Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:41 PM GMT

PDB ID	:	1YA6
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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	Percentile Ranks	Value
Rfree		0.275
Clashscore		22
Ramachandran outliers		1.3%
Sidechain outliers		3.0%
RSRZ outliers		6.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
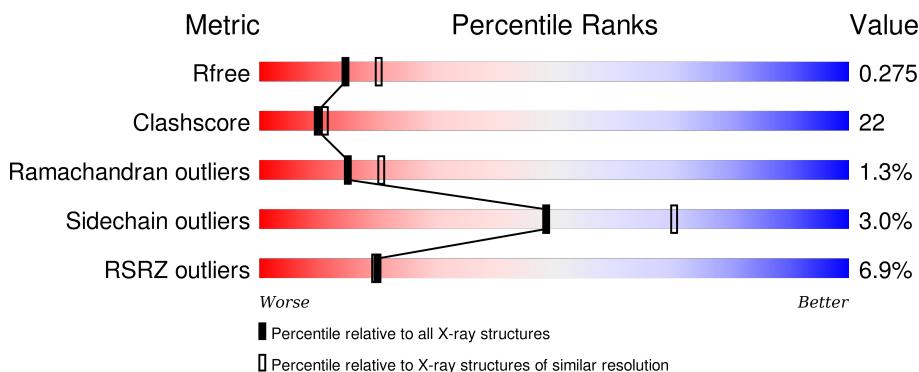
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	12	50% 42% 8%
2	D	12	75% 25%
3	A	403	7% 60% 32% • 6%
3	B	403	6% 51% 40% • 6%

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
4	NCO	B	3002	-	-	-	X

2 Entry composition (i)

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 246	C 119	N 49	O 67	P 11	0	0	0

- 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 242	C 118	N 41	O 72	P 11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	380	Total 3118	C 1986	N 532	O 584	S 16	0	0	0
3	B	377	Total 3091	C 1970	N 527	O 577	S 17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).
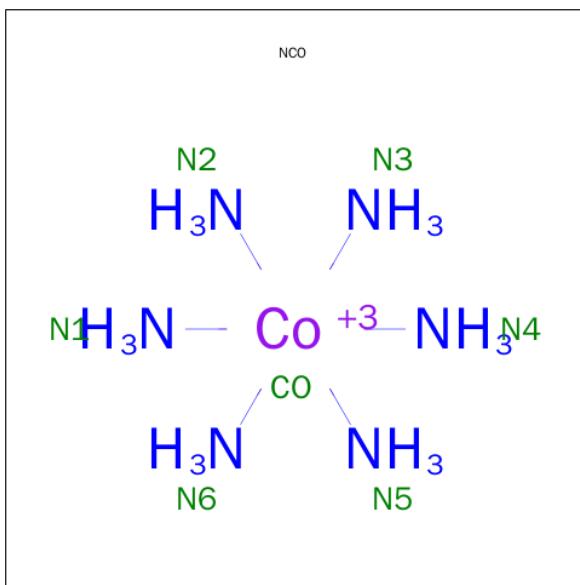
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	Co 1	N 6	0	0
4	B	1	Total 7	Co 1	N 6	0	0
4	A	1	Total 7	Co 1	N 6	0	0
4	B	1	Total 7	Co 1	N 6	0	0
4	D	1	Total 7	Co 1	N 6	0	0
4	B	1	Total 7	Co 1	N 6	0	0
4	A	1	Total 7	Co 1	N 6	0	0

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).
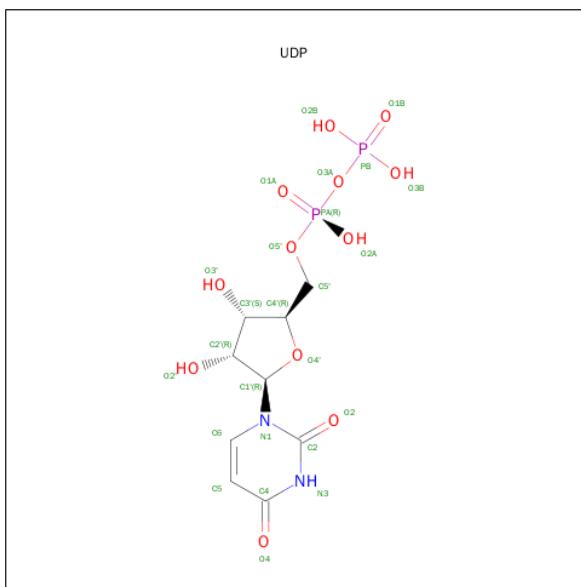
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
5	B	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 6 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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'
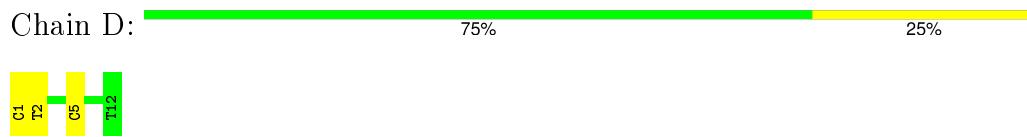
Chain D:

- Molecule 3: DNA alpha-glucosyltransferase

Chain A:

- Molecule 3: DNA alpha-glucosyltransferase

Chain B:
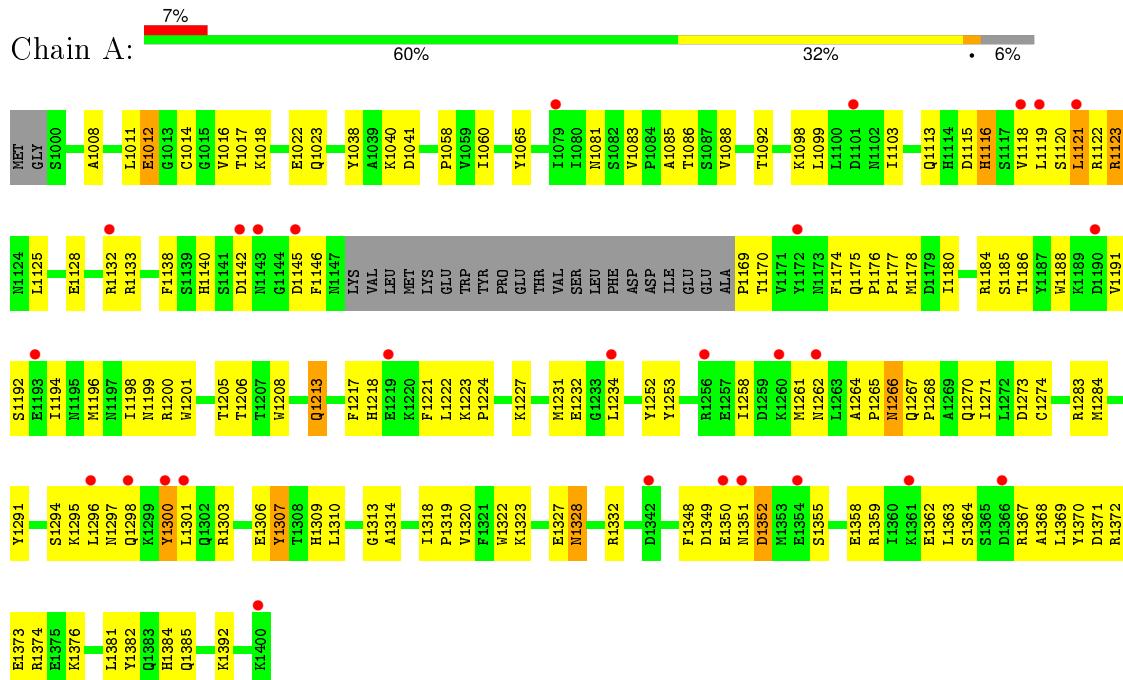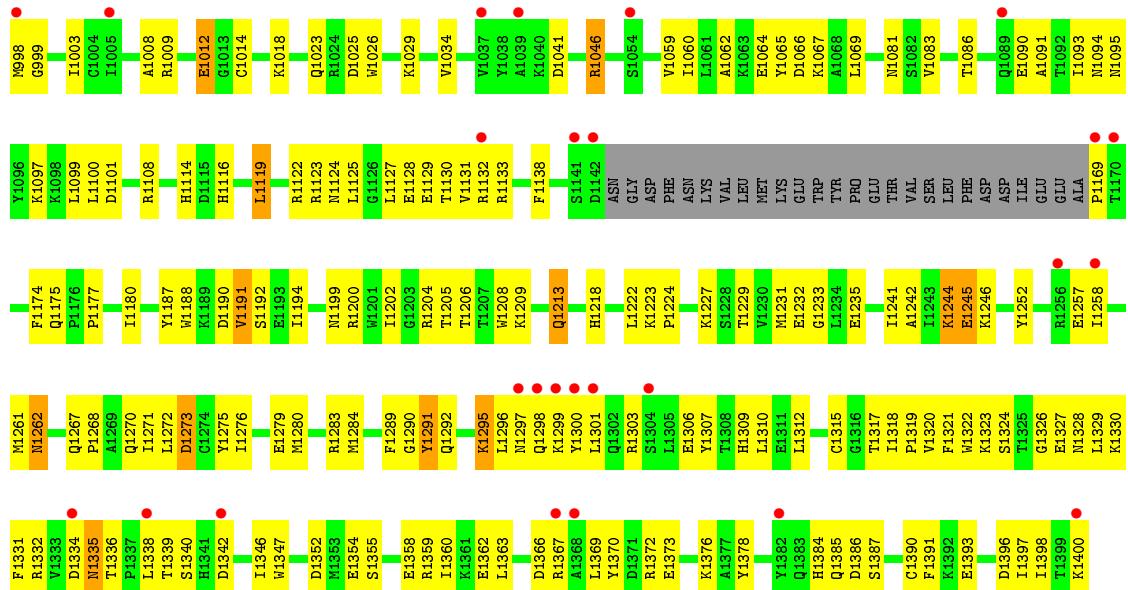
4 Data and refinement statistics (i)

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 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 99.9 (19.98-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.280 0.227 , 0.275	Depositor DCC
R_{free} test set	1795 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.6	EDS
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 36229 reflections	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.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, 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	0.48	0/277	0.76	0/426
2	D	0.44	0/270	0.71	0/415
3	A	0.41	0/3190	0.63	0/4301
3	B	0.39	0/3162	0.62	0/4262
All	All	0.41	0/6899	0.64	0/9404

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.

There are no bond angle outliers.

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 (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	246	0	137	4	0
2	D	242	0	139	6	0
3	A	3118	0	3060	143	0
3	B	3091	0	3044	141	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
6	D	6	0	0	0	0
All	All	6977	0	6402	290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (290) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1298:GLN:HA	3:A:1301:LEU:HD12	1.76	0.68
3:B:1327:GLU:C	3:B:1328:ASN:HD22	1.97	0.68
3:A:1296:LEU:O	3:A:1301:LEU:HD11	1.93	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
3:A:1368:ALA:O	3:A:1372:ARG:HG3	1.94	0.66
3:B:1129:GLU:OE1	3:B:1129:GLU:N	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:1120:SER:C	3:A:1122:ARG:H	2.01	0.63
3:A:1201:TRP:HB3	3:A:1231:MET:HG2	1.80	0.63
3:A:1327:GLU:C	3:A:1328:ASN:HD22	2.02	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: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:B:1323:LYS:HE2	3:B:1327:GLU:OE1	2.01	0.61
3:A:1169:PRO:HG2	3:A:1170:THR:H	1.64	0.61
3:A:1012:GLU:OE1	3:A:1016:VAL:HB	2.01	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1060:ILE:CD1	3:B:1245:GLU:HG3	2.32	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: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
3:B:1297:ASN:OD1	3:B:1299:LYS:HG2	2.02	0.58
2:D:1:DC:H5'	3:B:1241:ILE:HG22	1.83	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:1310:LEU:HD11	3:B:1385:GLN:NE2	2.19	0.57
3:B:1208:TRP:HA	3:B:1295:LYS:HD3	1.87	0.57
3:A:1351:ASN:O	3:A:1352:ASP:HB2	2.05	0.57
3:B:1003:ILE:HB	3:B:1034:VAL:HG22	1.86	0.57
3:A:1119:LEU:HD23	3:A:1119:LEU:O	2.03	0.57
3:B:1122:ARG:HG3	3:B:1122:ARG:HH21	1.69	0.57
3:A:1175:GLN:HE21	3:A:1303:ARG:CZ	2.16	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
3:B:1328:ASN:N	3:B:1328:ASN:HD22	2.03	0.56
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:1221:PHE:C	3:A:1224:PRO:HD2	2.26	0.56
3:A:1200:ARG:HD2	3:A:1284:MET:HE2	1.87	0.56
3:B:1199:ASN:HB3	3:B:1291:TYR:CE2	2.41	0.56
3:A:1206:THR:HG21	3:A:1208:TRP:NE1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:A:1200:ARG:HD3	3:A:1232:GLU:OE2	2.09	0.53
3:A:1085:ALA:O	3:A:1088:VAL:HG22	2.08	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:1200:ARG:HB3	3:A:1284:MET:HE1	1.92	0.52
3:A:1138:PHE:HB3	3:A:1174:PHE:CD2	2.44	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:1213:GLN:HE21	3:A:1213:GLN:N	2.05	0.51
3:B:1023:GLN:NE2	3:B:1081:ASN:HD21	2.07	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: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
3:B:1086:THR:HA	3:B:1125:LEU:HG	1.92	0.50
1:C:2:DA:H2'	1:C:3:DT:H72	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1352:ASP:CG	3:B:1355:SER:HB2	2.32	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:B:1393:GLU:O	3:B:1397:ILE:HG13	2.10	0.49
3:A:1253:TYR:CZ	3:A:1261:MET:HA	2.47	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:HG2	3:A:1040:LYS:O	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
3:B:1177:PRO:HG2	3:B:1391:PHE:CE1	2.47	0.48
3:A:1099:LEU:O	3:A:1103:ILE:HG13	2.13	0.48
3:B:1328:ASN:ND2	3:B:1328:ASN:N	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:1175:GLN:NE2	3:B:1303:ARG:HD2	2.29	0.48
3:B:1008:ALA:HB3	3:B:1083:VAL:HA	1.94	0.48
3:A:1180:ILE:HD12	3:A:1382:TYR:HA	1.95	0.47
3:B:1252:TYR:CZ	3:B:1273:ASP:HB3	2.50	0.47
3:B:1206:THR:HG21	3:B:1208:TRP:NE1	2.30	0.47
3:A:1318:ILE:HG12	3:A:1370:TYR:HE1	1.75	0.47
3:A:1265:PRO:O	3:A:1267:GLN:HG2	2.14	0.47
1:C:2:DA:H2'	1:C:3:DT:C7	2.44	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:B:1100:LEU:HD13	3:B:1130:THR:HA	1.96	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:A:1120:SER:C	3:A:1122:ARG:N	2.67	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:1373:GLU:OE2	3:A:1376:LYS:HE2	2.16	0.46
3:A:1332:ARG:H	3:A:1384:HIS:CD2	2.26	0.46
3:A:1258:ILE:HG12	3:A:1258:ILE:O	2.15	0.46
3:A:1350:GLU:HG3	3:A:1351:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:DC:H2'	2:D:2:DT:C7	2.43	0.46
3:A:1265:PRO:O	3:A:1266:ASN:C	2.53	0.46
3:A:1060:ILE:HD11	3:B:1245:GLU:HG3	1.98	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:1295:LYS:N	3:B:1295:LYS:HD2	2.31	0.45
3:B:1108:ARG:NH1	3:B:1398:ILE:O	2.49	0.45
3:B:1299:LYS:HE2	3:B:1300:TYR:CE1	2.51	0.45
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:1244:LYS:HG2	3:B:1245:GLU:N	2.31	0.45
3:B:1223:LYS:HB3	3:B:1224:PRO:HD3	1.97	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:B:1334:ASP:O	3:B:1335:ASN:C	2.54	0.45
3:A:1298:GLN:CA	3:A:1301:LEU:HD12	2.46	0.45
3:A:1116:HIS:HE1	4:A:2002:NCO:N3	2.08	0.45
3:A:1133:ARG:HG3	3:A:1133:ARG:O	2.17	0.45
3:B:1086:THR:HG23	3:B:1123:ARG:C	2.37	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:1329:LEU:HB2	3:B:1338:LEU:HD12	1.99	0.44
3:B:1188:TRP:CZ3	3:B:1378:TYR:HB2	2.52	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:1113:GLN:NE2	3:A:1115:ASP:CB	2.76	0.44
3:B:1194:ILE:HD12	3:B:1370:TYR:HE2	1.82	0.44
3:A:1371:ASP:HA	3:A:1374:ARG:HG2	1.98	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
3:B:1298:GLN:HG3	3:B:1328:ASN:CB	2.47	0.44
3:B:1291:TYR:CD2	3:B:1291:TYR:N	2.84	0.44
2:D:5:DC:C3'	3:B:1122:ARG:HH22	2.31	0.44
3:B:1367:ARG:O	3:B:1370:TYR:HB3	2.18	0.44
3:B:1065:TYR:CE1	3:B:1069:LEU:HD22	2.53	0.44
3:A:1140:HIS:HE1	3:A:1176:PRO:HD3	1.82	0.44
3:A:1217:PHE:HD2	3:A:1222:LEU:HD11	1.83	0.44
3:A:1231:MET:HB2	3:A:1271:ILE:HD12	2.00	0.43
3:A:1318:ILE:HA	3:A:1319:PRO:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1217:PHE:CE2	3:A:1222:LEU:HD21	2.54	0.43
3:B:1218:HIS:CD2	3:B:1229:THR:OG1	2.70	0.43
3:A:1273:ASP:O	3:A:1274:CYS:C	2.56	0.43
3:B:1018:LYS:HG2	3:B:1307:TYR:CG	2.54	0.43
3:B:998:MET:HB3	3:B:999:GLY:H	1.64	0.43
3:B:1124:ASN:ND2	6:B:37:HOH:O	2.51	0.43
3:A:1258:ILE:HD11	3:A:1283:ARG:CD	2.42	0.43
3:B:1296:LEU:CB	3:B:1301:LEU:HD21	2.49	0.43
3:A:1217:PHE:CD2	3:A:1222:LEU:HD11	2.54	0.43
3:B:1331:PHE:CE1	3:B:1384:HIS:HB2	2.54	0.43
3:B:1180:ILE:HB	3:B:1386:ASP:OD1	2.18	0.43
3:A:1120:SER:HB2	3:A:1123:ARG:NH2	2.32	0.43
3:A:1253:TYR:CE2	3:A:1261:MET:HA	2.53	0.43
3:A:1128:GLU:O	3:A:1132:ARG:HG3	2.19	0.43
3:A:1011:LEU:HD21	3:A:1017:THR:HG21	2.00	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:1065:TYR:CE2	3:A:1098:LYS:HB3	2.51	0.43
3:A:1038:TYR:CZ	3:A:1058:PRO:HB3	2.54	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: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:1295:LYS:H	3:B:1295:LYS:HD2	1.83	0.42
3:A:1184:ARG:C	3:A:1186:THR:H	2.23	0.42
3:B:1009:ARG:HB2	3:B:1083:VAL:O	2.19	0.42
3:B:1099:LEU:C	3:B:1101:ASP:H	2.22	0.42
3:B:1046:ARG:NH2	3:B:1235:GLU:OE2	2.51	0.42
3:B:1359:ARG:O	3:B:1363:LEU:CD1	2.68	0.42
3:B:1190:ASP:C	3:B:1192:SER:H	2.23	0.42
3:B:1218:HIS:HA	3:B:1222:LEU:HB2	2.00	0.42
3:A:1018:LYS:HG2	3:A:1307:TYR:CG	2.54	0.42
3:B:1397:ILE:HA	3:B:1400:LYS:HE3	2.00	0.42
3:B:1090:GLU:O	3:B:1094:ASN:HB2	2.19	0.42
3:B:1332:ARG:N	3:B:1384:HIS:HD2	2.17	0.42
3:A:1012:GLU:HG3	3:A:1012:GLU:H	1.56	0.42
3:B:1062:ALA:HA	3:B:1095:ASN:HD22	1.84	0.42
3:A:1191:VAL:HG13	3:A:1192:SER:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1234:LEU:HD12	3:A:1271:ILE:CG2	2.50	0.42
3:B:1187:TYR:O	3:B:1188:TRP:C	2.58	0.42
3:B:1289:PHE:CE2	3:B:1360:ILE:HG23	2.54	0.42
3:B:1261:MET:CE	3:B:1272:LEU:HB2	2.50	0.42
3:A:1310:LEU:HD11	3:A:1385:GLN:HB3	2.01	0.42
3:B:1123:ARG:HG2	3:B:1123:ARG:HH21	1.85	0.41
3:A:1041:ASP:OD1	3:A:1092:THR:HG23	2.20	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:B:1366:ASP:O	3:B:1367:ARG:C	2.58	0.41
3:A:1194:ILE:HD12	3:A:1370:TYR:HE2	1.86	0.41
3:A:1184:ARG:O	3:A:1186:THR:N	2.54	0.41
3:B:1369:LEU:O	3:B:1373:GLU:HG2	2.20	0.41
3:B:1242:ALA:O	3:B:1246:LYS:HG3	2.21	0.41
3:A:1008:ALA:HB3	3:A:1083:VAL:HA	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:A:1191:VAL:HG21	3:A:1367:ARG:HB3	2.02	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:1329:LEU:HB2	3:B:1338:LEU:CD1	2.52	0.40
3:B:1190:ASP:C	3:B:1192:SER:N	2.74	0.40
3:B:1258:ILE:HD11	3:B:1283:ARG:CZ	2.51	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

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	376/403 (93%)	336 (89%)	36 (10%)	4 (1%)	17	25
3	B	373/403 (93%)	336 (90%)	31 (8%)	6 (2%)	12	16
All	All	749/806 (93%)	672 (90%)	67 (9%)	10 (1%)	15	21

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 (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	347/368 (94%)	338 (97%)	9 (3%)	54	74
3	B	344/368 (94%)	332 (96%)	12 (4%)	43	64
All	All	691/736 (94%)	670 (97%)	21 (3%)	48	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1012	GLU
3	A	1116	HIS
3	A	1123	ARG

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Mol	Chain	Res	Type
3	A	1205	THR
3	A	1213	GLN
3	A	1262	ASN
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	1262	ASN
3	B	1291	TYR
3	B	1292	GLN
3	B	1295	LYS
3	B	1340	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1023	GLN
3	A	1089	GLN
3	A	1094	ASN
3	A	1102	ASN
3	A	1113	GLN
3	A	1175	GLN
3	A	1199	ASN
3	A	1213	GLN
3	A	1218	HIS
3	A	1262	ASN
3	A	1267	GLN
3	A	1270	GLN
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	1052	HIS

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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	1199	ASN
3	B	1213	GLN
3	B	1218	HIS
3	B	1255	ASN
3	B	1267	GLN
3	B	1270	GLN
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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
5	UDP	A	2001	-	18,26,26	1.06	1 (5%)	26,40,40	2.77	3 (11%)
4	NCO	A	2002	-	6,6,6	1.14	0	0,15,15	0.00	-
4	NCO	A	2003	-	6,6,6	1.35	0	0,15,15	0.00	-
4	NCO	A	2004	-	6,6,6	1.28	0	0,15,15	0.00	-
5	UDP	B	3001	-	18,26,26	1.07	2 (11%)	26,40,40	2.71	3 (11%)
4	NCO	B	3002	-	6,6,6	1.22	0	0,15,15	0.00	-
4	NCO	B	3003	-	6,6,6	1.29	0	0,15,15	0.00	-
4	NCO	B	3004	-	6,6,6	1.30	0	0,15,15	0.00	-
4	NCO	D	1003	-	6,6,6	1.39	0	0,15,15	0.00	-

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	A	2001	-	-	0/12/32/32	0/2/2/2
4	NCO	A	2002	-	-	0/0/0/0	0/0/0/0
4	NCO	A	2003	-	-	0/0/0/0	0/0/0/0
4	NCO	A	2004	-	-	0/0/0/0	0/0/0/0
5	UDP	B	3001	-	-	0/12/32/32	0/2/2/2
4	NCO	B	3002	-	-	0/0/0/0	0/0/0/0
4	NCO	B	3003	-	-	0/0/0/0	0/0/0/0
4	NCO	B	3004	-	-	0/0/0/0	0/0/0/0
4	NCO	D	1003	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3001	UDP	C6-C5	-2.02	1.33	1.38
5	A	2001	UDP	C4-N3	2.67	1.38	1.33
5	B	3001	UDP	C4-N3	2.67	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	UDP	C5-C4-N3	-3.40	114.39	123.12
5	B	3001	UDP	C5-C4-N3	-3.29	114.68	123.12
5	B	3001	UDP	O2B-PB-O1B	2.68	119.22	110.58
5	A	2001	UDP	O2B-PB-O1B	2.76	119.46	110.58
5	B	3001	UDP	C4-N3-C2	12.76	126.78	114.14
5	A	2001	UDP	C4-N3-C2	13.13	127.15	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	12/12 (100%)	0.22	0	100	100	38, 62, 71, 72	0
2	D	12/12 (100%)	-0.18	0	100	100	50, 60, 74, 74	0
3	A	380/403 (94%)	0.34	28 (7%)	17	17	34, 60, 87, 100	0
3	B	377/403 (93%)	0.39	26 (6%)	20	19	39, 65, 84, 97	0
All	All	781/830 (94%)	0.36	54 (6%)	20	19	34, 62, 86, 100	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1143	ASN	7.3
3	A	1145	ASP	5.5
3	B	1300	TYR	4.5
3	A	1296	LEU	4.0
3	B	1132	ARG	3.6
3	B	1400	LYS	3.5
3	A	1298	GLN	3.2
3	B	998	MET	3.2
3	B	1256	ARG	3.1
3	A	1300	TYR	3.1
3	B	1367	ARG	3.0
3	B	1169	PRO	3.0
3	A	1361	LYS	3.0
3	B	1301	LEU	3.0
3	B	1342	ASP	2.9
3	B	1368	ALA	2.9
3	A	1193	GLU	2.8
3	B	1298	GLN	2.8
3	B	1299	LYS	2.8
3	A	1256	ARG	2.8
3	B	1054	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	1142	ASP	2.7
3	A	1118	VAL	2.7
3	A	1079	ILE	2.7
3	B	1382	TYR	2.7
3	A	1119	LEU	2.6
3	A	1354	GLU	2.6
3	B	1037	VAL	2.6
3	B	1338	LEU	2.6
3	A	1132	ARG	2.5
3	B	1334	ASP	2.5
3	A	1172	TYR	2.5
3	A	1190	ASP	2.4
3	A	1121	LEU	2.4
3	B	1297	ASN	2.4
3	B	1089	GLN	2.4
3	A	1234	LEU	2.4
3	A	1301	LEU	2.4
3	A	1350	GLU	2.4
3	A	1101	ASP	2.3
3	A	1400	LYS	2.3
3	A	1260	LYS	2.3
3	A	1366	ASP	2.2
3	A	1142	ASP	2.2
3	A	1262	ASN	2.2
3	B	1039	ALA	2.1
3	A	1219	GLU	2.1
3	B	1304	SER	2.1
3	B	1258	ILE	2.1
3	B	1170	THR	2.1
3	A	1342	ASP	2.1
3	B	1141	SER	2.0
3	B	1005	ILE	2.0
3	A	1351	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

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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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	NCO	B	3002	7/7	0.93	0.22	3.63	78,79,79,79	0
4	NCO	A	2002	7/7	0.96	0.19	0.32	63,63,65,66	0
4	NCO	A	2004	7/7	0.93	0.19	0.19	92,92,93,93	7
4	NCO	B	3003	7/7	0.94	0.17	-0.47	98,99,99,99	0
4	NCO	D	1003	7/7	0.97	0.14	-0.49	88,89,89,91	0
4	NCO	A	2003	7/7	0.96	0.15	-0.51	81,82,84,84	0
5	UDP	B	3001	25/25	0.98	0.10	-1.24	37,43,47,49	0
5	UDP	A	2001	25/25	0.98	0.08	-1.40	38,44,46,48	0
4	NCO	B	3004	7/7	0.92	0.20	-	71,71,71,73	7

6.5 Other polymers (i)

There are no such residues in this entry.