



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:09 am BST

PDB ID : 2OH2
Title : Ternary Complex of Human DNA Polymerase
Authors : Lone, S.; Townson, S.A.; Uljon, S.N.; Prakash, S.; Prakash, L.; Aggarwal, A.K.
Deposited on : 2007-01-09
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

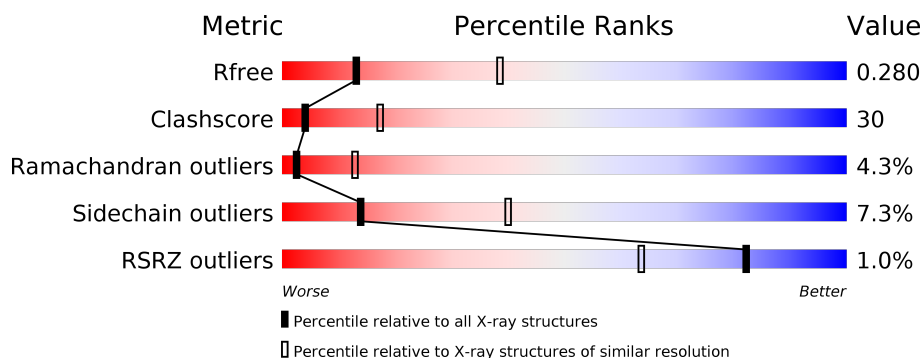
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	P	13	<div> <div></div> <div>85% 8% 8%</div> </div>
1	S	13	<div> <div></div> <div>69% 8% 23%</div> </div>
2	Q	18	<div> <div></div> <div>28% 39% 6% 28%</div> </div>
2	T	18	<div> <div></div> <div>39% 44% 17%</div> </div>
3	A	508	<div> <div>%</div> <div>46% 33% 5% 16%</div> </div>
3	B	508	<div> <div>%</div> <div>46% 35% 6% 13%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7583 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*GP*G*GP*GP*AP*AP*GP*GP*AP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	10	Total	C	N	O	P	0	0	0
			204	97	44	54	9			
1	P	12	Total	C	N	O	P	0	0	0
			248	117	54	66	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	13	Total	C	N	O	P	0	0	0
			258	124	44	78	12			
2	T	15	Total	C	N	O	P	0	0	0
			296	142	50	90	14			

- Molecule 3 is a protein called DNA polymerase kappa.

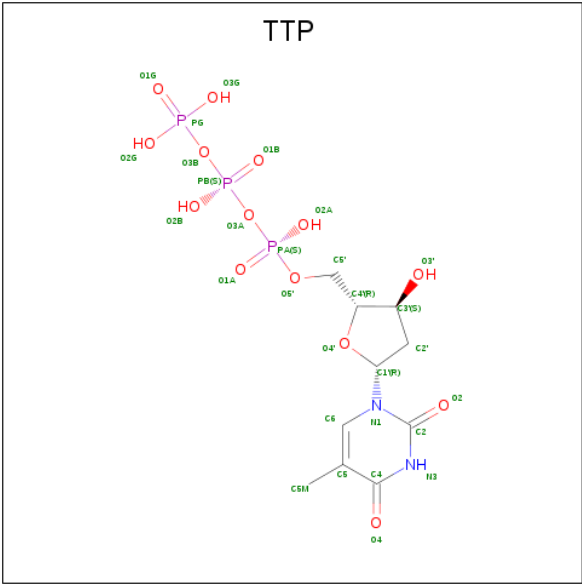
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	428	Total	C	N	O	S	0	0	0
			3225	2044	566	595	20			
3	B	440	Total	C	N	O	S	0	0	0
			3271	2069	572	610	20			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:

C₁₀H₁₇N₂O₁₄P₃).

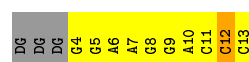


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
5	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total	O	0	0
			1	1		
6	Q	1	Total	O	0	0
			1	1		
6	P	1	Total	O	0	0
			1	1		
6	A	9	Total	O	0	0
			9	9		
6	B	9	Total	O	0	0
			9	9		

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



- | | |
|-----|--|
| DG | |
| G2 | |
| G3 | |
| G4 | |
| G5 | |
| A6 | |
| A7 | |
| G8 | |
| G9 | |
| A10 | |
| C11 | |
| C12 | |
| C13 | |

- | | | | | | | | | | | | | | | | |
|----|----|----|----|--|----|----|--|-----|-----|-----|-----|-----|----|----|----|
| DT | DT | C3 | C4 | | G7 | G8 | | C11 | T12 | T13 | C14 | C15 | DC | DC | DC |
|----|----|----|----|--|----|----|--|-----|-----|-----|-----|-----|----|----|----|

- | |
|-----|
| DT |
| DT |
| C3 |
| C4 |
| G7 |
| G8 |
| T9 |
| C10 |
| C11 |
| T12 |
| T13 |
| C14 |
| C17 |
| DC |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|-----|------|-----|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET | GLY | LEU | ASN | ASP | ASN | LYS | ALA | GLY | MET | GLU | GLY | LEU | ASP | K33 | K32 | K34 | K35 | I36 | K37 | K38 | I39 | K45 | I54 | K62 | K63 | I64 | K65 | K66 | K67 | K71 | I74 | T75 | K78 | L79 | K82 | K83 | L84 | K85 | K86 | D87 | K88 | K92 | L93 | K94 | K95 | K98 | L99 | S100 | K105 | L106 | | |
| D107 | M108 | D109 | A110 | F111 | Y112 | A113 | | M117 | | M120 | P121 | E122 | L123 | K124 | D125 | K126 | P127 | I128 | A129 | V130 | | L136 | S137 | T138 | S139 | I140 | Y141 | H142 | A143 | R144 | G147 | L156 | A157 | K158 | R159 | I165 | L166 | V167 | F171 | Y174 | V177 | S178 | K179 | E180 | V181 | K182 | E183 | L184 | L185 | L188 | D189 | L190 |

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	116.15Å 152.47Å 217.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.05 38.95 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.05) 93.6 (38.95-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.294 0.223 , 0.280	Depositor DCC
R_{free} test set	3531 reflections (8.99%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7583	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: MG, TTP

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	P	0.48	0/280	0.76	0/431
1	S	0.56	0/230	0.80	0/353
2	Q	0.60	0/287	0.84	0/440
2	T	0.40	0/329	0.79	0/504
3	A	0.42	0/3276	0.69	1/4436 (0.0%)
3	B	0.37	0/3324	0.63	0/4509
All	All	0.42	0/7726	0.68	1/10673 (0.0%)

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	P	0	1
1	S	0	1
2	Q	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	192	PHE	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	12	DC	Sidechain
2	Q	8	DG	Sidechain
1	S	12	DC	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	P	248	0	132	22	0
1	S	204	0	110	18	0
2	Q	258	0	148	13	0
2	T	296	0	170	10	0
3	A	3225	0	3159	178	0
3	B	3271	0	3121	210	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	29	0	10	2	0
5	B	29	0	10	3	0
6	A	9	0	0	1	0
6	B	9	0	0	2	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	S	1	0	0	0	0
All	All	7583	0	6860	431	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 30.

All (431) 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)
2:Q:12:DT:H2''	2:Q:13:DT:H5'	1.26	1.16
3:B:455:THR:HG23	3:B:473:THR:HG22	1.32	1.08
3:B:457:THR:HG23	3:B:471:ALA:HB2	1.44	0.98
3:A:128:ILE:HG12	3:A:140:ASN:HD22	1.28	0.96
3:A:141:TYR:HA	3:A:144:ARG:HD3	1.53	0.91
3:A:478:VAL:HG12	3:A:479:SER:H	1.35	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:180:GLU:HG3	3:A:304:LYS:HE2	1.55	0.89
3:A:203:ASN:ND2	3:A:205:THR:HG22	1.87	0.88
3:A:461:LYS:HB3	3:A:508:LEU:HB3	1.55	0.88
3:B:298:ARG:HH21	3:B:330:ASN:ND2	1.76	0.83
3:B:64:ILE:HG12	3:B:364:MET:HG2	1.63	0.81
3:A:500:PHE:HB2	3:A:501:PRO:HD3	1.61	0.81
3:A:445:ASP:HA	3:A:448:LYS:HE2	1.63	0.81
3:A:128:ILE:HG12	3:A:140:ASN:ND2	1.97	0.80
3:B:149:ARG:H	3:B:152:MET:HE3	1.48	0.79
3:B:141:TYR:HA	3:B:144:ARG:HD3	1.65	0.78
1:S:12:DC:H2''	1:S:13:DC:H5'	1.63	0.78
2:Q:12:DT:OP1	2:Q:12:DT:H4'	1.84	0.78
3:A:62:GLN:HE21	3:A:66:ASN:HD21	1.31	0.77
3:B:141:TYR:HE1	3:B:329:PRO:HA	1.48	0.77
3:B:214:TRP:HB2	3:B:219:ARG:HD3	1.65	0.77
3:A:420:ARG:O	3:A:508:LEU:HD22	1.85	0.77
3:A:478:VAL:HG12	3:A:479:SER:N	1.99	0.76
3:B:500:PHE:HB2	3:B:501:PRO:HD3	1.65	0.76
1:S:11:DC:OP1	3:A:361:THR:HG23	1.85	0.76
1:P:6:DA:OP1	3:B:472:SER:HA	1.85	0.76
3:A:192:PHE:O	3:A:193:MET:HB3	1.84	0.76
3:A:500:PHE:HB2	3:A:501:PRO:CD	2.17	0.75
3:A:177:VAL:O	3:A:181:VAL:HG12	1.86	0.75
3:B:108:MET:HB2	3:B:198:ASP:HB2	1.68	0.74
3:A:98:ASN:ND2	3:A:100:SER:H	1.85	0.74
1:P:7:DA:H2''	1:P:8:DG:H5'	1.70	0.74
3:A:86:VAL:HG11	3:A:380:ARG:HB2	1.69	0.74
3:B:298:ARG:HH21	3:B:330:ASN:HD21	1.35	0.74
3:A:128:ILE:H	3:A:140:ASN:ND2	1.86	0.73
3:A:480:THR:OG1	3:A:483:GLU:HG3	1.88	0.72
3:B:316:ASN:HD22	3:B:318:MET:H	1.38	0.72
3:B:455:THR:CG2	3:B:473:THR:HG22	2.15	0.72
1:P:11:DC:OP1	3:B:361:THR:HG22	1.91	0.71
3:A:508:LEU:HD13	3:A:509:MET:N	2.05	0.71
3:B:141:TYR:OH	3:B:328:LYS:HG3	1.90	0.71
3:B:317:THR:HG21	3:B:404:SER:HB2	1.71	0.70
3:B:500:PHE:HB2	3:B:501:PRO:CD	2.22	0.70
3:B:208:LEU:HD21	3:B:293:VAL:HG11	1.74	0.69
1:P:3:DG:H2''	1:P:4:DG:C8	2.27	0.69
2:Q:4:DC:H5'	3:A:507:ARG:HH22	1.56	0.69
3:B:478:VAL:HG13	3:B:483:GLU:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:95:GLN:NE2	3:B:84:LEU:HB2	2.07	0.69
1:S:4:DG:H2''	1:S:5:DG:O5'	1.91	0.69
3:B:155:PHE:CE1	3:B:156:ILE:HG13	2.27	0.69
3:A:366:LYS:HG3	3:A:371:ILE:HD11	1.74	0.69
3:B:148:VAL:HG13	3:B:157:ALA:HB1	1.74	0.69
1:P:8:DG:H1'	1:P:9:DG:H5'	1.74	0.68
3:A:212:GLN:HA	3:A:288:THR:HG21	1.76	0.67
3:B:137:SER:O	3:B:138:THR:HG23	1.93	0.67
3:A:394:TYR:O	3:A:398:ILE:HD13	1.95	0.67
3:B:478:VAL:HG13	3:B:483:GLU:CB	2.24	0.67
3:B:177:VAL:HG11	3:B:307:LEU:HD12	1.75	0.67
3:B:50:TYR:CE2	3:B:54:LEU:HD21	2.30	0.67
3:A:317:THR:HG22	3:A:318:MET:N	2.09	0.67
3:B:317:THR:HG22	3:B:404:SER:H	1.59	0.67
3:B:75:THR:OG1	3:B:78:GLN:HG3	1.94	0.67
3:B:181:VAL:HG23	3:B:301:ILE:HG12	1.76	0.66
1:S:11:DC:P	3:A:358:GLY:HA3	2.34	0.66
3:B:460:LEU:HD22	3:B:506:LEU:HD21	1.77	0.66
3:A:178:SER:O	3:A:182:LYS:HG3	1.95	0.66
3:B:201:TYR:C	3:B:202:LEU:HD12	2.15	0.66
3:B:140:ASN:ND2	3:B:142:HIS:HB3	2.11	0.66
2:Q:7:DG:H2''	2:Q:8:DG:H5'	1.78	0.66
2:Q:12:DT:H2''	2:Q:13:DT:C5'	2.15	0.66
1:P:10:DA:H2''	1:P:11:DC:OP2	1.96	0.66
1:P:6:DA:OP2	3:B:473:THR:HG23	1.96	0.66
2:T:12:DT:H2''	2:T:13:DT:H71	1.77	0.66
3:A:460:LEU:HD22	3:A:506:LEU:HD21	1.78	0.65
3:A:83:GLN:NE2	3:A:381:ALA:HB2	2.11	0.65
3:B:98:ASN:ND2	3:B:100:SER:H	1.95	0.65
3:A:108:MET:HB2	3:A:198:ASP:HB2	1.79	0.65
3:A:98:ASN:HD22	3:A:99:LEU:N	1.94	0.65
3:A:128:ILE:H	3:A:140:ASN:HD21	1.43	0.65
3:A:463:VAL:HG23	3:A:505:ARG:O	1.97	0.65
1:P:10:DA:H1'	1:P:11:DC:H5'	1.78	0.64
3:A:83:GLN:HE21	3:A:381:ALA:HB2	1.63	0.64
3:B:446:LEU:HD21	3:B:513:ILE:HD13	1.80	0.64
1:S:10:DA:H2''	1:S:11:DC:H5'	1.78	0.64
3:A:84:LEU:HD11	3:A:88:ARG:NH2	2.13	0.63
3:A:98:ASN:C	3:A:98:ASN:HD22	2.02	0.63
3:A:453:GLY:H	3:A:513:ILE:HD11	1.63	0.63
3:A:472:SER:HB2	3:A:491:LEU:HD21	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:318:MET:HE3	3:B:354:VAL:HG22	1.80	0.63
3:B:317:THR:CG2	3:B:404:SER:HB2	2.29	0.63
3:A:398:ILE:N	3:A:398:ILE:HD12	2.14	0.62
3:B:81:LYS:O	3:B:85:GLN:HG3	1.99	0.62
1:S:8:DG:H1'	1:S:9:DG:H5''	1.80	0.62
3:B:177:VAL:O	3:B:181:VAL:HG12	2.00	0.62
3:B:419:GLU:HB2	3:B:508:LEU:HD21	1.82	0.61
1:P:11:DC:H2''	1:P:12:DC:OP2	2.00	0.61
1:S:11:DC:O5'	3:A:358:GLY:HA3	2.00	0.61
3:A:434:LEU:O	3:A:438:LEU:HG	1.99	0.61
3:B:141:TYR:CE1	3:B:329:PRO:HA	2.35	0.61
3:B:351:ILE:HD11	3:B:376:LEU:HD22	1.82	0.61
3:B:508:LEU:HD22	3:B:509:MET:N	2.15	0.61
3:A:458:ILE:HG12	3:A:459:LYS:N	2.15	0.61
3:A:480:THR:HG23	3:A:483:GLU:OE1	2.00	0.61
3:A:138:THR:HG21	5:A:873:TTP:O1B	2.01	0.61
3:A:36:ILE:HD13	3:A:147:GLY:HA3	1.83	0.61
3:B:149:ARG:H	3:B:152:MET:CE	2.14	0.61
3:B:119:ASP:OD2	3:B:173:LYS:HD2	2.01	0.60
3:B:328:LYS:HE2	3:B:328:LYS:HA	1.82	0.60
3:A:504:LEU:HB3	3:A:506:LEU:HD13	1.81	0.60
1:S:6:DA:H2''	1:S:7:DA:OP2	2.01	0.60
3:A:120:ASN:HD21	3:A:122:GLU:HG2	1.67	0.60
3:A:421:THR:OG1	3:A:508:LEU:HD23	2.01	0.60
3:B:422:PHE:HD1	3:B:423:SER:O	1.85	0.60
3:B:71:LYS:O	3:B:74:ILE:HG13	2.02	0.60
3:B:115:VAL:C	3:B:117:MET:H	2.06	0.59
3:B:380:ARG:HH11	3:B:380:ARG:HG2	1.68	0.59
3:B:472:SER:HB2	3:B:491:LEU:HD21	1.84	0.59
3:A:478:VAL:CG1	3:A:479:SER:H	2.10	0.59
3:B:483:GLU:O	3:B:486:ALA:HB3	2.02	0.59
3:A:203:ASN:ND2	3:A:205:THR:CG2	2.63	0.59
3:B:299:PHE:O	3:B:302:GLU:HB3	2.03	0.59
3:A:500:PHE:CB	3:A:501:PRO:HD3	2.32	0.59
3:A:391:SER:O	3:A:394:TYR:HB3	2.03	0.58
3:B:215:PRO:HG2	3:B:218:LYS:HB2	1.84	0.58
3:A:452:LYS:HB3	3:A:477:VAL:HG12	1.86	0.58
3:B:476:SER:O	3:B:477:VAL:HB	2.04	0.58
2:Q:12:DT:C2'	2:Q:13:DT:H5'	2.18	0.58
3:B:173:LYS:O	3:B:176:ALA:HB3	2.04	0.58
3:A:461:LYS:HD3	3:A:467:VAL:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:317:THR:HG22	3:B:404:SER:N	2.19	0.58
1:S:6:DA:P	3:A:473:THR:HG22	2.44	0.57
3:B:148:VAL:HG13	3:B:157:ALA:CB	2.33	0.57
3:A:75:THR:OG1	3:A:78:GLN:HG3	2.04	0.57
3:A:212:GLN:HA	3:A:288:THR:CG2	2.33	0.57
2:Q:4:DC:H5'	3:A:507:ARG:NH2	2.19	0.57
3:B:461:LYS:HB3	3:B:508:LEU:HB3	1.85	0.57
3:B:165:ILE:HD12	3:B:165:ILE:N	2.19	0.57
3:A:308:THR:HB	3:A:330:ASN:ND2	2.19	0.57
3:B:22:ASN:O	3:B:23:ASP:CB	2.53	0.57
3:A:208:LEU:HD11	3:A:290:ALA:HB2	1.85	0.57
3:B:156:ILE:O	3:B:160:LEU:HD13	2.05	0.56
3:B:298:ARG:NH2	3:B:330:ASN:ND2	2.52	0.56
3:A:461:LYS:HD3	3:A:467:VAL:CG2	2.36	0.56
1:P:2:DG:H2''	1:P:3:DG:O5'	2.06	0.56
3:B:287:GLY:HA3	3:B:292:GLU:HG3	1.88	0.55
3:A:478:VAL:CG1	3:A:479:SER:N	2.70	0.55
3:A:95:GLN:HE22	3:B:84:LEU:HB2	1.72	0.55
3:B:210:GLU:O	3:B:212:GLN:N	2.39	0.55
3:A:221:TYR:HE1	3:A:296:GLU:OE2	1.90	0.55
3:B:453:GLY:H	3:B:513:ILE:HD11	1.71	0.55
3:A:171:PHE:HA	3:A:174:TYR:CD1	2.41	0.55
3:A:356:GLY:HA3	3:A:394:TYR:OH	2.07	0.55
3:A:504:LEU:HB3	3:A:506:LEU:CD1	2.37	0.55
3:B:192:PHE:O	3:B:192:PHE:CG	2.60	0.54
2:Q:7:DG:H2''	2:Q:8:DG:C5'	2.38	0.54
3:B:118:ARG:O	3:B:121:PRO:HD3	2.08	0.54
3:A:62:GLN:NE2	3:A:66:ASN:HD21	2.03	0.54
3:B:120:ASN:N	3:B:121:PRO:HD3	2.23	0.54
3:B:62:GLN:HE21	3:B:66:ASN:HD21	1.55	0.54
3:B:442:LEU:HD21	3:B:513:ILE:HG22	1.89	0.54
3:A:289:SER:O	3:A:293:VAL:HG12	2.07	0.54
3:A:74:ILE:HA	3:A:78:GLN:OE1	2.08	0.54
1:P:5:DG:H1'	1:P:6:DA:H5'	1.90	0.53
3:A:316:ASN:HB2	3:A:404:SER:O	2.08	0.53
3:A:35:LYS:O	3:A:39:ILE:HG13	2.08	0.53
1:P:7:DA:C2'	1:P:8:DG:H5'	2.37	0.53
3:B:89:PHE:CE2	3:B:93:LEU:HD11	2.44	0.53
3:B:460:LEU:HD22	3:B:506:LEU:CD2	2.38	0.53
3:B:461:LYS:HB2	3:B:508:LEU:HD12	1.90	0.53
3:A:326:LYS:NZ	6:A:874:HOH:O	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:128:ILE:N	3:A:140:ASN:HD21	2.05	0.52
3:B:204:ILE:O	3:B:204:ILE:HG13	2.10	0.52
3:B:339:ARG:HG2	3:B:339:ARG:HH11	1.74	0.52
3:B:98:ASN:C	3:B:98:ASN:ND2	2.63	0.52
3:A:290:ALA:HA	3:A:293:VAL:CG1	2.39	0.52
3:A:338:ASN:ND2	3:A:341:ALA:H	2.06	0.52
3:A:500:PHE:CB	3:A:501:PRO:CD	2.86	0.52
3:B:508:LEU:C	3:B:508:LEU:HD13	2.30	0.52
3:A:129:ALA:HA	3:A:139:SER:HA	1.92	0.52
3:A:458:ILE:HD11	3:A:460:LEU:HD21	1.91	0.52
3:B:98:ASN:HD22	3:B:98:ASN:C	2.12	0.52
3:A:476:SER:O	3:A:477:VAL:HB	2.10	0.52
3:B:148:VAL:CG1	3:B:157:ALA:HB1	2.40	0.52
3:B:500:PHE:CB	3:B:501:PRO:CD	2.87	0.52
3:B:446:LEU:CD2	3:B:513:ILE:HD13	2.40	0.52
3:A:199:GLU:OE2	3:A:321:LYS:NZ	2.43	0.51
3:B:313:ILE:O	3:B:334:GLN:HA	2.10	0.51
2:Q:11:DC:H2''	2:Q:12:DT:O5'	2.09	0.51
3:B:86:VAL:HG11	3:B:380:ARG:HB2	1.92	0.51
3:B:288:THR:O	3:B:288:THR:HG22	2.10	0.51
3:B:294:VAL:HG12	3:B:332:GLN:OE1	2.10	0.51
3:B:350:PRO:HB2	3:B:353:LYS:HG2	1.92	0.51
3:A:98:ASN:C	3:A:98:ASN:ND2	2.63	0.51
3:B:305:THR:O	3:B:306:THR:CB	2.58	0.51
3:B:203:ASN:HB2	3:B:407:LEU:HD12	1.93	0.51
3:B:126:LYS:O	3:B:128:ILE:HG23	2.10	0.51
3:A:514:SER:O	3:A:515:SER:HB2	2.10	0.51
3:B:305:THR:O	3:B:306:THR:HB	2.11	0.51
3:B:480:THR:OG1	3:B:483:GLU:HG3	2.10	0.51
3:B:99:LEU:HD12	3:B:99:LEU:N	2.26	0.51
3:A:201:TYR:O	3:A:202:LEU:HD12	2.10	0.50
3:B:500:PHE:CB	3:B:501:PRO:HD3	2.36	0.50
3:B:140:ASN:HD21	3:B:142:HIS:HB3	1.76	0.50
3:B:218:LYS:C	3:B:220:ARG:H	2.14	0.50
3:B:144:ARG:NH2	5:B:874:TTP:O1G	2.44	0.50
3:B:192:PHE:O	3:B:409:ARG:NH1	2.45	0.50
3:B:477:VAL:HG13	3:B:477:VAL:O	2.10	0.50
3:A:156:ILE:O	3:A:159:ARG:HB2	2.10	0.50
3:B:177:VAL:HG11	3:B:307:LEU:CD1	2.40	0.50
3:B:389:GLU:O	3:B:393:HIS:HB2	2.12	0.50
3:B:434:LEU:O	3:B:434:LEU:HD13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:13:DC:C6	1:S:13:DC:H5'	2.46	0.50
3:B:434:LEU:HD12	3:B:509:MET:SD	2.51	0.50
3:B:44:THR:HG22	3:B:50:TYR:HB2	1.93	0.50
3:A:366:LYS:HG3	3:A:371:ILE:CD1	2.41	0.50
1:P:10:DA:H1'	1:P:11:DC:C5'	2.41	0.50
1:P:4:DG:C5	1:P:5:DG:C6	2.99	0.50
2:T:9:DT:H2''	2:T:10:DC:H5'	1.94	0.50
3:B:105:HIS:O	3:B:311:ALA:HA	2.12	0.50
3:A:442:LEU:O	3:A:446:LEU:HB2	2.12	0.49
3:A:318:MET:CE	3:A:319:LEU:HD23	2.42	0.49
3:B:208:LEU:C	3:B:210:GLU:N	2.66	0.49
3:B:115:VAL:C	3:B:117:MET:N	2.65	0.49
3:B:329:PRO:O	3:B:330:ASN:HB3	2.12	0.49
3:A:452:LYS:HB3	3:A:477:VAL:CG1	2.42	0.49
3:B:127:PRO:HG3	3:B:142:HIS:CD2	2.47	0.49
3:B:212:GLN:HG3	3:B:213:ASN:OD1	2.13	0.49
3:A:478:VAL:HG13	3:A:483:GLU:HB3	1.94	0.49
3:B:141:TYR:OH	3:B:328:LYS:CG	2.59	0.49
3:B:120:ASN:O	3:B:122:GLU:N	2.46	0.49
3:B:184:ILE:HD11	3:B:304:LYS:HD3	1.95	0.49
3:A:379:GLN:NE2	3:B:340:GLN:NE2	2.60	0.48
3:A:185:LEU:HD13	3:A:202:LEU:HD11	1.95	0.48
3:A:398:ILE:N	3:A:398:ILE:CD1	2.75	0.48
2:Q:7:DG:H1'	2:Q:8:DG:H5''	1.95	0.48
3:A:483:GLU:O	3:A:486:ALA:HB3	2.13	0.48
3:B:328:LYS:O	3:B:330:ASN:N	2.40	0.48
3:B:482:GLU:CD	3:B:482:GLU:H	2.17	0.48
3:B:346:ILE:HA	3:B:346:ILE:HD12	1.73	0.48
3:B:458:ILE:HG12	3:B:459:LYS:N	2.27	0.48
3:A:74:ILE:HG21	3:A:385:LEU:HD13	1.96	0.48
3:A:379:GLN:NE2	3:B:340:GLN:HE21	2.11	0.48
3:B:201:TYR:O	3:B:202:LEU:HD12	2.13	0.48
3:A:305:THR:O	3:A:306:THR:CB	2.62	0.48
3:B:111:PHE:CD2	3:B:198:ASP:HB3	2.49	0.48
3:B:158:LYS:C	3:B:160:LEU:H	2.17	0.48
3:B:62:GLN:HE21	3:B:66:ASN:ND2	2.11	0.48
3:A:106:ILE:HD11	3:A:297:ILE:HG21	1.95	0.47
3:B:143:ALA:O	3:B:148:VAL:HB	2.14	0.47
3:B:478:VAL:HG12	3:B:479:SER:N	2.29	0.47
3:B:138:THR:HG23	5:B:874:TTP:H2'2	1.96	0.47
3:A:192:PHE:HD1	3:A:193:MET:N	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:TYR:C	3:A:202:LEU:HD12	2.34	0.47
3:A:128:ILE:N	3:A:140:ASN:ND2	2.58	0.47
3:B:118:ARG:NH1	3:B:305:THR:O	2.46	0.47
3:B:327:ASN:OD1	3:B:332:GLN:O	2.33	0.47
3:B:335:ILE:O	3:B:336:LEU:C	2.53	0.47
3:B:208:LEU:HD11	3:B:290:ALA:HB2	1.96	0.47
2:Q:14:DC:H2''	2:Q:15:DC:O5'	2.15	0.47
3:A:110:ALA:HA	5:A:873:TTP:O1B	2.15	0.47
3:B:470:ARG:HG3	3:B:495:GLU:OE2	2.14	0.47
3:B:380:ARG:NH1	3:B:380:ARG:HG2	2.30	0.47
3:B:478:VAL:HG13	3:B:483:GLU:HB3	1.94	0.47
1:P:5:DG:H2''	1:P:6:DA:OP2	2.15	0.47
2:T:13:DT:H2''	2:T:14:DC:H5''	1.96	0.47
3:B:297:ILE:O	3:B:301:ILE:HG13	2.15	0.46
3:A:366:LYS:HB2	3:A:366:LYS:HE3	1.79	0.46
3:B:116:GLU:O	3:B:123:LEU:HD11	2.15	0.46
3:B:32:ASP:C	3:B:34:GLU:H	2.19	0.46
3:A:192:PHE:CD1	3:A:193:MET:N	2.83	0.46
3:B:316:ASN:HD22	3:B:318:MET:N	2.10	0.46
3:B:382:LEU:O	3:B:382:LEU:HD22	2.16	0.46
3:A:36:ILE:C	3:A:38:LYS:H	2.19	0.46
3:B:313:ILE:HB	3:B:334:GLN:HB2	1.98	0.46
3:A:120:ASN:C	3:A:120:ASN:HD22	2.18	0.46
3:A:506:LEU:HD23	3:A:509:MET:CE	2.46	0.46
3:A:71:LYS:O	3:A:74:ILE:HG13	2.16	0.46
3:A:83:GLN:HE21	3:A:381:ALA:CB	2.28	0.46
3:A:382:LEU:HD22	3:A:386:LEU:HG	1.98	0.46
3:A:516:PHE:HB3	3:A:517:PRO:CD	2.46	0.46
3:B:180:GLU:O	3:B:183:GLU:HB3	2.15	0.46
3:B:208:LEU:C	3:B:210:GLU:H	2.19	0.46
1:S:11:DC:H2''	1:S:12:DC:OP2	2.15	0.46
3:A:126:LYS:NZ	3:A:165:ILE:HD11	2.31	0.46
3:B:136:LEU:HG	3:B:152:MET:O	2.15	0.46
1:S:13:DC:H6	1:S:13:DC:H5'	1.81	0.46
3:A:462:ASN:HB3	3:A:464:ASN:H	1.81	0.45
3:B:221:TYR:CD1	3:B:221:TYR:N	2.84	0.45
1:P:8:DG:OP2	3:B:469:THR:HG22	2.16	0.45
3:A:120:ASN:C	3:A:120:ASN:ND2	2.69	0.45
3:A:188:TYR:N	3:A:188:TYR:CD1	2.84	0.45
3:B:149:ARG:N	3:B:152:MET:HE3	2.26	0.45
3:A:420:ARG:C	3:A:508:LEU:HD22	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:188:TYR:CD1	3:B:188:TYR:N	2.85	0.45
3:B:293:VAL:O	3:B:297:ILE:HG13	2.15	0.45
3:B:28:MET:HB2	3:B:31:LEU:HD11	1.99	0.45
3:A:64:ILE:O	3:A:67:MET:HB3	2.16	0.45
3:A:84:LEU:HD11	3:A:88:ARG:HH21	1.79	0.45
3:B:146:PHE:HB2	3:B:148:VAL:HG23	1.99	0.45
3:B:71:LYS:NZ	6:B:876:HOH:O	2.49	0.45
3:A:208:LEU:HD21	3:A:290:ALA:HA	1.99	0.45
3:A:377:TYR:HB2	3:A:399:SER:HB2	1.98	0.45
3:A:79:LEU:O	3:A:82:ALA:HB3	2.17	0.45
3:B:135:MET:SD	3:B:151:ALA:HA	2.57	0.45
3:B:141:TYR:HE1	3:B:329:PRO:CA	2.24	0.45
2:T:7:DG:H1'	2:T:8:DG:H5''	1.99	0.45
3:A:98:ASN:HD21	3:A:100:SER:H	1.62	0.45
3:A:346:ILE:O	3:A:373:CYS:HB2	2.17	0.45
3:B:181:VAL:O	3:B:185:LEU:HG	2.17	0.45
3:B:462:ASN:O	3:B:465:PHE:N	2.45	0.45
3:B:138:THR:HG21	5:B:874:TTP:O1B	2.17	0.45
3:B:181:VAL:C	3:B:183:GLU:H	2.21	0.45
3:B:288:THR:N	6:B:879:HOH:O	2.35	0.45
3:B:94:GLU:OE2	3:B:339:ARG:NH2	2.50	0.45
1:P:6:DA:P	3:B:473:THR:HG23	2.57	0.45
3:A:92:GLU:O	3:A:93:LEU:C	2.54	0.45
3:B:210:GLU:C	3:B:212:GLN:H	2.20	0.45
3:B:463:VAL:HG12	3:B:463:VAL:O	2.16	0.45
2:Q:12:DT:C4'	2:Q:12:DT:OP1	2.59	0.44
3:B:101:ASN:HA	3:B:205:THR:OG1	2.16	0.44
3:A:398:ILE:CD1	3:A:398:ILE:H	2.30	0.44
2:T:12:DT:C2'	2:T:13:DT:H71	2.45	0.44
3:B:139:SER:O	3:B:144:ARG:HD2	2.18	0.44
3:B:36:ILE:C	3:B:38:LYS:H	2.20	0.44
3:A:206:LYS:HD3	3:A:206:LYS:HA	1.78	0.44
3:A:105:HIS:HD2	3:A:201:TYR:CE1	2.36	0.44
3:A:310:SER:HB2	3:A:328:LYS:HE2	1.98	0.44
3:B:427:LYS:O	3:B:431:GLN:HG3	2.18	0.44
1:P:3:DG:H2''	1:P:4:DG:N7	2.32	0.44
3:A:113:ALA:O	3:A:117:MET:HG3	2.17	0.44
3:B:293:VAL:O	3:B:296:GLU:HB3	2.18	0.44
3:B:94:GLU:CD	3:B:339:ARG:HE	2.21	0.44
1:S:5:DG:H2''	1:S:6:DA:C8	2.53	0.44
3:B:351:ILE:HD12	3:B:351:ILE:HA	1.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:44:THR:O	3:B:45:LYS:C	2.55	0.44
3:A:92:GLU:O	3:A:95:GLN:N	2.49	0.43
3:A:370:ILE:O	3:A:371:ILE:HD13	2.18	0.43
3:B:75:THR:HG23	3:B:78:GLN:OE1	2.19	0.43
1:P:5:DG:H1'	1:P:6:DA:C5'	2.47	0.43
2:T:4:DC:O4'	3:B:153:PRO:HG3	2.18	0.43
3:B:115:VAL:O	3:B:117:MET:N	2.51	0.43
3:B:349:LEU:HD12	3:B:350:PRO:HD2	1.99	0.43
1:S:12:DC:H2''	1:S:13:DC:C5'	2.39	0.43
3:A:184:ILE:CD1	3:A:301:ILE:HA	2.48	0.43
3:B:455:THR:HA	3:B:473:THR:HA	2.00	0.43
3:B:50:TYR:CD2	3:B:54:LEU:HD21	2.53	0.43
1:S:7:DA:H1'	1:S:8:DG:H5'	2.00	0.43
3:B:105:HIS:CD2	3:B:201:TYR:CE1	3.07	0.43
3:B:461:LYS:HE3	3:B:507:ARG:HD3	2.00	0.43
3:A:351:ILE:CD1	3:A:376:LEU:HD22	2.49	0.43
3:A:496:ILE:HG12	3:A:504:LEU:HD12	1.99	0.43
3:B:203:ASN:C	3:B:205:THR:H	2.21	0.43
3:B:316:ASN:HB2	3:B:404:SER:O	2.18	0.43
3:B:408:THR:O	3:B:409:ARG:C	2.57	0.43
3:B:49:PHE:O	3:B:53:GLU:HG2	2.18	0.43
1:P:12:DC:H1'	1:P:13:DC:H5'	2.01	0.43
2:Q:12:DT:C6	2:Q:13:DT:H72	2.54	0.43
3:A:128:ILE:CG1	3:A:140:ASN:ND2	2.75	0.43
3:B:181:VAL:C	3:B:183:GLU:N	2.70	0.43
3:B:219:ARG:HB2	3:B:219:ARG:HE	1.69	0.43
3:B:462:ASN:OD1	3:B:468:LYS:NZ	2.51	0.43
3:A:120:ASN:HA	3:A:121:PRO:HD2	1.77	0.43
3:B:453:GLY:N	3:B:513:ILE:HD11	2.34	0.43
3:A:319:LEU:CD1	3:A:342:VAL:HG22	2.49	0.42
3:A:421:THR:HG22	3:A:422:PHE:N	2.34	0.42
3:A:66:ASN:HD22	3:A:66:ASN:N	2.17	0.42
3:B:478:VAL:CG1	3:B:479:SER:N	2.82	0.42
3:B:417:SER:HB3	3:B:512:ARG:CB	2.49	0.42
3:A:351:ILE:HD11	3:A:376:LEU:HD22	2.00	0.42
1:S:6:DA:C2'	3:A:471:ALA:HB3	2.50	0.42
3:A:136:LEU:HD11	3:A:157:ALA:CB	2.50	0.42
3:B:203:ASN:O	3:B:205:THR:N	2.47	0.42
3:B:396:LEU:O	3:B:400:LEU:HG	2.18	0.42
3:A:126:LYS:HB3	3:A:126:LYS:HZ2	1.84	0.42
3:A:506:LEU:CD2	3:A:509:MET:HE2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:168:PRO:HA	3:B:169:PRO:HD3	1.93	0.42
3:A:508:LEU:HD13	3:A:508:LEU:C	2.39	0.42
3:A:98:ASN:HD22	3:A:100:SER:H	1.62	0.42
3:A:282:ASN:N	3:A:282:ASN:HD22	2.16	0.42
3:A:327:ASN:O	3:A:329:PRO:N	2.53	0.42
3:B:147:GLY:O	3:B:152:MET:HE1	2.19	0.42
3:B:98:ASN:HD22	3:B:99:LEU:N	2.17	0.42
3:A:319:LEU:HD11	3:A:342:VAL:HG22	2.02	0.42
3:A:310:SER:OG	3:A:328:LYS:O	2.25	0.42
3:B:110:ALA:O	3:B:111:PHE:C	2.58	0.42
3:B:150:ALA:O	3:B:151:ALA:HB3	2.20	0.42
3:B:328:LYS:HB3	3:B:329:PRO:HD3	2.01	0.42
3:B:89:PHE:HE2	3:B:93:LEU:HD11	1.84	0.42
3:A:473:THR:O	3:A:473:THR:HG23	2.20	0.42
3:B:446:LEU:HD22	3:B:513:ILE:HG21	2.01	0.42
3:A:139:SER:O	3:A:144:ARG:HD2	2.19	0.41
3:A:127:PRO:HB3	3:A:142:HIS:CD2	2.55	0.41
3:A:328:LYS:HE2	3:A:328:LYS:O	2.20	0.41
3:B:30:GLY:O	3:B:31:LEU:HD23	2.19	0.41
3:B:32:ASP:O	3:B:34:GLU:N	2.53	0.41
1:P:12:DC:H2''	1:P:13:DC:H6	1.85	0.41
2:T:8:DG:C8	2:T:9:DT:H72	2.54	0.41
3:A:178:SER:O	3:A:181:VAL:HG13	2.19	0.41
3:A:317:THR:HB	3:A:404:SER:HB2	2.02	0.41
3:B:208:LEU:O	3:B:210:GLU:N	2.53	0.41
1:S:12:DC:C2'	1:S:13:DC:H5'	2.44	0.41
2:T:12:DT:H2''	2:T:13:DT:C7	2.47	0.41
3:A:305:THR:C	3:A:306:THR:OG1	2.56	0.41
3:A:318:MET:HE1	3:A:319:LEU:HD23	2.02	0.41
3:B:476:SER:O	3:B:477:VAL:CB	2.66	0.41
2:T:13:DT:C2'	2:T:14:DC:H5''	2.50	0.41
3:A:130:VAL:HA	3:A:167:VAL:O	2.20	0.41
3:A:106:ILE:CD1	3:A:297:ILE:HG21	2.51	0.41
1:P:11:DC:OP1	3:B:361:THR:CG2	2.66	0.41
1:S:11:DC:P	3:A:360:VAL:HB	2.61	0.41
3:A:221:TYR:CE1	3:A:296:GLU:OE2	2.73	0.41
3:A:452:LYS:HG2	3:A:479:SER:HB2	2.02	0.41
3:A:311:ALA:O	3:A:332:GLN:HA	2.21	0.41
3:A:334:GLN:HG2	3:A:335:ILE:N	2.35	0.41
3:A:334:GLN:CG	3:A:335:ILE:N	2.83	0.41
3:A:286:PHE:CD1	3:A:296:GLU:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:346:ILE:HD12	3:A:346:ILE:HA	1.88	0.41
3:A:36:ILE:C	3:A:38:LYS:N	2.73	0.41
2:T:4:DC:C4	3:B:49:PHE:CE2	3.09	0.41
3:A:299:PHE:CE2	3:A:303:GLN:HG3	2.55	0.41
3:B:129:ALA:HA	3:B:139:SER:HA	2.01	0.41
3:A:421:THR:CG2	3:A:422:PHE:N	2.83	0.40
3:A:514:SER:O	3:A:515:SER:CB	2.69	0.40
3:B:207:HIS:CE1	3:B:211:ARG:HH11	2.38	0.40
3:B:377:TYR:CE1	3:B:400:LEU:HD21	2.55	0.40
3:A:189:ASP:HA	3:A:190:PRO:HD2	1.92	0.40
3:A:219:ARG:O	3:A:285:VAL:HA	2.22	0.40
3:A:120:ASN:HD21	3:A:122:GLU:CG	2.34	0.40
3:A:297:ILE:O	3:A:301:ILE:HG13	2.20	0.40
3:B:316:ASN:HD21	3:B:318:MET:HB3	1.86	0.40
3:B:146:PHE:N	3:B:146:PHE:CD1	2.90	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	424/508 (84%)	364 (86%)	44 (10%)	16 (4%)	3	15
3	B	436/508 (86%)	357 (82%)	58 (13%)	21 (5%)	2	11
All	All	860/1016 (85%)	721 (84%)	102 (12%)	37 (4%)	2	13

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	328	LYS
3	A	500	PHE
3	B	23	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	45	LYS
3	B	111	PHE
3	B	204	ILE
3	B	476	SER
3	B	477	VAL
3	B	500	PHE
3	A	45	LYS
3	A	479	SER
3	B	30	GLY
3	B	148	VAL
3	B	211	ARG
3	B	407	LEU
3	B	411	GLY
3	A	124	LYS
3	A	462	ASN
3	A	472	SER
3	B	33	LYS
3	B	121	PRO
3	B	410	ASP
3	A	477	VAL
3	B	192	PHE
3	B	337	PRO
3	B	472	SER
3	A	111	PHE
3	A	411	GLY
3	B	116	GLU
3	B	328	LYS
3	A	469	THR
3	A	515	SER
3	B	37	ASN
3	A	501	PRO
3	A	337	PRO
3	A	204	ILE
3	A	478	VAL

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	330/454 (73%)	303 (92%)	27 (8%)	11	35
3	B	324/454 (71%)	303 (94%)	21 (6%)	17	44
All	All	654/908 (72%)	606 (93%)	48 (7%)	14	40

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	54	LEU
3	A	87	ASP
3	A	98	ASN
3	A	120	ASN
3	A	138	THR
3	A	181	VAL
3	A	198	ASP
3	A	203	ASN
3	A	293	VAL
3	A	306	THR
3	A	317	THR
3	A	325	ASP
3	A	328	LYS
3	A	343	MET
3	A	346	ILE
3	A	361	THR
3	A	379	GLN
3	A	382	LEU
3	A	390	THR
3	A	393	HIS
3	A	423	SER
3	A	458	ILE
3	A	468	LYS
3	A	469	THR
3	A	487	ILE
3	A	508	LEU
3	A	513	ILE
3	B	29	GLU
3	B	54	LEU
3	B	98	ASN
3	B	99	LEU
3	B	119	ASP
3	B	198	ASP
3	B	203	ASN
3	B	293	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	318	MET
3	B	328	LYS
3	B	330	ASN
3	B	343	MET
3	B	361	THR
3	B	379	GLN
3	B	393	HIS
3	B	421	THR
3	B	454	ARG
3	B	458	ILE
3	B	469	THR
3	B	473	THR
3	B	508	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	66	ASN
3	A	83	GLN
3	A	95	GLN
3	A	98	ASN
3	A	101	ASN
3	A	105	HIS
3	A	120	ASN
3	A	140	ASN
3	A	142	HIS
3	A	163	GLN
3	A	203	ASN
3	A	282	ASN
3	A	316	ASN
3	A	327	ASN
3	A	330	ASN
3	A	338	ASN
3	A	340	GLN
3	A	378	GLN
3	A	379	GLN
3	A	397	HIS
3	A	431	GLN
3	B	66	ASN
3	B	98	ASN
3	B	105	HIS
3	B	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	316	ASN
3	B	327	ASN
3	B	330	ASN
3	B	340	GLN
3	B	378	GLN
3	B	379	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TTP	A	873	4	23,30,30	6.29	6 (26%)	29,47,47	2.37	9 (31%)
5	TTP	B	874	4	23,30,30	6.24	9 (39%)	29,47,47	2.48	10 (34%)

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	TTP	A	873	4	-	6/19/34/34	0/2/2/2
5	TTP	B	874	4	-	4/19/34/34	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	873	TTP	C5M-C5	-28.36	0.97	1.51
5	B	874	TTP	C5M-C5	-28.15	0.97	1.51
5	A	873	TTP	PA-O5'	-5.22	1.38	1.59
5	A	873	TTP	PA-O1A	-5.20	1.32	1.50
5	B	874	TTP	PA-O1A	-4.83	1.33	1.50
5	B	874	TTP	PA-O5'	-4.63	1.40	1.59
5	A	873	TTP	O5'-C5'	4.21	1.61	1.44
5	B	874	TTP	O5'-C5'	4.15	1.60	1.44
5	A	873	TTP	C1'-N1	3.32	1.59	1.49
5	B	874	TTP	O4-C4	3.11	1.32	1.24
5	B	874	TTP	C1'-N1	3.06	1.58	1.49
5	A	873	TTP	O4-C4	2.53	1.30	1.24
5	B	874	TTP	PG-O1G	2.26	1.57	1.50
5	B	874	TTP	C4-N3	2.22	1.36	1.33
5	B	874	TTP	PB-O1B	2.03	1.58	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	873	TTP	C4-N3-C2	6.40	120.54	115.14
5	B	874	TTP	C4-N3-C2	6.32	120.48	115.14
5	B	874	TTP	C2'-C1'-N1	-5.74	101.04	114.27
5	A	873	TTP	C2'-C1'-N1	-5.43	101.75	114.27
5	A	873	TTP	C6-N1-C1'	4.36	129.03	119.24
5	B	874	TTP	C6-N1-C1'	4.31	128.91	119.24
5	B	874	TTP	PB-O3B-PG	-3.98	119.17	132.83
5	B	874	TTP	O2A-PA-O5'	3.66	124.77	107.75
5	A	873	TTP	PB-O3B-PG	-3.48	120.88	132.83
5	B	874	TTP	PB-O3A-PA	-3.43	121.06	132.83
5	A	873	TTP	O2A-PA-O5'	3.25	122.84	107.75
5	B	874	TTP	O5'-C5'-C4'	3.10	119.67	108.99
5	A	873	TTP	PB-O3A-PA	-3.02	122.47	132.83
5	A	873	TTP	O5'-C5'-C4'	2.66	118.16	108.99
5	B	874	TTP	O4'-C4'-C5'	2.49	117.56	109.37
5	B	874	TTP	O2A-PA-O1A	-2.19	101.42	112.24
5	B	874	TTP	O3G-PG-O3B	2.18	111.93	104.64
5	A	873	TTP	O2A-PA-O1A	-2.16	101.54	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	873	TTP	O4'-C4'-C5'	2.04	116.08	109.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

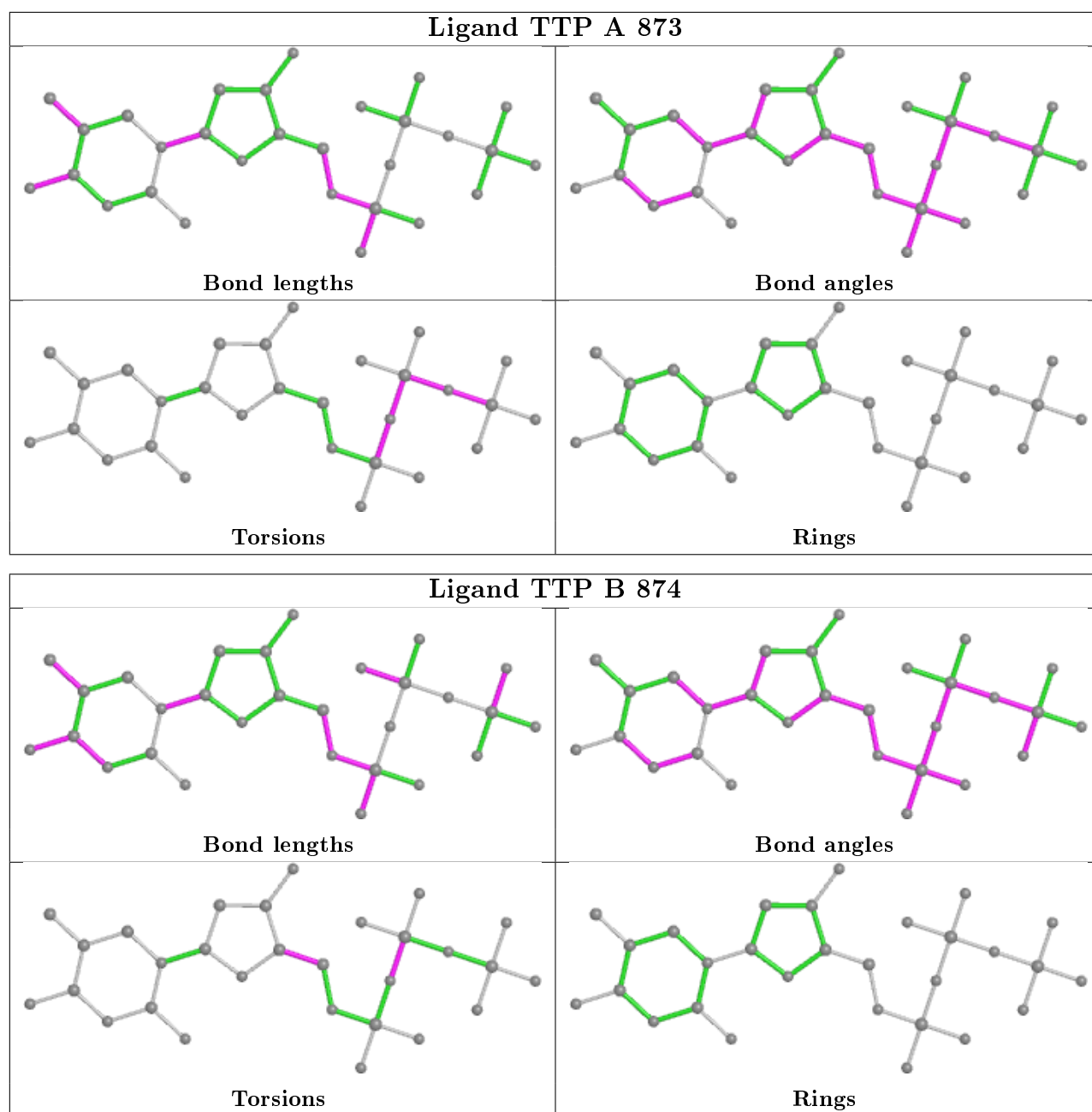
Mol	Chain	Res	Type	Atoms
5	A	873	TTP	PB-O3B-PG-O3G
5	B	874	TTP	O4'-C4'-C5'-O5'
5	B	874	TTP	C3'-C4'-C5'-O5'
5	A	873	TTP	PA-O3A-PB-O1B
5	A	873	TTP	PG-O3B-PB-O1B
5	A	873	TTP	PB-O3A-PA-O1A
5	B	874	TTP	PA-O3A-PB-O2B
5	A	873	TTP	PB-O3A-PA-O2A
5	B	874	TTP	PA-O3A-PB-O1B
5	A	873	TTP	PB-O3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	873	TTP	2	0
5	B	874	TTP	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 [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	P	12/13 (92%)	-0.10	0 100 100	38, 65, 121, 123	0
1	S	10/13 (76%)	-0.07	0 100 100	37, 59, 91, 100	0
2	Q	13/18 (72%)	-0.23	0 100 100	36, 54, 113, 129	0
2	T	15/18 (83%)	-0.04	0 100 100	51, 73, 109, 159	0
3	A	428/508 (84%)	-0.40	4 (0%) 84 66	12, 49, 95, 140	0
3	B	440/508 (86%)	-0.27	5 (1%) 80 60	26, 62, 120, 171	0
All	All	918/1078 (85%)	-0.32	9 (0%) 82 63	12, 57, 111, 171	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	478	VAL	2.7
3	B	410	ASP	2.6
3	A	475	SER	2.5
3	A	217	ASP	2.5
3	B	22	ASN	2.4
3	B	217	ASP	2.4
3	A	223	ILE	2.4
3	B	282	ASN	2.4
3	B	165	ILE	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](#)

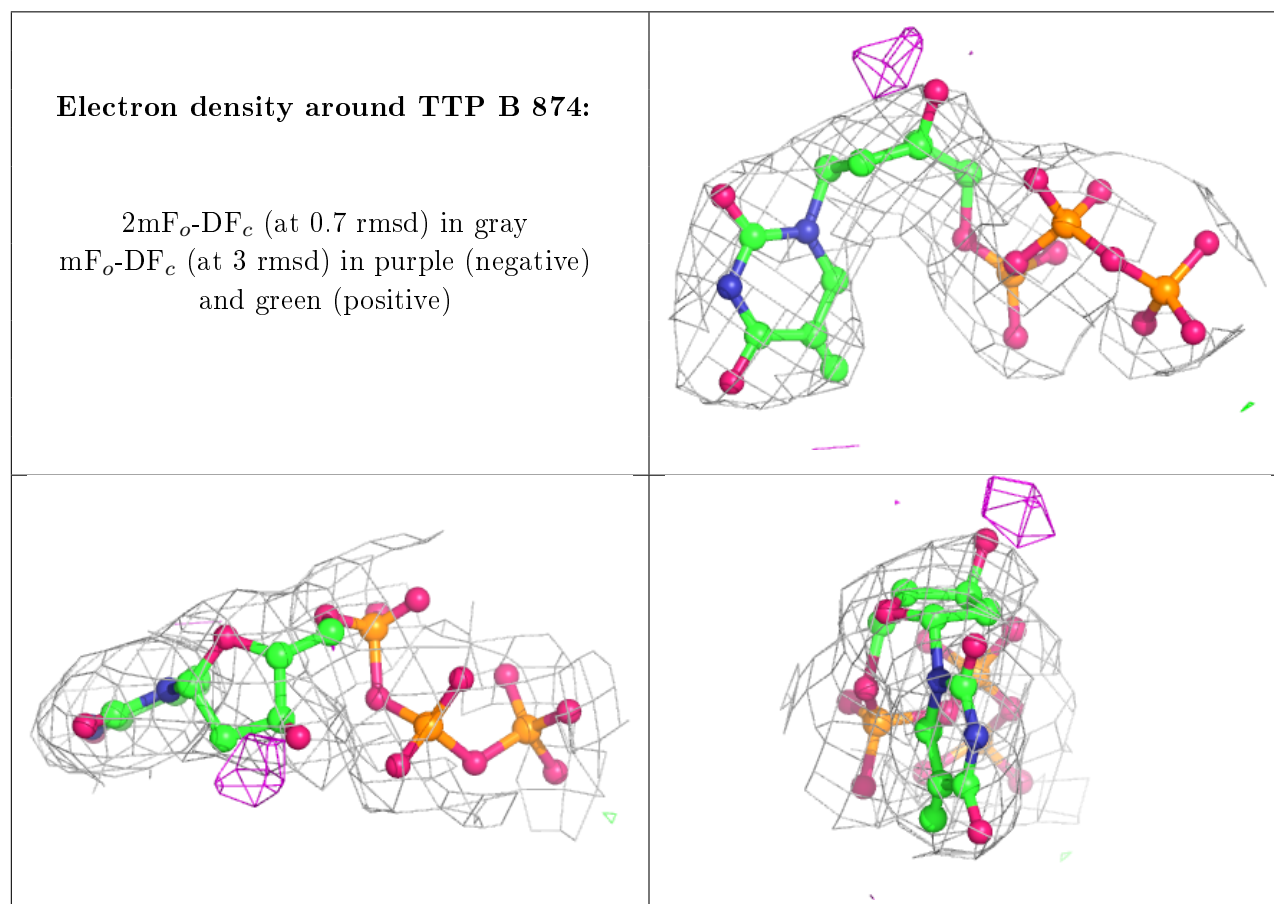
There are no carbohydrates in this entry.

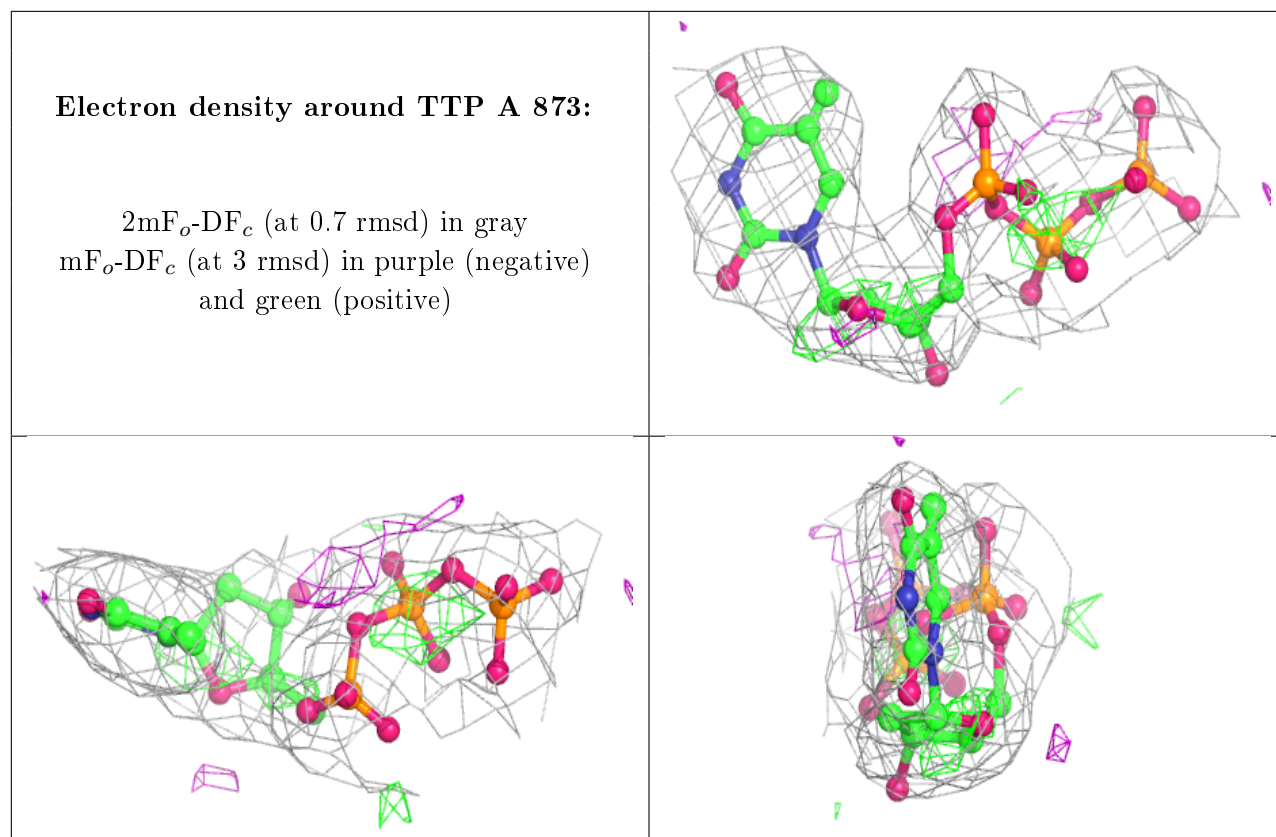
6.4 Ligands [i](#)

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	MG	A	872	1/1	0.94	0.16	51,51,51,51	0
4	MG	B	873	1/1	0.96	0.15	56,56,56,56	0
5	TTP	B	874	29/29	0.97	0.17	53,53,53,53	0
5	TTP	A	873	29/29	0.98	0.23	55,55,55,55	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.