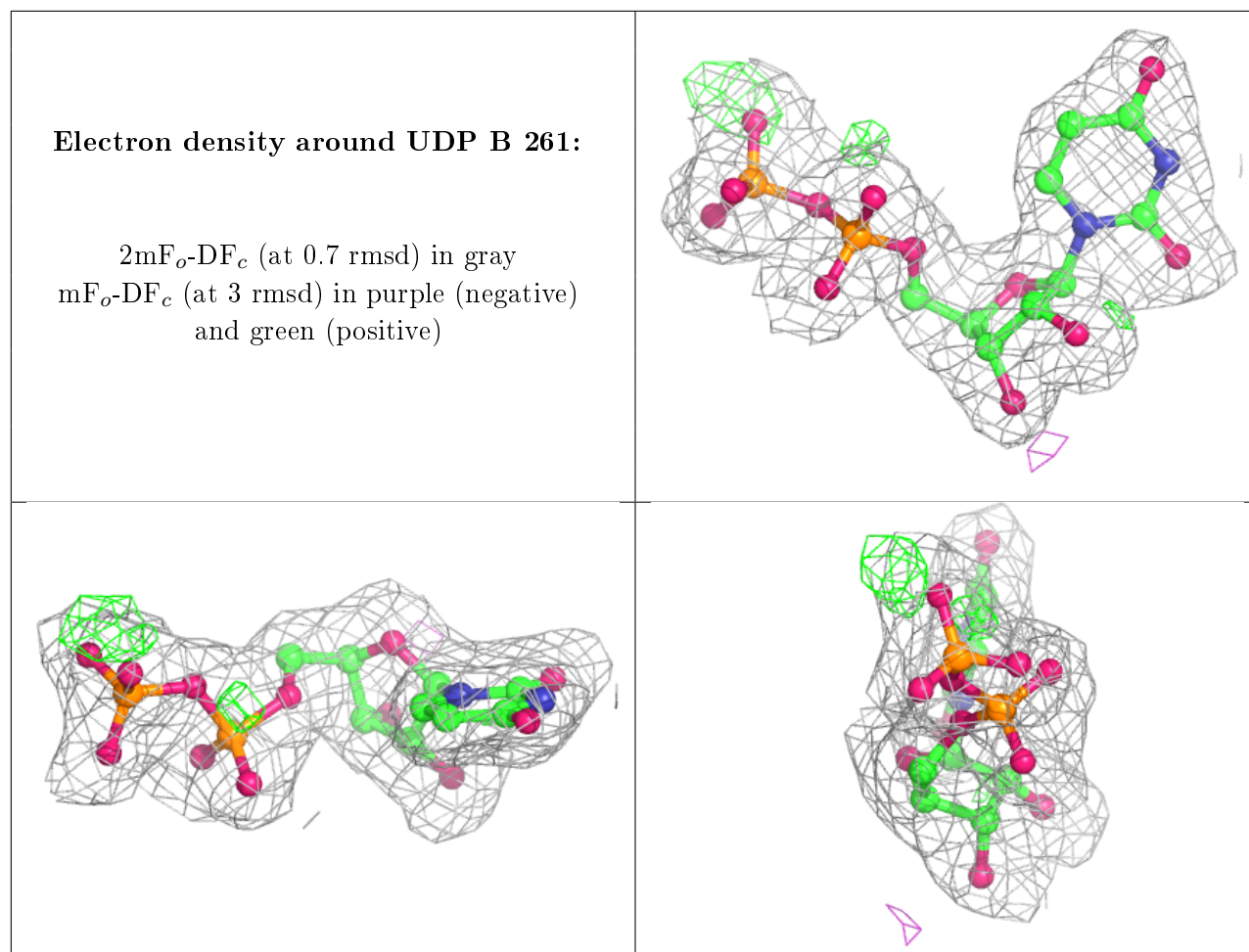
Electron density around UDP C 501:

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

**Electron density around UDP A 261:**

$2mF_o-DF_c$ (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.