Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 01:27 PM EDT

PDB ID	:	2A2Z
Title	:	Crystal Structure of human deoxycytidine kinase in complex with deoxycytidine and uridine diphosphate
Authors	:	Godsey, M.H.; Ort, S.; Sabini, E.; Konrad, M.; Lavie, A.
Deposited on	:	2005-06-23
Resolution	:	3.02 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:

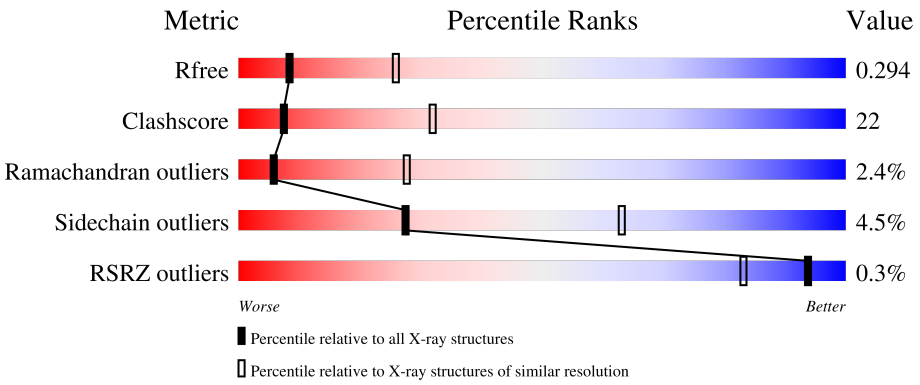
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	248	54% 33% • 10%
1	B	248	48% 38% • 11%
1	C	248	52% 34% • 10%
1	D	248	% 49% 37% • 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7406 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	222	1796	1156	299	332	9	0	0	0
1	B	221	1795	1156	295	335	9	0	0	0
1	C	222	1800	1158	299	334	9	0	0	0
1	D	220	1778	1148	293	328	9	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P27707
A	-1	SER	-	cloning artifact	UNP P27707
A	0	HIS	-	cloning artifact	UNP P27707
A	?	-	GLN	deletion	UNP P27707
A	?	-	ASP	deletion	UNP P27707
A	?	-	GLU	deletion	UNP P27707
A	?	-	PHE	deletion	UNP P27707
A	?	-	GLU	deletion	UNP P27707
A	?	-	GLU	deletion	UNP P27707
A	?	-	LEU	deletion	UNP P27707
A	?	-	THR	deletion	UNP P27707
A	?	-	MET	deletion	UNP P27707
A	?	-	SER	deletion	UNP P27707
A	?	-	GLN	deletion	UNP P27707
A	?	-	LYS	deletion	UNP P27707
A	?	-	ASN	deletion	UNP P27707
A	?	-	GLY	deletion	UNP P27707
A	?	-	GLY	deletion	UNP P27707
B	-2	GLY	-	cloning artifact	UNP P27707
B	-1	SER	-	cloning artifact	UNP P27707
B	0	HIS	-	cloning artifact	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P27707
B	?	-	ASP	deletion	UNP P27707
B	?	-	GLU	deletion	UNP P27707
B	?	-	PHE	deletion	UNP P27707
B	?	-	GLU	deletion	UNP P27707
B	?	-	GLU	deletion	UNP P27707
B	?	-	LEU	deletion	UNP P27707
B	?	-	THR	deletion	UNP P27707
B	?	-	MET	deletion	UNP P27707
B	?	-	SER	deletion	UNP P27707
B	?	-	GLN	deletion	UNP P27707
B	?	-	LYS	deletion	UNP P27707
B	?	-	ASN	deletion	UNP P27707
B	?	-	GLY	deletion	UNP P27707
B	?	-	GLY	deletion	UNP P27707
C	-2	GLY	-	cloning artifact	UNP P27707
C	-1	SER	-	cloning artifact	UNP P27707
C	0	HIS	-	cloning artifact	UNP P27707
C	?	-	GLN	deletion	UNP P27707
C	?	-	ASP	deletion	UNP P27707
C	?	-	GLU	deletion	UNP P27707
C	?	-	PHE	deletion	UNP P27707
C	?	-	GLU	deletion	UNP P27707
C	?	-	GLU	deletion	UNP P27707
C	?	-	LEU	deletion	UNP P27707
C	?	-	THR	deletion	UNP P27707
C	?	-	MET	deletion	UNP P27707
C	?	-	SER	deletion	UNP P27707
C	?	-	GLN	deletion	UNP P27707
C	?	-	LYS	deletion	UNP P27707
C	?	-	ASN	deletion	UNP P27707
C	?	-	GLY	deletion	UNP P27707
C	?	-	GLY	deletion	UNP P27707
D	-2	GLY	-	cloning artifact	UNP P27707
D	-1	SER	-	cloning artifact	UNP P27707
D	0	HIS	-	cloning artifact	UNP P27707
D	?	-	GLN	deletion	UNP P27707
D	?	-	ASP	deletion	UNP P27707
D	?	-	GLU	deletion	UNP P27707
D	?	-	PHE	deletion	UNP P27707
D	?	-	GLU	deletion	UNP P27707
D	?	-	GLU	deletion	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP P27707
D	?	-	THR	deletion	UNP P27707
D	?	-	MET	deletion	UNP P27707
D	?	-	SER	deletion	UNP P27707
D	?	-	GLN	deletion	UNP P27707
D	?	-	LYS	deletion	UNP P27707
D	?	-	ASN	deletion	UNP P27707
D	?	-	GLY	deletion	UNP P27707
D	?	-	GLY	deletion	UNP P27707

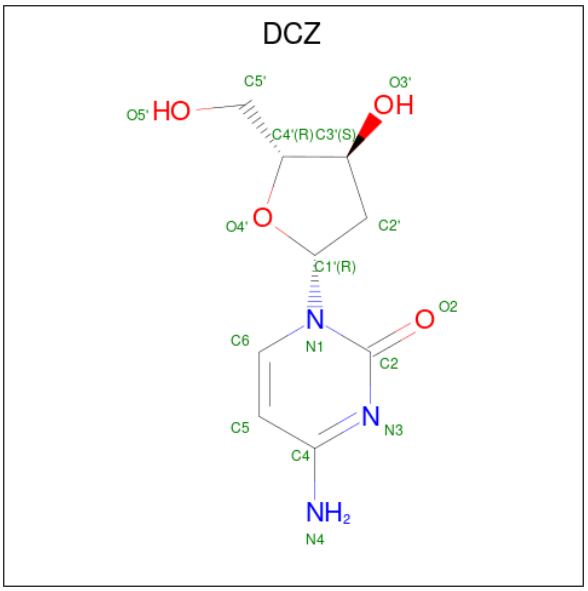
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

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

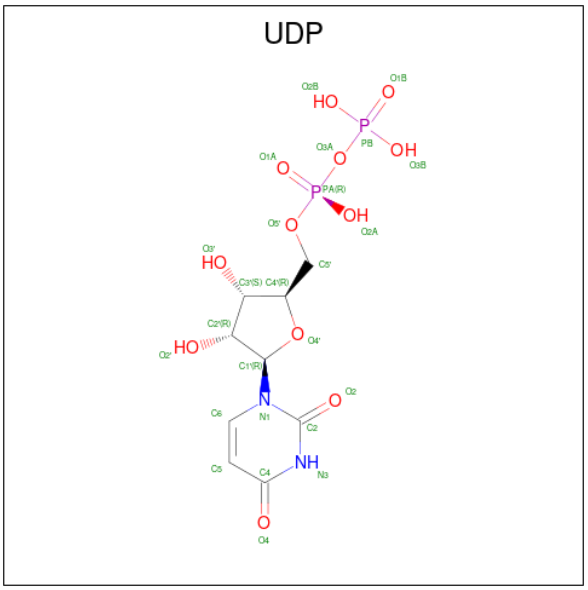
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 2'-DEOXYCYTIDINE (three-letter code: DCZ) (formula: $C_9H_{13}N_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	16	9	3	4	0	0
			Total	C	N	O		
4	B	1	16	9	3	4	0	0
			Total	C	N	O		
4	C	1	16	9	3	4	0	0
			Total	C	N	O		
4	D	1	16	9	3	4	0	0

- Molecule 5 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		
5	A	1	25	9	2	12	2	0	0
5	B	1	25	9	2	12	2	0	0
5	C	1	25	9	2	12	2	0	0
5	D	1	25	9	2	12	2	0	0

- Molecule 6 is water.

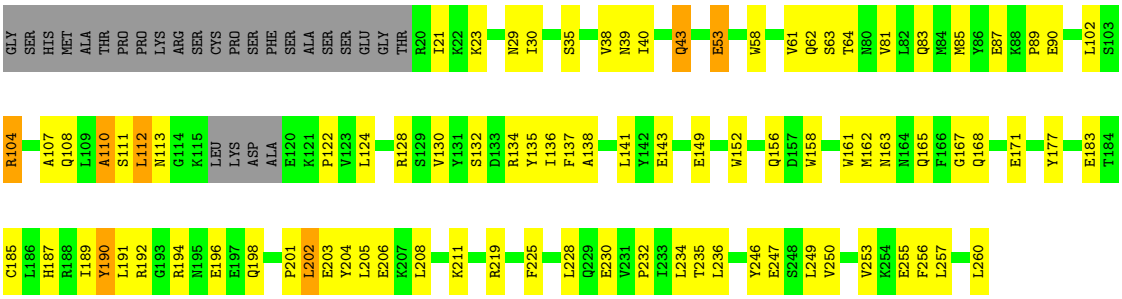
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	23	23	23	0	0
6	B	15	15	15	0	0
6	C	22	22	22	0	0
6	D	7	7	7	0	0

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.

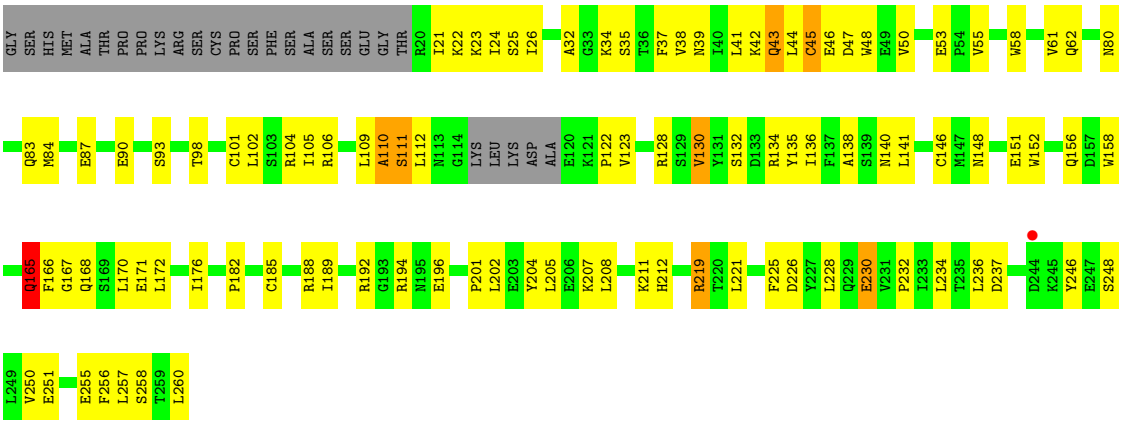
• Molecule 1: Deoxycytidine kinase

Chain A: 54% 33% • 10%



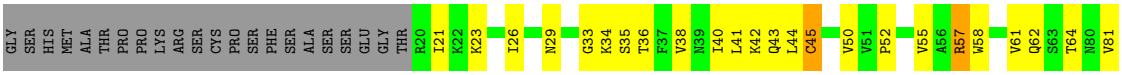
• Molecule 1: Deoxycytidine kinase

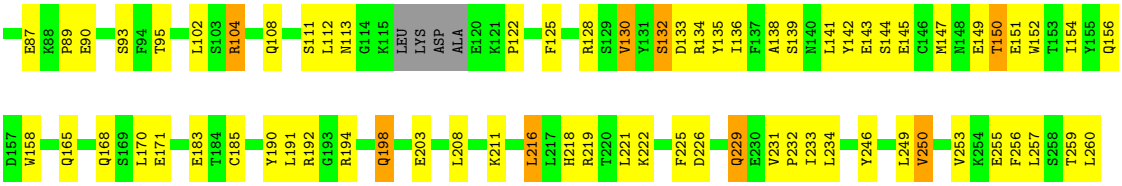
Chain B: 48% 38% • 11%



• Molecule 1: Deoxycytidine kinase

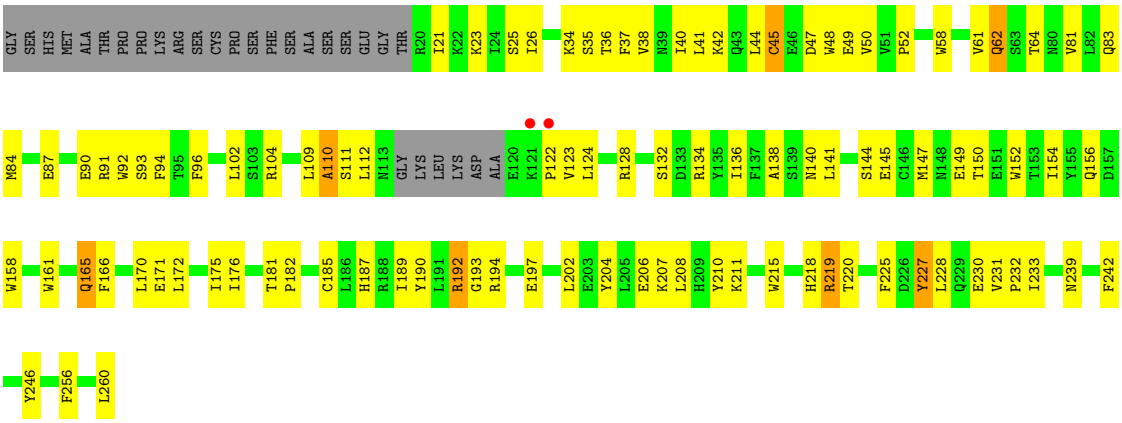
Chain C: 52% 34% • 10%





• Molecule 1: Deoxycytidine kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.18Å 110.85Å 155.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.66 – 3.02 29.66 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.66-3.02) 99.4 (29.66-3.02)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.300 0.245 , 0.294	Depositor DCC
R_{free} test set	2244 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7406	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 53.89 % 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 3.9513e-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: UDP, DCZ, MG, CA

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	0.47	0/1841	0.64	0/2505
1	B	0.46	1/1840 (0.1%)	0.62	0/2502
1	C	0.46	0/1845	0.63	0/2510
1	D	0.44	0/1823	0.61	0/2481
All	All	0.46	1/7349 (0.0%)	0.62	0/9998

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	CYS	CB-SG	-5.03	1.73	1.81

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	1796	0	1694	70	0
1	B	1795	0	1699	88	0
1	C	1800	0	1698	82	0
1	D	1778	0	1679	83	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	13	0	0
4	B	16	0	13	0	0
4	C	16	0	13	0	0
4	D	16	0	13	0	0
5	A	25	0	11	0	0
5	B	25	0	11	2	0
5	C	25	0	11	3	0
5	D	25	0	11	0	0
6	A	23	0	0	4	0
6	B	15	0	0	1	0
6	C	22	0	0	2	0
6	D	7	0	0	1	0
All	All	7406	0	6866	315	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 22.

All (315) 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:C:257:LEU:HA	1:C:260:LEU:HD12	1.48	0.92
1:C:246:TYR:O	1:C:250:VAL:HG23	1.73	0.88
1:A:21:ILE:HG23	1:A:122:PRO:HB2	1.58	0.86
1:D:150:THR:O	1:D:154:ILE:HG13	1.78	0.84
1:A:234:LEU:HG	1:A:236:LEU:HD21	1.60	0.83
1:C:35:SER:O	1:C:38:VAL:HG12	1.81	0.81
1:A:168:GLN:O	1:A:171:GLU:HG3	1.83	0.79
1:C:58:TRP:O	1:C:81:VAL:HG12	1.83	0.78
1:A:134:ARG:HD3	1:A:135:TYR:CE1	2.18	0.77
1:D:185:CYS:O	1:D:189:ILE:HG13	1.84	0.77
1:A:58:TRP:O	1:A:81:VAL:HG12	1.84	0.77
1:B:219:ARG:HB3	1:B:219:ARG:HH11	1.47	0.76
1:A:202:LEU:O	1:A:206:GLU:HG3	1.86	0.76
1:C:219:ARG:NH2	1:C:231:VAL:O	2.19	0.75
1:D:219:ARG:NE	1:D:233:ILE:HD12	2.03	0.74
1:C:194:ARG:O	1:C:198:GLN:NE2	2.21	0.74
1:C:26:ILE:HD11	1:C:125:PHE:HD2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:VAL:HG22	6:C:521:HOH:O	1.88	0.72
1:A:257:LEU:HD23	1:A:260:LEU:HD12	1.72	0.72
1:C:249:LEU:O	1:C:253:VAL:HG23	1.89	0.72
1:C:23:LYS:HE2	1:C:171:GLU:O	1.89	0.71
1:D:35:SER:O	1:D:38:VAL:HG12	1.90	0.71
1:B:101:CYS:SG	1:B:130:VAL:HG12	2.31	0.71
1:C:62:GLN:HG3	1:C:62:GLN:O	1.90	0.71
1:A:23:LYS:HE2	1:A:171:GLU:O	1.91	0.71
1:D:44:LEU:O	1:D:45:CYS:HB2	1.89	0.70
1:B:128:ARG:HG3	1:B:128:ARG:HH11	1.57	0.69
1:B:136:ILE:HD13	1:B:211:LYS:HB3	1.72	0.69
1:C:232:PRO:HG2	1:C:260:LEU:HD21	1.75	0.69
1:B:134:ARG:NH2	1:B:156:GLN:HB3	2.08	0.68
1:D:136:ILE:HD13	1:D:211:LYS:HB3	1.75	0.68
1:B:26:ILE:HD13	1:B:176:ILE:HB	1.76	0.67
1:A:192:ARG:HG2	1:A:194:ARG:H	1.58	0.67
1:B:219:ARG:HH11	1:B:219:ARG:CB	2.06	0.67
1:D:48:TRP:CD1	1:D:123:VAL:HB	2.30	0.67
1:B:202:LEU:HA	1:B:205:LEU:HD12	1.77	0.67
1:B:134:ARG:HD3	1:B:135:TYR:CE1	2.30	0.66
1:D:81:VAL:HG13	1:D:96:PHE:HD1	1.60	0.66
1:D:161:TRP:CE2	1:D:165:GLN:NE2	2.64	0.66
1:C:149:GLU:HB3	1:D:62:GLN:HG2	1.77	0.66
1:B:45:CYS:C	1:B:47:ASP:H	2.00	0.66
1:C:104:ARG:NH1	1:C:128:ARG:HB2	2.10	0.65
1:D:90:GLU:H	1:D:90:GLU:CD	1.99	0.65
1:B:45:CYS:SG	1:B:47:ASP:HB2	2.36	0.65
1:D:175:ILE:HD12	1:D:231:VAL:HG11	1.78	0.65
1:B:44:LEU:O	1:B:45:CYS:HB2	1.97	0.65
1:A:104:ARG:O	1:A:108:GLN:HG3	1.96	0.65
1:B:80:ASN:O	1:B:84:MET:HG3	1.97	0.64
1:B:37:PHE:O	1:B:41:LEU:HD13	1.99	0.64
1:B:246:TYR:O	1:B:250:VAL:HG12	1.96	0.64
1:C:134:ARG:HD3	1:C:135:TYR:CE1	2.34	0.63
1:A:234:LEU:HD22	1:A:256:PHE:HB2	1.80	0.63
1:B:39:ASN:HD22	1:B:42:LYS:HE2	1.63	0.63
1:B:55:VAL:HG21	1:B:194:ARG:NH1	2.14	0.63
1:A:149:GLU:HB3	1:B:62:GLN:HG2	1.82	0.62
1:B:35:SER:O	1:B:38:VAL:HG12	1.99	0.62
1:C:41:LEU:C	1:C:43:GLN:H	2.03	0.62
1:C:104:ARG:HH12	1:C:128:ARG:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:OD1	1:B:151:GLU:HG3	2.01	0.61
1:B:130:VAL:HG22	6:B:418:HOH:O	2.01	0.61
1:C:21:ILE:HG23	1:C:122:PRO:HB2	1.83	0.61
1:C:62:GLN:O	1:C:64:THR:HG23	2.00	0.61
1:A:234:LEU:CG	1:A:236:LEU:HD21	2.29	0.60
1:C:190:TYR:HA	1:C:198:GLN:OE1	2.02	0.60
1:B:22:LYS:HE3	1:B:123:VAL:HG22	1.83	0.60
1:B:194:ARG:HG2	1:B:196:GLU:OE1	2.02	0.60
1:A:187:HIS:CE1	1:A:191:LEU:HD22	2.37	0.60
1:B:128:ARG:HG3	1:B:128:ARG:NH1	2.16	0.60
1:A:62:GLN:O	1:A:62:GLN:HG3	2.02	0.59
1:A:194:ARG:O	1:A:198:GLN:NE2	2.33	0.59
1:C:192:ARG:HB2	5:C:501:UDP:H4'	1.84	0.59
1:D:140:ASN:ND2	1:D:207:LYS:HB3	2.17	0.59
1:D:34:LYS:NZ	1:D:128:ARG:NH2	2.50	0.59
1:A:136:ILE:CD1	1:A:211:LYS:HB3	2.33	0.59
1:A:35:SER:O	1:A:38:VAL:HG12	2.01	0.59
1:C:62:GLN:HG2	1:D:149:GLU:HB3	1.85	0.59
1:C:150:THR:O	1:C:154:ILE:HG13	2.03	0.59
1:A:204:TYR:CE2	1:A:208:LEU:HD11	2.38	0.59
1:B:53:GLU:HG3	1:B:104:ARG:NH1	2.19	0.58
1:B:32:ALA:O	1:B:188:ARG:NH1	2.36	0.58
1:B:152:TRP:O	1:B:156:GLN:HG3	2.03	0.58
1:C:93:SER:HB3	1:C:141:LEU:HD13	1.85	0.58
1:D:187:HIS:O	1:D:190:TYR:HB3	2.03	0.58
1:D:140:ASN:HD21	1:D:207:LYS:HB3	1.68	0.58
1:D:26:ILE:HD12	1:D:176:ILE:HB	1.85	0.58
1:A:234:LEU:HG	1:A:236:LEU:CD2	2.34	0.56
1:A:201:PRO:HB2	1:A:203:GLU:OE1	2.05	0.56
1:A:62:GLN:O	1:A:64:THR:HG23	2.06	0.56
1:D:50:VAL:HG12	1:D:52:PRO:HD3	1.86	0.56
1:A:30:ILE:O	1:A:185:CYS:HB3	2.06	0.55
1:B:34:LYS:N	5:B:401:UDP:O3B	2.39	0.55
1:B:219:ARG:HH11	1:B:219:ARG:CG	2.19	0.55
1:C:95:THR:HG23	1:D:94:PHE:CE2	2.42	0.55
1:C:158:TRP:HD1	1:D:102:LEU:HD22	1.72	0.55
1:D:37:PHE:O	1:D:41:LEU:HD13	2.06	0.55
1:B:35:SER:HA	1:B:38:VAL:HG12	1.88	0.55
1:B:23:LYS:HE2	1:B:171:GLU:O	2.07	0.55
1:C:102:LEU:HD22	1:D:158:TRP:HD1	1.71	0.55
1:D:182:PRO:HB2	1:D:202:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:SER:O	1:A:136:ILE:HB	2.06	0.55
1:D:204:TYR:CE2	1:D:208:LEU:HD11	2.41	0.54
1:C:136:ILE:HD13	1:C:211:LYS:HB3	1.90	0.54
1:A:107:ALA:O	1:A:110:ALA:HB3	2.07	0.54
1:B:39:ASN:HD22	1:B:42:LYS:CE	2.20	0.54
1:B:165:GLN:N	1:B:165:GLN:HE21	2.05	0.54
1:B:90:GLU:CD	1:B:90:GLU:H	2.10	0.54
1:C:111:SER:C	1:C:113:ASN:H	2.11	0.54
1:C:90:GLU:H	1:C:90:GLU:CD	2.11	0.53
1:C:218:HIS:O	1:C:219:ARG:HB2	2.07	0.53
1:B:182:PRO:HB2	1:B:202:LEU:HD11	1.90	0.53
1:D:182:PRO:HB2	1:D:202:LEU:CD1	2.39	0.53
1:D:35:SER:HA	1:D:38:VAL:HG12	1.89	0.53
1:B:93:SER:OG	1:B:141:LEU:HD22	2.09	0.53
1:A:249:LEU:O	1:A:253:VAL:HG23	2.09	0.53
1:A:192:ARG:HD3	1:A:194:ARG:HB2	1.90	0.53
1:C:234:LEU:HD22	1:C:256:PHE:HB2	1.91	0.52
1:A:143:GLU:HG3	6:A:318:HOH:O	2.09	0.52
1:C:192:ARG:HD2	6:C:523:HOH:O	2.08	0.52
1:B:225:PHE:CD1	1:B:225:PHE:N	2.77	0.52
1:C:57:ARG:O	1:C:57:ARG:HG3	2.09	0.52
1:D:192:ARG:HD3	1:D:197:GLU:OE1	2.10	0.52
1:C:229:GLN:CA	1:C:229:GLN:HE21	2.22	0.52
1:D:192:ARG:HG2	1:D:194:ARG:H	1.75	0.52
1:D:219:ARG:HE	1:D:233:ILE:CD1	2.23	0.52
1:D:37:PHE:O	1:D:41:LEU:CD1	2.58	0.52
1:D:132:SER:O	1:D:136:ILE:HB	2.10	0.52
1:C:152:TRP:CD1	1:C:156:GLN:NE2	2.77	0.52
1:C:168:GLN:HE21	1:C:168:GLN:HA	1.75	0.52
1:B:109:LEU:O	1:B:112:LEU:HB2	2.10	0.51
1:D:219:ARG:HE	1:D:233:ILE:HD12	1.72	0.51
1:B:21:ILE:HG23	1:B:122:PRO:HB2	1.92	0.51
1:B:38:VAL:HG22	1:B:50:VAL:HG21	1.92	0.51
1:B:102:LEU:O	1:B:106:ARG:HG3	2.11	0.51
1:C:216:LEU:HD12	1:C:233:ILE:HD13	1.92	0.51
1:B:48:TRP:CD1	1:B:123:VAL:HB	2.45	0.51
1:D:206:GLU:HG2	1:D:210:TYR:CE2	2.45	0.51
1:A:40:ILE:HD13	1:A:246:TYR:CD2	2.46	0.51
1:B:80:ASN:HB3	1:B:83:GLN:HB3	1.93	0.51
1:C:139:SER:HA	1:C:152:TRP:CH2	2.45	0.51
1:C:41:LEU:O	1:C:43:GLN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:HA	1:C:138:ALA:HB3	1.93	0.51
1:C:38:VAL:HG22	1:C:50:VAL:HG21	1.92	0.50
1:C:142:TYR:OH	1:C:149:GLU:OE2	2.23	0.50
1:A:29:ASN:HB3	1:A:185:CYS:SG	2.51	0.50
1:A:134:ARG:HD3	1:A:135:TYR:CZ	2.46	0.50
1:B:132:SER:O	1:B:136:ILE:HB	2.12	0.50
1:A:136:ILE:HD12	1:A:211:LYS:HB3	1.93	0.50
1:B:221:LEU:HD23	1:B:221:LEU:C	2.32	0.50
1:C:35:SER:HA	1:C:38:VAL:HG12	1.93	0.50
1:C:40:ILE:HD13	1:C:246:TYR:CD2	2.46	0.50
1:A:85:MET:O	1:A:89:PRO:HD3	2.12	0.50
1:A:128:ARG:HD3	6:A:315:HOH:O	2.12	0.50
1:B:192:ARG:HG2	1:B:194:ARG:H	1.77	0.50
1:D:109:LEU:HD23	1:D:170:LEU:HD21	1.94	0.49
1:D:232:PRO:HG2	1:D:260:LEU:HD21	1.93	0.49
1:B:34:LYS:HE3	1:B:128:ARG:HG2	1.94	0.49
1:C:234:LEU:HB2	1:C:256:PHE:CD2	2.47	0.49
1:A:104:ARG:HH12	1:A:128:ARG:HB2	1.77	0.49
1:A:235:THR:C	1:A:236:LEU:HD23	2.32	0.49
1:D:215:TRP:O	1:D:219:ARG:HD2	2.12	0.49
1:D:218:HIS:O	1:D:220:THR:HG23	2.12	0.49
1:A:104:ARG:NH1	1:A:128:ARG:HB2	2.27	0.49
1:A:128:ARG:HH11	1:A:128:ARG:HG3	1.77	0.49
1:C:33:GLY:N	5:C:501:UDP:O3B	2.39	0.49
1:B:136:ILE:CD1	1:B:211:LYS:HB3	2.43	0.49
1:B:185:CYS:O	1:B:189:ILE:HG13	2.13	0.49
1:A:190:TYR:HD2	1:A:190:TYR:O	1.95	0.49
1:B:165:GLN:HB3	1:B:166:PHE:H	1.41	0.49
1:C:36:THR:O	1:C:40:ILE:HG13	2.13	0.49
1:C:132:SER:O	1:C:136:ILE:HB	2.12	0.49
1:D:225:PHE:CD1	1:D:225:PHE:N	2.81	0.48
1:B:38:VAL:HG22	1:B:50:VAL:CG2	2.43	0.48
1:B:45:CYS:C	1:B:47:ASP:N	2.66	0.48
1:D:36:THR:O	1:D:40:ILE:HG13	2.13	0.48
1:D:81:VAL:HG13	1:D:96:PHE:CD1	2.45	0.48
1:D:34:LYS:HZ2	1:D:128:ARG:HH21	1.62	0.48
1:D:109:LEU:HD11	1:D:166:PHE:CB	2.43	0.48
1:A:90:GLU:H	1:A:90:GLU:CD	2.17	0.48
1:B:62:GLN:O	1:B:62:GLN:HG3	2.13	0.48
1:C:90:GLU:OE2	1:C:90:GLU:N	2.37	0.48
1:D:23:LYS:CE	1:D:171:GLU:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:O	1:A:250:VAL:HG12	2.14	0.48
1:B:25:SER:HB3	1:B:172:LEU:HD13	1.95	0.48
1:C:29:ASN:HB3	1:C:185:CYS:SG	2.54	0.48
1:D:47:ASP:O	1:D:48:TRP:HD1	1.96	0.48
1:D:62:GLN:O	1:D:62:GLN:HG3	2.13	0.48
1:A:111:SER:C	1:A:113:ASN:H	2.17	0.48
1:B:61:VAL:O	1:B:62:GLN:HB3	2.14	0.48
1:D:175:ILE:HD12	1:D:231:VAL:CG1	2.44	0.48
1:D:23:LYS:HE2	1:D:171:GLU:O	2.13	0.48
1:D:34:LYS:HZ2	1:D:128:ARG:NH2	2.12	0.48
1:D:104:ARG:NH1	1:D:128:ARG:HB2	2.29	0.48
1:C:136:ILE:HG22	1:C:208:LEU:HD22	1.95	0.48
1:C:221:LEU:C	1:C:221:LEU:HD23	2.34	0.47
1:B:248:SER:O	1:B:251:GLU:HB3	2.14	0.47
1:C:143:GLU:CD	1:C:211:LYS:HZ1	2.17	0.47
1:D:25:SER:HB3	1:D:172:LEU:HD13	1.96	0.47
1:A:130:VAL:HG21	1:A:163:ASN:HD21	1.80	0.47
1:A:137:PHE:O	1:A:141:LEU:HG	2.14	0.47
1:C:226:ASP:O	1:C:229:GLN:HB2	2.15	0.47
1:D:49:GLU:O	1:D:124:LEU:HD12	2.15	0.47
1:D:91:ARG:NH1	1:D:92:TRP:CZ3	2.83	0.47
1:B:232:PRO:HB2	1:B:256:PHE:CE2	2.50	0.47
1:C:150:THR:HG23	1:D:64:THR:OG1	2.14	0.47
1:A:134:ARG:HA	1:A:138:ALA:HB3	1.97	0.47
1:A:158:TRP:HE1	1:A:162:MET:HE3	1.80	0.47
1:B:228:LEU:O	1:B:230:GLU:N	2.44	0.47
1:D:227:TYR:CG	1:D:228:LEU:N	2.83	0.47
1:A:102:LEU:HD22	1:B:158:TRP:HD1	1.79	0.47
1:C:203:GLU:CD	1:C:203:GLU:H	2.18	0.47
1:C:61:VAL:O	1:C:62:GLN:HB3	2.15	0.46
1:C:108:GLN:HB3	1:C:170:LEU:HD21	1.96	0.46
1:A:53:GLU:OE1	1:A:128:ARG:HG3	2.15	0.46
1:C:34:LYS:HE3	1:C:128:ARG:CZ	2.45	0.46
1:C:50:VAL:HG12	1:C:52:PRO:HD3	1.98	0.46
1:B:232:PRO:HG2	1:B:260:LEU:HD21	1.98	0.46
1:C:104:ARG:HD2	1:C:108:GLN:HE22	1.81	0.46
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.72	0.45
1:B:140:ASN:ND2	1:B:207:LYS:HB3	2.30	0.45
1:C:136:ILE:CD1	1:C:211:LYS:HB3	2.46	0.45
1:D:21:ILE:HA	1:D:122:PRO:HG2	1.96	0.45
1:A:63:SER:HB3	6:A:327:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLN:HG3	1:A:196:GLU:HG3	1.99	0.45
1:D:83:GLN:O	1:D:87:GLU:HB2	2.17	0.45
1:A:219:ARG:NH2	1:A:228:LEU:O	2.49	0.45
1:B:140:ASN:HD21	1:B:207:LYS:HB3	1.82	0.45
1:C:147:MET:HA	1:C:151:GLU:OE1	2.15	0.45
1:B:136:ILE:HG21	1:B:212:HIS:CE1	2.51	0.45
1:D:35:SER:CA	1:D:38:VAL:HG12	2.46	0.45
1:B:55:VAL:HA	1:B:58:TRP:CE3	2.52	0.45
1:B:134:ARG:HA	1:B:138:ALA:HB3	1.98	0.45
1:C:229:GLN:NE2	1:C:229:GLN:HA	2.32	0.45
1:B:42:LYS:HG3	1:B:43:GLN:HG2	1.98	0.45
1:C:229:GLN:CA	1:C:229:GLN:NE2	2.79	0.45
1:A:161:TRP:CZ3	1:A:162:MET:HE1	2.52	0.45
1:C:130:VAL:O	1:C:133:ASP:HB2	2.17	0.45
1:A:136:ILE:HD13	1:A:211:LYS:HB3	1.99	0.44
1:B:39:ASN:HD22	1:B:42:LYS:NZ	2.14	0.44
1:D:58:TRP:O	1:D:81:VAL:HG12	2.17	0.44
1:A:192:ARG:HD3	1:A:194:ARG:CB	2.47	0.44
1:B:104:ARG:NH1	1:B:128:ARG:HB2	2.32	0.44
1:D:26:ILE:HD13	1:D:26:ILE:N	2.32	0.44
1:A:43:GLN:H	1:A:43:GLN:HG3	1.57	0.44
1:B:204:TYR:HE2	1:B:208:LEU:HD11	1.82	0.44
1:B:234:LEU:HD21	1:B:236:LEU:HD11	1.98	0.44
1:C:111:SER:O	1:C:113:ASN:N	2.49	0.44
1:D:93:SER:OG	1:D:141:LEU:HD22	2.17	0.44
1:B:53:GLU:HG3	1:B:104:ARG:HH12	1.83	0.44
1:C:41:LEU:C	1:C:43:GLN:N	2.70	0.44
1:D:50:VAL:HG12	1:D:52:PRO:CD	2.48	0.44
1:D:110:ALA:O	1:D:112:LEU:N	2.51	0.44
1:C:225:PHE:CD1	1:C:225:PHE:N	2.85	0.44
1:C:38:VAL:HG22	1:C:50:VAL:CG2	2.48	0.43
1:C:108:GLN:HB3	1:C:170:LEU:CD2	2.48	0.43
1:D:242:PHE:O	1:D:246:TYR:HD2	2.00	0.43
1:A:211:LYS:HE3	6:A:311:HOH:O	2.18	0.43
1:A:232:PRO:HB2	1:A:256:PHE:CE2	2.52	0.43
1:B:237:ASP:C	1:B:237:ASP:OD2	2.56	0.43
1:A:225:PHE:CD1	1:A:225:PHE:N	2.86	0.43
1:B:24:ILE:HG13	1:B:257:LEU:HD21	2.01	0.43
1:B:232:PRO:HB2	1:B:256:PHE:HE2	1.83	0.43
1:D:48:TRP:HD1	1:D:123:VAL:HB	1.83	0.43
1:D:134:ARG:HA	1:D:138:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ARG:HG2	1:D:193:GLY:N	2.33	0.43
1:C:233:ILE:O	1:C:233:ILE:HG22	2.19	0.43
1:D:147:MET:HG2	6:D:610:HOH:O	2.17	0.43
1:D:34:LYS:HE3	1:D:128:ARG:CZ	2.49	0.43
1:D:161:TRP:CD2	1:D:165:GLN:NE2	2.87	0.43
1:B:219:ARG:CG	1:B:219:ARG:NH1	2.79	0.43
1:A:112:LEU:HD23	1:A:124:LEU:CD2	2.49	0.43
1:C:152:TRP:NE1	1:C:156:GLN:NE2	2.66	0.43
1:D:218:HIS:O	1:D:219:ARG:C	2.57	0.42
1:A:128:ARG:HG3	1:A:128:ARG:NH1	2.33	0.42
1:C:144:SER:O	1:C:145:GLU:HB2	2.20	0.42
1:A:111:SER:O	1:A:113:ASN:N	2.53	0.42
1:B:182:PRO:HB2	1:B:202:LEU:CD1	2.50	0.42
1:B:83:GLN:O	1:B:87:GLU:HB2	2.20	0.42
1:B:105:ILE:HG22	1:B:109:LEU:HD12	2.00	0.42
1:C:192:ARG:HA	5:C:501:UDP:O3'	2.19	0.42
1:A:177:TYR:CD1	1:A:177:TYR:C	2.93	0.42
1:A:185:CYS:O	1:A:189:ILE:HG13	2.20	0.42
1:B:201:PRO:HG2	1:B:204:TYR:HB2	2.02	0.42
1:D:152:TRP:O	1:D:156:GLN:HG3	2.20	0.42
1:B:45:CYS:O	1:B:47:ASP:N	2.53	0.41
1:C:168:GLN:HA	1:C:168:GLN:NE2	2.34	0.41
1:D:35:SER:HA	1:D:38:VAL:CG1	2.50	0.41
1:D:42:LYS:NZ	1:D:42:LYS:CB	2.83	0.41
1:B:225:PHE:O	1:B:228:LEU:HB2	2.21	0.41
1:A:152:TRP:CD1	1:A:156:GLN:NE2	2.89	0.41
1:B:83:GLN:HB2	1:B:196:GLU:HG2	2.02	0.41
1:B:110:ALA:O	1:B:112:LEU:N	2.53	0.41
1:D:144:SER:O	1:D:145:GLU:HB2	2.20	0.41
1:D:232:PRO:HB2	1:D:256:PHE:CZ	2.55	0.41
1:B:192:ARG:NH2	5:B:401:UDP:PB	2.93	0.41
1:A:83:GLN:O	1:A:87:GLU:HB2	2.21	0.41
1:C:43:GLN:C	1:C:45:CYS:H	2.23	0.41
1:D:227:TYR:O	1:D:228:LEU:C	2.59	0.41
1:B:39:ASN:O	1:B:42:LYS:HG2	2.21	0.41
1:C:183:GLU:H	1:C:183:GLU:HG2	1.54	0.41
1:D:25:SER:C	1:D:26:ILE:HD13	2.41	0.41
1:C:221:LEU:HD23	1:C:222:LYS:N	2.37	0.41
1:D:61:VAL:O	1:D:62:GLN:HB3	2.21	0.41
1:A:62:GLN:HA	1:A:62:GLN:HE21	1.85	0.40
1:A:236:LEU:HD23	1:A:236:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:O	1:B:258:SER:OG	2.37	0.40
1:D:47:ASP:O	1:D:48:TRP:CD1	2.74	0.40
1:D:84:MET:HB3	1:D:92:TRP:CD1	2.56	0.40
1:B:35:SER:CA	1:B:38:VAL:HG12	2.50	0.40
1:C:89:PRO:HG2	1:C:90:GLU:OE2	2.21	0.40
1:C:104:ARG:CD	1:C:108:GLN:HE22	2.34	0.40
1:D:232:PRO:HB2	1:D:256:PHE:CE2	2.56	0.40
1:A:61:VAL:O	1:A:62:GLN:HB3	2.21	0.40
1:D:181:THR:HG23	1:D:239:ASN:OD1	2.22	0.40
1:A:183:GLU:CD	1:A:183:GLU:H	2.25	0.40
1:B:167:GLY:HA2	1:B:170:LEU:HD12	2.04	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	218/248 (88%)	187 (86%)	27 (12%)	4 (2%)	8 35
1	B	217/248 (88%)	183 (84%)	27 (12%)	7 (3%)	4 21
1	C	218/248 (88%)	192 (88%)	21 (10%)	5 (2%)	6 29
1	D	216/248 (87%)	192 (89%)	19 (9%)	5 (2%)	6 29
All	All	869/992 (88%)	754 (87%)	94 (11%)	21 (2%)	6 28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	GLU
1	D	45	CYS
1	D	230	GLU
1	B	45	CYS

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Mol	Chain	Res	Type
1	B	110	ALA
1	B	165	GLN
1	D	111	SER
1	A	112	LEU
1	B	111	SER
1	B	168	GLN
1	C	42	LYS
1	C	45	CYS
1	C	112	LEU
1	D	110	ALA
1	A	110	ALA
1	A	165	GLN
1	B	46	GLU
1	C	165	GLN
1	D	165	GLN
1	A	167	GLY
1	C	44	LEU

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	189/228 (83%)	180 (95%)	9 (5%)	25	60
1	B	191/228 (84%)	184 (96%)	7 (4%)	34	69
1	C	190/228 (83%)	176 (93%)	14 (7%)	13	42
1	D	187/228 (82%)	183 (98%)	4 (2%)	53	81
All	All	757/912 (83%)	723 (96%)	34 (4%)	27	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	43	GLN
1	A	53	GLU
1	A	104	ARG

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Mol	Chain	Res	Type
1	A	190	TYR
1	A	202	LEU
1	A	205	LEU
1	A	230	GLU
1	A	255	GLU
1	B	43	GLN
1	B	98	THR
1	B	111	SER
1	B	130	VAL
1	B	165	GLN
1	B	219	ARG
1	B	226	ASP
1	C	55	VAL
1	C	57	ARG
1	C	87	GLU
1	C	104	ARG
1	C	130	VAL
1	C	132	SER
1	C	150	THR
1	C	191	LEU
1	C	198	GLN
1	C	216	LEU
1	C	229	GLN
1	C	250	VAL
1	C	255	GLU
1	C	259	THR
1	D	62	GLN
1	D	192	ARG
1	D	219	ARG
1	D	227	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	140	ASN
1	A	156	GLN
1	A	163	ASN
1	A	165	GLN
1	B	39	ASN
1	B	43	GLN
1	B	62	GLN

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Mol	Chain	Res	Type
1	B	140	ASN
1	B	165	GLN
1	B	224	ASN
1	C	62	GLN
1	C	108	GLN
1	C	156	GLN
1	C	165	GLN
1	C	168	GLN
1	C	229	GLN
1	D	43	GLN
1	D	62	GLN
1	D	140	ASN
1	D	163	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)

Of 14 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
4	DCZ	A	304	-	17,17,17	1.55	2 (11%)	24,24,24	1.96	7 (29%)
5	UDP	D	601	3	24,26,26	1.72	4 (16%)	37,40,40	1.04	3 (8%)
4	DCZ	D	604	-	17,17,17	1.66	2 (11%)	24,24,24	1.95	5 (20%)
5	UDP	C	501	3	24,26,26	1.60	5 (20%)	37,40,40	1.15	5 (13%)
5	UDP	B	401	3	24,26,26	1.71	6 (25%)	37,40,40	1.13	6 (16%)
4	DCZ	B	404	-	17,17,17	1.67	3 (17%)	24,24,24	1.85	7 (29%)
5	UDP	A	301	3	24,26,26	1.57	2 (8%)	37,40,40	1.06	4 (10%)
4	DCZ	C	504	-	17,17,17	1.57	2 (11%)	24,24,24	1.76	6 (25%)

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
4	DCZ	A	304	-	-	0/6/18/18	0/2/2/2
5	UDP	D	601	3	-	1/16/32/32	0/2/2/2
4	DCZ	D	604	-	-	1/6/18/18	0/2/2/2
5	UDP	C	501	3	-	2/16/32/32	0/2/2/2
5	UDP	B	401	3	-	1/16/32/32	0/2/2/2
4	DCZ	B	404	-	-	0/6/18/18	0/2/2/2
5	UDP	A	301	3	-	0/16/32/32	0/2/2/2
4	DCZ	C	504	-	-	2/6/18/18	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	UDP	C6-C5	4.85	1.46	1.35
5	B	401	UDP	C6-C5	4.74	1.46	1.35
5	A	301	UDP	C6-C5	4.50	1.45	1.35
5	C	501	UDP	C6-C5	4.44	1.45	1.35
4	D	604	DCZ	O2-C2	4.39	1.31	1.23
4	A	304	DCZ	O2-C2	4.31	1.31	1.23
4	B	404	DCZ	O2-C2	4.29	1.31	1.23
4	C	504	DCZ	O2-C2	4.29	1.31	1.23
5	D	601	UDP	C5-C4	4.02	1.52	1.43
4	B	404	DCZ	C5-C4	-3.80	1.34	1.42
5	A	301	UDP	C5-C4	3.79	1.52	1.43
4	D	604	DCZ	C5-C4	-3.74	1.34	1.42
5	B	401	UDP	C5-C4	3.60	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	DCZ	C5-C4	-3.56	1.34	1.42
5	C	501	UDP	C5-C4	3.48	1.51	1.43
4	A	304	DCZ	C5-C4	-3.29	1.35	1.42
5	B	401	UDP	C2-N1	2.47	1.42	1.38
5	D	601	UDP	C2-N1	2.45	1.42	1.38
5	C	501	UDP	C4-N3	2.42	1.42	1.38
5	D	601	UDP	C1'-N1	2.29	1.54	1.47
5	B	401	UDP	O4-C4	-2.29	1.20	1.24
5	B	401	UDP	C4-N3	2.28	1.42	1.38
5	C	501	UDP	O4-C4	-2.21	1.20	1.24
5	C	501	UDP	C6-N1	2.17	1.43	1.38
5	B	401	UDP	C1'-N1	2.15	1.53	1.47
4	B	404	DCZ	C1'-N1	2.15	1.53	1.48

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	304	DCZ	O2-C2-N3	-5.66	113.12	122.33
4	D	604	DCZ	O2-C2-N3	-5.60	113.22	122.33
4	B	404	DCZ	O2-C2-N3	-5.34	113.64	122.33
4	C	504	DCZ	O2-C2-N3	-4.89	114.38	122.33
4	D	604	DCZ	C2'-C1'-N1	4.07	123.15	113.77
4	A	304	DCZ	C2'-C1'-N1	3.56	121.97	113.77
4	B	404	DCZ	C2'-C1'-N1	3.27	121.29	113.77
4	C	504	DCZ	C2'-C1'-N1	3.12	120.95	113.77
4	C	504	DCZ	C4-N3-C2	-3.11	115.23	120.25
4	D	604	DCZ	C4-N3-C2	-2.99	115.42	120.25
5	D	601	UDP	PA-O3A-PB	-2.97	122.64	132.83
4	A	304	DCZ	C6-C5-C4	2.77	121.97	117.50
4	D	604	DCZ	O2-C2-N1	2.73	124.54	118.89
4	B	404	DCZ	C4-N3-C2	-2.72	115.86	120.25
4	A	304	DCZ	C4-N3-C2	-2.71	115.88	120.25
4	D	604	DCZ	C6-C5-C4	2.66	121.79	117.50
5	B	401	UDP	PA-O3A-PB	-2.62	123.83	132.83
4	B	404	DCZ	C6-C5-C4	2.62	121.72	117.50
5	B	401	UDP	O4'-C1'-C2'	-2.60	100.97	106.64
4	C	504	DCZ	C6-C5-C4	2.56	121.63	117.50
5	C	501	UDP	C6-C5-C4	-2.53	116.06	119.52
5	C	501	UDP	C2'-C1'-N1	-2.51	106.11	113.22
4	A	304	DCZ	O2-C2-N1	2.44	123.93	118.89
4	B	404	DCZ	O2-C2-N1	2.35	123.75	118.89
5	A	301	UDP	C2'-C1'-N1	-2.32	106.66	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	501	UDP	O4-C4-C5	-2.31	121.10	125.16
5	C	501	UDP	PA-O3A-PB	-2.29	124.97	132.83
4	A	304	DCZ	N1-C2-N3	2.28	122.95	118.81
5	B	401	UDP	O4-C4-C5	-2.23	121.25	125.16
5	B	401	UDP	C6-C5-C4	-2.21	116.50	119.52
5	A	301	UDP	PA-O3A-PB	-2.17	125.38	132.83
5	A	301	UDP	C6-C5-C4	-2.14	116.60	119.52
5	B	401	UDP	C2'-C1'-N1	-2.13	107.17	113.22
4	B	404	DCZ	N1-C2-N3	2.09	122.61	118.81
5	B	401	UDP	O4-C4-N3	2.08	122.36	119.31
5	D	601	UDP	O3B-PB-O2B	2.07	115.54	107.64
4	C	504	DCZ	O2-C2-N1	2.07	123.16	118.89
5	C	501	UDP	O4-C4-N3	2.06	122.33	119.31
5	D	601	UDP	O4'-C1'-C2'	-2.06	102.15	106.64
5	A	301	UDP	O4-C4-C5	-2.06	121.55	125.16
4	B	404	DCZ	C6-N1-C2	-2.05	116.94	120.49
4	A	304	DCZ	C6-N1-C2	-2.01	117.01	120.49
4	C	504	DCZ	N1-C2-N3	2.01	122.47	118.81

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	504	DCZ	O4'-C4'-C5'-O5'
4	C	504	DCZ	C3'-C4'-C5'-O5'
4	D	604	DCZ	O4'-C4'-C5'-O5'
5	D	601	UDP	O4'-C4'-C5'-O5'
5	C	501	UDP	PB-O3A-PA-O1A
5	C	501	UDP	PB-O3A-PA-O2A
5	B	401	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

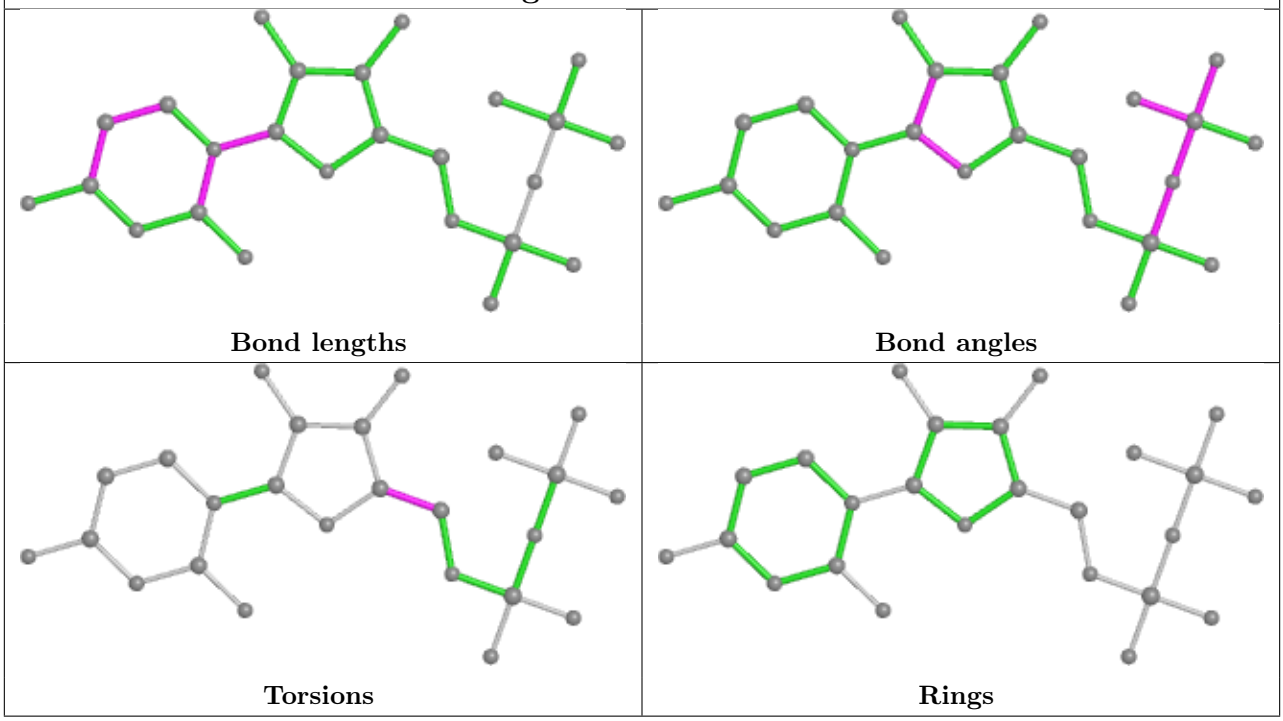
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	UDP	3	0
5	B	401	UDP	2	0

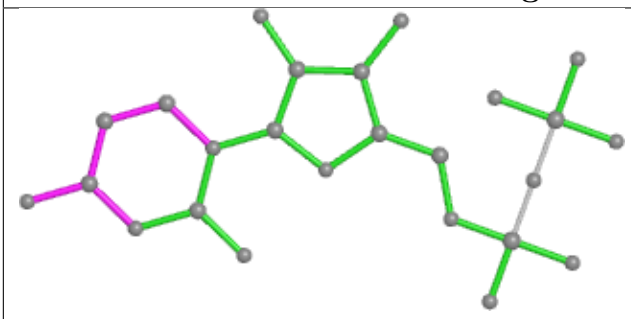
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

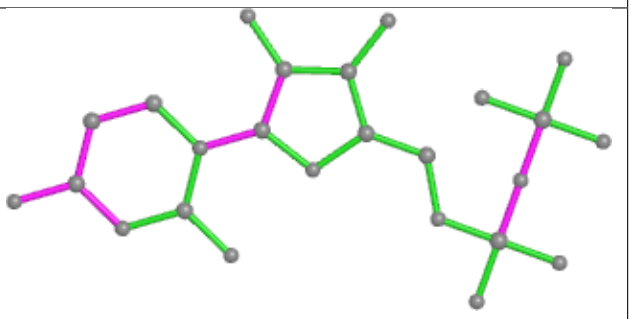
Ligand UDP D 601



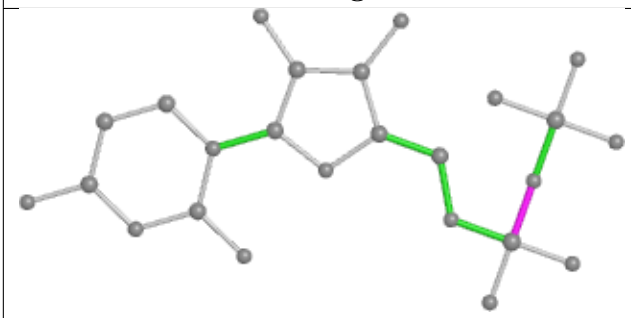
Ligand UDP C 501



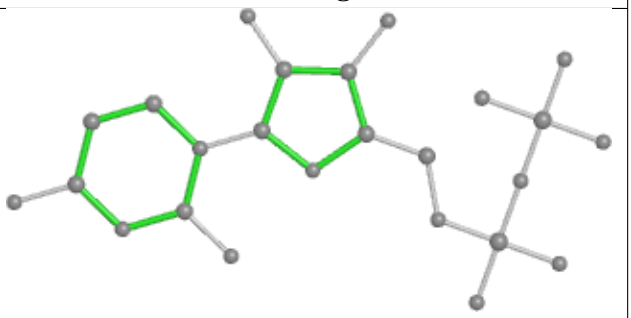
Bond lengths



Bond angles

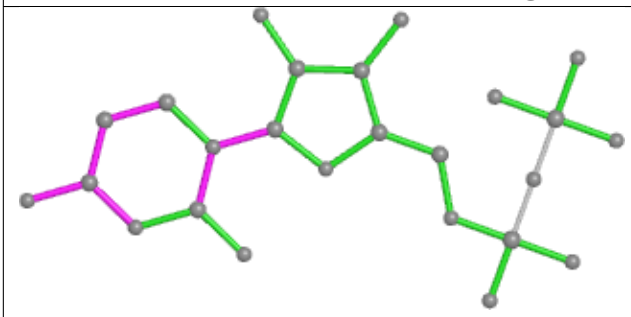


Torsions

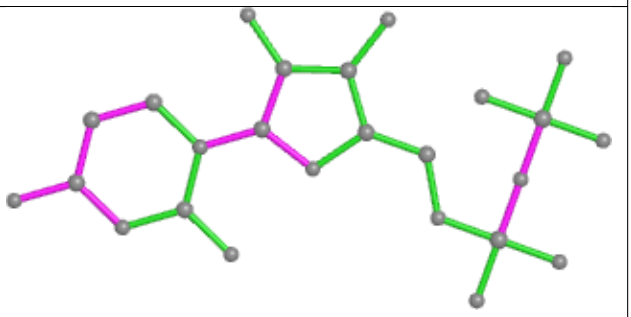


Rings

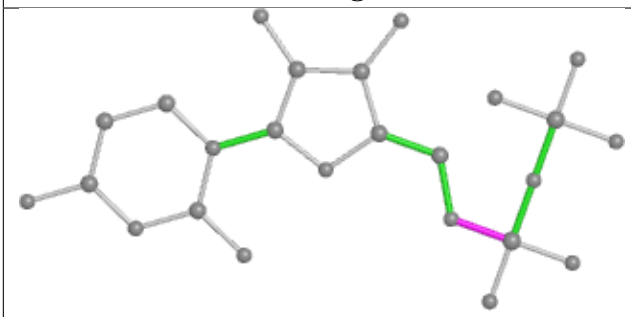
Ligand UDP B 401



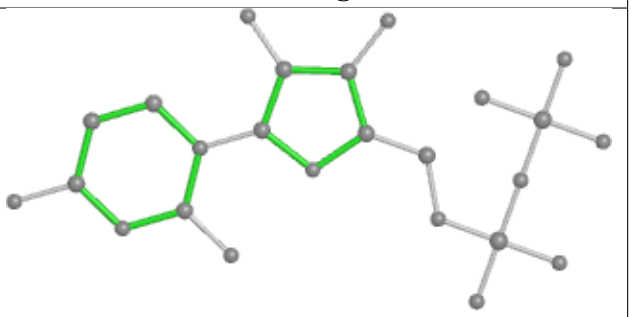
Bond lengths



Bond angles

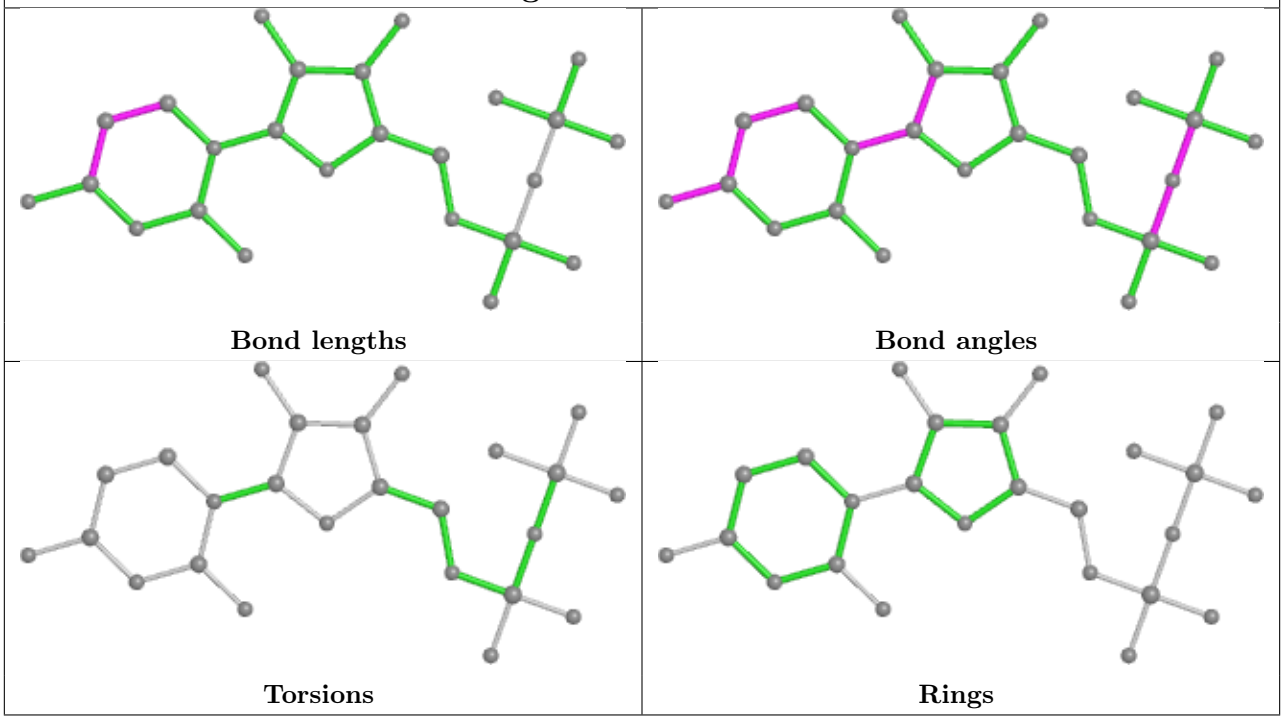


Torsions



Rings

Ligand UDP A 301



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	222/248 (89%)	-0.45	0 100 100	20, 41, 67, 78	0
1	B	221/248 (89%)	-0.30	1 (0%) 91 75	23, 44, 68, 77	0
1	C	222/248 (89%)	-0.46	0 100 100	19, 40, 68, 80	0
1	D	220/248 (88%)	-0.29	2 (0%) 84 62	26, 48, 74, 85	0
All	All	885/992 (89%)	-0.38	3 (0%) 94 83	19, 43, 71, 85	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	PRO	2.1
1	D	121	LYS	2.1
1	B	244	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

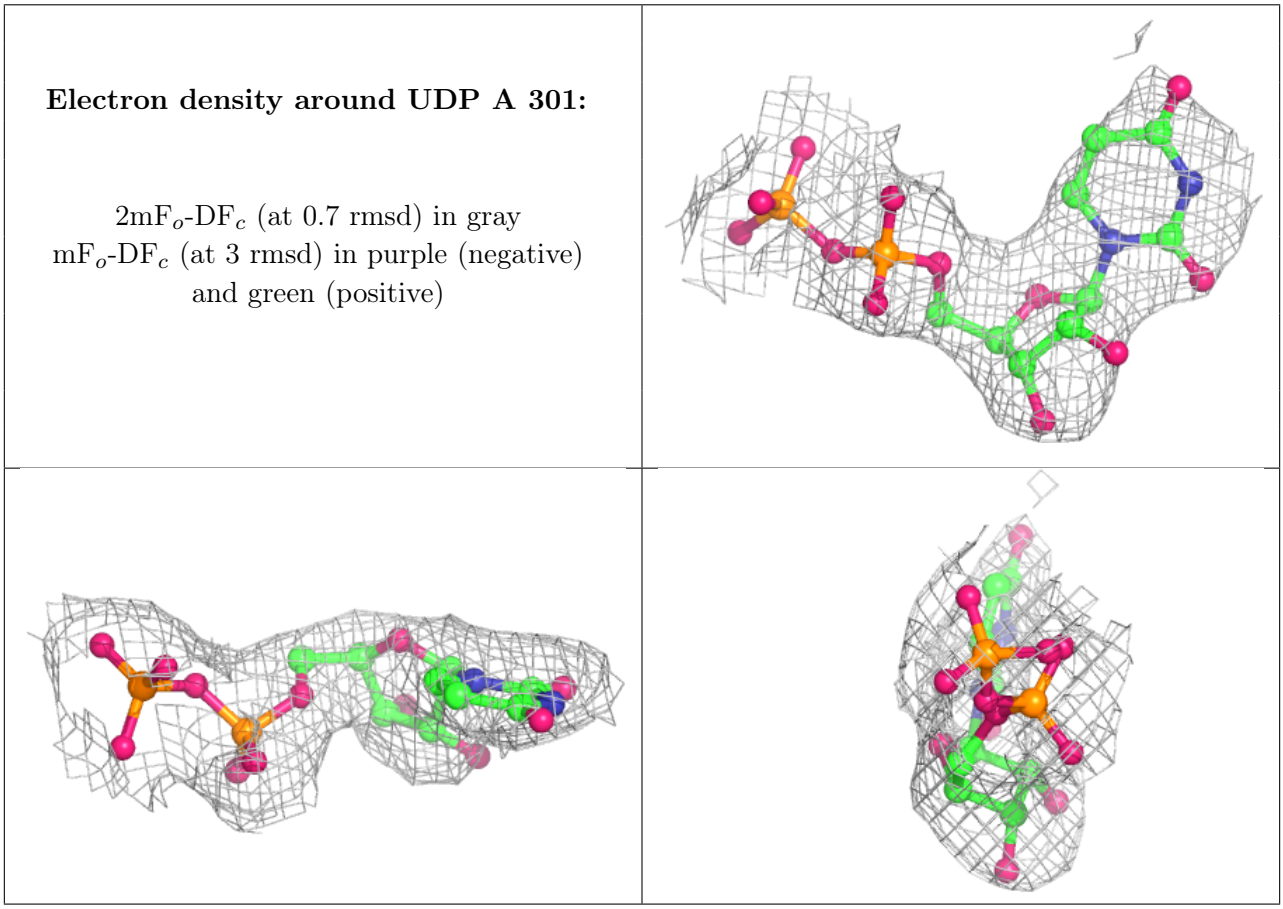
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	602	1/1	0.78	0.17	35,35,35,35	0
3	MG	B	402	1/1	0.88	0.27	39,39,39,39	0
3	MG	C	502	1/1	0.89	0.17	38,38,38,38	0
3	MG	A	302	1/1	0.89	0.18	46,46,46,46	0
2	CA	A	261	1/1	0.92	0.11	61,61,61,61	0
5	UDP	A	301	25/25	0.93	0.18	33,52,59,62	0
5	UDP	D	601	25/25	0.93	0.15	41,55,62,63	0
2	CA	C	261	1/1	0.94	0.09	59,59,59,59	0
5	UDP	C	501	25/25	0.94	0.19	37,53,60,61	0
4	DCZ	B	404	16/16	0.94	0.24	40,43,46,50	0
4	DCZ	A	304	16/16	0.95	0.17	13,16,21,21	0
5	UDP	B	401	25/25	0.95	0.13	34,43,48,51	0
4	DCZ	C	504	16/16	0.96	0.22	22,24,26,29	0
4	DCZ	D	604	16/16	0.96	0.19	36,40,44,46	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.

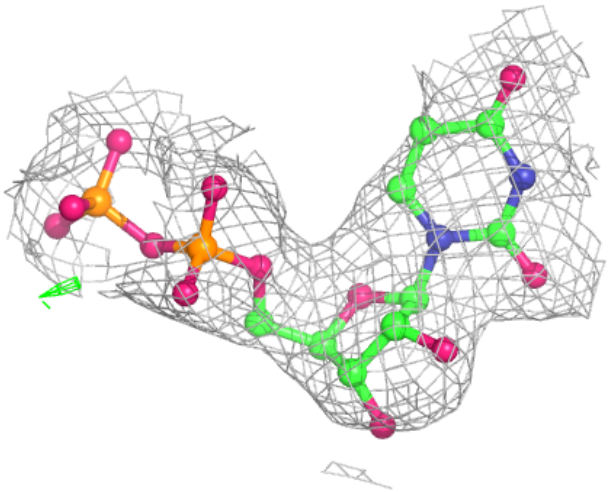
Electron density around UDP A 301:

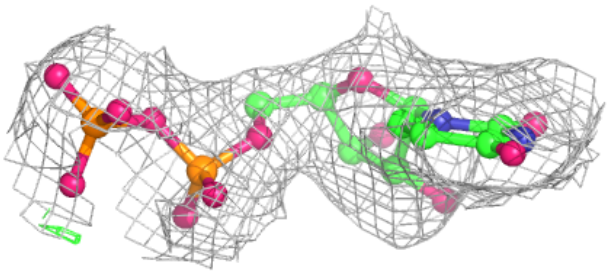
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

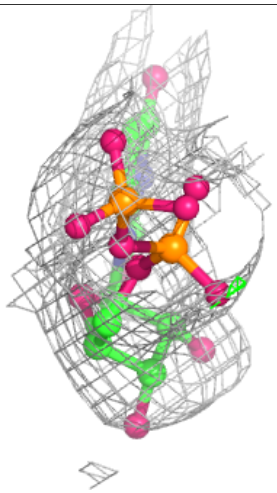


Electron density around UDP D 601:

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

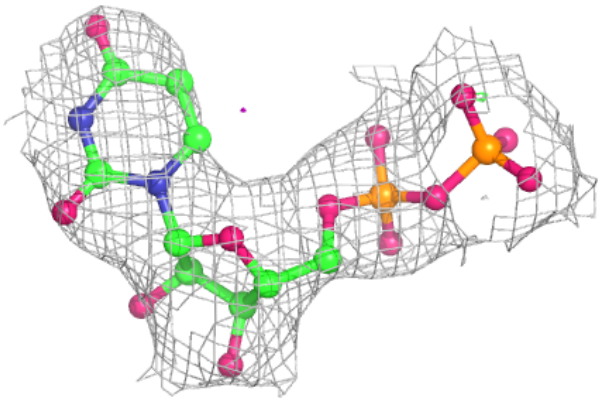


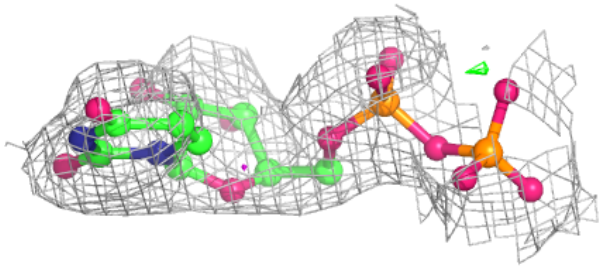


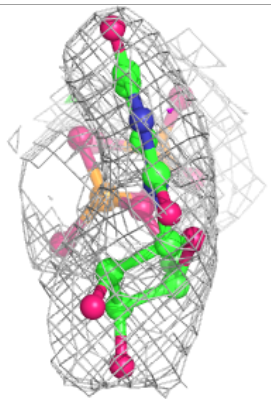


Electron density around UDP C 501:

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

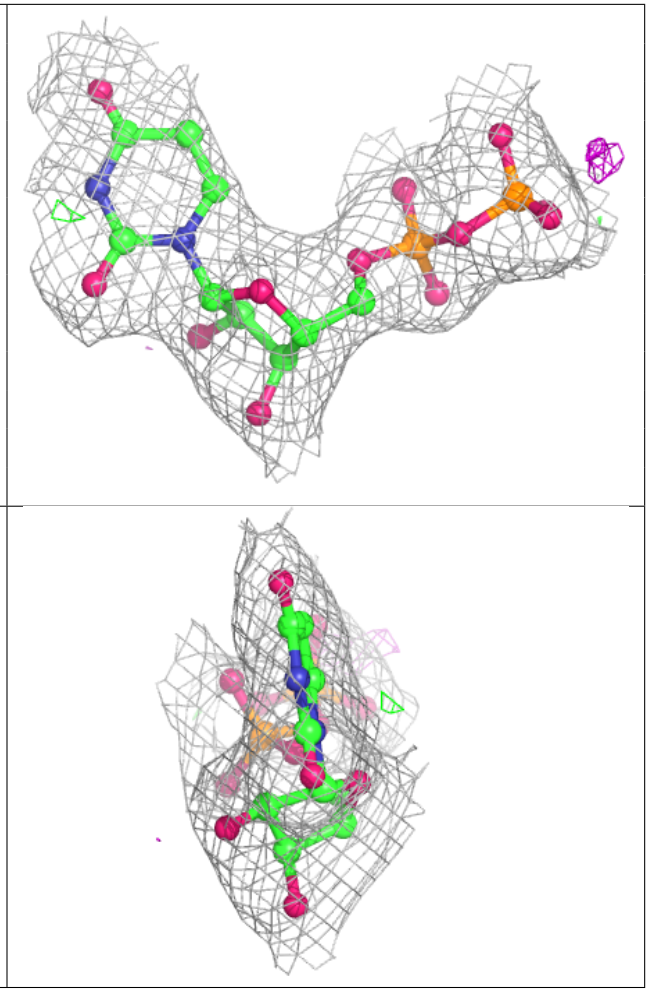






Electron density around UDP B 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.