



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:58 AM BST

PDB ID : 1TAU  
Title : TAQ POLYMERASE (E.C.2.7.7.7)/DNA/B-OCTYLGLUCOSIDE COMPLEX  
Authors : Eom, S.H.; Wang, J.; Steitz, T.A.  
Deposited on : 1996-06-17  
Resolution : 3.00 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](mailto: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.

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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	:	2.13.1
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)	:	2.13.1

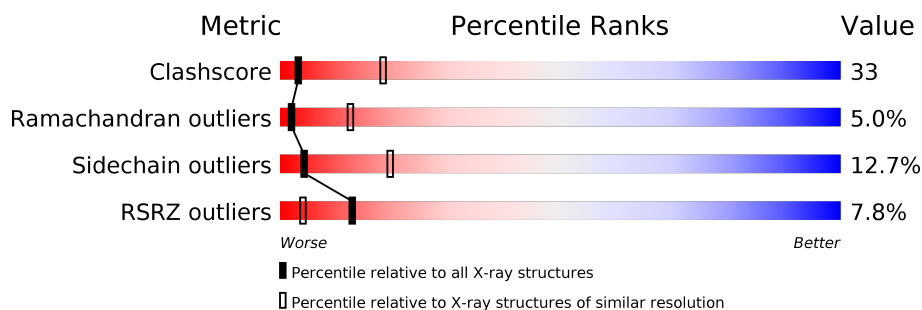
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	T	8	<div> <div>75%</div> <div>100%</div> </div>
2	P	8	<div> <div>75%</div> <div>100%</div> </div>
3	A	832	<div> <div>6%</div> <div>41%</div> <div>45%</div> <div>9%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8122 atoms, of which 1448 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 DNA (5'-D(\*GP\*CP\*GP\*AP\*TP\*CP\*CP\*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	T	8	Total	C	H	N	O	P	0	0	0
			181	77	20	31	46	7			

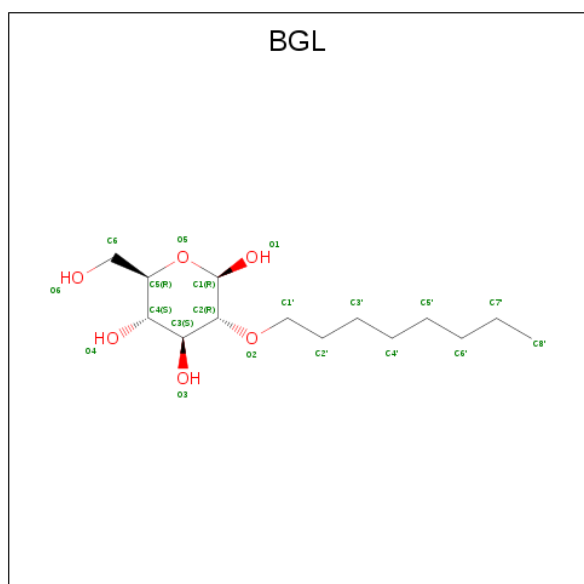
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*GP\*AP\*TP\*CP\*GP\*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	8	Total	C	H	N	O	P	0	0	0
			181	77	20	31	46	7			

- Molecule 3 is a protein called PROTEIN (TAQ POLYMERASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	793	Total	C	H	N	O	S	0	0	0
			7739	4039	1408	1125	1153	14			

- Molecule 4 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		

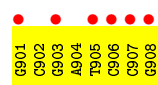
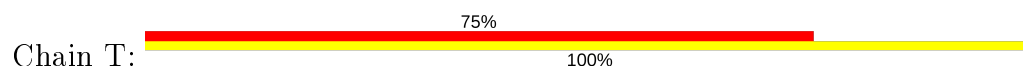
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

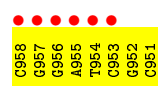
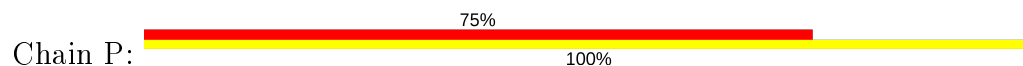
### 3 Residue-property plots [i](#)

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.

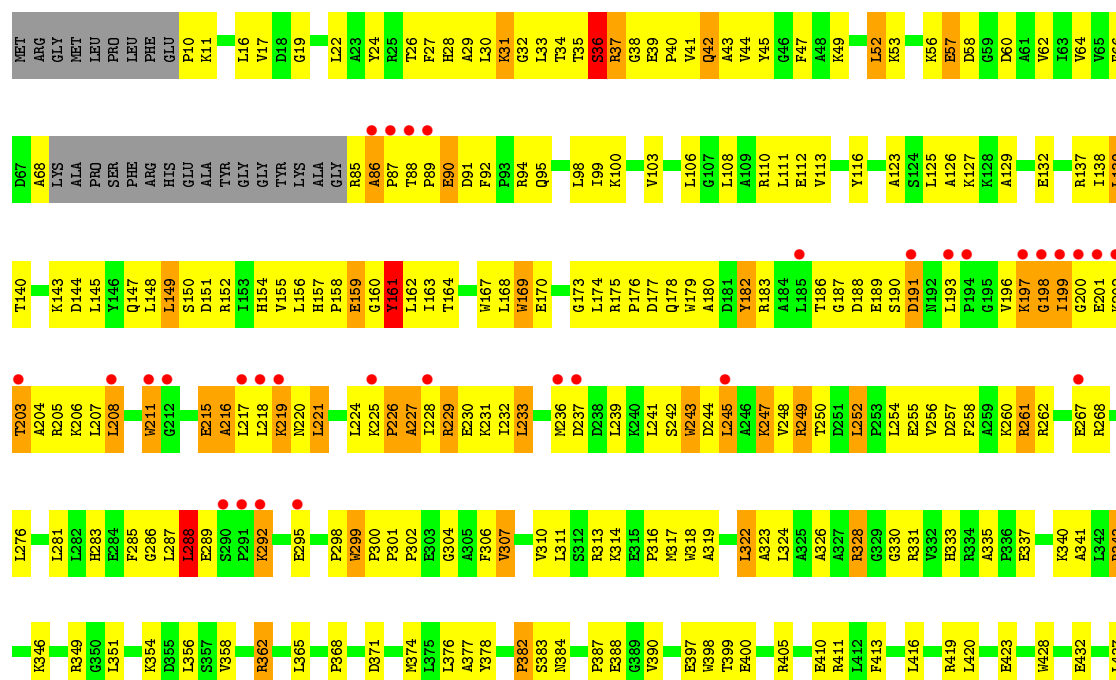
- Molecule 1: DNA (5'-D(\*GP\*CP\*GP\*AP\*TP\*CP\*CP\*G)-3')



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



- Molecule 3: PROTEIN (TAQ POLYMERASE)



V806	E734	K663	Q582	LYS	S438
M607	A735	T664	M583	ARG	
E808	R736	I665	I584	SS13	A442
G809	V737	N666	P585	TS14	
V810	K738	N667	V586	SS15	T447
Y811	S739	F667	R587	AS16	G448
P812	V740	G668	T588	AS17	V449
	R741	V669	P589	V518	R450
V815	E742	L670	L590	L519	V453
P816	A743	G671	G591	E520	
L817	A744	G672	Q592	AS21	
	E745	M673	R593	L522	L456
E820	R746	S674	T594	R523	
V821	M747	A675	R595	E524	A464
G822	A748	H676		AS25	E466
I823	F749	R677	A600	H526	I467
	N750		E601	P527	A468
D826	M751	Q680	E602	I528	R469
H827	P752	E681	G603	V529	L470
L828	V753	L682	M604	E530	E471
	Q754	A683	L605	K531	A472
K831	G755	I684	L606	I532	E473
E832	T756	P685	V607	L533	V474
	A757	Y686	A608	O534	F475
	A758	E687	L609	Y535	R476
		E688	H610	R536	L477
	K762		Y611	E537	A478
	K767	A691		L538	G479
	L768	F692	I614	TS39	H480
	F769	E694	R617	K540	F481
	P770	R695	V618	L541	F482
	R771		L619		M483
		S699		TS44	N485
	E774	F700	G624	Y546	L484
		P701	D625	D547	S486
	R778	K702	E626	P548	R487
M779			I627	L549	D488
L780		W706	L628	P550	Q489
L781		I707	L629	D551	L490
Q782		E708	R630	L552	E491
V783		K709	V631	I553	R492
H784			F632	H554	V493
D785			Q633	P555	L494
		E712	E634	R556	F495
	E790	E713	G635		D496
		R715	R636	L560	E497
K793		G714	D637	H561	L498
E794		R716	I638	TS62	GLY
R795		R717	H639		LEU
A796		G718	T640	Q566	PRO
E797		Y719	E641	TS67	ALA
			T642	A568	ILE
		T722			GLY
A798		L723			LYS
V799			R651	H573	THR
A800				L574	
R801		R727			GLU
L802		R728	V654		LYS
A803		Y729	D655	P579	THR
				N580	GLY
K804				L581	
E805		L733	M658		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.60Å 107.60Å 170.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00 45.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.00) 88.0 (45.46-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.244 , 0.305 0.267 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 92.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	T	0.74	0/180	1.08	0/276
2	P	0.87	0/180	0.87	0/276
3	A	0.46	0/6464	0.76	5/8749 (0.1%)
All	All	0.49	0/6824	0.78	5/9301 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	781	LEU	CA-CB-CG	6.48	130.21	115.30
3	A	151	ASP	N-CA-C	-5.34	96.58	111.00
3	A	568	ALA	N-CA-C	5.13	124.85	111.00
3	A	281	LEU	CA-CB-CG	5.11	127.04	115.30
3	A	191	ASP	N-CA-C	-5.09	97.27	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	T	161	20	91	36	0
2	P	161	20	91	57	0
3	A	6331	1408	6407	381	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	26	1	0
5	A	1	0	0	0	0
All	All	6674	1448	6615	441	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 33.

All (441) 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:P:954:DT:H2'	2:P:953:DC:C6	1.74	1.23
2:P:954:DT:H2'	2:P:953:DC:C5	1.77	1.20
1:T:905:DT:H4'	3:A:580:ASN:HB2	1.29	1.13
2:P:955:DA:H2''	2:P:954:DT:C7	1.78	1.12
1:T:906:DC:H4'	3:A:544:THR:HG23	1.19	1.10
1:T:902:DC:H2'	1:T:903:DG:C8	1.86	1.10
2:P:954:DT:H4'	3:A:537:GLU:OE2	1.54	1.07
3:A:780:LEU:HD11	3:A:790:GLU:HB2	1.38	1.05
2:P:955:DA:C2'	2:P:954:DT:H71	1.85	1.05
2:P:955:DA:H2''	2:P:954:DT:H71	1.36	1.04
2:P:955:DA:H2''	2:P:954:DT:C5	1.93	1.03
3:A:207:LEU:HB3	3:A:211:TRP:HE1	1.22	1.02
2:P:953:DC:H2''	2:P:952:DG:H5'	1.37	1.00
3:A:34:THR:HG22	3:A:40:PRO:HA	1.46	0.96
3:A:217:LEU:HG	3:A:218:LEU:HG	1.47	0.94
1:T:902:DC:H2'	1:T:903:DG:H8	1.27	0.92
3:A:728:ARG:HG2	3:A:751:MET:HG3	1.53	0.90
2:P:955:DA:C2'	2:P:954:DT:C7	2.45	0.90
2:P:954:DT:C2'	2:P:953:DC:C6	2.56	0.88
3:A:317:MET:HE1	3:A:362:ARG:HB3	1.57	0.86
2:P:952:DG:H2'	2:P:951:DC:C6	2.11	0.84
2:P:953:DC:H4'	3:A:585:PRO:HB3	1.59	0.84
2:P:953:DC:H1'	3:A:583:ASN:ND2	1.92	0.84
2:P:953:DC:H2'	2:P:952:DG:H8	1.42	0.84
1:T:908:DG:H21	2:P:958:DC:H41	1.23	0.84
3:A:34:THR:HB	3:A:38:GLY:O	1.79	0.83
3:A:300:PRO:HA	3:A:301:PRO:N	1.93	0.83
2:P:953:DC:H1'	3:A:583:ASN:HD22	1.44	0.83
3:A:340:LYS:HD2	3:A:343:ARG:HD2	1.59	0.82
3:A:137:ARG:HB3	3:A:156:LEU:HD13	1.60	0.82
1:T:901:DG:O5'	3:A:677:ARG:HD2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:955:DA:H5''	3:A:519:LEU:HG	1.60	0.81
3:A:207:LEU:HB3	3:A:211:TRP:NE1	1.94	0.81
3:A:302:PRO:HG3	3:A:331:ARG:NH2	1.95	0.81
2:P:953:DC:H2''	2:P:952:DG:C5'	2.11	0.81
3:A:89:PRO:HB2	3:A:92:PHE:HB2	1.63	0.80
3:A:640:THR:HG23	3:A:654:VAL:HG21	1.64	0.80
3:A:198:GLY:HA2	3:A:203:THR:HA	1.62	0.79
3:A:547:ASP:O	3:A:550:PRO:HD2	1.82	0.79
3:A:180:ALA:HA	3:A:245:LEU:HD12	1.66	0.78
2:P:958:DC:H2''	2:P:957:DG:C8	2.18	0.78
2:P:952:DG:H4'	3:A:784:HIS:CE1	2.20	0.77
3:A:292:LYS:HA	3:A:292:LYS:HE2	1.67	0.77
2:P:955:DA:H5''	3:A:519:LEU:CD2	2.15	0.77
2:P:951:DC:H5'	3:A:784:HIS:ND1	2.00	0.77
3:A:673:MET:HA	3:A:677:ARG:HH11	1.49	0.77
3:A:111:LEU:HD23	3:A:125:LEU:HD11	1.67	0.76
3:A:706:TRP:CZ3	3:A:749:PHE:HB2	2.21	0.76
3:A:750:ASN:C	3:A:750:ASN:HD22	1.90	0.75
1:T:906:DC:H4'	3:A:544:THR:CG2	2.10	0.75
3:A:202:LYS:HB2	3:A:207:LEU:HG	1.69	0.75
1:T:905:DT:H4'	3:A:580:ASN:CB	2.14	0.74
2:P:955:DA:H5''	3:A:519:LEU:CG	2.15	0.74
2:P:952:DG:O3'	3:A:784:HIS:CE1	2.41	0.74
3:A:634:GLU:OE1	3:A:636:ARG:HD2	1.87	0.73
3:A:695:ARG:HG2	4:A:1001:BGL:H3	1.70	0.73
1:T:905:DT:C4	1:T:906:DC:N4	2.56	0.73
3:A:374:MET:HE1	3:A:387:PRO:HA	1.70	0.73
3:A:182:TYR:CZ	3:A:208:LEU:HD13	2.24	0.73
1:T:906:DC:H1'	1:T:907:DC:O5'	1.90	0.72
3:A:324:LEU:HD23	3:A:341:ALA:HB3	1.72	0.71
3:A:808:GLU:HG3	3:A:817:LEU:O	1.91	0.71
3:A:607:VAL:HG12	3:A:609:LEU:HD11	1.70	0.71
1:T:904:DA:H2''	1:T:905:DT:C5'	2.21	0.71
3:A:673:MET:HA	3:A:677:ARG:HD3	1.72	0.70
2:P:953:DC:H2'	2:P:952:DG:C8	2.26	0.70
3:A:399:THR:O	3:A:405:ARG:HD2	1.90	0.70
3:A:684:ILE:HG23	3:A:685:PRO:HD3	1.73	0.70
3:A:651:ARG:O	3:A:654:VAL:HG22	1.91	0.70
1:T:908:DG:H21	2:P:958:DC:N4	1.90	0.69
3:A:140:THR:HG21	3:A:145:LEU:HD12	1.74	0.69
2:P:955:DA:H2''	2:P:954:DT:C6	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:902:DC:C2'	1:T:903:DG:H8	2.04	0.69
3:A:244:ASP:O	3:A:247:LYS:HB2	1.92	0.69
3:A:44:VAL:HG21	3:A:98:LEU:HD12	1.75	0.69
3:A:719:TYR:CD2	3:A:727:ARG:HG3	2.27	0.69
2:P:954:DT:C2'	2:P:953:DC:C5	2.69	0.69
3:A:464:ALA:O	3:A:467:ILE:HG12	1.91	0.68
3:A:487:ARG:O	3:A:491:GLU:HG3	1.94	0.68
2:P:958:DC:H2''	2:P:957:DG:H8	1.57	0.68
3:A:244:ASP:HA	3:A:247:LYS:HG3	1.75	0.68
3:A:68:ALA:HA	3:A:85:ARG:HH22	1.59	0.67
3:A:516:ALA:O	3:A:520:GLU:HG2	1.95	0.67
3:A:157:HIS:HB3	3:A:160:GLY:O	1.95	0.67
1:T:904:DA:H2''	1:T:905:DT:H5'	1.76	0.66
3:A:738:LYS:O	3:A:742:GLU:HG2	1.95	0.66
3:A:204:ALA:O	3:A:208:LEU:HG	1.96	0.66
2:P:955:DA:C5'	3:A:519:LEU:CD2	2.74	0.66
3:A:60:ASP:HB3	3:A:260:LYS:HG2	1.78	0.66
3:A:317:MET:HE2	3:A:358:VAL:HG12	1.77	0.66
3:A:10:PRO:HG3	3:A:152:ARG:HH12	1.61	0.65
3:A:317:MET:CE	3:A:362:ARG:HB3	2.26	0.65
2:P:952:DG:H4'	3:A:784:HIS:HE1	1.60	0.65
3:A:609:LEU:HG	3:A:821:VAL:HG12	1.78	0.65
3:A:202:LYS:HA	3:A:206:LYS:HB3	1.79	0.64
3:A:605:LEU:HD21	3:A:793:LYS:HD3	1.80	0.64
3:A:377:ALA:HB2	3:A:416:LEU:HD21	1.80	0.64
3:A:202:LYS:CB	3:A:207:LEU:HG	2.28	0.63
3:A:667:PHE:CZ	3:A:671:TYR:HE2	2.16	0.63
3:A:600:ALA:HB2	3:A:606:LEU:HG	1.79	0.63
3:A:211:TRP:N	3:A:211:TRP:CD1	2.66	0.63
1:T:907:DC:H2''	1:T:908:DG:C8	2.34	0.63
3:A:302:PRO:HG3	3:A:331:ARG:HH22	1.63	0.63
1:T:901:DG:H2'	1:T:902:DC:C6	2.33	0.63
3:A:665:ILE:HD11	3:A:692:PHE:HB3	1.80	0.63
3:A:388:GLU:HG3	3:A:398:TRP:CD1	2.34	0.62
3:A:127:LYS:HG3	3:A:250:THR:HB	1.82	0.62
3:A:200:GLY:O	3:A:201:GLU:HG2	2.00	0.62
1:T:902:DC:C2'	1:T:903:DG:C8	2.74	0.62
1:T:905:DT:H2''	1:T:906:DC:OP2	2.00	0.62
3:A:147:GLN:CD	3:A:248:VAL:HG21	2.19	0.62
3:A:354:LYS:O	3:A:358:VAL:HG23	1.99	0.62
2:P:951:DC:O3'	3:A:573:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:953:DC:C6	2:P:953:DC:OP2	2.53	0.61
1:T:908:DG:N2	2:P:958:DC:H41	1.96	0.61
3:A:52:LEU:HD11	3:A:285:PHE:CE1	2.35	0.61
3:A:810:VAL:HG13	3:A:811:TYR:H	1.66	0.61
3:A:248:VAL:O	3:A:248:VAL:HG23	2.00	0.61
3:A:68:ALA:HB2	3:A:112:GLU:HB2	1.82	0.61
3:A:545:TYR:O	3:A:549:LEU:HD13	2.00	0.61
3:A:526:HIS:O	3:A:529:VAL:HG22	2.00	0.61
3:A:673:MET:HA	3:A:677:ARG:NH1	2.15	0.61
2:P:953:DC:C2	2:P:952:DG:C8	2.89	0.61
3:A:655:ASP:OD1	3:A:658:MET:HB2	2.00	0.61
3:A:346:LYS:O	3:A:368:PRO:HD2	2.01	0.60
3:A:24:TYR:HA	3:A:92:PHE:HE1	1.64	0.60
1:T:904:DA:H2''	1:T:905:DT:O5'	2.00	0.60
3:A:607:VAL:HG12	3:A:609:LEU:CD1	2.31	0.60
3:A:482:PHE:HE2	3:A:490:LEU:HD23	1.67	0.59
3:A:480:HIS:HE1	3:A:493:VAL:HG13	1.67	0.59
3:A:57:GLU:HB3	3:A:137:ARG:HH12	1.66	0.59
3:A:317:MET:CE	3:A:358:VAL:HG12	2.31	0.59
3:A:351:LEU:HD23	3:A:398:TRP:CZ3	2.37	0.59
3:A:149:LEU:HD11	3:A:163:ILE:O	2.03	0.59
3:A:465:GLU:HG3	3:A:469:ARG:NH2	2.18	0.58
3:A:449:VAL:HG12	3:A:780:LEU:HD13	1.85	0.58
3:A:85:ARG:N	3:A:88:THR:HG1	2.01	0.58
3:A:227:ALA:N	3:A:230:GLU:HB3	2.19	0.58
3:A:287:LEU:O	3:A:288:LEU:HD23	2.03	0.58
3:A:541:LEU:HD23	3:A:590:LEU:HD12	1.84	0.58
3:A:230:GLU:O	3:A:233:LEU:HD12	2.03	0.58
3:A:154:HIS:CD2	3:A:164:THR:HG22	2.38	0.58
1:T:906:DC:C4'	3:A:544:THR:HG23	2.12	0.58
3:A:286:GLY:O	3:A:289:GLU:HG2	2.04	0.57
3:A:673:MET:HG3	3:A:677:ARG:NH1	2.19	0.57
2:P:953:DC:O2	2:P:952:DG:C8	2.58	0.57
3:A:631:VAL:HG11	3:A:638:ILE:HA	1.85	0.57
3:A:523:ARG:HA	3:A:529:VAL:HG21	1.87	0.57
3:A:163:ILE:HG23	3:A:167:TRP:CD1	2.39	0.57
3:A:595:ARG:NH2	3:A:828:LEU:HD12	2.20	0.57
3:A:149:LEU:HD21	3:A:163:ILE:HG22	1.86	0.56
1:T:907:DC:H1'	1:T:908:DG:H5'	1.86	0.56
3:A:797:GLU:O	3:A:801:ARG:HG3	2.04	0.56
1:T:907:DC:H3'	1:T:907:DC:OP1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:906:DC:H2''	1:T:907:DC:OP2	2.05	0.56
3:A:358:VAL:HG22	3:A:442:ALA:HA	1.88	0.56
3:A:103:VAL:HG11	3:A:110:ARG:HG3	1.87	0.56
3:A:22:LEU:O	3:A:26:THR:HG23	2.06	0.56
3:A:224:LEU:HB3	3:A:229:ARG:HB2	1.88	0.56
3:A:769:PHE:HB3	3:A:770:PRO:HD3	1.87	0.56
3:A:802:LEU:O	3:A:806:VAL:HG23	2.06	0.56
3:A:95:GLN:O	3:A:99:ILE:HG12	2.06	0.56
3:A:471:GLU:O	3:A:474:VAL:HG22	2.07	0.56
3:A:211:TRP:N	3:A:211:TRP:HD1	2.04	0.55
3:A:688:GLU:O	3:A:691:ALA:HB3	2.05	0.55
3:A:310:VAL:HG21	3:A:400:GLU:O	2.06	0.55
3:A:484:LEU:HD23	3:A:485:ASN:H	1.71	0.55
3:A:586:VAL:HG12	3:A:587:ARG:HG3	1.89	0.55
3:A:196:VAL:HB	3:A:204:ALA:HB2	1.89	0.55
2:P:951:DC:H2'	3:A:754:GLN:NE2	2.21	0.55
3:A:10:PRO:HG3	3:A:152:ARG:NH1	2.21	0.55
3:A:35:THR:O	3:A:37:ARG:N	2.39	0.55
3:A:673:MET:HG3	3:A:677:ARG:HH11	1.72	0.55
3:A:709:LYS:O	3:A:712:GLU:HB3	2.07	0.55
3:A:179:TRP:CZ3	3:A:183:ARG:HG3	2.42	0.55
3:A:605:LEU:CD2	3:A:793:LYS:HA	2.36	0.55
3:A:116:TYR:CZ	3:A:252:LEU:HD12	2.41	0.55
3:A:217:LEU:CG	3:A:218:LEU:HG	2.29	0.54
3:A:227:ALA:H	3:A:230:GLU:HB3	1.73	0.54
3:A:475:PHE:CE1	3:A:482:PHE:O	2.61	0.54
3:A:30:LEU:HB2	3:A:42:GLN:HB2	1.88	0.54
3:A:474:VAL:HG12	3:A:531:LYS:HB2	1.89	0.54
3:A:722:THR:HG22	3:A:755:GLY:HA3	1.90	0.54
3:A:535:TYR:O	3:A:539:THR:HG23	2.08	0.54
2:P:953:DC:C2'	2:P:952:DG:C5'	2.82	0.54
3:A:723:LEU:HB3	3:A:756:THR:HG23	1.88	0.54
3:A:197:LYS:HD3	3:A:227:ALA:HB2	1.90	0.54
3:A:249:ARG:HG3	3:A:252:LEU:HD21	1.89	0.54
3:A:58:ASP:HB2	3:A:261:ARG:NH2	2.23	0.54
2:P:955:DA:C5'	3:A:519:LEU:HD21	2.38	0.53
3:A:53:LYS:HA	3:A:56:LYS:HD3	1.90	0.53
3:A:682:LEU:HB3	3:A:685:PRO:HD2	1.89	0.53
3:A:211:TRP:H	3:A:211:TRP:HD1	1.57	0.53
3:A:147:GLN:OE1	3:A:248:VAL:HG21	2.09	0.53
3:A:562:THR:HG23	3:A:579:PRO:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:TRP:CH2	3:A:183:ARG:HG3	2.44	0.53
3:A:298:PRO:O	3:A:333:HIS:HD2	1.92	0.53
3:A:465:GLU:HG3	3:A:469:ARG:CZ	2.38	0.53
3:A:149:LEU:HD13	3:A:155:VAL:HG23	1.91	0.53
3:A:595:ARG:HH21	3:A:828:LEU:HD12	1.74	0.53
3:A:24:TYR:HA	3:A:92:PHE:CE1	2.43	0.53
1:T:907:DC:C5	1:T:908:DG:C6	2.97	0.53
3:A:592:GLN:HE21	3:A:828:LEU:HD11	1.74	0.53
3:A:34:THR:HG22	3:A:40:PRO:CA	2.29	0.52
2:P:955:DA:H2'	2:P:954:DT:C7	2.36	0.52
1:T:902:DC:OP2	1:T:902:DC:H6	1.92	0.52
3:A:155:VAL:HB	3:A:163:ILE:HB	1.90	0.52
3:A:45:TYR:HE1	3:A:49:LYS:HD3	1.74	0.52
3:A:19:GLY:HA2	3:A:47:PHE:HE2	1.72	0.52
2:P:953:DC:C2'	2:P:952:DG:O5'	2.58	0.52
3:A:243:TRP:HD1	3:A:244:ASP:N	2.07	0.52
3:A:306:PHE:HA	3:A:349:ARG:O	2.09	0.52
3:A:554:HIS:CE1	3:A:556:ARG:HB2	2.45	0.52
2:P:955:DA:C3'	2:P:954:DT:H71	2.40	0.52
3:A:371:ASP:HB3	3:A:413:PHE:CE2	2.45	0.52
3:A:664:THR:HG21	3:A:682:LEU:HD22	1.92	0.52
3:A:149:LEU:CD2	3:A:163:ILE:HG22	2.40	0.51
3:A:482:PHE:CD2	3:A:493:VAL:HG21	2.45	0.51
3:A:183:ARG:NH1	3:A:188:ASP:HB2	2.25	0.51
3:A:580:ASN:OD1	3:A:582:GLN:HB2	2.10	0.51
3:A:609:LEU:HD21	3:A:803:ALA:HB3	1.91	0.51
3:A:40:PRO:HD2	3:A:94:ARG:NH1	2.25	0.51
3:A:226:PRO:O	3:A:228:ILE:N	2.43	0.51
3:A:453:VAL:HA	3:A:456:LEU:HB2	1.93	0.51
2:P:958:DC:C2'	2:P:957:DG:C8	2.90	0.51
3:A:307:VAL:HG21	3:A:356:LEU:HD22	1.92	0.51
3:A:183:ARG:HE	3:A:245:LEU:HD21	1.74	0.51
3:A:377:ALA:HB2	3:A:416:LEU:CD2	2.40	0.51
3:A:143:LYS:HE3	3:A:183:ARG:HH11	1.75	0.51
3:A:750:ASN:C	3:A:750:ASN:ND2	2.63	0.51
1:T:907:DC:H2''	1:T:908:DG:O5'	2.10	0.51
3:A:642:THR:HG23	3:A:700:PHE:HE2	1.76	0.51
3:A:36:SER:O	3:A:37:ARG:HG3	2.11	0.50
3:A:632:PHE:HB2	3:A:815:VAL:HG11	1.94	0.50
3:A:22:LEU:HD11	3:A:139:LEU:HD22	1.93	0.50
2:P:952:DG:OP1	3:A:586:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:164:THR:O	3:A:167:TRP:HB3	2.11	0.50
3:A:552:LEU:HB3	3:A:560:LEU:HD13	1.93	0.50
3:A:547:ASP:HB2	3:A:548:PRO:HD3	1.92	0.50
3:A:514:THR:O	3:A:519:LEU:N	2.44	0.50
1:T:901:DG:N7	3:A:677:ARG:NH2	2.60	0.50
3:A:322:LEU:O	3:A:323:ALA:HB3	2.11	0.50
3:A:699:SER:O	3:A:701:PRO:HD3	2.12	0.50
3:A:218:LEU:O	3:A:219:LYS:HB2	2.11	0.49
3:A:682:LEU:HB3	3:A:685:PRO:HG2	1.93	0.49
3:A:665:ILE:O	3:A:669:VAL:HG23	2.12	0.49
2:P:951:DC:H2'	3:A:754:GLN:HE22	1.77	0.49
3:A:215:GLU:O	3:A:216:ALA:HB3	2.11	0.49
3:A:528:ILE:O	3:A:532:ILE:HG23	2.13	0.49
3:A:585:PRO:O	3:A:591:GLY:HA3	2.12	0.49
3:A:682:LEU:HB3	3:A:685:PRO:CD	2.42	0.49
3:A:301:PRO:HG2	3:A:326:ALA:HB3	1.94	0.49
3:A:595:ARG:HH22	3:A:831:LYS:HA	1.78	0.49
3:A:639:HIS:CD2	3:A:663:LYS:HA	2.48	0.49
2:P:957:DG:H2''	2:P:956:DG:OP2	2.11	0.49
3:A:199:ILE:HD12	3:A:225:LYS:HE3	1.94	0.49
3:A:706:TRP:HE3	3:A:707:ILE:HD13	1.77	0.49
3:A:199:ILE:HG13	3:A:226:PRO:O	2.12	0.49
3:A:68:ALA:HB3	3:A:113:VAL:O	2.13	0.48
3:A:164:THR:H	3:A:167:TRP:HB3	1.79	0.48
3:A:186:THR:OG1	3:A:208:LEU:HD21	2.13	0.48
3:A:742:GLU:O	3:A:745:GLU:HB2	2.12	0.48
2:P:953:DC:C5	2:P:953:DC:OP2	2.66	0.48
3:A:173:GLY:C	3:A:174:LEU:HD22	2.33	0.48
3:A:249:ARG:HE	3:A:252:LEU:HD11	1.78	0.48
3:A:605:LEU:HD23	3:A:793:LYS:HA	1.95	0.48
3:A:706:TRP:CE3	3:A:707:ILE:HD13	2.47	0.48
3:A:729:TYR:N	3:A:729:TYR:CD1	2.81	0.48
3:A:52:LEU:HD11	3:A:285:PHE:CD1	2.48	0.48
3:A:420:LEU:O	3:A:423:GLU:HB2	2.13	0.48
3:A:750:ASN:ND2	3:A:754:GLN:HG3	2.29	0.48
3:A:123:ALA:HB1	3:A:148:LEU:HD21	1.96	0.48
3:A:465:GLU:O	3:A:468:ALA:HB3	2.13	0.48
3:A:595:ARG:NH2	3:A:828:LEU:HA	2.29	0.48
2:P:953:DC:OP2	2:P:953:DC:H6	1.95	0.48
3:A:611:TYR:HB2	3:A:785:ASP:HB3	1.95	0.47
3:A:625:ASP:HB2	3:A:702:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:149:LEU:O	3:A:176:PRO:HG2	2.13	0.47
3:A:625:ASP:OD2	3:A:700:PHE:HD1	1.97	0.47
3:A:795:ARG:O	3:A:799:VAL:HG23	2.14	0.47
3:A:810:VAL:HG13	3:A:811:TYR:N	2.29	0.47
3:A:86:ALA:HB3	3:A:87:PRO:CD	2.44	0.47
3:A:169:TRP:O	3:A:173:GLY:HA2	2.14	0.47
3:A:437:LEU:HD22	3:A:762:LYS:HG2	1.97	0.47
3:A:625:ASP:O	3:A:627:ASN:N	2.47	0.47
3:A:699:SER:C	3:A:701:PRO:HD3	2.35	0.47
3:A:632:PHE:HB2	3:A:815:VAL:CG1	2.45	0.47
3:A:86:ALA:HB3	3:A:87:PRO:HD3	1.96	0.47
3:A:41:VAL:HG22	3:A:41:VAL:O	2.15	0.47
3:A:713:GLU:HB3	3:A:717:ARG:HH11	1.79	0.47
3:A:228:ILE:O	3:A:232:ILE:HG13	2.15	0.47
3:A:140:THR:O	3:A:158:PRO:HD3	2.14	0.46
3:A:187:GLY:O	3:A:191:ASP:HB3	2.16	0.46
3:A:26:THR:OG1	3:A:43:ALA:HA	2.15	0.46
3:A:673:MET:HE2	3:A:681:GLU:OE2	2.15	0.46
1:T:903:DG:O6	2:P:954:DT:C4	2.68	0.46
3:A:313:ARG:HD3	3:A:318:TRP:O	2.15	0.46
3:A:589:PRO:HB3	3:A:593:ARG:NH1	2.30	0.46
2:P:951:DC:C2'	3:A:754:GLN:NE2	2.79	0.46
1:T:902:DC:H2''	1:T:903:DG:O4'	2.15	0.46
3:A:351:LEU:HD23	3:A:398:TRP:HZ3	1.80	0.46
3:A:611:TYR:HB3	3:A:614:ILE:HB	1.98	0.46
3:A:654:VAL:O	3:A:654:VAL:HG23	2.16	0.46
3:A:183:ARG:CZ	3:A:188:ASP:HB2	2.46	0.46
3:A:478:ALA:HA	3:A:497:GLU:OE2	2.15	0.46
3:A:90:GLU:HG3	3:A:91:ASP:H	1.80	0.46
3:A:216:ALA:HB2	3:A:221:LEU:HD12	1.96	0.46
3:A:604:TRP:HZ3	3:A:778:ARG:HG2	1.79	0.46
3:A:743:ALA:O	3:A:746:ARG:HB3	2.15	0.46
3:A:300:PRO:O	3:A:301:PRO:HA	2.16	0.46
3:A:771:ARG:HA	3:A:774:GLU:CD	2.37	0.45
3:A:112:GLU:HG3	3:A:112:GLU:O	2.16	0.45
3:A:317:MET:HE1	3:A:362:ARG:CB	2.36	0.45
3:A:607:VAL:CG1	3:A:609:LEU:HD11	2.44	0.45
3:A:639:HIS:CD2	3:A:666:ASN:HD22	2.34	0.45
3:A:157:HIS:CE1	3:A:159:GLU:HB2	2.51	0.45
3:A:306:PHE:O	3:A:326:ALA:HA	2.17	0.45
3:A:514:THR:HA	3:A:518:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:VAL:HG11	3:A:108:LEU:HD22	1.98	0.45
3:A:737:VAL:O	3:A:740:VAL:HG12	2.16	0.45
3:A:137:ARG:HB3	3:A:156:LEU:CD1	2.39	0.45
3:A:207:LEU:HD13	3:A:211:TRP:CZ2	2.51	0.45
3:A:19:GLY:HA2	3:A:47:PHE:CE2	2.51	0.45
3:A:26:THR:HA	3:A:29:ALA:HB3	1.99	0.45
3:A:826:ASP:OD1	3:A:828:LEU:HB3	2.17	0.45
3:A:160:GLY:O	3:A:161:TYR:CD1	2.70	0.45
3:A:193:LEU:HD13	3:A:242:SER:OG	2.17	0.45
3:A:226:PRO:HA	3:A:230:GLU:HB2	1.99	0.45
3:A:410:GLU:HG3	3:A:411:ARG:N	2.32	0.45
3:A:497:GLU:O	3:A:498:LEU:HG	2.17	0.45
1:T:906:DC:H1'	1:T:907:DC:C5'	2.47	0.45
3:A:324:LEU:HD23	3:A:341:ALA:CB	2.42	0.44
3:A:482:PHE:H	3:A:482:PHE:HD1	1.65	0.44
3:A:607:VAL:HG13	3:A:823:ILE:HG12	1.99	0.44
3:A:202:LYS:HA	3:A:206:LYS:CB	2.44	0.44
3:A:605:LEU:CD2	3:A:793:LYS:HD3	2.47	0.44
3:A:532:ILE:HG13	3:A:533:LEU:N	2.32	0.44
3:A:800:ALA:CB	3:A:823:ILE:HD11	2.47	0.44
2:P:951:DC:C6	2:P:951:DC:OP2	2.70	0.44
3:A:16:LEU:HD12	3:A:138:ILE:HG12	1.99	0.44
3:A:229:ARG:NH1	3:A:233:LEU:HD11	2.33	0.44
2:P:951:DC:OP2	2:P:951:DC:C5	2.71	0.44
3:A:28:HIS:HA	3:A:31:LYS:HE2	2.00	0.44
3:A:527:PRO:O	3:A:531:LYS:HG2	2.18	0.44
3:A:11:LYS:HD2	3:A:11:LYS:HA	1.83	0.44
3:A:90:GLU:HG3	3:A:91:ASP:N	2.33	0.44
3:A:217:LEU:HD12	3:A:239:LEU:CD1	2.48	0.43
3:A:319:ALA:O	3:A:362:ARG:NH2	2.51	0.43
1:T:905:DT:C4'	3:A:580:ASN:HD22	2.31	0.43
3:A:236:MET:O	3:A:237:ASP:HB2	2.19	0.43
3:A:382:PRO:HB2	3:A:728:ARG:NH2	2.34	0.43
3:A:627:ASN:O	3:A:630:ARG:HB3	2.18	0.43
3:A:751:MET:HB3	3:A:752:PRO:HD3	2.01	0.43
3:A:538:LEU:HD23	3:A:538:LEU:HA	1.83	0.43
3:A:140:THR:HG21	3:A:145:LEU:CD1	2.44	0.43
3:A:100:LYS:HB3	3:A:110:ARG:HD2	2.01	0.43
3:A:16:LEU:HD11	3:A:126:ALA:CA	2.49	0.43
3:A:438:SER:HA	3:A:566:GLN:NE2	2.33	0.43
2:P:953:DC:P	2:P:953:DC:H6	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:123:ALA:HA	3:A:148:LEU:HD11	1.99	0.43
3:A:382:PRO:C	3:A:384:ASN:H	2.22	0.43
3:A:473:GLU:O	3:A:476:ARG:HB3	2.19	0.43
3:A:17:VAL:HB	3:A:64:VAL:HG22	2.01	0.43
3:A:267:GLU:HG3	3:A:268:ARG:N	2.34	0.43
3:A:376:LEU:HD22	3:A:420:LEU:HD13	2.01	0.43
3:A:428:TRP:NE1	3:A:432:GLU:HG3	2.34	0.43
3:A:624:GLY:HA2	3:A:629:ILE:HD11	2.00	0.43
2:P:954:DT:OP2	2:P:954:DT:H71	2.19	0.43
3:A:201:GLU:O	3:A:206:LYS:HE2	2.18	0.42
3:A:30:LEU:O	3:A:32:GLY:N	2.52	0.42
3:A:33:LEU:HB2	3:A:42:GLN:HB3	2.01	0.42
3:A:137:ARG:HA	3:A:154:HIS:O	2.19	0.42
3:A:52:LEU:HA	3:A:52:LEU:HD12	1.77	0.42
3:A:523:ARG:HH21	3:A:530:GLU:HG3	1.84	0.42
3:A:715:ARG:HB2	3:A:734:GLU:HG2	2.01	0.42
3:A:106:LEU:HD11	3:A:285:PHE:HE1	1.84	0.42
3:A:335:ALA:HB1	3:A:341:ALA:HB2	2.01	0.42
3:A:351:LEU:HD11	3:A:374:MET:HE2	2.02	0.42
3:A:605:LEU:HD23	3:A:793:LYS:O	2.19	0.42
3:A:628:LEU:HD13	3:A:700:PHE:CE1	2.54	0.42
3:A:811:TYR:HA	3:A:812:PRO:HD3	1.84	0.42
1:T:902:DC:OP2	1:T:902:DC:C6	2.72	0.42
3:A:224:LEU:HG	3:A:225:LYS:N	2.34	0.42
3:A:518:VAL:HG12	3:A:518:VAL:O	2.19	0.42
3:A:692:PHE:CD1	3:A:692:PHE:N	2.87	0.42
3:A:581:LEU:HB2	3:A:783:VAL:HG13	2.01	0.42
3:A:231:LYS:HD3	3:A:231:LYS:HA	1.86	0.42
3:A:465:GLU:O	3:A:469:ARG:HG3	2.19	0.42
3:A:378:TYR:CZ	3:A:567:THR:HA	2.54	0.42
3:A:670:LEU:H	3:A:670:LEU:HD22	1.84	0.42
3:A:239:LEU:C	3:A:241:LEU:H	2.23	0.42
3:A:287:LEU:C	3:A:288:LEU:HD23	2.40	0.42
3:A:295:GLU:H	3:A:295:GLU:CD	2.23	0.42
3:A:311:LEU:HB3	3:A:319:ALA:HB1	2.00	0.42
3:A:43:ALA:HB3	3:A:95:GLN:OE1	2.20	0.42
3:A:758:ALA:O	3:A:762:LYS:HD3	2.20	0.42
3:A:299:TRP:HB3	3:A:300:PRO:HD3	2.02	0.42
3:A:175:ARG:HB2	3:A:177:ASP:OD1	2.20	0.41
3:A:183:ARG:NE	3:A:245:LEU:HD21	2.35	0.41
3:A:450:ARG:HH12	3:A:602:GLU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:66:PHE:HZ	3:A:99:ILE:HG22	1.83	0.41
3:A:692:PHE:HD1	3:A:692:PHE:N	2.18	0.41
1:T:907:DC:C2'	1:T:908:DG:C8	3.02	0.41
3:A:218:LEU:O	3:A:219:LYS:CB	2.68	0.41
3:A:447:THR:HG22	3:A:448:GLY:O	2.19	0.41
3:A:625:ASP:CB	3:A:702:LYS:HB2	2.49	0.41
3:A:198:GLY:HA2	3:A:203:THR:CA	2.42	0.41
3:A:682:LEU:HB3	3:A:685:PRO:CG	2.51	0.41
3:A:733:LEU:HA	3:A:733:LEU:HD23	1.89	0.41
3:A:722:THR:CG2	3:A:755:GLY:HA3	2.49	0.41
3:A:495:PHE:N	3:A:495:PHE:CD1	2.86	0.41
3:A:17:VAL:HB	3:A:64:VAL:HA	2.02	0.41
3:A:778:ARG:HG3	3:A:790:GLU:HB3	2.02	0.41
3:A:314:LYS:O	3:A:316:PRO:HD3	2.20	0.41
2:P:951:DC:H5'	3:A:784:HIS:CG	2.55	0.41
1:T:904:DA:C2'	1:T:905:DT:O5'	2.66	0.41
3:A:667:PHE:CE2	3:A:671:TYR:HE2	2.38	0.41
3:A:524:GLU:HG3	3:A:526:HIS:HB2	2.02	0.41
2:P:951:DC:C2'	3:A:754:GLN:HE22	2.33	0.41
3:A:202:LYS:CA	3:A:206:LYS:HB3	2.49	0.41
3:A:225:LYS:HE3	3:A:225:LYS:HB3	1.87	0.41
3:A:276:LEU:N	3:A:276:LEU:HD23	2.36	0.41
3:A:684:ILE:CG2	3:A:685:PRO:HD3	2.47	0.41
3:A:749:PHE:C	3:A:752:PRO:HD2	2.41	0.41
3:A:328:ARG:C	3:A:330:GLY:H	2.25	0.41
3:A:767:LYS:O	3:A:770:PRO:HD2	2.21	0.41
1:T:905:DT:C2	1:T:906:DC:C5	3.09	0.41
3:A:574:LEU:HD12	3:A:782:GLN:HE21	1.86	0.41
3:A:518:VAL:HA	3:A:521:ALA:HB3	2.03	0.40
3:A:733:LEU:HD11	3:A:748:ALA:HB2	2.02	0.40
2:P:955:DA:H5"	3:A:519:LEU:HD23	2.00	0.40
3:A:299:TRP:HB3	3:A:300:PRO:CD	2.52	0.40
3:A:552:LEU:HB3	3:A:560:LEU:CD1	2.52	0.40
3:A:609:LEU:HD21	3:A:803:ALA:CB	2.51	0.40
3:A:129:ALA:HB2	3:A:258:PHE:CE2	2.56	0.40
3:A:27:PHE:HA	3:A:43:ALA:HB2	2.02	0.40
3:A:106:LEU:HD21	3:A:285:PHE:CD1	2.56	0.40
3:A:304:GLY:O	3:A:349:ARG:NH1	2.55	0.40
3:A:470:LEU:HD13	3:A:470:LEU:HA	1.93	0.40
3:A:143:LYS:HE3	3:A:183:ARG:NH1	2.37	0.40
3:A:609:LEU:N	3:A:609:LEU:HD12	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	785/832 (94%)	653 (83%)	93 (12%)	39 (5%)	2	12

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	LYS
3	A	37	ARG
3	A	86	ALA
3	A	161	TYR
3	A	220	ASN
3	A	221	LEU
3	A	496	ASP
3	A	517	ALA
3	A	626	GLU
3	A	674	SER
3	A	675	ALA
3	A	793	LYS
3	A	36	SER
3	A	190	SER
3	A	208	LEU
3	A	215	GLU
3	A	216	ALA
3	A	219	LYS
3	A	227	ALA
3	A	487	ARG
3	A	625	ASP
3	A	203	THR
3	A	486	SER
3	A	149	LEU
3	A	288	LEU

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Mol	Chain	Res	Type
3	A	516	ALA
3	A	602	GLU
3	A	132	GLU
3	A	197	LYS
3	A	199	ILE
3	A	567	THR
3	A	637	ASP
3	A	683	ALA
3	A	39	GLU
3	A	299	TRP
3	A	256	VAL
3	A	198	GLY
3	A	226	PRO
3	A	382	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
3	A	655/683 (96%)	572 (87%)	83 (13%)	4 19

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	36	SER
3	A	42	GLN
3	A	52	LEU
3	A	57	GLU
3	A	90	GLU
3	A	139	LEU
3	A	144	ASP
3	A	150	SER
3	A	159	GLU
3	A	161	TYR
3	A	162	LEU
3	A	168	LEU

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Mol	Chain	Res	Type
3	A	169	TRP
3	A	170	GLU
3	A	178	GLN
3	A	182	TYR
3	A	189	GLU
3	A	205	ARG
3	A	211	TRP
3	A	229	ARG
3	A	233	LEU
3	A	243	TRP
3	A	245	LEU
3	A	247	LYS
3	A	249	ARG
3	A	252	LEU
3	A	254	LEU
3	A	255	GLU
3	A	257	ASP
3	A	261	ARG
3	A	262	ARG
3	A	283	HIS
3	A	288	LEU
3	A	292	LYS
3	A	307	VAL
3	A	322	LEU
3	A	328	ARG
3	A	337	GLU
3	A	343	ARG
3	A	362	ARG
3	A	365	LEU
3	A	383	SER
3	A	390	VAL
3	A	397	GLU
3	A	419	ARG
3	A	456	LEU
3	A	519	LEU
3	A	523	ARG
3	A	524	GLU
3	A	526	HIS
3	A	541	LEU
3	A	579	PRO
3	A	583	ASN
3	A	590	LEU

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Mol	Chain	Res	Type
3	A	593	ARG
3	A	617	ARG
3	A	619	LEU
3	A	633	GLN
3	A	636	ARG
3	A	658	MET
3	A	670	LEU
3	A	680	GLN
3	A	681	GLU
3	A	682	LEU
3	A	686	TYR
3	A	694	GLU
3	A	699	SER
3	A	728	ARG
3	A	736	ARG
3	A	745	GLU
3	A	746	ARG
3	A	747	MET
3	A	750	ASN
3	A	751	MET
3	A	752	PRO
3	A	781	LEU
3	A	782	GLN
3	A	783	VAL
3	A	795	ARG
3	A	805	GLU
3	A	815	VAL
3	A	817	LEU
3	A	820	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	20	HIS
3	A	154	HIS
3	A	333	HIS
3	A	489	GLN
3	A	566	GLN
3	A	583	ASN
3	A	592	GLN
3	A	633	GLN
3	A	639	HIS

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Mol	Chain	Res	Type
3	A	750	ASN
3	A	782	GLN
3	A	784	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
4	BGL	A	1001	-	20,20,20	1.17	3 (15%)	24,25,25	2.59	12 (50%)

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
4	BGL	A	1001	-	-	3/11/31/31	0/1/1/1



All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	BGL	O3-C3	-3.12	1.35	1.43
4	A	1001	BGL	O4-C4	-2.48	1.37	1.43
4	A	1001	BGL	C4-C3	2.32	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	BGL	O2-C2-C3	5.54	121.41	109.83
4	A	1001	BGL	C1-O5-C5	-5.36	103.55	113.66
4	A	1001	BGL	C6-C5-C4	4.20	122.83	113.00
4	A	1001	BGL	O3-C3-C4	-4.02	101.05	110.35
4	A	1001	BGL	C4-C3-C2	3.73	118.20	109.68
4	A	1001	BGL	O1-C1-O5	-3.64	99.47	110.38
4	A	1001	BGL	O6-C6-C5	-2.62	102.29	111.29
4	A	1001	BGL	O1-C1-C2	2.45	120.96	110.04
4	A	1001	BGL	O5-C1-C2	-2.41	102.37	109.93
4	A	1001	BGL	C1'-O2-C2	2.09	119.31	114.32
4	A	1001	BGL	C3'-C2'-C1'	2.09	122.75	113.49
4	A	1001	BGL	C3-C4-C5	-2.00	106.67	110.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	BGL	C3-C2-O2-C1'
4	A	1001	BGL	O2-C1'-C2'-C3'
4	A	1001	BGL	C3'-C4'-C5'-C6'

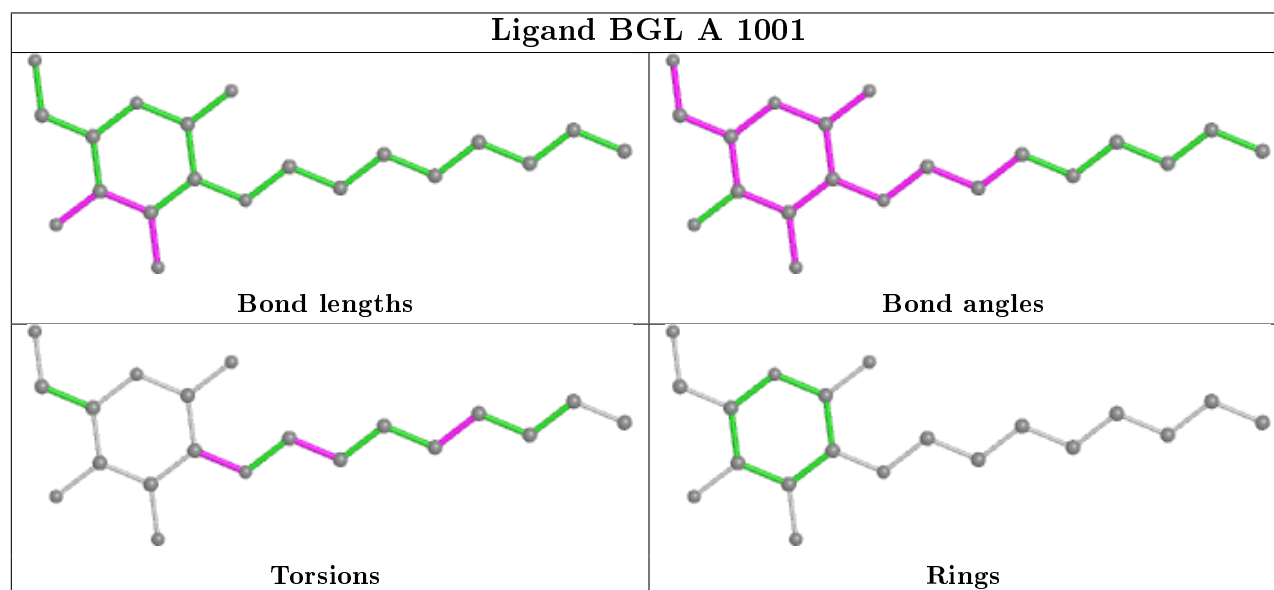
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	BGL	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	300:PRO	C	301:PRO	N	3.05

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	T	8/8 (100%)	3.00	6 (75%) 0 0	57, 59, 61, 61	0
2	P	8/8 (100%)	3.50	6 (75%) 0 0	57, 60, 62, 62	0
3	A	793/832 (95%)	0.14	51 (6%) 19 6	10, 37, 95, 100	0
All	All	809/848 (95%)	0.20	63 (7%) 13 4	10, 38, 95, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	517	ALA	10.6
3	A	211	TRP	7.7
3	A	194	PRO	7.6
3	A	518	VAL	7.4
3	A	516	ALA	6.8
3	A	217	LEU	6.7
2	P	958	DC	6.5
3	A	674	SER	6.2
3	A	197	LYS	5.9
3	A	200	GLY	5.8
3	A	228	ILE	5.7
1	T	907	DC	5.2
3	A	199	ILE	5.1
3	A	198	GLY	5.1
3	A	236	MET	4.8
1	T	908	DG	4.7
3	A	497	GLU	4.7
2	P	954	DT	4.6
3	A	203	THR	4.5
3	A	88	THR	4.4
3	A	498	LEU	4.3
2	P	955	DA	4.1
3	A	218	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	A	212	GLY	3.9
2	P	957	DG	3.9
3	A	513	SER	3.9
3	A	201	GLU	3.7
3	A	515	SER	3.7
3	A	794	GLU	3.5
2	P	956	DG	3.4
2	P	953	DC	3.2
3	A	86	ALA	3.2
3	A	291	PRO	3.2
3	A	514	THR	3.1
1	T	903	DG	3.1
3	A	202	LYS	3.0
3	A	89	PRO	3.0
3	A	520	GLU	2.9
1	T	901	DG	2.8
3	A	290	SER	2.8
1	T	906	DC	2.8
3	A	487	ARG	2.7
3	A	482	PHE	2.7
3	A	191	ASP	2.7
3	A	87	PRO	2.7
3	A	245	LEU	2.5
1	T	905	DT	2.5
3	A	267	GLU	2.5
3	A	488	ASP	2.5
3	A	292	LYS	2.4
3	A	522	LEU	2.3
3	A	526	HIS	2.3
3	A	193	LEU	2.3
3	A	686	TYR	2.3
3	A	295	GLU	2.2
3	A	219	LYS	2.2
3	A	208	LEU	2.2
3	A	237	ASP	2.1
3	A	225	LYS	2.1
3	A	478	ALA	2.0
3	A	525	ALA	2.0
3	A	185	LEU	2.0
3	A	671	TYR	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](#)

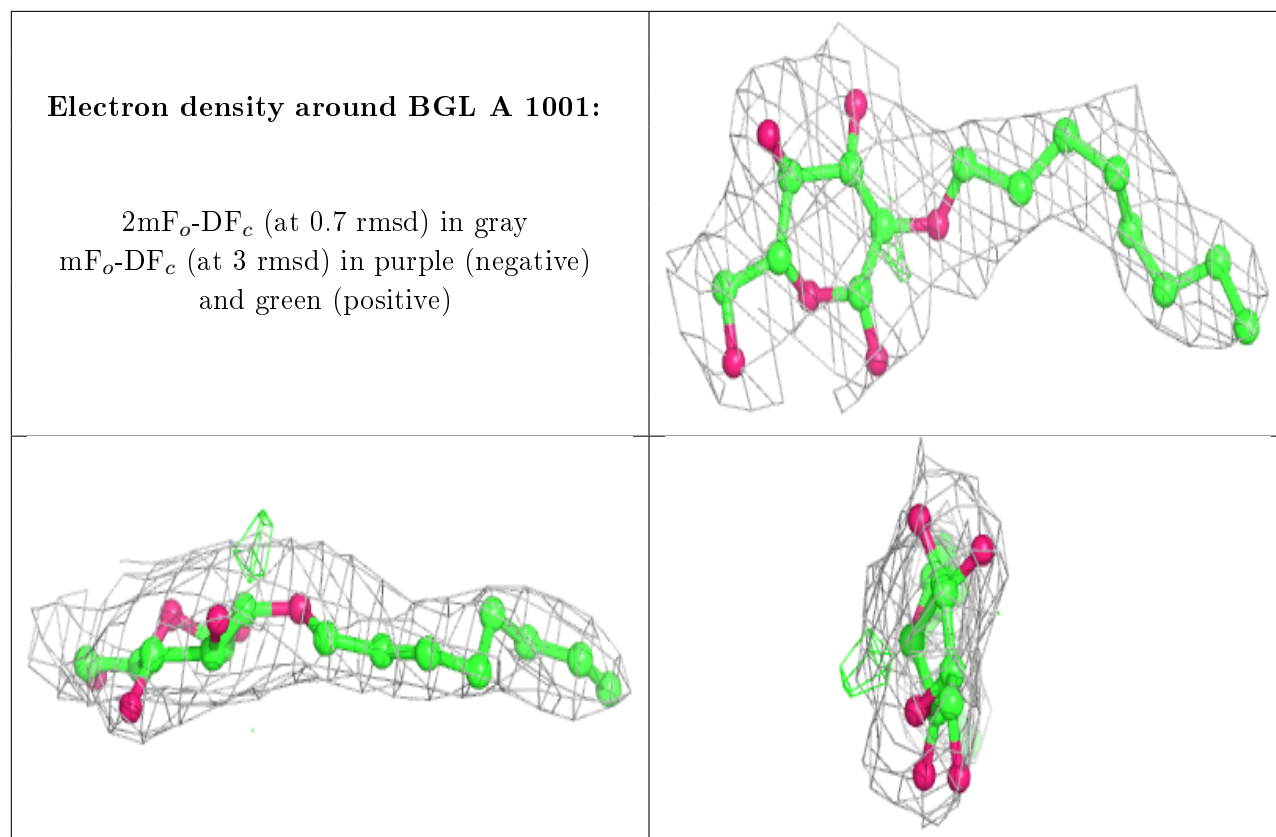
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
4	BGL	A	1001	20/20	0.94	0.21	10,22,41,46	0
5	ZN	A	900	1/1	0.97	0.08	58,58,58,58	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.