



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:30 AM UTC

PDB ID : 8B7E / pdb_00008b7e
Title : The crystal structure of N828V variant of DNA Pol Epsilon containing UTP
in the polymerase active site
Authors : Parkash, V.; Johansson, E.
Deposited on : 2022-09-29
Resolution : 2.60 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

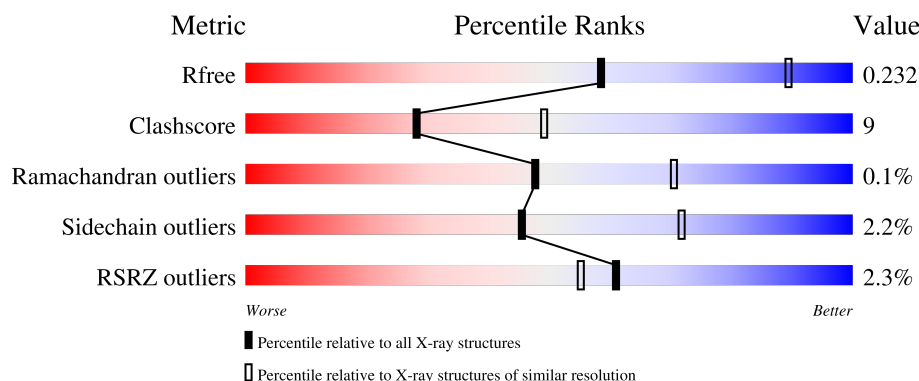
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

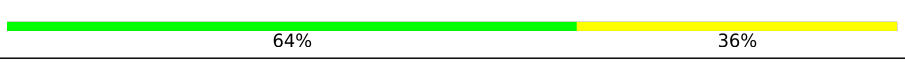
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	A	1191	 2% 75% 19% • 6%
1	B	1191	 3% 72% 21% • 6%
2	C	11	 64% 36%
2	P	11	 55% 45%
3	D	16	 62% 31% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	T	16	50% 44% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18824 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 protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1118	Total	C	N	O	S	0	0	0
			8878	5699	1473	1662	44			
1	B	1122	Total	C	N	O	S	0	0	0
			8744	5608	1457	1636	43			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P21951
A	-3	GLY	-	expression tag	UNP P21951
A	-2	ASP	-	expression tag	UNP P21951
A	-1	PRO	-	expression tag	UNP P21951
A	0	HIS	-	expression tag	UNP P21951
A	290	ALA	ASP	engineered mutation	UNP P21951
A	292	ALA	GLU	engineered mutation	UNP P21951
A	828	VAL	ASN	engineered mutation	UNP P21951
B	-4	GLY	-	expression tag	UNP P21951
B	-3	GLY	-	expression tag	UNP P21951
B	-2	ASP	-	expression tag	UNP P21951
B	-1	PRO	-	expression tag	UNP P21951
B	0	HIS	-	expression tag	UNP P21951
B	290	ALA	ASP	engineered mutation	UNP P21951
B	292	ALA	GLU	engineered mutation	UNP P21951
B	828	VAL	ASN	engineered mutation	UNP P21951

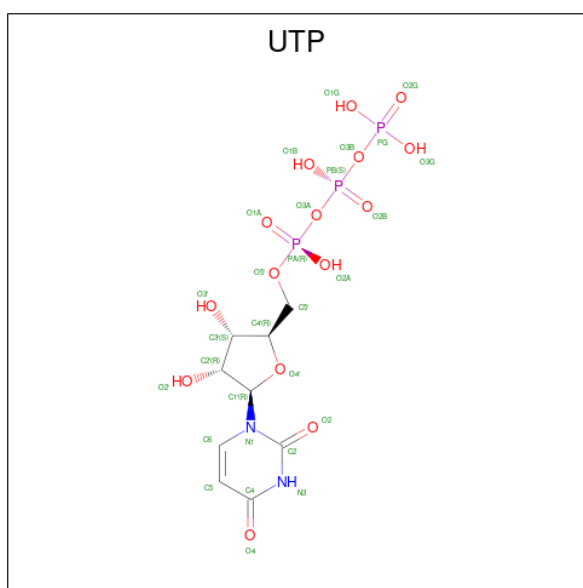
- Molecule 2 is a DNA chain called Primer DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			217	106	38	63	10			
2	P	11	Total	C	N	O	P	0	0	0
			217	106	38	63	10			

- Molecule 3 is a DNA chain called Template DNA sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	15	Total	C	N	O	P	0	0	0
			309	147	57	90	15			
3	T	15	Total	C	N	O	P	0	0	0
			309	147	57	90	15			

- Molecule 4 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

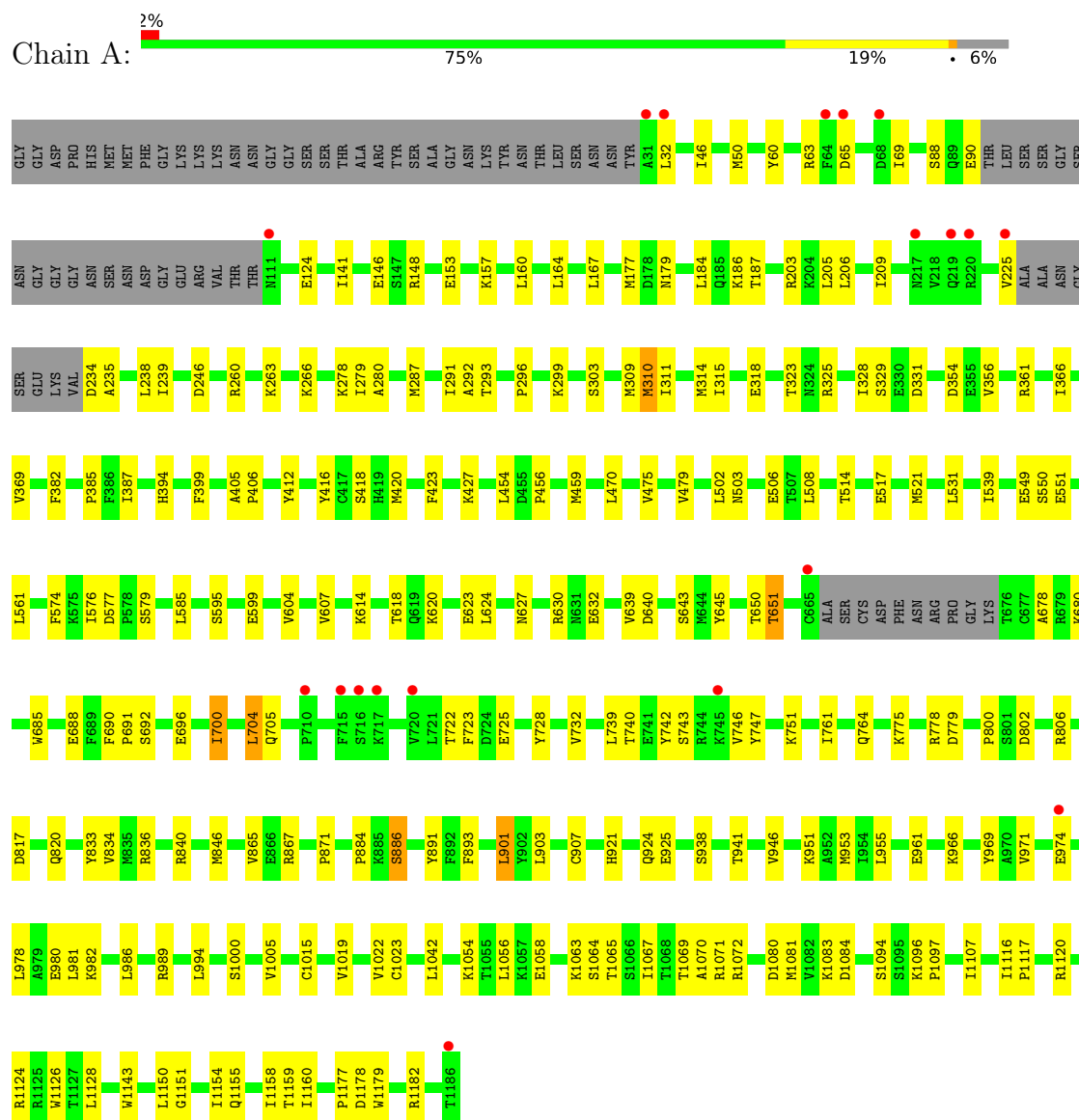
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total	O	0	0
			42	42		
7	B	26	Total	O	0	0
			26	26		
7	D	5	Total	O	0	0
			5	5		
7	P	3	Total	O	0	0
			3	3		
7	T	6	Total	O	0	0
			6	6		

3 Residue-property plots [i](#)

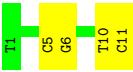
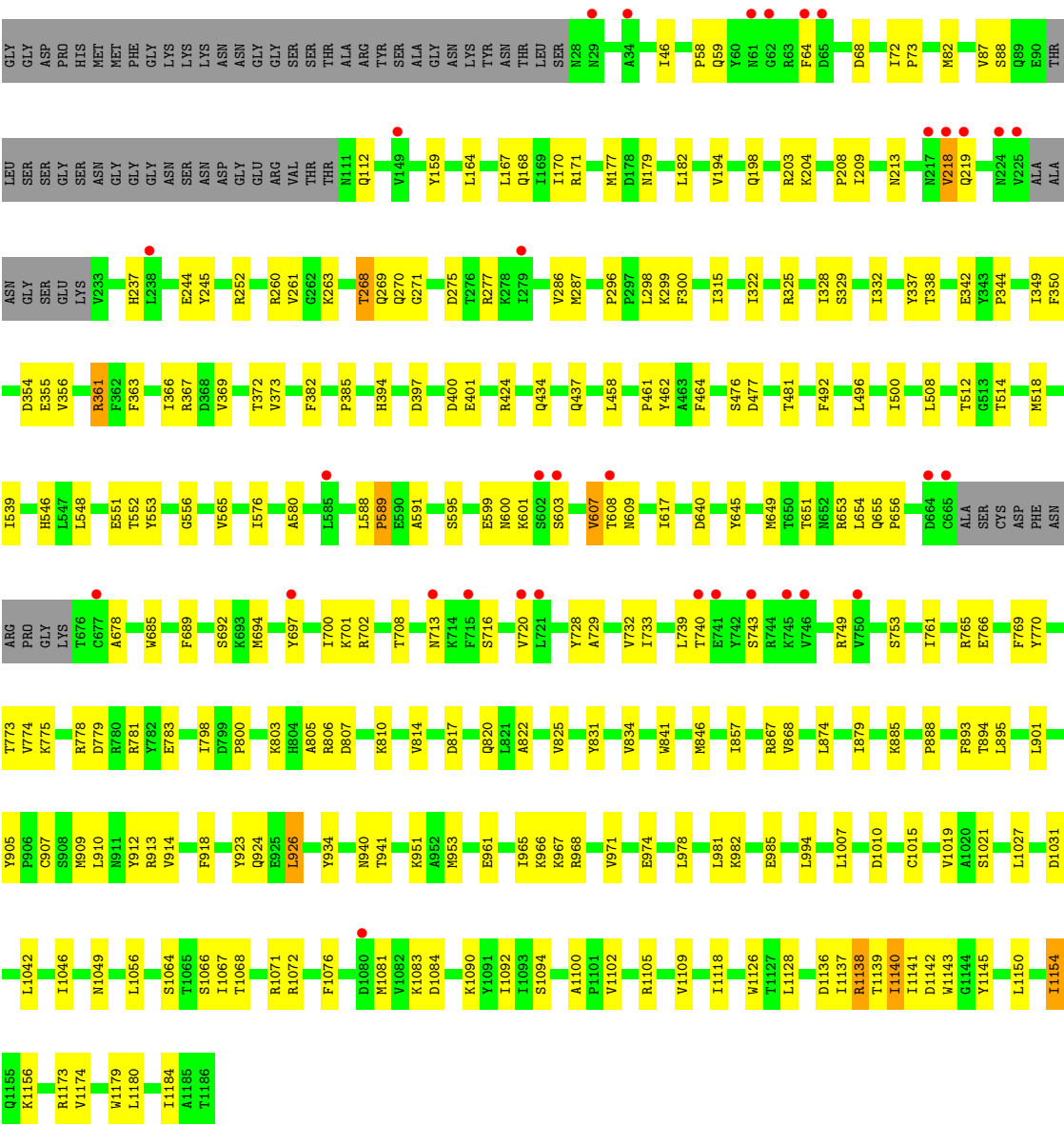
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA polymerase epsilon catalytic subunit A

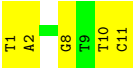


- Molecule 1: DNA polymerase epsilon catalytic subunit A





• Molecule 2: Primer DNA sequence



• Molecule 3: Template DNA sequence

Chain D:  62% 31% 6%



● Molecule 3: Template DNA sequence

Chain T:  50% 44% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.36Å 69.99Å 158.32Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	26.75 – 2.60 26.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (26.75-2.60) 98.6 (26.75-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.230 0.204 , 0.232	Depositor DCC
R_{free} test set	4771 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18824	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4669e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UTP, GOL, DOC, CA

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	A	0.30	0/9084	0.51	0/12321
1	B	0.32	0/8946	0.55	5/12148 (0.0%)
2	C	0.38	0/222	0.63	0/341
2	P	0.40	0/222	0.65	0/341
3	D	0.34	0/346	0.49	0/532
3	T	0.38	0/346	0.59	0/532
All	All	0.31	0/19166	0.54	5/26215 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	VAL	N-CA-C	8.06	120.26	109.37
1	B	601	LYS	N-CA-C	6.13	119.70	111.24
1	B	218	VAL	N-CA-C	6.12	122.07	109.34
1	B	219	GLN	N-CA-CB	-5.65	103.55	112.08
1	B	868	VAL	N-CA-C	-5.57	108.42	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8878	0	8576	147	0
1	B	8744	0	8324	170	0
2	C	217	0	123	3	0
2	P	217	0	123	4	0
3	D	309	0	170	3	0
3	T	309	0	170	5	0
4	A	29	0	11	3	0
4	B	29	0	11	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	T	6	0	8	1	0
7	A	42	0	0	1	0
7	B	26	0	0	4	0
7	D	5	0	0	0	0
7	P	3	0	0	0	0
7	T	6	0	0	0	0
All	All	18824	0	17516	324	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 9.

All (324) 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)
1:B:1092:ILE:HD12	1:B:1141:ILE:CD1	1.74	1.17
1:B:1092:ILE:HD12	1:B:1141:ILE:HD11	1.51	0.91
1:B:1064:SER:HB3	1:B:1067:ILE:HG13	1.53	0.90
1:B:1092:ILE:HD12	1:B:1141:ILE:HD13	1.53	0.88
1:B:895:LEU:HD21	1:B:901:LEU:HG	1.56	0.85
1:B:1137:ILE:O	1:B:1141:ILE:HG12	1.76	0.84
1:A:146:GLU:HG2	1:A:187:THR:HB	1.61	0.83
1:A:260:ARG:HB2	1:A:263:LYS:HD2	1.68	0.76
1:B:300:PHE:H	1:B:1081:MET:HE1	1.51	0.75
1:A:356:VAL:HG22	1:A:394:HIS:CG	2.22	0.75
1:A:627:ASN:HB2	1:A:630:ARG:NH2	2.03	0.74
1:B:367:ARG:HH12	1:B:401:GLU:HG3	1.52	0.74
1:B:708:THR:OG1	1:B:720:VAL:HG23	1.88	0.74
1:B:1092:ILE:CD1	1:B:1141:ILE:HD11	2.18	0.74
1:B:1156:LYS:NZ	7:B:1301:HOH:O	2.22	0.73
1:A:953:MET:HG3	1:A:971:VAL:HG22	1.71	0.72
1:A:164:LEU:HD21	1:A:167:LEU:HD13	1.71	0.71
1:B:905:TYR:O	1:B:909:MET:HG2	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ASN:HB2	1:A:630:ARG:HH21	1.55	0.70
1:A:921:HIS:HD1	1:A:938:SER:HG	1.40	0.69
1:A:148:ARG:HH22	1:A:234:ASP:HB3	1.58	0.68
1:B:765:ARG:NH1	1:B:924:GLN:OE1	2.27	0.67
1:A:246:ASP:OD1	1:A:840:ARG:NH2	2.26	0.67
1:B:59:GLN:HG3	1:B:269:GLN:HE21	1.59	0.67
1:B:1137:ILE:HG23	1:B:1141:ILE:HD11	1.76	0.67
1:B:268:THR:HG22	1:B:270:GLN:H	1.60	0.66
1:B:1118:ILE:HD12	1:B:1118:ILE:H	1.61	0.65
1:B:800:PRO:HA	1:B:806:ARG:HD2	1.79	0.65
1:B:1136:ASP:O	1:B:1139:THR:HG22	1.98	0.64
1:B:1049:ASN:HD22	1:B:1090:LYS:HE3	1.64	0.63
1:A:521:MET:HG2	1:A:531:LEU:HD21	1.79	0.63
1:B:1042:LEU:HD11	1:B:1143:TRP:HH2	1.64	0.63
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.33	0.63
1:B:1138:ARG:HH21	1:B:1138:ARG:HB2	1.62	0.62
1:B:607:VAL:HA	1:B:894:THR:O	1.98	0.62
1:B:655:GLN:HA	1:B:846:MET:HE2	1.82	0.62
1:B:580:ALA:HB2	1:B:867:ARG:HE	1.65	0.62
1:A:456:PRO:HA	1:A:459:MET:HG3	1.82	0.62
1:B:778:ARG:NH1	1:B:779:ASP:OD1	2.32	0.62
1:A:60:TYR:HE2	1:A:63:ARG:HA	1.64	0.61
1:A:650:THR:HB	1:A:775:LYS:HE2	1.81	0.61
1:B:332:ILE:HB	1:B:349:ILE:HG21	1.82	0.61
3:T:13:DG:H2'	3:T:14:DT:H71	1.82	0.61
1:A:982:LYS:HB3	2:P:10:DT:H5''	1.82	0.60
1:B:367:ARG:NH1	1:B:401:GLU:HG3	2.16	0.60
1:B:539:ILE:HD12	1:B:539:ILE:H	1.66	0.60
1:A:418:SER:HB3	1:A:420:MET:HE3	1.84	0.60
1:B:1056:LEU:HD21	1:B:1071:ARG:HG2	1.84	0.60
1:B:329:SER:HB3	1:B:464:PHE:HA	1.83	0.59
1:B:653:ARG:HG3	1:B:923:TYR:CE2	2.37	0.59
1:B:831:TYR:O	1:B:834:VAL:HG22	2.02	0.59
1:B:260:ARG:HB2	1:B:263:LYS:HD2	1.83	0.59
1:B:1150:LEU:O	1:B:1154:ILE:HD12	2.02	0.58
1:A:1072:ARG:HB3	1:A:1126:TRP:CZ2	2.39	0.58
1:A:1064:SER:OG	1:A:1067:ILE:HD12	2.05	0.57
1:A:539:ILE:H	1:A:539:ILE:HD12	1.69	0.57
1:A:454:LEU:HD23	1:A:459:MET:HG2	1.87	0.57
1:B:961:GLU:HG3	1:B:1179:TRP:CE3	2.39	0.57
1:B:653:ARG:HG3	1:B:923:TYR:CZ	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PRO:HG2	1:B:73:PRO:HB2	1.86	0.56
1:A:981:LEU:HD21	1:A:986:LEU:HD23	1.86	0.56
1:B:296:PRO:HB2	1:B:299:LYS:HB2	1.88	0.56
1:A:623:GLU:OE1	1:A:630:ARG:NH2	2.38	0.56
1:A:287:MET:HE1	1:A:366:ILE:HG12	1.87	0.56
1:A:742:TYR:CE1	1:A:746:VAL:HG21	2.40	0.56
1:A:696:GLU:HG2	1:A:742:TYR:CE2	2.40	0.56
1:B:653:ARG:NH1	1:B:766:GLU:O	2.39	0.56
1:A:1072:ARG:HD3	1:A:1126:TRP:CE2	2.41	0.55
1:A:1083:LYS:HG3	1:A:1084:ASP:OD1	2.06	0.55
1:A:1151:GLY:O	1:A:1155:GLN:HG3	2.06	0.55
1:A:1056:LEU:HD13	1:A:1070:ALA:HB3	1.90	0.54
1:A:475:VAL:O	1:A:479:VAL:HG23	2.07	0.54
1:B:338:THR:HG23	1:B:344:PRO:HA	1.89	0.54
1:B:546:HIS:ND1	1:B:692:SER:O	2.36	0.54
1:A:1155:GLN:HB3	1:A:1160:ILE:HD12	1.89	0.54
2:C:10:DT:H2''	2:C:11:DOC:H5'	1.90	0.54
1:A:836:ARG:HB2	3:T:5:DA:H4'	1.89	0.54
1:B:213:ASN:OD1	1:B:237:HIS:HA	2.07	0.54
1:B:82:MET:HE3	1:B:261:VAL:HG23	1.90	0.54
1:B:170:ILE:HD12	1:B:171:ARG:H	1.73	0.54
1:B:1100:ALA:O	1:B:1105:ARG:NH1	2.40	0.54
1:B:728:TYR:O	1:B:732:VAL:HG13	2.07	0.54
1:A:639:VAL:HG12	1:A:946:VAL:HG22	1.89	0.53
1:A:1005:VAL:HG21	1:A:1022:VAL:HG21	1.88	0.53
1:A:1023:CYS:HB3	1:A:1154:ILE:HD13	1.89	0.53
1:B:548:LEU:HD23	1:B:689:PHE:HB3	1.90	0.53
1:B:778:ARG:HG2	1:B:778:ARG:HH11	1.73	0.53
1:B:354:ASP:OD1	1:B:354:ASP:N	2.40	0.53
1:A:989:ARG:HH21	2:P:8:DG:P	2.31	0.53
1:B:893:PHE:HB2	1:B:901:LEU:HB2	1.90	0.53
1:A:153:GLU:O	1:A:157:LYS:HB2	2.09	0.53
1:A:406:PRO:HG3	1:A:412:TYR:CZ	2.44	0.53
1:B:1072:ARG:HB3	1:B:1126:TRP:CZ2	2.43	0.53
1:A:1178:ASP:O	1:A:1182:ARG:HG3	2.10	0.52
1:B:551:GLU:HG2	1:B:685:TRP:HE1	1.74	0.52
1:A:296:PRO:HG2	1:A:299:LYS:HB3	1.91	0.52
1:B:112:GLN:OE1	1:B:198:GLN:NE2	2.42	0.52
1:B:275:ASP:OD1	1:B:277:ARG:HD3	2.10	0.52
1:B:342:GLU:OE1	1:B:342:GLU:N	2.32	0.52
1:A:63:ARG:HG2	1:A:65:ASP:H	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG21	1:A:239:ILE:HD12	1.90	0.52
1:A:980:GLU:HB3	1:A:982:LYS:HE2	1.91	0.52
1:A:423:PHE:O	1:A:427:LYS:HG3	2.10	0.52
1:B:743:SER:HB3	1:B:749:ARG:O	2.09	0.52
1:B:286:VAL:HG22	1:B:373:VAL:HB	1.92	0.52
1:B:769:PHE:O	1:B:773:THR:OG1	2.23	0.52
1:A:315:ILE:HD13	1:A:369:VAL:HG21	1.91	0.52
1:B:167:LEU:HD23	1:B:168:GLN:N	2.25	0.52
1:A:325:ARG:HD3	1:A:331:ASP:OD1	2.10	0.51
1:B:496:LEU:HG	1:B:500:ILE:HD12	1.92	0.51
1:A:865:VAL:HG12	1:A:871:PRO:HD3	1.93	0.51
1:B:508:LEU:HD12	7:B:1302:HOH:O	2.09	0.51
1:A:279:ILE:HG13	1:A:280:ALA:N	2.24	0.51
1:A:299:LYS:NZ	1:A:1080:ASP:HB2	2.26	0.51
1:A:561:LEU:HD13	1:A:871:PRO:HB2	1.92	0.51
1:A:700:ILE:O	1:A:704:LEU:HD13	2.10	0.51
1:B:492:PHE:CZ	1:B:822:ALA:HB1	2.46	0.51
1:B:244:GLU:OE1	1:B:252:ARG:NH2	2.44	0.51
3:D:11:DC:H2"	3:D:12:DG:C8	2.45	0.51
1:B:552:THR:OG1	1:B:553:TYR:N	2.44	0.51
1:B:588:LEU:HB3	1:B:589:PRO:HD3	1.92	0.51
1:B:600:ASN:HB3	1:B:901:LEU:HD13	1.93	0.51
1:B:591:ALA:HA	1:B:912:TYR:CD2	2.46	0.50
1:A:141:ILE:HD11	1:A:206:LEU:HD11	1.93	0.50
2:C:5:DC:H2"	2:C:6:DG:C8	2.46	0.50
1:B:434:GLN:HA	1:B:437:GLN:HG3	1.94	0.50
1:B:781:ARG:NH2	1:B:820:GLN:OE1	2.44	0.50
1:A:630:ARG:NH1	1:A:632:GLU:OE2	2.38	0.50
1:A:978:LEU:HD21	1:A:981:LEU:HB2	1.94	0.50
1:A:966:LYS:HD3	3:T:9:DC:H5"	1.93	0.50
1:B:656:PRO:HG2	1:B:841:TRP:HB3	1.93	0.50
1:B:1094:SER:HA	1:B:1140:ILE:O	2.12	0.50
1:A:614:LYS:O	1:A:618:THR:OG1	2.22	0.50
1:A:696:GLU:HB3	1:A:742:TYR:CE2	2.47	0.50
1:A:1097:PRO:HG3	1:A:1128:LEU:HB2	1.92	0.49
1:B:576:ILE:HD12	1:B:576:ILE:H	1.77	0.49
1:A:179:ASN:HB2	1:A:184:LEU:HD12	1.94	0.49
1:A:705:GLN:HA	1:A:723:PHE:HB3	1.94	0.49
1:A:1094:SER:HB3	1:A:1107:ILE:HD12	1.93	0.49
1:B:325:ARG:NH1	1:B:328:ILE:O	2.45	0.49
1:A:604:VAL:O	1:A:607:VAL:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PRO:HA	1:A:806:ARG:HD2	1.95	0.49
1:B:653:ARG:HD2	1:B:923:TYR:CE1	2.48	0.49
1:B:729:ALA:O	1:B:732:VAL:HG22	2.12	0.49
1:B:909:MET:O	1:B:913:ARG:HG3	2.12	0.48
1:B:1137:ILE:CG2	1:B:1141:ILE:HD11	2.43	0.48
1:A:292:ALA:HB3	1:A:310:MET:HG3	1.95	0.48
1:A:951:LYS:HB2	1:A:974:GLU:HA	1.95	0.48
1:B:1042:LEU:O	1:B:1046:ILE:HG12	2.13	0.48
1:B:159:TYR:CE2	1:B:209:ILE:HD11	2.49	0.48
1:B:729:ALA:O	1:B:733:ILE:HG12	2.13	0.48
1:B:1027:LEU:HD11	1:B:1174:VAL:HG23	1.96	0.48
1:A:680:LYS:HB2	1:A:680:LYS:HE3	1.66	0.48
3:D:14:DT:H2'	3:D:15:DT:H71	1.95	0.48
1:A:382:PHE:O	1:A:385:PRO:HD2	2.13	0.48
1:A:834:VAL:HG21	1:A:846:MET:HE2	1.96	0.47
1:B:512:THR:HG21	1:B:825:VAL:HG22	1.95	0.47
1:A:50:MET:HE2	1:A:416:TYR:CE2	2.49	0.47
1:A:577:ASP:OD1	1:A:579:SER:OG	2.29	0.47
1:A:764:GLN:O	1:A:924:GLN:HB2	2.15	0.47
1:A:690:PHE:HE2	1:A:740:THR:HG22	1.79	0.47
1:B:617:ILE:HG12	1:B:888:PRO:HB3	1.97	0.47
1:B:1139:THR:CG2	1:B:1140:ILE:HG13	2.45	0.47
1:B:1139:THR:HG23	1:B:1140:ILE:HG13	1.97	0.47
1:A:514:THR:OG1	1:A:836:ARG:NH2	2.47	0.47
1:B:382:PHE:C	1:B:385:PRO:HD2	2.40	0.47
1:B:287:MET:HE1	1:B:366:ILE:HG12	1.97	0.47
1:B:551:GLU:HG2	1:B:685:TRP:NE1	2.29	0.47
1:B:580:ALA:CA	1:B:867:ARG:HH21	2.28	0.47
1:A:46:ILE:HG13	1:A:399:PHE:CE1	2.50	0.47
1:B:337:TYR:HE2	1:B:476:SER:HA	1.80	0.47
1:B:951:LYS:HD3	1:B:1007:LEU:HD22	1.97	0.47
1:B:951:LYS:HB2	1:B:974:GLU:HA	1.97	0.46
1:B:64:PHE:CB	1:B:68:ASP:HB2	2.45	0.46
1:B:458:LEU:HD13	1:B:462:TYR:CZ	2.50	0.46
1:A:893:PHE:HB2	1:A:901:LEU:HB2	1.97	0.46
1:B:355:GLU:HB3	1:B:394:HIS:HE1	1.80	0.46
1:B:1180:LEU:O	1:B:1184:ILE:HG13	2.16	0.46
1:A:88:SER:OG	1:A:90:GLU:HG3	2.15	0.46
1:B:968:ARG:HH22	1:B:985:GLU:CD	2.24	0.46
1:A:299:LYS:HD3	1:A:1081:MET:SD	2.56	0.46
1:A:577:ASP:HB3	1:A:867:ARG:HB3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LEU:C	1:B:461:PRO:HD2	2.40	0.46
1:B:477:ASP:O	1:B:481:THR:HG23	2.16	0.46
1:B:609:ASN:ND2	1:B:894:THR:HG23	2.31	0.45
1:B:803:LYS:HE3	1:B:807:ASP:OD2	2.16	0.45
1:A:160:LEU:HD23	1:A:205:LEU:HD12	1.96	0.45
1:B:194:VAL:HG12	1:B:198:GLN:HG3	1.97	0.45
1:B:978:LEU:HD21	1:B:981:LEU:HB2	1.97	0.45
1:B:1031:ASP:OD2	1:B:1173:ARG:NH2	2.46	0.45
1:A:291:ILE:HG22	1:A:311:ILE:HG12	1.97	0.45
1:A:549:GLU:HG2	1:A:690:PHE:CE1	2.52	0.45
1:B:68:ASP:O	1:B:72:ILE:HG13	2.16	0.45
1:B:363:PHE:CD2	1:B:401:GLU:HG2	2.51	0.45
1:B:595:SER:HA	1:B:599:GLU:HB2	1.98	0.45
1:B:1092:ILE:HG23	1:B:1109:VAL:HG12	1.99	0.45
1:B:775:LYS:HE2	1:B:779:ASP:OD2	2.17	0.45
1:B:965:ILE:HD11	1:B:1156:LYS:HD2	1.99	0.45
2:P:1:DT:H2''	2:P:2:DA:C8	2.52	0.45
1:B:514:THR:O	1:B:518:MET:HG2	2.17	0.45
1:B:1083:LYS:HG3	1:B:1084:ASP:N	2.31	0.45
1:B:591:ALA:HA	1:B:912:TYR:HD2	1.81	0.45
1:A:722:THR:OG1	1:A:725:GLU:HG3	2.17	0.45
1:A:651:THR:OG1	1:A:941:THR:HG22	2.17	0.44
1:A:700:ILE:HG13	1:A:739:LEU:HD12	1.98	0.44
1:B:798:ILE:HD13	1:B:805:ALA:HB1	1.99	0.44
1:A:696:GLU:OE1	1:A:747:TYR:OH	2.34	0.44
1:A:574:PHE:CG	1:A:884:PRO:HG3	2.52	0.44
1:A:645:TYR:CD2	4:A:1201:UTP:O2'	2.71	0.44
1:B:87:VAL:HG12	1:B:88:SER:O	2.17	0.44
1:A:503:ASN:OD1	1:A:506:GLU:HG3	2.18	0.44
1:B:651:THR:OG1	1:B:941:THR:HG22	2.17	0.44
1:B:678:ALA:HB1	1:B:761:ILE:HG23	1.98	0.44
1:B:961:GLU:HG3	1:B:1179:TRP:CZ3	2.53	0.44
1:A:1065:THR:O	1:A:1069:THR:OG1	2.33	0.44
1:A:1177:PRO:HB2	1:A:1179:TRP:CD1	2.53	0.44
1:A:817:ASP:O	1:A:820:GLN:HG3	2.18	0.44
1:A:1054:LYS:HE3	1:A:1058:GLU:HB2	2.00	0.44
1:B:600:ASN:CB	1:B:901:LEU:HD13	2.48	0.44
1:B:700:ILE:HD13	1:B:739:LEU:HA	1.98	0.44
1:A:177:MET:HE1	1:A:186:LYS:HA	2.00	0.44
1:B:1142:ASP:O	1:B:1145:TYR:N	2.49	0.44
1:A:502:LEU:HB3	1:A:506:GLU:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:TYR:HB2	1:A:903:LEU:HD23	2.00	0.43
1:B:713:ASN:O	1:B:716:SER:OG	2.33	0.43
1:A:961:GLU:HB2	1:A:1179:TRP:CD2	2.53	0.43
1:B:46:ILE:HD13	1:B:46:ILE:HA	1.88	0.43
1:B:164:LEU:HD21	1:B:167:LEU:HD12	1.99	0.43
1:B:203:ARG:HD2	1:B:245:TYR:HB2	1.99	0.43
1:A:1019:VAL:CG1	1:A:1158:ILE:HG12	2.49	0.43
1:A:1081:MET:HE3	1:A:1081:MET:HB3	1.84	0.43
1:A:1155:GLN:HA	1:A:1159:THR:OG1	2.18	0.43
1:B:397:ASP:HB3	1:B:400:ASP:HB2	2.00	0.43
1:A:643:SER:HA	4:A:1201:UTP:O2B	2.18	0.43
1:A:994:LEU:HD21	1:A:1150:LEU:HB2	2.00	0.43
1:B:953:MET:HG3	1:B:971:VAL:HG22	1.99	0.43
1:A:969:TYR:OH	2:P:11:DOC:OP1	2.34	0.43
3:T:15:DT:H2"	3:T:16:DA:C8	2.53	0.43
1:A:508:LEU:HD12	7:A:1301:HOH:O	2.17	0.43
1:A:595:SER:HA	1:A:599:GLU:HB2	2.00	0.43
1:A:778:ARG:NH1	1:A:779:ASP:OD1	2.51	0.43
1:B:59:GLN:HG3	1:B:269:GLN:NE2	2.31	0.43
1:B:315:ILE:HD13	1:B:369:VAL:HG11	1.99	0.43
1:B:322:ILE:HA	1:B:350:PHE:O	2.18	0.43
1:B:1092:ILE:CD1	1:B:1141:ILE:CD1	2.65	0.43
1:A:691:PRO:HG2	1:A:743:SER:HB3	2.00	0.43
1:B:361:ARG:HD3	1:B:361:ARG:HA	1.78	0.43
1:B:967:LYS:O	1:B:968:ARG:HG3	2.19	0.43
1:B:1027:LEU:HD23	1:B:1027:LEU:HA	1.75	0.43
1:A:356:VAL:HG22	1:A:394:HIS:CB	2.49	0.42
1:A:356:VAL:CG2	1:A:394:HIS:CG	2.96	0.42
1:A:620:LYS:HE2	1:A:886:SER:O	2.19	0.42
1:A:696:GLU:HG2	1:A:742:TYR:HE2	1.83	0.42
1:B:857:ILE:HG12	1:B:918:PHE:CD2	2.54	0.42
1:A:323:THR:HB	1:A:328:ILE:HG13	2.01	0.42
1:B:778:ARG:NH1	1:B:778:ARG:HG2	2.33	0.42
1:B:179:ASN:HA	1:B:182:LEU:HD23	2.01	0.42
1:B:1068:THR:O	1:B:1072:ARG:HG3	2.19	0.42
1:B:1102:VAL:HG23	7:B:1320:HOH:O	2.18	0.42
1:A:953:MET:SD	1:A:955:LEU:HD11	2.60	0.42
1:B:177:MET:HE3	1:B:177:MET:HB2	1.85	0.42
1:B:765:ARG:HG3	1:B:924:GLN:OE1	2.20	0.42
1:B:770:TYR:O	1:B:774:VAL:HG23	2.19	0.42
1:A:32:LEU:O	1:A:32:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:MET:HA	1:A:318:GLU:O	2.20	0.42
1:A:1120:ARG:HD2	1:A:1124:ARG:CZ	2.50	0.42
1:A:585:LEU:HD23	1:A:585:LEU:HA	1.74	0.42
1:A:761:ILE:HD12	1:A:761:ILE:N	2.35	0.42
1:A:585:LEU:HD22	1:A:618:THR:HG23	2.02	0.42
1:A:1042:LEU:HD11	1:A:1143:TRP:HH2	1.85	0.42
1:B:810:LYS:O	1:B:814:VAL:HG23	2.20	0.42
1:B:885:LYS:O	1:B:885:LYS:HG3	2.20	0.42
1:A:69:ILE:HD11	1:A:266:LYS:HB2	2.01	0.41
1:A:287:MET:HA	1:A:314:MET:O	2.20	0.41
1:A:551:GLU:HG2	1:A:685:TRP:HE1	1.85	0.41
1:B:700:ILE:HD13	1:B:739:LEU:CA	2.50	0.41
1:A:688:GLU:CD	1:A:751:LYS:HD3	2.45	0.41
1:B:268:THR:HB	1:B:271:GLY:O	2.21	0.41
3:T:12:DG:N7	6:T:101:GOL:O3	2.42	0.41
1:A:678:ALA:HB1	1:A:761:ILE:HG23	2.03	0.41
1:A:802:ASP:O	1:A:806:ARG:HG3	2.20	0.41
1:B:556:GLY:HA2	7:B:1313:HOH:O	2.19	0.41
1:A:354:ASP:OD1	1:A:354:ASP:N	2.52	0.41
1:A:576:ILE:CD1	1:A:624:LEU:HD22	2.51	0.41
1:A:1064:SER:OG	1:A:1067:ILE:HB	2.21	0.41
1:A:1116:ILE:N	1:A:1117:PRO:HD2	2.35	0.41
1:B:649:MET:HA	1:B:654:LEU:HB2	2.03	0.41
1:A:1071:ARG:NH1	1:A:1071:ARG:HG3	2.36	0.41
1:B:458:LEU:HD23	1:B:458:LEU:HA	1.84	0.41
1:B:926:LEU:HD13	1:B:934:TYR:CZ	2.56	0.41
1:B:700:ILE:CD1	1:B:739:LEU:HD13	2.50	0.41
1:B:874:LEU:HD12	1:B:879:ILE:HG12	2.02	0.41
1:B:910:LEU:O	1:B:914:VAL:HG23	2.21	0.41
1:A:203:ARG:HE	1:A:203:ARG:HB3	1.71	0.41
1:A:309:MET:CE	1:A:470:LEU:HD21	2.50	0.41
1:A:399:PHE:HD2	1:A:405:ALA:HB2	1.86	0.41
1:A:624:LEU:HD23	1:A:630:ARG:CZ	2.51	0.41
1:A:700:ILE:HG13	1:A:739:LEU:CD1	2.51	0.41
1:A:739:LEU:HD12	1:A:739:LEU:HA	1.97	0.41
1:A:969:TYR:CE1	1:A:982:LYS:HG3	2.56	0.41
1:A:1071:ARG:HG3	1:A:1071:ARG:HH11	1.86	0.41
1:B:655:GLN:HB2	1:B:770:TYR:HB3	2.03	0.41
1:B:1015:CYS:O	1:B:1019:VAL:HG23	2.21	0.41
1:A:517:GLU:HB2	1:A:833:TYR:CE1	2.56	0.41
1:B:700:ILE:CD1	1:B:739:LEU:HA	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:ASP:O	1:B:820:GLN:HG3	2.21	0.41
1:A:907:CYS:SG	1:A:946:VAL:HG23	2.62	0.40
1:B:694:MET:HA	1:B:697:TYR:HB3	2.04	0.40
1:B:701:LYS:O	1:B:702:ARG:C	2.63	0.40
1:A:278:LYS:HE3	1:A:278:LYS:HB3	1.93	0.40
1:A:643:SER:HA	4:A:1201:UTP:PB	2.61	0.40
1:B:645:TYR:CD2	4:B:1201:UTP:O2'	2.74	0.40
1:B:966:LYS:HD3	3:D:9:DC:H5''	2.02	0.40
1:B:982:LYS:HB3	2:C:10:DT:H5''	2.03	0.40
1:A:291:ILE:HG21	1:A:387:ILE:HD11	2.02	0.40
1:A:728:TYR:O	1:A:732:VAL:HG13	2.21	0.40
1:A:1096:LYS:NZ	1:B:1010:ASP:OD2	2.41	0.40
1:B:252:ARG:HA	1:B:252:ARG:HD3	1.80	0.40
1:B:424:ARG:HD2	1:B:424:ARG:HA	1.74	0.40
1:B:588:LEU:N	1:B:589:PRO:CD	2.85	0.40
1:B:918:PHE:O	1:B:940:ASN:ND2	2.55	0.40
1:B:1128:LEU:HD23	1:B:1128:LEU:HA	1.90	0.40
1:A:235:ALA:HA	1:A:238:LEU:HD12	2.02	0.40
1:B:204:LYS:O	1:B:208:PRO:HD2	2.21	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	
1	A	1110/1191 (93%)	1072 (97%)	38 (3%)	0	100	100
1	B	1114/1191 (94%)	1069 (96%)	43 (4%)	2 (0%)	43	66
All	All	2224/2382 (93%)	2141 (96%)	81 (4%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	VAL
1	B	589	PRO

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	
1	A	946/1065 (89%)	927 (98%)	19 (2%)	48	74
1	B	909/1065 (85%)	888 (98%)	21 (2%)	44	71
All	All	1855/2130 (87%)	1815 (98%)	40 (2%)	45	72

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	225	VAL
1	A	293	THR
1	A	303	SER
1	A	310	MET
1	A	329	SER
1	A	361	ARG
1	A	550	SER
1	A	640	ASP
1	A	651	THR
1	A	692	SER
1	A	700	ILE
1	A	704	LEU
1	A	886	SER
1	A	901	LEU
1	A	925	GLU
1	A	1000	SER
1	A	1015	CYS
1	A	1063	LYS
1	B	268	THR
1	B	298	LEU
1	B	356	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	361	ARG
1	B	372	THR
1	B	565	VAL
1	B	603	SER
1	B	608	THR
1	B	640	ASP
1	B	740	THR
1	B	753	SER
1	B	783	GLU
1	B	907	CYS
1	B	926	LEU
1	B	994	LEU
1	B	1021	SER
1	B	1066	SER
1	B	1076	PHE
1	B	1138	ARG
1	B	1140	ILE
1	B	1154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	616	GLN
1	A	859	GLN
1	B	112	GLN
1	B	198	GLN
1	B	269	GLN
1	B	394	HIS
1	B	468	GLN
1	B	523	GLN
1	B	528	ASN
1	B	535	HIS
1	B	734	HIS
1	B	859	GLN
1	B	973	ASN
1	B	1033	HIS
1	B	1176	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DOC	C	11	3,2	16,19,20	0.42	0	20,26,29	0.31	0
2	DOC	P	11	3,2	16,19,20	0.42	0	20,26,29	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	C	11	3,2	-	2/7/18/19	0/2/2/2
2	DOC	P	11	3,2	-	2/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	11	DOC	C3'-C4'-C5'-O5'
2	C	11	DOC	O4'-C4'-C5'-O5'
2	P	11	DOC	C3'-C4'-C5'-O5'
2	P	11	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	DOC	1	0
2	P	11	DOC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	T	101	-	5,5,5	1.11	0	5,5,5	1.04	0
4	UTP	A	1201	5	29,30,30	0.57	0	43,47,47	0.59	0
4	UTP	B	1201	5	29,30,30	0.60	0	43,47,47	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	T	101	-	-	2/4/4/4	-
4	UTP	A	1201	5	-	9/22/38/38	0/2/2/2
4	UTP	B	1201	5	-	5/22/38/38	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

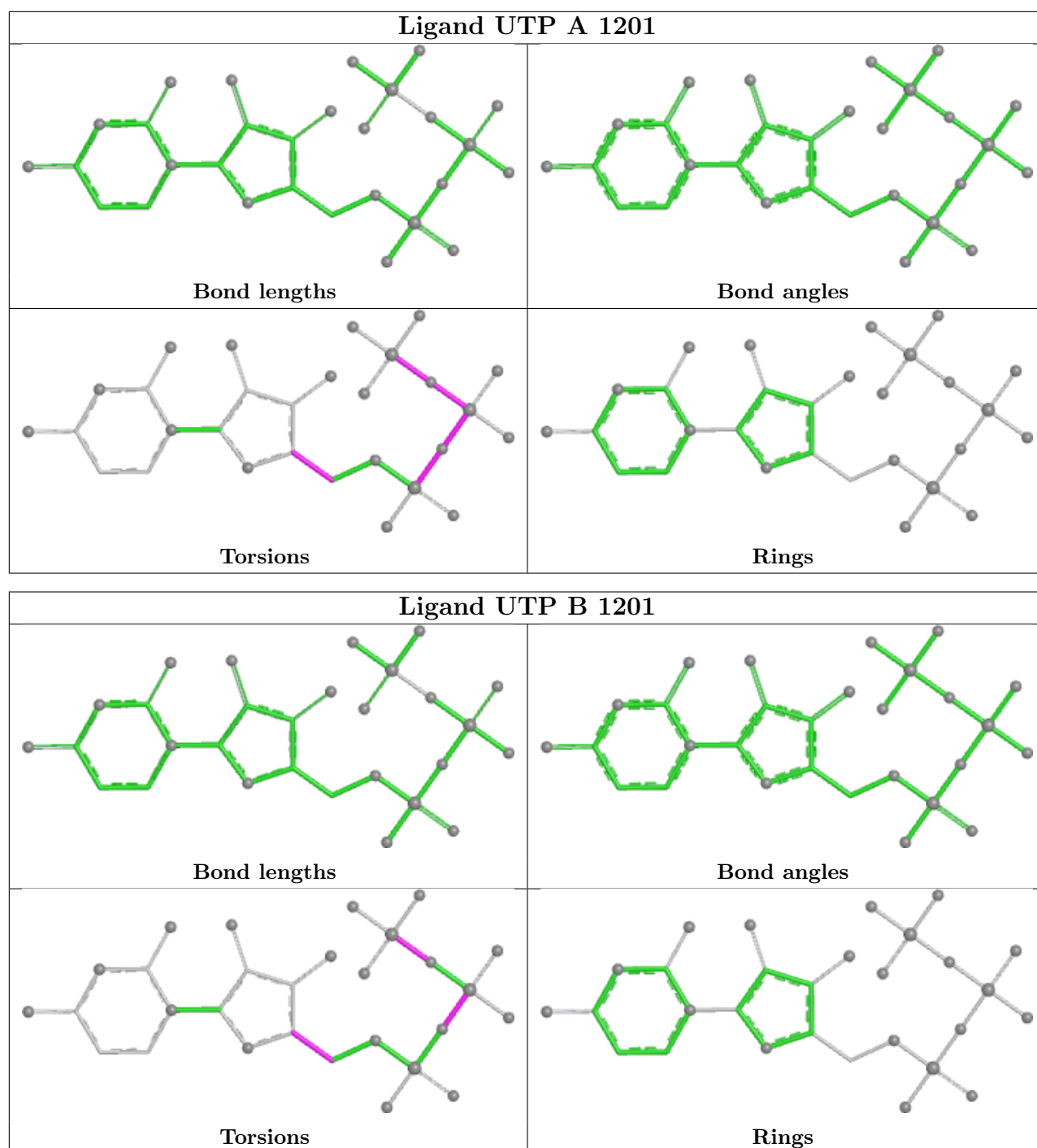
Mol	Chain	Res	Type	Atoms
4	A	1201	UTP	PB-O3B-PG-O1G
6	T	101	GOL	C1-C2-C3-O3
6	T	101	GOL	O2-C2-C3-O3
4	A	1201	UTP	O4'-C4'-C5'-O5'
4	B	1201	UTP	O4'-C4'-C5'-O5'
4	A	1201	UTP	PB-O3A-PA-O1A
4	A	1201	UTP	C3'-C4'-C5'-O5'
4	A	1201	UTP	PB-O3B-PG-O2G
4	A	1201	UTP	PB-O3A-PA-O2A
4	A	1201	UTP	PA-O3A-PB-O2B
4	B	1201	UTP	C3'-C4'-C5'-O5'
4	B	1201	UTP	PB-O3B-PG-O2G
4	B	1201	UTP	PB-O3B-PG-O3G
4	A	1201	UTP	PA-O3A-PB-O1B
4	A	1201	UTP	PG-O3B-PB-O1B
4	B	1201	UTP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	T	101	GOL	1	0
4	A	1201	UTP	3	0
4	B	1201	UTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1118/1191 (93%)	-0.17	19 (1%) 69 64	26, 55, 85, 118	0
1	B	1122/1191 (94%)	0.01	33 (2%) 53 48	29, 59, 94, 115	0
2	C	10/11 (90%)	-0.76	0 100 100	38, 47, 65, 67	0
2	P	10/11 (90%)	-0.83	0 100 100	36, 45, 64, 69	0
3	D	15/16 (93%)	-0.77	0 100 100	34, 47, 73, 85	0
3	T	15/16 (93%)	-0.70	0 100 100	31, 44, 72, 86	0
All	All	2290/2436 (94%)	-0.10	52 (2%) 61 55	26, 57, 89, 118	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	665	CYS	7.0
1	A	665	CYS	5.1
1	A	64	PHE	4.7
1	B	743	SER	4.0
1	A	716	SER	3.8
1	B	29	ASN	3.8
1	A	715	PHE	3.5
1	B	218	VAL	3.4
1	A	219	GLN	3.3
1	A	220	ARG	3.2
1	A	225	VAL	3.2
1	B	225	VAL	3.2
1	A	68	ASP	3.0
1	B	279	ILE	2.9
1	B	745	LYS	2.8
1	A	217	ASN	2.8
1	B	677	CYS	2.7
1	B	750	VAL	2.7
1	B	664	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	741	GLU	2.7
1	A	32	LEU	2.6
1	A	717	LYS	2.6
1	B	64	PHE	2.6
1	B	746	VAL	2.6
1	A	31	ALA	2.6
1	B	149	VAL	2.5
1	B	219	GLN	2.5
1	B	217	ASN	2.5
1	A	720	VAL	2.5
1	B	740	THR	2.4
1	B	1080	ASP	2.4
1	A	710	PRO	2.4
1	B	721	LEU	2.4
1	B	585	LEU	2.4
1	A	65	ASP	2.4
1	A	745	LYS	2.4
1	B	715	PHE	2.3
1	B	608	THR	2.3
1	B	720	VAL	2.3
1	B	65	ASP	2.3
1	B	713	ASN	2.2
1	B	62	GLY	2.2
1	B	603	SER	2.2
1	B	238	LEU	2.1
1	B	61	ASN	2.1
1	B	34	ALA	2.1
1	A	111	ASN	2.1
1	B	697	TYR	2.1
1	B	602	SER	2.0
1	A	1186	THR	2.0
1	A	974	GLU	2.0
1	B	224	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
2	DOC	C	11	18/19	0.97	0.07	24,33,42,43	0
2	DOC	P	11	18/19	0.97	0.07	23,32,39,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

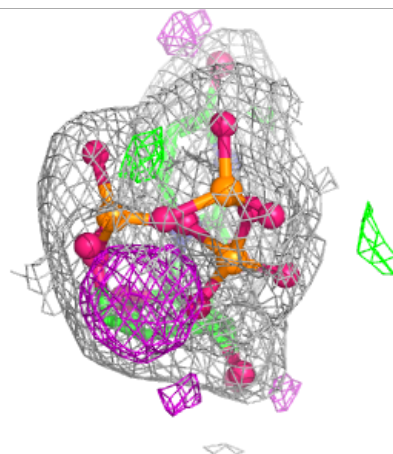
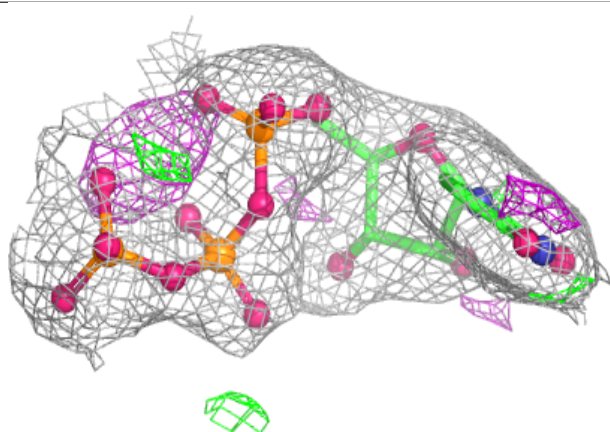
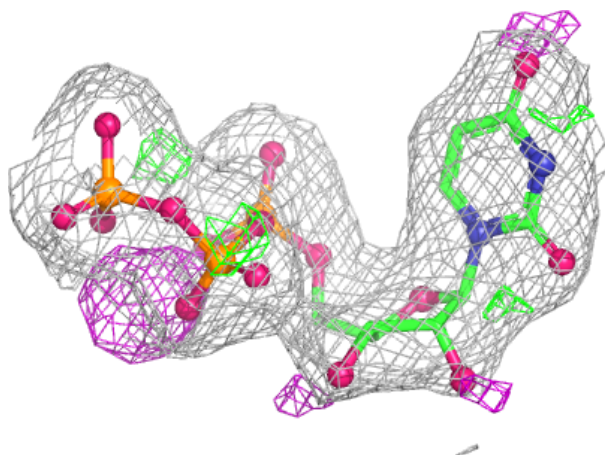
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

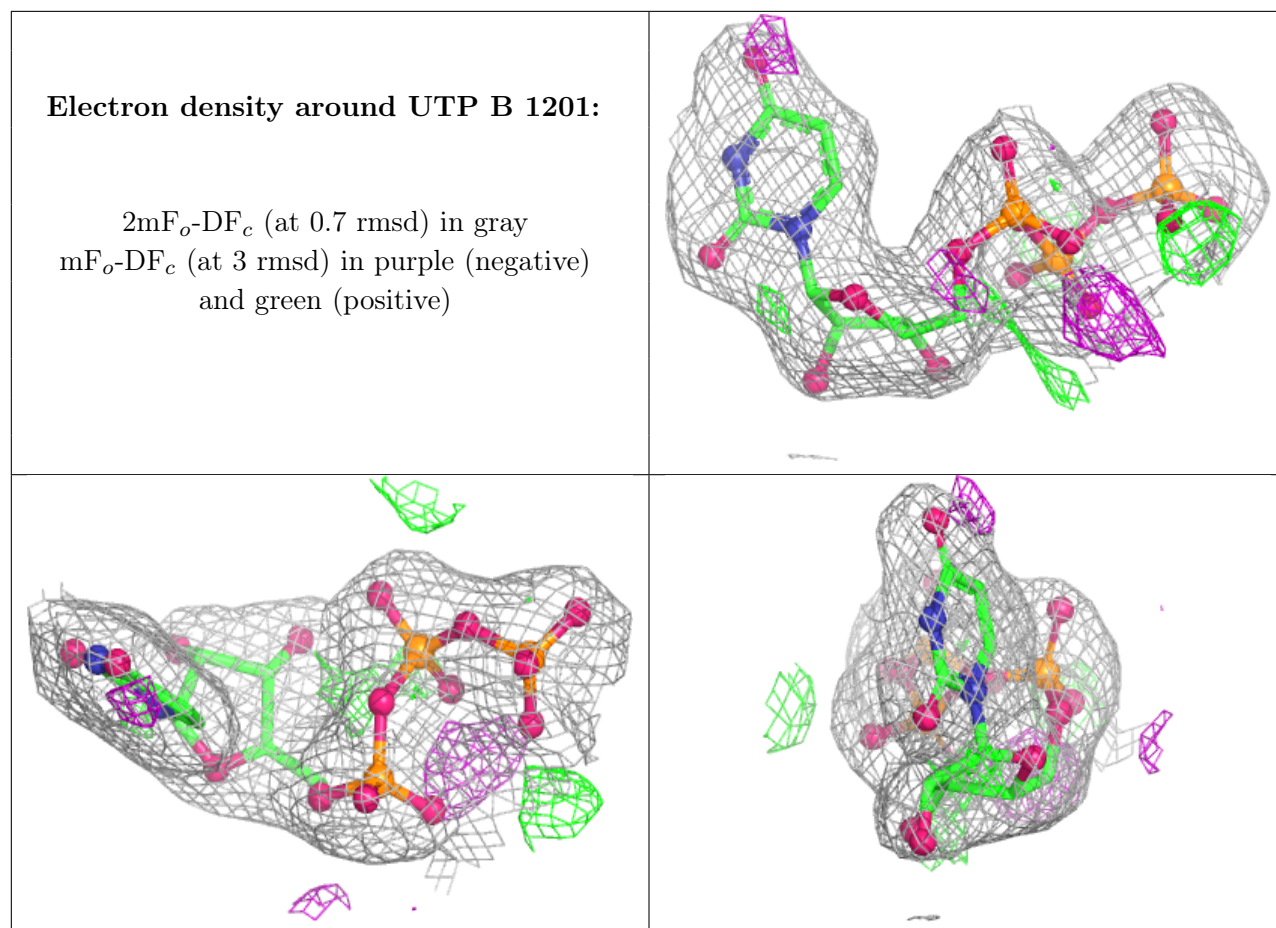
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	B	1203	1/1	0.86	0.11	84,84,84,84	0
6	GOL	T	101	6/6	0.87	0.14	57,63,66,67	0
5	CA	B	1202	1/1	0.91	0.09	42,42,42,42	0
4	UTP	A	1201	29/29	0.95	0.08	26,34,48,50	0
5	CA	A	1202	1/1	0.95	0.12	36,36,36,36	0
5	CA	A	1203	1/1	0.95	0.07	79,79,79,79	0
4	UTP	B	1201	29/29	0.97	0.07	27,36,49,55	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.

Electron density around UTP A 1201:

$2mF_o-DF_c$ (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.