Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 06:58 PM EST

PDB ID	:	1Y6F
Title	:	alpha-glucosyltransferase in complex with UDP-glucose and DNA containing an abasic site
Authors	:	Lariviere, L.; Sommer, N.; Morera, S.
Deposited on	:	2004-12-06
Resolution	:	2.40 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:

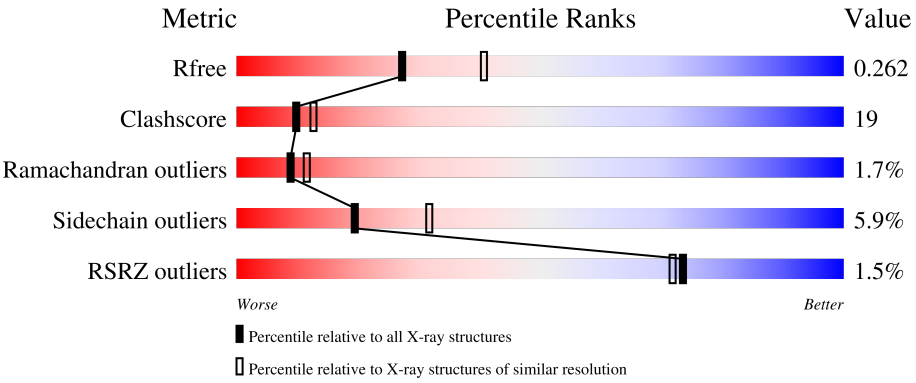
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	C	13	8% 54% 46%
2	D	13	38% 62%
3	A	403	% 58% 37%
3	B	403	% 61% 33%

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
5	GOL	A	701	-	X	-	-
5	GOL	A	702	-	X	-	-
5	GOL	B	602	-	X	-	-
5	GOL	B	703	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7311 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*(3DR)P*AP*GP*AP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	13	258	124	49	73	12	7	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	13	261	127	44	78	12	0	0	0

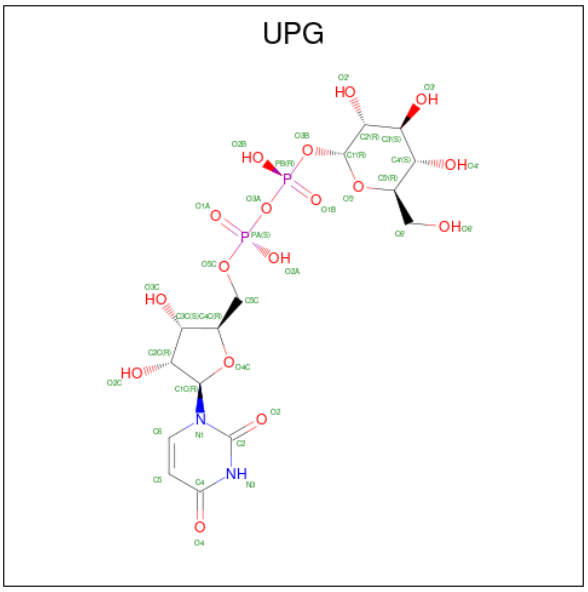
- Molecule 3 is a protein called DNA alpha-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	394	3236	2064	549	605	18	0	0	0
3	B	394	Total	C	N	O	S	0	0	0
			3233	2062	549	605	17			

There are 6 discrepancies between the modelled and reference sequences:

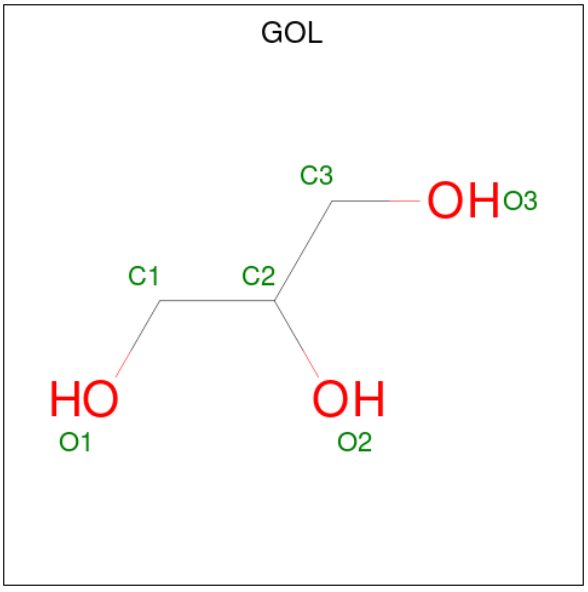
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	MET	-	cloning artifact	UNP P04519
A	999	GLY	-	cloning artifact	UNP P04519
A	1000	SER	-	cloning artifact	UNP P04519
B	998	MET	-	cloning artifact	UNP P04519
B	999	GLY	-	cloning artifact	UNP P04519
B	1000	SER	-	cloning artifact	UNP P04519

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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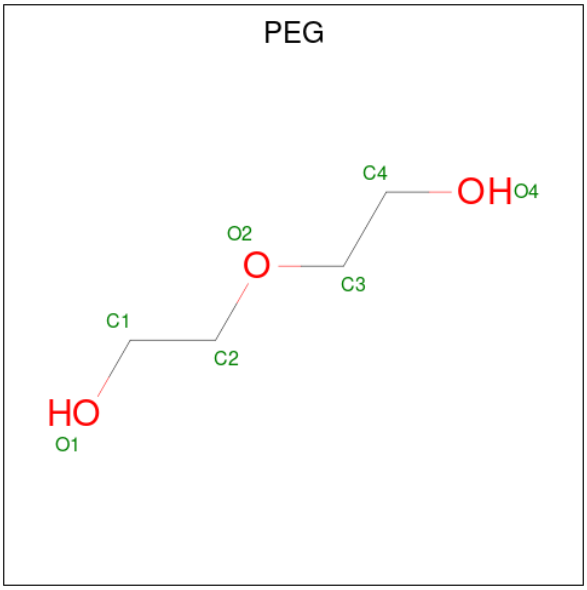
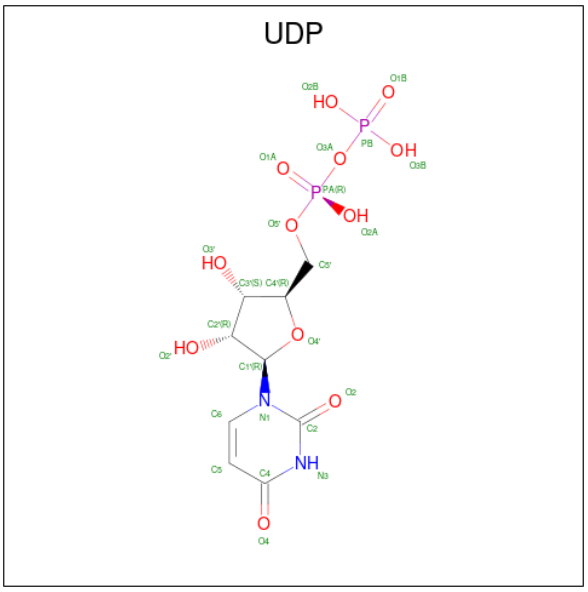
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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

- Molecule 8 is water.

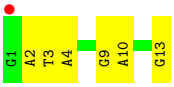
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	3	Total	O	0	0
			3	3		
8	D	11	Total	O	0	0
			11	11		
8	A	115	Total	O	0	0
			115	115		
8	B	95	Total	O	0	0
			95	95		

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.

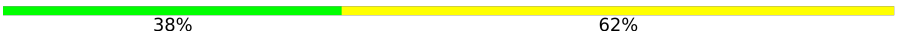
• Molecule 1: 5'-D(*GP*AP*TP*AP*CP*TP*(3DR)P*AP*GP*AP*TP*AP*G)-3'

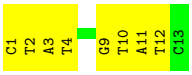
Chain C:



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

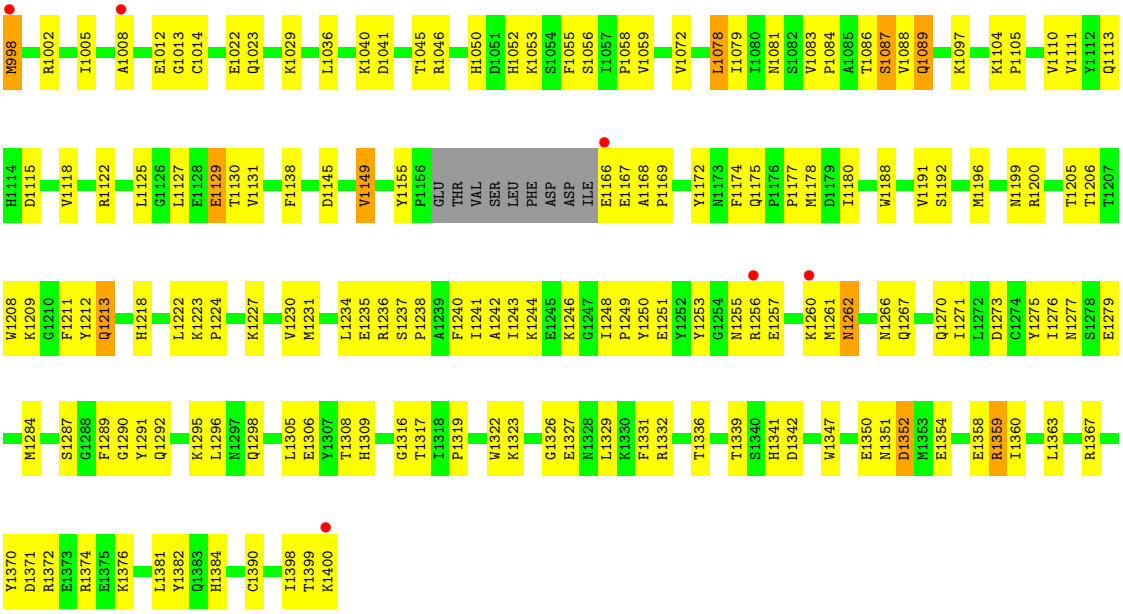
Chain D:





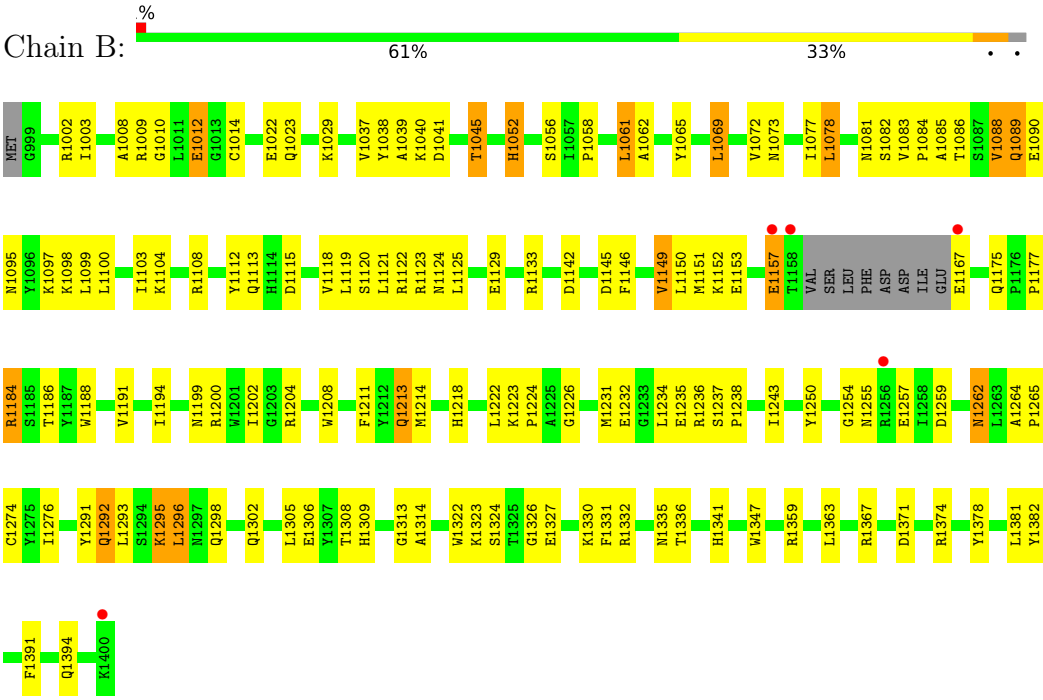
• Molecule 3: DNA alpha-glucosyltransferase

Chain A:



• Molecule 3: DNA alpha-glucosyltransferase

Chain B:


%
61%
33%
MET G999 R1002 I1003 A1008 R1009 G1010 L1011 E1012 G1013 C1014 E1022 Q1023 K1029 V1037 Y1038 A1039 K1040 D1041 T1045 H1052 S1056 I1057 P1058 L1061 A1062 Y1065 L1069 V1072 N1073 I1077 L1078 N1081 S1082 V1083 P1084 A1085 T1086 S1087 V1088 Q1089 E1090 A1091 T1092 I1093 N1094
N1095 Y1096 K1097 K1098 L1099 L1100 I1103 K1104 R1108 Y1112 Q1113 H1114 D1115 V1118 L1119 S1120 L1121 R1122 R1123 N1124 L1125 E1129 R1133 D1142 D1145 F1146 Y1149 L1150 M1151 K1152 E1153 E1157 T1158 VAL SER LEU PHE ASP ASP ILE GLU E1167 Q1175 P1176 P1177 M1178 D1179 I1180
R1184 S1185 T1186 Y1187 W1188 V1191 I1194 N1199 R1200 W1201 I1202 G1203 R1204 W1208 F1211 Y1212 Q1213 M1214 H1218 L1222 K1223 P1224 A1225 G1226 M1231 E1232 G1233 L1234 E1235 R1236 S1237 P1238 I1243 Y1250 G1254 N1255 R1256 E1257 I1258 D1259 N1262 L1263 A1264 P1265 Q1270 D1273
C1274 Y1275 I1276 Y1291 Q1292 L1293 S1294 K1295 L1296 N1297 Q1298 Q1302 L1305 E1306 Y1307 T1308 H1309 G1313 A1314 W1322 K1323 S1324 T1325 G1326 E1327 K1330 F1331 R1332 N1335 T1336 H1341 W1347 R1359 L1363 R1367 D1371 R1374 Y1378 L1381 Y1382 Q1383 H1384 S1387
F1391 Q1394 K1400

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.36Å 123.96Å 86.63Å 90.00° 101.83° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 99.6 (19.87-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.274 0.189 , 0.262	Depositor DCC
R_{free} test set	1888 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, UDP, 3DR, UPG

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	0.38	0/277	0.67	0/424
2	D	0.39	0/291	0.73	0/447
3	A	0.39	0/3312	0.64	0/4466
3	B	0.39	0/3309	0.64	0/4463
All	All	0.39	0/7189	0.64	0/9800

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

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	258	0	146	7	0
2	D	261	0	150	11	0
3	A	3236	0	3175	128	0
3	B	3233	0	3168	120	0
4	A	36	0	22	4	0
5	A	12	0	6	0	0
5	B	12	0	6	0	0
6	A	7	0	10	0	0
6	B	7	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	25	0	11	1	0
8	A	115	0	0	1	0
8	B	95	0	0	3	0
8	C	3	0	0	1	0
8	D	11	0	0	1	0
All	All	7311	0	6704	265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (265) 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:1306:GLU:H	3:B:1309:HIS:HD2	0.96	0.95
3:B:1306:GLU:H	3:B:1309:HIS:CD2	1.87	0.93
3:A:1306:GLU:H	3:A:1309:HIS:HD2	1.18	0.91
3:A:1113:GLN:HE21	3:A:1115:ASP:H	1.18	0.88
3:B:1237:SER:OG	3:B:1238:PRO:HD2	1.78	0.83
3:A:1118:VAL:HG23	3:A:1145:ASP:OD1	1.79	0.81
3:A:1022:GLU:HG2	3:A:1178:MET:HA	1.62	0.81
3:A:1211:PHE:HE2	3:A:1243:ILE:HD11	1.47	0.79
3:A:1127:LEU:O	3:A:1131:VAL:HG23	1.82	0.79
3:A:1113:GLN:NE2	3:A:1115:ASP:H	1.81	0.78
3:B:1088:VAL:O	3:B:1089:GLN:HB3	1.84	0.77
3:B:1223:LYS:HB3	3:B:1224:PRO:HD3	1.67	0.77
3:A:1223:LYS:HB3	3:A:1224:PRO:HD3	1.66	0.77
3:B:1113:GLN:HE21	3:B:1115:ASP:H	1.32	0.76
3:A:1306:GLU:H	3:A:1309:HIS:CD2	2.01	0.75
3:B:1175:GLN:O	3:B:1177:PRO:HD3	1.88	0.74
3:B:1177:PRO:HG2	3:B:1391:PHE:CE1	2.25	0.72
3:B:1023:GLN:HE22	3:B:1081:ASN:HD21	1.36	0.72
3:B:1332:ARG:H	3:B:1384:HIS:HD2	1.35	0.71
1:C:2:DA:H2"	1:C:3:DT:H5'	1.71	0.71
3:B:1083:VAL:HG13	3:B:1084:PRO:HD2	1.74	0.70
3:A:1008:ALA:HB3	3:A:1083:VAL:HA	1.72	0.70
3:A:1088:VAL:O	3:A:1089:GLN:HB3	1.90	0.70
3:B:1313:GLY:HA3	3:B:1381:LEU:HD12	1.74	0.69
3:A:1237:SER:OG	3:A:1238:PRO:HD2	1.92	0.69
3:A:1208:TRP:CE3	3:A:1296:LEU:HD13	2.28	0.69
3:B:1113:GLN:HG2	3:B:1146:PHE:CD1	2.27	0.69
2:D:1:DC:H3'	8:D:21:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1262:ASN:HB3	3:A:1267:GLN:HE21	1.59	0.68
3:A:1359:ARG:HH11	3:A:1363:LEU:HG	1.58	0.68
3:B:1213:GLN:H	3:B:1213:GLN:NE2	1.92	0.68
2:D:11:DA:H2"	2:D:12:DT:H5'	1.74	0.68
2:D:3:DA:OP1	3:A:1256:ARG:HG3	1.93	0.68
3:A:1086:THR:O	3:A:1086:THR:HG23	1.93	0.68
3:B:1022:GLU:HG2	3:B:1178:MET:HA	1.77	0.67
3:B:1226:GLY:O	3:B:1265:PRO:HB3	1.95	0.67
3:B:1359:ARG:CZ	3:B:1363:LEU:HD11	2.23	0.67
3:A:1205:THR:OG1	3:A:1234:LEU:HD22	1.95	0.66
3:A:1241:ILE:HD12	3:A:1242:ALA:N	2.10	0.65
3:A:1331:PHE:HA	3:A:1384:HIS:HD2	1.61	0.65
3:B:1052:HIS:HD2	3:B:1056:SER:CB	2.09	0.65
3:A:1262:ASN:H	3:A:1270:GLN:NE2	1.94	0.65
3:A:1022:GLU:CG	3:A:1178:MET:HA	2.26	0.65
3:B:1359:ARG:NH2	3:B:1363:LEU:HD11	2.11	0.64
3:B:1077:ILE:HD13	3:B:1108:ARG:HB3	1.79	0.64
3:A:1236:ARG:HG2	3:A:1240:PHE:CD2	2.32	0.64
3:B:1002:ARG:C	3:B:1003:ILE:HD12	2.18	0.64
3:B:1112:TYR:OH	3:B:1394:GLN:NE2	2.31	0.64
3:A:1110:VAL:HG21	3:A:1398:ILE:HD13	1.81	0.63
3:B:1180:ILE:HD12	3:B:1382:TYR:HA	1.81	0.63
3:B:1052:HIS:HD2	3:B:1056:SER:HB2	1.63	0.63
3:B:1330:LYS:HD3	3:B:1335:ASN:OD1	1.98	0.63
3:A:1145:ASP:O	3:A:1149:VAL:HG13	1.99	0.62
3:B:1213:GLN:H	3:B:1213:GLN:HE21	1.45	0.62
3:B:1292:GLN:HG2	3:B:1309:HIS:ND1	2.14	0.62
3:A:1211:PHE:CE2	3:A:1243:ILE:HD11	2.33	0.62
3:B:1149:VAL:CG2	3:B:1150:LEU:N	2.63	0.62
3:B:1273:ASP:OD2	3:B:1274:CYS:N	2.33	0.62
3:B:1306:GLU:N	3:B:1309:HIS:HD2	1.82	0.62
3:B:1085:ALA:O	3:B:1088:VAL:HG22	2.00	0.61
3:B:1276:ILE:N	3:B:1276:ILE:HD12	2.16	0.61
3:B:1086:THR:HA	3:B:1125:LEU:HG	1.83	0.60
3:B:1072:VAL:HG13	3:B:1078:LEU:HG	1.83	0.59
3:A:1199:ASN:HB3	3:A:1291:TYR:CE2	2.38	0.59
3:B:1184:ARG:HG3	3:B:1378:TYR:CE2	2.38	0.59
3:B:1149:VAL:HG23	3:B:1150:LEU:N	2.17	0.58
3:A:1155:TYR:CE1	3:A:1169:PRO:HD3	2.38	0.58
3:A:1240:PHE:CE2	3:A:1244:LYS:HD3	2.39	0.58
3:B:1003:ILE:HD12	3:B:1003:ILE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:DG:H5'	8:C:42:HOH:O	2.03	0.57
3:A:1088:VAL:O	3:A:1089:GLN:CB	2.52	0.56
3:A:1191:VAL:HG21	3:A:1371:ASP:HB2	1.87	0.56
3:B:1113:GLN:NE2	3:B:1115:ASP:H	2.01	0.56
3:B:1009:ARG:HH21	3:B:1123:ARG:HH12	1.54	0.56
3:A:1260:LYS:NZ	3:A:1260:LYS:HB3	2.21	0.56
3:B:1086:THR:HA	3:B:1125:LEU:CD1	2.36	0.56
3:A:1331:PHE:HA	3:A:1384:HIS:CD2	2.41	0.55
2:D:1:DC:H2'	2:D:2:DT:H72	1.87	0.55
3:B:1145:ASP:O	3:B:1149:VAL:HG22	2.06	0.55
3:B:1332:ARG:H	3:B:1384:HIS:CD2	2.21	0.55
2:D:9:DG:H2"	2:D:10:DT:OP2	2.05	0.55
3:A:1205:THR:HB	3:A:1235:GLU:OE2	2.07	0.55
3:A:1013:GLY:HA3	3:A:1046:ARG:O	2.06	0.55
3:A:1104:LYS:HB2	3:A:1105:PRO:HD2	1.89	0.55
3:B:1199:ASN:HB3	3:B:1291:TYR:CE2	2.41	0.55
3:A:1306:GLU:N	3:A:1309:HIS:HD2	1.98	0.55
3:B:1099:LEU:O	3:B:1103:ILE:HG13	2.08	0.54
2:D:1:DC:C6	2:D:2:DT:H72	2.43	0.53
3:A:1083:VAL:HB	3:A:1084:PRO:HD2	1.90	0.53
3:A:1118:VAL:HG23	3:A:1145:ASP:CG	2.29	0.53
3:A:1253:TYR:CE2	3:A:1261:MET:HA	2.43	0.53
3:B:1276:ILE:N	3:B:1276:ILE:CD1	2.71	0.53
3:A:1113:GLN:HE21	3:A:1115:ASP:N	1.97	0.53
3:A:1040:LYS:HD2	3:A:1058:PRO:HB2	1.91	0.53
3:B:1088:VAL:O	3:B:1089:GLN:CB	2.51	0.53
3:B:1208:TRP:CE3	3:B:1296:LEU:HD13	2.44	0.53
3:A:1354:GLU:O	3:A:1358:GLU:HG2	2.08	0.53
3:A:1276:ILE:HD12	3:A:1279:GLU:OE2	2.09	0.52
3:A:1284:MET:HE3	3:A:1287:SER:HB2	1.92	0.52
3:A:1372:ARG:HG3	3:A:1372:ARG:HH11	1.73	0.52
3:B:1065:TYR:CE2	3:B:1098:LYS:HG3	2.43	0.52
3:B:1200:ARG:NH1	3:B:1232:GLU:OE2	2.43	0.52
3:B:1177:PRO:HB2	3:B:1387:SER:HA	1.92	0.52
3:A:1223:LYS:HE3	3:A:1267:GLN:N	2.25	0.52
3:A:1199:ASN:ND2	3:A:1291:TYR:OH	2.42	0.52
3:A:1236:ARG:HG2	3:A:1240:PHE:CE2	2.45	0.51
3:A:998:MET:HE1	3:A:1399:THR:HG21	1.93	0.51
3:A:1200:ARG:NH1	3:A:1230:VAL:HG11	2.25	0.51
3:B:1264:ALA:HB1	3:B:1265:PRO:HD2	1.92	0.51
3:A:1072:VAL:HG13	3:A:1078:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1086:THR:HA	3:A:1125:LEU:HD11	1.92	0.51
3:B:1008:ALA:HB3	3:B:1082:SER:O	2.11	0.51
3:B:1202:ILE:HD12	3:B:1308:THR:HG22	1.91	0.51
3:B:1038:TYR:HE1	3:B:1056:SER:OG	1.93	0.50
3:B:1295:LYS:HB3	3:B:1322:TRP:CD1	2.46	0.50
3:B:1118:VAL:HG13	3:B:1119:LEU:N	2.25	0.50
3:A:1200:ARG:HB3	3:A:1284:MET:CE	2.41	0.50
3:A:1097:LYS:HE2	3:A:1129:GLU:HG3	1.93	0.50
2:D:1:DC:H2'	2:D:2:DT:C7	2.42	0.49
3:A:1005:ILE:HB	3:A:1036:LEU:HD12	1.92	0.49
3:B:1038:TYR:CE1	3:B:1056:SER:OG	2.64	0.49
1:C:2:DA:C2'	1:C:3:DT:H5'	2.40	0.49
3:A:1029:LYS:O	3:A:1029:LYS:HG2	2.11	0.49
3:A:1177:PRO:HB3	3:A:1390:CYS:HB2	1.95	0.49
3:A:1359:ARG:NH1	3:A:1363:LEU:HG	2.26	0.49
3:B:1022:GLU:HG3	8:B:34:HOH:O	2.12	0.49
3:B:1089:GLN:O	3:B:1091:ALA:N	2.45	0.49
3:A:1086:THR:O	3:A:1087:SER:HB3	2.12	0.49
3:A:1212:TYR:HB2	3:A:1213:GLN:OE1	2.12	0.49
2:D:10:DT:OP2	2:D:10:DT:H6	1.96	0.49
3:A:1284:MET:CE	3:A:1287:SER:HB2	2.43	0.49
3:B:1052:HIS:CD2	3:B:1056:SER:HB2	2.47	0.49
3:B:1121:LEU:HB3	3:B:1150:LEU:HD11	1.94	0.49
3:A:1231:MET:HB2	3:A:1271:ILE:CD1	2.42	0.48
3:B:1234:LEU:O	3:B:1273:ASP:HA	2.13	0.48
3:A:1323:LYS:HE2	3:A:1327:GLU:OE1	2.14	0.48
3:A:1213:GLN:HG3	3:A:1322:TRP:CZ3	2.49	0.48
3:A:1213:GLN:NE2	3:A:1295:LYS:HZ2	2.11	0.48
3:B:1099:LEU:O	3:B:1099:LEU:HD23	2.13	0.48
3:B:1262:ASN:H	3:B:1270:GLN:NE2	2.11	0.48
3:B:1191:VAL:HG12	3:B:1367:ARG:HD3	1.95	0.48
3:B:1118:VAL:HG13	3:B:1119:LEU:HD12	1.95	0.48
3:A:1175:GLN:O	3:A:1177:PRO:HD3	2.14	0.47
3:B:1323:LYS:HE2	3:B:1327:GLU:OE1	2.13	0.47
3:B:1069:LEU:HD22	3:B:1073:ASN:ND2	2.29	0.47
3:A:998:MET:HE3	3:A:998:MET:N	2.29	0.47
3:A:1111:VAL:HG21	3:A:1130:THR:HG22	1.96	0.47
3:A:1305:LEU:HD13	3:A:1329:LEU:HD13	1.96	0.47
3:A:1014:CYS:HB3	4:A:501:UPG:O2B	2.15	0.47
3:A:1118:VAL:HG22	3:A:1145:ASP:HB3	1.96	0.47
3:B:1029:LYS:HG3	8:B:182:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1223:LYS:HE2	3:A:1266:ASN:HD22	1.80	0.47
3:A:1332:ARG:H	3:A:1384:HIS:CD2	2.33	0.47
3:B:1194:ILE:HD11	3:B:1374:ARG:NH1	2.30	0.47
3:B:1211:PHE:CE2	3:B:1243:ILE:HD11	2.50	0.47
3:A:1079:ILE:HG12	3:A:1110:VAL:HB	1.97	0.47
1:C:13:DG:OP1	3:B:1120:SER:HB2	2.14	0.47
3:A:1052:HIS:HD2	3:A:1056:SER:OG	1.97	0.47
3:A:1342:ASP:OD1	3:A:1376:LYS:NZ	2.41	0.47
3:B:1359:ARG:O	3:B:1363:LEU:HD13	2.15	0.47
3:A:1238:PRO:O	3:A:1241:ILE:HG13	2.14	0.47
3:B:1038:TYR:CZ	3:B:1058:PRO:HB3	2.50	0.47
3:B:1180:ILE:HG23	3:B:1314:ALA:HB2	1.97	0.46
3:A:1008:ALA:HB1	3:A:1084:PRO:HD3	1.98	0.46
3:B:1250:TYR:OH	6:B:801:PEG:H42	2.16	0.46
3:B:1326:GLY:HA3	3:B:1347:TRP:CZ3	2.51	0.46
3:A:1180:ILE:HD12	3:A:1382:TYR:HA	1.98	0.46
3:A:1289:PHE:CZ	3:A:1360:ILE:HG23	2.50	0.46
3:A:1138:PHE:HB3	3:A:1174:PHE:CD2	2.51	0.46
3:A:1236:ARG:HG2	3:A:1240:PHE:CG	2.50	0.46
3:A:1086:THR:HA	3:A:1125:LEU:CD1	2.46	0.46
3:A:1118:VAL:O	3:A:1122:ARG:HG2	2.15	0.46
3:B:1038:TYR:HE1	3:B:1056:SER:HG	1.64	0.46
3:A:1222:LEU:HB3	3:A:1227:LYS:HB2	1.96	0.46
3:A:1363:LEU:HD22	3:A:1370:TYR:HA	1.97	0.46
3:B:1086:THR:HA	3:B:1125:LEU:CG	2.45	0.46
3:B:1213:GLN:HG2	3:B:1322:TRP:CZ3	2.50	0.46
3:B:1305:LEU:HD22	3:B:1309:HIS:CG	2.51	0.46
3:B:1008:ALA:HB1	3:B:1084:PRO:HD3	1.98	0.45
3:A:1138:PHE:HA	3:A:1172:TYR:O	2.16	0.45
3:A:1231:MET:HB2	3:A:1271:ILE:HD13	1.97	0.45
3:A:1251:GLU:O	3:A:1253:TYR:CD1	2.70	0.45
3:B:1065:TYR:HB2	3:B:1095:ASN:ND2	2.31	0.45
3:B:1142:ASP:H	3:B:1302:GLN:NE2	2.15	0.45
3:A:1155:TYR:CD1	3:A:1168:ALA:HA	2.51	0.45
3:A:1213:GLN:NE2	3:A:1295:LYS:NZ	2.64	0.45
3:A:1262:ASN:CB	3:A:1267:GLN:HE21	2.26	0.45
3:A:1050:HIS:HD2	8:A:73:HOH:O	2.00	0.45
3:B:1218:HIS:HA	3:B:1222:LEU:HB2	1.98	0.45
3:A:1240:PHE:CD2	3:A:1244:LYS:HD3	2.51	0.45
3:B:1236:ARG:HA	6:B:801:PEG:O1	2.17	0.45
1:C:9:DG:H2"	1:C:10:DA:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1177:PRO:HG2	3:B:1391:PHE:CZ	2.52	0.44
3:B:1313:GLY:HA3	3:B:1381:LEU:CD1	2.46	0.44
3:A:1248:ILE:HA	3:A:1249:PRO:HD3	1.80	0.44
3:A:1275:TYR:CE1	4:A:501:UPG:C2	3.01	0.44
3:A:1257:GLU:OE1	3:A:1257:GLU:N	2.45	0.44
3:A:1023:GLN:HE22	3:A:1081:ASN:HD21	1.64	0.44
3:B:1093:ILE:CG1	3:B:1097:LYS:HE3	2.48	0.44
3:B:1184:ARG:HG2	3:B:1188:TRP:CE3	2.52	0.44
3:B:1292:GLN:CG	3:B:1309:HIS:CE1	3.01	0.44
1:C:2:DA:H1'	1:C:3:DT:C5'	2.48	0.44
3:B:1009:ARG:HB2	3:B:1083:VAL:O	2.18	0.44
4:A:501:UPG:O1B	4:A:501:UPG:O2'	2.32	0.43
3:B:1040:LYS:HE3	3:B:1058:PRO:HB2	2.00	0.43
2:D:3:DA:C8	2:D:4:DT:H72	2.54	0.43
3:A:1262:ASN:OD1	3:A:1267:GLN:NE2	2.52	0.43
3:B:1100:LEU:HA	3:B:1103:ILE:CD1	2.48	0.43
3:A:1200:ARG:O	3:A:1290:GLY:HA2	2.18	0.43
3:B:1040:LYS:O	3:B:1041:ASP:C	2.57	0.43
3:B:1122:ARG:C	3:B:1124:ASN:H	2.22	0.43
3:A:1223:LYS:CE	3:A:1266:ASN:HA	2.49	0.43
3:A:1262:ASN:N	3:A:1270:GLN:NE2	2.66	0.43
3:A:1242:ALA:O	3:A:1246:LYS:HG3	2.18	0.43
3:B:1097:LYS:HD3	3:B:1129:GLU:OE2	2.19	0.43
3:A:1262:ASN:H	3:A:1270:GLN:HE21	1.64	0.43
3:B:1331:PHE:CE1	3:B:1384:HIS:HB2	2.54	0.43
3:B:1093:ILE:HG23	3:B:1094:ASN:N	2.34	0.42
3:A:998:MET:CE	3:A:1399:THR:HG21	2.49	0.42
3:B:1083:VAL:HG13	3:B:1084:PRO:CD	2.46	0.42
3:A:1058:PRO:O	3:A:1059:VAL:HG23	2.20	0.42
3:B:1041:ASP:OD2	3:B:1061:LEU:HB2	2.20	0.42
3:B:1081:ASN:OD1	3:B:1112:TYR:HB2	2.20	0.42
2:D:1:DC:H2"	2:D:2:DT:O5'	2.18	0.42
2:D:11:DA:C2'	2:D:12:DT:H5'	2.47	0.42
3:A:1218:HIS:CE1	3:A:1223:LYS:HB2	2.54	0.42
3:A:1052:HIS:HA	3:A:1055:PHE:CZ	2.55	0.42
3:A:1188:TRP:CZ3	3:A:1316:GLY:HA2	2.54	0.42
3:A:1192:SER:HA	3:A:1367:ARG:NH1	2.34	0.42
3:A:1322:TRP:CH2	3:A:1350:GLU:HB2	2.55	0.42
3:A:1277:ASN:ND2	4:A:501:UPG:O2C	2.53	0.42
3:B:1003:ILE:HG13	3:B:1077:ILE:HB	2.02	0.42
3:B:1204:ARG:NH2	7:B:601:UDP:O1B	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1251:GLU:O	3:A:1253:TYR:HD1	2.03	0.42
3:B:1103:ILE:O	3:B:1104:LYS:C	2.58	0.42
3:A:1260:LYS:HB3	3:A:1260:LYS:HZ2	1.85	0.41
3:A:1306:GLU:HB2	3:A:1309:HIS:CD2	2.55	0.41
3:B:1295:LYS:HB3	3:B:1322:TRP:NE1	2.36	0.41
3:B:1062:ALA:HA	3:B:1091:ALA:O	2.19	0.41
3:B:1149:VAL:O	3:B:1153:GLU:HG3	2.20	0.41
1:C:3:DT:H2"	1:C:4:DA:OP2	2.20	0.41
3:A:1336:THR:OG1	3:A:1341:HIS:HE1	2.03	0.41
3:B:1100:LEU:HA	3:B:1103:ILE:HD11	2.03	0.41
3:B:1336:THR:OG1	3:B:1341:HIS:HE1	2.02	0.41
3:A:1317:THR:O	3:A:1319:PRO:HD3	2.20	0.41
3:A:1326:GLY:HA3	3:A:1347:TRP:CZ3	2.55	0.41
3:B:1302:GLN:HE21	3:B:1302:GLN:HB2	1.73	0.41
3:A:1113:GLN:NE2	3:A:1115:ASP:HB2	2.36	0.41
3:A:1250:TYR:CD1	3:A:1250:TYR:C	2.94	0.41
3:A:1084:PRO:HG2	3:A:1125:LEU:O	2.21	0.41
3:A:1305:LEU:HD12	3:A:1305:LEU:HA	1.83	0.41
3:B:1010:GLY:HA2	3:B:1039:ALA:O	2.21	0.41
3:B:1254:GLY:O	3:B:1257:GLU:HG2	2.21	0.41
3:A:1316:GLY:O	3:A:1374:ARG:CD	2.68	0.41
3:A:1351:ASN:O	3:A:1352:ASP:HB2	2.20	0.41
3:A:1289:PHE:CD1	3:A:1289:PHE:N	2.89	0.40
3:A:1372:ARG:HH11	3:A:1372:ARG:CG	2.34	0.40
3:B:1012:GLU:OE1	3:B:1014:CYS:HB2	2.22	0.40
3:B:1146:PHE:O	3:B:1151:MET:HG2	2.21	0.40
3:A:1206:THR:O	3:A:1209:LYS:HB2	2.21	0.40
3:B:1298:GLN:NE2	8:B:47:HOH:O	2.54	0.40
3:B:1322:TRP:CD1	3:B:1324:SER:HB3	2.57	0.40
3:B:1022:GLU:HG2	3:B:1177:PRO:O	2.22	0.40
3:B:1149:VAL:CG2	3:B:1150:LEU:H	2.34	0.40
3:B:1214:MET:HB3	3:B:1231:MET:CE	2.52	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	390/403 (97%)	346 (89%)	37 (10%)	7 (2%)	8 10
3	B	390/403 (97%)	354 (91%)	30 (8%)	6 (2%)	10 14
All	All	780/806 (97%)	700 (90%)	67 (9%)	13 (2%)	9 11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1087	SER
3	A	1089	GLN
3	A	1352	ASP
3	B	1090	GLU
3	B	1157	GLU
3	B	1045	THR
3	A	1298	GLN
3	B	1089	GLN
3	B	1186	THR
3	A	1273	ASP
3	B	1052	HIS
3	A	1167	GLU
3	A	1196	MET

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	359/368 (98%)	340 (95%)	19 (5%)	22 37
3	B	358/368 (97%)	335 (94%)	23 (6%)	17 28
All	All	717/736 (97%)	675 (94%)	42 (6%)	19 32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	998	MET
3	A	1002	ARG
3	A	1012	GLU
3	A	1041	ASP
3	A	1045	THR
3	A	1053	LYS
3	A	1078	LEU
3	A	1129	GLU
3	A	1149	VAL
3	A	1166	GLU
3	A	1213	GLN
3	A	1255	ASN
3	A	1262	ASN
3	A	1292	GLN
3	A	1308	THR
3	A	1339	THR
3	A	1359	ARG
3	A	1381	LEU
3	A	1400	LYS
3	B	1012	GLU
3	B	1037	VAL
3	B	1045	THR
3	B	1061	LEU
3	B	1069	LEU
3	B	1078	LEU
3	B	1088	VAL
3	B	1133	ARG
3	B	1149	VAL
3	B	1152	LYS
3	B	1157	GLU
3	B	1167	GLU
3	B	1184	ARG
3	B	1213	GLN
3	B	1235	GLU
3	B	1255	ASN
3	B	1259	ASP
3	B	1262	ASN
3	B	1292	GLN
3	B	1293	LEU
3	B	1295	LYS
3	B	1296	LEU
3	B	1371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46)

such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1023	GLN
3	A	1030	ASN
3	A	1050	HIS
3	A	1052	HIS
3	A	1094	ASN
3	A	1095	ASN
3	A	1113	GLN
3	A	1124	ASN
3	A	1175	GLN
3	A	1199	ASN
3	A	1213	GLN
3	A	1218	HIS
3	A	1255	ASN
3	A	1262	ASN
3	A	1266	ASN
3	A	1267	GLN
3	A	1270	GLN
3	A	1277	ASN
3	A	1309	HIS
3	A	1328	ASN
3	A	1341	HIS
3	A	1351	ASN
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	1094	ASN
3	B	1113	GLN
3	B	1175	GLN
3	B	1199	ASN
3	B	1213	GLN
3	B	1218	HIS
3	B	1255	ASN
3	B	1262	ASN
3	B	1270	GLN
3	B	1292	GLN
3	B	1298	GLN
3	B	1302	GLN
3	B	1309	HIS
3	B	1328	ASN

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Mol	Chain	Res	Type
3	B	1341	HIS
3	B	1351	ASN
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	3DR	C	7	1	8,11,12	0.33	0	9,14,17	0.71	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
1	3DR	C	7	1	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PEG	B	801	-	6,6,6	0.67	0	5,5,5	0.34	0
5	GOL	A	702	-	5,5,5	4.25	5 (100%)	5,5,5	2.13	2 (40%)
4	UPG	A	501	-	35,38,38	0.58	0	53,58,58	0.88	2 (3%)
5	GOL	B	703	-	5,5,5	4.23	5 (100%)	5,5,5	2.09	2 (40%)
6	PEG	A	802	-	6,6,6	0.72	0	5,5,5	0.36	0
5	GOL	A	701	-	5,5,5	4.33	5 (100%)	5,5,5	2.13	2 (40%)
5	GOL	B	602	-	5,5,5	4.28	5 (100%)	5,5,5	2.08	2 (40%)
7	UDP	B	601	-	24,26,26	0.58	0	37,40,40	0.67	1 (2%)

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	PEG	B	801	-	-	3/4/4/4	-
5	GOL	A	702	-	-	3/4/4/4	-
4	UPG	A	501	-	-	10/23/59/59	0/3/3/3
5	GOL	B	703	-	-	4/4/4/4	-
6	PEG	A	802	-	-	2/4/4/4	-
5	GOL	A	701	-	-	1/4/4/4	-
5	GOL	B	602	-	-	2/4/4/4	-
7	UDP	B	601	-	-	3/16/32/32	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	GOL	C3-C2	-5.23	1.30	1.51
5	A	701	GOL	C1-C2	-5.22	1.30	1.51
5	B	602	GOL	C1-C2	-5.22	1.30	1.51
5	B	703	GOL	C1-C2	-5.13	1.30	1.51
5	A	702	GOL	C3-C2	-5.10	1.30	1.51
5	B	703	GOL	C3-C2	-5.08	1.30	1.51
5	A	701	GOL	C3-C2	-5.03	1.31	1.51
5	A	702	GOL	C1-C2	-5.00	1.31	1.51
5	A	701	GOL	O1-C1	4.11	1.59	1.42
5	A	702	GOL	O1-C1	4.03	1.59	1.42
5	A	701	GOL	O3-C3	4.02	1.59	1.42
5	B	703	GOL	O1-C1	3.95	1.59	1.42
5	A	702	GOL	O3-C3	3.95	1.59	1.42
5	B	703	GOL	O3-C3	3.91	1.58	1.42
5	B	602	GOL	O1-C1	3.82	1.58	1.42
5	B	602	GOL	O3-C3	3.81	1.58	1.42
5	A	701	GOL	O2-C2	-2.82	1.35	1.43
5	B	602	GOL	O2-C2	-2.79	1.35	1.43
5	A	702	GOL	O2-C2	-2.76	1.35	1.43
5	B	703	GOL	O2-C2	-2.57	1.35	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	UPG	O3B-C1'-C2'	3.82	115.37	108.38
5	A	702	GOL	O1-C1-C2	3.39	126.43	110.20
5	B	602	GOL	O1-C1-C2	3.32	126.14	110.20
5	A	701	GOL	O1-C1-C2	3.32	126.12	110.20
5	A	701	GOL	O3-C3-C2	3.30	126.03	110.20
5	B	703	GOL	O3-C3-C2	3.25	125.80	110.20
5	A	702	GOL	O3-C3-C2	3.25	125.79	110.20
5	B	703	GOL	O1-C1-C2	3.22	125.65	110.20
5	B	602	GOL	O3-C3-C2	3.05	124.80	110.20
4	A	501	UPG	O5'-C1'-O3B	-2.89	107.59	111.36
7	B	601	UDP	O2B-PB-O1B	2.33	119.82	110.68

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	UPG	C2'-C1'-O3B-PB

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Mol	Chain	Res	Type	Atoms
4	A	501	UPG	O5'-C1'-O3B-PB
5	A	702	GOL	C1-C2-C3-O3
5	B	703	GOL	O1-C1-C2-C3
5	B	703	GOL	C1-C2-C3-O3
7	B	601	UDP	PA-O3A-PB-O3B
4	A	501	UPG	C4'-C5'-C6'-O6'
4	A	501	UPG	O5'-C5'-C6'-O6'
6	A	802	PEG	O2-C3-C4-O4
6	B	801	PEG	O1-C1-C2-O2
6	B	801	PEG	O2-C3-C4-O4
5	B	602	GOL	C1-C2-C3-O3
5	B	703	GOL	O1-C1-C2-O2
5	B	703	GOL	O2-C2-C3-O3
4	A	501	UPG	C1'-O3B-PB-O3A
5	A	702	GOL	O2-C2-C3-O3
4	A	501	UPG	PA-O3A-PB-O3B
4	A	501	UPG	O4C-C4C-C5C-O5C
6	B	801	PEG	C1-C2-O2-C3
4	A	501	UPG	PA-O3A-PB-O1B
4	A	501	UPG	C1'-O3B-PB-O2B
5	A	701	GOL	O1-C1-C2-C3
5	A	702	GOL	O1-C1-C2-C3
6	A	802	PEG	C1-C2-O2-C3
7	B	601	UDP	PA-O3A-PB-O1B
7	B	601	UDP	O4'-C4'-C5'-O5'
4	A	501	UPG	C3C-C4C-C5C-O5C
5	B	602	GOL	O2-C2-C3-O3

There are no ring outliers.

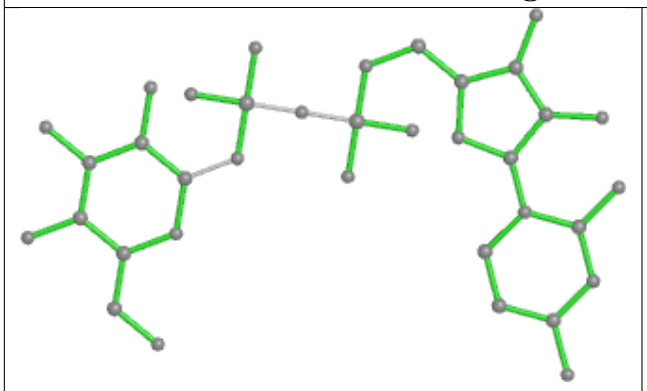
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	801	PEG	2	0
4	A	501	UPG	4	0
7	B	601	UDP	1	0

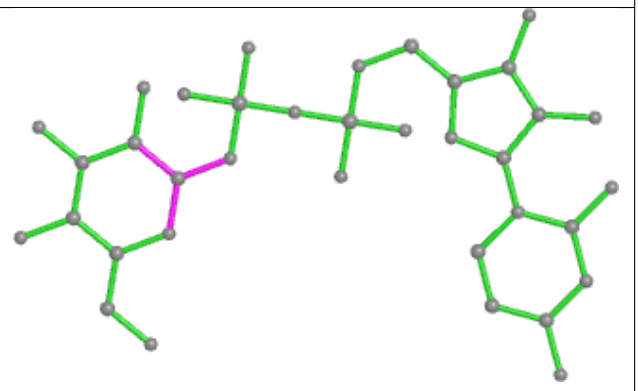
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

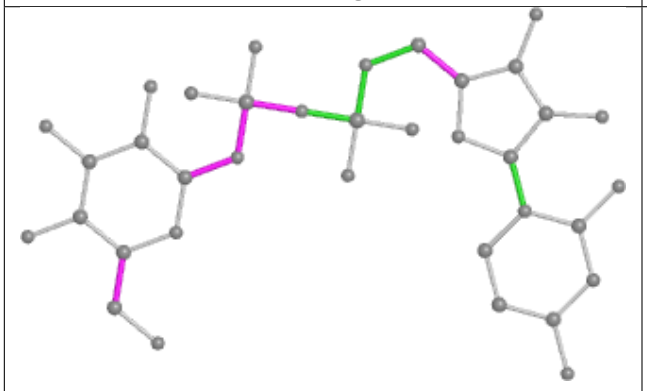
Ligand UPG A 501



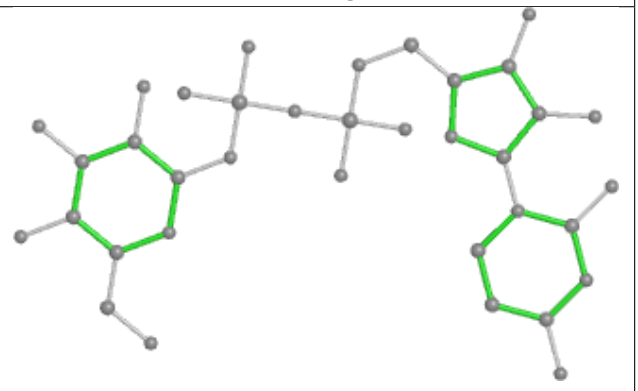
Bond lengths



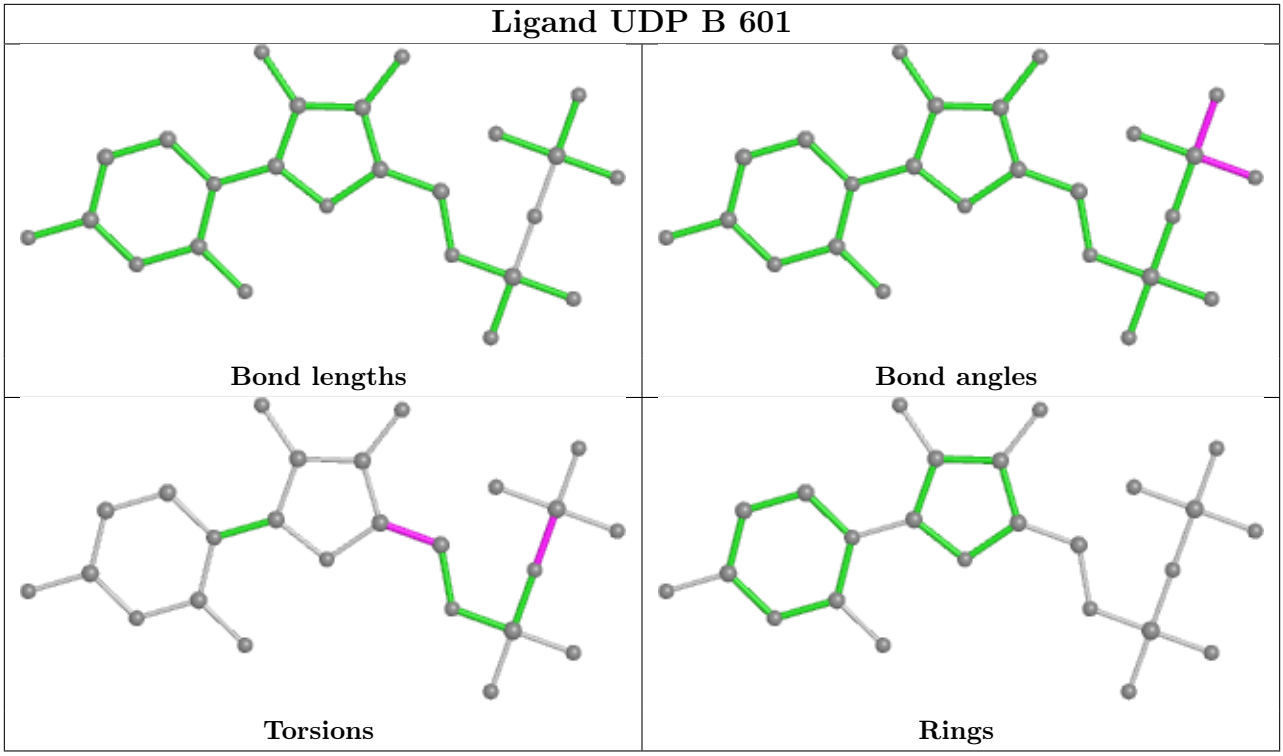
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	7:3DR	O3'	8:DA	P	3.54

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, 95^{th} 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%)	0.46	1 (8%) 11 10	55, 73, 78, 82	0
2	D	13/13 (100%)	0.50	0 100 100	61, 70, 80, 83	0
3	A	394/403 (97%)	-0.12	6 (1%) 73 72	24, 50, 76, 94	0
3	B	394/403 (97%)	-0.21	5 (1%) 77 75	26, 49, 74, 99	0
All	All	813/832 (97%)	-0.15	12 (1%) 73 72	24, 50, 76, 99	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1158	THR	3.1
3	A	1400	LYS	3.1
3	A	1166	GLU	3.1
3	B	1157	GLU	2.9
3	B	1400	LYS	2.7
3	B	1167	GLU	2.5
3	A	1008	ALA	2.5
3	A	1260	LYS	2.5
3	B	1256	ARG	2.5
3	A	1256	ARG	2.4
1	C	1	DG	2.4
3	A	998	MET	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	3DR	C	7	11/12	0.89	0.13	82,91,97,98	7

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

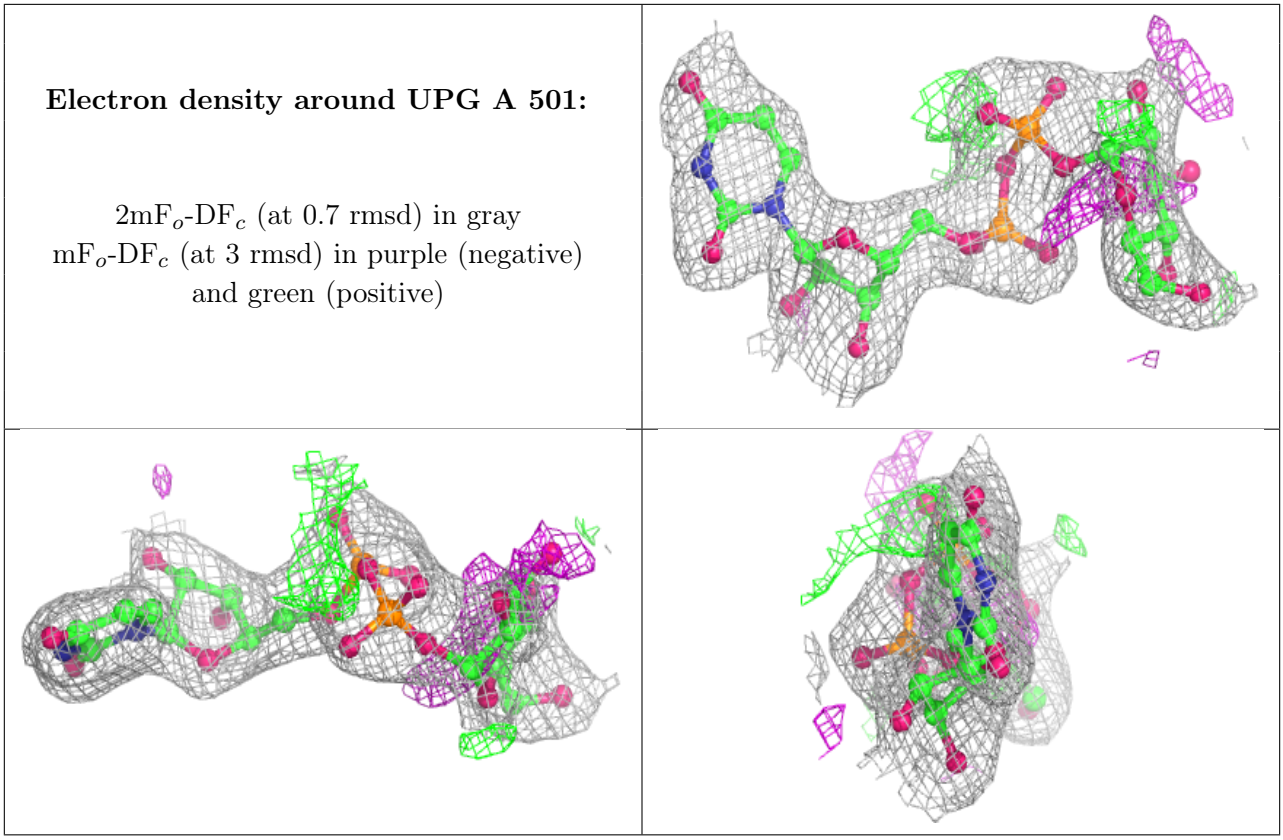
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	GOL	A	702	6/6	0.79	0.23	80,96,98,98	0
6	PEG	A	802	7/7	0.84	0.29	82,84,85,85	0
5	GOL	B	703	6/6	0.90	0.23	54,68,72,73	0
6	PEG	B	801	7/7	0.90	0.16	45,60,78,82	0
5	GOL	A	701	6/6	0.91	0.17	44,66,69,78	0
5	GOL	B	602	6/6	0.94	0.15	40,50,53,53	0
4	UPG	A	501	36/36	0.94	0.14	21,48,77,79	0
7	UDP	B	601	25/25	0.98	0.10	30,43,53,56	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.

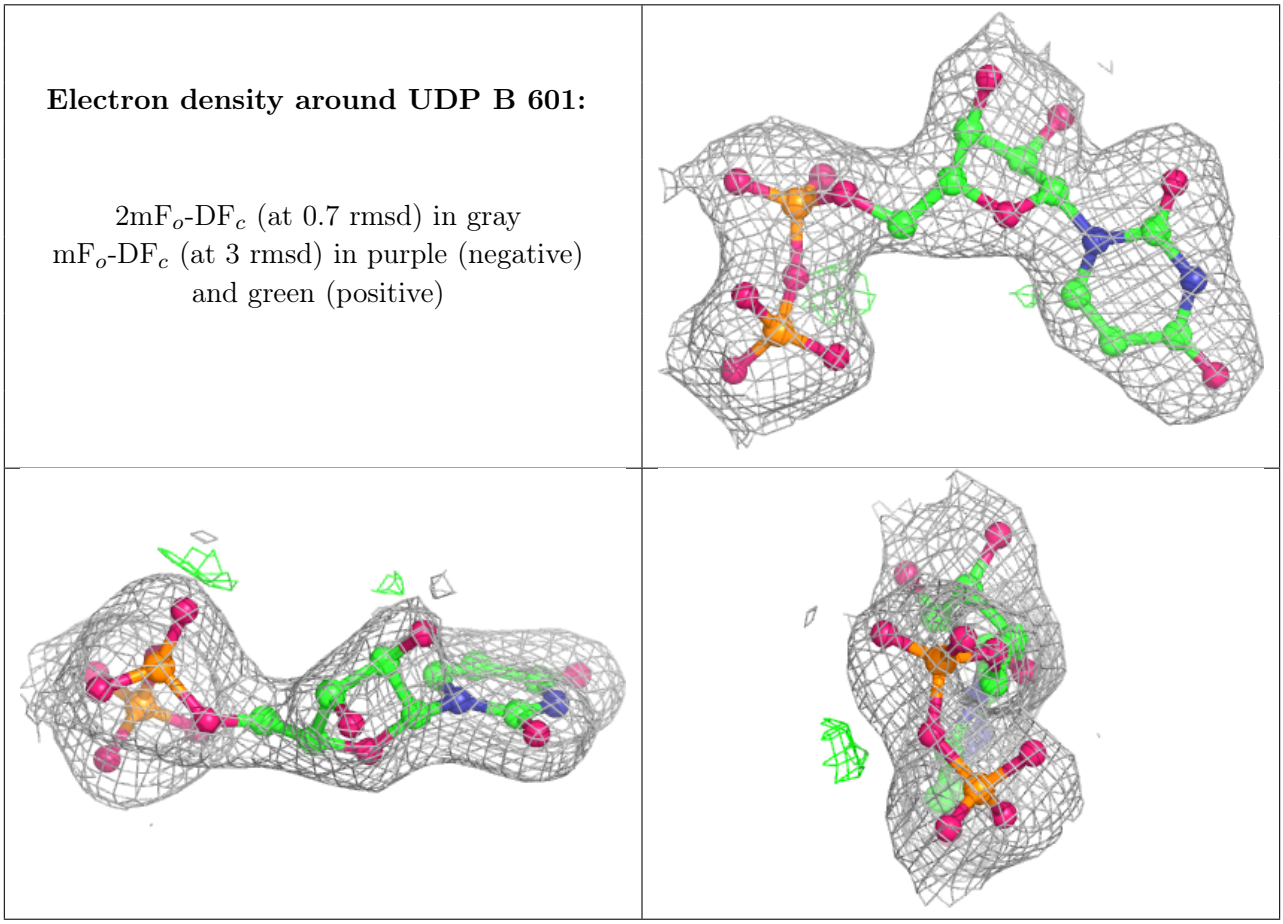
Electron density around UPG A 501:

$2mF_o$-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 601:

$2mF_o$-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.