



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:09 PM BST

PDB ID : 1Y6G
Title : alpha-glucosyltransferase in complex with UDP and a 13_mer DNA containing a HMU base at 2.8 Å resolution
Authors : Lariviere, L.; Sommer, N.; Morera, S.
Deposited on : 2004-12-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

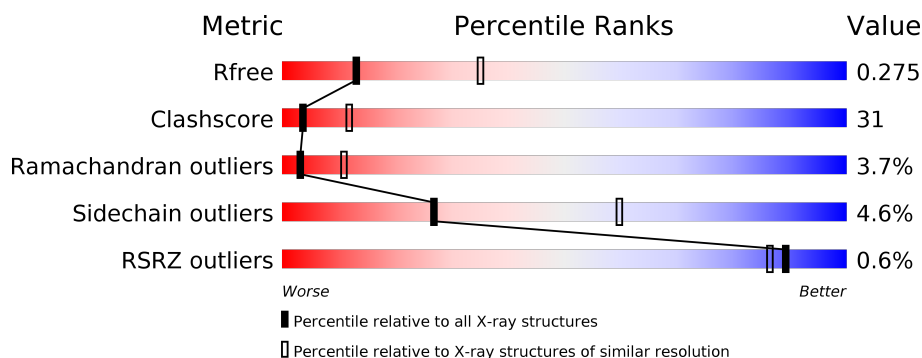
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	13	<div> <div>15%</div> <div>23%</div> <div>69%</div> <div>8%</div> </div>
2	D	12	<div> <div>8%</div> <div>17%</div> <div>83%</div> </div>
3	A	403	<div> <div>38%</div> <div>52%</div> <div>7%</div> <div>•</div> </div>
3	B	403	<div> <div>55%</div> <div>39%</div> <div>• •</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7132 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 DNA chain called 5'-D(*GP*AP*TP*AP*CP*TP*(5HU)P*AP*GP*AP*T P*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	13	Total	C	N	O	P	0	0	0
			268	129	51	76	12			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*GP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			242	118	41	72	11			

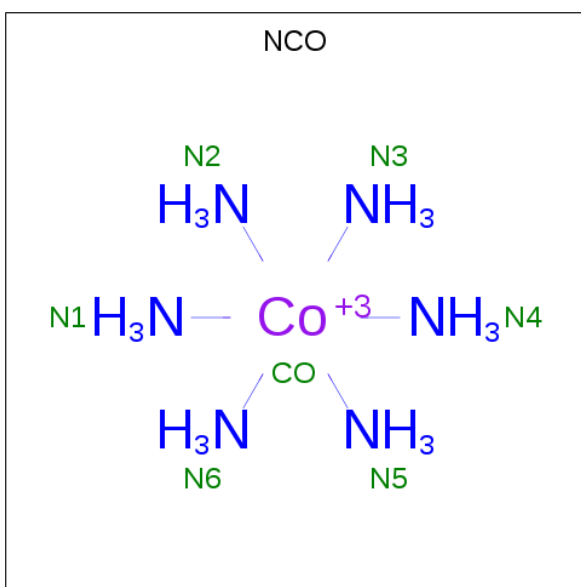
- Molecule 3 is a protein called DNA alpha-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	392	Total	C	N	O	S	0	0	0
			3212	2051	544	599	18			
3	B	393	Total	C	N	O	S	0	0	0
			3227	2059	548	602	18			

There are 6 discrepancies between the modelled and reference sequences:

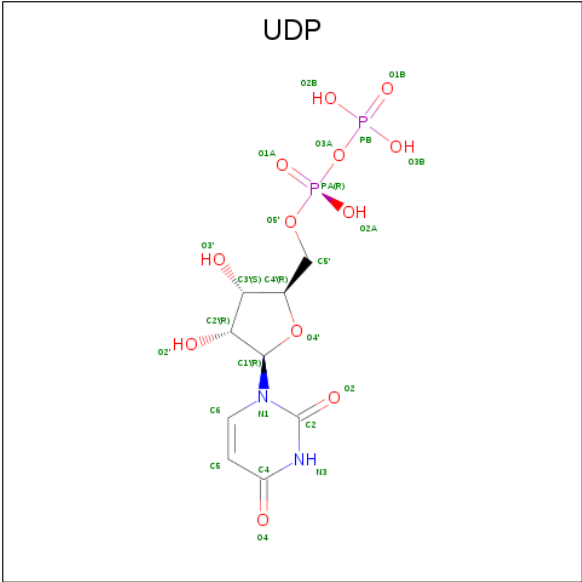
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	MET	-	cloning artifact	UNP P04519
A	999	GLY	-	cloning artifact	UNP P04519
A	1000	SER	-	cloning artifact	UNP P04519
B	998	MET	-	cloning artifact	UNP P04519
B	999	GLY	-	cloning artifact	UNP P04519
B	1000	SER	-	cloning artifact	UNP P04519

- Molecule 4 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: CoH₁₈N₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	Co	N	0	0
			7	1	6		
4	A	1	Total	Co	N	0	0
			7	1	6		
4	A	1	Total	Co	N	0	0
			7	1	6		
4	A	1	Total	Co	N	0	0
			7	1	6		
4	B	1	Total	Co	N	0	0
			7	1	6		
4	B	1	Total	Co	N	0	0
			7	1	6		
4	B	1	Total	Co	N	0	0
			7	1	6		

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

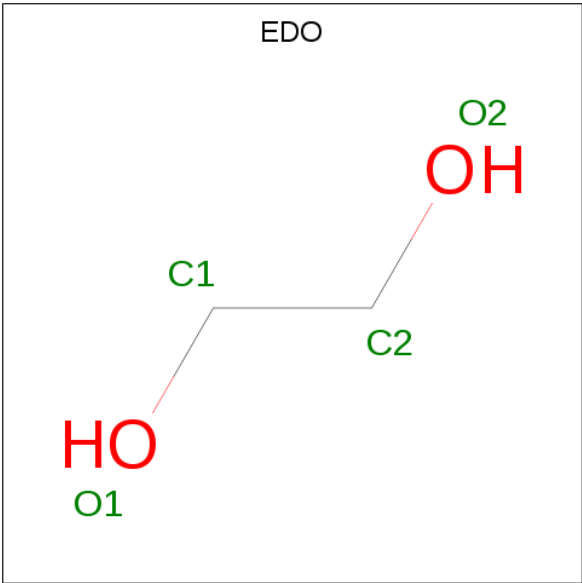


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

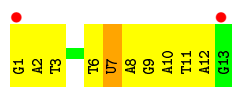
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	O	0	0
			1	1		
8	A	30	Total	O	0	0
			30	30		
8	B	48	Total	O	0	0
			48	48		

3 Residue-property plots

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.

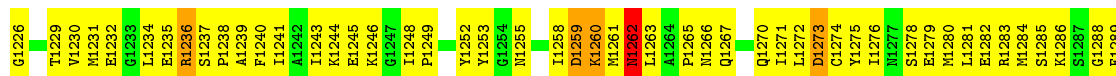
- Molecule 1: 5'-D(*GP*AP*TP*AP*CP*TP*(5HU)P*AP*GP*AP*TP*AP*G)-3'



- Molecule 2: 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*GP*TP*AP*T)-3'

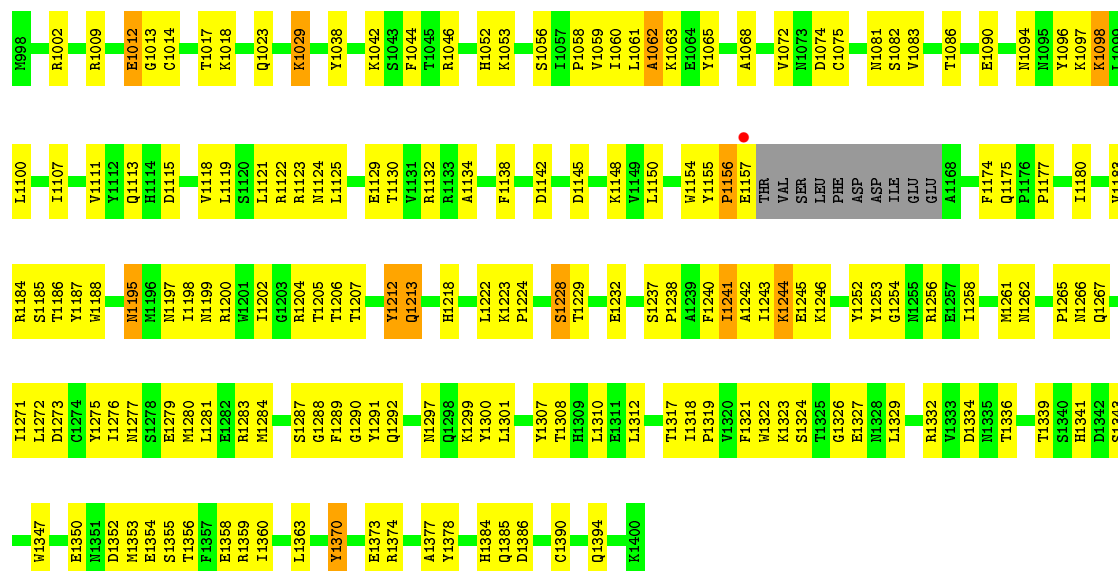


- Molecule 3: DNA alpha-glucosyltransferase



● Molecule 3: DNA alpha-glucosyltransferase

Chain B:  55% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.99 Å 120.52 Å 86.81 Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 99.2 (29.62-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.68 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.287 0.214 , 0.275	Depositor DCC
R_{free} test set	1120 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.827	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7132	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, 5HU, EDO, NCO, CL

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	C	0.41	0/277	0.70	0/424
2	D	0.42	0/270	0.70	0/415
3	A	0.40	0/3288	0.64	0/4435
3	B	0.44	0/3303	0.68	0/4454
All	All	0.42	0/7138	0.66	0/9728

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	C	268	0	149	22	0
2	D	242	0	139	13	0
3	A	3212	0	3152	260	0
3	B	3227	0	3169	146	0
4	A	21	0	0	2	0
4	B	21	0	0	1	0
4	D	7	0	0	0	0
5	A	25	0	11	1	0
5	B	25	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	B	4	0	6	0	0
8	A	30	0	0	1	0
8	B	48	0	0	1	0
8	D	1	0	0	0	0
All	All	7132	0	6637	429	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 31.

All (429) 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:2:DA:H2''	1:C:3:DT:H5'	1.30	1.06
3:A:1213:GLN:H	3:A:1213:GLN:HE21	1.07	1.02
3:A:1252:TYR:OH	3:A:1273:ASP:HB3	1.59	1.02
1:C:7:5HU:H5A1	3:A:1237:SER:HA	1.43	0.98
3:A:1218:HIS:HA	3:A:1222:LEU:HB2	1.50	0.94
3:A:1236:ARG:HG2	3:A:1236:ARG:HH11	1.34	0.93
3:B:1242:ALA:O	3:B:1246:LYS:HB2	1.71	0.90
3:A:1113:GLN:HE21	3:A:1115:ASP:H	1.17	0.90
1:C:8:DA:OP2	1:C:8:DA:H2'	1.73	0.89
3:B:1118:VAL:HG13	3:B:1145:ASP:HB3	1.52	0.89
3:A:1332:ARG:H	3:A:1384:HIS:HD2	1.20	0.87
3:A:1175:GLN:O	3:A:1177:PRO:HD3	1.74	0.87
3:A:1065:TYR:HB2	3:A:1095:ASN:HD22	1.40	0.84
3:B:1312:LEU:HD12	3:B:1321:PHE:HE1	1.42	0.82
3:A:1012:GLU:OE2	3:A:1016:VAL:HG12	1.82	0.80
3:A:1184:ARG:HD2	3:A:1378:TYR:CE2	2.17	0.80
3:A:1213:GLN:HE21	3:A:1213:GLN:N	1.79	0.80
3:A:1332:ARG:H	3:A:1384:HIS:CD2	1.99	0.79
3:A:1085:ALA:O	3:A:1088:VAL:HG22	1.82	0.79
3:A:1285:SER:HB3	3:A:1315:CYS:HB2	1.65	0.79
3:B:1129:GLU:N	3:B:1129:GLU:OE1	2.18	0.77
3:A:1359:ARG:O	3:A:1363:LEU:HD13	1.86	0.76
3:A:1218:HIS:O	3:A:1223:LYS:HB2	1.86	0.75
3:A:1321:PHE:HB2	3:A:1347:TRP:HZ3	1.52	0.75
3:A:1236:ARG:CG	3:A:1236:ARG:HH11	2.00	0.75
3:A:1113:GLN:NE2	3:A:1115:ASP:H	1.85	0.75
3:A:1199:ASN:HD22	3:A:1291:TYR:HE2	1.35	0.74
3:A:1319:PRO:O	3:A:1345:ILE:HG23	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1296:LEU:CD1	3:A:1300:TYR:HB2	2.18	0.74
3:A:1148:LYS:HA	3:A:1152:LYS:HE3	1.70	0.74
3:A:1280:MET:HE3	3:A:1281:LEU:HG	1.68	0.74
3:A:1201:TRP:HB3	3:A:1231:MET:HG2	1.70	0.73
3:A:1065:TYR:HB2	3:A:1095:ASN:ND2	2.03	0.73
3:B:1213:GLN:H	3:B:1213:GLN:NE2	1.87	0.73
3:A:1366:ASP:HB3	3:A:1369:LEU:HB3	1.70	0.72
3:A:1110:VAL:HG13	3:A:1136:VAL:HB	1.70	0.72
3:A:1301:LEU:HD22	3:A:1329:LEU:HD21	1.72	0.72
3:B:1213:GLN:H	3:B:1213:GLN:HE21	1.37	0.71
3:A:1234:LEU:HD12	3:A:1271:ILE:HD12	1.73	0.70
3:B:1184:ARG:HD2	3:B:1378:TYR:CE2	2.26	0.70
3:A:1235:GLU:HB3	8:A:2063:HOH:O	1.91	0.69
3:A:1146:PHE:O	3:A:1151:MET:HG2	1.92	0.69
3:B:1111:VAL:HG21	3:B:1130:THR:HG22	1.75	0.69
3:B:1323:LYS:HE2	3:B:1327:GLU:OE1	1.93	0.69
3:B:1199:ASN:OD1	3:B:1222:LEU:HD22	1.93	0.69
3:A:1116:HIS:ND1	3:A:1300:TYR:HB3	2.07	0.68
3:A:1213:GLN:H	3:A:1213:GLN:NE2	1.85	0.68
3:A:1194:ILE:O	3:A:1196:MET:HE2	1.93	0.68
3:A:1038:TYR:CZ	3:A:1058:PRO:HB3	2.29	0.68
3:A:1240:PHE:CE1	3:A:1243:ILE:HD12	2.29	0.68
3:B:1322:TRP:CD1	3:B:1324:SER:HB3	2.29	0.67
3:A:1305:LEU:HD22	3:A:1309:HIS:ND1	2.10	0.67
3:B:1336:THR:OG1	3:B:1341:HIS:HE1	1.78	0.67
2:D:1:DC:H2'	2:D:2:DT:H72	1.76	0.66
3:B:1113:GLN:NE2	3:B:1115:ASP:H	1.93	0.66
3:A:1321:PHE:HB2	3:A:1347:TRP:CZ3	2.30	0.66
3:B:1332:ARG:HD3	3:B:1384:HIS:O	1.95	0.66
3:A:1200:ARG:HD2	3:A:1284:MET:HE2	1.78	0.65
3:A:1221:PHE:C	3:A:1224:PRO:HD2	2.17	0.65
1:C:7:5HU:C5A	3:A:1237:SER:HA	2.23	0.65
1:C:2:DA:H2''	1:C:3:DT:C5'	2.18	0.65
1:C:7:5HU:HC6	3:A:1238:PRO:HD3	1.77	0.65
3:A:1199:ASN:HB3	3:A:1291:TYR:HE2	1.62	0.65
3:A:1113:GLN:NE2	3:A:1115:ASP:HB2	2.12	0.64
3:A:1184:ARG:O	3:A:1186:THR:N	2.30	0.64
3:A:1008:ALA:HB3	3:A:1083:VAL:HA	1.78	0.64
3:B:1240:PHE:O	3:B:1241:ILE:C	2.35	0.64
1:C:10:DA:H1'	1:C:11:DT:H5'	1.78	0.64
3:A:1298:GLN:HB2	3:A:1328:ASN:ND2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1253:TYR:OH	3:A:1270:GLN:NE2	2.31	0.63
3:A:1175:GLN:NE2	3:A:1303:ARG:HD2	2.14	0.62
3:A:1180:ILE:HD12	3:A:1382:TYR:HA	1.81	0.62
3:B:1177:PRO:HB3	3:B:1390:CYS:HB2	1.80	0.62
1:C:2:DA:C2'	1:C:3:DT:H5'	2.19	0.62
3:B:1111:VAL:CG2	3:B:1130:THR:HG22	2.30	0.62
3:B:1332:ARG:H	3:B:1384:HIS:HD2	1.48	0.62
3:A:1113:GLN:HE21	3:A:1115:ASP:N	1.94	0.62
3:B:1322:TRP:CH2	3:B:1350:GLU:HB2	2.35	0.62
1:C:2:DA:H61	2:D:12:DT:H3	1.48	0.62
3:A:1226:GLY:O	3:A:1265:PRO:HB3	2.00	0.61
3:B:1363:LEU:HD21	3:B:1373:GLU:HG3	1.80	0.61
3:B:1332:ARG:N	3:B:1384:HIS:HD2	1.98	0.61
3:A:1018:LYS:HD3	3:A:1050:HIS:CD2	2.36	0.61
3:A:1322:TRP:NE1	3:A:1324:SER:HB2	2.16	0.61
3:A:1201:TRP:HZ2	3:A:1209:LYS:O	1.83	0.61
3:A:1293:LEU:HD23	3:A:1322:TRP:HE3	1.66	0.61
3:A:1240:PHE:CD1	3:A:1243:ILE:HD12	2.35	0.60
3:B:1218:HIS:HA	3:B:1222:LEU:HB2	1.82	0.60
3:B:1326:GLY:C	3:B:1339:THR:HG23	2.22	0.60
3:A:1011:LEU:HD12	3:A:1038:TYR:CG	2.37	0.60
3:A:1322:TRP:HE1	3:A:1324:SER:HB2	1.67	0.59
3:B:1276:ILE:HB	3:B:1279:GLU:HG3	1.85	0.59
3:A:1202:ILE:HD12	3:A:1308:THR:HB	1.83	0.59
3:A:1310:LEU:HD11	3:A:1385:GLN:NE2	2.18	0.59
3:A:998:MET:HB2	3:A:1395:PHE:HE1	1.68	0.59
3:A:1317:THR:O	3:A:1319:PRO:HD3	2.02	0.59
3:B:1223:LYS:HB3	3:B:1224:PRO:HD3	1.84	0.59
3:B:1390:CYS:O	3:B:1394:GLN:HG3	2.03	0.58
3:B:1297:ASN:HB3	3:B:1300:TYR:CD2	2.38	0.58
1:C:12:DA:H4'	3:B:1123:ARG:HE	1.67	0.58
3:B:1138:PHE:HD2	3:B:1174:PHE:HB3	1.69	0.57
3:B:1326:GLY:HA3	3:B:1347:TRP:CH2	2.40	0.57
3:A:1074:ASP:O	3:A:1075:CYS:HB3	2.05	0.57
3:A:1246:LYS:NZ	3:A:1246:LYS:HB2	2.20	0.57
3:A:1262:ASN:OD1	3:A:1267:GLN:NE2	2.38	0.57
3:B:1334:ASP:OD1	3:B:1336:THR:HG23	2.05	0.57
3:A:1293:LEU:HA	3:A:1322:TRP:HB2	1.87	0.56
3:A:1306:GLU:HB3	5:A:1404:UDP:O2A	2.05	0.56
3:B:1200:ARG:O	3:B:1290:GLY:HA2	2.06	0.56
3:A:1116:HIS:HB3	3:A:1300:TYR:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1366:ASP:C	3:A:1368:ALA:H	2.08	0.56
3:B:1202:ILE:HG22	3:B:1232:GLU:HB2	1.86	0.56
3:A:1213:GLN:NE2	3:A:1213:GLN:N	2.48	0.56
3:A:1236:ARG:NH1	3:A:1236:ARG:HG2	2.14	0.56
3:A:1097:LYS:HE2	3:A:1129:GLU:HG2	1.88	0.56
3:B:1012:GLU:OE1	3:B:1014:CYS:HB2	2.06	0.56
3:B:1252:TYR:CE2	3:B:1273:ASP:HB3	2.41	0.56
3:A:1202:ILE:HD13	3:A:1312:LEU:HD21	1.89	0.56
3:B:1052:HIS:HD2	3:B:1056:SER:OG	1.88	0.56
3:B:1121:LEU:N	3:B:1121:LEU:HD23	2.20	0.56
3:B:1187:TYR:CE2	3:B:1281:LEU:HB2	2.41	0.56
3:A:1208:TRP:CH2	3:A:1209:LYS:HE2	2.40	0.55
3:A:1009:ARG:HB2	3:A:1083:VAL:O	2.07	0.55
3:A:1116:HIS:HD1	3:A:1300:TYR:HB3	1.72	0.55
3:A:1120:SER:C	3:A:1122:ARG:H	2.10	0.55
3:A:1232:GLU:HG2	3:A:1272:LEU:HD23	1.88	0.55
3:B:1090:GLU:O	3:B:1094:ASN:HB2	2.06	0.55
3:A:1312:LEU:HD12	3:A:1321:PHE:HE1	1.72	0.55
3:B:1198:ILE:HD13	3:B:1228:SER:HB3	1.87	0.55
3:B:1352:ASP:CG	3:B:1355:SER:HB2	2.26	0.55
3:A:1208:TRP:CE3	3:A:1296:LEU:HD23	2.42	0.55
2:D:7:DG:H1'	3:A:1241:ILE:HD13	1.88	0.55
3:B:1086:THR:HG22	3:B:1125:LEU:HG	1.89	0.55
3:B:1318:ILE:HG12	3:B:1370:TYR:CE1	2.42	0.55
3:A:1248:ILE:HG23	3:A:1249:PRO:HD2	1.89	0.55
3:B:1175:GLN:O	3:B:1177:PRO:HD3	2.07	0.55
3:B:1177:PRO:HG3	3:B:1390:CYS:HB3	1.89	0.55
2:D:6:DT:OP1	3:B:1122:ARG:NH2	2.39	0.55
3:A:1175:GLN:CD	3:A:1303:ARG:HD2	2.28	0.55
1:C:1:DG:H2''	1:C:2:DA:O5'	2.07	0.55
3:A:1011:LEU:HD12	3:A:1038:TYR:CD2	2.42	0.54
3:A:1288:GLY:C	3:A:1289:PHE:CD1	2.81	0.54
3:A:1175:GLN:HE21	3:A:1303:ARG:NH2	2.05	0.54
3:B:1083:VAL:HG22	3:B:1124:ASN:ND2	2.22	0.54
3:A:1011:LEU:HD22	3:A:1052:HIS:NE2	2.21	0.54
3:A:1340:SER:O	3:A:1341:HIS:ND1	2.39	0.54
3:B:1356:THR:O	3:B:1360:ILE:HG13	2.07	0.54
3:B:1184:ARG:C	3:B:1186:THR:H	2.11	0.54
3:B:1218:HIS:CD2	3:B:1229:THR:OG1	2.61	0.54
3:B:1142:ASP:O	3:B:1148:LYS:HE2	2.07	0.54
3:A:1194:ILE:HG21	3:A:1370:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1012:GLU:OE2	3:A:1017:THR:N	2.41	0.53
3:B:1002:ARG:O	3:B:1075:CYS:HB2	2.09	0.53
3:A:1150:LEU:O	3:A:1153:GLU:HB3	2.08	0.53
3:A:1232:GLU:OE1	3:A:1283:ARG:NH2	2.42	0.53
3:A:1200:ARG:HB3	3:A:1284:MET:CE	2.39	0.53
3:A:1336:THR:O	3:A:1337:PRO:C	2.46	0.53
3:B:1059:VAL:HG21	3:B:1068:ALA:HB2	1.90	0.53
3:B:1156:PRO:O	3:B:1157:GLU:HB2	2.08	0.53
3:B:1018:LYS:HG2	3:B:1307:TYR:CG	2.44	0.53
3:B:1038:TYR:CZ	3:B:1058:PRO:HB3	2.43	0.53
3:A:998:MET:HB2	3:A:1395:PHE:CE1	2.43	0.53
3:B:1062:ALA:O	3:B:1063:LYS:HG3	2.09	0.53
3:B:1029:LYS:O	3:B:1029:LYS:HG2	2.09	0.53
3:A:1069:LEU:HD11	3:A:1073:ASN:ND2	2.24	0.52
3:A:1086:THR:HA	3:A:1125:LEU:HG	1.90	0.52
3:A:1291:TYR:CE1	3:A:1320:VAL:HG11	2.44	0.52
3:B:1096:TYR:CE1	3:B:1100:LEU:HD11	2.45	0.52
1:C:7:5HU:H5A1	3:A:1237:SER:CA	2.28	0.52
3:A:1147:ASN:O	3:A:1151:MET:HB2	2.09	0.52
3:B:1083:VAL:HG22	3:B:1124:ASN:HD22	1.74	0.52
1:C:7:5HU:O2	1:C:7:5HU:H2"	2.09	0.52
3:B:1138:PHE:CD2	3:B:1174:PHE:HB3	2.44	0.52
3:B:1183:VAL:HG13	3:B:1281:LEU:HD13	1.90	0.52
3:A:1279:GLU:O	3:A:1282:GLU:HB3	2.09	0.52
3:A:1230:VAL:HG22	3:A:1270:GLN:HB2	1.91	0.52
3:B:1138:PHE:HB3	3:B:1174:PHE:CD2	2.44	0.52
3:A:1332:ARG:NH2	3:A:1389:PHE:CD1	2.78	0.52
3:B:1118:VAL:HG13	3:B:1145:ASP:CB	2.32	0.52
4:B:2019:NCO:N5	5:B:2021:UDP:O1B	2.42	0.52
3:A:1150:LEU:HD23	3:A:1154:TRP:CH2	2.45	0.52
3:A:1347:TRP:CE3	3:A:1347:TRP:HA	2.43	0.52
3:A:1232:GLU:HB3	3:A:1275:TYR:CD2	2.45	0.52
3:A:1175:GLN:HE21	3:A:1303:ARG:HH21	1.59	0.51
3:A:1356:THR:O	3:A:1360:ILE:HG13	2.10	0.51
3:B:1042:LYS:HG2	3:B:1044:PHE:CE1	2.45	0.51
3:B:1237:SER:HB2	3:B:1238:PRO:HD2	1.92	0.51
1:C:12:DA:H4'	3:B:1123:ARG:NE	2.26	0.51
3:A:1022:GLU:OE1	3:A:1178:MET:HG3	2.10	0.51
3:A:1296:LEU:HD12	3:A:1300:TYR:HB2	1.89	0.51
3:A:1322:TRP:CD1	3:A:1324:SER:HB2	2.45	0.51
3:B:1275:TYR:CD1	3:B:1280:MET:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1317:THR:O	3:B:1319:PRO:HD3	2.11	0.51
3:B:1354:GLU:O	3:B:1358:GLU:HG2	2.11	0.51
3:B:1065:TYR:CZ	3:B:1098:LYS:HE3	2.46	0.51
3:B:1267:GLN:HA	3:B:1267:GLN:NE2	2.25	0.51
3:B:1283:ARG:HG3	3:B:1283:ARG:HH11	1.74	0.51
1:C:8:DA:H2"	1:C:9:DG:OP2	2.10	0.51
3:A:1184:ARG:C	3:A:1186:THR:H	2.15	0.50
3:A:1236:ARG:NH1	3:A:1236:ARG:CG	2.68	0.50
3:A:1293:LEU:CA	3:A:1322:TRP:HB2	2.40	0.50
3:B:1132:ARG:NH1	3:B:1155:TYR:CE1	2.80	0.50
3:A:1319:PRO:HB2	3:A:1345:ILE:HG12	1.94	0.50
3:B:1177:PRO:HG3	3:B:1390:CYS:CB	2.42	0.50
3:B:1200:ARG:HH12	3:B:1283:ARG:HD2	1.76	0.50
3:A:1322:TRP:HE1	3:A:1324:SER:CB	2.24	0.50
3:B:1086:THR:HG23	3:B:1123:ARG:O	2.11	0.50
3:B:1065:TYR:HE2	3:B:1098:LYS:HB3	1.76	0.50
3:A:1110:VAL:HG11	3:A:1398:ILE:HG12	1.94	0.50
3:A:1199:ASN:HB3	3:A:1291:TYR:CE2	2.45	0.50
3:A:1366:ASP:O	3:A:1368:ALA:N	2.44	0.50
3:B:1012:GLU:OE2	3:B:1017:THR:N	2.45	0.50
2:D:1:DC:H2'	2:D:2:DT:C7	2.41	0.50
3:A:1329:LEU:O	3:A:1338:LEU:HG	2.12	0.49
3:A:1223:LYS:HB3	3:A:1224:PRO:HD3	1.94	0.49
3:B:1385:GLN:O	3:B:1385:GLN:HG2	2.12	0.49
3:A:1028:ILE:O	3:A:1031:GLY:N	2.38	0.49
3:B:1065:TYR:CE2	3:B:1098:LYS:HB3	2.48	0.49
3:A:1201:TRP:CB	3:A:1231:MET:HG2	2.41	0.49
3:A:1138:PHE:HB3	3:A:1174:PHE:CD2	2.47	0.49
3:A:1221:PHE:O	3:A:1224:PRO:HD2	2.11	0.49
3:A:1187:TYR:O	3:A:1189:LYS:N	2.46	0.49
3:A:1190:ASP:C	3:A:1192:SER:H	2.15	0.49
3:A:1259:ASP:C	3:A:1261:MET:H	2.16	0.49
3:B:1258:ILE:HG13	3:B:1261:MET:CE	2.43	0.49
3:A:1150:LEU:HD12	3:A:1150:LEU:N	2.28	0.49
3:A:1323:LYS:O	3:A:1324:SER:C	2.50	0.49
3:B:1199:ASN:ND2	3:B:1291:TYR:OH	2.46	0.49
3:A:1222:LEU:HD13	3:A:1229:THR:OG1	2.13	0.49
3:B:1359:ARG:O	3:B:1363:LEU:HD13	2.12	0.49
3:A:1306:GLU:O	3:A:1309:HIS:HB2	2.13	0.48
3:A:1008:ALA:O	3:A:1039:ALA:HB3	2.13	0.48
3:A:1200:ARG:HA	3:A:1230:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1290:GLY:O	3:A:1320:VAL:HG23	2.13	0.48
3:A:1175:GLN:NE2	3:A:1303:ARG:HH21	2.11	0.48
3:A:1293:LEU:HB3	3:A:1322:TRP:HB2	1.96	0.48
3:A:1177:PRO:HB2	3:A:1391:PHE:CE1	2.48	0.48
3:A:1232:GLU:OE1	3:A:1272:LEU:HD23	2.12	0.48
3:A:1297:ASN:OD1	3:A:1298:GLN:N	2.47	0.48
3:A:1339:THR:HG22	3:A:1347:TRP:CE2	2.49	0.48
3:B:1200:ARG:CZ	3:B:1283:ARG:HB3	2.43	0.48
3:B:1068:ALA:O	3:B:1072:VAL:HG22	2.14	0.48
3:B:1184:ARG:HG3	3:B:1188:TRP:CE3	2.48	0.48
3:B:1258:ILE:HG13	3:B:1261:MET:HE3	1.95	0.48
3:A:1184:ARG:HB2	3:A:1378:TYR:HE2	1.78	0.48
3:B:1292:GLN:HB2	3:B:1312:LEU:HD11	1.96	0.48
3:A:1202:ILE:CD1	3:A:1312:LEU:HD21	2.44	0.48
3:A:1218:HIS:O	3:A:1218:HIS:CD2	2.67	0.48
3:B:1086:THR:HG22	3:B:1125:LEU:CD2	2.44	0.48
2:D:1:DC:C2	3:B:1238:PRO:HB2	2.49	0.48
3:A:1253:TYR:CE1	3:A:1261:MET:HG3	2.49	0.48
3:A:1116:HIS:HB3	3:A:1300:TYR:CG	2.48	0.48
3:A:1133:ARG:HH21	3:A:1133:ARG:HG3	1.78	0.48
3:A:1190:ASP:O	3:A:1192:SER:N	2.46	0.48
3:A:1338:LEU:O	3:A:1340:SER:N	2.47	0.48
3:B:1200:ARG:NH1	3:B:1283:ARG:HD2	2.29	0.48
3:A:1170:THR:HG21	3:A:1172:TYR:CZ	2.49	0.48
3:B:1312:LEU:HD12	3:B:1321:PHE:CE1	2.34	0.47
3:B:1074:ASP:O	3:B:1075:CYS:HB3	2.14	0.47
3:B:1097:LYS:HE2	3:B:1129:GLU:OE2	2.15	0.47
3:B:1297:ASN:OD1	3:B:1299:LYS:HG2	2.14	0.47
2:D:7:DG:H1'	3:A:1241:ILE:CD1	2.43	0.47
3:B:1204:ARG:O	3:B:1206:THR:N	2.39	0.47
3:B:1271:ILE:HG22	3:B:1272:LEU:H	1.79	0.47
3:A:1178:MET:HG2	3:A:1179:ASP:N	2.29	0.47
3:A:1289:PHE:CD2	3:A:1318:ILE:HB	2.49	0.47
3:A:1347:TRP:HE3	3:A:1347:TRP:HA	1.79	0.47
3:B:1343:SER:O	3:B:1377:ALA:N	2.48	0.47
3:A:1011:LEU:HD22	3:A:1052:HIS:CE1	2.50	0.47
3:A:1083:VAL:CG2	3:A:1124:ASN:HB3	2.45	0.47
3:B:1352:ASP:OD2	3:B:1355:SER:HB2	2.15	0.47
3:A:1113:GLN:HE21	3:A:1115:ASP:HB2	1.79	0.47
3:A:1072:VAL:HG21	3:A:1099:LEU:HD22	1.97	0.47
3:B:1013:GLY:HA3	3:B:1046:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1018:LYS:HD3	3:A:1050:HIS:NE2	2.30	0.46
3:A:1093:ILE:HG23	3:A:1094:ASN:N	2.30	0.46
3:A:1214:MET:O	3:A:1217:PHE:N	2.48	0.46
3:A:1003:ILE:HB	3:A:1034:VAL:HG22	1.97	0.46
3:A:1281:LEU:HD21	3:A:1311:GLU:HB3	1.97	0.46
3:B:1271:ILE:HG22	3:B:1272:LEU:N	2.30	0.46
3:B:1353:MET:O	3:B:1356:THR:N	2.48	0.46
3:A:1292:GLN:OE1	3:A:1309:HIS:NE2	2.49	0.46
3:B:1180:ILE:HB	3:B:1386:ASP:OD1	2.16	0.46
3:B:1276:ILE:O	3:B:1277:ASN:C	2.54	0.46
3:A:1266:ASN:O	3:A:1267:GLN:OE1	2.34	0.46
3:A:1323:LYS:CE	3:A:1327:GLU:OE1	2.64	0.46
3:B:1253:TYR:CZ	3:B:1261:MET:HA	2.51	0.46
3:A:1037:VAL:HG22	3:A:1071:LEU:HD13	1.98	0.46
3:A:1120:SER:O	3:A:1122:ARG:N	2.49	0.46
3:A:1255:ASN:ND2	3:A:1274:CYS:O	2.48	0.46
3:A:1189:LYS:HG3	3:A:1286:LYS:HG2	1.98	0.46
3:B:1265:PRO:O	3:B:1267:GLN:HG2	2.16	0.46
3:A:1291:TYR:CD1	3:A:1320:VAL:HG11	2.51	0.45
3:A:1259:ASP:OD2	3:A:1260:LYS:HG3	2.17	0.45
3:B:1283:ARG:HG3	3:B:1283:ARG:NH1	2.31	0.45
3:B:1252:TYR:CZ	3:B:1273:ASP:HB3	2.51	0.45
3:A:1133:ARG:NH2	3:A:1133:ARG:HG3	2.31	0.45
3:B:1198:ILE:CD1	3:B:1228:SER:HB3	2.46	0.45
3:B:1310:LEU:HD11	3:B:1385:GLN:HE21	1.81	0.45
3:A:1086:THR:HA	3:A:1125:LEU:CD1	2.47	0.45
3:A:1103:ILE:O	3:A:1104:LYS:C	2.54	0.45
3:A:1145:ASP:HA	3:A:1149:VAL:HG23	1.97	0.45
3:A:1201:TRP:CZ2	3:A:1209:LYS:O	2.66	0.45
3:A:1116:HIS:NE2	4:A:1403:NCO:N3	2.64	0.45
3:A:1293:LEU:HB3	3:A:1322:TRP:CE3	2.51	0.45
3:A:1298:GLN:NE2	3:A:1299:LYS:HA	2.31	0.45
3:A:1150:LEU:HD12	3:A:1150:LEU:H	1.82	0.45
3:A:1342:ASP:OD2	3:A:1376:LYS:NZ	2.47	0.45
3:A:1187:TYR:O	3:A:1189:LYS:HG2	2.17	0.45
3:A:1293:LEU:HD23	3:A:1322:TRP:CE3	2.49	0.45
3:A:1350:GLU:HG3	3:A:1351:ASN:HD22	1.82	0.45
3:A:1373:GLU:OE2	3:A:1376:LYS:NZ	2.50	0.45
3:A:1026:TRP:CD2	3:A:1391:PHE:HB3	2.52	0.45
3:B:1195:ASN:OD1	3:B:1197:ASN:HB2	2.17	0.45
3:B:1238:PRO:O	3:B:1241:ILE:HB	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:DG:H2"	2:D:10:DT:OP2	2.15	0.44
3:A:1293:LEU:HB3	3:A:1322:TRP:HE3	1.82	0.44
3:A:1296:LEU:HD11	3:A:1300:TYR:HB2	1.95	0.44
3:B:1118:VAL:CG1	3:B:1145:ASP:HB3	2.37	0.44
3:B:1289:PHE:CD2	3:B:1318:ILE:HB	2.53	0.44
3:A:1284:MET:HG3	3:A:1315:CYS:SG	2.58	0.44
3:B:1288:GLY:C	3:B:1289:PHE:CD1	2.91	0.44
1:C:9:DG:H1'	1:C:10:DA:H5'	1.98	0.44
3:A:1199:ASN:ND2	3:A:1291:TYR:OH	2.51	0.44
3:A:1322:TRP:NE1	3:A:1324:SER:CB	2.81	0.44
3:A:1366:ASP:C	3:A:1368:ALA:N	2.71	0.44
3:A:1184:ARG:HD2	3:A:1378:TYR:CD2	2.51	0.44
2:D:7:DG:N7	3:A:1244:LYS:NZ	2.62	0.44
3:A:1065:TYR:CE2	3:A:1098:LYS:HD2	2.53	0.44
3:A:1092:THR:O	3:A:1093:ILE:C	2.56	0.44
3:B:1279:GLU:HB3	3:B:1283:ARG:HH12	1.83	0.44
3:A:1065:TYR:CZ	3:A:1098:LYS:HD2	2.52	0.44
3:A:1132:ARG:O	4:A:1401:NCO:N1	2.51	0.44
3:A:1200:ARG:HB3	3:A:1284:MET:HE1	2.00	0.44
3:A:1378:TYR:C	3:A:1378:TYR:CD1	2.91	0.44
3:B:1187:TYR:CZ	3:B:1281:LEU:HD12	2.53	0.44
3:A:1002:ARG:HB2	3:A:1075:CYS:HA	2.00	0.44
3:B:1276:ILE:HG22	8:B:2026:HOH:O	2.18	0.44
3:A:1240:PHE:HD2	3:A:1244:LYS:HE3	1.81	0.44
3:A:1276:ILE:HB	3:A:1279:GLU:HG3	2.00	0.43
3:A:1199:ASN:ND2	3:A:1291:TYR:HE2	2.10	0.43
1:C:9:DG:H2"	1:C:10:DA:OP2	2.17	0.43
3:A:1009:ARG:NH1	3:A:1085:ALA:HA	2.34	0.43
3:A:1261:MET:O	3:A:1263:LEU:N	2.51	0.43
3:A:1118:VAL:HG23	3:A:1119:LEU:N	2.34	0.43
3:B:1060:ILE:O	3:B:1061:LEU:C	2.55	0.43
3:B:1327:GLU:HG3	3:B:1339:THR:HG21	2.00	0.43
3:A:1118:VAL:HG13	3:A:1145:ASP:OD1	2.18	0.43
3:A:1292:GLN:CD	3:A:1309:HIS:CD2	2.92	0.43
3:B:1002:ARG:HB2	3:B:1075:CYS:HA	2.00	0.43
3:A:1205:THR:HG22	3:A:1239:ALA:HB3	2.00	0.43
3:A:1289:PHE:CD1	3:A:1289:PHE:N	2.87	0.43
3:A:1291:TYR:HA	3:A:1320:VAL:HB	1.99	0.43
3:B:1284:MET:O	3:B:1287:SER:HB2	2.19	0.43
3:A:1284:MET:O	3:A:1317:THR:HB	2.18	0.43
3:A:1261:MET:O	3:A:1263:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1213:GLN:HG2	3:A:1322:TRP:HZ3	1.84	0.43
3:A:1393:GLU:O	3:A:1397:ILE:HG13	2.18	0.43
3:A:1175:GLN:O	3:A:1177:PRO:CD	2.57	0.43
3:A:1202:ILE:HD12	3:A:1308:THR:CB	2.49	0.43
3:A:1370:TYR:CD2	3:A:1370:TYR:C	2.92	0.43
3:A:1148:LYS:O	3:A:1152:LYS:HD2	2.19	0.42
3:B:1184:ARG:HD2	3:B:1378:TYR:CZ	2.54	0.42
3:A:1117:SER:O	3:A:1121:LEU:HG	2.19	0.42
3:A:1323:LYS:HG2	3:A:1327:GLU:OE1	2.19	0.42
3:A:1201:TRP:CZ2	3:A:1211:PHE:HB3	2.55	0.42
3:A:1258:ILE:HD13	3:A:1283:ARG:NH1	2.34	0.42
3:A:1253:TYR:O	3:A:1272:LEU:HD12	2.19	0.42
3:B:1083:VAL:CG2	3:B:1124:ASN:HD22	2.32	0.42
3:A:1320:VAL:HG12	3:A:1348:PHE:HB2	2.01	0.42
3:B:1023:GLN:HE22	3:B:1081:ASN:HD21	1.67	0.42
3:A:1258:ILE:CD1	3:A:1283:ARG:NH1	2.83	0.42
3:A:1305:LEU:HA	3:A:1305:LEU:HD23	1.87	0.42
3:A:1184:ARG:NH2	3:A:1375:GLU:OE1	2.36	0.42
3:A:1009:ARG:HH21	3:A:1124:ASN:HD22	1.68	0.42
3:A:1399:THR:O	3:A:1400:LYS:C	2.57	0.42
3:B:1254:GLY:C	3:B:1256:ARG:H	2.23	0.42
3:B:1359:ARG:O	3:B:1363:LEU:CD1	2.68	0.42
1:C:6:DT:H6	1:C:6:DT:H5'	1.84	0.42
2:D:4:DT:H1'	2:D:5:DC:H5'	2.02	0.42
3:A:1180:ILE:CD1	3:A:1382:TYR:HA	2.49	0.42
3:B:1132:ARG:HH11	3:B:1132:ARG:HG2	1.84	0.42
3:B:1155:TYR:O	3:B:1157:GLU:N	2.51	0.42
3:A:1191:VAL:HA	3:A:1194:ILE:HD12	2.02	0.42
3:A:1232:GLU:CG	3:A:1272:LEU:HD23	2.49	0.42
3:B:1009:ARG:HB2	3:B:1082:SER:HB2	2.02	0.42
3:B:1111:VAL:HG23	3:B:1134:ALA:HB2	2.00	0.42
3:B:1244:LYS:C	3:B:1246:LYS:H	2.23	0.42
3:B:1212:TYR:HE2	3:B:1243:ILE:HG12	1.85	0.42
3:B:1301:LEU:HB3	3:B:1329:LEU:CD2	2.49	0.42
1:C:8:DA:C6	1:C:9:DG:O6	2.73	0.42
2:D:3:DA:H2''	2:D:4:DT:H71	2.00	0.42
3:A:1177:PRO:HB3	3:A:1390:CYS:HB2	2.01	0.41
3:A:1216:ASP:O	3:A:1219:GLU:HB3	2.20	0.41
3:B:1175:GLN:O	3:B:1177:PRO:CD	2.67	0.41
3:A:1113:GLN:NE2	3:A:1115:ASP:N	2.60	0.41
3:B:1280:MET:O	3:B:1281:LEU:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1009:ARG:HH12	3:A:1085:ALA:HA	1.86	0.41
3:A:1191:VAL:HG22	3:A:1191:VAL:O	2.21	0.41
3:A:1248:ILE:CG2	3:A:1249:PRO:HD2	2.50	0.41
3:A:1293:LEU:N	3:A:1293:LEU:HD12	2.35	0.41
3:B:1223:LYS:HE3	3:B:1266:ASN:C	2.41	0.41
3:A:1012:GLU:OE1	3:A:1014:CYS:HB2	2.19	0.41
3:A:1178:MET:HB2	3:A:1307:TYR:CE2	2.56	0.41
3:B:1370:TYR:O	3:B:1373:GLU:N	2.53	0.41
3:B:1318:ILE:HD13	3:B:1374:ARG:HB3	2.03	0.41
3:A:1037:VAL:HG21	3:A:1071:LEU:HB3	2.03	0.41
3:A:1332:ARG:HD3	3:A:1384:HIS:O	2.21	0.41
2:D:2:DT:H2"	2:D:3:DA:OP2	2.20	0.41
3:B:1332:ARG:HB2	3:B:1384:HIS:CD2	2.55	0.41
1:C:11:DT:H2"	1:C:12:DA:OP2	2.21	0.41
3:A:1086:THR:HA	3:A:1125:LEU:CG	2.50	0.41
3:A:1120:SER:C	3:A:1122:ARG:N	2.74	0.41
3:A:1241:ILE:O	3:A:1245:GLU:HG3	2.21	0.41
3:B:1308:THR:O	3:B:1312:LEU:HG	2.21	0.41
3:A:1009:ARG:HH11	3:A:1085:ALA:HB2	1.84	0.41
3:A:1041:ASP:OD2	3:A:1061:LEU:N	2.54	0.41
3:A:1085:ALA:O	3:A:1125:LEU:HD12	2.21	0.41
3:A:1361:LYS:HA	3:A:1364:SER:HG	1.86	0.41
3:A:1168:ALA:HA	3:A:1169:PRO:HA	1.82	0.40
1:C:2:DA:C8	1:C:3:DT:H72	2.56	0.40
3:B:1138:PHE:HB3	3:B:1174:PHE:HD2	1.84	0.40
3:B:1240:PHE:O	3:B:1243:ILE:N	2.54	0.40
3:A:1069:LEU:HD13	3:A:1099:LEU:HD23	2.03	0.40
3:B:1198:ILE:HA	3:B:1198:ILE:HD13	1.94	0.40
1:C:8:DA:H61	2:D:5:DC:H42	1.69	0.40
3:A:1017:THR:O	3:A:1021:LEU:HG	2.20	0.40
3:A:1052:HIS:HA	3:A:1055:PHE:CE1	2.57	0.40
3:B:1150:LEU:HD23	3:B:1154:TRP:CZ2	2.56	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	
3	A	388/403 (96%)	308 (79%)	61 (16%)	19 (5%)	2	7
3	B	389/403 (96%)	326 (84%)	53 (14%)	10 (3%)	5	18
All	All	777/806 (96%)	634 (82%)	114 (15%)	29 (4%)	3	11

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1185	SER
3	A	1188	TRP
3	A	1339	THR
3	A	1367	ARG
3	B	1244	LYS
3	A	1121	LEU
3	A	1149	VAL
3	A	1191	VAL
3	A	1225	ALA
3	A	1260	LYS
3	A	1262	ASN
3	A	1273	ASP
3	B	1062	ALA
3	B	1195	ASN
3	B	1205	THR
3	A	1303	ARG
3	B	1053	LYS
3	B	1185	SER
3	A	1046	ARG
3	B	1370	TYR
3	A	1052	HIS
3	A	1323	LYS
3	A	1324	SER
3	A	1338	LEU
3	B	1156	PRO
3	A	1337	PRO
3	B	1241	ILE
3	B	1107	ILE
3	A	1169	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	356/368 (97%)	333 (94%)	23 (6%)	17	44
3	B	358/368 (97%)	348 (97%)	10 (3%)	43	77
All	All	714/736 (97%)	681 (95%)	33 (5%)	27	60

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	998	MET
3	A	1011	LEU
3	A	1012	GLU
3	A	1016	VAL
3	A	1036	LEU
3	A	1048	SER
3	A	1066	ASP
3	A	1110	VAL
3	A	1124	ASN
3	A	1129	GLU
3	A	1169	PRO
3	A	1186	THR
3	A	1212	TYR
3	A	1213	GLN
3	A	1236	ARG
3	A	1259	ASP
3	A	1262	ASN
3	A	1278	SER
3	A	1293	LEU
3	A	1296	LEU
3	A	1298	GLN
3	A	1370	TYR
3	A	1375	GLU
3	B	1012	GLU
3	B	1029	LYS
3	B	1098	LYS
3	B	1119	LEU

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Mol	Chain	Res	Type
3	B	1207	THR
3	B	1212	TYR
3	B	1213	GLN
3	B	1228	SER
3	B	1245	GLU
3	B	1262	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1094	ASN
3	A	1095	ASN
3	A	1102	ASN
3	A	1113	GLN
3	A	1114	HIS
3	A	1175	GLN
3	A	1199	ASN
3	A	1213	GLN
3	A	1218	HIS
3	A	1267	GLN
3	A	1270	GLN
3	A	1298	GLN
3	A	1351	ASN
3	A	1383	GLN
3	A	1384	HIS
3	A	1394	GLN
3	B	1023	GLN
3	B	1052	HIS
3	B	1094	ASN
3	B	1102	ASN
3	B	1113	GLN
3	B	1124	ASN
3	B	1147	ASN
3	B	1175	GLN
3	B	1199	ASN
3	B	1213	GLN
3	B	1218	HIS
3	B	1267	GLN
3	B	1270	GLN
3	B	1277	ASN
3	B	1328	ASN
3	B	1341	HIS

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Mol	Chain	Res	Type
3	B	1351	ASN
3	B	1383	GLN
3	B	1384	HIS
3	B	1394	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
1	5HU	C	7	1	16,22,23	1.17	2 (12%)	19,31,34	3.66	3 (15%)

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
1	5HU	C	7	1	-	4/6/23/24	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	5HU	C4-N3	3.74	1.39	1.33
1	C	7	5HU	C6-C5	2.48	1.42	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	5HU	C4-N3-C2	14.52	127.40	115.14
1	C	7	5HU	C5-C4-N3	-5.42	117.31	125.25
1	C	7	5HU	C5A-C5-C6	2.52	121.62	119.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	7	5HU	O4'-C1'-N1-C6
1	C	7	5HU	C4-C5-C5A-O5B
1	C	7	5HU	C6-C5-C5A-O5B
1	C	7	5HU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	7	5HU	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
5	UDP	B	2021	-	20,26,26	1.08	1 (5%)	25,40,40	1.11	2 (8%)
5	UDP	A	1404	-	20,26,26	1.11	2 (10%)	25,40,40	1.06	2 (8%)
4	NCO	A	1401	-	6,6,6	1.33	0	-		
4	NCO	B	2018	-	6,6,6	1.31	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NCO	A	1402	-	6,6,6	1.37	0	-		
4	NCO	B	2020	-	6,6,6	1.43	0	-		
4	NCO	B	2019	-	6,6,6	1.47	0	-		
4	NCO	A	1403	-	6,6,6	1.48	0	-		
7	EDO	B	2022	-	3,3,3	0.70	0	2,2,2	0.01	0
4	NCO	D	1003	-	6,6,6	1.38	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	UDP	B	2021	-	-	4/14/32/32	0/2/2/2
5	UDP	A	1404	-	-	8/14/32/32	0/2/2/2
7	EDO	B	2022	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1404	UDP	C4-N3	3.23	1.38	1.33
5	B	2021	UDP	C4-N3	3.21	1.38	1.33
5	A	1404	UDP	C6-C5	-2.13	1.33	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2021	UDP	C5-C4-N3	-4.06	114.38	123.31
5	A	1404	UDP	C5-C4-N3	-3.94	114.64	123.31
5	B	2021	UDP	O2B-PB-O1B	2.31	119.72	110.68
5	A	1404	UDP	O2B-PB-O1B	2.30	119.70	110.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2021	UDP	C5'-O5'-PA-O1A
5	B	2021	UDP	C5'-O5'-PA-O2A
5	B	2021	UDP	C5'-O5'-PA-O3A
5	A	1404	UDP	C2'-C1'-N1-C6
5	A	1404	UDP	O4'-C1'-N1-C6

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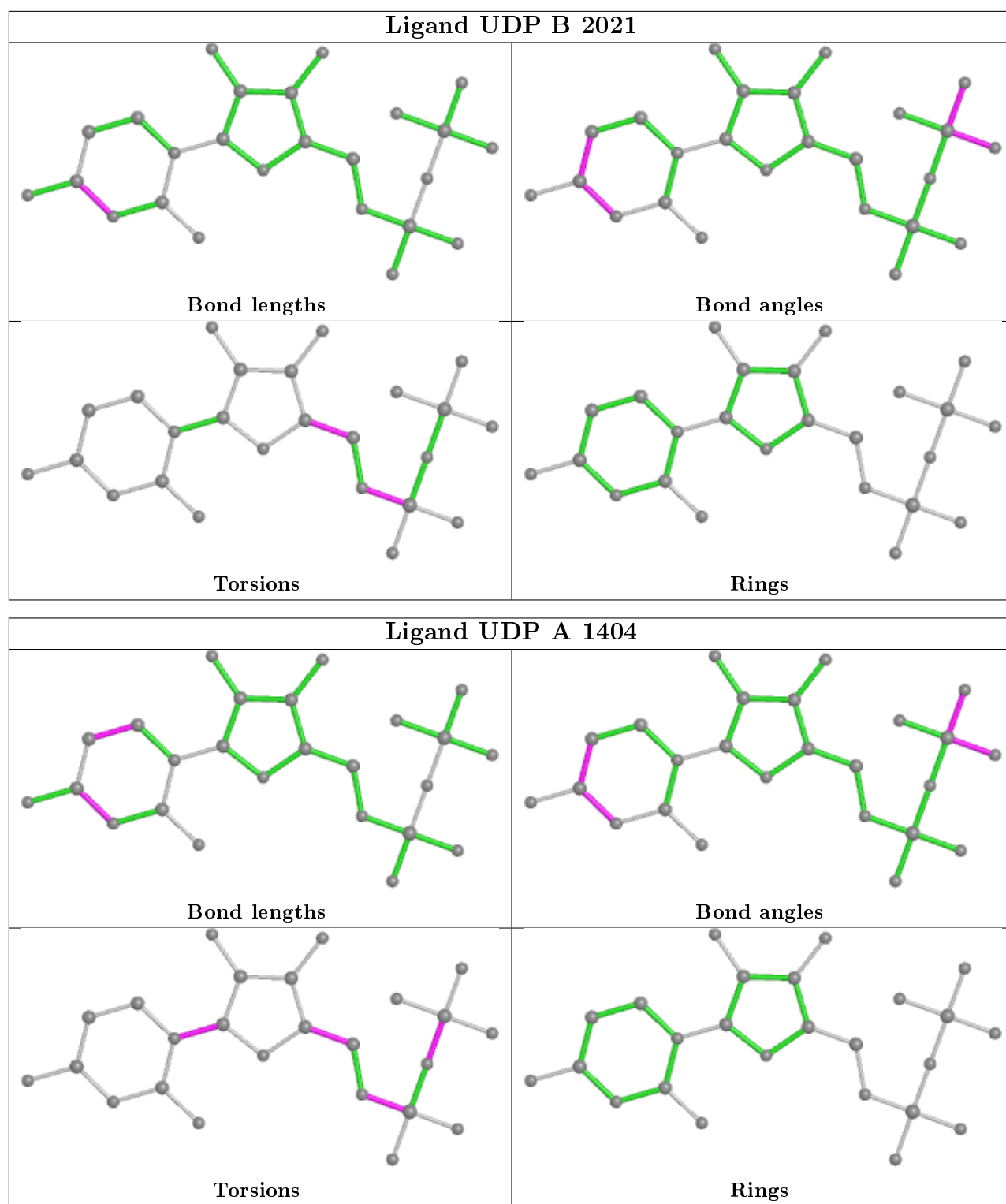
Mol	Chain	Res	Type	Atoms
5	A	1404	UDP	C5'-O5'-PA-O3A
5	A	1404	UDP	PA-O3A-PB-O2B
7	B	2022	EDO	O1-C1-C2-O2
5	A	1404	UDP	PA-O3A-PB-O3B
5	A	1404	UDP	C5'-O5'-PA-O1A
5	A	1404	UDP	C5'-O5'-PA-O2A
5	B	2021	UDP	O4'-C4'-C5'-O5'
5	A	1404	UDP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2021	UDP	1	0
5	A	1404	UDP	1	0
4	A	1401	NCO	1	0
4	B	2019	NCO	1	0
4	A	1403	NCO	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	C	12/13 (92%)	1.01	2 (16%) 1 1	53, 98, 100, 100	0
2	D	12/12 (100%)	0.03	1 (8%) 11 6	64, 88, 100, 100	0
3	A	392/403 (97%)	-0.21	1 (0%) 94 93	32, 62, 89, 96	0
3	B	393/403 (97%)	-0.41	1 (0%) 94 93	27, 50, 68, 91	0
All	All	809/831 (97%)	-0.28	5 (0%) 89 86	27, 56, 87, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	DG	5.6
3	B	1157	GLU	3.5
2	D	1	DC	2.7
1	C	13	DG	2.2
3	A	1320	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	5HU	C	7	21/22	0.85	0.21	85,98,99,99	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

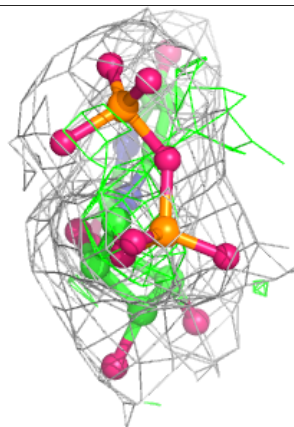
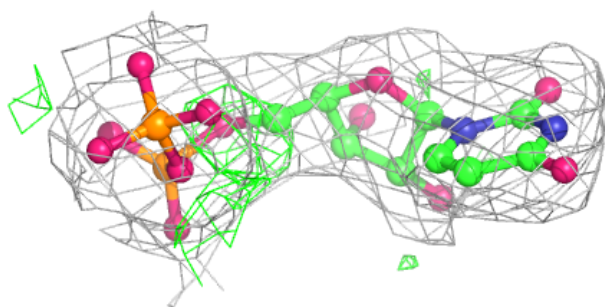
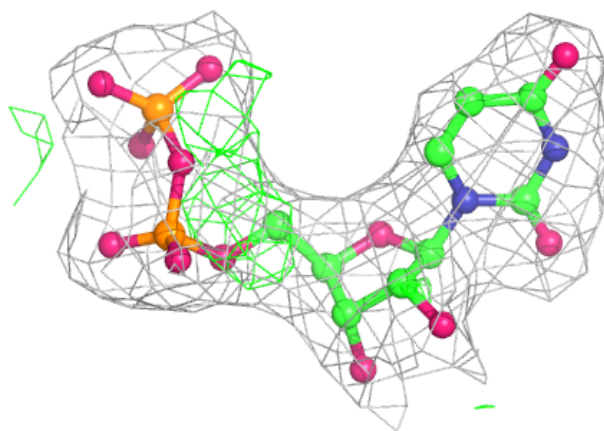
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NCO	A	1402	7/7	0.85	0.26	99,99,99,99	7
4	NCO	B	2019	7/7	0.87	1.12	98,98,99,99	7
4	NCO	A	1403	7/7	0.90	1.04	99,99,99,99	7
6	CL	B	2017	1/1	0.90	0.44	65,65,65,65	0
4	NCO	B	2020	7/7	0.93	0.48	99,99,99,99	7
7	EDO	B	2022	4/4	0.94	0.28	64,64,65,65	0
4	NCO	D	1003	7/7	0.95	0.19	92,92,93,93	0
5	UDP	A	1404	25/25	0.95	0.24	39,46,55,56	0
5	UDP	B	2021	25/25	0.96	0.22	35,39,42,43	0
4	NCO	A	1401	7/7	0.96	0.13	93,94,94,95	0
4	NCO	B	2018	7/7	0.98	0.10	84,84,85,85	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.

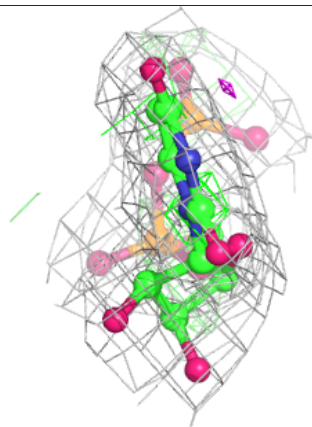
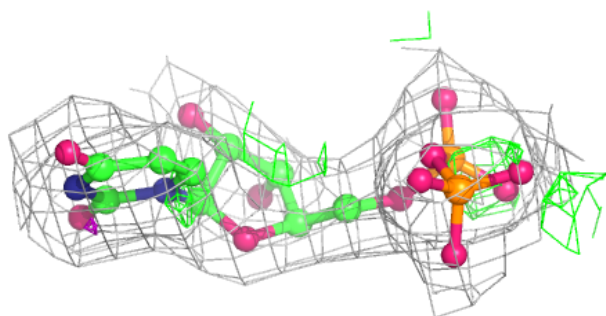
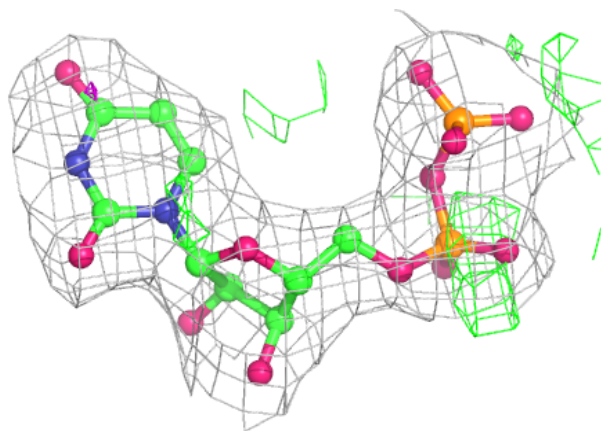
Electron density around UDP A 1404:

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



Electron density around UDP B 2021:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.