



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2017 – 05:27 AM EST

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

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

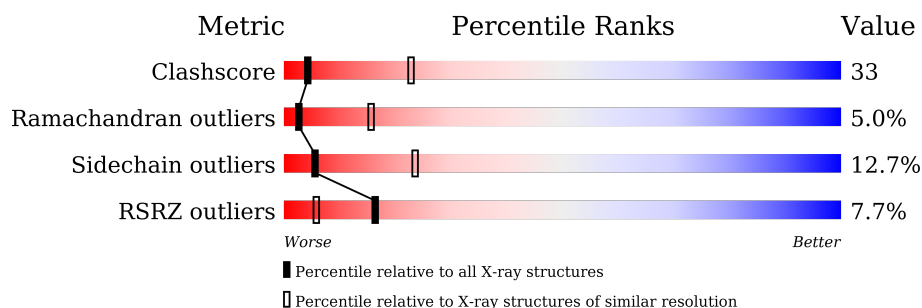
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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			

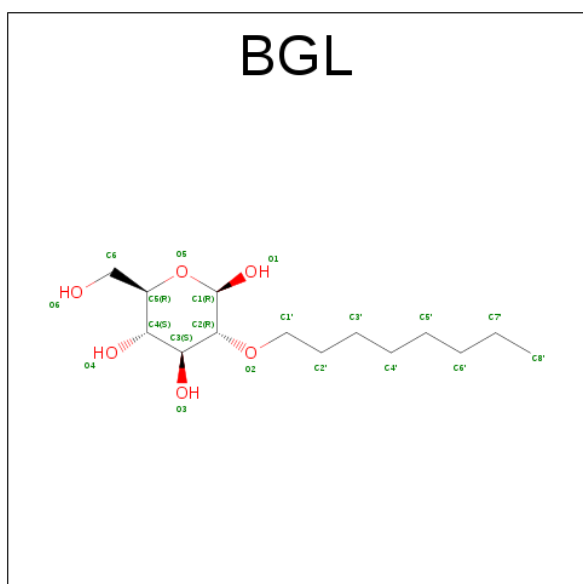
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*GP*AP*TP*CP*GP*C)-3').

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 SUGAR (B-2-OCTYLGLUCOSIDE) (three-letter code: BGL) (formula: C₁₄H₂₈O₆).



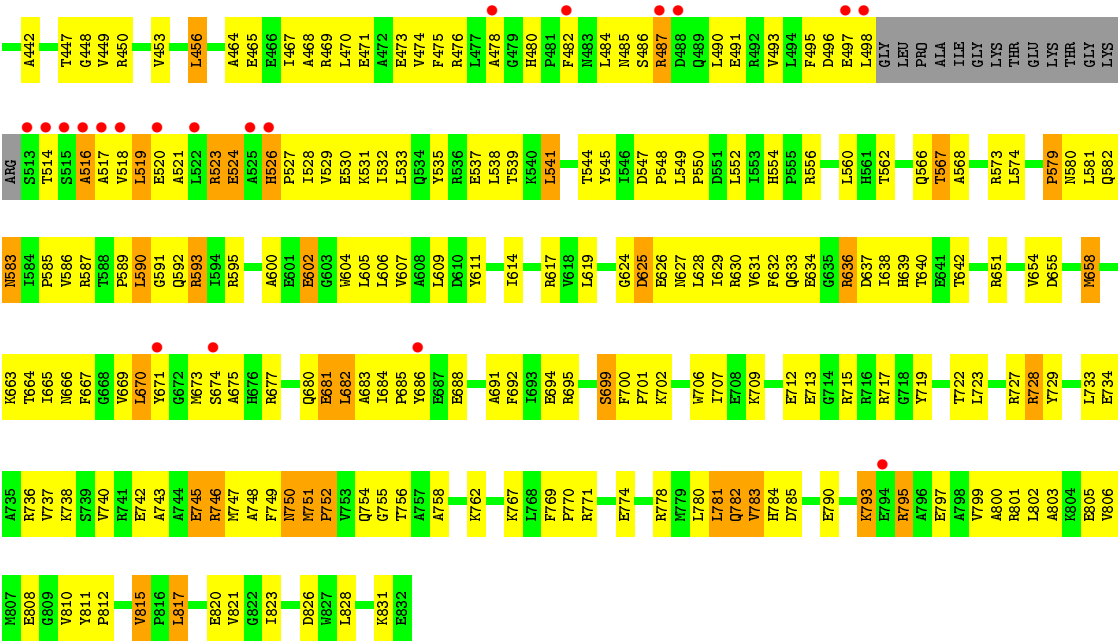
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		

- 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		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 3.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.244 , 0.305 0.262 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.030 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 ²)	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.*

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 [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:68:ALA:HB2	3:A:112:GLU:HB2	1.82	0.61
3:A:248:VAL:O	3:A:248:VAL:HG23	2.00	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:24:TYR:HA	3:A:92:PHE:HE1	1.64	0.60
3:A:346:LYS:O	3:A:368:PRO:HD2	2.01	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:480:HIS:HE1	3:A:493:VAL:HG13	1.67	0.59
3:A:482:PHE:HE2	3:A:490:LEU:HD23	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:906:DC:H2''	1:T:907:DC:OP2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:907:DC:H3'	1:T:907:DC:OP1	2.04	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:40:PRO:HD2	3:A:94:ARG:NH1	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: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:639:HIS:CD2	3:A:663:LYS:HA	2.48	0.49
3:A:595:ARG:HH22	3:A:831:LYS:HA	1.78	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:743:ALA:O	3:A:746:ARG:HB3	2.15	0.46
3:A:604:TRP:HZ3	3:A:778:ARG:HG2	1.79	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:26:THR:HA	3:A:29:ALA:HB3	1.99	0.45
3:A:19:GLY:HA2	3:A:47:PHE:CE2	2.51	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: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
3:A:17:VAL:HB	3:A:64:VAL:HG22	2.01	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:523:ARG:HH21	3:A:530:GLU:HG3	1.84	0.42
3:A:52:LEU:HA	3:A:52:LEU:HD12	1.77	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:722:THR:CG2	3:A:755:GLY:HA3	2.49	0.41
3:A:733:LEU:HA	3:A:733:LEU:HD23	1.89	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%)	3	15

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%)	5 23

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 carbohydrates 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	-	19,20,20	1.18	3 (15%)	23,25,25	2.96	9 (39%)

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	-	-	0/11/31/31	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	-3.11	1.35	1.43
4	A	1001	BGL	O4-C4	-2.47	1.37	1.43
4	A	1001	BGL	C4-C3	2.22	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	BGL	C1-C2-C3	-7.37	97.72	110.49
4	A	1001	BGL	C1-O5-C5	-5.22	103.55	113.54
4	A	1001	BGL	O3-C3-C4	-4.13	101.05	110.36
4	A	1001	BGL	O1-C1-O5	-3.90	99.47	110.33
4	A	1001	BGL	O6-C6-C5	-2.70	102.29	111.30
4	A	1001	BGL	C3'-C2'-C1'	2.05	122.75	113.47
4	A	1001	BGL	C4-C3-C2	3.88	118.20	109.63
4	A	1001	BGL	C6-C5-C4	3.93	122.83	112.99
4	A	1001	BGL	O2-C2-C3	5.46	121.41	109.97

There are no chirality outliers.

There are no torsion outliers.

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

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	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%)	0.15	50 (6%) 23 9	10, 37, 95, 100	0
All	All	809/848 (95%)	0.21	62 (7%) 16 6	10, 38, 95, 100	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	517	ALA	10.9
3	A	194	PRO	7.9
3	A	518	VAL	7.6
3	A	211	TRP	7.5
3	A	516	ALA	7.1
3	A	217	LEU	6.7
2	P	958	DC	6.5
3	A	674	SER	6.3
3	A	197	LYS	5.7
3	A	228	ILE	5.7
3	A	200	GLY	5.7
1	T	907	DC	5.3
3	A	199	ILE	5.0
3	A	198	GLY	5.0
3	A	236	MET	4.9
3	A	497	GLU	4.8
1	T	908	DG	4.7
3	A	203	THR	4.6
3	A	498	LEU	4.6
2	P	954	DT	4.5
3	A	88	THR	4.4
3	A	218	LEU	4.1
2	P	955	DA	4.1

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Mol	Chain	Res	Type	RSRZ
3	A	513	SER	4.1
2	P	957	DG	3.9
3	A	212	GLY	3.9
3	A	515	SER	3.8
3	A	201	GLU	3.6
2	P	956	DG	3.5
3	A	794	GLU	3.4
3	A	86	ALA	3.2
3	A	514	THR	3.2
3	A	291	PRO	3.2
2	P	953	DC	3.1
3	A	202	LYS	3.0
3	A	520	GLU	3.0
3	A	89	PRO	3.0
1	T	903	DG	3.0
1	T	901	DG	2.9
3	A	290	SER	2.8
3	A	482	PHE	2.8
1	T	906	DC	2.8
3	A	191	ASP	2.7
3	A	487	ARG	2.6
3	A	87	PRO	2.6
3	A	267	GLU	2.5
3	A	245	LEU	2.5
1	T	905	DT	2.5
3	A	488	ASP	2.5
3	A	292	LYS	2.4
3	A	526	HIS	2.4
3	A	193	LEU	2.3
3	A	522	LEU	2.3
3	A	237	ASP	2.3
3	A	686	TYR	2.3
3	A	219	LYS	2.2
3	A	225	LYS	2.2
3	A	295	GLU	2.2
3	A	208	LEU	2.1
3	A	525	ALA	2.1
3	A	478	ALA	2.1
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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BGL	A	1001	20/20	0.94	0.21	1.81	10,22,41,46	0
5	ZN	A	900	1/1	0.97	0.08	-2.80	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.