



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 07:18 PM EDT

PDB ID : 1Y8Z
Title : alpha-glucosyltransferase in complex with UDP and a 13-mer DNA containing a HMU base at 1.9 Å resolution
Authors : Lariviere, L.; Sommer, N.; Morera, S.
Deposited on : 2004-12-14
Resolution : 1.90 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

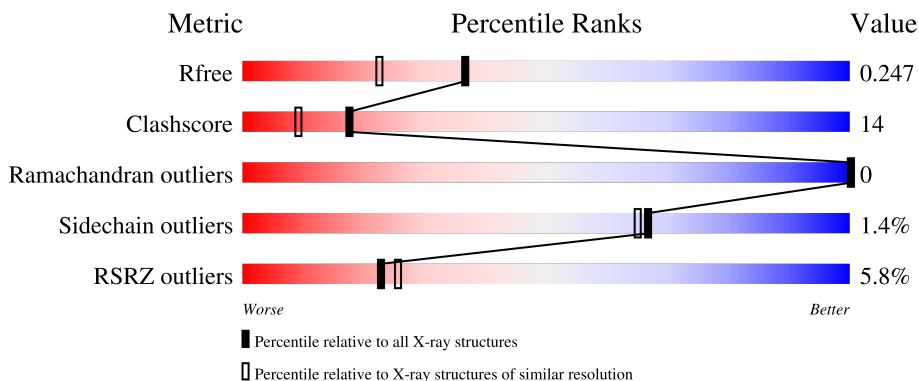
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	
2	D	9	
3	A	402	
3	B	402	

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
6	GOL	A	5001	-	X	-	-
6	GOL	A	5002	-	X	-	-
6	GOL	A	5003	-	X	-	-
6	GOL	B	5004	-	X	-	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7340 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*TP*AP*G)-3'.

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

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	9	181	88	32	53	8	0	0	0

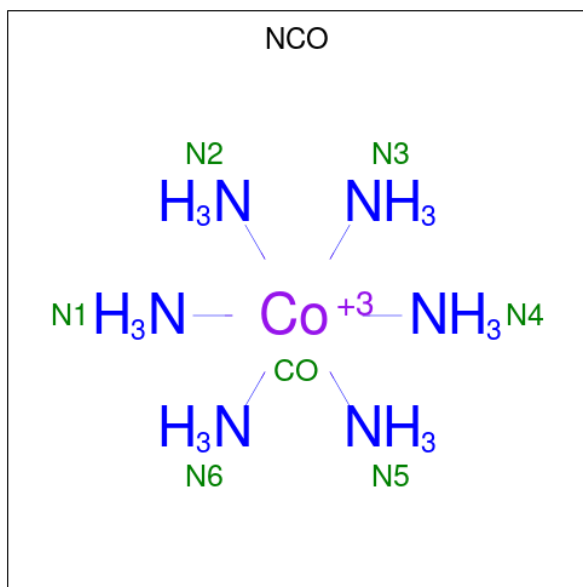
- Molecule 3 is a protein called DNA alpha-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	391	3218	2053	546	600	19	0	0	0
3	B	373	3069	1956	523	572	18	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

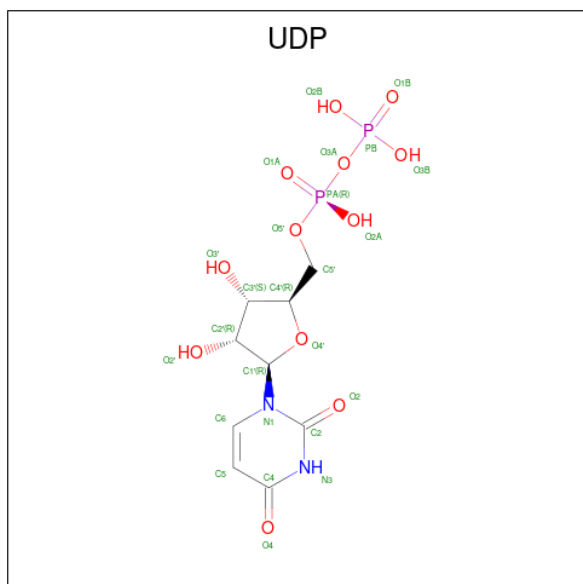
Chain	Residue	Modelled	Actual	Comment	Reference
A	999	GLY	-	cloning artifact	UNP P04519
A	1000	SER	-	cloning artifact	UNP P04519
A	1014	CME	CYS	modified residue	UNP P04519
A	1274	CME	CYS	modified residue	UNP P04519
B	999	GLY	-	cloning artifact	UNP P04519
B	1000	SER	-	cloning artifact	UNP P04519
B	1014	CME	CYS	modified residue	UNP P04519
B	1274	CME	CYS	modified residue	UNP P04519

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



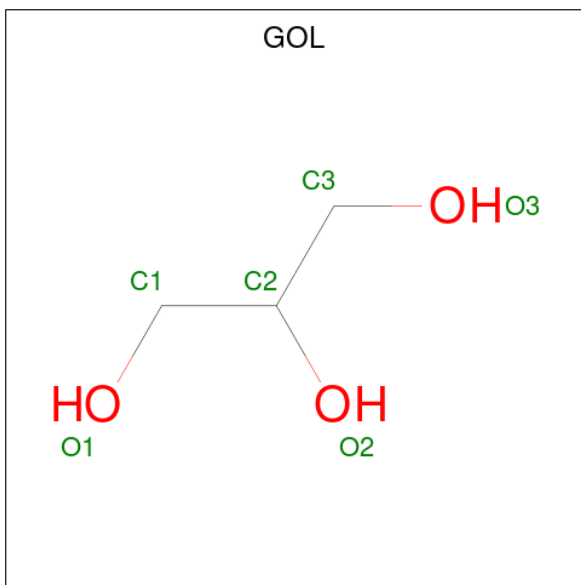
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Co N 7 1 6	0	0
4	A	1	Total Co N 7 1 6	0	0
4	A	1	Total Co N 7 1 6	0	0
4	B	1	Total Co N 7 1 6	0	0
4	B	1	Total Co N 7 1 6	0	0

- 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
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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	21	Total O 21 21	0	0
8	D	8	Total O 8 8	0	0
8	A	266	Total O 266 266	0	0
8	B	199	Total O 199 199	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.

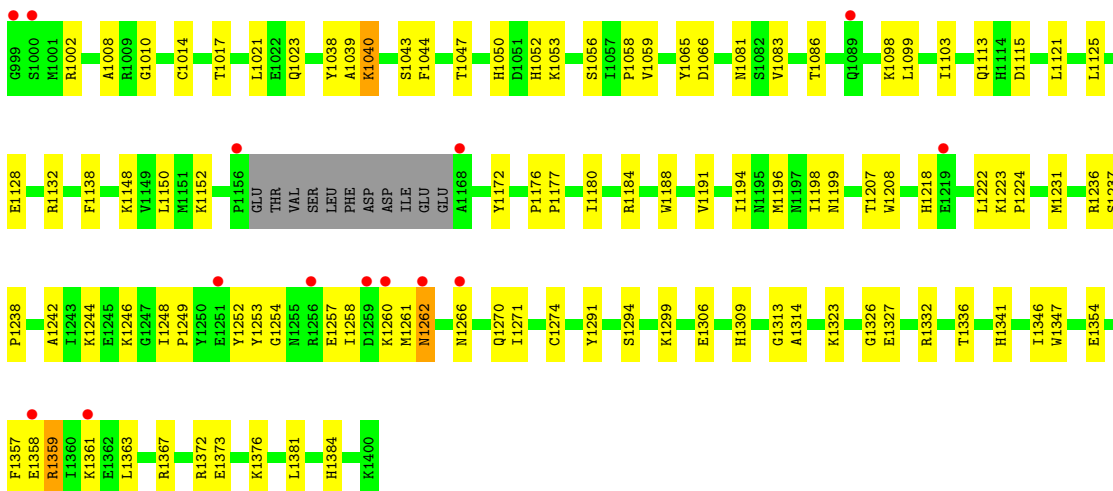
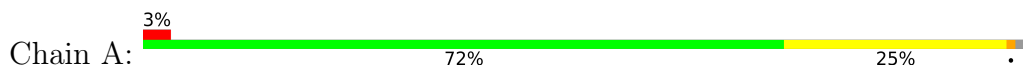
- Molecule 1: 5'-D(*GP*AP*TP*AP*CP*TP*(5HU)P*AP*GP*AP*TP*AP*G)-3'



- Molecule 2: 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*G)-3'

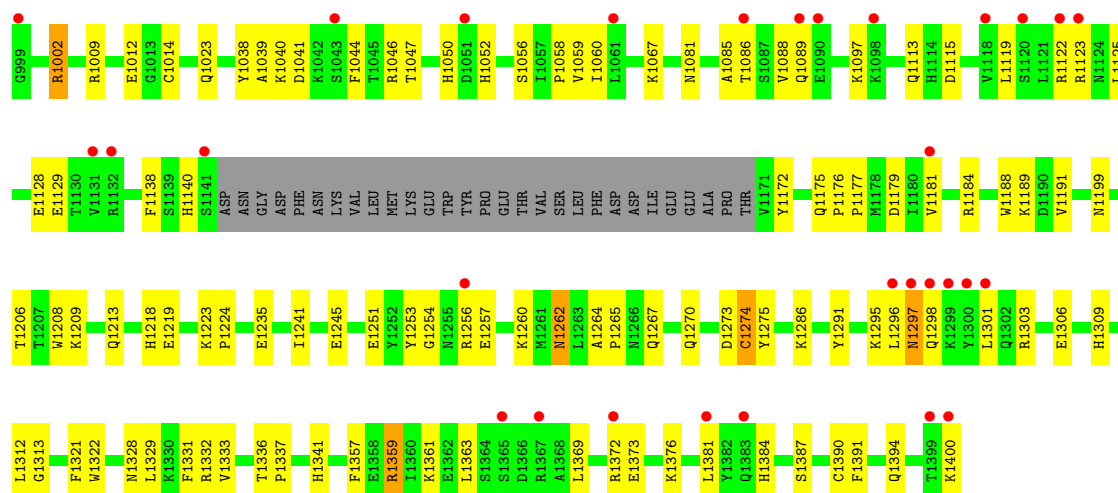


- Molecule 3: DNA alpha-glucosyltransferase



- Molecule 3: DNA alpha-glucosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.26Å 114.66Å 86.14Å 90.00° 89.49° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.90) 99.1 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.90Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.250 0.204 , 0.247	Depositor DCC
R_{free} test set	3141 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.247	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7340	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: 5HU, GOL, CL, UDP, NCO, CME

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	0.24	0/277	0.63	0/424
2	D	0.25	0/202	0.69	0/310
3	A	0.34	0/3272	0.60	0/4410
3	B	0.32	0/3117	0.57	0/4198
All	All	0.32	0/6868	0.59	0/9342

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	9	0
2	D	181	0	104	5	0
3	A	3218	0	3158	77	0
3	B	3069	0	3020	97	0
4	A	14	0	0	0	0
4	B	14	0	0	0	0
4	D	7	0	0	0	0
5	A	25	0	11	0	0
5	B	25	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	18	0	9	0	0
6	B	6	0	3	0	0
7	B	1	0	0	1	0
8	A	266	0	0	9	0
8	B	199	0	0	8	0
8	C	21	0	0	0	0
8	D	8	0	0	0	0
All	All	7340	0	6465	182	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 (182) 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)
3:B:1002:ARG:HH21	3:B:1002:ARG:HB3	1.13	1.11
3:A:1306:GLU:H	3:A:1309:HIS:HD2	1.07	0.97
3:B:1306:GLU:H	3:B:1309:HIS:HD2	1.04	0.95
3:B:1002:ARG:HB3	3:B:1002:ARG:NH2	1.85	0.92
3:A:1113:GLN:HE21	3:A:1115:ASP:H	1.16	0.87
3:A:1237:SER:HB2	3:A:1238:PRO:HD2	1.62	0.82
3:A:1306:GLU:H	3:A:1309:HIS:CD2	1.96	0.80
3:B:1306:GLU:H	3:B:1309:HIS:CD2	1.96	0.79
3:B:1113:GLN:HE21	3:B:1115:ASP:H	1.30	0.79
3:B:1002:ARG:HH21	3:B:1002:ARG:CB	1.95	0.78
3:B:1175:GLN:O	3:B:1177:PRO:HD3	1.84	0.77
3:B:1357:PHE:CE2	3:B:1361:LYS:HD2	2.19	0.77
3:A:1323:LYS:HE2	3:A:1327:GLU:OE1	1.87	0.74
3:B:1067:LYS:HE3	3:B:1067:LYS:HA	1.68	0.73
3:A:1332:ARG:H	3:A:1384:HIS:HD2	1.37	0.72
1:C:8:DA:H8	1:C:8:DA:H5'	1.56	0.70
3:B:1332:ARG:H	3:B:1384:HIS:HD2	1.44	0.66
1:C:3:DT:C3'	1:C:4:DA:H5'	2.26	0.65
3:A:1040:LYS:HB2	3:A:1040:LYS:NZ	2.12	0.65
3:B:1009:ARG:HH12	3:B:1044:PHE:HE2	1.43	0.65
3:B:1336:THR:OG1	3:B:1341:HIS:HE1	1.79	0.65
3:A:1354:GLU:O	3:A:1358:GLU:HG2	1.98	0.64
3:A:1242:ALA:O	3:A:1246:LYS:HG2	1.98	0.63
3:A:1313:GLY:HA3	3:A:1381:LEU:HD12	1.81	0.63
2:D:1:DC:H2'	2:D:2:DT:H72	1.80	0.62
3:A:1184:ARG:HG3	3:A:1188:TRP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1099:LEU:O	3:A:1103:ILE:HG13	1.98	0.62
3:B:1241:ILE:O	3:B:1245:GLU:HG3	2.00	0.61
3:A:1044:PHE:O	3:A:1047:THR:HG23	2.01	0.60
3:B:1286:LYS:NZ	3:B:1286:LYS:HB2	2.16	0.60
3:A:1113:GLN:NE2	3:A:1115:ASP:H	1.94	0.59
1:C:8:DA:H5'	1:C:8:DA:C8	2.38	0.59
3:B:1297:ASN:HD22	3:B:1298:GLN:H	1.51	0.59
3:B:1359:ARG:HH12	3:B:1363:LEU:HD21	1.68	0.59
3:B:1313:GLY:HA3	3:B:1381:LEU:HD12	1.83	0.59
3:B:1122:ARG:HG2	3:B:1122:ARG:HH21	1.68	0.58
3:A:1218:HIS:HA	3:A:1222:LEU:HB2	1.85	0.58
3:A:1357:PHE:O	3:A:1361:LYS:HG3	2.05	0.56
1:C:12:DA:H4'	3:B:1123:ARG:HE	1.70	0.56
3:B:1177:PRO:HB3	3:B:1390:CYS:HB2	1.88	0.56
3:A:1052:HIS:HD2	3:A:1056:SER:OG	1.88	0.56
3:B:1297:ASN:HD22	3:B:1298:GLN:N	2.04	0.55
3:A:1373:GLU:HA	3:A:1376:LYS:HD3	1.88	0.55
3:B:1223:LYS:HB3	3:B:1224:PRO:HD3	1.88	0.55
3:B:1050:HIS:HD2	8:B:95:HOH:O	1.89	0.55
3:B:1206:THR:HG22	3:B:1209:LYS:HG2	1.87	0.55
3:B:1023:GLN:HE22	3:B:1081:ASN:HD21	1.56	0.54
3:A:1191:VAL:HG23	8:A:74:HOH:O	2.06	0.54
3:A:1262:ASN:H	3:A:1270:GLN:NE2	2.05	0.54
3:B:1177:PRO:HB2	3:B:1387:SER:HA	1.89	0.54
3:B:1301:LEU:HD22	3:B:1329:LEU:HD21	1.89	0.54
3:B:1296:LEU:HD22	3:B:1296:LEU:N	2.23	0.54
3:B:1359:ARG:NH1	3:B:1363:LEU:HD21	2.22	0.54
3:A:1121:LEU:HB3	3:A:1150:LEU:HD11	1.89	0.53
3:A:1332:ARG:H	3:A:1384:HIS:CD2	2.23	0.53
3:B:1312:LEU:HD12	3:B:1321:PHE:HE1	1.73	0.53
3:B:1206:THR:CG2	3:B:1209:LYS:HG2	2.38	0.53
3:B:1336:THR:OG1	3:B:1341:HIS:CE1	2.61	0.53
3:B:1219:GLU:HG3	8:B:312:HOH:O	2.08	0.53
3:A:1223:LYS:HB3	3:A:1224:PRO:HD3	1.91	0.53
3:B:1119:LEU:HD12	3:B:1119:LEU:H	1.74	0.53
3:B:1332:ARG:H	3:B:1384:HIS:CD2	2.25	0.52
3:B:1097:LYS:HG2	3:B:1129:GLU:HG3	1.91	0.52
3:B:1286:LYS:HB2	3:B:1286:LYS:HZ2	1.74	0.52
3:A:1336:THR:OG1	3:A:1341:HIS:CE1	2.63	0.52
3:B:1128:GLU:HB3	3:B:1129:GLU:OE1	2.10	0.52
3:B:1184:ARG:HG3	3:B:1188:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1331:PHE:CE2	3:B:1333:VAL:HB	2.45	0.52
3:B:1009:ARG:NH1	3:B:1044:PHE:CE2	2.78	0.52
3:A:1346:ILE:HD11	3:A:1363:LEU:HD12	1.91	0.52
3:B:1295:LYS:HB2	8:B:468:HOH:O	2.09	0.52
3:B:1296:LEU:HB2	3:B:1301:LEU:HD21	1.92	0.52
3:B:1089:GLN:HG2	8:B:85:HOH:O	2.10	0.52
2:D:1:DC:H5 ⁷	3:B:1245:GLU:OE1	2.09	0.51
3:A:1260:LYS:NZ	3:A:1260:LYS:HB3	2.24	0.51
3:B:1040:LYS:HG3	3:B:1060:ILE:HG12	1.92	0.51
3:A:1372:ARG:O	3:A:1376:LYS:HG3	2.10	0.51
3:B:1047:THR:O	3:B:1052:HIS:HE1	1.93	0.51
3:B:1012:GLU:HG2	3:B:1044:PHE:CE2	2.46	0.51
3:B:1119:LEU:HD12	3:B:1119:LEU:N	2.25	0.51
3:B:1191:VAL:HG23	8:B:99:HOH:O	2.10	0.51
3:A:1148:LYS:O	3:A:1152:LYS:HD2	2.11	0.51
3:B:1179:ASP:OD1	3:B:1181:VAL:HG22	2.11	0.51
3:B:1122:ARG:HG2	3:B:1122:ARG:NH2	2.26	0.50
3:B:1257:GLU:HG2	3:B:1257:GLU:O	2.12	0.50
3:A:1023:GLN:HE22	3:A:1081:ASN:HD21	1.58	0.50
3:A:1357:PHE:CE2	3:A:1361:LYS:HD2	2.47	0.50
3:A:1010:GLY:HA2	3:A:1039:ALA:O	2.11	0.50
3:B:1189:LYS:HD3	8:B:289:HOH:O	2.10	0.50
3:A:1336:THR:OG1	3:A:1341:HIS:HE1	1.94	0.50
3:B:1046:ARG:NH2	3:B:1235:GLU:OE2	2.45	0.50
3:A:1198:ILE:HD12	8:A:341:HOH:O	2.11	0.49
3:B:1140:HIS:CE1	3:B:1176:PRO:HD3	2.46	0.49
3:A:1128:GLU:O	3:A:1132:ARG:HG3	2.12	0.49
3:B:1273:ASP:OD2	3:B:1274:CME:N	2.45	0.49
3:A:1040:LYS:HB2	3:A:1040:LYS:HZ1	1.76	0.49
3:A:1313:GLY:HA3	3:A:1381:LEU:CD1	2.43	0.49
3:B:1260:LYS:HB3	3:B:1260:LYS:NZ	2.27	0.49
3:A:1309:HIS:HE1	8:A:8:HOH:O	1.95	0.49
3:B:1213:GLN:HG2	3:B:1322:TRP:CZ3	2.47	0.49
3:A:1053:LYS:HE2	8:A:344:HOH:O	2.12	0.49
3:B:1052:HIS:HD2	3:B:1056:SER:OG	1.96	0.49
3:B:1002:ARG:HD3	8:B:155:HOH:O	2.14	0.48
3:A:1050:HIS:HD2	8:A:62:HOH:O	1.97	0.48
3:A:1196:MET:HE3	3:A:1367:ARG:NH1	2.28	0.48
3:B:1177:PRO:HG2	3:B:1391:PHE:CE1	2.48	0.48
3:B:1208:TRP:HA	3:B:1295:LYS:HE3	1.95	0.48
3:A:1236:ARG:HG3	3:A:1252:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1199:ASN:HB3	3:B:1291:TYR:CE2	2.49	0.47
2:D:1:DC:C2'	2:D:2:DT:H72	2.43	0.47
3:A:1047:THR:O	3:A:1052:HIS:HE1	1.97	0.47
1:C:11:DT:O4'	3:B:1119:LEU:HD22	2.15	0.47
3:A:1199:ASN:HB3	3:A:1291:TYR:CE2	2.50	0.47
3:B:1012:GLU:HB2	7:B:4001:CL:CL	2.51	0.47
3:B:1113:GLN:NE2	3:B:1115:ASP:H	2.04	0.47
3:A:1231:MET:HB2	3:A:1271:ILE:CD1	2.45	0.47
3:B:1296:LEU:HB2	3:B:1301:LEU:CG	2.45	0.47
3:A:1326:GLY:HA3	3:A:1347:TRP:CZ3	2.50	0.47
3:A:1113:GLN:HE21	3:A:1115:ASP:N	1.99	0.46
3:B:1067:LYS:HA	3:B:1067:LYS:CE	2.41	0.46
3:B:1251:GLU:HG2	3:B:1253:TYR:OH	2.14	0.46
3:B:1303:ARG:O	3:B:1384:HIS:CE1	2.67	0.46
3:A:1180:ILE:HG23	3:A:1314:ALA:HB2	1.96	0.46
1:C:3:DT:H3'	1:C:4:DA:H5'	1.95	0.46
1:C:3:DT:H3'	1:C:4:DA:C5'	2.44	0.46
3:B:1140:HIS:HE1	3:B:1176:PRO:HD3	1.79	0.46
3:A:1299:LYS:HE2	8:A:254:HOH:O	2.17	0.45
3:B:1372:ARG:O	3:B:1376:LYS:HG3	2.16	0.45
3:B:1039:ALA:HA	3:B:1059:VAL:O	2.16	0.45
3:B:1086:THR:HA	3:B:1125:LEU:CD1	2.47	0.45
3:A:1254:GLY:H	3:A:1257:GLU:CD	2.20	0.45
3:A:1199:ASN:ND2	3:A:1291:TYR:OH	2.49	0.44
3:B:1254:GLY:C	3:B:1256:ARG:H	2.19	0.44
3:B:1297:ASN:ND2	3:B:1298:GLN:N	2.65	0.44
1:C:3:DT:H5'	3:A:1207:THR:HG21	1.98	0.44
3:A:1086:THR:HA	3:A:1125:LEU:HG	1.99	0.44
3:A:1065:TYR:CZ	3:A:1098:LYS:HD2	2.52	0.44
2:D:8:DA:C2	3:A:1238:PRO:HB2	2.53	0.44
3:B:1085:ALA:O	3:B:1088:VAL:HG22	2.18	0.44
3:B:1086:THR:HA	3:B:1125:LEU:HD11	2.00	0.43
3:B:1113:GLN:NE2	3:B:1115:ASP:HB2	2.33	0.43
3:B:1369:LEU:CD1	3:B:1372:ARG:HH11	2.31	0.43
3:A:1040:LYS:NZ	3:A:1040:LYS:CB	2.80	0.43
3:A:1306:GLU:N	3:A:1309:HIS:HD2	1.92	0.43
3:A:1038:TYR:CZ	3:A:1058:PRO:HB3	2.54	0.43
3:B:1206:THR:HG22	3:B:1209:LYS:CG	2.49	0.43
3:A:1002:ARG:NH2	8:A:87:HOH:O	2.51	0.43
3:B:1262:ASN:H	3:B:1270:GLN:NE2	2.16	0.43
3:B:1275:TYR:CE1	5:B:2001:UDP:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1301:LEU:HD22	3:B:1329:LEU:CG	2.49	0.43
3:A:1231:MET:HB2	3:A:1271:ILE:HD12	1.99	0.43
1:C:3:DT:C3'	1:C:4:DA:C5'	2.97	0.42
3:A:1254:GLY:H	3:A:1257:GLU:CG	2.32	0.42
3:A:1258:ILE:O	3:A:1261:MET:HB2	2.19	0.42
3:A:1244:LYS:HA	8:A:399:HOH:O	2.19	0.42
3:B:1329:LEU:O	3:B:1337:PRO:HA	2.19	0.42
3:A:1194:ILE:O	3:A:1196:MET:HE2	2.20	0.42
3:B:1331:PHE:HE1	3:B:1384:HIS:HB2	1.85	0.42
2:D:2:DT:OP2	3:A:1043:SER:CB	2.68	0.42
3:B:1301:LEU:HD12	3:B:1328:ASN:HB2	2.02	0.42
3:B:1138:PHE:HA	3:B:1172:TYR:O	2.20	0.41
3:B:1264:ALA:HB1	3:B:1265:PRO:HD2	2.02	0.41
3:A:1208:TRP:O	3:A:1294:SER:HA	2.20	0.41
3:B:1309:HIS:HE1	8:B:51:HOH:O	2.03	0.41
3:B:1331:PHE:CE1	3:B:1384:HIS:HB2	2.55	0.41
3:A:1359:ARG:NH1	3:A:1363:LEU:HD21	2.36	0.41
3:A:1138:PHE:HA	3:A:1172:TYR:O	2.20	0.41
3:B:1038:TYR:CZ	3:B:1058:PRO:HB3	2.55	0.41
3:B:1373:GLU:O	3:B:1376:LYS:HB2	2.21	0.41
3:A:1039:ALA:HA	3:A:1059:VAL:O	2.21	0.41
3:A:1306:GLU:O	3:A:1309:HIS:HB2	2.21	0.41
3:B:1390:CYS:O	3:B:1394:GLN:HG3	2.21	0.41
3:A:1008:ALA:HB3	3:A:1083:VAL:HA	2.03	0.41
3:A:1017:THR:O	3:A:1021:LEU:HG	2.21	0.41
3:A:1359:ARG:HH11	3:A:1363:LEU:HG	1.86	0.41
3:A:1363:LEU:HD21	3:A:1373:GLU:HG3	2.03	0.41
3:B:1113:GLN:HE21	3:B:1115:ASP:N	2.07	0.41
3:A:1253:TYR:OH	3:A:1270:GLN:NE2	2.53	0.40
3:A:1066:ASP:HB3	8:A:77:HOH:O	2.20	0.40
3:A:1176:PRO:HA	3:A:1177:PRO:HD3	1.91	0.40
3:A:1248:ILE:HA	3:A:1249:PRO:HD3	1.89	0.40
3:B:1218:HIS:HE1	3:B:1267:GLN:O	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	
3	A	385/402 (96%)	365 (95%)	20 (5%)	0	100	100
3	B	367/402 (91%)	354 (96%)	13 (4%)	0	100	100
All	All	752/804 (94%)	719 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	A	354/365 (97%)	350 (99%)	4 (1%)	73	73
3	B	338/365 (93%)	332 (98%)	6 (2%)	59	55
All	All	692/730 (95%)	682 (99%)	10 (1%)	67	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1040	LYS
3	A	1262	ASN
3	A	1266	ASN
3	A	1359	ARG
3	B	1002	ARG
3	B	1041	ASP
3	B	1262	ASN
3	B	1297	ASN

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Mol	Chain	Res	Type
3	B	1359	ARG
3	B	1400	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1023	GLN
3	A	1050	HIS
3	A	1052	HIS
3	A	1094	ASN
3	A	1102	ASN
3	A	1113	GLN
3	A	1124	ASN
3	A	1175	GLN
3	A	1199	ASN
3	A	1218	HIS
3	A	1262	ASN
3	A	1266	ASN
3	A	1267	GLN
3	A	1270	GLN
3	A	1309	HIS
3	A	1328	ASN
3	A	1341	HIS
3	A	1351	ASN
3	A	1383	GLN
3	A	1384	HIS
3	A	1394	GLN
3	B	1023	GLN
3	B	1030	ASN
3	B	1050	HIS
3	B	1052	HIS
3	B	1089	GLN
3	B	1094	ASN
3	B	1102	ASN
3	B	1113	GLN
3	B	1124	ASN
3	B	1175	GLN
3	B	1199	ASN
3	B	1218	HIS
3	B	1262	ASN
3	B	1266	ASN
3	B	1267	GLN

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Mol	Chain	Res	Type
3	B	1270	GLN
3	B	1297	ASN
3	B	1302	GLN
3	B	1309	HIS
3	B	1328	ASN
3	B	1341	HIS
3	B	1351	ASN
3	B	1384	HIS
3	B	1394	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](#)

5 non-standard protein/DNA/RNA residues 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
3	CME	A	1274	3	8,9,10	1.07	1 (12%)	5,9,11	0.44	0
3	CME	A	1014	3	8,9,10	1.10	1 (12%)	5,9,11	0.60	0
3	CME	B	1014	3	8,9,10	1.07	1 (12%)	5,9,11	0.38	0
3	CME	B	1274	3	8,9,10	1.06	1 (12%)	5,9,11	0.50	0
1	5HU	C	7	1	19,22,23	0.41	0	26,31,34	0.76	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CME	A	1274	3	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CME	A	1014	3	-	2/5/8/10	-
3	CME	B	1014	3	-	1/5/8/10	-
3	CME	B	1274	3	-	1/5/8/10	-
1	5HU	C	7	1	-	0/9/23/24	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1014	CME	OH-CZ	-2.90	1.27	1.42
3	B	1014	CME	OH-CZ	-2.84	1.27	1.42
3	B	1274	CME	OH-CZ	-2.74	1.27	1.42
3	A	1274	CME	OH-CZ	-2.73	1.28	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	5HU	C5A-C5-C6	2.68	123.37	119.33
1	C	7	5HU	O5B-C5A-C5	-2.28	105.09	111.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1014	CME	SD-CE-CZ-OH
3	B	1014	CME	CE-SD-SG-CB
3	A	1014	CME	CZ-CE-SD-SG
3	B	1274	CME	CZ-CE-SD-SG
3	A	1274	CME	CA-CB-SG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1274	CME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
6	GOL	A	5001	-	5,5,5	4.27	5 (100%)	5,5,5	2.12	2 (40%)
4	NCO	A	3005	-	6,6,6	1.31	0	-		
6	GOL	A	5003	-	5,5,5	4.27	5 (100%)	5,5,5	2.12	2 (40%)
4	NCO	A	3001	-	6,6,6	1.34	0	-		
5	UDP	A	3006	-	24,26,26	0.62	0	37,40,40	0.60	1 (2%)
6	GOL	B	5004	-	5,5,5	4.28	5 (100%)	5,5,5	2.11	2 (40%)
6	GOL	A	5002	-	5,5,5	4.27	5 (100%)	5,5,5	2.08	2 (40%)
4	NCO	D	3003	-	6,6,6	1.32	0	-		
4	NCO	B	3004	-	6,6,6	1.30	0	-		
5	UDP	B	2001	-	24,26,26	0.58	0	37,40,40	0.58	1 (2%)
4	NCO	B	3002	-	6,6,6	1.35	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
6	GOL	A	5001	-	-	4/4/4/4	-
6	GOL	A	5003	-	-	2/4/4/4	-
5	UDP	A	3006	-	-	4/16/32/32	0/2/2/2
6	GOL	B	5004	-	-	2/4/4/4	-
6	GOL	A	5002	-	-	2/4/4/4	-
5	UDP	B	2001	-	-	4/16/32/32	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5002	GOL	C1-C2	-5.17	1.30	1.51
6	B	5004	GOL	C3-C2	-5.15	1.30	1.51
6	A	5002	GOL	C3-C2	-5.14	1.30	1.51
6	A	5001	GOL	C1-C2	-5.12	1.30	1.51
6	A	5003	GOL	C3-C2	-5.11	1.30	1.51
6	A	5001	GOL	C3-C2	-5.11	1.30	1.51
6	B	5004	GOL	C1-C2	-5.08	1.30	1.51
6	A	5003	GOL	C1-C2	-5.06	1.30	1.51
6	B	5004	GOL	O1-C1	3.99	1.59	1.42
6	A	5003	GOL	O1-C1	3.98	1.59	1.42
6	A	5001	GOL	O3-C3	3.97	1.59	1.42
6	A	5001	GOL	O1-C1	3.94	1.59	1.42
6	B	5004	GOL	O3-C3	3.93	1.59	1.42
6	A	5002	GOL	O1-C1	3.91	1.58	1.42
6	A	5002	GOL	O3-C3	3.90	1.58	1.42
6	A	5003	GOL	O3-C3	3.89	1.58	1.42
6	A	5003	GOL	O2-C2	-2.89	1.34	1.43
6	B	5004	GOL	O2-C2	-2.80	1.35	1.43
6	A	5002	GOL	O2-C2	-2.78	1.35	1.43
6	A	5001	GOL	O2-C2	-2.76	1.35	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5003	GOL	O1-C1-C2	3.34	126.20	110.20
6	B	5004	GOL	O1-C1-C2	3.32	126.11	110.20
6	A	5001	GOL	O3-C3-C2	3.30	126.03	110.20
6	A	5001	GOL	O1-C1-C2	3.28	125.93	110.20
6	A	5003	GOL	O3-C3-C2	3.25	125.77	110.20
6	B	5004	GOL	O3-C3-C2	3.24	125.73	110.20
6	A	5002	GOL	O3-C3-C2	3.24	125.73	110.20
6	A	5002	GOL	O1-C1-C2	3.21	125.61	110.20
5	A	3006	UDP	O2B-PB-O1B	2.24	119.44	110.68
5	B	2001	UDP	O2B-PB-O1B	2.19	119.27	110.68

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3006	UDP	PA-O3A-PB-O3B
5	B	2001	UDP	PA-O3A-PB-O3B
6	A	5001	GOL	C1-C2-C3-O3

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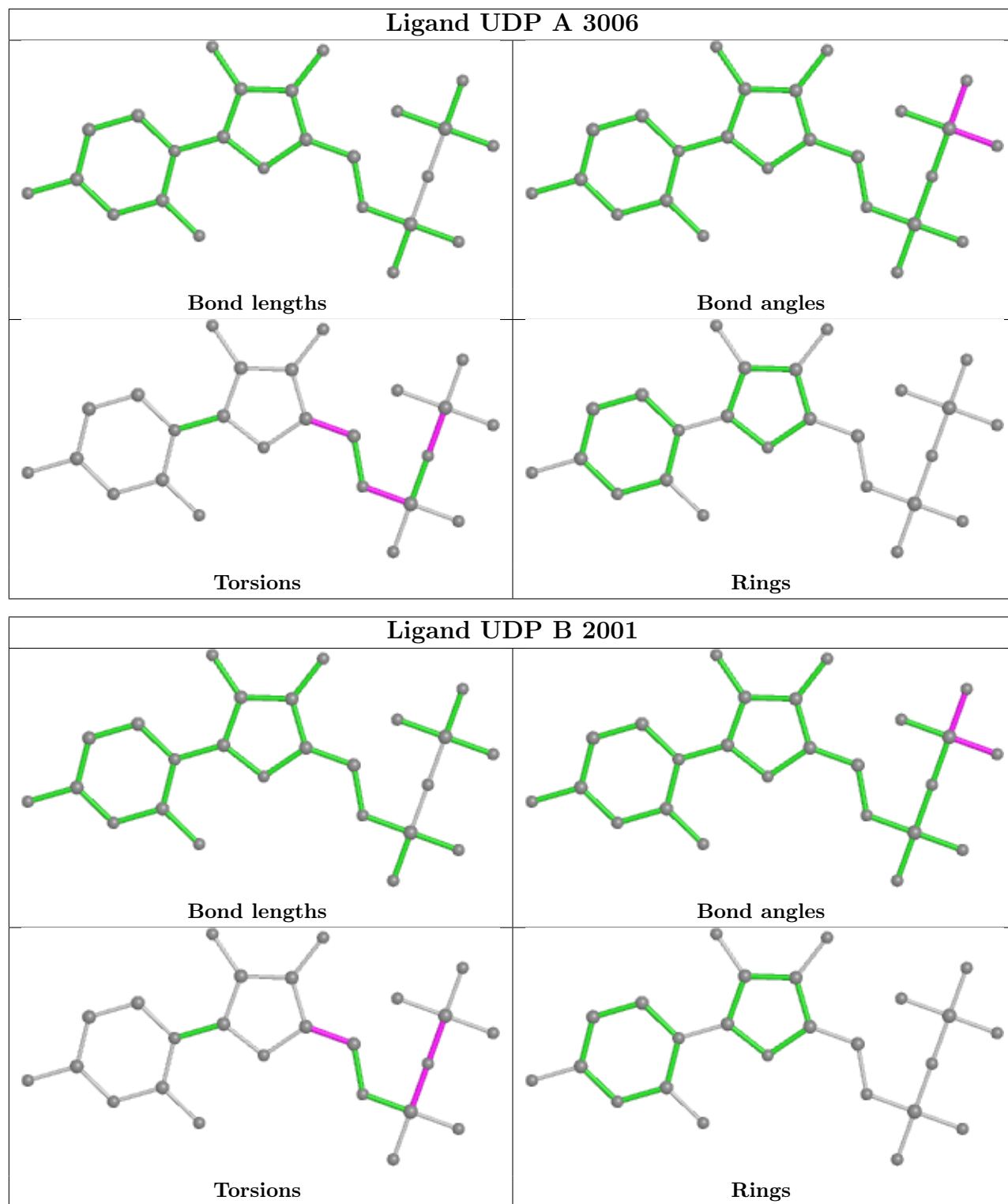
Mol	Chain	Res	Type	Atoms
6	B	5004	GOL	O1-C1-C2-C3
6	A	5001	GOL	O2-C2-C3-O3
6	A	5002	GOL	C1-C2-C3-O3
6	A	5003	GOL	O1-C1-C2-C3
6	A	5002	GOL	O2-C2-C3-O3
6	A	5003	GOL	O1-C1-C2-O2
6	B	5004	GOL	O1-C1-C2-O2
5	B	2001	UDP	PB-O3A-PA-O5'
5	A	3006	UDP	C5'-O5'-PA-O3A
6	A	5001	GOL	O1-C1-C2-O2
5	A	3006	UDP	O4'-C4'-C5'-O5'
5	B	2001	UDP	O4'-C4'-C5'-O5'
6	A	5001	GOL	O1-C1-C2-C3
5	A	3006	UDP	PA-O3A-PB-O2B
5	B	2001	UDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	UDP	1	0

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

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.78	1 (8%) 11 13	24, 46, 59, 74	0
2	D	9/9 (100%)	0.56	0 100 100	41, 47, 50, 50	0
3	A	389/402 (96%)	0.34	14 (3%) 42 45	11, 25, 43, 60	0
3	B	371/402 (92%)	0.54	30 (8%) 12 13	16, 30, 50, 67	0
All	All	781/826 (94%)	0.45	45 (5%) 23 25	11, 28, 48, 74	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1300	TYR	6.1
3	B	1400	LYS	5.4
3	A	1168	ALA	5.2
3	B	1301	LEU	5.0
1	C	1	DG	4.8
3	B	1256	ARG	4.2
3	A	1256	ARG	4.0
3	B	1132	ARG	4.0
3	B	1043	SER	3.9
3	B	1297	ASN	3.8
3	B	1141	SER	3.3
3	B	1299	LYS	3.3
3	A	1266	ASN	3.2
3	A	1156	PRO	3.2
3	B	1090	GLU	2.9
3	A	999	GLY	2.9
3	A	1262	ASN	2.9
3	B	1296	LEU	2.9
3	A	1259	ASP	2.8
3	B	1123	ARG	2.8
3	A	1089	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	1089	GLN	2.8
3	A	1260	LYS	2.8
3	B	1298	GLN	2.7
3	A	1361	LYS	2.7
3	A	1358	GLU	2.6
3	B	1399	THR	2.6
3	B	1365	SER	2.5
3	B	1372	ARG	2.4
3	B	1383	GLN	2.4
3	A	1251	GLU	2.3
3	B	1051	ASP	2.3
3	A	1000	SER	2.2
3	B	1120	SER	2.2
3	B	1367	ARG	2.2
3	B	1181	VAL	2.2
3	B	1118	VAL	2.1
3	B	1086	THR	2.1
3	B	1381	LEU	2.1
3	B	1131	VAL	2.1
3	B	999	GLY	2.1
3	B	1098	LYS	2.1
3	B	1122	ARG	2.1
3	B	1061	LEU	2.1
3	A	1219	GLU	2.0

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
3	CME	A	1274	10/11	0.84	0.16	28,37,49,51	0
3	CME	B	1274	10/11	0.87	0.16	25,32,45,46	0
1	5HU	C	7	21/22	0.91	0.13	33,47,49,50	0
3	CME	B	1014	10/11	0.93	0.13	23,29,42,46	0
3	CME	A	1014	10/11	0.93	0.12	13,22,38,39	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

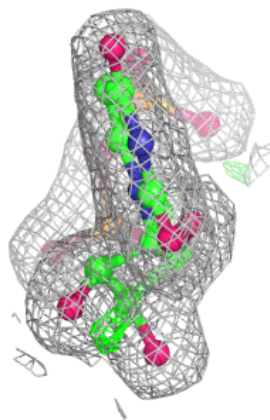
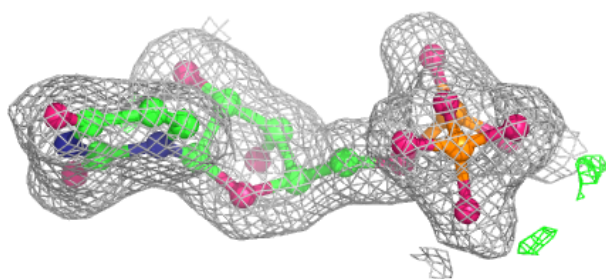
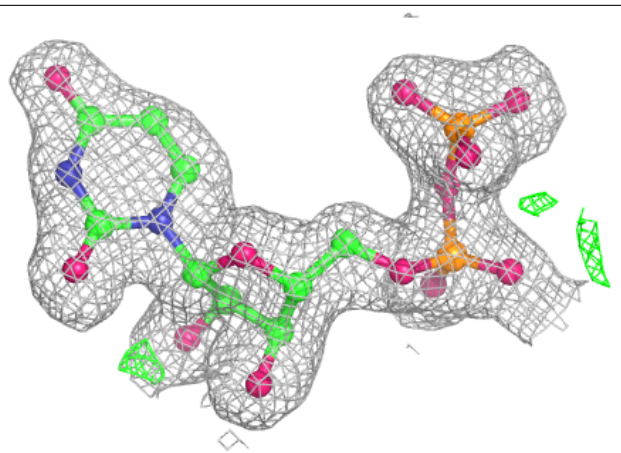
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

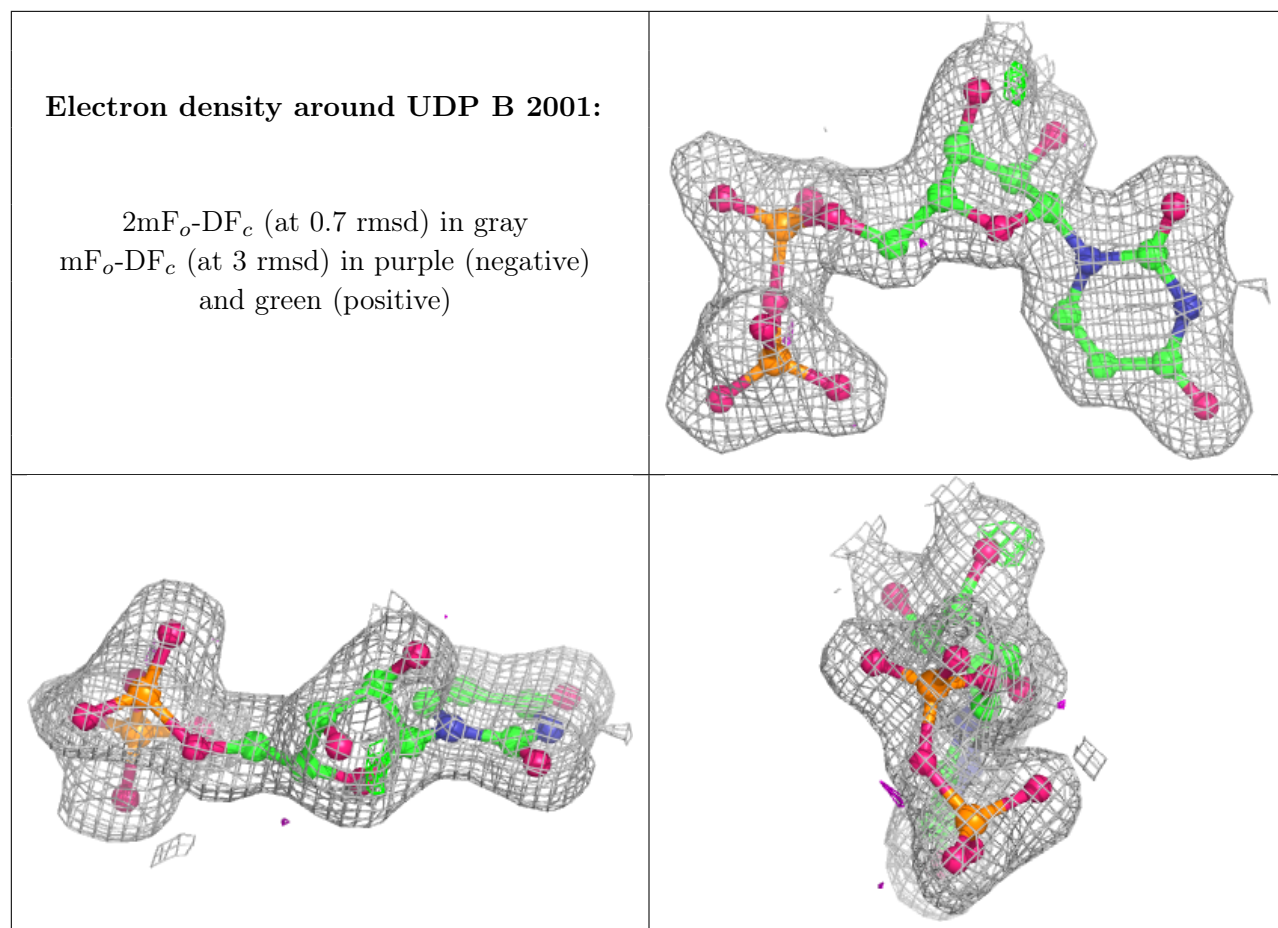
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	5004	6/6	0.62	0.30	67,68,68,69	0
6	GOL	A	5003	6/6	0.63	0.28	62,63,63,64	0
6	GOL	A	5002	6/6	0.70	0.21	63,63,63,64	0
4	NCO	B	3004	7/7	0.82	0.23	53,53,53,54	7
6	GOL	A	5001	6/6	0.84	0.17	72,72,72,72	0
4	NCO	A	3005	7/7	0.91	0.22	45,45,45,46	7
4	NCO	B	3002	7/7	0.96	0.19	43,44,44,45	0
4	NCO	D	3003	7/7	0.96	0.16	58,58,59,59	0
5	UDP	A	3006	25/25	0.97	0.08	13,16,20,22	0
5	UDP	B	2001	25/25	0.97	0.07	17,20,23,25	0
4	NCO	A	3001	7/7	0.97	0.14	43,44,44,45	0
7	CL	B	4001	1/1	0.98	0.07	36,36,36,36	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 3006:

$2mF_o-DF_c$ (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.