Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 04:02 PM EDT

PDB ID	:	2QRO
Title	:	Human Deoxycytidine kinase dAMP, UDP, Mg ion product complex
Authors	:	Ealick, S.E.; Soriano, E.V.
Deposited on	:	2007-07-28
Resolution	:	3.45 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:

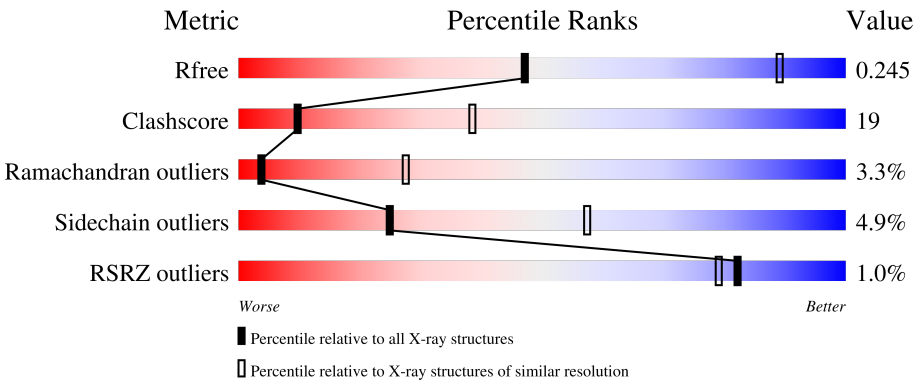
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	280	2%, 50%, 27%, •, 19%
1	B	280	49%, 28%, 5%, 19%
1	C	280	51%, 26%, 5%, 19%
1	D	280	51%, 26%, •, 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7816 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
			Total	C	N	O	S			
1	A	228	1906	1223	317	357	9	0	0	0
1	B	228	1906	1223	317	357	9	0	0	0
1	C	228	1906	1223	317	357	9	0	0	0
1	D	228	1906	1223	317	357	9	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27707
A	-18	GLY	-	expression tag	UNP P27707
A	-17	SER	-	expression tag	UNP P27707
A	-16	SER	-	expression tag	UNP P27707
A	-15	HIS	-	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	SER	-	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
B	-19	MET	-	expression tag	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P27707
B	-17	SER	-	expression tag	UNP P27707
B	-16	SER	-	expression tag	UNP P27707
B	-15	HIS	-	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	SER	-	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
C	-19	MET	-	expression tag	UNP P27707
C	-18	GLY	-	expression tag	UNP P27707
C	-17	SER	-	expression tag	UNP P27707
C	-16	SER	-	expression tag	UNP P27707
C	-15	HIS	-	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	SER	-	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
C	-1	SER	-	expression tag	UNP P27707
C	0	HIS	-	expression tag	UNP P27707
D	-19	MET	-	expression tag	UNP P27707
D	-18	GLY	-	expression tag	UNP P27707
D	-17	SER	-	expression tag	UNP P27707

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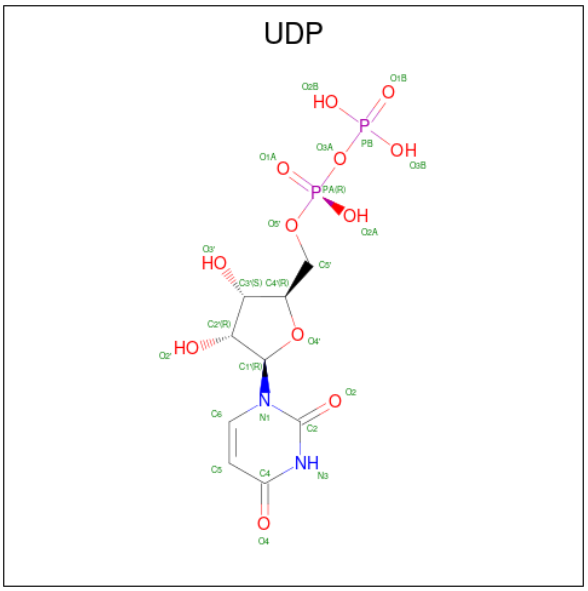
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P27707
D	-15	HIS	-	expression tag	UNP P27707
D	-14	HIS	-	expression tag	UNP P27707
D	-13	HIS	-	expression tag	UNP P27707
D	-12	HIS	-	expression tag	UNP P27707
D	-11	HIS	-	expression tag	UNP P27707
D	-10	HIS	-	expression tag	UNP P27707
D	-9	SER	-	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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

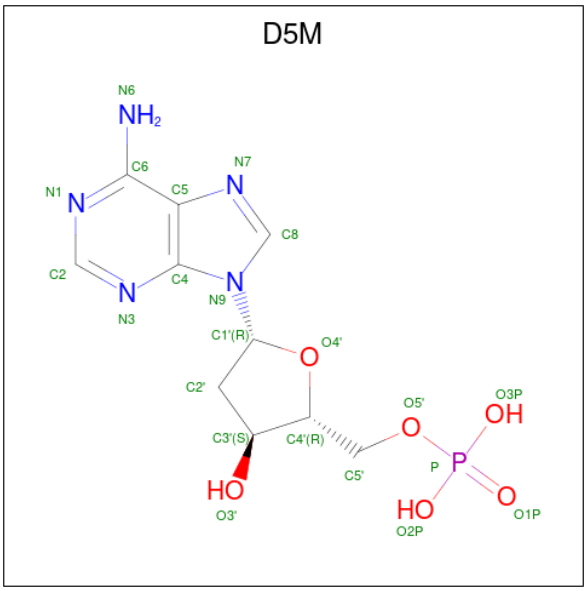
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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

- Molecule 4 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	22	10	5	6	1	0	0
			Total	C	N	O	P		
4	B	1	22	10	5	6	1	0	0
			Total	C	N	O	P		
4	C	1	22	10	5	6	1	0	0
			Total	C	N	O	P		
4	D	1	22	10	5	6	1	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: 2% 50% 27% • 19%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA THR PRO PRO LYS ARG SER CYS PRO SER PHE SER ALA SER SER GLU GLY THR R20 I21 K22 K23 I24 S25 I26 I30 K34 S35 L44 C45 E46 D47 W48 E49 V50 V51

P52 E53 P54 V55 A56 R57 W58 C59 N60 V61 Q62 S63 THR GLN ASP GLU PHE GLU GLU LEU THR MET SER GLN LYS N77 G78 G79 N80 Q83 E90 R91 Q97 L102 S103 R104 I105 R106 A107 Q108 L112 K115 L116 K117 D118 A119 E120 K121 P122 V123 L124 E127 R128

S129 V130 D133 R134 Y135 I136 F137 A138 S139 E143 N148 E149 T150 E151 W152 T153 I154 Y155 Q156 D157 W158 W161 M162 N163 F166 G167 Q168 L178 Q179 A180 I189 R192 G193 R194 E197 E203 Y204 L205 H212 W215 L221 K222 T223 D226 Y227

L234 D237 V238 N239 E240 D241 F242 Y246 E247 V250 F256 L257 S258 T259 L260

• Molecule 1: Deoxycytidine kinase

Chain B: 49% 28% 5% 19%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA THR PRO PRO LYS ARG SER CYS PRO SER PHE SER ALA SER SER GLU GLY THR R20 I21 S25 I26 I30 A31 K34 S35 Q43 L44 C45 E46 D47 W48 E49 V50 V51

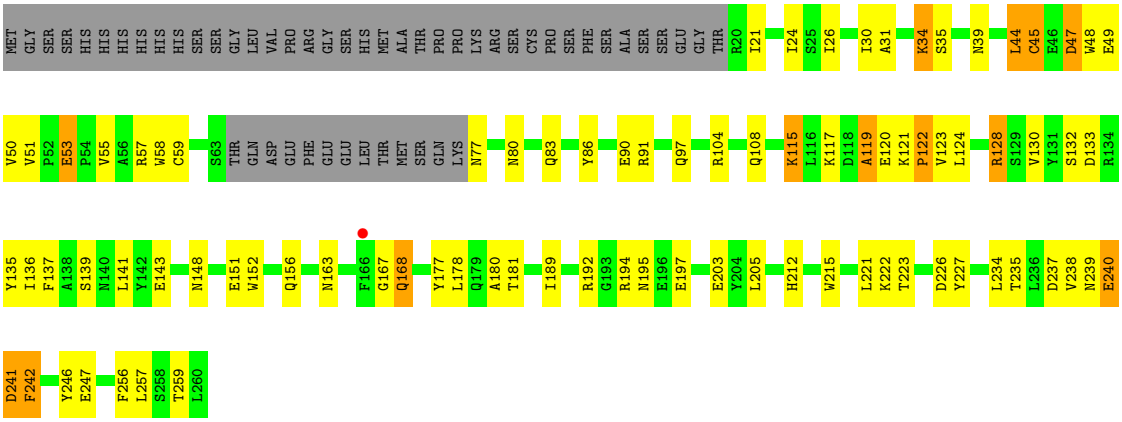
P52 E53 P54 V55 A56 R57 W58 C59 N60 V61 Q62 S63 THR GLN ASP GLU PHE GLU GLU LEU THR MET SER GLN LYS N77 N80 V81 L82 Q83 M84 M85 Y86 E90 R91 W92 S93 F96 Q97 T98 Y99 L102 S103 R104 I105 R106 A107 Q108 K115 L116 K117 D118 A119 E120 K121

P122 V123 L124 E127 R128 S129 V130 D133 R134 Y135 I136 F137 A138 S139 E143 N148 E151 W152 Q156 D157 W158 W161 M162 N163 F166 G167 Q168 L172 L178 Q179 A180 I189 R192 G193 R194 E197 E203 Y204 L205 E206 K207 H212 W215

L221 K222 T223 D226 Y227 L234 D237 V238 N239 E240 D241 F242 Y246 E247 F256 T259 L260

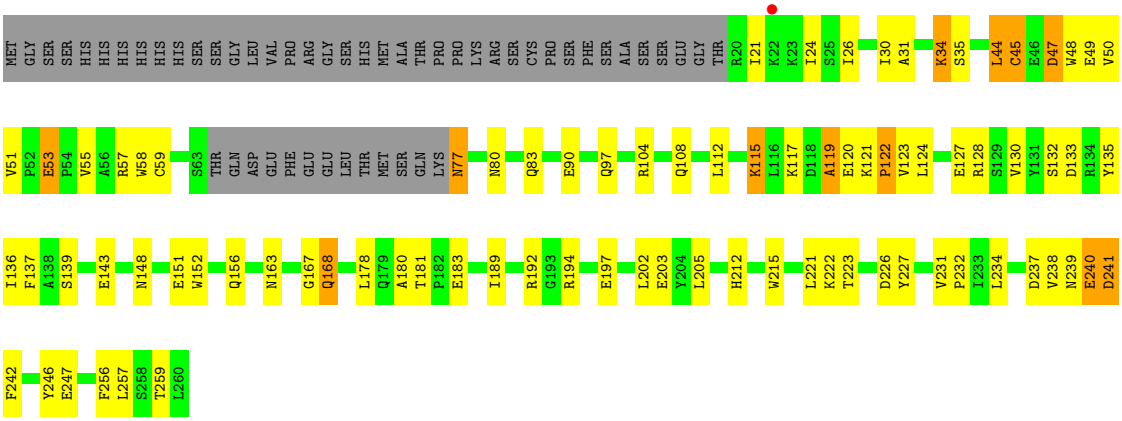
• Molecule 1: Deoxycytidine kinase

Chain C: 51% 26% 5% 19%



- Molecule 1: Deoxycytidine kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.69Å 93.69Å 332.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.60 – 3.45 47.69 – 3.17	Depositor EDS
% Data completeness (in resolution range)	86.5 (38.60-3.45) 86.5 (47.69-3.17)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.200 , 0.257 0.186 , 0.245	Depositor DCC
R_{free} test set	1260 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7816	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: MG, D5M, 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	0.39	0/1952	0.59	0/2641
1	B	0.38	0/1952	0.59	0/2641
1	C	0.37	0/1952	0.58	0/2641
1	D	0.39	0/1952	0.59	0/2641
All	All	0.38	0/7808	0.59	0/10564

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	1906	0	1854	83	0
1	B	1906	0	1855	87	0
1	C	1906	0	1855	79	0
1	D	1906	0	1854	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	11	4	0
3	C	25	0	11	4	0
3	D	25	0	11	4	0
4	A	22	0	12	6	0
4	B	22	0	12	3	0
4	C	22	0	12	6	0
4	D	22	0	12	4	0
All	All	7816	0	7510	296	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 19.

All (296) 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:43:GLN:HE22	1:C:195:ASN:HB2	1.13	1.12
1:B:43:GLN:NE2	1:C:195:ASN:HB2	1.77	0.99
1:B:43:GLN:HE22	1:C:195:ASN:CB	1.91	0.81
1:A:59:CYS:HA	1:A:80:ASN:OD1	1.81	0.79
1:D:53:GLU:OE1	1:D:128:ARG:HD2	1.82	0.79
1:B:59:CYS:HA	1:B:80:ASN:OD1	1.83	0.79
1:C:59:CYS:HA	1:C:80:ASN:OD1	1.82	0.77
1:C:53:GLU:OE1	1:C:128:ARG:HD2	1.86	0.76
1:B:148:ASN:OD1	1:B:151:GLU:HG3	1.87	0.75
1:C:152:TRP:O	1:C:156:GLN:HG3	1.87	0.75
1:B:53:GLU:OE1	1:B:128:ARG:HD2	1.86	0.75
1:C:148:ASN:OD1	1:C:151:GLU:HG3	1.87	0.75
1:C:128:ARG:HH21	1:C:137:PHE:HZ	1.34	0.75
1:D:59:CYS:HA	1:D:80:ASN:OD1	1.87	0.74
1:D:128:ARG:HH21	1:D:137:PHE:HZ	1.33	0.74
1:D:152:TRP:O	1:D:156:GLN:HG3	1.87	0.73
1:C:57:ARG:HB2	1:C:57:ARG:NH1	2.04	0.73
1:B:152:TRP:O	1:B:156:GLN:HG3	1.88	0.73
1:A:53:GLU:OE1	1:A:128:ARG:HD2	1.87	0.73
1:D:57:ARG:NH1	1:D:57:ARG:HB2	2.05	0.72
1:A:128:ARG:HH21	1:A:137:PHE:HZ	1.36	0.71
1:A:152:TRP:O	1:A:156:GLN:HG3	1.91	0.71
1:A:57:ARG:NH1	1:A:57:ARG:HB2	2.06	0.71
1:C:34:LYS:H	1:C:34:LYS:HD3	1.55	0.71
1:B:57:ARG:NH1	1:B:57:ARG:HB2	2.05	0.71
1:D:34:LYS:H	1:D:34:LYS:HD3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:H	1:A:34:LYS:HD3	1.55	0.70
1:B:34:LYS:HD3	1:B:34:LYS:H	1.55	0.70
1:B:128:ARG:HH21	1:B:137:PHE:HZ	1.38	0.70
1:A:148:ASN:OD1	1:A:151:GLU:HG3	1.91	0.70
1:B:130:VAL:HG21	1:B:163:ASN:HD21	1.55	0.70
1:C:53:GLU:HG3	1:C:104:ARG:HH12	1.57	0.70
1:A:53:GLU:HG3	1:A:104:ARG:HH12	1.58	0.68
1:B:115:LYS:HB2	1:C:39:ASN:ND2	2.08	0.68
1:A:97:GLN:HE22	4:A:503:D5M:C2	2.06	0.68
1:B:53:GLU:HG3	1:B:104:ARG:HH12	1.58	0.68
1:A:130:VAL:HG21	1:A:163:ASN:HD21	1.60	0.67
1:D:53:GLU:HG3	1:D:104:ARG:HH12	1.57	0.67
1:B:80:ASN:ND2	1:B:83:GLN:HB2	2.09	0.66
1:D:97:GLN:HE22	4:D:503:D5M:H2	1.60	0.66
1:D:130:VAL:HG21	1:D:163:ASN:HD21	1.59	0.66
1:A:136:ILE:HG21	1:A:212:HIS:CE1	2.31	0.65
1:C:136:ILE:HG21	1:C:212:HIS:CE1	2.31	0.65
1:B:43:GLN:NE2	1:C:195:ASN:CB	2.53	0.65
1:C:130:VAL:HG21	1:C:163:ASN:HD21	1.60	0.64
1:A:61:VAL:HG22	1:A:79:GLY:O	1.97	0.64
1:A:97:GLN:HE22	4:A:503:D5M:H2	1.60	0.64
1:B:120:GLU:HG3	1:B:121:LYS:H	1.63	0.63
1:D:136:ILE:HG21	1:D:212:HIS:CE1	2.33	0.63
1:D:148:ASN:OD1	1:D:151:GLU:HG3	1.98	0.63
1:D:77:ASN:N	1:D:77:ASN:HD22	1.96	0.63
1:A:120:GLU:HG3	1:A:121:LYS:H	1.64	0.63
1:D:80:ASN:ND2	1:D:83:GLN:HB2	2.13	0.62
1:C:80:ASN:ND2	1:C:83:GLN:HB2	2.14	0.62
1:C:115:LYS:H	1:C:115:LYS:HD3	1.64	0.62
1:C:120:GLU:HG3	1:C:121:LYS:H	1.64	0.61
1:B:61:VAL:HG23	1:B:62:GLN:H	1.66	0.61
1:D:120:GLU:HG3	1:D:121:LYS:H	1.65	0.61
1:A:80:ASN:ND2	1:A:83:GLN:HB2	2.16	0.61
1:A:166:PHE:CZ	1:B:166:PHE:CZ	2.90	0.60
1:B:192:ARG:NH1	1:B:197:GLU:OE1	2.31	0.60
1:B:115:LYS:H	1:B:115:LYS:HD3	1.68	0.59
1:D:133:ASP:OD1	4:D:503:D5M:N6	2.36	0.59
1:A:104:ARG:O	1:A:108:GLN:HG3	2.02	0.59
1:D:192:ARG:NH1	1:D:197:GLU:OE1	2.33	0.59
1:B:136:ILE:HG21	1:B:212:HIS:CE1	2.38	0.58
1:A:115:LYS:H	1:A:115:LYS:HD3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HD12	1:A:205:LEU:HD11	1.85	0.58
1:D:135:TYR:CE2	1:D:223:THR:HA	2.39	0.58
1:A:161:TRP:CE2	1:B:106:ARG:HG2	2.39	0.58
1:C:241:ASP:HA	3:C:402:UDP:O4	2.04	0.58
1:D:115:LYS:H	1:D:115:LYS:HD3	1.68	0.58
1:B:49:GLU:O	1:B:124:LEU:HD12	2.04	0.57
1:C:49:GLU:O	1:C:124:LEU:HD12	2.04	0.57
1:C:104:ARG:O	1:C:108:GLN:HG3	2.04	0.57
1:D:49:GLU:O	1:D:124:LEU:HD12	2.04	0.57
1:A:117:LYS:NZ	1:A:117:LYS:HB3	2.20	0.56
1:C:192:ARG:NH1	1:C:197:GLU:OE1	2.34	0.56
1:B:135:TYR:CE2	1:B:223:THR:HA	2.41	0.55
1:D:34:LYS:HZ1	1:D:128:ARG:NH1	2.04	0.55
1:A:49:GLU:O	1:A:124:LEU:HD12	2.06	0.55
1:B:47:ASP:OD2	1:B:119:ALA:HB1	2.07	0.54
1:B:34:LYS:N	3:B:402:UDP:O3B	2.40	0.54
1:A:178:LEU:HD22	1:A:238:VAL:HG11	1.89	0.54
1:B:117:LYS:NZ	1:B:117:LYS:HB3	2.23	0.54
1:B:130:VAL:HG21	1:B:163:ASN:ND2	2.21	0.54
1:A:34:LYS:N	3:A:402:UDP:O3B	2.41	0.54
1:A:221:LEU:C	1:A:221:LEU:HD23	2.28	0.54
1:D:117:LYS:NZ	1:D:117:LYS:HB3	2.22	0.53
1:A:158:TRP:HD1	1:B:102:LEU:HD22	1.72	0.53
1:A:241:ASP:HA	3:A:402:UDP:O4	2.09	0.53
1:C:26:ILE:HG22	1:C:34:LYS:HG3	1.90	0.53
1:C:47:ASP:OD2	1:C:119:ALA:HB1	2.09	0.53
1:D:26:ILE:HG22	1:D:34:LYS:HG3	1.90	0.53
1:A:26:ILE:HG22	1:A:34:LYS:HG3	1.89	0.53
1:D:57:ARG:NH1	1:D:57:ARG:CB	2.71	0.53
1:B:26:ILE:HG22	1:B:34:LYS:HG3	1.90	0.53
1:C:135:TYR:CE2	1:C:223:THR:HA	2.44	0.53
1:B:104:ARG:O	1:B:108:GLN:HG3	2.09	0.52
1:D:130:VAL:HG21	1:D:163:ASN:ND2	2.23	0.52
1:B:241:ASP:HA	3:B:402:UDP:O4	2.09	0.52
1:C:221:LEU:C	1:C:221:LEU:HD23	2.29	0.52
1:B:60:ASN:O	1:B:61:VAL:C	2.47	0.52
1:B:221:LEU:HD23	1:B:221:LEU:C	2.30	0.52
1:C:104:ARG:NE	1:C:133:ASP:OD2	2.32	0.52
1:C:117:LYS:NZ	1:C:117:LYS:HB3	2.25	0.52
1:C:34:LYS:N	3:C:402:UDP:O3B	2.43	0.52
1:D:77:ASN:N	1:D:77:ASN:ND2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ARG:CB	1:D:57:ARG:HH11	2.23	0.52
1:D:47:ASP:OD2	1:D:119:ALA:HB1	2.10	0.51
1:D:90:GLU:OE1	1:D:90:GLU:N	2.43	0.51
1:B:57:ARG:NH1	1:B:57:ARG:CB	2.72	0.51
1:A:57:ARG:NH1	1:A:57:ARG:CB	2.73	0.51
1:C:57:ARG:NH1	1:C:57:ARG:CB	2.71	0.51
1:C:57:ARG:CB	1:C:57:ARG:HH11	2.23	0.51
1:C:34:LYS:HZ1	1:C:128:ARG:NH1	2.09	0.51
1:D:104:ARG:O	1:D:108:GLN:HG3	2.10	0.51
1:A:47:ASP:OD2	1:A:119:ALA:HB1	2.11	0.51
1:C:57:ARG:HB2	1:C:57:ARG:CZ	2.41	0.51
1:C:178:LEU:HD22	1:C:238:VAL:HG11	1.92	0.51
1:A:57:ARG:HB2	1:A:57:ARG:CZ	2.41	0.51
1:D:57:ARG:HB2	1:D:57:ARG:CZ	2.41	0.51
1:B:57:ARG:HB2	1:B:57:ARG:CZ	2.41	0.50
1:A:130:VAL:HG21	1:A:163:ASN:ND2	2.24	0.50
1:C:203:GLU:CD	1:C:203:GLU:H	2.15	0.50
1:B:57:ARG:CB	1:B:57:ARG:HH11	2.24	0.50
1:A:161:TRP:CD1	1:B:106:ARG:NE	2.80	0.50
1:B:34:LYS:CE	1:B:128:ARG:HH12	2.24	0.50
1:D:221:LEU:C	1:D:221:LEU:HD23	2.32	0.50
1:C:130:VAL:HG21	1:C:163:ASN:ND2	2.26	0.50
1:B:90:GLU:OE1	1:B:90:GLU:N	2.44	0.50
1:B:189:ILE:HD12	1:B:205:LEU:HD11	1.93	0.50
1:A:135:TYR:CE2	1:A:223:THR:HA	2.47	0.49
1:D:241:ASP:HA	3:D:402:UDP:O4	2.12	0.49
1:A:57:ARG:CB	1:A:57:ARG:HH11	2.25	0.49
1:A:90:GLU:OE1	1:A:90:GLU:N	2.44	0.49
1:A:203:GLU:CD	1:A:203:GLU:H	2.15	0.49
1:B:104:ARG:NE	1:B:133:ASP:OD2	2.36	0.49
1:C:180:ALA:HA	1:C:239:ASN:ND2	2.28	0.49
1:B:61:VAL:HG23	1:B:62:GLN:N	2.25	0.49
1:C:128:ARG:CZ	4:C:503:D5M:O1P	2.60	0.49
1:D:189:ILE:HD12	1:D:205:LEU:HD11	1.95	0.49
1:B:192:ARG:HD3	1:B:194:ARG:HG3	1.94	0.49
1:B:128:ARG:CZ	4:B:503:D5M:O1P	2.61	0.49
1:C:189:ILE:HD12	1:C:205:LEU:HD11	1.95	0.49
1:B:203:GLU:CD	1:B:203:GLU:H	2.16	0.49
1:C:90:GLU:OE1	1:C:90:GLU:N	2.45	0.48
1:A:102:LEU:HD22	1:B:158:TRP:HD1	1.78	0.48
1:A:166:PHE:HZ	1:B:166:PHE:CZ	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NH1	1:A:197:GLU:OE1	2.36	0.48
1:B:180:ALA:HA	1:B:239:ASN:ND2	2.29	0.48
1:A:106:ARG:HG2	1:B:161:TRP:CE2	2.49	0.48
1:C:139:SER:O	1:C:143:GLU:HG3	2.14	0.48
1:D:104:ARG:NE	1:D:133:ASP:OD2	2.33	0.48
1:A:161:TRP:CD1	1:B:106:ARG:CZ	2.97	0.48
1:B:167:GLY:O	1:B:168:GLN:C	2.52	0.48
1:C:34:LYS:CE	1:C:128:ARG:HH12	2.26	0.48
1:B:115:LYS:CB	1:C:39:ASN:ND2	2.74	0.47
1:A:234:LEU:HB2	1:A:256:PHE:CD2	2.50	0.47
1:A:166:PHE:CZ	1:B:166:PHE:HZ	2.30	0.47
1:A:167:GLY:O	1:A:168:GLN:C	2.52	0.47
1:C:167:GLY:O	1:C:168:GLN:C	2.52	0.47
1:D:34:LYS:N	3:D:402:UDP:O3B	2.47	0.47
1:D:180:ALA:HA	1:D:239:ASN:ND2	2.29	0.47
1:C:242:PHE:O	1:C:246:TYR:HD2	1.98	0.47
1:C:45:CYS:SG	1:C:47:ASP:HB2	2.54	0.47
1:C:234:LEU:HB2	1:C:256:PHE:CD2	2.50	0.47
1:B:234:LEU:HB2	1:B:256:PHE:CD2	2.50	0.47
1:D:34:LYS:CE	1:D:128:ARG:HH12	2.28	0.47
1:D:167:GLY:O	1:D:168:GLN:C	2.54	0.47
1:D:178:LEU:HD22	1:D:238:VAL:HG11	1.97	0.47
1:A:34:LYS:HZ2	1:A:34:LYS:HB2	1.81	0.46
1:A:154:ILE:HG23	1:B:99:TYR:CD1	2.50	0.46
1:B:45:CYS:SG	1:B:47:ASP:HB2	2.56	0.46
1:C:97:GLN:HE22	4:C:503:D5M:H2	1.80	0.46
1:A:180:ALA:HA	1:A:239:ASN:ND2	2.31	0.46
1:B:31:ALA:HA	3:B:402:UDP:O3A	2.16	0.46
1:D:45:CYS:SG	1:D:47:ASP:HB2	2.56	0.46
1:D:203:GLU:H	1:D:203:GLU:CD	2.18	0.46
1:A:215:TRP:HB2	1:A:221:LEU:HD13	1.98	0.46
1:B:178:LEU:HD22	1:B:238:VAL:HG11	1.97	0.46
1:B:139:SER:O	1:B:143:GLU:HG3	2.16	0.45
1:C:215:TRP:HB2	1:C:221:LEU:HD13	1.97	0.45
1:A:139:SER:O	1:A:143:GLU:HG3	2.16	0.45
1:B:30:ILE:HD13	4:B:503:D5M:H1	1.97	0.45
1:B:43:GLN:NE2	1:C:195:ASN:CG	2.69	0.45
1:D:34:LYS:HZ1	1:D:128:ARG:HH12	1.62	0.45
1:C:242:PHE:CD1	1:C:242:PHE:N	2.79	0.45
1:D:97:GLN:HE22	4:D:503:D5M:C2	2.27	0.45
1:D:234:LEU:HB2	1:D:256:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:OH	4:B:503:D5M:H2'1	2.17	0.45
1:C:91:ARG:HD2	1:C:91:ARG:O	2.17	0.45
1:D:215:TRP:HB2	1:D:221:LEU:HD13	1.97	0.45
1:A:35:SER:N	3:A:402:UDP:O3B	2.49	0.45
1:A:104:ARG:NE	1:A:133:ASP:OD2	2.33	0.45
1:A:34:LYS:CE	1:A:128:ARG:HH12	2.30	0.44
1:B:242:PHE:O	1:B:246:TYR:HD2	2.00	0.44
1:C:35:SER:N	3:C:402:UDP:O3B	2.49	0.44
1:A:128:ARG:NH1	4:A:503:D5M:O1P	2.50	0.44
1:B:34:LYS:HZ1	1:B:128:ARG:NH1	2.16	0.44
1:D:21:ILE:HA	1:D:122:PRO:HG2	1.99	0.44
1:D:55:VAL:HA	1:D:58:TRP:CE3	2.52	0.44
1:A:45:CYS:SG	1:A:47:ASP:HB2	2.58	0.44
1:A:102:LEU:HD11	1:B:161:TRP:CZ3	2.52	0.44
1:C:240:GLU:O	1:C:241:ASP:HB2	2.18	0.44
1:B:55:VAL:HA	1:B:58:TRP:CE3	2.52	0.44
1:B:240:GLU:O	1:B:241:ASP:HB2	2.18	0.44
1:D:30:ILE:HD13	4:D:503:D5M:H1	2.00	0.44
1:D:139:SER:O	1:D:143:GLU:HG3	2.18	0.44
1:A:50:VAL:HG12	1:A:51:VAL:N	2.33	0.44
1:A:242:PHE:O	1:A:246:TYR:HD2	2.01	0.44
1:C:34:LYS:HZ1	1:C:128:ARG:HH12	1.65	0.44
1:A:55:VAL:HA	1:A:58:TRP:CE3	2.52	0.43
1:D:31:ALA:HA	3:D:402:UDP:O3A	2.18	0.43
1:D:117:LYS:HB3	1:D:117:LYS:HZ3	1.83	0.43
1:A:91:ARG:HD2	1:A:91:ARG:O	2.18	0.43
1:A:192:ARG:HD3	1:A:194:ARG:HG3	1.99	0.43
1:D:44:LEU:O	1:D:45:CYS:HB2	2.19	0.43
1:D:127:GLU:O	1:D:128:ARG:HB2	2.17	0.43
1:A:150:THR:HG23	1:B:61:VAL:HG11	2.00	0.43
1:A:44:LEU:O	1:A:45:CYS:HB2	2.19	0.43
1:B:34:LYS:HB2	1:B:34:LYS:HZ2	1.84	0.43
1:C:31:ALA:HA	3:C:402:UDP:O3A	2.18	0.43
1:C:115:LYS:HD3	1:C:115:LYS:N	2.33	0.43
1:B:44:LEU:O	1:B:45:CYS:HB2	2.18	0.43
1:C:181:THR:H	1:C:239:ASN:HD21	1.66	0.43
1:D:240:GLU:O	1:D:241:ASP:HB2	2.18	0.43
1:D:242:PHE:O	1:D:246:TYR:HD2	2.02	0.43
1:A:106:ARG:CZ	1:B:161:TRP:CD1	3.02	0.43
1:A:128:ARG:CZ	4:A:503:D5M:O1P	2.67	0.43
1:A:30:ILE:HD13	4:A:503:D5M:H1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:O	1:C:45:CYS:HB2	2.19	0.43
1:D:48:TRP:CD1	1:D:123:VAL:HB	2.54	0.43
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.83	0.43
1:A:48:TRP:CD1	1:A:123:VAL:HB	2.54	0.43
1:C:55:VAL:HA	1:C:58:TRP:CE3	2.54	0.43
1:C:86:TYR:OH	4:C:503:D5M:H2'1	2.18	0.43
1:C:115:LYS:H	1:C:115:LYS:CD	2.32	0.43
1:C:24:ILE:HG13	1:C:257:LEU:HD21	2.01	0.42
1:D:192:ARG:HD3	1:D:194:ARG:HG3	2.01	0.42
1:A:106:ARG:HG2	1:B:161:TRP:CZ2	2.54	0.42
1:B:237:ASP:OD2	1:B:239:ASN:HB2	2.19	0.42
1:C:117:LYS:HB3	1:C:117:LYS:HZ3	1.85	0.42
1:C:21:ILE:HA	1:C:122:PRO:HG2	2.01	0.42
1:C:234:LEU:HD22	1:C:256:PHE:HB2	2.01	0.42
1:B:21:ILE:HA	1:B:122:PRO:HG2	2.01	0.42
1:A:24:ILE:HG13	1:A:257:LEU:HD21	2.02	0.42
1:A:34:LYS:HZ1	1:A:128:ARG:HH12	1.68	0.42
1:A:34:LYS:HZ1	1:A:128:ARG:NH1	2.16	0.42
1:D:242:PHE:H	1:D:242:PHE:HD1	1.62	0.42
1:C:120:GLU:O	1:C:122:PRO:HD3	2.20	0.42
1:D:50:VAL:HG12	1:D:51:VAL:N	2.35	0.42
1:A:34:LYS:O	1:A:35:SER:C	2.59	0.42
1:D:24:ILE:HG13	1:D:257:LEU:HD21	2.02	0.42
1:D:181:THR:H	1:D:239:ASN:HD21	1.66	0.42
1:B:127:GLU:O	1:B:128:ARG:HB2	2.18	0.41
1:A:136:ILE:HG21	1:A:212:HIS:HE1	1.81	0.41
1:A:221:LEU:HD23	1:A:221:LEU:O	2.20	0.41
1:A:237:ASP:OD2	1:A:239:ASN:HB2	2.20	0.41
1:B:35:SER:N	3:B:402:UDP:O3B	2.51	0.41
1:D:231:VAL:HA	1:D:232:PRO:HD3	1.95	0.41
1:A:97:GLN:OE1	4:A:503:D5M:N1	2.53	0.41
1:B:50:VAL:HG12	1:B:51:VAL:N	2.35	0.41
1:C:128:ARG:NH1	4:C:503:D5M:O1P	2.53	0.41
1:A:240:GLU:O	1:A:241:ASP:HB2	2.20	0.41
1:C:177:TYR:CD2	1:C:235:THR:HG23	2.56	0.41
1:A:127:GLU:O	1:A:128:ARG:HB2	2.21	0.41
1:A:246:TYR:O	1:A:250:VAL:HG23	2.21	0.41
1:C:48:TRP:CD1	1:C:123:VAL:HB	2.55	0.41
1:C:192:ARG:HD3	1:C:194:ARG:HG3	2.02	0.41
1:C:237:ASP:OD2	1:C:239:ASN:HB2	2.19	0.41
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:SER:O	1:D:136:ILE:HB	2.21	0.41
1:A:21:ILE:HA	1:A:122:PRO:HG2	2.02	0.41
1:A:120:GLU:O	1:A:122:PRO:HD3	2.21	0.41
1:B:91:ARG:HD2	1:B:91:ARG:O	2.21	0.41
1:B:93:SER:O	1:B:97:GLN:HB2	2.21	0.41
1:B:203:GLU:O	1:B:207:LYS:HG3	2.20	0.41
1:C:30:ILE:HD13	4:C:503:D5M:H1	2.02	0.41
1:D:237:ASP:OD2	1:D:239:ASN:HB2	2.21	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.84	0.41
1:C:34:LYS:HD3	1:C:34:LYS:N	2.31	0.41
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.91	0.41
1:B:34:LYS:HZ1	1:B:128:ARG:HH12	1.68	0.40
1:B:60:ASN:O	1:B:61:VAL:O	2.39	0.40
1:B:81:VAL:HA	1:B:84:MET:HG3	2.03	0.40
1:B:215:TRP:HB2	1:B:221:LEU:HD13	2.03	0.40
1:C:50:VAL:HG12	1:C:51:VAL:N	2.35	0.40
1:C:97:GLN:HE22	4:C:503:D5M:C2	2.35	0.40
1:D:183:GLU:OE2	1:D:202:LEU:HD21	2.21	0.40
1:C:34:LYS:O	1:C:35:SER:C	2.59	0.40
1:C:132:SER:HA	1:C:136:ILE:HG12	2.03	0.40
1:D:35:SER:N	3:D:402:UDP:O3B	2.52	0.40
1:A:234:LEU:HD22	1:A:256:PHE:HB2	2.03	0.40
1:B:96:PHE:CD2	1:B:96:PHE:C	2.94	0.40
1:B:25:SER:HB3	1:B:172:LEU:HD13	2.03	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	224/280 (80%)	191 (85%)	26 (12%)	7 (3%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	224/280 (80%)	190 (85%)	25 (11%)	9 (4%)	3	23
1	C	224/280 (80%)	190 (85%)	27 (12%)	7 (3%)	4	29
1	D	224/280 (80%)	191 (85%)	26 (12%)	7 (3%)	4	29
All	All	896/1120 (80%)	762 (85%)	104 (12%)	30 (3%)	4	27

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ALA
1	A	240	GLU
1	B	61	VAL
1	B	119	ALA
1	B	240	GLU
1	C	119	ALA
1	C	240	GLU
1	D	119	ALA
1	D	240	GLU
1	A	168	GLN
1	A	226	ASP
1	A	241	ASP
1	B	168	GLN
1	B	226	ASP
1	B	241	ASP
1	C	226	ASP
1	C	241	ASP
1	D	226	ASP
1	D	241	ASP
1	A	45	CYS
1	B	45	CYS
1	C	45	CYS
1	C	168	GLN
1	D	45	CYS
1	D	168	GLN
1	A	259	THR
1	B	60	ASN
1	B	259	THR
1	C	259	THR
1	D	259	THR

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	210/256 (82%)	201 (96%)	9 (4%)	29	61
1	B	210/256 (82%)	200 (95%)	10 (5%)	25	58
1	C	210/256 (82%)	198 (94%)	12 (6%)	20	52
1	D	210/256 (82%)	200 (95%)	10 (5%)	25	58
All	All	840/1024 (82%)	799 (95%)	41 (5%)	25	57

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	44	LEU
1	A	47	ASP
1	A	53	GLU
1	A	115	LYS
1	A	122	PRO
1	A	222	LYS
1	A	227	TYR
1	A	247	GLU
1	B	34	LYS
1	B	44	LEU
1	B	47	ASP
1	B	53	GLU
1	B	77	ASN
1	B	115	LYS
1	B	122	PRO
1	B	222	LYS
1	B	227	TYR
1	B	247	GLU
1	C	34	LYS
1	C	44	LEU
1	C	47	ASP
1	C	53	GLU
1	C	77	ASN

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Mol	Chain	Res	Type
1	C	115	LYS
1	C	122	PRO
1	C	128	ARG
1	C	222	LYS
1	C	227	TYR
1	C	242	PHE
1	C	247	GLU
1	D	34	LYS
1	D	44	LEU
1	D	47	ASP
1	D	53	GLU
1	D	77	ASN
1	D	115	LYS
1	D	122	PRO
1	D	222	LYS
1	D	227	TYR
1	D	247	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	77	ASN
1	A	97	GLN
1	A	163	ASN
1	A	224	ASN
1	B	43	GLN
1	B	77	ASN
1	B	80	ASN
1	B	97	GLN
1	B	163	ASN
1	C	39	ASN
1	C	43	GLN
1	C	62	GLN
1	C	77	ASN
1	C	97	GLN
1	C	156	GLN
1	C	163	ASN
1	D	43	GLN
1	D	62	GLN
1	D	97	GLN
1	D	156	GLN

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Mol	Chain	Res	Type
1	D	163	ASN
1	D	224	ASN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	UDP	A	402	2	24,26,26	0.98	0	37,40,40	1.99	7 (18%)
4	D5M	C	503	-	22,24,24	1.03	3 (13%)	24,36,36	1.65	4 (16%)
4	D5M	A	503	-	22,24,24	0.93	1 (4%)	24,36,36	1.73	4 (16%)
3	UDP	B	402	2	24,26,26	0.95	1 (4%)	37,40,40	1.99	7 (18%)
3	UDP	D	402	2	24,26,26	1.04	1 (4%)	37,40,40	1.99	7 (18%)
4	D5M	B	503	-	22,24,24	1.03	3 (13%)	24,36,36	1.76	4 (16%)
4	D5M	D	503	-	22,24,24	0.97	2 (9%)	24,36,36	1.64	4 (16%)
3	UDP	C	402	2	24,26,26	0.98	1 (4%)	37,40,40	1.99	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
3	UDP	A	402	2	-	0/16/32/32	0/2/2/2
4	D5M	C	503	-	-	0/6/22/22	0/3/3/3
4	D5M	A	503	-	-	0/6/22/22	0/3/3/3
3	UDP	B	402	2	-	0/16/32/32	0/2/2/2
3	UDP	D	402	2	-	0/16/32/32	0/2/2/2
4	D5M	B	503	-	-	0/6/22/22	0/3/3/3
4	D5M	D	503	-	-	0/6/22/22	0/3/3/3
3	UDP	C	402	2	-	0/16/32/32	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	503	D5M	C8-N7	-2.45	1.30	1.34
4	D	503	D5M	P-O3P	2.39	1.64	1.54
4	A	503	D5M	C8-N7	-2.28	1.30	1.34
3	D	402	UDP	O5'-C5'	-2.28	1.36	1.44
4	C	503	D5M	P-O3P	2.28	1.63	1.54
4	C	503	D5M	P-O2P	2.19	1.63	1.54
4	D	503	D5M	C8-N7	-2.17	1.30	1.34
4	B	503	D5M	C8-N7	-2.17	1.30	1.34
4	B	503	D5M	P-O3P	2.11	1.63	1.54
4	B	503	D5M	P-O2P	2.05	1.62	1.54
3	C	402	UDP	PB-O2B	-2.03	1.47	1.54
3	B	402	UDP	PB-O2B	-2.01	1.47	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	UDP	PA-O3A-PB	-7.46	107.22	132.83
3	A	402	UDP	PA-O3A-PB	-7.43	107.34	132.83
3	B	402	UDP	PA-O3A-PB	-7.41	107.39	132.83
3	D	402	UDP	PA-O3A-PB	-7.37	107.53	132.83
4	B	503	D5M	P-O5'-C5'	-5.19	104.01	118.30
4	A	503	D5M	N3-C2-N1	-4.87	121.07	128.68
4	B	503	D5M	N3-C2-N1	-4.85	121.10	128.68
4	C	503	D5M	N3-C2-N1	-4.78	121.21	128.68
4	D	503	D5M	N3-C2-N1	-4.77	121.22	128.68
3	B	402	UDP	C4-N3-C2	-4.77	120.29	126.58
3	C	402	UDP	C4-N3-C2	-4.77	120.29	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	UDP	C4-N3-C2	-4.73	120.34	126.58
3	A	402	UDP	C4-N3-C2	-4.69	120.39	126.58
4	A	503	D5M	P-O5'-C5'	-4.63	105.54	118.30
3	D	402	UDP	N3-C2-N1	4.51	120.87	114.89
4	D	503	D5M	P-O5'-C5'	-4.49	105.93	118.30
3	A	402	UDP	N3-C2-N1	4.44	120.78	114.89
3	C	402	UDP	N3-C2-N1	4.43	120.78	114.89
3	B	402	UDP	N3-C2-N1	4.40	120.72	114.89
4	C	503	D5M	P-O5'-C5'	-4.32	106.40	118.30
3	D	402	UDP	C5-C4-N3	3.02	119.36	114.84
3	B	402	UDP	C5-C4-N3	3.01	119.34	114.84
3	C	402	UDP	C5-C4-N3	2.99	119.31	114.84
3	A	402	UDP	C5-C4-N3	2.98	119.30	114.84
4	A	503	D5M	O4'-C1'-C2'	2.96	111.83	106.25
3	D	402	UDP	O4-C4-C5	-2.80	120.23	125.16
3	A	402	UDP	O4-C4-C5	-2.77	120.29	125.16
3	B	402	UDP	O4-C4-C5	-2.75	120.32	125.16
3	C	402	UDP	O4-C4-C5	-2.73	120.35	125.16
3	C	402	UDP	PA-O5'-C5'	-2.51	106.96	121.68
3	B	402	UDP	PA-O5'-C5'	-2.48	107.16	121.68
3	D	402	UDP	O2-C2-N1	-2.47	119.50	122.79
3	A	402	UDP	PA-O5'-C5'	-2.46	107.23	121.68
3	A	402	UDP	O2-C2-N1	-2.46	119.52	122.79
3	D	402	UDP	PA-O5'-C5'	-2.45	107.34	121.68
4	C	503	D5M	O4'-C1'-C2'	2.38	110.74	106.25
3	C	402	UDP	O2-C2-N1	-2.37	119.63	122.79
3	B	402	UDP	O2-C2-N1	-2.37	119.64	122.79
4	B	503	D5M	O4'-C1'-C2'	2.33	110.65	106.25
4	B	503	D5M	C2-N1-C6	2.13	122.40	118.75
4	D	503	D5M	O4'-C1'-C2'	2.09	110.19	106.25
4	C	503	D5M	C4-C5-N7	-2.04	107.27	109.40
4	A	503	D5M	C4-C5-N7	-2.04	107.27	109.40
4	D	503	D5M	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	UDP	3	0

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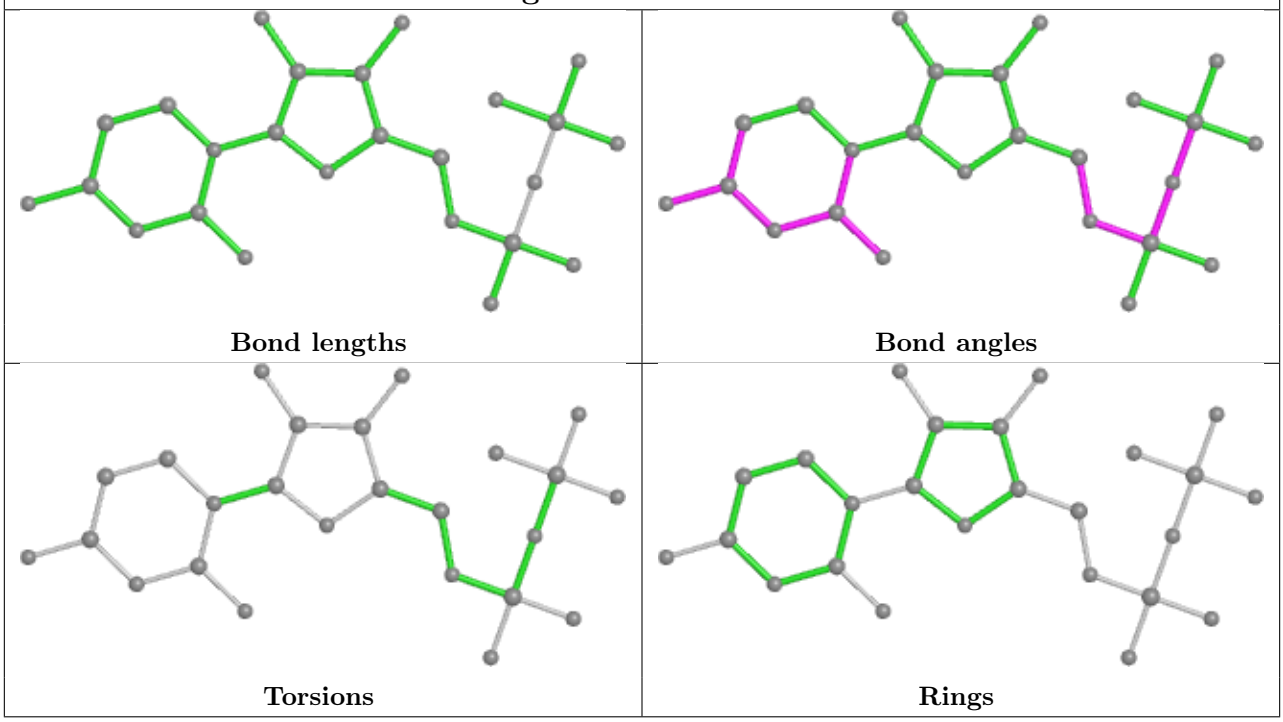
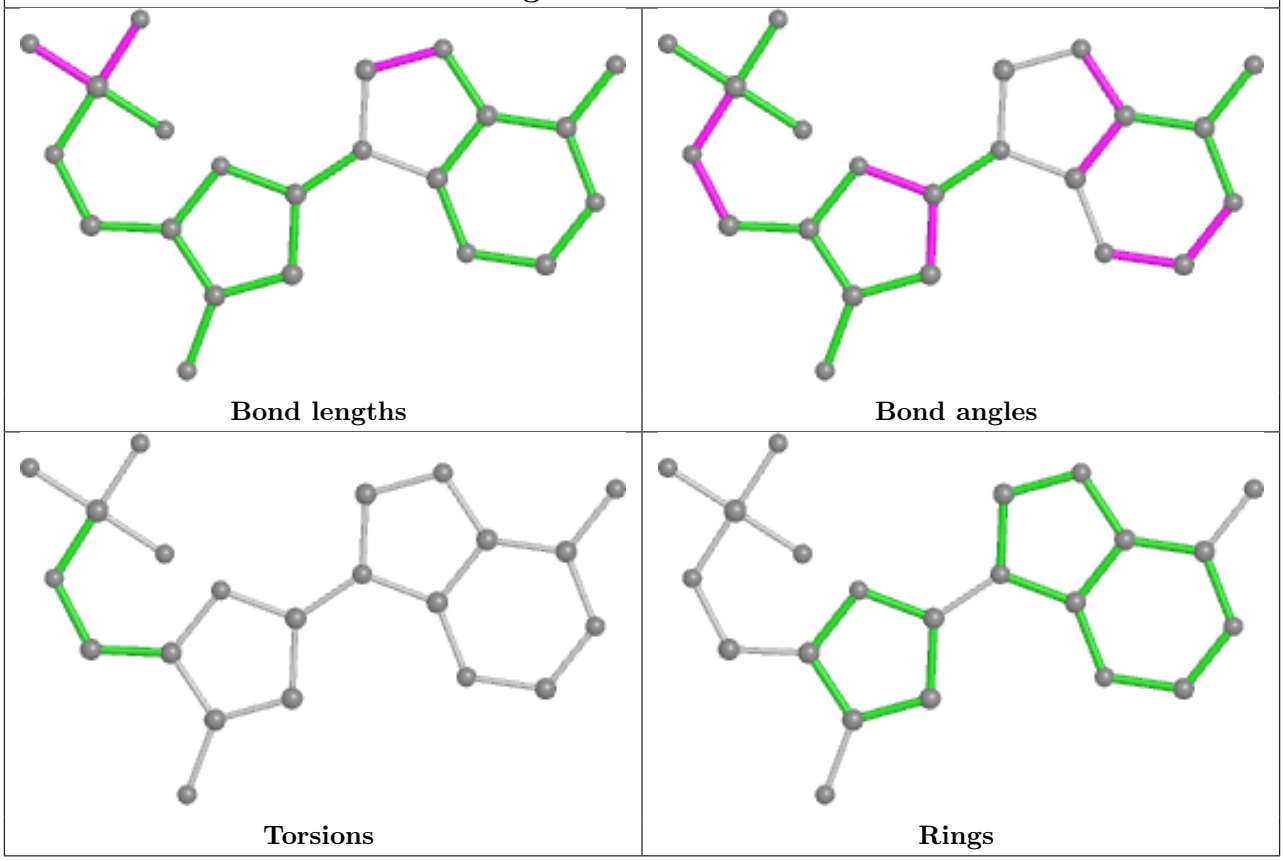
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	D5M	6	0
4	A	503	D5M	6	0
3	B	402	UDP	4	0
3	D	402	UDP	4	0
4	B	503	D5M	3	0
4	D	503	D5M	4	0
3	C	402	UDP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

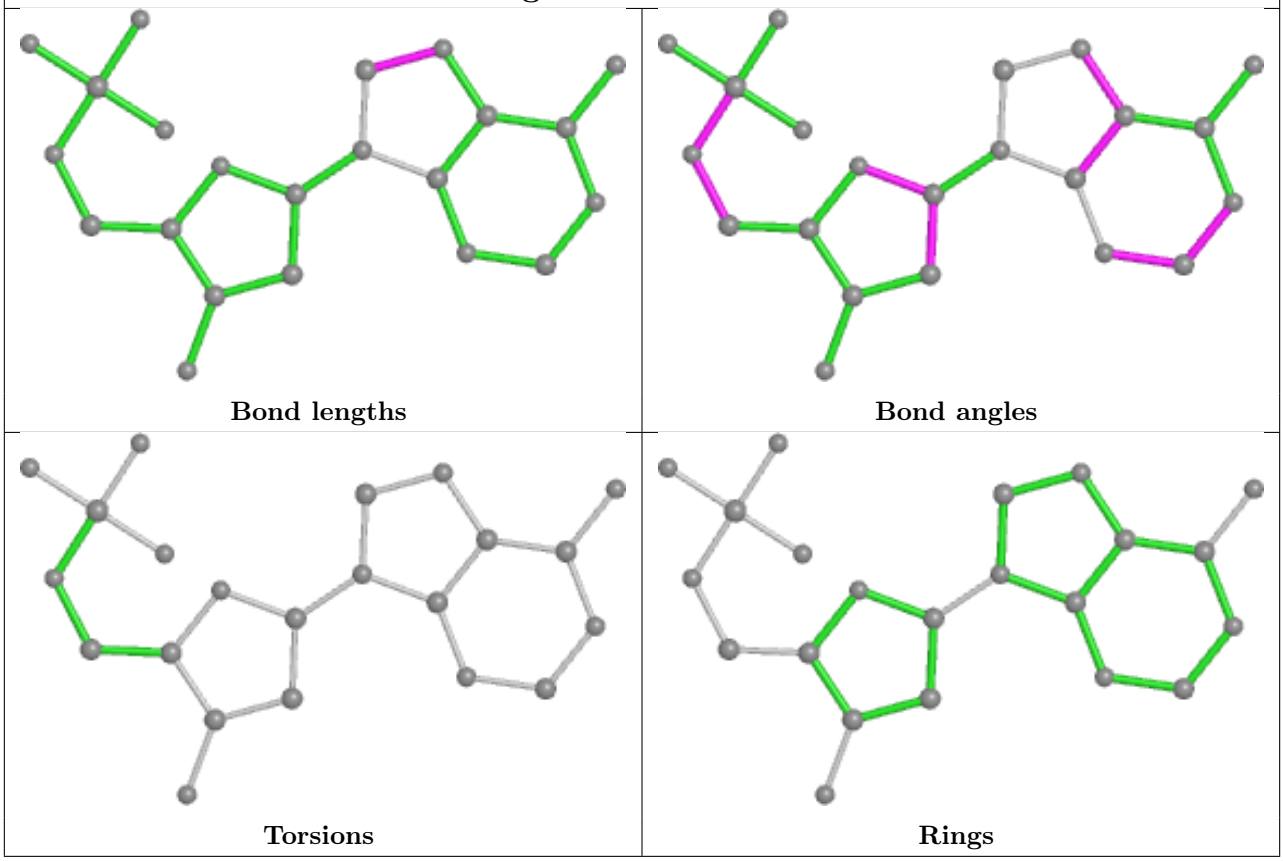
Ligand UDP A 402



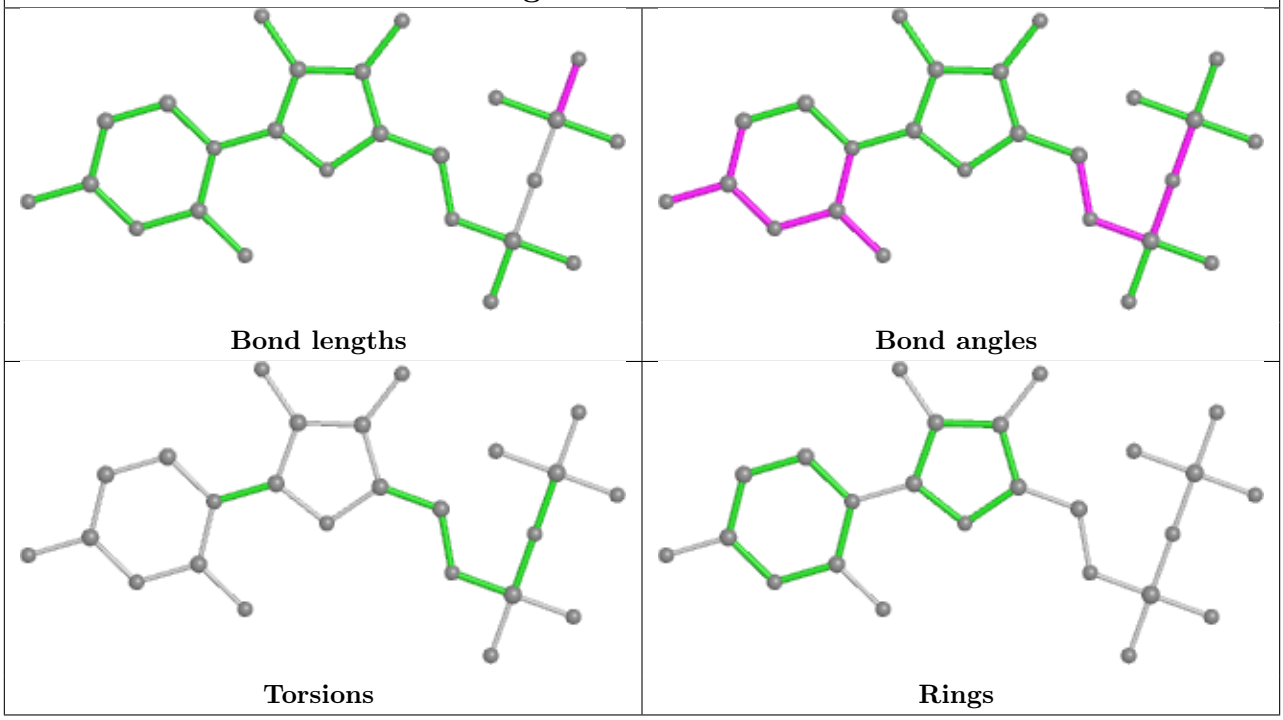
Ligand D5M C 503



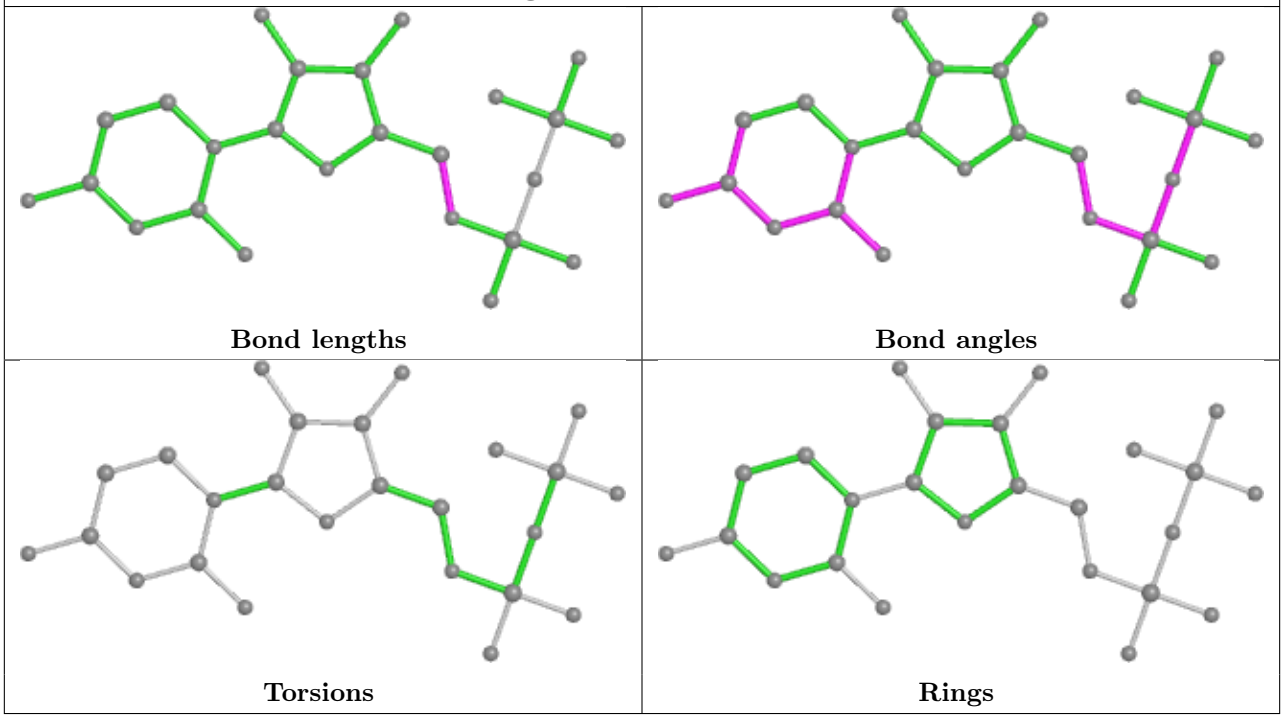
Ligand D5M A 503



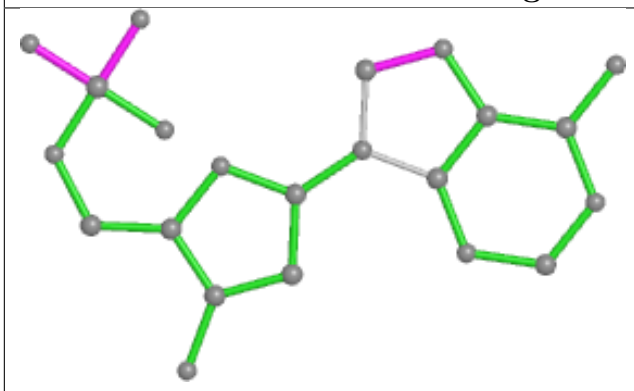
Ligand UDP B 402



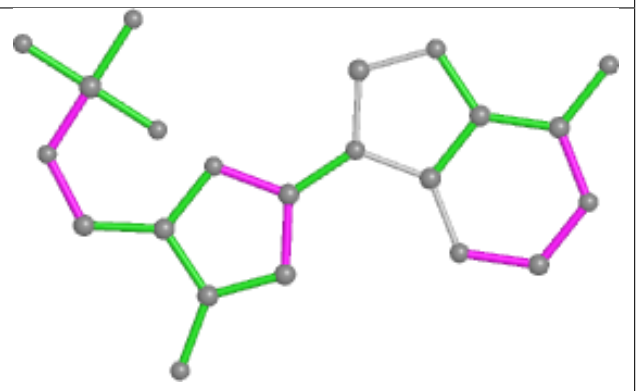
Ligand UDP D 402



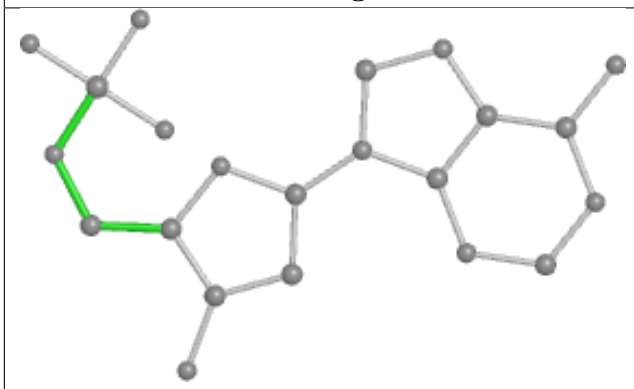
Ligand D5M B 503



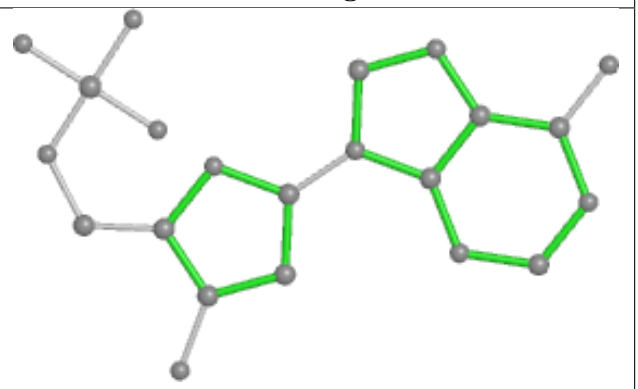
Bond lengths



Bond angles

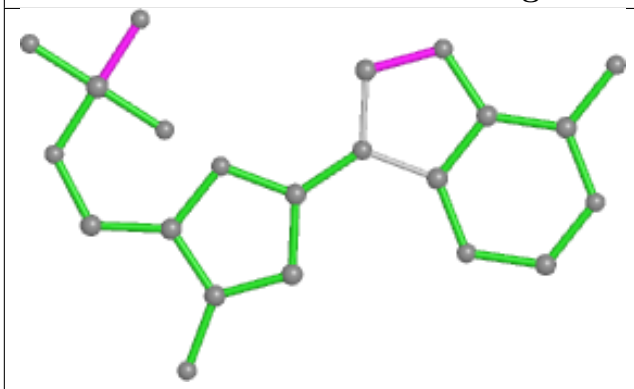


Torsions

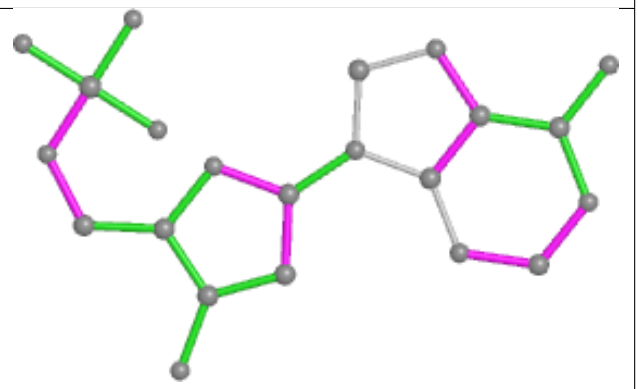


Rings

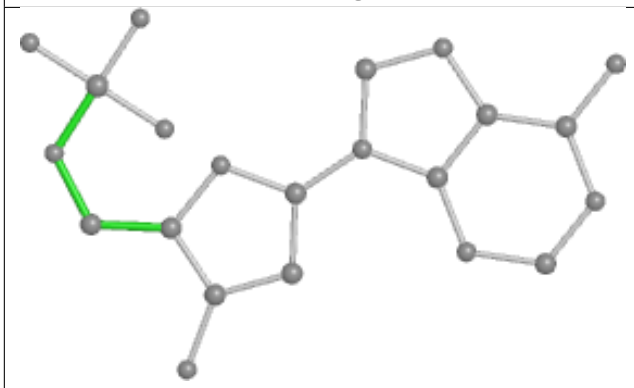
Ligand D5M D 503



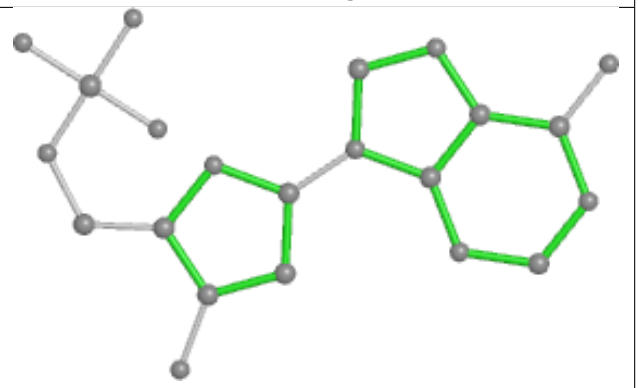
Bond lengths



Bond angles

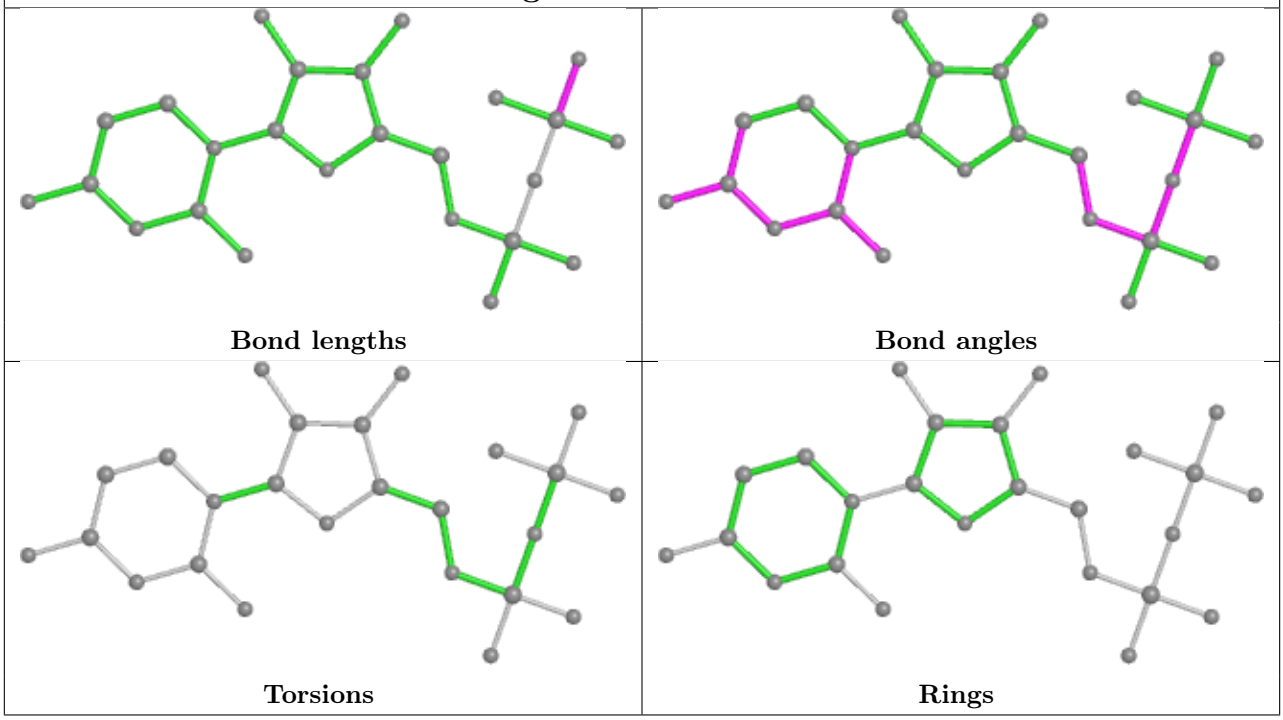


Torsions



Rings

Ligand UDP C 402



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	228/280 (81%)	-0.20	7 (3%) 49 47	43, 76, 140, 207	0
1	B	228/280 (81%)	-0.36	0 100 100	45, 74, 144, 187	0
1	C	228/280 (81%)	-0.40	1 (0%) 92 90	42, 72, 143, 197	0
1	D	228/280 (81%)	-0.40	1 (0%) 92 90	43, 71, 139, 180	0
All	All	912/1120 (81%)	-0.34	9 (0%) 82 79	42, 74, 143, 207	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ILE	3.3
1	A	46	GLU	2.5
1	A	22	LYS	2.5
1	C	166	PHE	2.4
1	A	49	GLU	2.4
1	A	121	LYS	2.3
1	D	22	LYS	2.1
1	A	63	SER	2.1
1	A	47	ASP	2.1

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)

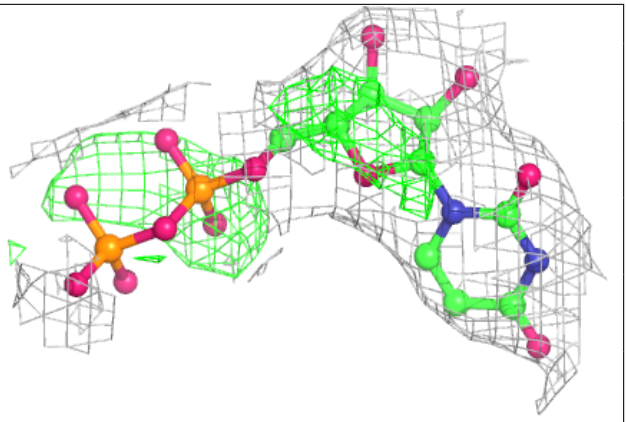
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

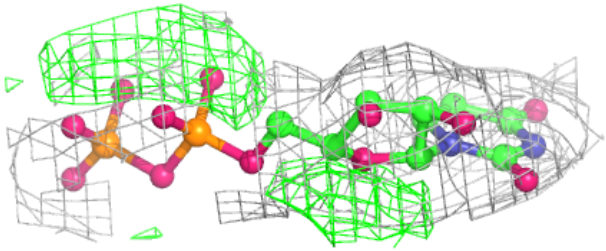
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	401	1/1	0.88	0.27	75,75,75,75	0
3	UDP	B	402	25/25	0.91	0.15	75,75,75,75	0
3	UDP	C	402	25/25	0.91	0.22	75,75,75,75	0
3	UDP	A	402	25/25	0.92	0.16	75,75,75,75	0
3	UDP	D	402	25/25	0.93	0.18	75,75,75,75	0
4	D5M	B	503	22/22	0.93	0.20	75,75,75,75	0
4	D5M	C	503	22/22	0.93	0.19	75,75,75,75	0
4	D5M	D	503	22/22	0.94	0.16	75,75,75,75	0
2	MG	C	401	1/1	0.96	0.23	75,75,75,75	0
2	MG	A	401	1/1	0.96	0.10	75,75,75,75	0
4	D5M	A	503	22/22	0.96	0.17	75,75,75,75	0
2	MG	B	401	1/1	0.97	0.12	75,75,75,75	0

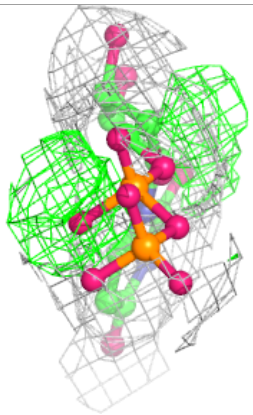
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP B 402:

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

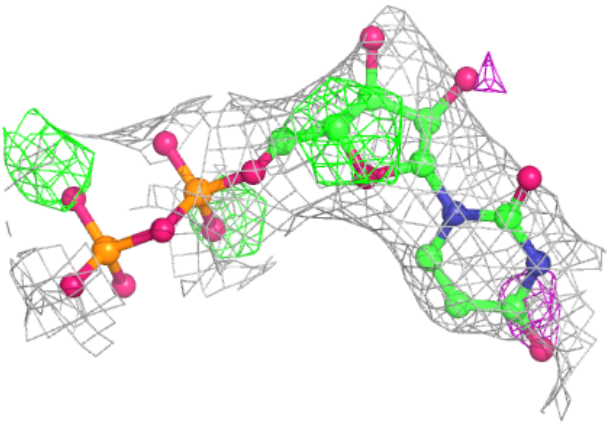


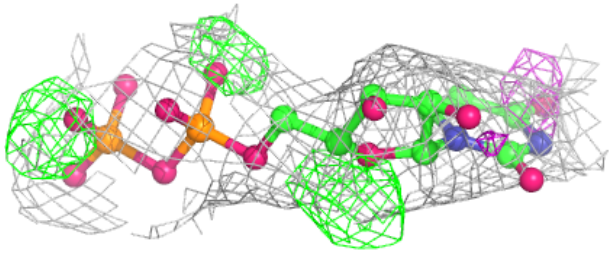


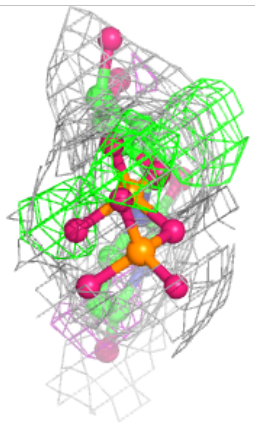


Electron density around UDP C 402:

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

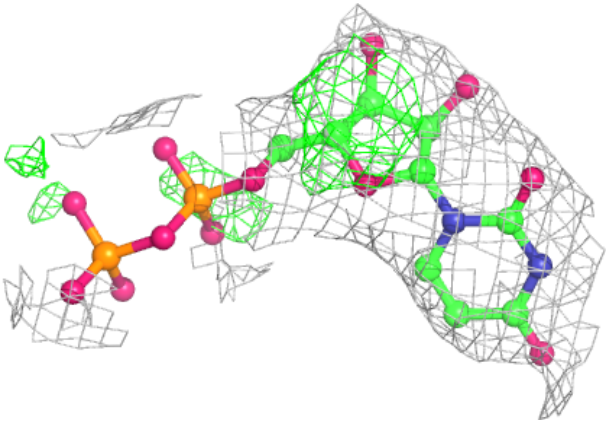


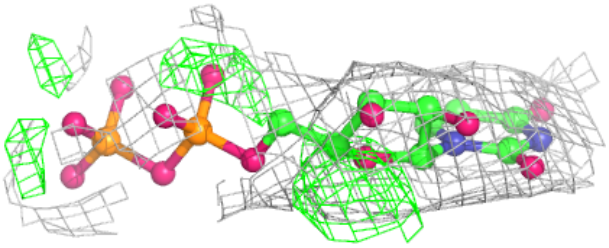


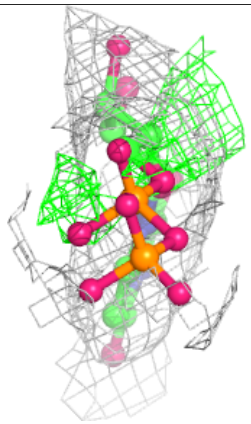


Electron density around UDP A 402:

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

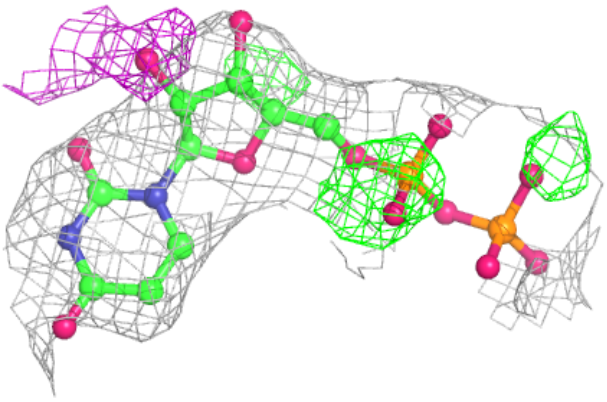


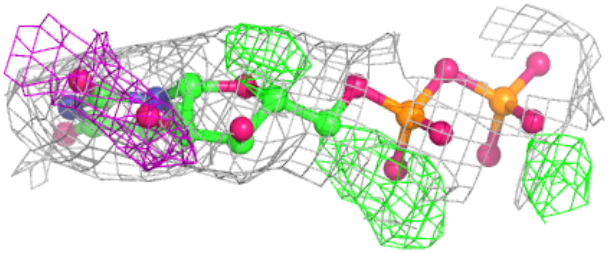


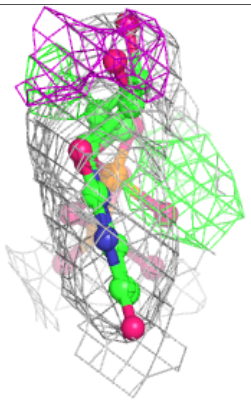


Electron density around UDP D 402:

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

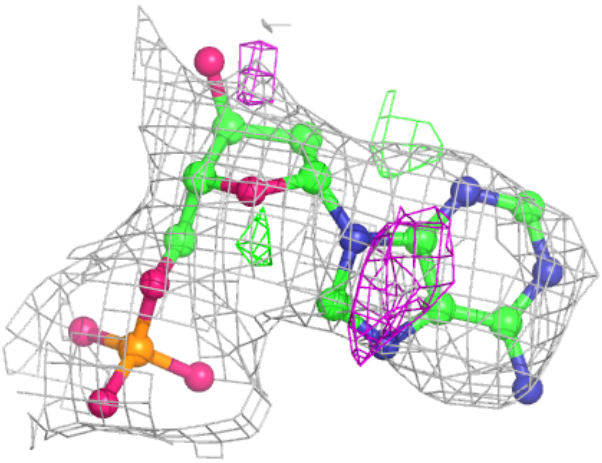


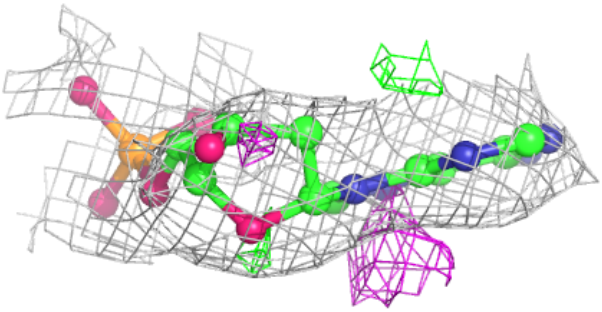


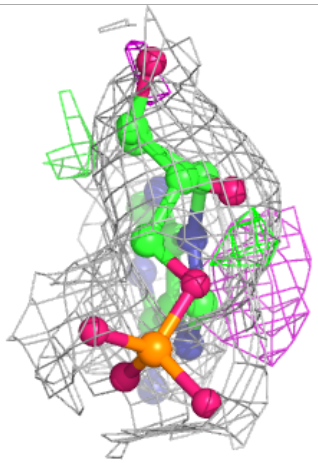


Electron density around D5M B 503:

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

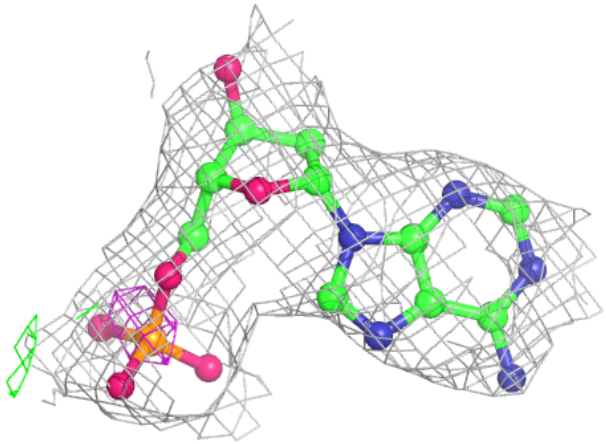


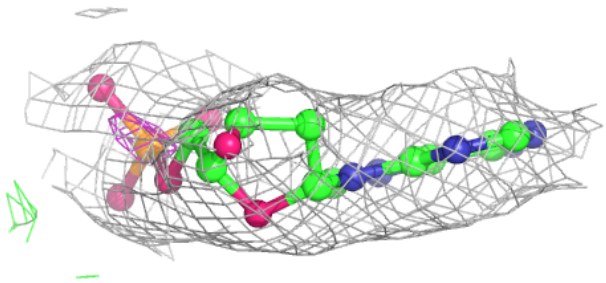


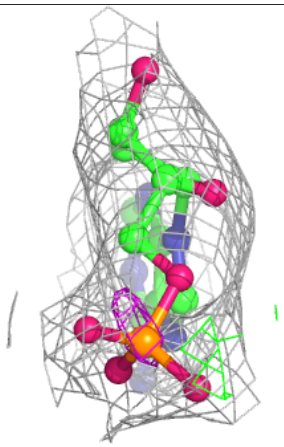


Electron density around D5M C 503:

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

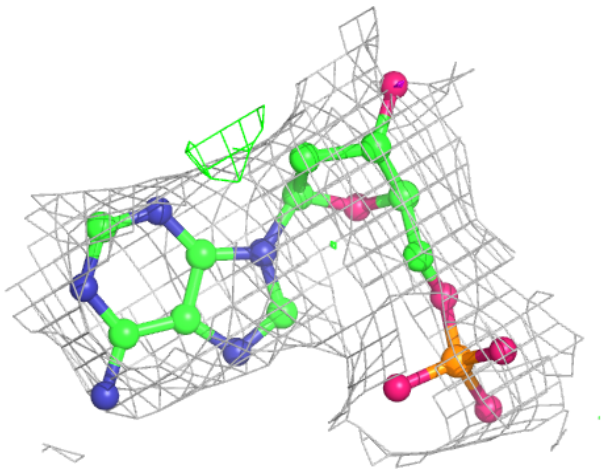


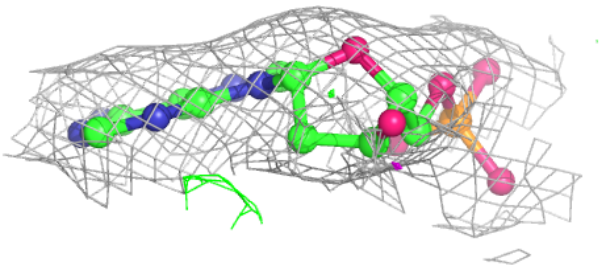


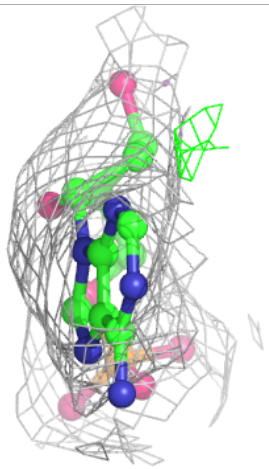


Electron density around D5M D 503:

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

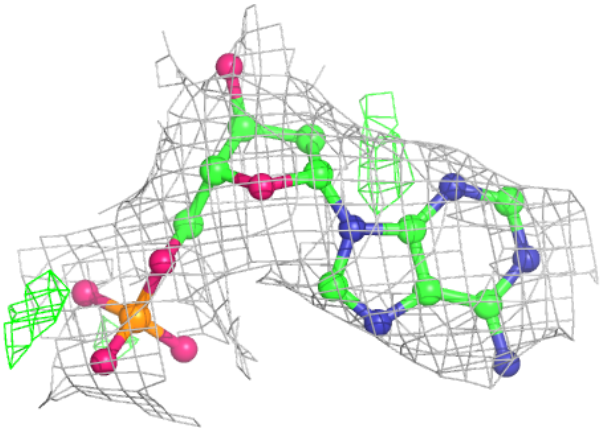


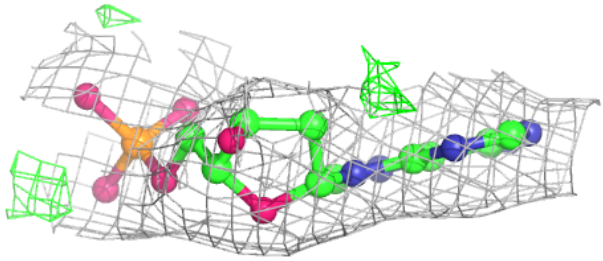


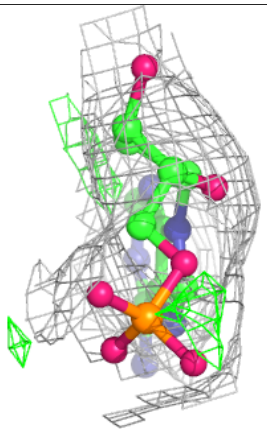


Electron density around D5M A 503:

$2mF_o$-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.