Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 02:56 am GMT

PDB ID	:	5MQL
Title	:	Crystal structure of dCK mutant C3S in complex with masitinib and UDP
Authors	:	Rebuffet, E.; Hammam, K.; Saez-Ayala, M.; Gros, L.; Lopez, S.; Hajem, B.; Humbert, M.; Baudelet, E.; Audebert, S.; Betzi, S.; Lugari, A.; Combes, S.; Pez, D.; Letard, S.; Mansfield, C.; Moussy, A.; de Sepulveda, P.; Morelli, X.; Dubreuil, P.
Deposited on	:	2016-12-20
Resolution	:	3.25 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 (1)) were used in the production of this report:

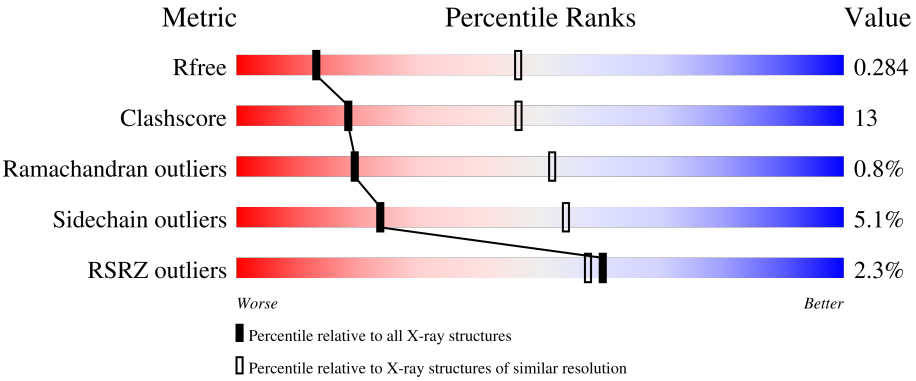
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	289	62% 17% 20%
1	B	289	3% 58% 20% 21%
1	C	289	56% 21% 21%
1	D	289	2% 58% 18% 22%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G65	A	302	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7527 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	231	Total	C	N	O	S	0	0	0
			1858	1192	305	353	8			
1	B	227	Total	C	N	O	S	0	0	0
			1806	1167	299	333	7			
1	C	228	Total	C	N	O	S	0	0	0
			1853	1190	308	348	7			
1	D	225	Total	C	N	O	S	0	0	0
			1815	1169	294	345	7			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	initiating methionine	UNP P27707
A	-27	SER	-	expression tag	UNP P27707
A	-26	TYR	-	expression tag	UNP P27707
A	-25	TYR	-	expression tag	UNP P27707
A	-24	HIS	-	expression tag	UNP P27707
A	-23	HIS	-	expression tag	UNP P27707
A	-22	HIS	-	expression tag	UNP P27707
A	-21	HIS	-	expression tag	UNP P27707
A	-20	HIS	-	expression tag	UNP P27707
A	-19	HIS	-	expression tag	UNP P27707
A	-18	LEU	-	expression tag	UNP P27707
A	-17	GLU	-	expression tag	UNP P27707
A	-16	SER	-	expression tag	UNP P27707
A	-15	THR	-	expression tag	UNP P27707
A	-14	SER	-	expression tag	UNP P27707
A	-13	LEU	-	expression tag	UNP P27707
A	-12	TYR	-	expression tag	UNP P27707
A	-11	LYS	-	expression tag	UNP P27707
A	-10	LYS	-	expression tag	UNP P27707
A	-9	ALA	-	expression tag	UNP P27707
A	-8	GLY	-	expression tag	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP P27707
A	-6	GLU	-	expression tag	UNP P27707
A	-5	ASN	-	expression tag	UNP P27707
A	-4	LEU	-	expression tag	UNP P27707
A	-3	TYR	-	expression tag	UNP P27707
A	-2	PHE	-	expression tag	UNP P27707
A	-1	GLN	-	expression tag	UNP P27707
A	0	GLY	-	expression tag	UNP P27707
A	9	SER	CYS	engineered mutation	UNP P27707
A	45	SER	CYS	engineered mutation	UNP P27707
A	59	SER	CYS	engineered mutation	UNP P27707
B	-28	MET	-	initiating methionine	UNP P27707
B	-27	SER	-	expression tag	UNP P27707
B	-26	TYR	-	expression tag	UNP P27707
B	-25	TYR	-	expression tag	UNP P27707
B	-24	HIS	-	expression tag	UNP P27707
B	-23	HIS	-	expression tag	UNP P27707
B	-22	HIS	-	expression tag	UNP P27707
B	-21	HIS	-	expression tag	UNP P27707
B	-20	HIS	-	expression tag	UNP P27707
B	-19	HIS	-	expression tag	UNP P27707
B	-18	LEU	-	expression tag	UNP P27707
B	-17	GLU	-	expression tag	UNP P27707
B	-16	SER	-	expression tag	UNP P27707
B	-15	THR	-	expression tag	UNP P27707
B	-14	SER	-	expression tag	UNP P27707
B	-13	LEU	-	expression tag	UNP P27707
B	-12	TYR	-	expression tag	UNP P27707
B	-11	LYS	-	expression tag	UNP P27707
B	-10	LYS	-	expression tag	UNP P27707
B	-9	ALA	-	expression tag	UNP P27707
B	-8	GLY	-	expression tag	UNP P27707
B	-7	LEU	-	expression tag	UNP P27707
B	-6	GLU	-	expression tag	UNP P27707
B	-5	ASN	-	expression tag	UNP P27707
B	-4	LEU	-	expression tag	UNP P27707
B	-3	TYR	-	expression tag	UNP P27707
B	-2	PHE	-	expression tag	UNP P27707
B	-1	GLN	-	expression tag	UNP P27707
B	0	GLY	-	expression tag	UNP P27707
B	9	SER	CYS	engineered mutation	UNP P27707
B	45	SER	CYS	engineered mutation	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
B	59	SER	CYS	engineered mutation	UNP P27707
C	-28	MET	-	initiating methionine	UNP P27707
C	-27	SER	-	expression tag	UNP P27707
C	-26	TYR	-	expression tag	UNP P27707
C	-25	TYR	-	expression tag	UNP P27707
C	-24	HIS	-	expression tag	UNP P27707
C	-23	HIS	-	expression tag	UNP P27707
C	-22	HIS	-	expression tag	UNP P27707
C	-21	HIS	-	expression tag	UNP P27707
C	-20	HIS	-	expression tag	UNP P27707
C	-19	HIS	-	expression tag	UNP P27707
C	-18	LEU	-	expression tag	UNP P27707
C	-17	GLU	-	expression tag	UNP P27707
C	-16	SER	-	expression tag	UNP P27707
C	-15	THR	-	expression tag	UNP P27707
C	-14	SER	-	expression tag	UNP P27707
C	-13	LEU	-	expression tag	UNP P27707
C	-12	TYR	-	expression tag	UNP P27707
C	-11	LYS	-	expression tag	UNP P27707
C	-10	LYS	-	expression tag	UNP P27707
C	-9	ALA	-	expression tag	UNP P27707
C	-8	GLY	-	expression tag	UNP P27707
C	-7	LEU	-	expression tag	UNP P27707
C	-6	GLU	-	expression tag	UNP P27707
C	-5	ASN	-	expression tag	UNP P27707
C	-4	LEU	-	expression tag	UNP P27707
C	-3	TYR	-	expression tag	UNP P27707
C	-2	PHE	-	expression tag	UNP P27707
C	-1	GLN	-	expression tag	UNP P27707
C	0	GLY	-	expression tag	UNP P27707
C	9	SER	CYS	engineered mutation	UNP P27707
C	45	SER	CYS	engineered mutation	UNP P27707
C	59	SER	CYS	engineered mutation	UNP P27707
D	-28	MET	-	initiating methionine	UNP P27707
D	-27	SER	-	expression tag	UNP P27707
D	-26	TYR	-	expression tag	UNP P27707
D	-25	TYR	-	expression tag	UNP P27707
D	-24	HIS	-	expression tag	UNP P27707
D	-23	HIS	-	expression tag	UNP P27707
D	-22	HIS	-	expression tag	UNP P27707
D	-21	HIS	-	expression tag	UNP P27707
D	-20	HIS	-	expression tag	UNP P27707

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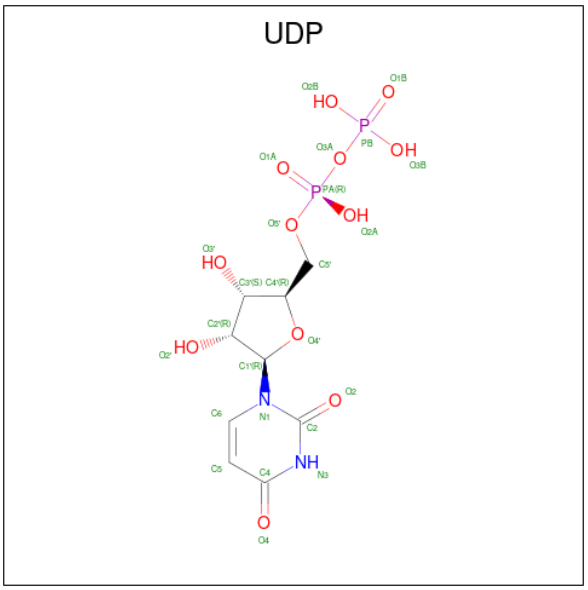
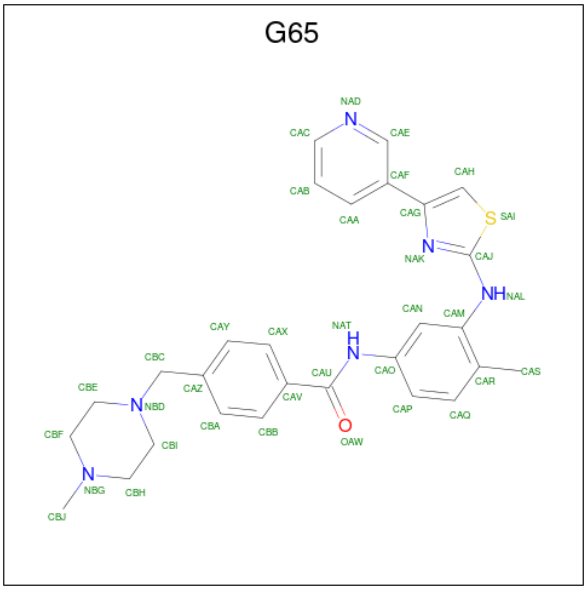
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	HIS	-	expression tag	UNP P27707
D	-18	LEU	-	expression tag	UNP P27707
D	-17	GLU	-	expression tag	UNP P27707
D	-16	SER	-	expression tag	UNP P27707
D	-15	THR	-	expression tag	UNP P27707
D	-14	SER	-	expression tag	UNP P27707
D	-13	LEU	-	expression tag	UNP P27707
D	-12	TYR	-	expression tag	UNP P27707
D	-11	LYS	-	expression tag	UNP P27707
D	-10	LYS	-	expression tag	UNP P27707
D	-9	ALA	-	expression tag	UNP P27707
D	-8	GLY	-	expression tag	UNP P27707
D	-7	LEU	-	expression tag	UNP P27707
D	-6	GLU	-	expression tag	UNP P27707
D	-5	ASN	-	expression tag	UNP P27707
D	-4	LEU	-	expression tag	UNP P27707
D	-3	TYR	-	expression tag	UNP P27707
D	-2	PHE	-	expression tag	UNP P27707
D	-1	GLN	-	expression tag	UNP P27707
D	0	GLY	-	expression tag	UNP P27707
D	9	SER	CYS	engineered mutation	UNP P27707
D	45	SER	CYS	engineered mutation	UNP P27707
D	59	SER	CYS	engineered mutation	UNP P27707

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



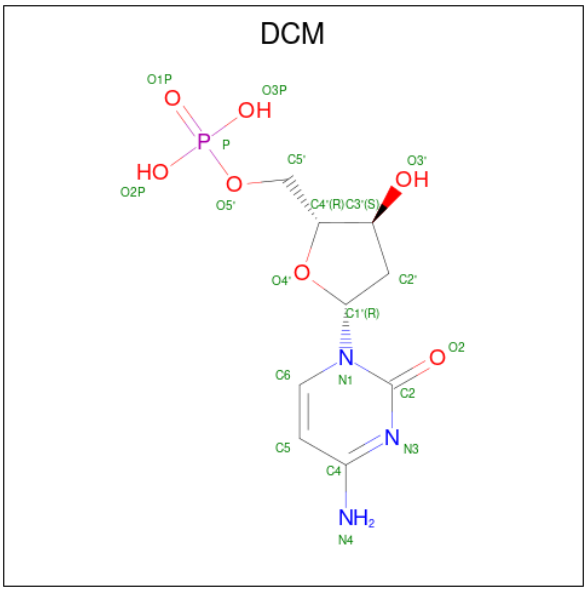
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is Masitinib (three-letter code: G65) (formula: $C_{28}H_{30}N_6OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			36	28	6	1	1		

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DCM) (formula: $C_9H_{14}N_3O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 20 9 3 7 1	0	0
4	C	1	Total C N O P 20 9 3 7 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is water.

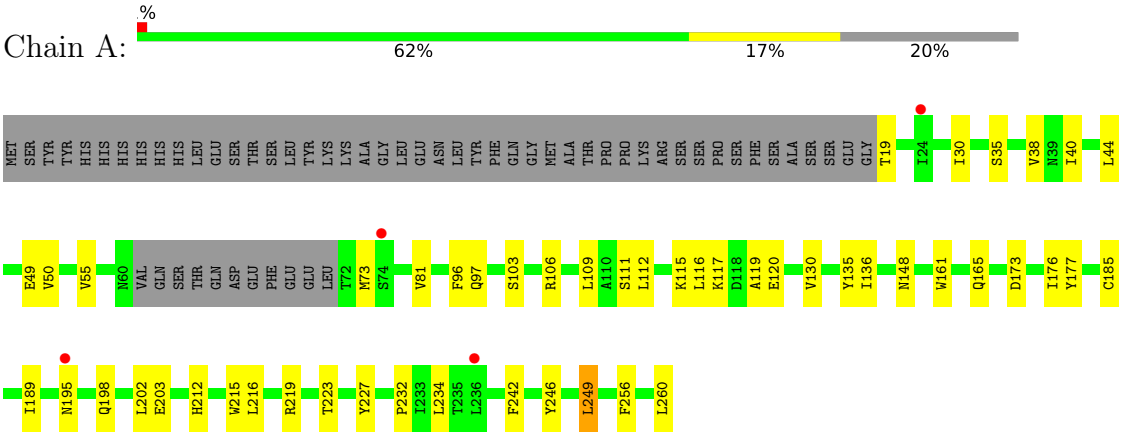
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total O 5 5	0	0
6	B	3	Total O 3 3	0	0
6	C	5	Total O 5 5	0	0
6	D	5	Total O 5 5	0	0

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.

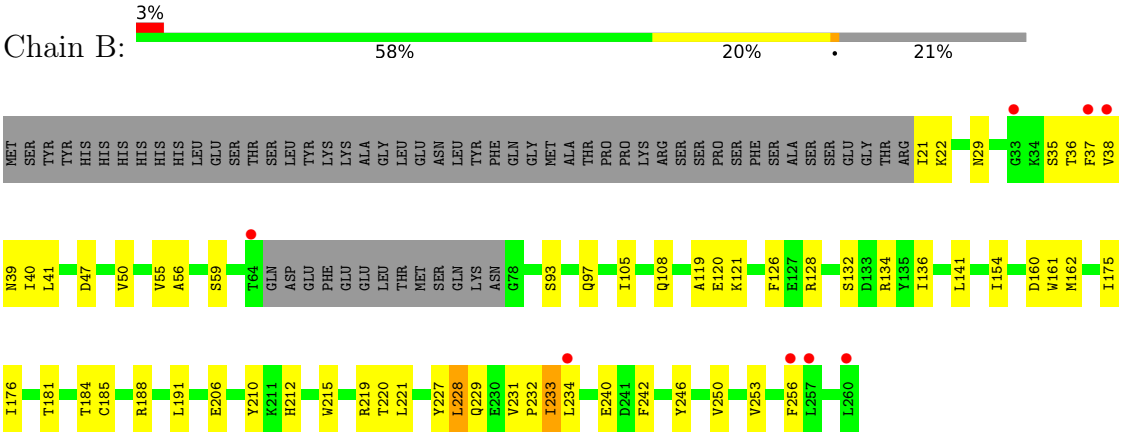
• Molecule 1: Deoxycytidine kinase

Chain A:



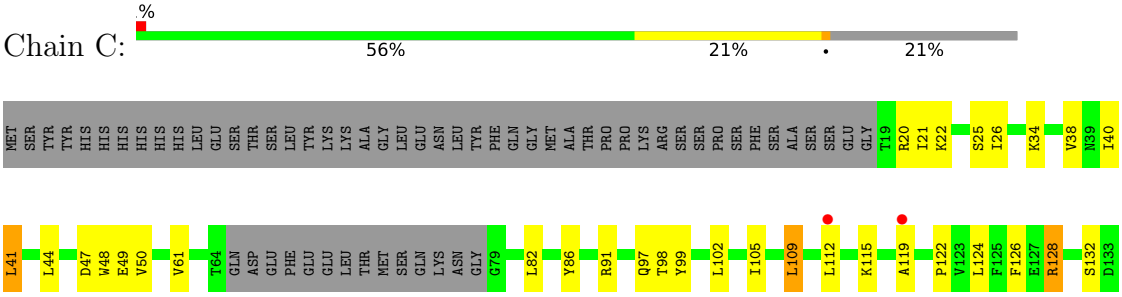
• Molecule 1: Deoxycytidine kinase

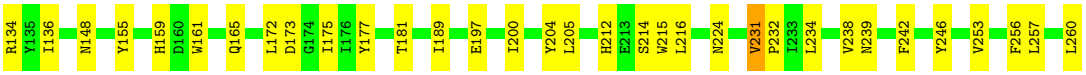
Chain B:



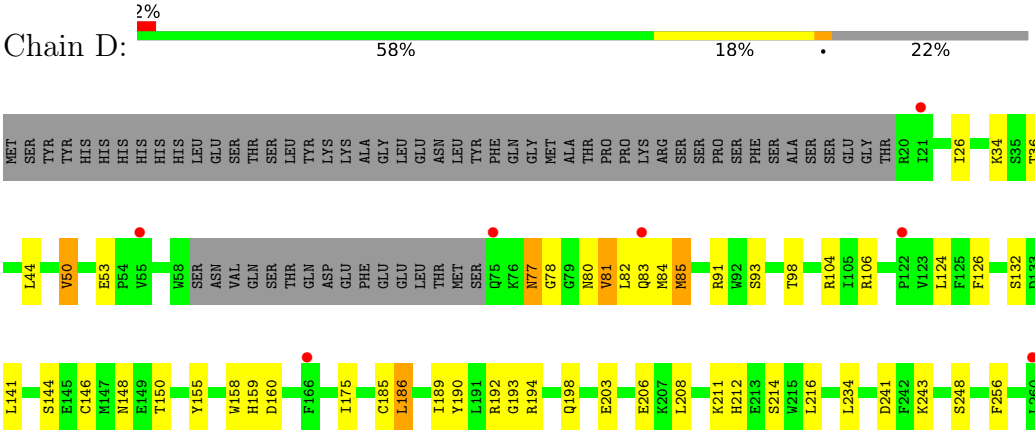
• Molecule 1: Deoxycytidine kinase

Chain C:





• Molecule 1: Deoxycytidine kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.33Å 88.33Å 342.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 3.25 47.95 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.80-3.25) 99.9 (47.95-3.25)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.215 , 0.277 0.225 , 0.284	Depositor DCC
R_{free} test set	1120 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	100.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 97.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7527	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: UDP, MG, G65, DCM

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	0.56	0/1904	0.74	0/2590
1	B	0.52	0/1852	0.72	0/2521
1	C	0.57	0/1899	0.73	0/2581
1	D	0.56	0/1861	0.73	0/2532
All	All	0.55	0/7516	0.73	0/10224

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

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	1858	0	1734	39	0
1	B	1806	0	1690	61	0
1	C	1853	0	1750	58	0
1	D	1815	0	1688	44	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	1	0
2	D	25	0	11	1	0
3	A	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	12	1	0
4	C	20	0	12	1	0
5	C	1	0	0	0	0
6	A	5	0	0	0	0
6	B	3	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
All	All	7527	0	6930	192	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 13.

All (192) 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:219:ARG:NH1	1:B:233:ILE:HD12	1.32	1.38
1:B:219:ARG:HH11	1:B:233:ILE:CD1	1.40	1.34
1:B:219:ARG:NH1	1:B:233:ILE:CD1	1.91	1.30
1:B:47:ASP:OD1	1:B:119:ALA:HB1	1.36	1.25
1:C:41:LEU:HD11	1:C:48:TRP:CZ3	1.80	1.15
1:D:85:MET:CE	1:D:93:SER:HA	1.85	1.06
1:B:47:ASP:OD1	1:B:119:ALA:CB	2.05	1.04
1:B:35:SER:O	1:B:38:VAL:HG12	1.56	1.02
1:C:41:LEU:HD11	1:C:48:TRP:HZ3	1.12	0.98
1:A:49:GLU:HB2	1:A:116:LEU:HD11	1.46	0.97
1:D:85:MET:HE3	1:D:93:SER:HA	1.45	0.95
1:B:21:ILE:HG22	1:B:21:ILE:O	1.70	0.90
1:C:41:LEU:CD1	1:C:48:TRP:HZ3	1.89	0.85
1:B:219:ARG:HH12	1:B:233:ILE:HD12	1.37	0.85
1:C:41:LEU:CD1	1:C:48:TRP:CZ3	2.60	0.85
1:B:219:ARG:NH1	1:B:233:ILE:HD13	1.92	0.84
1:D:85:MET:HE2	1:D:93:SER:HA	1.59	0.82
1:C:38:VAL:HG11	1:C:50:VAL:HG11	1.62	0.81
1:C:38:VAL:CG1	1:C:50:VAL:HG11	2.10	0.80
1:C:41:LEU:HD12	1:C:41:LEU:O	1.81	0.79
1:B:219:ARG:HH11	1:B:233:ILE:HD12	1.04	0.78
1:B:38:VAL:HG22	1:B:50:VAL:HG21	1.65	0.78
1:D:194:ARG:O	1:D:198:GLN:HG2	1.84	0.78
1:A:97:GLN:HE22	3:A:302:G65:CAE	1.98	0.76
1:A:203:GLU:N	1:A:203:GLU:OE2	2.21	0.74
1:D:85:MET:CE	1:D:93:SER:CA	2.65	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HD13	1:A:246:TYR:CG	2.24	0.72
1:A:202:LEU:HD12	1:A:202:LEU:O	1.90	0.71
1:C:197:GLU:O	1:C:200:ILE:HG13	1.91	0.71
1:B:35:SER:C	1:B:38:VAL:HG12	2.12	0.70
1:B:35:SER:HA	1:B:38:VAL:CG1	2.21	0.69
1:B:108:GLN:NE2	1:B:126:PHE:HB3	2.06	0.69
1:B:97:GLN:HE22	4:B:302:DCM:HN41	1.41	0.69
1:C:61:VAL:HG11	1:D:150:THR:HG23	1.74	0.69
1:D:85:MET:HE2	1:D:93:SER:CA	2.23	0.69
1:A:185:CYS:O	1:A:189:ILE:HG13	1.93	0.69
1:B:35:SER:HA	1:B:38:VAL:HG12	1.75	0.68
1:C:175:ILE:HG21	1:C:216:LEU:HD22	1.76	0.67
1:D:134:ARG:NH1	1:D:160:ASP:OD1	2.28	0.67
1:A:232:PRO:HG2	1:A:260:LEU:CD2	2.24	0.66
1:B:219:ARG:HH11	1:B:233:ILE:HD11	1.52	0.66
1:A:173:ASP:O	1:A:260:LEU:HD22	1.95	0.66
1:C:44:LEU:HD23	1:C:44:LEU:N	2.10	0.66
1:B:105:ILE:HD13	1:B:162:MET:HE3	1.76	0.65
1:B:38:VAL:HG22	1:B:50:VAL:CG2	2.26	0.65
1:A:232:PRO:HG2	1:A:260:LEU:HD21	1.77	0.65
1:C:41:LEU:HD21	1:C:253:VAL:HG11	1.79	0.65
1:D:93:SER:OG	1:D:141:LEU:HD13	1.97	0.64
1:B:21:ILE:O	1:B:21:ILE:CG2	2.44	0.63
1:A:40:ILE:HD13	1:A:246:TYR:CD2	2.34	0.62
1:D:80:ASN:O	1:D:83:GLN:N	2.34	0.61
1:B:35:SER:CA	1:B:38:VAL:HG12	2.32	0.59
1:C:38:VAL:HG11	1:C:50:VAL:CG1	2.34	0.58
1:C:238:VAL:HG23	1:C:238:VAL:O	2.01	0.58
1:C:136:ILE:HD11	1:C:215:TRP:HE3	1.68	0.57
1:C:161:TRP:CD1	1:D:106:ARG:HD3	2.39	0.57
1:B:108:GLN:NE2	1:B:126:PHE:CG	2.73	0.57
1:B:38:VAL:HG13	1:B:39:ASN:N	2.18	0.57
1:C:38:VAL:HG13	1:C:50:VAL:HG21	1.87	0.57
1:C:161:TRP:CD1	1:D:106:ARG:CD	2.88	0.57
1:B:121:LYS:HG3	1:B:121:LYS:O	2.06	0.56
1:B:38:VAL:CG1	1:B:39:ASN:N	2.69	0.56
1:C:246:TYR:CD1	1:C:246:TYR:N	2.73	0.56
1:D:193:GLY:O	1:D:194:ARG:C	2.45	0.54
1:D:26:ILE:HG13	1:D:38:VAL:HG23	1.88	0.54
1:A:109:LEU:HA	1:A:112:LEU:HD12	1.90	0.53
1:B:47:ASP:OD1	1:B:119:ALA:HB3	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:O	1:C:109:LEU:HB2	2.09	0.52
1:C:41:LEU:CD1	1:C:48:TRP:CE3	2.92	0.52
1:C:189:ILE:HD12	1:C:205:LEU:HD11	1.91	0.52
1:A:177:TYR:HB2	1:A:216:LEU:HD13	1.92	0.52
1:B:40:ILE:HD13	1:B:246:TYR:CD2	2.44	0.52
1:C:38:VAL:CG1	1:C:50:VAL:CG1	2.87	0.52
1:A:116:LEU:O	1:A:117:LYS:C	2.47	0.52
1:D:81:VAL:CG1	1:D:82:LEU:N	2.73	0.52
1:D:136:ILE:HG21	1:D:212:HIS:CE1	2.45	0.52
1:C:97:GLN:HE22	4:C:303:DCM:HN41	1.59	0.51
1:B:232:PRO:HB2	1:B:256:PHE:HE1	1.76	0.51
1:D:77:ASN:ND2	1:D:77:ASN:H	2.08	0.51
1:C:41:LEU:HD11	1:C:48:TRP:CE3	2.43	0.51
1:A:116:LEU:HD23	1:A:116:LEU:N	2.26	0.50
1:C:21:ILE:HG23	1:C:122:PRO:HB2	1.93	0.50
1:C:41:LEU:HD12	1:C:41:LEU:C	2.31	0.50
1:B:227:TYR:CD1	1:B:227:TYR:C	2.85	0.50
1:C:119:ALA:HB3	1:C:122:PRO:HB3	1.94	0.50
1:A:81:VAL:HG12	1:A:96:PHE:HD1	1.76	0.49
1:A:136:ILE:HD13	1:A:212:HIS:CE1	2.47	0.49
1:C:242:PHE:CD1	2:C:302:UDP:O4	2.65	0.49
1:A:116:LEU:O	1:A:119:ALA:HB3	2.12	0.49
1:C:161:TRP:CD1	1:D:106:ARG:HD2	2.48	0.49
1:B:40:ILE:HD12	1:B:41:LEU:HD23	1.94	0.48
1:B:108:GLN:HE22	1:B:126:PHE:HB3	1.77	0.48
1:D:134:ARG:NH2	1:D:135:TYR:OH	2.45	0.48
1:D:77:ASN:ND2	1:D:77:ASN:N	2.60	0.48
1:A:44:LEU:N	1:A:44:LEU:HD23	2.28	0.48
1:B:128:ARG:HD3	1:B:132:SER:OG	2.14	0.48
1:D:36:THR:O	1:D:40:ILE:HG13	2.13	0.48
1:B:234:LEU:HD13	1:B:256:PHE:HB2	1.95	0.48
1:B:215:TRP:HB2	1:B:221:LEU:HD22	1.96	0.47
1:B:250:VAL:HA	1:B:253:VAL:HG12	1.95	0.47
1:D:132:SER:HA	1:D:136:ILE:HD13	1.95	0.47
1:A:81:VAL:HG12	1:A:96:PHE:CD1	2.50	0.47
1:C:49:GLU:HB3	1:C:124:LEU:HD12	1.97	0.47
1:A:116:LEU:O	1:A:119:ALA:N	2.48	0.47
1:D:234:LEU:HD13	1:D:256:PHE:HB2	1.97	0.47
1:A:81:VAL:HG11	1:A:96:PHE:HA	1.96	0.47
1:B:56:ALA:HA	1:B:59:SER:HB2	1.96	0.47
1:C:173:ASP:O	1:C:260:LEU:HD22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PHE:HB2	1:A:249:LEU:HD21	1.96	0.46
1:D:26:ILE:HG22	1:D:34:LYS:HG2	1.98	0.46
1:C:200:ILE:HG23	1:C:204:TYR:HD2	1.80	0.46
1:D:134:ARG:HD3	1:D:159:HIS:ND1	2.31	0.46
1:B:188:ARG:HA	1:B:191:LEU:HD12	1.98	0.45
1:C:38:VAL:HG13	1:C:50:VAL:CG2	2.47	0.45
1:A:106:ARG:HG3	1:B:161:TRP:NE1	2.32	0.45
1:C:181:THR:HG23	1:C:239:ASN:HD21	1.81	0.45
1:C:136:ILE:HG21	1:C:212:HIS:CE1	2.52	0.45
1:A:35:SER:HA	1:A:38:VAL:HG22	1.98	0.45
1:A:176:ILE:HG12	1:A:234:LEU:HD23	1.99	0.45
1:C:91:ARG:CD	1:D:91:ARG:HD3	2.47	0.45
1:C:132:SER:O	1:C:136:ILE:HB	2.17	0.45
1:C:134:ARG:HB2	1:C:159:HIS:CD2	2.52	0.44
1:D:203:GLU:HA	1:D:206:GLU:HG2	1.99	0.44
1:D:185:CYS:O	1:D:189:ILE:HG12	2.17	0.44
1:A:161:TRP:CZ2	1:A:165:GLN:HG3	2.52	0.44
1:B:108:GLN:NE2	1:B:126:PHE:CB	2.78	0.44
1:A:115:LYS:O	1:A:116:LEU:C	2.56	0.44
1:C:136:ILE:HD11	1:C:215:TRP:CE3	2.51	0.44
1:C:161:TRP:NE1	1:D:106:ARG:HD3	2.31	0.44
1:C:161:TRP:O	1:C:165:GLN:HG2	2.18	0.44
1:C:200:ILE:CG2	1:C:204:TYR:HD2	2.31	0.44
1:B:93:SER:HB3	1:B:141:LEU:HD13	1.99	0.44
1:C:34:LYS:HE3	1:C:128:ARG:CZ	2.48	0.44
1:C:200:ILE:HG23	1:C:204:TYR:CD2	2.53	0.43
1:B:134:ARG:NH1	1:B:160:ASP:OD1	2.44	0.43
1:D:38:VAL:HG13	1:D:50:VAL:HG11	2.00	0.43
1:A:135:TYR:CE2	1:A:223:THR:HB	2.53	0.43
1:B:175:ILE:O	1:B:233:ILE:HA	2.17	0.43
1:A:97:GLN:NE2	3:A:302:G65:CAE	2.73	0.43
1:B:29:ASN:HB3	1:B:185:CYS:SG	2.59	0.43
1:C:47:ASP:O	1:C:122:PRO:HA	2.18	0.43
1:B:21:ILE:O	1:B:22:LYS:C	2.57	0.43
1:B:227:TYR:HE1	1:B:231:VAL:HG21	1.84	0.43
1:B:227:TYR:O	1:B:229:GLN:N	2.52	0.43
1:C:234:LEU:HD13	1:C:256:PHE:HB2	2.01	0.43
1:D:190:TYR:HA	1:D:198:GLN:HE22	1.83	0.43
1:B:35:SER:O	1:B:38:VAL:CG1	2.47	0.43
1:C:82:LEU:HD11	1:C:86:TYR:HE2	1.84	0.43
1:B:47:ASP:CG	1:B:120:GLU:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HG23	1:C:99:TYR:CE2	2.54	0.42
1:D:175:ILE:HG21	1:D:216:LEU:HD22	2.01	0.42
1:A:40:ILE:CD1	1:A:246:TYR:CD2	3.01	0.42
1:B:35:SER:HA	1:B:38:VAL:HG11	1.96	0.42
1:B:36:THR:O	1:B:40:ILE:HG23	2.19	0.42
1:B:206:GLU:HG2	1:B:210:TYR:CE2	2.54	0.42
1:C:124:LEU:HD23	1:C:126:PHE:HE1	1.84	0.42
1:A:30:ILE:O	1:A:185:CYS:HB3	2.20	0.42
1:B:176:ILE:HG12	1:B:234:LEU:HD23	2.01	0.42
1:D:77:ASN:HD22	1:D:78:GLY:H	1.67	0.42
1:D:80:ASN:O	1:D:81:VAL:C	2.55	0.42
1:D:81:VAL:HA	1:D:84:MET:HB2	2.00	0.42
1:A:81:VAL:CG1	1:A:96:PHE:HB2	2.49	0.42
1:D:192:ARG:HD3	2:D:500:UDP:H5'1	2.01	0.42
1:A:106:ARG:HG3	1:B:161:TRP:CD1	2.55	0.42
1:A:81:VAL:CG1	1:A:96:PHE:HD1	2.33	0.42
1:D:124:LEU:HD23	1:D:126:PHE:HE1	1.84	0.42
1:A:195:ASN:HA	1:A:198:GLN:HG2	2.02	0.42
1:A:232:PRO:HB2	1:A:256:PHE:HE1	1.84	0.42
1:C:25:SER:HB2	1:C:172:LEU:HD22	2.02	0.42
1:D:40:ILE:O	1:D:44:LEU:HG	2.19	0.42
1:A:215:TRP:O	1:A:219:ARG:HA	2.19	0.41
1:B:227:TYR:CD1	1:B:228:LEU:N	2.89	0.41
1:A:81:VAL:HG23	1:B:154:ILE:HD11	2.02	0.41
1:B:108:GLN:HE21	1:B:126:PHE:HB3	1.82	0.41
1:C:242:PHE:CD1	1:C:242:PHE:N	2.86	0.41
1:B:242:PHE:O	1:B:246:TYR:HB3	2.21	0.41
1:C:231:VAL:HA	1:C:232:PRO:HD3	1.88	0.41
1:B:38:VAL:HG21	1:B:50:VAL:CG1	2.51	0.41
1:B:136:ILE:HD13	1:B:212:HIS:CE1	2.56	0.41
1:C:177:TYR:HB2	1:C:216:LEU:HD13	2.03	0.41
1:C:98:THR:HG22	1:C:155:TYR:HD1	1.86	0.41
1:C:148:ASN:ND2	1:D:84:MET:HE1	2.36	0.41
1:D:53:GLU:HG3	1:D:104:ARG:HH22	1.86	0.41
1:D:155:TYR:O	1:D:158:TRP:HB3	2.21	0.41
1:A:55:VAL:HG21	3:A:302:G65:CAA	2.50	0.40
1:B:37:PHE:O	1:B:40:ILE:HG13	2.21	0.40
1:D:81:VAL:HG13	1:D:82:LEU:N	2.36	0.40
1:B:219:ARG:CZ	1:B:233:ILE:HD13	2.49	0.40
1:D:85:MET:CE	1:D:93:SER:CB	2.99	0.40
1:D:186:LEU:HD22	1:D:190:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:O	1:C:20:ARG:HG2	2.21	0.40
1:C:22:LYS:HA	1:C:173:ASP:OD2	2.21	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	227/289 (78%)	202 (89%)	24 (11%)	1 (0%)	34	67
1	B	223/289 (77%)	200 (90%)	21 (9%)	2 (1%)	17	50
1	C	224/289 (78%)	209 (93%)	13 (6%)	2 (1%)	17	50
1	D	221/289 (76%)	188 (85%)	31 (14%)	2 (1%)	17	50
All	All	895/1156 (77%)	799 (89%)	89 (10%)	7 (1%)	19	52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	ARG
1	C	115	LYS
1	A	120	GLU
1	B	228	LEU
1	D	241	ASP
1	D	243	LYS
1	B	55	VAL

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	195/265 (74%)	186 (95%)	9 (5%)	27	57
1	B	185/265 (70%)	180 (97%)	5 (3%)	44	70
1	C	196/265 (74%)	186 (95%)	10 (5%)	24	54
1	D	189/265 (71%)	174 (92%)	15 (8%)	12	37
All	All	765/1060 (72%)	726 (95%)	39 (5%)	24	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	50	VAL
1	A	73	MET
1	A	103	SER
1	A	111	SER
1	A	130	VAL
1	A	148	ASN
1	A	227	TYR
1	A	249	LEU
1	B	181	THR
1	B	184	THR
1	B	220	THR
1	B	233	ILE
1	B	240	GLU
1	C	26	ILE
1	C	40	ILE
1	C	41	LEU
1	C	102	LEU
1	C	109	LEU
1	C	112	LEU
1	C	214	SER
1	C	224	ASN
1	C	231	VAL
1	C	257	LEU
1	D	39	ASN
1	D	40	ILE
1	D	50	VAL
1	D	77	ASN
1	D	81	VAL
1	D	85	MET

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Mol	Chain	Res	Type
1	D	98	THR
1	D	144	SER
1	D	146	CYS
1	D	148	ASN
1	D	186	LEU
1	D	208	LEU
1	D	211	LYS
1	D	214	SER
1	D	248	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	B	97	GLN
1	B	108	GLN
1	B	163	ASN
1	B	212	HIS
1	C	97	GLN
1	C	108	GLN
1	C	148	ASN
1	C	156	GLN
1	D	77	ASN
1	D	97	GLN
1	D	218	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)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	D	500	-	24,26,26	0.40	0	37,40,40	0.74	1 (2%)
2	UDP	B	301	-	24,26,26	0.41	0	37,40,40	0.45	0
2	UDP	A	301	-	24,26,26	0.53	0	37,40,40	0.59	0
3	G65	A	302	-	37,40,40	2.41	7 (18%)	49,55,55	1.64	9 (18%)
4	DCM	B	302	-	21,21,21	0.49	0	31,31,31	0.53	0
4	DCM	C	303	5	21,21,21	0.61	0	31,31,31	0.43	0
2	UDP	C	302	-	24,26,26	0.39	0	37,40,40	0.44	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	D	500	-	-	0/16/32/32	0/2/2/2
2	UDP	B	301	-	-	0/16/32/32	0/2/2/2
2	UDP	A	301	-	-	0/16/32/32	0/2/2/2
3	G65	A	302	-	-	8/18/30/30	0/5/5/5
4	DCM	B	302	-	-	4/10/22/22	0/2/2/2
4	DCM	C	303	5	-	4/10/22/22	0/2/2/2
2	UDP	C	302	-	-	6/16/32/32	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	G65	CAF-CAG	-8.15	1.36	1.48
3	A	302	G65	CBC-CAZ	-6.37	1.40	1.51
3	A	302	G65	CAS-CAR	-5.94	1.39	1.51
3	A	302	G65	CAV-CAU	-5.23	1.39	1.50
3	A	302	G65	CAO-NAT	-3.64	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	G65	CAE-NAD	3.46	1.41	1.34
3	A	302	G65	CAC-NAD	2.32	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	G65	CBH-NBG-CBF	4.43	115.71	109.52
3	A	302	G65	CAH-CAG-CAF	-4.25	123.53	129.44
3	A	302	G65	CAS-CAR-CAM	3.58	125.31	121.25
3	A	302	G65	CBJ-NBG-CBH	-3.21	105.86	110.66
3	A	302	G65	CAG-CAH-SAI	-2.95	108.17	111.79
2	D	500	UDP	O2B-PB-O3A	2.90	114.35	104.64
3	A	302	G65	CBE-CBF-NBG	2.64	113.79	110.80
3	A	302	G65	CAS-CAR-CAQ	-2.32	115.79	120.31
3	A	302	G65	CAO-NAT-CAU	-2.29	120.64	126.58
3	A	302	G65	CAR-CAM-NAL	2.09	122.66	118.70

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	UDP	C5'-O5'-PA-O1A
2	C	302	UDP	PA-O3A-PB-O3B
4	B	302	DCM	C5'-O5'-P-O2P
4	B	302	DCM	C5'-O5'-P-O3P
4	C	303	DCM	C5'-O5'-P-O1P
4	C	303	DCM	C5'-O5'-P-O3P
3	A	302	G65	CAZ-CBC-NBD-CBE
3	A	302	G65	CAZ-CBC-NBD-CBI
3	A	302	G65	OAW-CAU-CAV-CAX
3	A	302	G65	NAT-CAU-CAV-CAX
3	A	302	G65	CAN-CAO-NAT-CAU
3	A	302	G65	NAT-CAU-CAV-CBB
3	A	302	G65	OAW-CAU-CAV-CBB
3	A	302	G65	CAP-CAO-NAT-CAU
4	B	302	DCM	C5'-O5'-P-O1P
4	C	303	DCM	O4'-C4'-C5'-O5'
2	C	302	UDP	PA-O3A-PB-O2B
2	C	302	UDP	C5'-O5'-PA-O3A
2	C	302	UDP	C5'-O5'-PA-O2A
4	B	302	DCM	C3'-C4'-C5'-O5'
4	C	303	DCM	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	C	302	UDP	C4'-C5'-O5'-PA

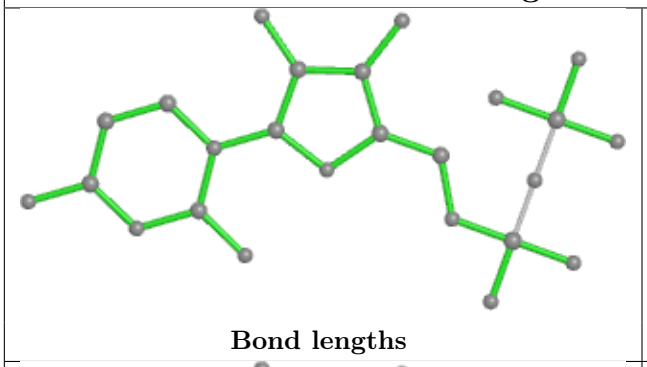
There are no ring outliers.

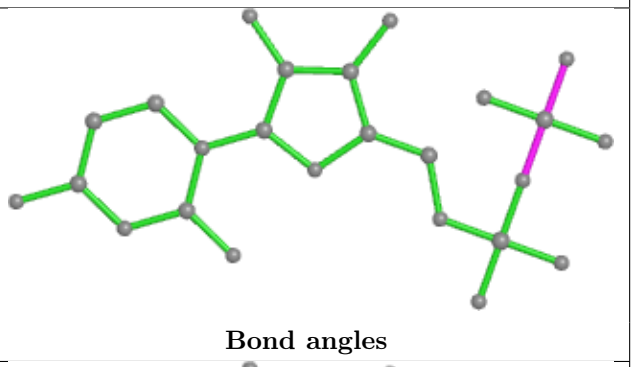
5 monomers are involved in 7 short contacts:

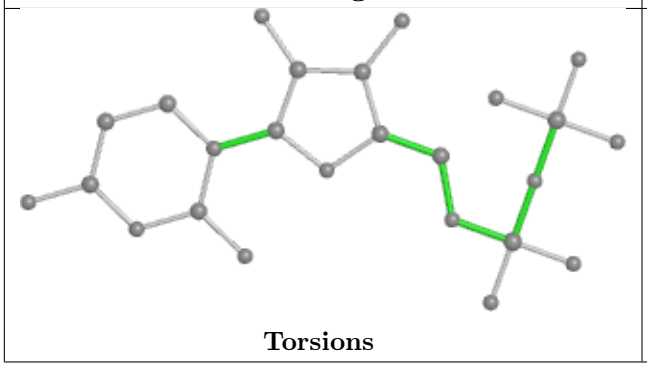
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	UDP	1	0
3	A	302	G65	3	0
4	B	302	DCM	1	0
4	C	303	DCM	1	0
2	C	302	UDP	1	0

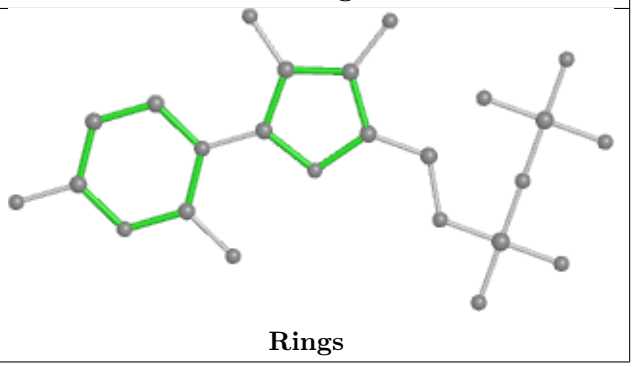
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 D 500

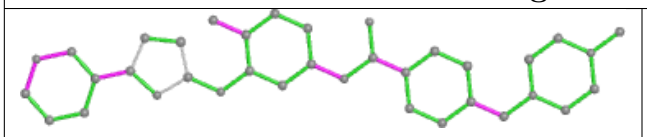

Bond lengths

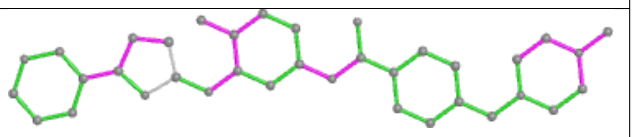

Bond angles

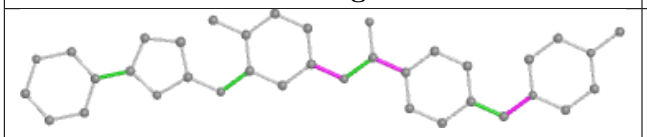

Torsions

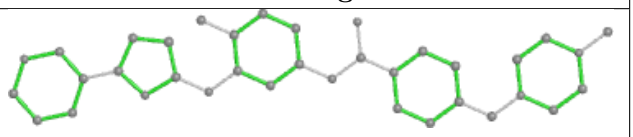

Rings

Ligand G65 A 302

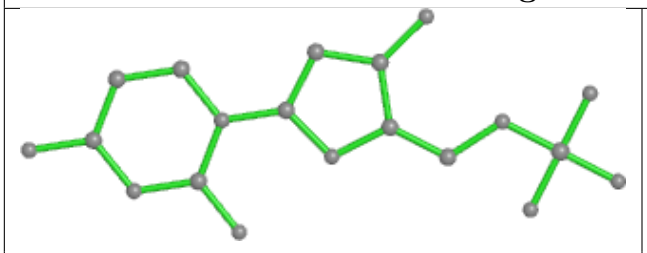

Bond lengths

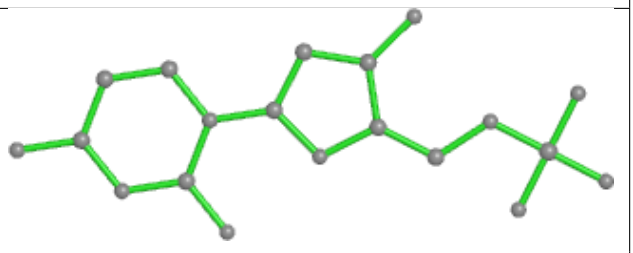

Bond angles

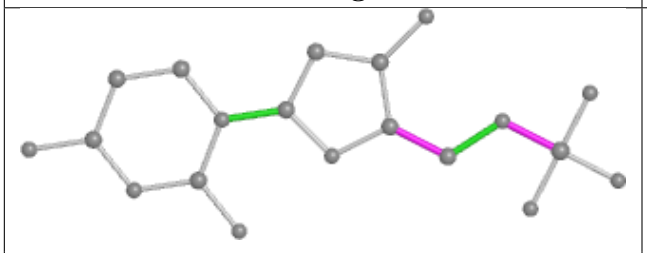

Torsions

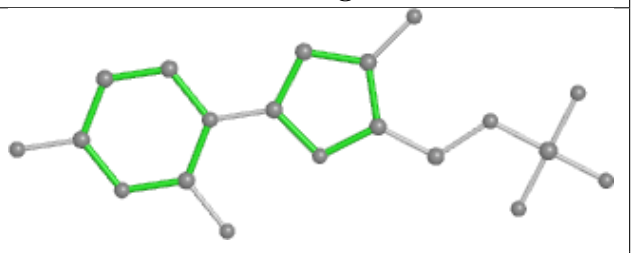

Rings

Ligand DCM B 302

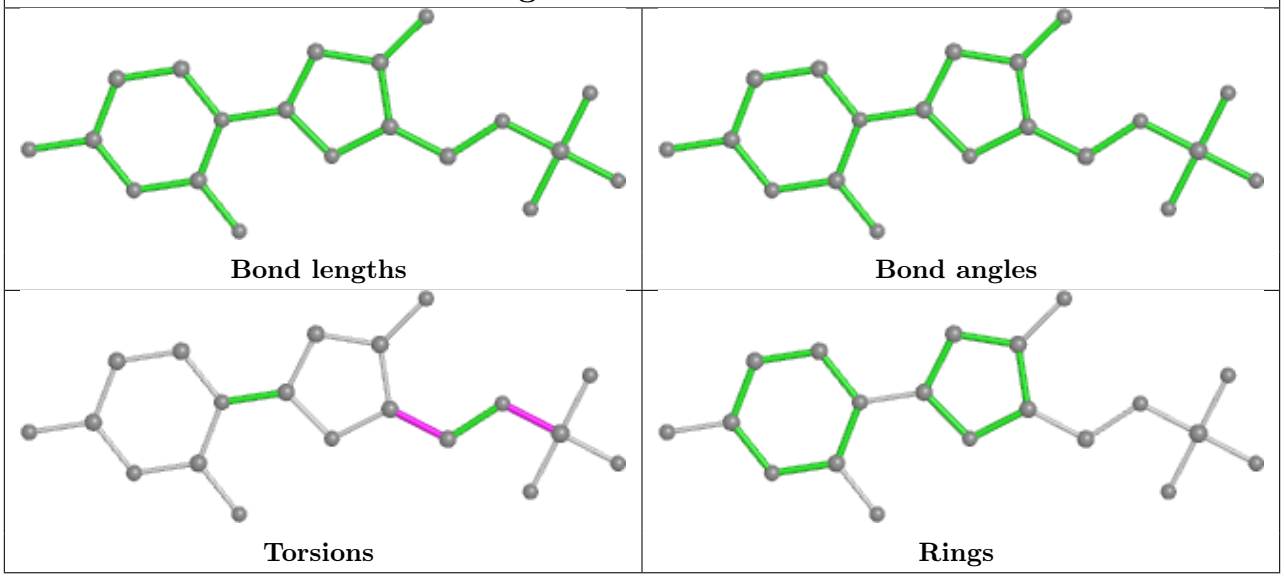

Bond lengths


Bond angles

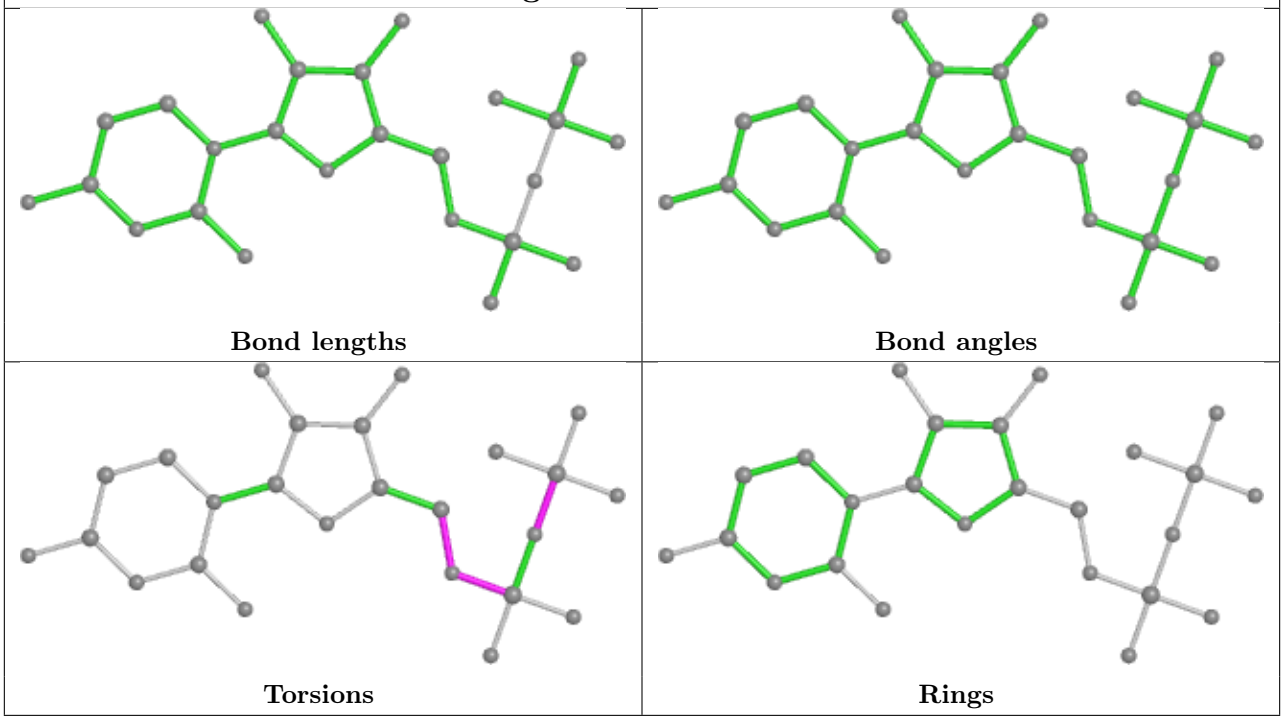

Torsions


Rings

Ligand DCM C 303



Ligand UDP C 302



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	231/289 (79%)	0.13	4 (1%)	70	67	75, 99, 128, 153	0
1	B	227/289 (78%)	0.41	8 (3%)	44	40	70, 96, 134, 145	0
1	C	228/289 (78%)	-0.03	2 (0%)	84	84	67, 88, 125, 170	0
1	D	225/289 (77%)	0.11	7 (3%)	49	47	72, 95, 127, 141	0
All	All	911/1156 (78%)	0.15	21 (2%)	60	58	67, 95, 129, 170	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	PHE	3.7
1	B	260	LEU	3.4
1	D	55	VAL	3.3
1	B	256	PHE	3.1
1	B	234	LEU	3.0
1	A	195	ASN	2.8
1	B	64	THR	2.7
1	A	24	ILE	2.7
1	B	257	LEU	2.6
1	D	75	GLN	2.5
1	C	112	LEU	2.5
1	D	83	GLN	2.3
1	D	21	ILE	2.3
1	A	74	SER	2.3
1	D	166	PHE	2.3
1	B	33	GLY	2.2
1	D	122	PRO	2.2
1	C	119	ALA	2.2
1	B	38	VAL	2.1
1	D	260	LEU	2.1
1	A	236	LEU	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)

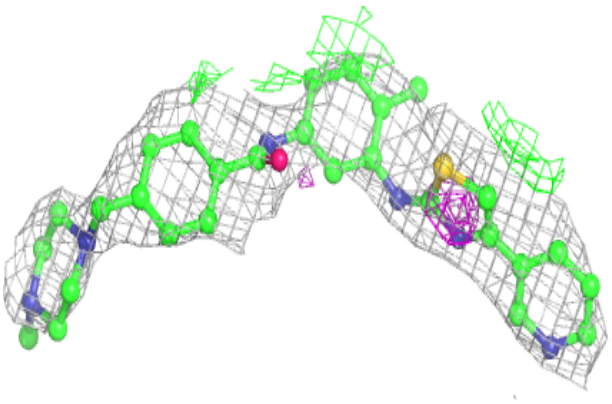
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

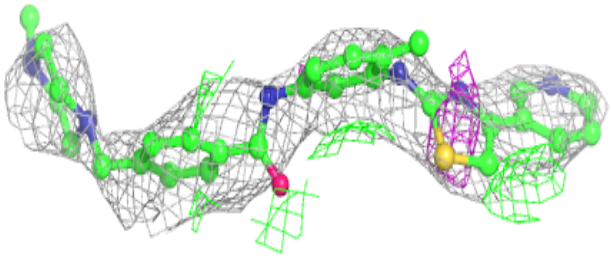
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	G65	A	302	36/36	0.75	0.43	122,133,142,143	0
4	DCM	B	302	20/20	0.90	0.27	105,114,127,129	0
2	UDP	B	301	25/25	0.93	0.24	106,109,111,111	0
2	UDP	D	500	25/25	0.93	0.21	98,100,104,106	0
2	UDP	C	302	25/25	0.94	0.23	91,95,105,107	0
2	UDP	A	301	25/25	0.94	0.26	113,119,124,125	0
5	MG	C	301	1/1	0.94	0.24	67,67,67,67	0
4	DCM	C	303	20/20	0.95	0.27	80,89,108,109	0

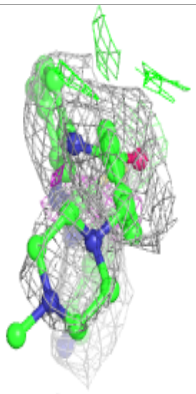
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G65 A 302:

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

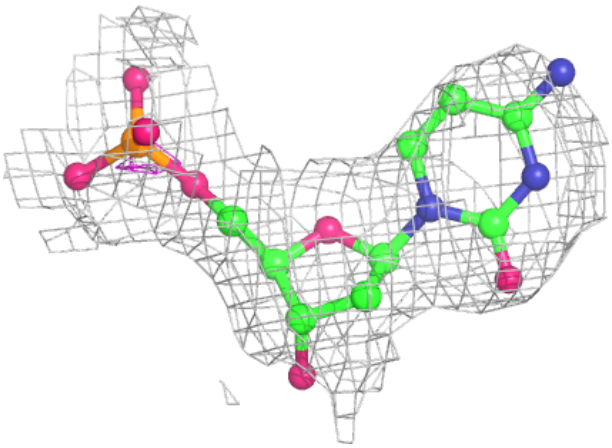


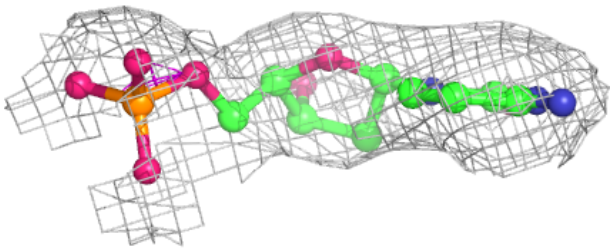


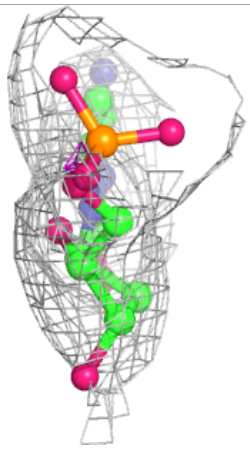


Electron density around DCM B 302:

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

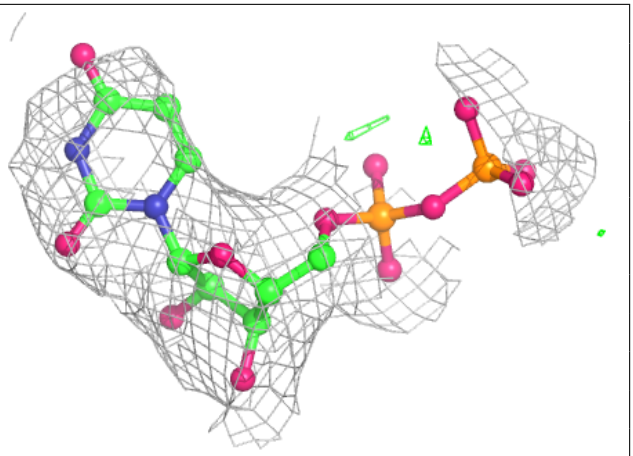


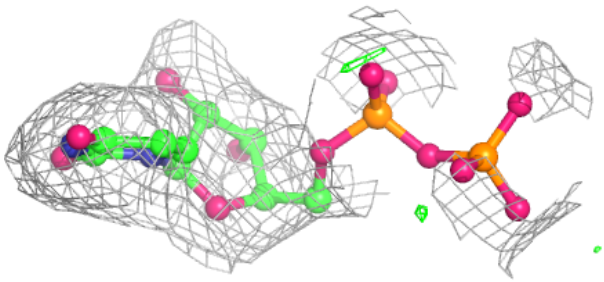


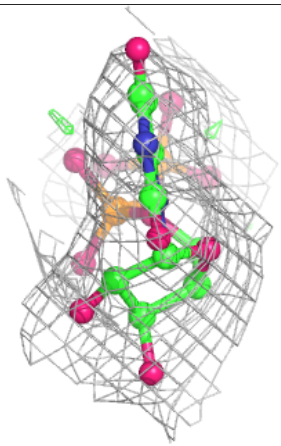


Electron density around UDP D 500:

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

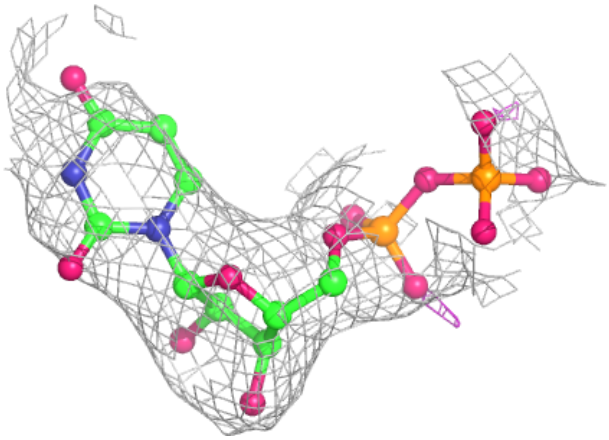


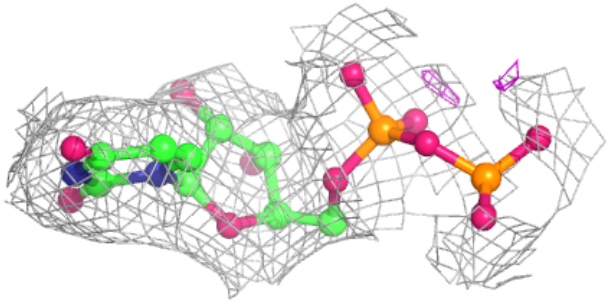


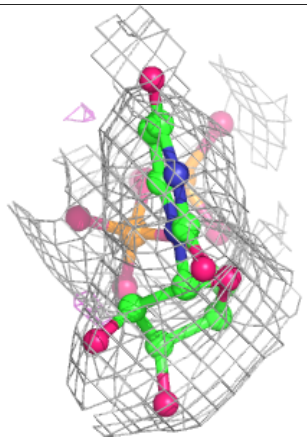


Electron density around UDP C 302:

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

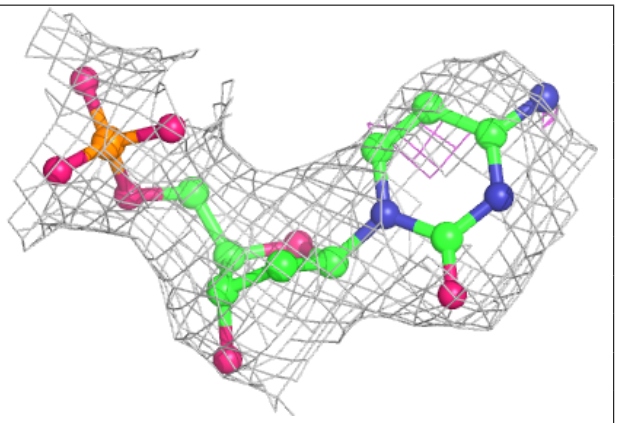


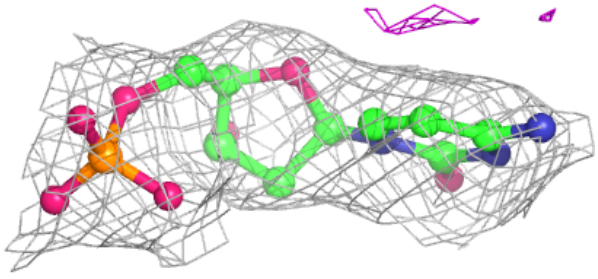


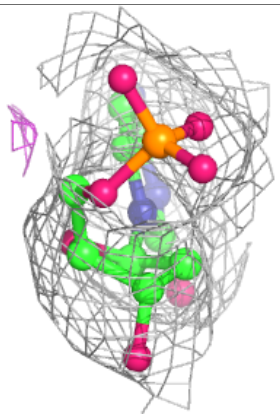


Electron density around DCM C 303:

$2mF_o$-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.