



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:04 AM EDT

PDB ID : 1YA6 / pdb_00001ya6
Title : alpha-glucosyltransferase in complex with UDP and a 13-mer DNA containing a central A:G mismatch
Authors : Lariviere, L.; Sommer, N.; Morera, S.
Deposited on : 2004-12-17
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

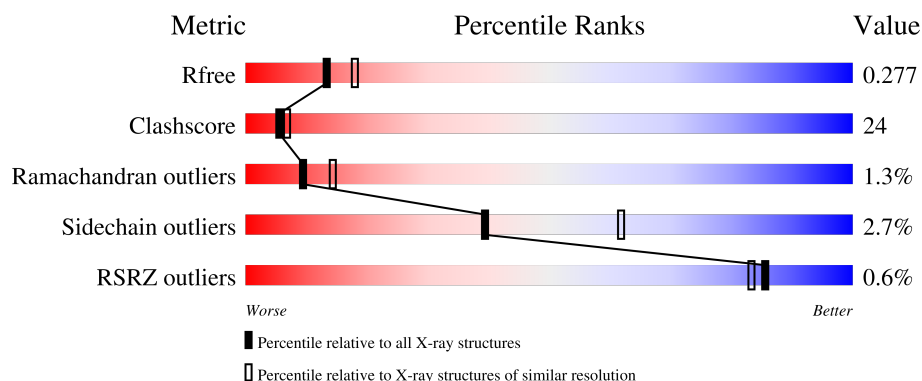
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	12	 50% 42% 8%
2	D	12	 75% 25%
3	A	403	 % 55% 36% • 6%
3	B	403	 48% 42% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6977 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(*AP*TP*AP*CP*TP*AP*AP*GP*AP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			246	119	49	67	11			

- 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	380	Total	C	N	O	S	0	0	0
			3118	1986	532	584	16			
3	B	377	Total	C	N	O	S	0	0	0
			3091	1970	527	577	17			

There are 6 discrepancies between the modelled and reference sequences:

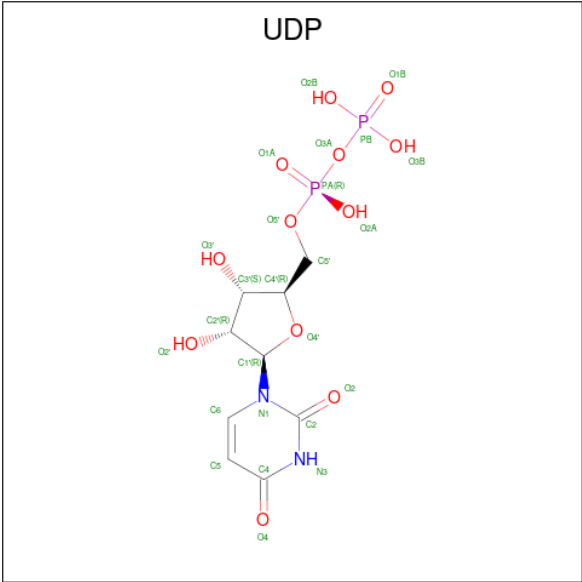
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	MET	-	cloning artifact	UNP P04519
A	999	GLY	-	cloning artifact	UNP P04519
A	1000	SER	-	cloning artifact	UNP P04519
B	998	MET	-	cloning artifact	UNP P04519
B	999	GLY	-	cloning artifact	UNP P04519
B	1000	SER	-	cloning artifact	UNP P04519

- Molecule 4 is COBALT HEXAMMINE(III) (CCD ID: 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 (CCD ID: 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	5	Total	O	0	0
			5	5		
6	D	6	Total	O	0	0
			6	6		
6	A	89	Total	O	0	0
			89	89		
6	B	81	Total	O	0	0
			81	81		

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.

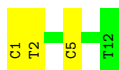
- Molecule 1: 5'-D(*AP*TP*AP*CP*TP*AP*AP*GP*AP*TP*AP*G)-3'

Chain C: 



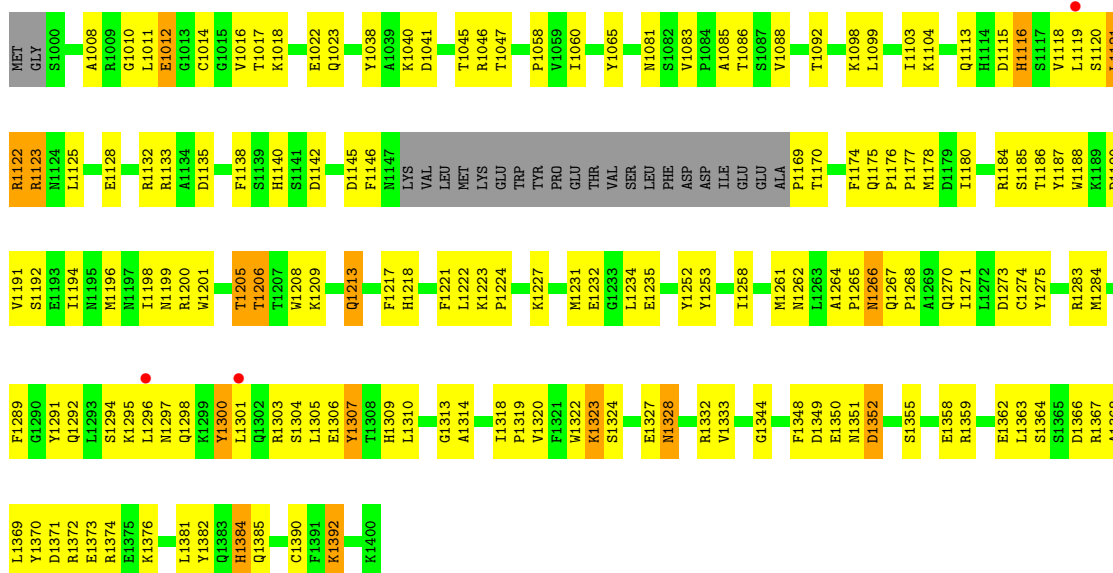
- Molecule 2: 5'-D(*CP*TP*AP*TP*CP*TP*GP*AP*GP*TP*AP*T)-3'

Chain D: 



- Molecule 3: DNA alpha-glucosyltransferase

Chain A: 



- Molecule 3: DNA alpha-glucosyltransferase

Chain B: 

K1330	M1261	P1177	I1103	K998
F1331	M1262	I1180	K1104	G999
V1333	Q1267	Y1187	R1108	I1003
D1334	P1268	W1188	H1114	A1008
N1335	A1269	K1189	D1115	R1009
T1336	Q1270	D1190	H1116	E1012
F1337	I1271	V1191	L1119	G1013
L1338	L1272	S1192	L1119	C1014
T1339	D1273	E1193	R1122	K1018
S1340	C1274	I1194	R1123	Q1023
H1341	Y1275	N1195	N1123	R1024
D1342	I1276	M1196	N1124	D1025
S1343	M1277	N1199	L1125	W1026
I1345	S1278	R1200	G1126	K1029
T1346	E1279	W1201	L1127	V1034
W1347	M1280	I1202	E1128	D1041
		G1203	E1129	R1046
D1352	R1283	R1204	T1130	T1047
M1353	M1284	T1205	V1131	S1048
E1354	F1289	T1206	R1132	V1059
S1355	G1290	T1207	R1133	I1060
E1358	Y1291	W1208	A1134	I1061
R1359	K1295	K1209	D1135	K1063
I1360	L1296	G1210	F1138	E1064
K1361	N1297	F1211	ASN	Y1065
E1362	Q1298	Y1212	D1142	D1066
L1363	K1299	Q1213	ASN	K1067
	Y1300	H1218	GLY	A1068
D1366	L1301	L1222	ASP	L1069
R1367	Q1302	K1223	GLY	I1069
A1368	R1303	P1224	PHE	I1061
L1369	S1304		ASN	L1061
Y1370	L1305		LYS	K1063
D1371	E1306		VAL	Y1065
R1372	Y1307		LEU	D1066
E1373	T1308		MET	K1067
	H1309		LYS	A1068
K1376	L1310		GLU	L1069
A1377	E1311		TRP	V1059
Y1378	L1312		TYR	I1060
			PRO	I1061
H1384	C1315		GLU	S1082
Q1385	G1316		THR	V1083
D1386	T1317		VAL	T1086
S1387	I1318		SER	T1086
	P1319		LEU	E1090
C1390	V1320		PHE	A1091
F1391	F1321		ASP	T1092
K1392	W1322		ASP	I1093
E1393	K1323		ILE	N1094
	S1324		GLU	N1095
D1396	T1325		GLU	Y1096
I1397	G1326		ALA	K1097
L1398	E1327		P1169	K1098
T1399	M1328			L1099
K1400	L1329		F1174	L1100
			Q1175	D1101
			P1176	N1102

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.85Å 119.32Å 86.81Å 90.00° 92.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 99.7 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.280 0.224 , 0.277	Depositor DCC
R_{free} test set	1795 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6977	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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

5.1 Standard geometry

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

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	0.35	0/277	0.76	0/426
2	D	0.31	0/270	0.78	0/415
3	A	0.45	0/3190	0.95	14/4301 (0.3%)
3	B	0.45	0/3162	0.93	9/4262 (0.2%)
All	All	0.44	0/6899	0.93	23/9404 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
3	A	0	1
All	All	0	2

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1304	SER	N-CA-C	8.98	122.59	108.67
3	B	1344	GLY	N-CA-C	-7.75	103.80	114.64
3	A	1390	CYS	N-CA-C	7.53	119.49	111.28
3	A	1205	THR	N-CA-C	7.18	121.82	110.70
3	A	1333	VAL	N-CA-C	6.96	117.57	110.82
3	A	1384	HIS	N-CA-C	6.35	119.50	111.69
3	A	1305	LEU	N-CA-C	-6.26	101.51	110.59
3	A	1304	SER	N-CA-C	6.03	118.48	109.25
3	A	1344	GLY	N-CA-C	-5.96	107.02	115.30
3	A	1209	LYS	N-CA-C	-5.76	106.20	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1305	LEU	N-CA-C	-5.64	102.40	110.59
3	A	1135	ASP	N-CA-C	-5.64	106.57	113.50
3	B	1254	GLY	N-CA-C	-5.61	105.08	112.82
3	A	1323	LYS	N-CA-C	5.57	117.80	111.11
3	B	1271	ILE	N-CA-C	5.56	116.31	108.36
3	A	1392	LYS	N-CA-C	-5.44	105.43	111.36
3	A	1122	ARG	N-CA-C	-5.29	105.10	112.45
3	B	1277	ASN	N-CA-C	5.24	118.45	111.75
3	B	1209	LYS	N-CA-C	-5.24	106.89	113.28
3	A	1289	PHE	N-CA-C	5.19	117.91	109.24
3	B	1135	ASP	N-CA-C	-5.11	107.43	113.97
3	A	1010	GLY	N-CA-C	-5.02	105.82	111.85
3	B	1200	ARG	N-CA-C	5.02	116.58	108.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1307	TYR	Sidechain
1	C	6	DT	Sidechain

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	246	0	137	4	0
2	D	242	0	139	6	0
3	A	3118	0	3060	156	0
3	B	3091	0	3044	148	0
4	A	21	0	0	3	0
4	B	21	0	0	4	0
4	D	7	0	0	0	0
5	A	25	0	11	0	0
5	B	25	0	11	1	0
6	A	89	0	0	3	0
6	B	81	0	0	3	0
6	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	6	0	0	0	0
All	All	6977	0	6402	310	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 24.

All (310) 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:A:1213:GLN:H	3:A:1213:GLN:NE2	1.68	0.92
3:A:1118:VAL:HG12	3:A:1145:ASP:HB2	1.55	0.87
3:A:1113:GLN:HE22	3:A:1115:ASP:HB2	1.40	0.85
3:A:1116:HIS:CE1	4:A:2002:NCO:N3	2.45	0.85
3:A:1318:ILE:HG12	3:A:1370:TYR:CE1	2.15	0.82
3:A:1113:GLN:NE2	3:A:1115:ASP:HB2	1.96	0.81
3:B:1132:ARG:HD2	6:B:41:HOH:O	1.79	0.81
3:A:1120:SER:HA	3:A:1123:ARG:HD2	1.60	0.80
3:A:1199:ASN:HB3	3:A:1291:TYR:CE2	2.21	0.76
3:A:1213:GLN:H	3:A:1213:GLN:HE21	1.31	0.76
3:B:1175:GLN:O	3:B:1177:PRO:HD3	1.84	0.76
3:A:1258:ILE:HD11	3:A:1283:ARG:HD3	1.69	0.74
3:A:1023:GLN:HE22	3:A:1081:ASN:HD21	1.34	0.74
3:A:1372:ARG:O	3:A:1376:LYS:HG3	1.89	0.73
3:B:1327:GLU:C	3:B:1328:ASN:HD22	1.97	0.73
3:B:1023:GLN:HE22	3:B:1081:ASN:HD21	1.35	0.72
3:B:1252:TYR:OH	3:B:1273:ASP:HB3	1.89	0.72
3:B:1231:MET:HB2	3:B:1271:ILE:HD12	1.72	0.71
3:B:1301:LEU:HD22	3:B:1329:LEU:HD21	1.71	0.71
3:A:1118:VAL:HA	3:A:1145:ASP:OD1	1.91	0.71
3:A:1199:ASN:ND2	3:A:1291:TYR:OH	2.23	0.70
3:A:1332:ARG:H	3:A:1384:HIS:HD2	1.40	0.70
3:A:1313:GLY:HA3	3:A:1381:LEU:HD12	1.74	0.70
3:A:1359:ARG:O	3:A:1363:LEU:HD13	1.91	0.70
3:B:1396:ASP:O	3:B:1400:LYS:HB2	1.93	0.69
3:B:1261:MET:HE1	3:B:1272:LEU:HB2	1.75	0.69
3:A:1298:GLN:HA	3:A:1301:LEU:HD12	1.76	0.68
3:A:1120:SER:C	3:A:1122:ARG:H	2.01	0.68
3:A:1296:LEU:O	3:A:1301:LEU:HD11	1.93	0.68
3:A:1327:GLU:C	3:A:1328:ASN:HD22	2.02	0.68
3:A:1199:ASN:HB3	3:A:1291:TYR:HE2	1.59	0.67
3:A:1196:MET:HB3	3:A:1364:SER:OG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1368:ALA:O	3:A:1372:ARG:HG3	1.94	0.66
3:B:1129:GLU:N	3:B:1129:GLU:OE1	2.29	0.66
3:B:1116:HIS:NE2	4:B:3002:NCO:N3	2.45	0.65
3:B:1119:LEU:HD23	3:B:1123:ARG:HH22	1.62	0.65
3:B:1175:GLN:NE2	3:B:1303:ARG:HB3	2.11	0.65
3:B:1093:ILE:HD13	3:B:1125:LEU:HB3	1.79	0.64
3:A:1120:SER:HA	3:A:1123:ARG:CD	2.28	0.64
3:A:1218:HIS:HA	3:A:1222:LEU:HB2	1.80	0.63
3:A:1201:TRP:HB3	3:A:1231:MET:HG2	1.80	0.63
3:B:1177:PRO:HB3	3:B:1390:CYS:HB2	1.81	0.62
3:B:1298:GLN:HG3	3:B:1328:ASN:HB3	1.81	0.62
3:A:1306:GLU:O	3:A:1309:HIS:HB2	2.00	0.62
3:A:1200:ARG:HB3	3:A:1284:MET:HE1	1.82	0.61
3:B:1128:GLU:HB3	3:B:1129:GLU:OE1	1.99	0.61
3:A:1115:ASP:HB3	3:A:1120:SER:CB	2.30	0.61
3:A:1328:ASN:HD22	3:A:1328:ASN:N	1.98	0.61
3:A:1116:HIS:NE2	4:A:2002:NCO:N3	2.47	0.61
3:A:1180:ILE:HG23	3:A:1314:ALA:HB2	1.81	0.61
3:B:1127:LEU:O	3:B:1131:VAL:HG23	2.00	0.61
3:A:1355:SER:HA	3:A:1358:GLU:HG2	1.82	0.61
3:A:1169:PRO:HG2	3:A:1170:THR:H	1.64	0.61
3:B:1323:LYS:HE2	3:B:1327:GLU:OE1	2.01	0.61
3:A:1012:GLU:OE1	3:A:1016:VAL:HB	2.01	0.61
3:A:1221:PHE:C	3:A:1224:PRO:HD2	2.26	0.61
3:A:1060:ILE:CD1	3:B:1245:GLU:HG3	2.32	0.60
3:B:1116:HIS:CE1	4:B:3002:NCO:N3	2.70	0.60
3:B:1332:ARG:H	3:B:1384:HIS:HD2	1.49	0.60
3:A:1142:ASP:HB3	6:A:134:HOH:O	2.00	0.60
3:A:1253:TYR:OH	3:A:1270:GLN:NE2	2.34	0.60
3:A:1322:TRP:CD1	3:A:1324:SER:HG	2.19	0.60
3:A:1224:PRO:HB2	6:A:108:HOH:O	2.01	0.59
3:A:1252:TYR:OH	3:A:1273:ASP:HB3	2.01	0.59
3:B:1326:GLY:HA3	3:B:1347:TRP:CZ3	2.38	0.59
3:A:1113:GLN:NE2	3:A:1115:ASP:H	2.01	0.59
3:B:1202:ILE:HG22	3:B:1232:GLU:HB2	1.85	0.59
3:A:1223:LYS:HB3	3:A:1224:PRO:HD3	1.84	0.59
3:B:1372:ARG:O	3:B:1376:LYS:HG3	2.02	0.59
3:B:1267:GLN:HE21	3:B:1268:PRO:HD2	1.67	0.59
2:D:1:DC:H2'	2:D:2:DT:H72	1.84	0.58
3:A:1065:TYR:HE2	3:A:1098:LYS:HB3	1.68	0.58
2:D:1:DC:H5'	3:B:1241:ILE:HG22	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1297:ASN:OD1	3:B:1299:LYS:HG2	2.02	0.58
3:B:1199:ASN:ND2	3:B:1291:TYR:OH	2.30	0.58
3:A:1022:GLU:OE1	3:A:1178:MET:HG3	2.04	0.58
3:B:1114:HIS:O	4:B:3002:NCO:N4	2.36	0.58
3:B:1358:GLU:O	3:B:1362:GLU:HG3	2.04	0.58
3:A:1120:SER:OG	3:A:1121:LEU:HG	2.04	0.57
3:B:1064:GLU:OE2	3:B:1067:LYS:HD3	2.04	0.57
3:B:1352:ASP:OD1	3:B:1355:SER:HB2	2.04	0.57
3:B:1208:TRP:HA	3:B:1295:LYS:HD3	1.87	0.57
3:B:1310:LEU:HD11	3:B:1385:GLN:NE2	2.19	0.57
3:A:1351:ASN:O	3:A:1352:ASP:HB2	2.05	0.57
3:A:1119:LEU:HD23	3:A:1119:LEU:O	2.03	0.57
3:A:1175:GLN:HE21	3:A:1303:ARG:CZ	2.16	0.57
3:B:1003:ILE:HB	3:B:1034:VAL:HG22	1.86	0.57
3:B:1122:ARG:HH21	3:B:1122:ARG:HG3	1.69	0.57
3:A:1222:LEU:O	3:A:1227:LYS:HB2	2.05	0.57
3:B:1169:PRO:HB2	6:B:42:HOH:O	2.05	0.57
3:B:1359:ARG:O	3:B:1363:LEU:HD13	2.04	0.57
1:C:9:DG:H2"	1:C:10:DA:OP2	2.05	0.56
3:B:1306:GLU:O	3:B:1309:HIS:HB2	2.05	0.56
3:A:1206:THR:HG21	3:A:1208:TRP:NE1	2.21	0.56
3:B:1199:ASN:HB3	3:B:1291:TYR:CE2	2.41	0.56
3:B:1317:THR:O	3:B:1319:PRO:HD3	2.06	0.55
3:B:1241:ILE:O	3:B:1245:GLU:HB2	2.07	0.55
3:A:1121:LEU:HB2	6:A:181:HOH:O	2.07	0.55
3:B:1231:MET:HB2	3:B:1271:ILE:CD1	2.36	0.55
3:A:1232:GLU:OE1	3:A:1283:ARG:NH2	2.31	0.55
3:A:1086:THR:HA	3:A:1125:LEU:HD11	1.88	0.55
3:B:1059:VAL:HG23	3:B:1067:LYS:HE3	1.89	0.55
3:A:1116:HIS:NE2	3:A:1296:LEU:HD11	2.22	0.54
3:A:1115:ASP:HB3	3:A:1120:SER:HB2	1.89	0.54
3:A:1120:SER:O	3:A:1122:ARG:N	2.38	0.54
3:B:1354:GLU:O	3:B:1358:GLU:HG2	2.07	0.54
3:B:1330:LYS:HA	3:B:1336:THR:O	2.07	0.54
3:B:1334:ASP:O	3:B:1336:THR:HG23	2.07	0.54
3:B:1352:ASP:CG	3:B:1355:SER:HB2	2.32	0.54
3:B:1177:PRO:HB2	3:B:1387:SER:HA	1.90	0.54
3:A:1120:SER:CB	3:A:1123:ARG:NH2	2.70	0.54
3:A:1060:ILE:HD13	3:B:1245:GLU:HG3	1.91	0.53
3:B:1284:MET:HG3	3:B:1315:CYS:SG	2.48	0.53
3:B:1190:ASP:O	3:B:1192:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1085:ALA:O	3:A:1088:VAL:HG22	2.08	0.53
3:A:1200:ARG:HD3	3:A:1232:GLU:OE2	2.09	0.53
3:B:1295:LYS:O	3:B:1295:LYS:HG2	2.08	0.53
3:A:1213:GLN:NE2	3:A:1213:GLN:N	2.50	0.52
3:A:1264:ALA:HB1	3:A:1265:PRO:CD	2.39	0.52
3:A:1298:GLN:HA	3:A:1301:LEU:CD1	2.40	0.52
3:A:1138:PHE:HB3	3:A:1174:PHE:CD2	2.44	0.52
3:B:1328:ASN:HD22	3:B:1328:ASN:N	2.03	0.52
3:A:1012:GLU:OE2	3:A:1014:CYS:HB2	2.09	0.52
3:A:1208:TRP:O	3:A:1294:SER:HA	2.10	0.51
3:A:1298:GLN:HA	3:A:1301:LEU:CG	2.40	0.51
3:A:1113:GLN:HG2	3:A:1146:PHE:CE1	2.45	0.51
3:B:1026:TRP:CD2	3:B:1391:PHE:HB3	2.45	0.51
3:B:1301:LEU:HB3	3:B:1329:LEU:HD23	1.93	0.51
3:B:1062:ALA:HB1	3:B:1091:ALA:HB3	1.92	0.51
3:A:1265:PRO:O	3:A:1266:ASN:C	2.53	0.51
3:A:1213:GLN:HE21	3:A:1213:GLN:N	2.05	0.51
3:A:1221:PHE:O	3:A:1224:PRO:HD2	2.11	0.51
3:B:1012:GLU:OE1	3:B:1014:CYS:HB2	2.11	0.51
3:B:1023:GLN:NE2	3:B:1081:ASN:HD21	2.07	0.51
3:B:1262:ASN:H	3:B:1270:GLN:NE2	2.09	0.51
3:A:1175:GLN:O	3:A:1177:PRO:HD3	2.11	0.50
3:B:1200:ARG:O	3:B:1290:GLY:HA2	2.12	0.50
3:A:1184:ARG:HG3	3:A:1188:TRP:HB2	1.92	0.50
1:C:2:DA:H2'	1:C:3:DT:H72	1.93	0.50
3:B:1086:THR:HA	3:B:1125:LEU:HG	1.92	0.50
3:B:1213:GLN:H	3:B:1213:GLN:NE2	2.10	0.50
3:A:1196:MET:HB3	3:A:1364:SER:HG	1.77	0.50
3:A:1320:VAL:HG12	3:A:1348:PHE:HB2	1.92	0.50
3:B:1093:ILE:HG13	3:B:1097:LYS:HE3	1.92	0.50
3:A:1253:TYR:CZ	3:A:1261:MET:HA	2.47	0.49
3:B:1393:GLU:O	3:B:1397:ILE:HG13	2.10	0.49
3:B:1334:ASP:O	3:B:1335:ASN:C	2.54	0.49
3:B:1086:THR:HG23	3:B:1123:ARG:C	2.37	0.49
3:B:1138:PHE:HB3	3:B:1174:PHE:CD2	2.46	0.49
3:B:1233:GLY:HA2	3:B:1273:ASP:O	2.12	0.49
3:B:1297:ASN:O	3:B:1301:LEU:HG	2.11	0.49
3:A:1040:LYS:O	3:A:1040:LYS:HG2	2.13	0.49
3:B:1331:PHE:HE1	3:B:1384:HIS:HB2	1.77	0.49
3:A:1298:GLN:HA	3:A:1301:LEU:HB2	1.95	0.48
3:A:1267:GLN:HE21	3:A:1268:PRO:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1099:LEU:O	3:A:1103:ILE:HG13	2.13	0.48
3:B:1177:PRO:HG2	3:B:1391:PHE:CE1	2.47	0.48
3:A:1273:ASP:O	3:A:1274:CYS:C	2.56	0.48
3:B:1328:ASN:N	3:B:1328:ASN:ND2	2.62	0.48
3:B:1133:ARG:HG3	3:B:1133:ARG:O	2.12	0.48
3:B:1062:ALA:HB1	3:B:1091:ALA:CB	2.44	0.48
3:B:1320:VAL:HA	3:B:1346:ILE:O	2.12	0.48
3:A:1318:ILE:HG12	3:A:1370:TYR:CD1	2.49	0.48
3:B:1008:ALA:HB3	3:B:1083:VAL:HA	1.94	0.48
3:B:1175:GLN:NE2	3:B:1303:ARG:HD2	2.29	0.48
3:A:1180:ILE:HD12	3:A:1382:TYR:HA	1.95	0.47
3:B:1206:THR:HG21	3:B:1208:TRP:NE1	2.30	0.47
3:B:1252:TYR:CZ	3:B:1273:ASP:HB3	2.50	0.47
1:C:2:DA:H2'	1:C:3:DT:C7	2.44	0.47
3:A:1265:PRO:O	3:A:1267:GLN:HG2	2.14	0.47
3:A:1318:ILE:HG12	3:A:1370:TYR:HE1	1.75	0.47
3:A:1184:ARG:C	3:A:1186:THR:H	2.23	0.47
3:B:1301:LEU:HD12	3:B:1328:ASN:HB2	1.97	0.47
2:D:1:DC:C6	2:D:2:DT:H72	2.50	0.47
3:A:1194:ILE:HG22	3:A:1196:MET:HE2	1.97	0.47
3:B:1099:LEU:C	3:B:1101:ASP:H	2.22	0.47
3:B:1100:LEU:HD13	3:B:1130:THR:HA	1.96	0.47
3:B:1190:ASP:C	3:B:1192:SER:H	2.23	0.47
3:A:1369:LEU:HA	3:A:1372:ARG:NH1	2.30	0.47
3:B:1312:LEU:HD12	3:B:1321:PHE:HE1	1.79	0.47
3:B:1233:GLY:CA	3:B:1273:ASP:O	2.63	0.47
3:B:1327:GLU:HG3	3:B:1339:THR:HG21	1.97	0.47
3:A:1332:ARG:H	3:A:1384:HIS:CD2	2.26	0.46
3:A:1373:GLU:OE2	3:A:1376:LYS:HE2	2.16	0.46
3:B:1187:TYR:O	3:B:1188:TRP:C	2.58	0.46
3:A:1200:ARG:HD2	3:A:1284:MET:HE2	1.97	0.46
3:A:1350:GLU:HG3	3:A:1351:ASN:ND2	2.31	0.46
2:D:1:DC:H2'	2:D:2:DT:C7	2.43	0.46
3:A:1060:ILE:HD11	3:B:1245:GLU:HG3	1.98	0.46
3:A:1258:ILE:HG12	3:A:1258:ILE:O	2.15	0.46
3:B:1366:ASP:O	3:B:1367:ARG:C	2.58	0.46
1:C:5:DC:H2''	1:C:6:DT:H5'	1.98	0.46
3:A:1295:LYS:HG2	3:A:1322:TRP:CD2	2.51	0.46
3:B:1108:ARG:NH1	3:B:1398:ILE:O	2.49	0.45
3:B:1295:LYS:HD2	3:B:1295:LYS:N	2.31	0.45
3:B:1299:LYS:HE2	3:B:1300:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1275:TYR:CD1	3:B:1280:MET:HB2	2.51	0.45
3:A:1234:LEU:HD12	3:A:1271:ILE:HG23	1.99	0.45
3:B:1223:LYS:HB3	3:B:1224:PRO:HD3	1.97	0.45
3:B:1244:LYS:HG2	3:B:1245:GLU:N	2.31	0.45
3:A:1113:GLN:HE22	3:A:1115:ASP:CB	2.20	0.45
3:B:1342:ASP:OD2	3:B:1376:LYS:NZ	2.49	0.45
3:A:1116:HIS:HE1	4:A:2002:NCO:N3	2.08	0.45
3:A:1133:ARG:O	3:A:1133:ARG:HG3	2.17	0.45
3:A:1298:GLN:CA	3:A:1301:LEU:HD12	2.46	0.45
3:B:1276:ILE:HB	3:B:1279:GLU:HB2	1.99	0.45
3:A:1297:ASN:O	3:A:1301:LEU:HG	2.17	0.45
4:B:3002:NCO:N1	5:B:3001:UDP:PB	2.90	0.45
3:A:1120:SER:HA	3:A:1123:ARG:NE	2.32	0.44
3:B:1188:TRP:CZ3	3:B:1378:TYR:HB2	2.52	0.44
3:B:1329:LEU:HB2	3:B:1338:LEU:HD12	1.99	0.44
3:A:1275:TYR:CD1	3:A:1275:TYR:C	2.95	0.44
3:B:1003:ILE:O	3:B:1034:VAL:HA	2.17	0.44
3:B:1191:VAL:HG23	3:B:1370:TYR:CD2	2.52	0.44
3:A:1045:THR:C	3:A:1047:THR:H	2.25	0.44
3:A:1113:GLN:NE2	3:A:1115:ASP:CB	2.76	0.44
3:A:1371:ASP:HA	3:A:1374:ARG:HG2	1.98	0.44
3:B:1194:ILE:HD12	3:B:1370:TYR:HE2	1.82	0.44
3:A:1120:SER:HA	3:A:1123:ARG:CZ	2.48	0.44
3:A:1323:LYS:HD3	3:A:1349:ASP:OD2	2.16	0.44
2:D:5:DC:C3'	3:B:1122:ARG:HH22	2.31	0.44
3:B:1291:TYR:N	3:B:1291:TYR:CD2	2.84	0.44
3:B:1298:GLN:HG3	3:B:1328:ASN:CB	2.47	0.44
3:A:1190:ASP:O	3:A:1191:VAL:C	2.61	0.44
3:B:1367:ARG:O	3:B:1370:TYR:HB3	2.18	0.44
3:A:1140:HIS:HE1	3:A:1176:PRO:HD3	1.82	0.44
3:B:1065:TYR:CE1	3:B:1069:LEU:HD22	2.53	0.44
3:A:1046:ARG:HH22	3:A:1235:GLU:CD	2.25	0.44
3:A:1217:PHE:HD2	3:A:1222:LEU:HD11	1.83	0.44
3:B:1190:ASP:C	3:B:1192:SER:N	2.74	0.44
3:A:1231:MET:HB2	3:A:1271:ILE:HD12	2.00	0.43
3:A:1217:PHE:CE2	3:A:1222:LEU:HD21	2.54	0.43
3:A:1318:ILE:HA	3:A:1319:PRO:HD3	1.82	0.43
3:B:1218:HIS:CD2	3:B:1229:THR:OG1	2.70	0.43
3:A:1366:ASP:C	3:A:1368:ALA:N	2.77	0.43
3:B:998:MET:HB3	3:B:999:GLY:H	1.64	0.43
3:B:1018:LYS:HG2	3:B:1307:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1124:ASN:ND2	6:B:37:HOH:O	2.51	0.43
3:A:1217:PHE:CD2	3:A:1222:LEU:HD11	2.54	0.43
3:A:1258:ILE:HD11	3:A:1283:ARG:CD	2.42	0.43
3:B:1180:ILE:HB	3:B:1386:ASP:OD1	2.18	0.43
3:B:1296:LEU:CB	3:B:1301:LEU:HD21	2.49	0.43
3:B:1331:PHE:CE1	3:B:1384:HIS:HB2	2.54	0.43
3:A:1011:LEU:HD21	3:A:1017:THR:HG21	2.00	0.43
3:A:1120:SER:HB2	3:A:1123:ARG:NH2	2.32	0.43
3:A:1128:GLU:O	3:A:1132:ARG:HG3	2.19	0.43
3:A:1253:TYR:CE2	3:A:1261:MET:HA	2.53	0.43
3:A:1115:ASP:OD1	3:A:1120:SER:HB2	2.19	0.43
3:A:1206:THR:CG2	3:A:1208:TRP:CD1	3.01	0.43
3:A:1038:TYR:CZ	3:A:1058:PRO:HB3	2.54	0.43
3:A:1065:TYR:CE2	3:A:1098:LYS:HB3	2.51	0.43
3:A:1103:ILE:O	3:A:1104:LYS:C	2.61	0.43
3:A:1113:GLN:NE2	3:A:1115:ASP:N	2.65	0.43
3:A:1116:HIS:HB2	3:A:1300:TYR:HB3	2.00	0.43
3:B:1211:PHE:HB2	3:B:1231:MET:HE1	2.00	0.43
3:A:1113:GLN:HG2	3:A:1146:PHE:CD1	2.54	0.42
3:A:1363:LEU:O	3:A:1370:TYR:HB2	2.19	0.42
3:B:1025:ASP:O	3:B:1029:LYS:HB2	2.18	0.42
3:B:1046:ARG:C	3:B:1048:SER:H	2.27	0.42
3:B:1295:LYS:HD2	3:B:1295:LYS:H	1.83	0.42
3:B:1009:ARG:HB2	3:B:1083:VAL:O	2.19	0.42
3:B:1046:ARG:NH2	3:B:1235:GLU:OE2	2.51	0.42
3:A:1018:LYS:HG2	3:A:1307:TYR:CG	2.54	0.42
3:B:1218:HIS:HA	3:B:1222:LEU:HB2	2.00	0.42
3:B:1273:ASP:CG	3:B:1274:CYS:H	2.27	0.42
3:B:1359:ARG:O	3:B:1363:LEU:CD1	2.68	0.42
3:B:1090:GLU:O	3:B:1094:ASN:HB2	2.19	0.42
3:B:1397:ILE:HA	3:B:1400:LYS:HE3	2.00	0.42
3:A:1120:SER:C	3:A:1122:ARG:N	2.67	0.42
3:A:1187:TYR:O	3:A:1188:TRP:C	2.61	0.42
3:B:1332:ARG:N	3:B:1384:HIS:HD2	2.17	0.42
3:A:1012:GLU:H	3:A:1012:GLU:HG3	1.56	0.42
3:A:1191:VAL:HG13	3:A:1192:SER:N	2.35	0.42
3:B:1062:ALA:HA	3:B:1095:ASN:HD22	1.84	0.42
3:A:1115:ASP:OD1	3:A:1123:ARG:NH2	2.52	0.42
3:A:1198:ILE:HG21	3:A:1200:ARG:NH2	2.35	0.42
3:A:1234:LEU:HD12	3:A:1271:ILE:CG2	2.50	0.42
3:A:1262:ASN:C	3:A:1262:ASN:HD22	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1310:LEU:HD11	3:A:1385:GLN:HB3	2.01	0.42
3:B:1289:PHE:CE2	3:B:1360:ILE:HG23	2.54	0.42
3:A:1041:ASP:OD1	3:A:1092:THR:HG23	2.20	0.41
3:B:1123:ARG:HH21	3:B:1123:ARG:HG2	1.85	0.41
3:B:1194:ILE:HG22	3:B:1196:MET:HE2	2.03	0.41
3:B:1204:ARG:HA	3:B:1233:GLY:O	2.20	0.41
3:B:1318:ILE:HG12	3:B:1370:TYR:CE1	2.55	0.41
3:B:1322:TRP:NE1	3:B:1324:SER:HB3	2.35	0.41
2:D:1:DC:H2''	2:D:2:DT:C6	2.56	0.41
3:A:1292:GLN:OE1	3:A:1292:GLN:C	2.63	0.41
3:A:1184:ARG:C	3:A:1186:THR:N	2.79	0.41
3:A:1194:ILE:HD12	3:A:1370:TYR:HE2	1.86	0.41
3:B:1103:ILE:O	3:B:1104:LYS:C	2.63	0.41
3:A:1008:ALA:HB3	3:A:1083:VAL:HA	2.02	0.41
3:A:1184:ARG:O	3:A:1186:THR:N	2.54	0.41
3:A:1348:PHE:CD1	3:A:1348:PHE:C	2.98	0.41
3:B:1242:ALA:O	3:B:1246:LYS:HG3	2.21	0.41
3:B:1298:GLN:HG3	3:B:1328:ASN:CG	2.45	0.41
3:B:1369:LEU:O	3:B:1373:GLU:HG2	2.20	0.41
3:A:1191:VAL:HG21	3:A:1367:ARG:HB3	2.02	0.41
3:A:1223:LYS:N	3:A:1224:PRO:CD	2.83	0.41
3:B:1060:ILE:HD12	3:B:1064:GLU:OE1	2.20	0.41
3:B:1322:TRP:CD1	3:B:1324:SER:HB3	2.56	0.41
3:A:1358:GLU:O	3:A:1362:GLU:HB2	2.21	0.40
3:A:1115:ASP:CB	3:A:1120:SER:HB2	2.50	0.40
3:B:1258:ILE:HD11	3:B:1283:ARG:CZ	2.51	0.40
3:B:1329:LEU:HB2	3:B:1338:LEU:CD1	2.52	0.40
3:A:1369:LEU:HD13	3:A:1372:ARG:NH2	2.37	0.40
3:B:1208:TRP:CH2	3:B:1209:LYS:HE2	2.56	0.40
3:B:1222:LEU:O	3:B:1227:LYS:HB2	2.22	0.40
3:B:1122:ARG:HG3	3:B:1122:ARG:NH2	2.35	0.40
3:B:1257:GLU:O	3:B:1258:ILE:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	376/403 (93%)	336 (89%)	36 (10%)	4 (1%)	11	18
3	B	373/403 (93%)	336 (90%)	31 (8%)	6 (2%)	7	11
All	All	749/806 (93%)	672 (90%)	67 (9%)	10 (1%)	9	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1352	ASP
3	B	1191	VAL
3	B	1335	ASN
3	A	1185	SER
3	B	1273	ASP
3	A	1121	LEU
3	A	1266	ASN
3	B	1041	ASP
3	B	1046	ARG
3	B	1205	THR

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	347/368 (94%)	338 (97%)	9 (3%)	40	63
3	B	344/368 (94%)	334 (97%)	10 (3%)	37	60
All	All	691/736 (94%)	672 (97%)	19 (3%)	39	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1012	GLU
3	A	1116	HIS

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Mol	Chain	Res	Type
3	A	1123	ARG
3	A	1205	THR
3	A	1206	THR
3	A	1213	GLN
3	A	1300	TYR
3	A	1328	ASN
3	A	1392	LYS
3	B	1012	GLU
3	B	1066	ASP
3	B	1119	LEU
3	B	1213	GLN
3	B	1244	LYS
3	B	1245	GLU
3	B	1257	GLU
3	B	1291	TYR
3	B	1295	LYS
3	B	1340	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1023	GLN
3	A	1089	GLN
3	A	1094	ASN
3	A	1113	GLN
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	1267	GLN
3	A	1270	GLN
3	A	1297	ASN
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	1052	HIS
3	B	1081	ASN

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Mol	Chain	Res	Type
3	B	1094	ASN
3	B	1095	ASN
3	B	1113	GLN
3	B	1124	ASN
3	B	1175	GLN
3	B	1197	ASN
3	B	1199	ASN
3	B	1213	GLN
3	B	1218	HIS
3	B	1255	ASN
3	B	1267	GLN
3	B	1270	GLN
3	B	1277	ASN
3	B	1328	ASN
3	B	1335	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
4	NCO	B	3003	-	6,6,6	1.49	0	-		
5	UDP	B	3001	-	25,26,26	1.02	1 (4%)	38,40,40	0.63	1 (2%)
4	NCO	A	2003	-	6,6,6	1.57	0	-		
4	NCO	B	3002	-	6,6,6	1.41	0	-		
4	NCO	B	3004	-	6,6,6	1.51	0	-		
4	NCO	A	2004	-	6,6,6	1.49	0	-		
4	NCO	D	1003	-	6,6,6	1.61	0	-		
4	NCO	A	2002	-	6,6,6	1.32	0	-		
5	UDP	A	2001	-	25,26,26	1.11	1 (4%)	38,40,40	0.59	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
5	UDP	B	3001	-	-	4/16/32/32	0/2/2/2
5	UDP	A	2001	-	-	3/16/32/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	UDP	PA-O3A	4.78	1.64	1.59
5	B	3001	UDP	PA-O3A	4.19	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	UDP	O2B-PB-O1B	2.21	119.46	110.83
5	B	3001	UDP	O2B-PB-O1B	2.15	119.22	110.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	UDP	PA-O3A-PB-O1B
5	A	2001	UDP	PB-O3A-PA-O5'

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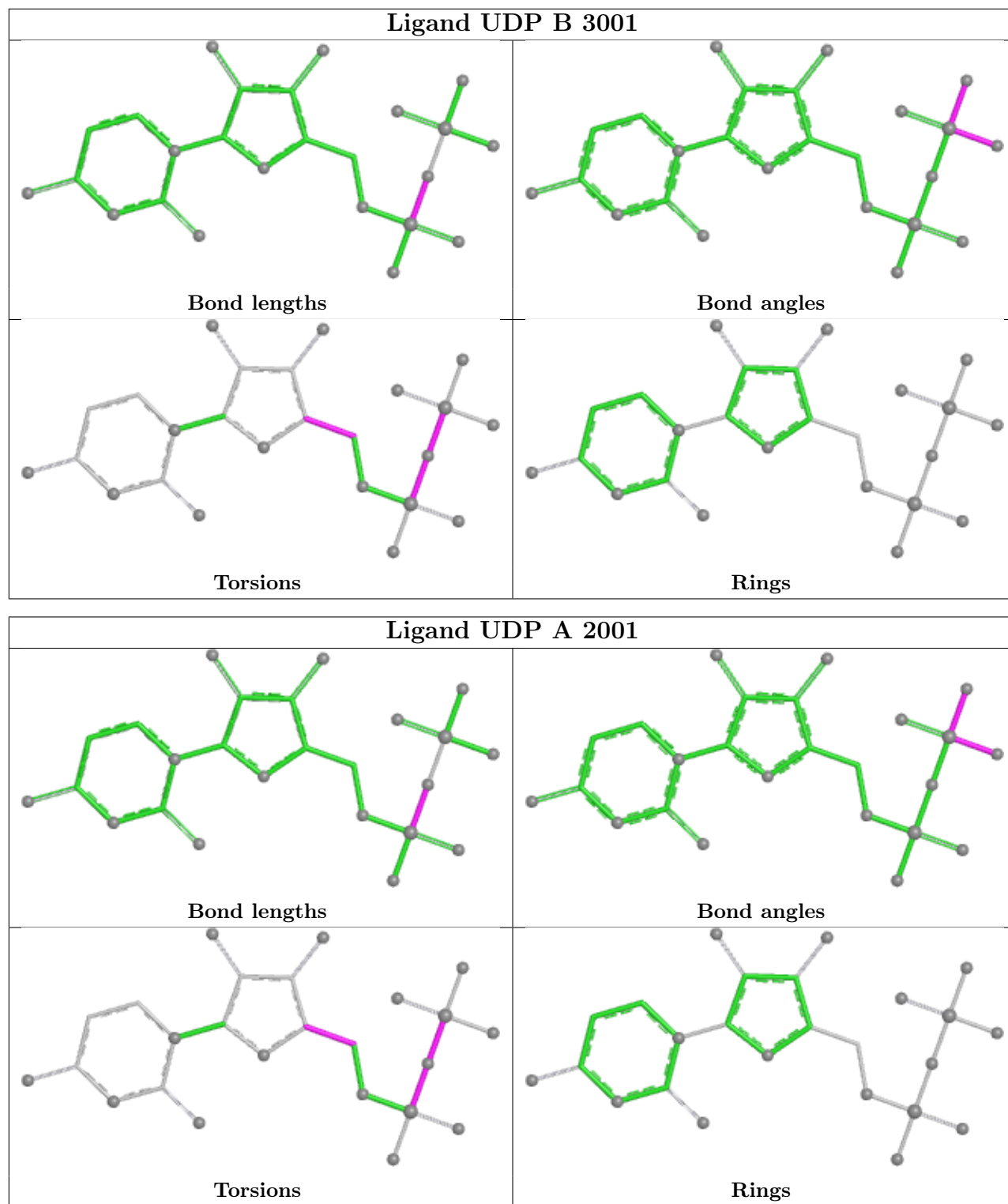
Mol	Chain	Res	Type	Atoms
5	B	3001	UDP	PB-O3A-PA-O5'
5	B	3001	UDP	PA-O3A-PB-O1B
5	B	3001	UDP	O4'-C4'-C5'-O5'
5	A	2001	UDP	O4'-C4'-C5'-O5'
5	B	3001	UDP	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3001	UDP	1	0
4	B	3002	NCO	4	0
4	A	2002	NCO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	12/12 (100%)	-0.30	0 100 100	38, 62, 71, 72	0
2	D	12/12 (100%)	-0.34	0 100 100	50, 60, 74, 74	0
3	A	380/403 (94%)	-0.03	3 (0%) 82 80	34, 60, 87, 100	0
3	B	377/403 (93%)	0.01	2 (0%) 87 85	39, 65, 84, 97	0
All	All	781/830 (94%)	-0.02	5 (0%) 85 83	34, 62, 86, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1296	LEU	3.5
3	A	1301	LEU	2.4
3	B	1300	TYR	2.4
3	B	1301	LEU	2.3
3	A	1119	LEU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

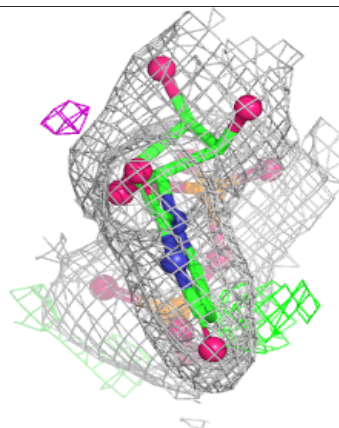
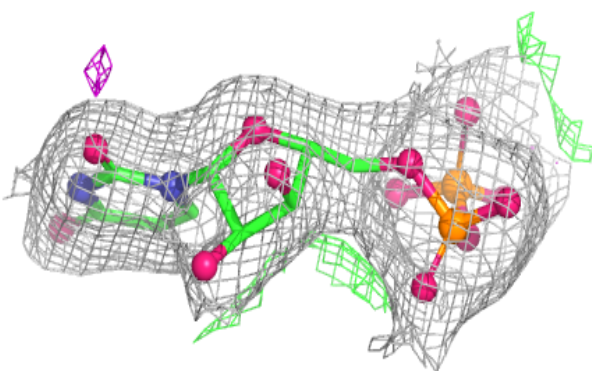
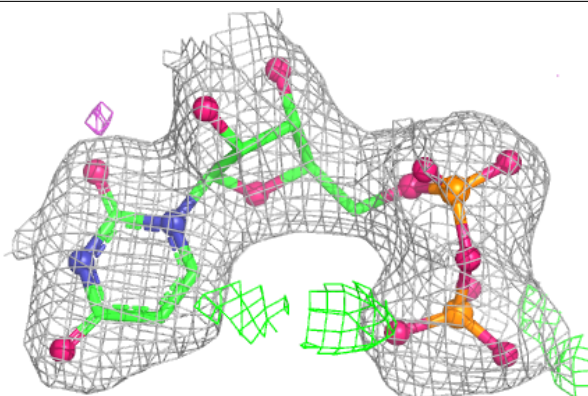
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NCO	B	3004	7/7	0.81	0.18	71,71,71,73	7
4	NCO	A	2004	7/7	0.89	0.19	92,92,93,93	7
4	NCO	B	3003	7/7	0.92	0.09	98,99,99,99	0
4	NCO	B	3002	7/7	0.93	0.13	78,79,79,79	0
4	NCO	D	1003	7/7	0.94	0.09	88,89,89,91	0
4	NCO	A	2002	7/7	0.95	0.14	63,63,65,66	0
4	NCO	A	2003	7/7	0.95	0.09	81,82,84,84	0
5	UDP	B	3001	25/25	0.97	0.05	37,43,47,49	0
5	UDP	A	2001	25/25	0.98	0.05	38,44,46,48	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.

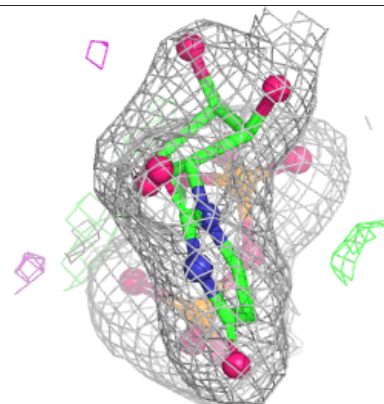
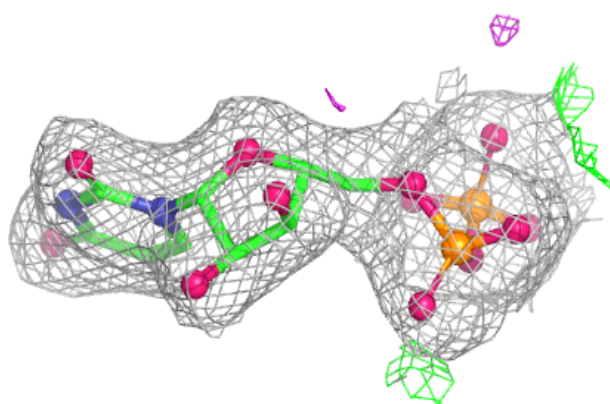
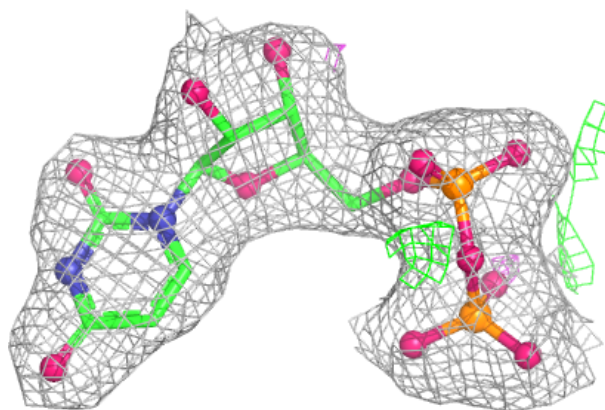
Electron density around UDP B 3001:

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



Electron density around UDP A 2001:

$2mF_o - DF_c$ (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.