Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 12:42 AM EDT

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

This is a 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:

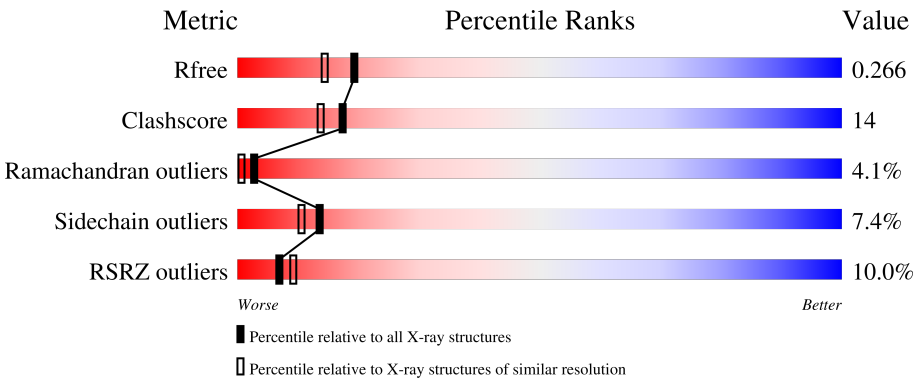
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	279	.%, 57%, 22%, •, 18%
1	B	279	61%, 18%, •, 19%
1	C	279	17%, 52%, 24%, •, 20%
1	D	279	14%, 46%, 30%, •, 21%

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
2	AC2	A	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7428 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Deoxycytidine kinase.

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

There are 92 discrepancies between the modelled and reference sequences:

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

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

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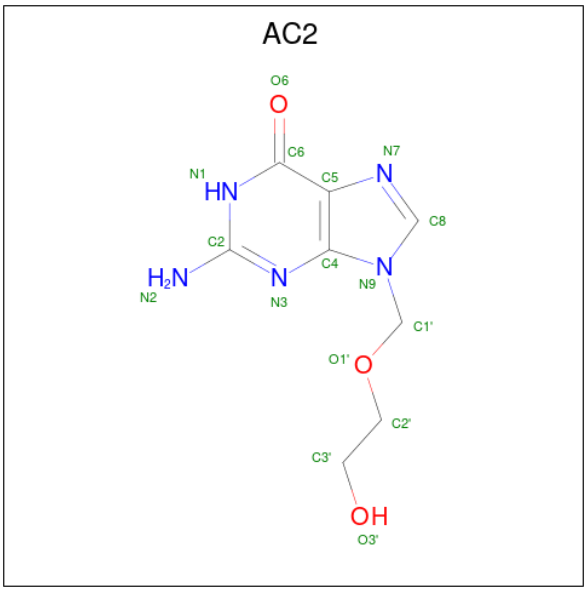
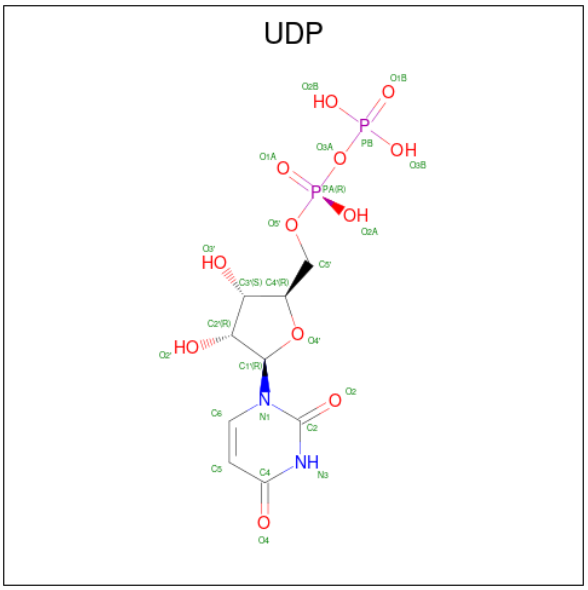
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP P27707
C	0	HIS	-	expression tag	UNP P27707
C	9	SER	CYS	conflict	UNP P27707
C	45	SER	CYS	conflict	UNP P27707
C	59	SER	CYS	conflict	UNP P27707
C	146	SER	CYS	conflict	UNP P27707
D	-18	MET	-	expression tag	UNP P27707
D	-17	GLY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

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



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

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

- Molecule 4 is water.

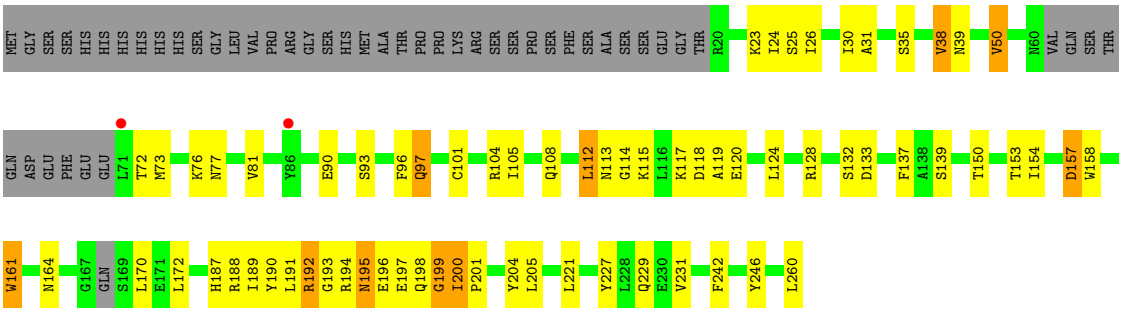
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	22	22	22	0	0
4	B	32	32	32	0	0
4	C	7	7	7	0	0
4	D	4	4	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

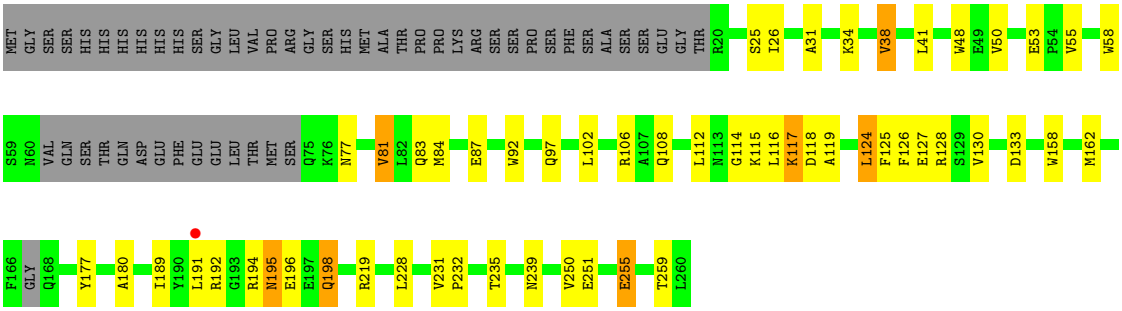
• Molecule 1: Deoxycytidine kinase

Chain A:



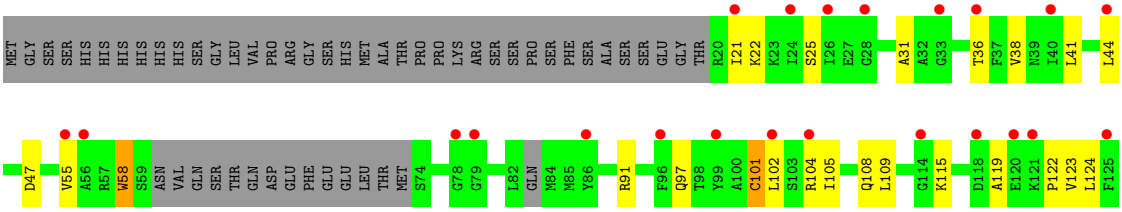
• Molecule 1: Deoxycytidine kinase

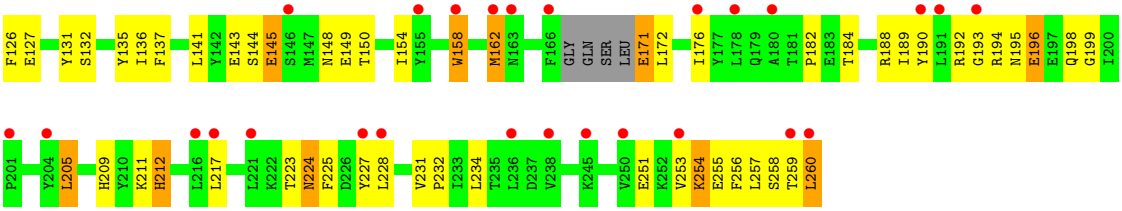
Chain B:



• Molecule 1: Deoxycytidine kinase

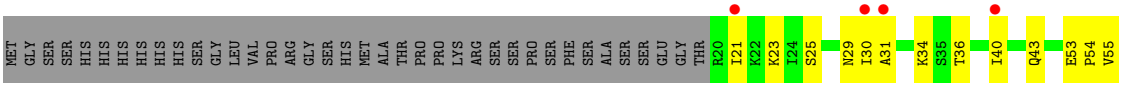
Chain C:

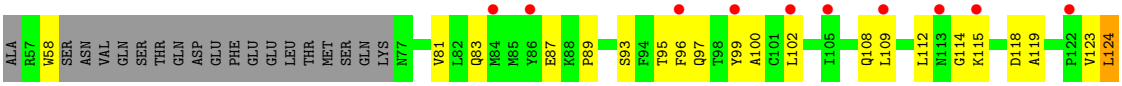


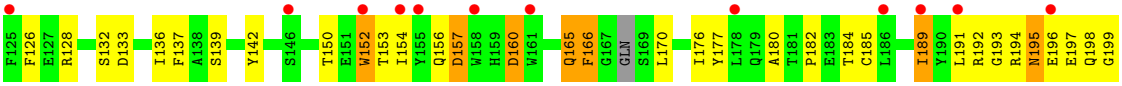


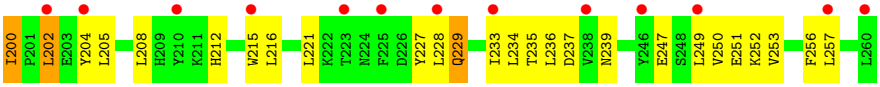
- Molecule 1: Deoxycytidine kinase

Chain D:









4 Data and refinement statistics (i)

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

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

[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: AC2, UDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.46	0/1910	0.62	0/2590
1	B	0.46	0/1857	0.63	0/2520
1	C	0.37	0/1796	0.56	1/2437 (0.0%)
1	D	0.38	0/1816	0.58	0/2462
All	All	0.42	0/7379	0.60	1/10009 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1866	0	1765	51	0
1	B	1815	0	1688	35	0
1	C	1757	0	1606	41	0
1	D	1777	0	1670	72	0
2	A	16	0	11	9	0
2	B	16	0	11	2	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:O	1:A:96:PHE:O	1.58	1.22
1:B:53:GLU:OE1	2:B:401:AC2:N2	1.71	1.21
1:A:200:ILE:HB	1:A:201:PRO:HD3	1.38	1.01
1:D:180:ALA:HA	1:D:239:ASN:HD21	1.27	0.95
1:A:38:VAL:HG22	1:A:50:VAL:HG22	1.51	0.93
1:D:198:GLN:HG3	1:D:199:GLY:H	1.38	0.89
1:B:108:GLN:OE1	4:B:293:HOH:O	1.96	0.83
1:D:133:ASP:OD1	2:D:601:AC2:O6	1.96	0.83
1:C:97:GLN:O	1:C:101:CYS:HB2	1.81	0.81
1:A:38:VAL:HG22	1:A:50:VAL:CG2	2.12	0.80
1:A:190:TYR:HA	1:A:194:ARG:HE	1.50	0.76
1:A:189:ILE:HG21	1:A:199:GLY:HA3	1.68	0.76
1:B:117:LYS:HA	1:B:119:ALA:N	2.02	0.75
1:A:200:ILE:HB	1:A:201:PRO:CD	2.18	0.72
1:D:165:GLN:HB3	1:D:166:PHE:CB	2.20	0.71
1:A:227:TYR:O	1:A:231:VAL:HG23	1.90	0.71
1:D:249:LEU:O	1:D:253:VAL:HG23	1.90	0.71
1:D:132:SER:O	1:D:136:ILE:HB	1.91	0.70
1:A:97:GLN:N	4:A:283:HOH:O	2.04	0.70
1:D:182:PRO:HB2	1:D:202:LEU:CD2	2.22	0.70
1:D:23:LYS:HG2	1:D:126:PHE:HE1	1.54	0.69
1:B:102:LEU:O	1:B:106:ARG:HG3	1.92	0.69
1:D:199:GLY:O	1:D:200:ILE:HB	1.94	0.67
1:B:158:TRP:CE2	1:B:162:MET:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:VAL:HA	1:C:41:LEU:HD12	1.78	0.66
1:D:247:GLU:HA	1:D:250:VAL:HG12	1.77	0.66
1:D:31:ALA:HB3	1:D:189:ILE:HG12	1.78	0.65
1:B:251:GLU:OE2	4:B:269:HOH:O	2.14	0.65
1:A:96:PHE:O	1:A:97:GLN:HB2	1.96	0.65
1:A:38:VAL:CG2	1:A:50:VAL:HG22	2.24	0.64
1:B:31:ALA:HB3	1:B:189:ILE:HG13	1.78	0.64
1:A:204:TYR:OH	2:A:301:AC2:H3'1	1.97	0.64
1:D:97:GLN:NE2	2:D:601:AC2:N7	2.45	0.64
1:D:132:SER:O	1:D:137:PHE:HD1	1.81	0.64
1:A:101:CYS:O	1:A:105:ILE:HG13	1.99	0.63
1:D:180:ALA:HA	1:D:239:ASN:ND2	2.07	0.63
1:A:96:PHE:HA	4:A:283:HOH:O	1.99	0.63
1:A:77:ASN:O	1:A:81:VAL:HG22	1.99	0.62
1:B:84:MET:HB3	1:B:92:TRP:CD1	2.34	0.62
1:C:256:PHE:HD1	4:C:262:HOH:O	1.82	0.62
1:C:21:ILE:HG22	1:C:22:LYS:H	1.65	0.61
1:D:29:ASN:HD21	1:D:205:LEU:HB3	1.64	0.61
1:D:177:TYR:HE1	1:D:212:HIS:HB3	1.66	0.61
1:C:195:ASN:O	1:C:196:GLU:HB2	2.01	0.61
1:D:53:GLU:O	1:D:55:VAL:N	2.33	0.61
1:D:192:ARG:HB2	3:D:261:UDP:H4'	1.84	0.60
1:B:77:ASN:O	1:B:81:VAL:HG22	2.02	0.60
1:D:182:PRO:HB2	1:D:202:LEU:HD21	1.83	0.59
1:A:204:TYR:OH	2:A:301:AC2:C3'	2.50	0.59
1:B:117:LYS:HA	1:B:119:ALA:H	1.66	0.59
1:C:198:GLN:HG3	1:C:199:GLY:H	1.68	0.58
1:C:253:VAL:HA	4:C:262:HOH:O	2.03	0.58
1:B:124:LEU:HD13	1:B:126:PHE:HE2	1.69	0.57
1:B:31:ALA:CB	1:B:189:ILE:HG13	2.34	0.57
1:D:185:CYS:O	1:D:189:ILE:HG13	2.05	0.57
1:A:25:SER:HB2	1:A:172:LEU:HD13	1.87	0.57
1:A:195:ASN:C	1:A:197:GLU:H	2.09	0.56
1:C:158:TRP:HB3	1:D:102:LEU:HD21	1.87	0.56
1:D:31:ALA:CB	1:D:189:ILE:HG12	2.35	0.56
1:C:192:ARG:HG2	1:C:193:GLY:H	1.71	0.56
1:A:96:PHE:O	1:A:97:GLN:CB	2.54	0.56
1:C:171:GLU:HA	1:C:227:TYR:OH	2.06	0.55
1:A:117:LYS:HA	1:A:118:ASP:C	2.27	0.55
1:D:177:TYR:CE1	1:D:212:HIS:HB3	2.42	0.55
1:B:130:VAL:HA	1:B:133:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:O	1:A:154:ILE:HG13	2.07	0.55
1:D:139:SER:HA	1:D:152:TRP:HZ2	1.72	0.55
1:A:128:ARG:HH11	2:A:301:AC2:HN22	1.54	0.55
1:D:176:ILE:HD13	1:D:253:VAL:HG22	1.88	0.54
1:D:21:ILE:CG2	1:D:124:LEU:HB2	2.38	0.54
1:D:23:LYS:HG2	1:D:126:PHE:CE1	2.41	0.54
1:A:153:THR:CG2	1:B:77:ASN:HD21	2.20	0.54
1:B:25:SER:HA	1:B:126:PHE:O	2.08	0.54
1:D:137:PHE:CD2	2:D:601:AC2:C5	2.91	0.54
1:B:41:LEU:O	1:B:48:TRP:HE3	1.91	0.54
1:D:55:VAL:HA	1:D:58:TRP:HA	1.88	0.54
1:C:176:ILE:HG12	1:C:234:LEU:HB3	1.90	0.53
1:D:198:GLN:CG	1:D:199:GLY:H	2.10	0.53
1:D:198:GLN:HG3	1:D:199:GLY:N	2.15	0.53
1:A:35:SER:O	1:A:39:ASN:ND2	2.42	0.52
1:D:123:VAL:HG21	1:D:257:LEU:HD21	1.91	0.52
1:C:251:GLU:HA	1:C:254:LYS:HE3	1.91	0.52
1:D:184:THR:HG21	1:D:239:ASN:HA	1.91	0.52
1:B:50:VAL:HG22	1:B:125:PHE:HB2	1.92	0.52
1:D:83:GLN:O	1:D:87:GLU:HG2	2.10	0.52
1:A:190:TYR:HA	1:A:194:ARG:NE	2.23	0.51
1:C:154:ILE:HG12	1:D:99:TYR:CD1	2.44	0.51
1:B:177:TYR:CD2	1:B:235:THR:HG23	2.45	0.51
1:D:177:TYR:HD2	1:D:235:THR:HG23	1.76	0.51
1:D:252:LYS:O	1:D:256:PHE:HB3	2.10	0.51
1:C:144:SER:O	1:C:145:GLU:HB2	2.10	0.51
1:D:95:THR:O	1:D:96:PHE:HB3	2.10	0.51
1:A:204:TYR:HH	2:A:301:AC2:C3'	2.23	0.51
1:B:195:ASN:O	1:B:196:GLU:HB3	2.11	0.50
1:A:73:MET:HA	1:A:76:LYS:HB3	1.93	0.50
1:C:132:SER:HA	1:C:136:ILE:HD12	1.92	0.50
1:C:102:LEU:HA	1:C:105:ILE:HD12	1.93	0.50
1:C:136:ILE:HD13	1:C:212:HIS:CE1	2.47	0.50
1:C:184:THR:HB	1:C:188:ARG:NH1	2.27	0.50
1:B:97:GLN:OE1	2:B:401:AC2:N7	2.45	0.49
1:D:157:ASP:HA	1:D:160:ASP:HB2	1.93	0.49
1:B:158:TRP:NE1	1:B:162:MET:CG	2.75	0.49
1:D:152:TRP:HE3	1:D:156:GLN:HG3	1.77	0.49
1:D:96:PHE:O	1:D:100:ALA:HB2	2.11	0.49
1:D:234:LEU:HD13	1:D:256:PHE:HB2	1.93	0.49
1:B:180:ALA:HA	1:B:239:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:O	1:B:117:LYS:CB	2.60	0.49
1:B:38:VAL:HG11	1:B:127:GLU:OE1	2.12	0.49
1:D:34:LYS:HE3	1:D:128:ARG:HE	1.77	0.49
1:C:135:TYR:OH	1:C:224:ASN:ND2	2.46	0.49
1:C:158:TRP:CD1	1:C:162:MET:HG3	2.47	0.49
1:D:108:GLN:O	1:D:112:LEU:HB2	2.13	0.49
1:A:128:ARG:NH1	2:A:301:AC2:N2	2.57	0.48
1:A:189:ILE:HD12	1:A:205:LEU:HD11	1.95	0.48
1:A:192:ARG:HD3	3:A:261:UDP:H5'1	1.96	0.48
1:D:36:THR:O	1:D:40:ILE:HG13	2.13	0.48
1:D:89:PRO:O	1:D:93:SER:HB2	2.14	0.48
1:A:137:PHE:HE2	2:A:301:AC2:HO'3	1.59	0.48
1:C:31:ALA:HB3	1:C:189:ILE:HG13	1.95	0.48
1:D:195:ASN:H	1:D:198:GLN:H	1.62	0.47
1:D:198:GLN:CG	1:D:199:GLY:N	2.75	0.47
1:B:83:GLN:O	1:B:87:GLU:HG2	2.12	0.47
1:D:227:TYR:C	1:D:229:GLN:H	2.18	0.47
1:B:250:VAL:HG23	4:B:269:HOH:O	2.15	0.47
1:D:215:TRP:HA	1:D:221:LEU:HB3	1.97	0.47
1:A:192:ARG:HA	3:A:261:UDP:O3'	2.15	0.46
1:A:23:LYS:HE2	1:A:112:LEU:HD11	1.97	0.46
1:B:26:ILE:HG22	1:B:34:LYS:HG2	1.96	0.46
1:A:117:LYS:HA	1:A:118:ASP:O	2.16	0.46
1:A:128:ARG:NH1	2:A:301:AC2:HN22	2.14	0.46
1:C:119:ALA:HB3	1:C:122:PRO:HG3	1.98	0.46
1:D:182:PRO:HB2	1:D:202:LEU:HD23	1.98	0.46
1:A:31:ALA:HB1	1:A:188:ARG:HB3	1.98	0.46
1:D:205:LEU:HA	1:D:208:LEU:HD12	1.98	0.45
1:D:109:LEU:HG	1:D:170:LEU:HD21	1.98	0.45
1:D:194:ARG:HB3	1:D:198:GLN:HA	1.98	0.45
1:D:236:LEU:HD13	1:D:249:LEU:HD22	1.99	0.45
1:C:131:TYR:HE1	1:C:172:LEU:HG	1.80	0.45
1:D:165:GLN:CB	1:D:166:PHE:CB	2.91	0.45
1:C:190:TYR:HA	1:C:194:ARG:HE	1.80	0.45
1:A:108:GLN:HB3	1:A:170:LEU:HD22	1.99	0.45
1:B:55:VAL:O	1:B:58:TRP:HB2	2.17	0.45
1:D:142:TYR:HB2	1:D:152:TRP:HE1	1.81	0.45
1:A:101:CYS:HB3	1:A:158:TRP:HH2	1.81	0.45
1:A:153:THR:HG21	1:B:77:ASN:HD21	1.81	0.45
1:B:219:ARG:NH2	1:B:228:LEU:O	2.50	0.45
1:C:223:THR:C	1:C:225:PHE:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLN:NE2	2:A:301:AC2:N7	2.64	0.45
1:A:101:CYS:HB3	1:A:158:TRP:CH2	2.52	0.44
1:D:234:LEU:HB2	1:D:256:PHE:CD2	2.51	0.44
1:C:225:PHE:HB2	1:C:228:LEU:HD12	1.99	0.44
1:D:152:TRP:CE3	1:D:156:GLN:HG3	2.53	0.44
1:D:216:LEU:HB3	1:D:233:ILE:HG21	1.99	0.44
1:B:128:ARG:HD3	4:B:275:HOH:O	2.16	0.44
1:D:139:SER:HA	1:D:152:TRP:CZ2	2.52	0.44
1:D:239:ASN:HD22	1:D:239:ASN:H	1.65	0.44
1:B:231:VAL:HA	1:B:232:PRO:HD3	1.80	0.44
1:D:237:ASP:OD1	1:D:239:ASN:ND2	2.51	0.43
1:D:133:ASP:HA	1:D:137:PHE:HB2	1.99	0.43
1:C:21:ILE:HG23	1:C:122:PRO:HB2	2.00	0.43
1:C:182:PRO:HD3	1:C:209:HIS:CE1	2.53	0.43
1:C:25:SER:HA	1:C:126:PHE:HB2	2.00	0.43
1:D:195:ASN:N	1:D:198:GLN:H	2.16	0.43
1:A:24:ILE:HD11	1:A:260:LEU:HD13	2.01	0.43
1:C:182:PRO:HG3	1:C:209:HIS:ND1	2.33	0.43
1:D:153:THR:HA	1:D:156:GLN:HB2	2.00	0.43
1:C:31:ALA:CB	1:C:189:ILE:HG13	2.49	0.42
1:D:21:ILE:HG21	1:D:124:LEU:HB2	2.01	0.42
1:D:176:ILE:HG12	1:D:234:LEU:HD23	2.01	0.42
1:A:24:ILE:HD11	1:A:260:LEU:CD1	2.50	0.42
1:D:150:THR:O	1:D:154:ILE:N	2.40	0.42
1:A:189:ILE:HG21	1:A:199:GLY:CA	2.43	0.42
1:A:242:PHE:O	1:A:246:TYR:HB3	2.18	0.42
1:C:104:ARG:O	1:C:108:GLN:HG3	2.20	0.42
1:C:123:VAL:HG13	4:C:263:HOH:O	2.19	0.42
1:B:255:GLU:O	1:B:259:THR:HG23	2.19	0.42
1:A:104:ARG:NE	1:A:133:ASP:OD2	2.44	0.42
1:D:25:SER:HA	1:D:126:PHE:O	2.20	0.42
1:B:158:TRP:CZ2	1:B:162:MET:HG3	2.54	0.41
1:A:30:ILE:HD11	2:A:301:AC2:O3'	2.19	0.41
1:A:194:ARG:HH11	1:A:198:GLN:NE2	2.19	0.41
1:C:211:LYS:H	1:C:211:LYS:HG3	1.69	0.41
1:C:231:VAL:HA	1:C:232:PRO:HD3	1.87	0.41
1:C:182:PRO:HB3	1:C:205:LEU:HD22	2.02	0.41
1:A:187:HIS:O	1:A:191:LEU:HG	2.21	0.41
1:C:91:ARG:O	1:C:91:ARG:HG3	2.20	0.41
1:C:137:PHE:O	1:C:141:LEU:HG	2.21	0.41
1:C:143:GLU:OE1	1:C:211:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:O	1:A:161:TRP:HB3	2.20	0.40
1:D:139:SER:CA	1:D:152:TRP:HZ2	2.32	0.40
1:B:158:TRP:CE2	1:B:162:MET:CG	3.03	0.40
1:C:55:VAL:HA	1:C:58:TRP:HB2	2.03	0.40
1:D:247:GLU:O	1:D:251:GLU:HG2	2.20	0.40
1:A:112:LEU:C	1:A:114:GLY:H	2.25	0.40
1:C:256:PHE:O	1:C:258:SER:N	2.54	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	224/279 (80%)	201 (90%)	11 (5%)	12 (5%)	2 0
1	B	220/279 (79%)	188 (86%)	24 (11%)	8 (4%)	3 1
1	C	214/279 (77%)	173 (81%)	36 (17%)	5 (2%)	6 2
1	D	213/279 (76%)	179 (84%)	23 (11%)	11 (5%)	2 0
All	All	871/1116 (78%)	741 (85%)	94 (11%)	36 (4%)	3 1

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	119	ALA
1	A	200	ILE
1	B	115	LYS
1	B	117	LYS
1	B	194	ARG
1	C	196	GLU
1	D	54	PRO

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Mol	Chain	Res	Type
1	D	119	ALA
1	D	166	PHE
1	D	200	ILE
1	A	112	LEU
1	A	192	ARG
1	A	193	GLY
1	A	195	ASN
1	C	127	GLU
1	C	145	GLU
1	C	257	LEU
1	A	199	GLY
1	D	118	ASP
1	D	195	ASN
1	D	228	LEU
1	A	72	THR
1	A	113	ASN
1	B	118	ASP
1	B	192	ARG
1	B	195	ASN
1	B	198	GLN
1	C	224	ASN
1	D	193	GLY
1	A	115	LYS
1	D	115	LYS
1	D	197	GLU
1	A	196	GLU
1	D	114	GLY
1	B	114	GLY

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	197/255 (77%)	184 (93%)	13 (7%)	16 14
1	B	187/255 (73%)	180 (96%)	7 (4%)	34 35
1	C	177/255 (69%)	156 (88%)	21 (12%)	5 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	185/255 (72%)	171 (92%)	14 (8%)	13	10
All	All	746/1020 (73%)	691 (93%)	55 (7%)	13	10

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	38	VAL
1	A	50	VAL
1	A	90	GLU
1	A	120	GLU
1	A	124	LEU
1	A	132	SER
1	A	139	SER
1	A	157	ASP
1	A	161	TRP
1	A	164	ASN
1	A	221	LEU
1	A	229	GLN
1	B	38	VAL
1	B	81	VAL
1	B	112	LEU
1	B	124	LEU
1	B	191	LEU
1	B	198	GLN
1	B	255	GLU
1	C	36	THR
1	C	44	LEU
1	C	47	ASP
1	C	58	TRP
1	C	101	CYS
1	C	109	LEU
1	C	115	LYS
1	C	124	LEU
1	C	148	ASN
1	C	149	GLU
1	C	150	THR
1	C	158	TRP
1	C	162	MET
1	C	171	GLU
1	C	205	LEU
1	C	212	HIS

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Mol	Chain	Res	Type
1	C	217	LEU
1	C	254	LYS
1	C	255	GLU
1	C	259	THR
1	C	260	LEU
1	D	30	ILE
1	D	43	GLN
1	D	81	VAL
1	D	124	LEU
1	D	152	TRP
1	D	157	ASP
1	D	160	ASP
1	D	165	GLN
1	D	189	ILE
1	D	191	LEU
1	D	196	GLU
1	D	202	LEU
1	D	204	TYR
1	D	229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	165	GLN
1	A	195	ASN
1	A	224	ASN
1	B	77	ASN
1	B	97	GLN
1	B	218	HIS
1	B	229	GLN
1	C	39	ASN
1	C	148	ASN
1	C	209	HIS
1	C	224	ASN
1	C	229	GLN
1	D	113	ASN
1	D	165	GLN

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)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AC2	A	301	-	12,17,17	2.31	2 (16%)	11,23,23	1.59	3 (27%)
3	UDP	D	261	-	24,26,26	0.91	0	37,40,40	1.64	5 (13%)
2	AC2	B	401	-	12,17,17	2.28	2 (16%)	11,23,23	1.73	4 (36%)
3	UDP	A	261	-	24,26,26	0.95	0	37,40,40	1.64	5 (13%)
3	UDP	B	261	-	24,26,26	0.98	1 (4%)	37,40,40	1.59	5 (13%)
2	AC2	D	601	-	12,17,17	2.30	2 (16%)	11,23,23	1.73	4 (36%)
3	UDP	C	501	-	24,26,26	0.94	0	37,40,40	1.60	5 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC2	A	301	-	-	1/3/5/5	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	D	261	-	-	4/16/32/32	0/2/2/2
2	AC2	B	401	-	-	1/3/5/5	0/2/2/2
3	UDP	A	261	-	-	0/16/32/32	0/2/2/2
3	UDP	B	261	-	-	3/16/32/32	0/2/2/2
2	AC2	D	601	-	-	1/3/5/5	0/2/2/2
3	UDP	C	501	-	-	4/16/32/32	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	AC2	O6-C6	6.53	1.36	1.23
2	D	601	AC2	O6-C6	6.34	1.36	1.23
2	B	401	AC2	O6-C6	6.26	1.36	1.23
2	D	601	AC2	C5-C6	-3.98	1.39	1.47
2	A	301	AC2	C5-C6	-3.69	1.39	1.47
2	B	401	AC2	C5-C6	-3.65	1.40	1.47
3	B	261	UDP	C6-C5	2.02	1.39	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	261	UDP	C4-N3-C2	-5.27	119.62	126.58
3	B	261	UDP	C4-N3-C2	-5.22	119.69	126.58
3	D	261	UDP	C4-N3-C2	-4.86	120.17	126.58
3	C	501	UDP	C4-N3-C2	-4.83	120.21	126.58
3	B	261	UDP	C5-C4-N3	4.17	121.07	114.84
3	C	501	UDP	N3-C2-N1	3.81	119.94	114.89
3	A	261	UDP	N3-C2-N1	3.77	119.89	114.89
3	B	261	UDP	N3-C2-N1	3.69	119.79	114.89
3	D	261	UDP	N3-C2-N1	3.69	119.79	114.89
3	A	261	UDP	C5-C4-N3	3.55	120.14	114.84
3	C	501	UDP	PA-O3A-PB	-3.40	121.14	132.83
2	D	601	AC2	C5-C6-N1	3.26	119.71	113.95
3	D	261	UDP	C5-C4-N3	3.15	119.56	114.84
3	A	261	UDP	PA-O3A-PB	-3.14	122.07	132.83
3	A	261	UDP	O4-C4-C5	-3.11	119.70	125.16
2	B	401	AC2	C5-C6-N1	3.08	119.39	113.95
3	C	501	UDP	C5-C4-N3	3.02	119.36	114.84
3	D	261	UDP	O4-C4-C5	-3.02	119.86	125.16
2	A	301	AC2	C5-C6-N1	2.94	119.14	113.95
2	B	401	AC2	C2-N1-C6	-2.81	119.92	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	UDP	O4-C4-C5	-2.80	120.24	125.16
2	B	401	AC2	C8-N7-C5	2.76	108.24	102.99
2	D	601	AC2	C2-N1-C6	-2.66	120.20	125.10
2	A	301	AC2	C8-N7-C5	2.62	107.99	102.99
3	B	261	UDP	O4-C4-C5	-2.62	120.56	125.16
2	D	601	AC2	C8-N7-C5	2.58	107.90	102.99
2	A	301	AC2	C2-N1-C6	-2.49	120.52	125.10
3	D	261	UDP	C3'-C2'-C1'	2.44	106.07	101.43
2	D	601	AC2	O6-C6-C5	-2.33	119.81	124.37
3	B	261	UDP	O4'-C1'-N1	2.21	113.42	108.36
2	B	401	AC2	O6-C6-N1	-2.01	118.28	120.65

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	UDP	C5'-O5'-PA-O1A
3	C	501	UDP	C5'-O5'-PA-O3A
3	D	261	UDP	C5'-O5'-PA-O1A
3	D	261	UDP	C5'-O5'-PA-O2A
3	C	501	UDP	C3'-C4'-C5'-O5'
3	C	501	UDP	O4'-C4'-C5'-O5'
2	A	301	AC2	C3'-C2'-O1'-C1'
2	B	401	AC2	C3'-C2'-O1'-C1'
2	D	601	AC2	C3'-C2'-O1'-C1'
3	D	261	UDP	C4'-C5'-O5'-PA
3	B	261	UDP	PA-O3A-PB-O1B
3	B	261	UDP	PA-O3A-PB-O2B
3	B	261	UDP	PA-O3A-PB-O3B
3	D	261	UDP	C5'-O5'-PA-O3A

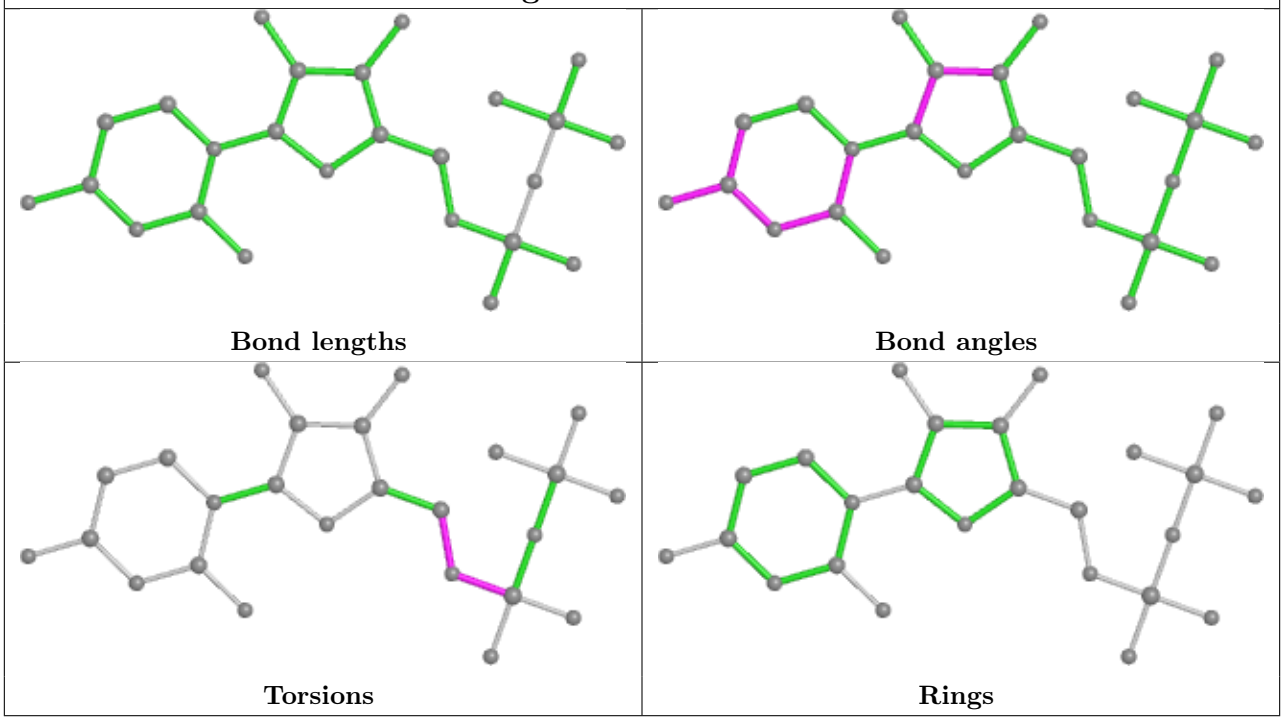
There are no ring outliers.

5 monomers are involved in 17 short contacts:

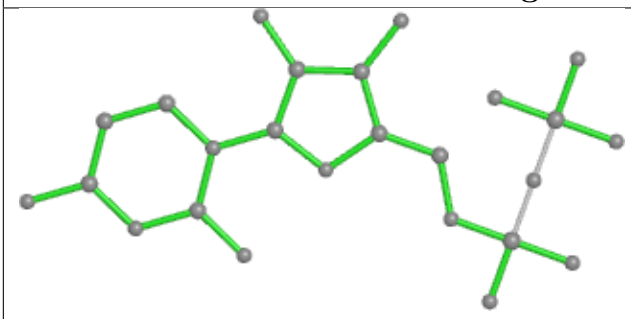
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AC2	9	0
3	D	261	UDP	1	0
2	B	401	AC2	2	0
3	A	261	UDP	2	0
2	D	601	AC2	3	0

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.

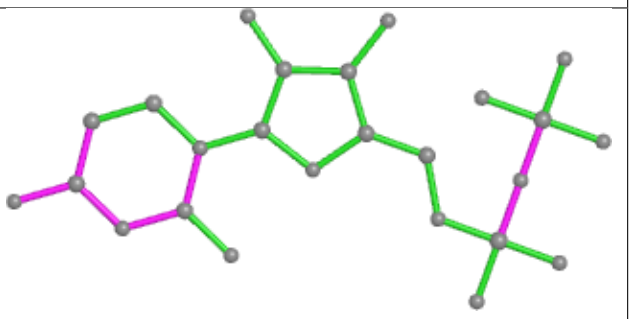
Ligand UDP D 261



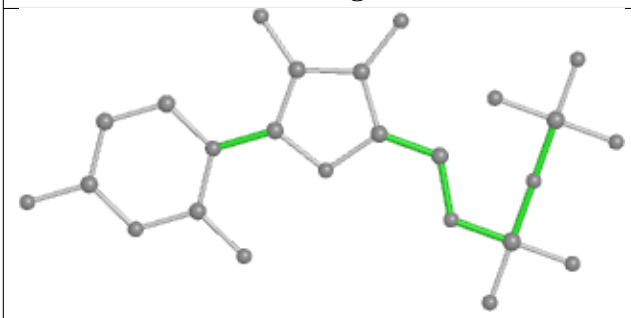
Ligand UDP A 261



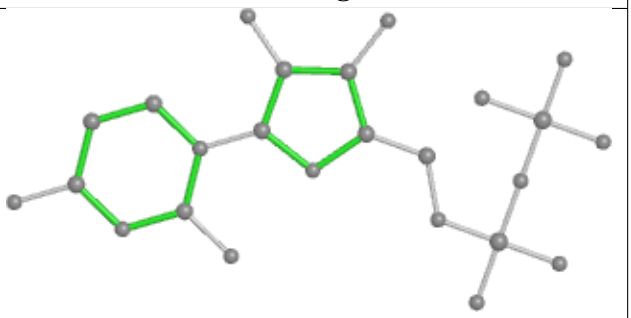
Bond lengths



Bond angles

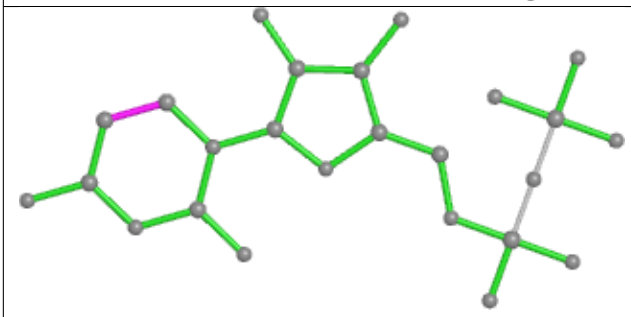


Torsions

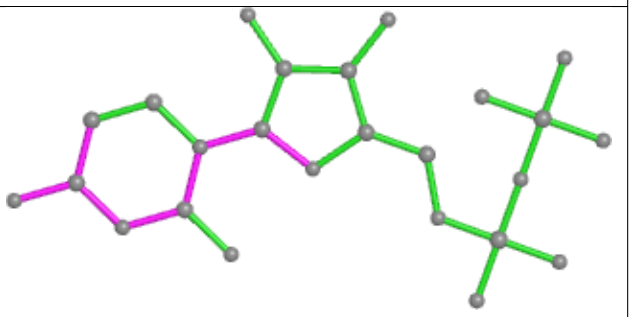


Rings

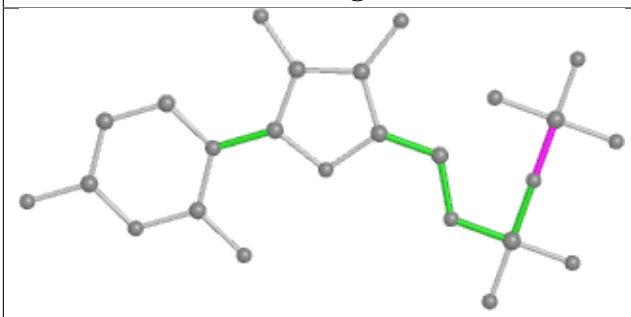
Ligand UDP B 261



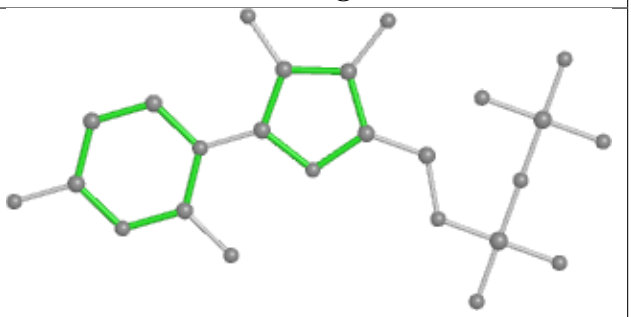
Bond lengths



Bond angles

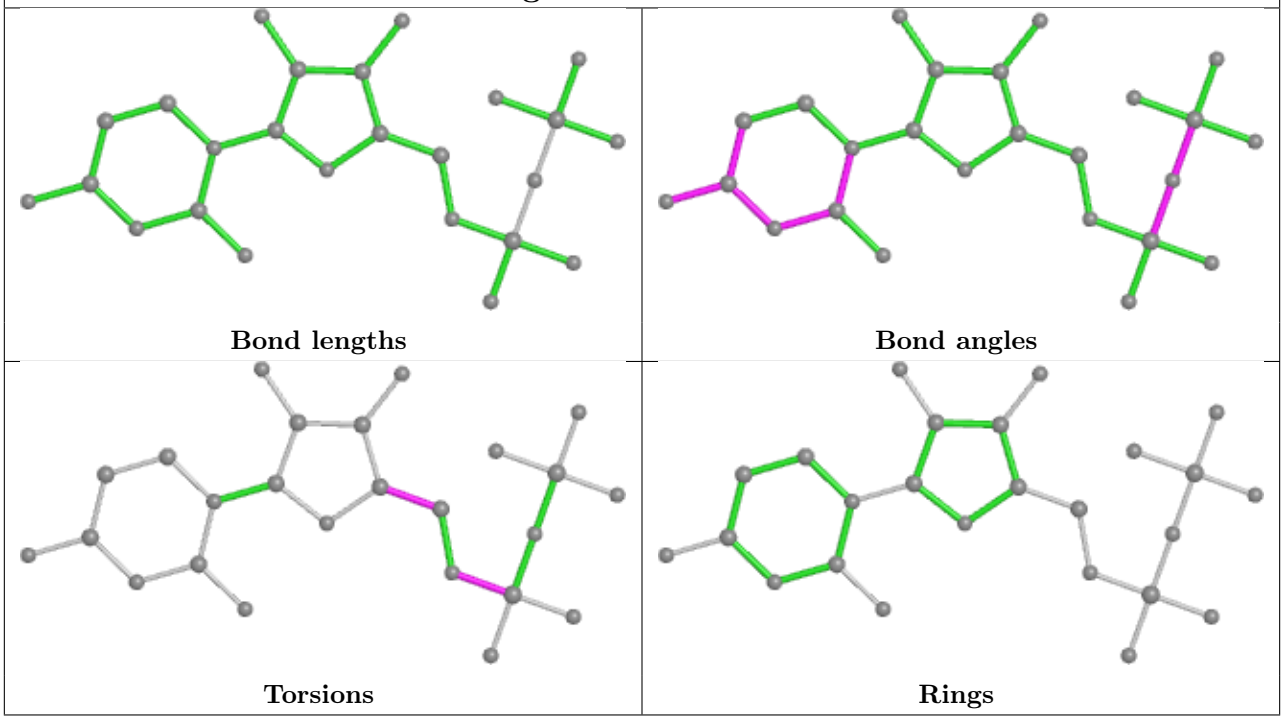


Torsions



Rings

Ligand UDP C 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/279 (82%)	0.26	2 (0%)	84	86	21, 32, 43, 49	0
1	B	226/279 (81%)	0.25	1 (0%)	92	93	21, 32, 43, 47	0
1	C	222/279 (79%)	1.17	48 (21%)	0	0	44, 55, 63, 65	0
1	D	221/279 (79%)	1.03	39 (17%)	1	1	45, 54, 59, 62	0
All	All	899/1116 (80%)	0.67	90 (10%)	7	9	21, 45, 60, 65	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	191	LEU	8.1
1	C	96	PHE	6.9
1	D	158	TRP	6.2
1	C	238	VAL	6.0
1	C	180	ALA	5.4
1	D	21	ILE	5.2
1	D	154	ILE	4.5
1	C	163	ASN	4.5
1	C	86	TYR	4.3
1	D	260	LEU	4.3
1	C	176	ILE	4.3
1	D	30	ILE	4.1
1	C	228	LEU	4.1
1	C	193	GLY	4.1
1	D	249	LEU	4.0
1	D	196	GLU	3.9
1	C	33	GLY	3.8
1	D	40	ILE	3.7
1	C	78	GLY	3.6
1	D	31	ALA	3.5
1	D	84	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	223	THR	3.4
1	D	257	LEU	3.4
1	C	221	LEU	3.4
1	C	216	LEU	3.4
1	D	109	LEU	3.3
1	C	236	LEU	3.3
1	D	152	TRP	3.3
1	C	114	GLY	3.2
1	C	56	ALA	3.1
1	C	204	TYR	3.1
1	C	250	VAL	3.1
1	C	158	TRP	3.1
1	C	178	LEU	3.1
1	D	225	PHE	3.0
1	C	36	THR	3.0
1	C	253	VAL	2.9
1	C	28	GLY	2.9
1	C	217	LEU	2.9
1	C	201	PRO	2.9
1	C	162	MET	2.9
1	C	26	ILE	2.8
1	C	21	ILE	2.8
1	D	202	LEU	2.8
1	D	215	TRP	2.8
1	D	86	TYR	2.7
1	C	260	LEU	2.7
1	D	186	LEU	2.7
1	C	259	THR	2.6
1	C	227	TYR	2.6
1	C	245	LYS	2.6
1	C	166	PHE	2.5
1	D	189	ILE	2.5
1	A	71	LEU	2.5
1	D	115	LYS	2.5
1	D	125	PHE	2.5
1	C	99	TYR	2.4
1	D	161	TRP	2.4
1	D	204	TYR	2.4
1	D	102	LEU	2.4
1	D	191	LEU	2.4
1	D	113	ASN	2.4
1	C	146	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	55	VAL	2.3
1	D	233	ILE	2.3
1	C	118	ASP	2.3
1	D	146	SER	2.3
1	D	122	PRO	2.2
1	C	155	TYR	2.2
1	C	120	GLU	2.2
1	C	24	ILE	2.2
1	C	44	LEU	2.2
1	D	96	PHE	2.1
1	D	228	LEU	2.1
1	D	238	VAL	2.1
1	C	125	PHE	2.1
1	D	105	ILE	2.1
1	C	102	LEU	2.1
1	D	178	LEU	2.1
1	D	99	TYR	2.1
1	C	40	ILE	2.1
1	C	121	LYS	2.1
1	D	246	TYR	2.1
1	C	79	GLY	2.1
1	B	191	LEU	2.0
1	C	190	TYR	2.0
1	D	210	TYR	2.0
1	A	86	TYR	2.0
1	D	155	TYR	2.0
1	C	104	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

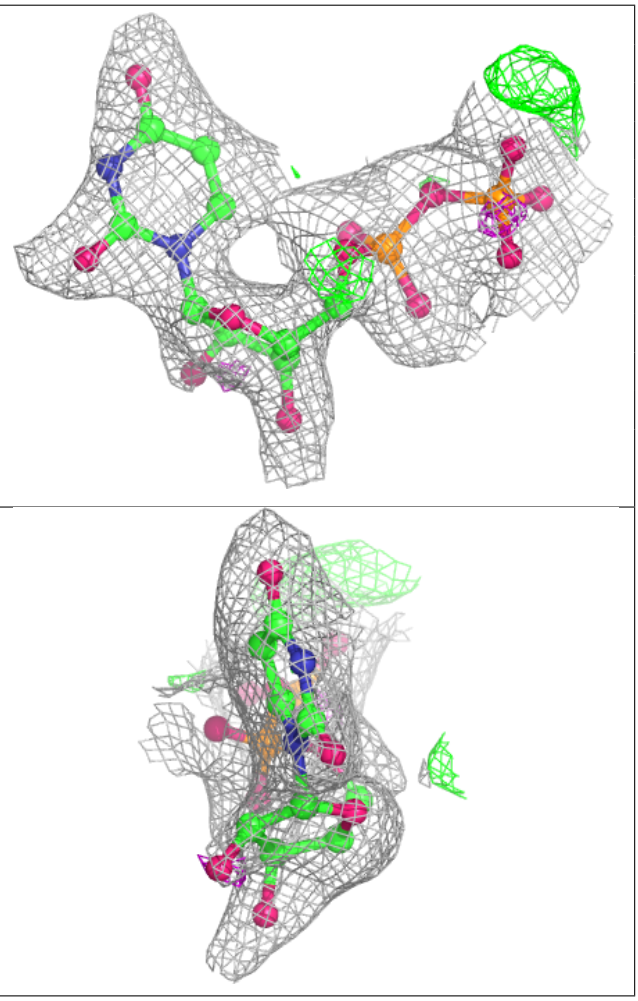
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

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

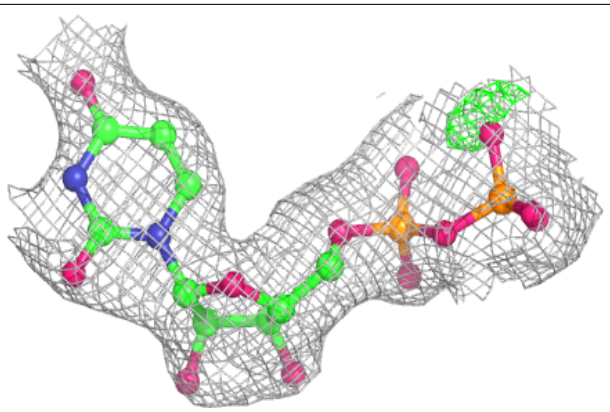
Electron density around UDP D 261:

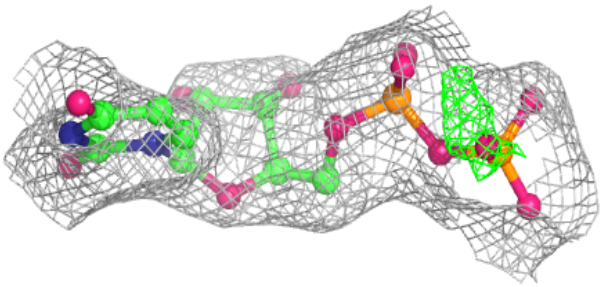
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

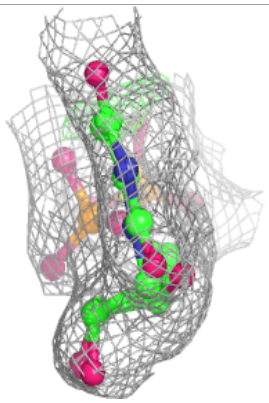


Electron density around UDP C 501:

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

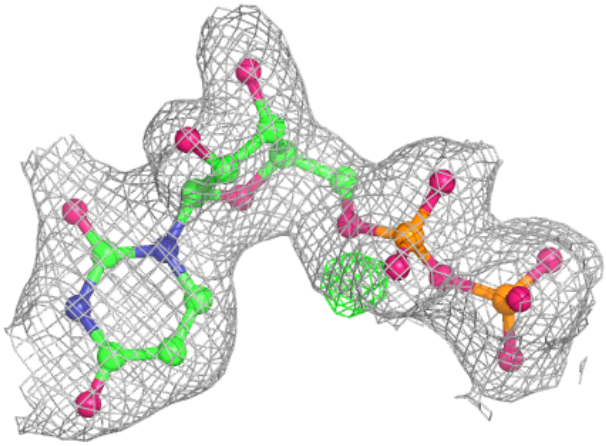


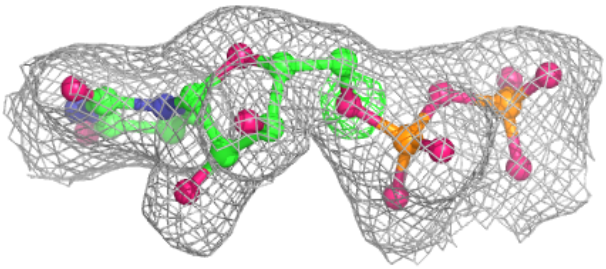


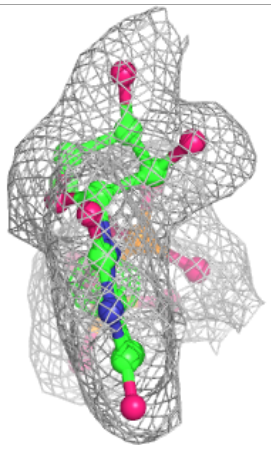


Electron density around UDP A 261:

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

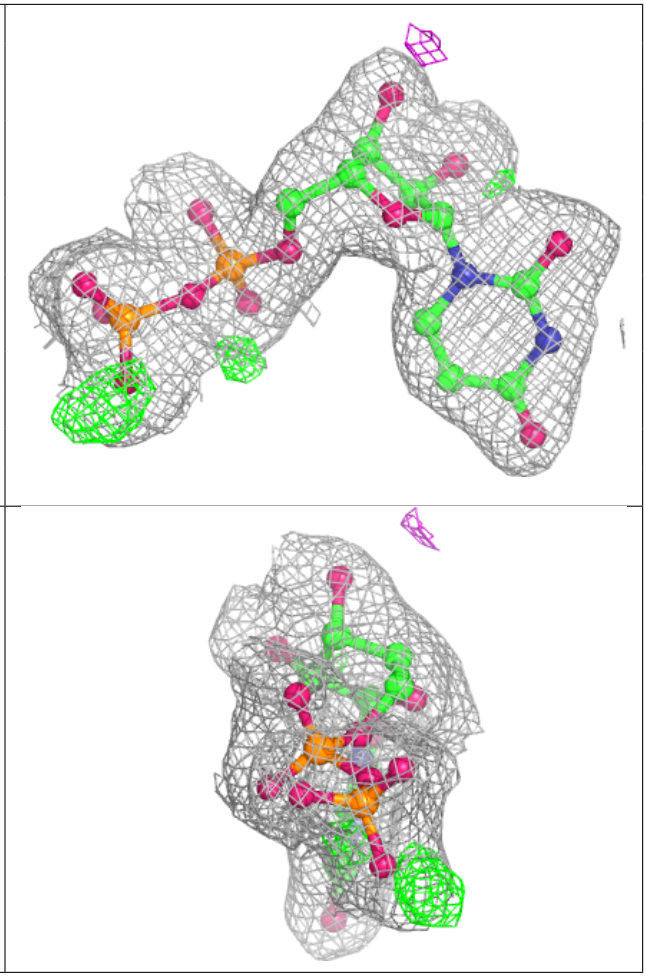






Electron density around UDP B 261:

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



6.5 Other polymers (i)

There are no such residues in this entry.