Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2023 – 12:52 AM EDT

PDB ID	:	1CLQ
Title	:	CRYSTAL STRUCTURE OF A REPLICATION FORK DNA POLYMERASE EDITING COMPLEX AT 2.7 A RESOLUTION
Authors	:	Shamoo, Y.; Steitz, T.A.
Deposited on	:	1999-04-30
Resolution	:	2.70 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:

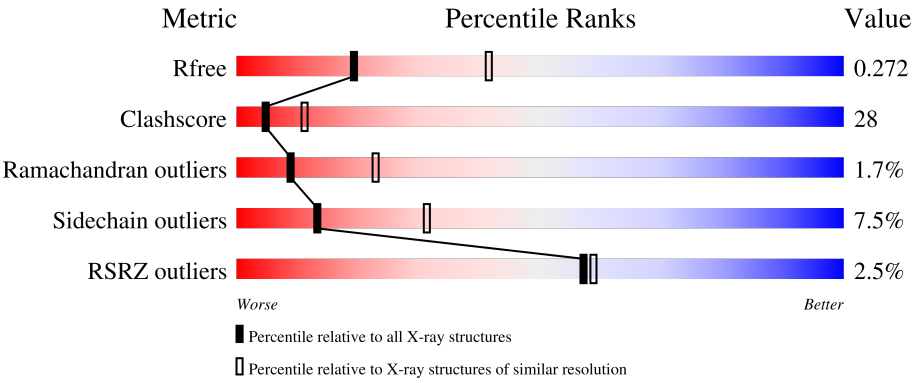
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	E	11	18% 91% 9%
2	D	12	33% 8% 50% 42%
3	A	903	2% 59% 37% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*AP*AP*CP*TP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	11	Total	C	N	O	P	0	0	0
			223	107	43	63	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			244	117	45	71	11			

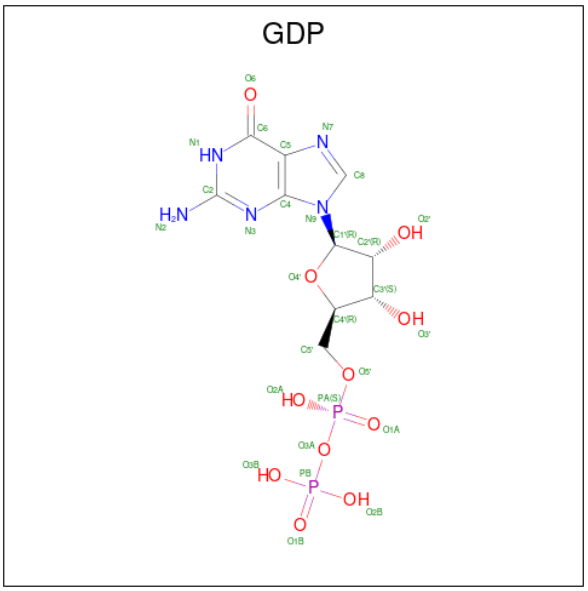
- Molecule 3 is a protein called PROTEIN (DNA POLYMERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	0	0
			7381	4739	1226	1383	33			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ca	0	0
			1	1		
4	D	2	Total	Ca	0	0
			2	2		
4	A	6	Total	Ca	0	0
			6	6		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is water.

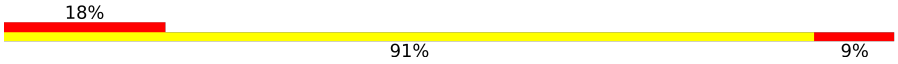
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	5	Total	O	0	0
			5	5		
6	D	4	Total	O	0	0
			4	4		
6	A	212	Total	O	0	0
			212	212		

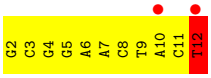
3 Residue-property plots (i)

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*GP*AP*AP*CP*TP*AP*CP*T)-3')

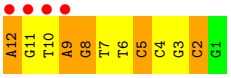
Chain E:





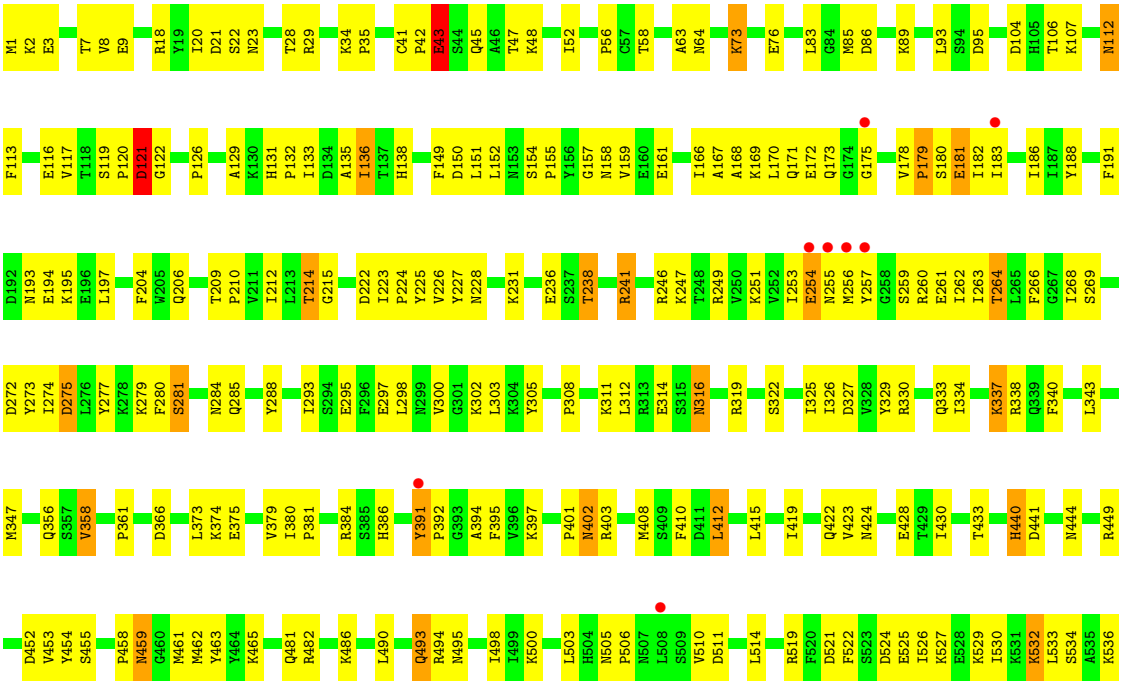
• Molecule 2: DNA (5'-D(*AP*GP*TP*AP*GP*TP*TP*CP*CP*GP*CP*G)-3')

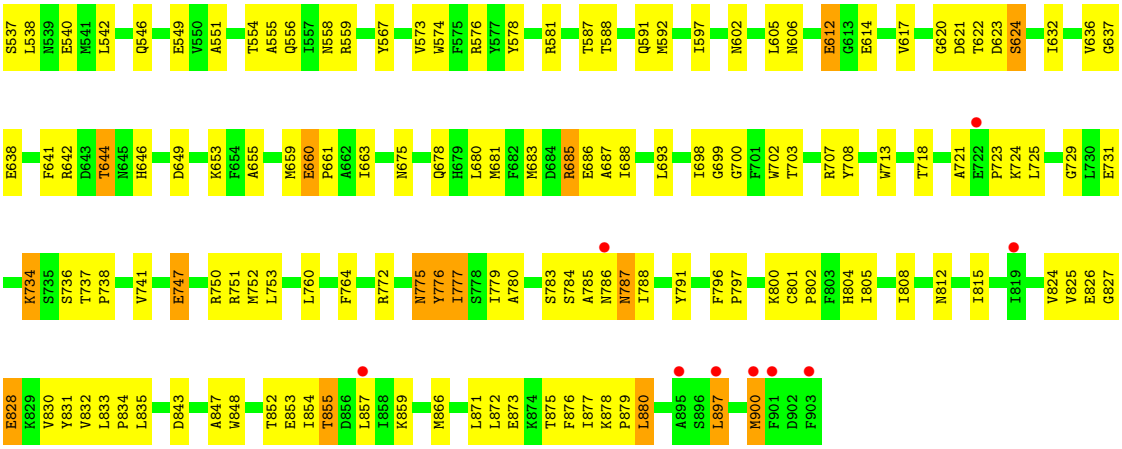
Chain D:



• Molecule 3: PROTEIN (DNA POLYMERASE)

Chain A:




S537 L538 N539 E540 M541 L542 Q546 E549 V550 A551 T554 A555 Q556 I557 N558 R559 Y567 V573 W574 F575 R576 Y577 Y578 R581 T587 T588 Q591 M592 I597 N602 L605 N606 E612 G613 E614 V617 G620 D621 T622 D623 S624 I632 V636 G637
E638 F641 R642 D643 T644 N645 H646 D649 K653 F654 A655 M659 E660 P661 A662 I663 N675 Q678 H679 L680 M681 F682 M683 D684 R685 E686 A687 I688 L693 I698 G699 G700 F701 W702 T703 R707 Y708 W713 T718 A721 E722 P723 K724 L725 G729 L730 E731
K734 S735 S736 T737 P738 V741 E747 R750 R751 M752 L753 L760 F764 R772 N775 Y776 I777 S778 I779 A780 S783 S784 A785 N786 N787 I788 Y791 F796 P797 K800 C801 P802 F803 H804 I805 I808 M812 I815 I819 V824 V825 E826 G827
E828 K829 V830 Y831 V832 L833 P834 L835 D843 A847 W848 T852 E853 I854 T855 D856 L857 I858 K859 M866 L871 L872 E873 K874 T875 F876 I877 K878 P879 L880 A895 S896 L897 M900 F901 D902 F903

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	209.74Å 209.74Å 114.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (40.00-2.70) 97.3 (39.64-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.284 0.219 , 0.272	Depositor DCC
R_{free} test set	4903 reflections (9.75%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, GDP

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	E	0.92	0/250	1.32	1/384 (0.3%)
2	D	1.07	2/273 (0.7%)	1.70	8/420 (1.9%)
3	A	0.43	0/7562	0.66	1/10217 (0.0%)
All	All	0.48	2/8085 (0.0%)	0.76	10/11021 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
3	A	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	DC	N1-C2	-5.61	1.34	1.40
2	D	12	DA	N9-C4	-5.56	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	12	DA	O4'-C1'-C2'	10.10	113.98	105.90
2	D	12	DA	O4'-C1'-N9	8.97	114.28	108.00
3	A	412	LEU	CA-CB-CG	8.55	134.96	115.30
2	D	12	DA	N9-C1'-C2'	8.07	127.94	112.60
2	D	12	DA	C8-N9-C1'	8.00	142.09	127.70
1	E	12	DT	O4'-C1'-N1	7.95	113.56	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	12	DA	C4-N9-C1'	-7.94	112.01	126.30
2	D	8	DG	O4'-C1'-C2'	5.91	110.62	105.90
2	D	9	DA	O4'-C1'-C2'	5.24	110.09	105.90
2	D	5	DC	O4'-C1'-C2'	5.20	110.06	105.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	567	TYR	Sidechain
1	E	12	DT	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	223	0	125	34	0
2	D	244	0	137	45	0
3	A	7381	0	7265	360	0
4	A	6	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	A	28	0	12	3	0
6	A	212	0	0	6	0
6	D	4	0	0	0	0
6	E	5	0	0	0	0
All	All	8106	0	7539	425	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 28.

All (425) 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:D:6:DT:H2"	2:D:5:DC:C5'	1.49	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:DC:N4	2:D:8:DG:H1	1.41	1.19
2:D:6:DT:H2"	2:D:5:DC:H5"	1.31	1.11
2:D:3:DG:H2"	2:D:2:DC:H5"	1.28	1.09
2:D:6:DT:H2"	2:D:5:DC:H5'	1.10	1.07
3:A:402:ASN:ND2	3:A:403:ARG:H	1.55	1.02
2:D:7:DT:H2"	2:D:6:DT:H5"	1.43	1.00
1:E:4:DG:H1'	1:E:5:DG:H5"	1.43	0.99
2:D:3:DG:H2"	2:D:2:DC:C5'	1.93	0.98
2:D:6:DT:C2'	2:D:5:DC:C5'	2.43	0.96
3:A:422:GLN:HG3	3:A:678:GLN:O	1.67	0.94
3:A:402:ASN:HD22	3:A:403:ARG:H	0.98	0.92
3:A:1:MET:HG2	3:A:2:LYS:H	1.35	0.91
1:E:2:DG:H2"	1:E:3:DC:H5'	1.49	0.91
3:A:402:ASN:HD22	3:A:403:ARG:N	1.70	0.89
2:D:6:DT:C2'	2:D:5:DC:H5"	2.03	0.88
2:D:6:DT:C2'	2:D:5:DC:H5'	2.02	0.88
3:A:277:TYR:O	3:A:281:SER:HB2	1.74	0.88
1:E:2:DG:O5'	3:A:255:ASN:N	2.07	0.88
3:A:316:ASN:HD21	3:A:319:ARG:H	1.22	0.88
1:E:11:DC:H4'	1:E:12:DT:OP1	1.73	0.87
3:A:224:PRO:HA	3:A:263:ILE:HD12	1.55	0.86
3:A:422:GLN:HE21	3:A:680:LEU:H	1.24	0.84
3:A:830:VAL:HG11	3:A:847:ALA:HB1	1.60	0.83
2:D:10:DT:H1'	2:D:9:DA:H5"	1.62	0.82
3:A:8:VAL:HG21	3:A:93:LEU:HD11	1.63	0.81
1:E:3:DC:H2'	1:E:3:DC:O2	1.80	0.81
3:A:126:PRO:HA	3:A:225:TYR:HD1	1.44	0.81
3:A:47:THR:HG22	3:A:48:LYS:N	1.96	0.81
2:D:11:DG:H2"	2:D:10:DT:O5'	1.79	0.81
3:A:606:ASN:OD1	3:A:614:GLU:HB3	1.81	0.80
3:A:392:PRO:O	3:A:587:THR:HG21	1.83	0.79
3:A:825:VAL:O	3:A:828:GLU:HG2	1.81	0.79
3:A:136:ILE:CG2	3:A:149:PHE:HB2	2.12	0.79
3:A:179:PRO:O	3:A:182:ILE:HG22	1.83	0.79
3:A:254:GLU:OE1	3:A:259:SER:HB2	1.83	0.79
3:A:524:ASP:HA	3:A:527:LYS:HD3	1.65	0.78
3:A:785:ALA:HB2	3:A:808:ILE:HD12	1.66	0.77
3:A:785:ALA:HB1	3:A:788:ILE:CG2	2.15	0.77
2:D:3:DG:C2'	2:D:2:DC:C5'	2.64	0.76
3:A:808:ILE:HG23	3:A:824:VAL:HG11	1.65	0.76
3:A:641:PHE:HD1	3:A:646:HIS:HD1	1.32	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:316:ASN:ND2	3:A:319:ARG:HB3	2.02	0.74
3:A:136:ILE:HG23	3:A:149:PHE:HB2	1.69	0.73
2:D:8:DG:H2"	2:D:7:DT:OP1	1.87	0.73
3:A:788:ILE:HG22	3:A:805:ILE:HD12	1.70	0.73
2:D:12:DA:H2"	2:D:11:DG:C8	2.24	0.73
3:A:322:SER:O	3:A:326:ILE:HG12	1.88	0.73
1:E:4:DG:C1'	1:E:5:DG:H5"	2.18	0.71
3:A:481:GLN:NE2	3:A:559:ARG:HH11	1.88	0.70
2:D:10:DT:H2"	2:D:9:DA:C5'	2.21	0.70
3:A:47:THR:HG22	3:A:48:LYS:H	1.54	0.70
3:A:303:LEU:HD11	3:A:326:ILE:HG21	1.72	0.70
1:E:12:DT:O4	2:D:12:DA:N1	2.25	0.70
3:A:150:ASP:HB3	3:A:188:TYR:HE1	1.56	0.69
3:A:663:ILE:HD13	3:A:683:MET:HE2	1.74	0.69
2:D:10:DT:H2"	2:D:9:DA:H5'	1.73	0.69
3:A:581:ARG:HG3	3:A:581:ARG:HH11	1.57	0.69
3:A:316:ASN:HD21	3:A:319:ARG:N	1.89	0.69
3:A:830:VAL:CG1	3:A:847:ALA:HB1	2.21	0.69
1:E:4:DG:H2"	1:E:5:DG:H5'	1.75	0.69
3:A:126:PRO:HA	3:A:225:TYR:CD1	2.28	0.69
3:A:253:ILE:C	3:A:254:GLU:HG2	2.12	0.68
3:A:180:SER:HA	3:A:183:ILE:CD1	2.23	0.68
2:D:12:DA:H2"	2:D:11:DG:N7	2.08	0.68
2:D:5:DC:H2"	2:D:4:DC:C6	2.27	0.68
2:D:7:DT:H5"	2:D:7:DT:H6	1.57	0.68
3:A:104:ASP:OD1	3:A:106:THR:HG22	1.93	0.68
3:A:655:ALA:HA	3:A:659:MET:HB2	1.75	0.68
3:A:514:LEU:HD11	3:A:533:LEU:HD21	1.74	0.68
3:A:830:VAL:HG13	3:A:848:TRP:O	1.94	0.68
3:A:724:LYS:NZ	3:A:724:LYS:HB3	2.09	0.66
2:D:3:DG:C2'	2:D:2:DC:H5'	2.26	0.66
3:A:775:ASN:OD1	3:A:777:ILE:HG23	1.96	0.66
3:A:410:PHE:CZ	3:A:659:MET:HG2	2.30	0.66
3:A:897:LEU:O	3:A:900:MET:HG3	1.96	0.66
3:A:455:SER:HA	3:A:675:ASN:O	1.96	0.66
3:A:636:VAL:HG12	3:A:636:VAL:O	1.95	0.66
3:A:83:LEU:HD12	3:A:83:LEU:H	1.60	0.66
1:E:10:DA:H4'	1:E:11:DC:OP1	1.96	0.65
3:A:494:ARG:NH1	3:A:521:ASP:OD1	2.28	0.65
3:A:621:ASP:HB2	3:A:624:SER:HB2	1.77	0.65
3:A:227:TYR:CD2	3:A:263:ILE:HD13	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:ASN:ND2	3:A:403:ARG:N	2.34	0.65
3:A:873:GLU:HG2	3:A:877:ILE:HD12	1.77	0.65
3:A:73:LYS:HE2	3:A:73:LYS:O	1.95	0.65
3:A:181:GLU:OE1	3:A:181:GLU:N	2.27	0.65
3:A:149:PHE:HB3	3:A:197:LEU:HD21	1.79	0.65
3:A:206:GLN:NE2	3:A:246:ARG:HH12	1.93	0.65
3:A:347:MET:CE	3:A:358:VAL:HG22	2.27	0.64
3:A:169:LYS:HE3	6:A:1154:HOH:O	1.96	0.64
3:A:737:THR:HG23	3:A:875:THR:HB	1.79	0.64
3:A:707:ARG:HG2	3:A:729:GLY:O	1.98	0.64
3:A:731:GLU:HG2	3:A:734:LYS:NZ	2.13	0.64
3:A:223:ILE:HB	3:A:224:PRO:HD3	1.79	0.64
1:E:4:DG:H1'	1:E:5:DG:C5'	2.26	0.64
2:D:11:DG:H1'	2:D:10:DT:H5'	1.80	0.64
3:A:453:VAL:HG23	3:A:454:TYR:CD2	2.33	0.64
3:A:800:LYS:HB2	3:A:800:LYS:NZ	2.12	0.64
3:A:152:LEU:HB2	3:A:191:PHE:O	1.98	0.64
1:E:4:DG:H2"	1:E:5:DG:C5'	2.28	0.63
3:A:180:SER:HA	3:A:183:ILE:HD11	1.80	0.63
3:A:612:GLU:HA	3:A:612:GLU:OE1	1.99	0.63
3:A:621:ASP:HB3	3:A:624:SER:H	1.64	0.62
1:E:2:DG:C2'	1:E:3:DC:H5'	2.25	0.62
3:A:785:ALA:HB2	3:A:808:ILE:CD1	2.29	0.62
1:E:9:DT:H2"	1:E:10:DA:O5'	2.00	0.62
2:D:5:DC:H2"	2:D:4:DC:C5	2.35	0.62
3:A:83:LEU:HD12	3:A:83:LEU:N	2.15	0.62
3:A:394:ALA:HB1	3:A:622:THR:OG1	1.99	0.61
1:E:5:DG:N2	1:E:6:DA:C2	2.69	0.61
3:A:316:ASN:HD21	3:A:319:ARG:HB3	1.65	0.61
3:A:171:GLN:C	3:A:173:GLN:H	2.03	0.61
3:A:117:VAL:HG13	3:A:132:PRO:O	2.00	0.61
3:A:380:ILE:HG12	5:A:999:GDP:O6	2.00	0.61
2:D:10:DT:C1'	2:D:9:DA:H5"	2.30	0.61
3:A:316:ASN:C	3:A:316:ASN:HD22	2.04	0.61
3:A:298:LEU:O	3:A:300:VAL:HG23	2.00	0.61
3:A:257:TYR:CD1	3:A:787:ASN:ND2	2.58	0.60
3:A:410:PHE:CE2	3:A:685:ARG:HB2	2.35	0.60
3:A:459:ASN:HD22	3:A:459:ASN:N	1.97	0.60
3:A:830:VAL:HG12	3:A:831:TYR:N	2.16	0.60
1:E:12:DT:O4	2:D:12:DA:C6	2.54	0.60
3:A:731:GLU:HG2	3:A:734:LYS:HZ2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:391:TYR:HB2	3:A:392:PRO:HD2	1.82	0.60
3:A:297:GLU:OE2	3:A:338:ARG:NH1	2.32	0.60
3:A:542:LEU:HD21	3:A:546:GLN:OE1	2.02	0.60
3:A:830:VAL:CG1	3:A:831:TYR:N	2.65	0.60
1:E:6:DA:H2"	1:E:7:DA:O5'	2.01	0.60
3:A:152:LEU:HD11	3:A:161:GLU:HG2	1.84	0.60
3:A:461:MET:CE	3:A:581:ARG:HD2	2.32	0.60
3:A:48:LYS:NZ	5:A:999:GDP:O1B	2.25	0.59
3:A:206:GLN:NE2	3:A:241:ARG:O	2.35	0.59
3:A:254:GLU:HB3	3:A:259:SER:CB	2.31	0.59
3:A:785:ALA:HB1	3:A:788:ILE:HG21	1.85	0.59
3:A:788:ILE:HG22	3:A:805:ILE:CD1	2.32	0.59
3:A:422:GLN:HE22	3:A:681:MET:HG2	1.68	0.59
3:A:597:ILE:HD11	3:A:663:ILE:HG23	1.84	0.59
3:A:897:LEU:O	3:A:900:MET:CG	2.50	0.59
3:A:279:LYS:HE3	6:A:1111:HOH:O	2.02	0.59
3:A:542:LEU:HD23	3:A:542:LEU:C	2.23	0.58
3:A:361:PRO:HD2	6:A:1036:HOH:O	2.03	0.58
3:A:542:LEU:HD23	3:A:542:LEU:O	2.03	0.58
3:A:104:ASP:CG	3:A:106:THR:HG22	2.24	0.58
3:A:272:ASP:OD1	3:A:274:ILE:HG22	2.04	0.58
3:A:257:TYR:CD1	3:A:257:TYR:O	2.56	0.58
3:A:214:THR:HG23	3:A:215:GLY:N	2.18	0.58
3:A:157:GLY:C	3:A:158:ASN:HD22	2.07	0.57
3:A:347:MET:HE1	3:A:358:VAL:HG22	1.86	0.57
3:A:852:THR:HG22	3:A:853:GLU:H	1.69	0.57
3:A:116:GLU:HB2	3:A:135:ALA:HB3	1.86	0.57
3:A:330:ARG:HG3	3:A:330:ARG:HH11	1.69	0.57
3:A:366:ASP:OD1	3:A:576:ARG:NH1	2.37	0.57
3:A:721:ALA:HB3	6:A:1077:HOH:O	2.04	0.57
3:A:206:GLN:HA	3:A:206:GLN:OE1	2.04	0.57
3:A:251:LYS:HD3	3:A:262:ILE:HD11	1.86	0.57
3:A:316:ASN:ND2	3:A:316:ASN:C	2.58	0.57
3:A:459:ASN:HD22	3:A:459:ASN:H	1.51	0.57
3:A:776:TYR:HD1	3:A:776:TYR:H	1.53	0.57
3:A:510:VAL:HG23	3:A:510:VAL:O	2.05	0.57
3:A:28:THR:HG22	3:A:29:ARG:N	2.19	0.57
3:A:872:LEU:HD22	3:A:877:ILE:HD11	1.86	0.56
3:A:1:MET:HG2	3:A:2:LYS:N	2.13	0.56
3:A:458:PRO:HG3	3:A:592:MET:SD	2.45	0.56
3:A:73:LYS:O	3:A:76:GLU:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:129:ALA:HA	3:A:225:TYR:CE1	2.41	0.56
3:A:737:THR:HG22	3:A:741:VAL:HB	1.87	0.56
3:A:288:TYR:HA	3:A:293:ILE:HD13	1.86	0.56
3:A:713:TRP:CZ3	3:A:723:PRO:HD3	2.40	0.56
1:E:3:DC:O2	1:E:3:DC:C2'	2.53	0.56
3:A:191:PHE:CD1	3:A:197:LEU:HD23	2.40	0.56
3:A:197:LEU:C	3:A:197:LEU:HD13	2.26	0.56
3:A:255:ASN:OD1	3:A:255:ASN:O	2.23	0.56
3:A:533:LEU:HB2	3:A:538:LEU:HD13	1.87	0.56
3:A:403:ARG:HH21	3:A:698:ILE:HG22	1.70	0.56
3:A:241:ARG:CB	3:A:241:ARG:HH11	2.20	0.55
3:A:312:LEU:HD12	3:A:312:LEU:O	2.07	0.55
3:A:337:LYS:HG3	3:A:338:ARG:N	2.21	0.55
3:A:300:VAL:CG1	3:A:330:ARG:NH2	2.70	0.55
3:A:808:ILE:HD13	3:A:824:VAL:HG21	1.89	0.55
3:A:175:GLY:O	3:A:319:ARG:NH2	2.40	0.54
3:A:700:GLY:HA2	3:A:753:LEU:HD22	1.89	0.54
3:A:461:MET:HE1	3:A:581:ARG:HD2	1.89	0.54
3:A:21:ASP:OD1	3:A:23:ASN:N	2.32	0.54
3:A:555:ALA:O	3:A:559:ARG:HG2	2.07	0.54
3:A:876:PHE:O	3:A:880:LEU:HB2	2.07	0.54
3:A:698:ILE:HG12	3:A:752:MET:O	2.08	0.54
3:A:21:ASP:OD1	3:A:22:SER:N	2.41	0.54
2:D:10:DT:C2'	2:D:9:DA:H5"	2.37	0.54
3:A:305:TYR:CD1	3:A:312:LEU:HD22	2.43	0.54
3:A:347:MET:HE2	3:A:358:VAL:HG22	1.90	0.54
3:A:206:GLN:NE2	3:A:246:ARG:NH1	2.56	0.53
3:A:171:GLN:O	3:A:173:GLN:N	2.41	0.53
3:A:247:LYS:O	3:A:266:PHE:HB2	2.09	0.53
3:A:222:ASP:O	3:A:226:VAL:HG23	2.09	0.53
3:A:241:ARG:HH11	3:A:241:ARG:HB3	1.74	0.53
2:D:11:DG:C8	2:D:10:DT:H72	2.44	0.53
3:A:89:LYS:HB2	3:A:89:LYS:NZ	2.24	0.53
3:A:852:THR:HG22	3:A:853:GLU:N	2.24	0.53
3:A:149:PHE:HB3	3:A:197:LEU:CD2	2.39	0.52
3:A:249:ARG:O	3:A:264:THR:HG23	2.10	0.52
3:A:700:GLY:HA2	3:A:753:LEU:CD2	2.40	0.52
1:E:2:DG:HO5'	3:A:255:ASN:N	2.04	0.52
3:A:511:ASP:OD2	3:A:533:LEU:HA	2.09	0.52
3:A:855:THR:HB	3:A:857:LEU:HB2	1.92	0.52
3:A:193:ASN:OD1	3:A:194:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:786:ASN:HA	3:A:826:GLU:OE2	2.10	0.52
3:A:786:ASN:OD1	3:A:827:GLY:HA2	2.10	0.52
3:A:408:MET:HE2	3:A:685:ARG:HG3	1.92	0.51
2:D:6:DT:C1'	2:D:5:DC:H5"	2.41	0.51
3:A:178:VAL:HA	3:A:326:ILE:HD11	1.91	0.51
3:A:300:VAL:HG12	3:A:330:ARG:NH2	2.26	0.51
3:A:288:TYR:HA	3:A:293:ILE:CD1	2.41	0.51
3:A:644:THR:HB	3:A:693:LEU:H	1.76	0.51
3:A:825:VAL:HB	3:A:828:GLU:CG	2.41	0.51
3:A:401:PRO:O	3:A:402:ASN:HB2	2.11	0.51
1:E:5:DG:H2"	1:E:6:DA:C8	2.46	0.51
3:A:764:PHE:CE1	3:A:876:PHE:HE2	2.28	0.51
3:A:85:MET:HA	3:A:380:ILE:HD11	1.93	0.51
3:A:42:PRO:HG2	3:A:45:GLN:HG2	1.93	0.50
3:A:458:PRO:HB2	3:A:588:THR:HG22	1.94	0.50
3:A:747:GLU:O	3:A:751:ARG:HG3	2.12	0.50
1:E:3:DC:H2"	1:E:4:DG:C8	2.46	0.50
2:D:10:DT:C2'	2:D:9:DA:C5'	2.88	0.50
3:A:490:LEU:O	3:A:494:ARG:HB2	2.12	0.50
3:A:514:LEU:N	3:A:514:LEU:HD12	2.26	0.50
3:A:255:ASN:O	3:A:257:TYR:N	2.45	0.50
3:A:503:LEU:HD23	3:A:538:LEU:HD23	1.93	0.50
3:A:872:LEU:O	3:A:872:LEU:HD23	2.12	0.50
3:A:493:GLN:HB2	3:A:549:GLU:CD	2.32	0.49
3:A:495:ASN:HB3	3:A:522:PHE:CE2	2.47	0.49
1:E:4:DG:C2'	1:E:5:DG:C5'	2.90	0.49
3:A:347:MET:HG3	3:A:558:ASN:OD1	2.13	0.49
3:A:602:ASN:OD1	3:A:617:VAL:HG23	2.13	0.49
3:A:878:LYS:N	3:A:879:PRO:HD2	2.28	0.49
3:A:402:ASN:ND2	3:A:403:ARG:HG2	2.28	0.49
2:D:11:DG:C2	2:D:10:DT:C2	3.01	0.49
3:A:384:ARG:HG3	3:A:384:ARG:HH11	1.77	0.49
3:A:482:ARG:CG	3:A:559:ARG:HB2	2.42	0.49
3:A:815:ILE:CG2	3:A:815:ILE:O	2.61	0.49
3:A:440:HIS:HB3	6:A:1132:HOH:O	2.11	0.49
1:E:4:DG:C2'	1:E:5:DG:H5"	2.42	0.49
2:D:6:DT:H1'	2:D:5:DC:H5"	1.94	0.49
2:D:9:DA:H2"	2:D:8:DG:O5'	2.13	0.48
3:A:663:ILE:HD13	3:A:683:MET:CE	2.42	0.48
3:A:854:ILE:HD12	3:A:859:LYS:HG3	1.95	0.48
3:A:170:LEU:HD22	3:A:170:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:534:SER:O	3:A:538:LEU:HB2	2.13	0.48
3:A:112:ASN:C	3:A:112:ASN:HD22	2.15	0.48
3:A:227:TYR:HB3	3:A:263:ILE:HD13	1.94	0.48
3:A:231:LYS:HE3	3:A:236:GLU:HB2	1.94	0.48
3:A:316:ASN:HD21	3:A:319:ARG:CB	2.27	0.48
3:A:686:GLU:HG3	3:A:687:ALA:N	2.28	0.48
3:A:83:LEU:HB3	3:A:379:VAL:HG12	1.94	0.48
3:A:274:ILE:HG23	3:A:275:ASP:N	2.29	0.48
3:A:655:ALA:HA	3:A:659:MET:CB	2.42	0.48
3:A:166:ILE:O	3:A:168:ALA:N	2.47	0.48
1:E:5:DG:N1	2:D:5:DC:O2	2.47	0.47
3:A:440:HIS:CD2	3:A:444:ASN:ND2	2.82	0.47
3:A:685:ARG:NH2	3:A:688:ILE:HG13	2.29	0.47
2:D:3:DG:H2'	2:D:2:DC:H5'	1.95	0.47
3:A:154:SER:HB2	3:A:155:PRO:HD2	1.96	0.47
3:A:724:LYS:HB3	3:A:724:LYS:HZ3	1.79	0.47
3:A:119:SER:HA	3:A:131:HIS:CD2	2.49	0.47
3:A:138:HIS:CD2	3:A:204:PHE:HE2	2.33	0.47
1:E:2:DG:O5'	3:A:255:ASN:CG	2.53	0.47
3:A:150:ASP:HB3	3:A:188:TYR:CE1	2.45	0.47
3:A:9:GLU:HG2	3:A:266:PHE:CD2	2.49	0.47
3:A:316:ASN:ND2	3:A:319:ARG:H	2.02	0.47
3:A:329:TYR:O	3:A:333:GLN:HG3	2.14	0.47
3:A:180:SER:C	3:A:182:ILE:H	2.17	0.46
3:A:254:GLU:HA	3:A:259:SER:HA	1.97	0.46
3:A:581:ARG:HG3	3:A:581:ARG:NH1	2.28	0.46
1:E:5:DG:C6	2:D:5:DC:N3	2.84	0.46
3:A:537:SER:O	3:A:540:GLU:HB3	2.14	0.46
1:E:5:DG:O6	2:D:5:DC:N3	2.48	0.46
3:A:212:ILE:HA	3:A:269:SER:O	2.16	0.46
3:A:433:THR:N	3:A:462:MET:HE2	2.30	0.46
3:A:791:TYR:CE2	3:A:802:PRO:HD3	2.51	0.46
3:A:224:PRO:HA	3:A:263:ILE:CD1	2.37	0.46
3:A:228:ASN:ND2	3:A:261:GLU:OE1	2.41	0.46
3:A:494:ARG:O	3:A:498:ILE:HD13	2.15	0.46
3:A:825:VAL:C	3:A:828:GLU:HG2	2.36	0.46
3:A:9:GLU:HG2	3:A:266:PHE:HD2	1.81	0.46
1:E:8:DC:N4	2:D:8:DG:N1	2.21	0.46
3:A:777:ILE:HD12	3:A:777:ILE:O	2.14	0.46
3:A:702:TRP:CD1	3:A:708:TYR:HB3	2.51	0.46
3:A:47:THR:CG2	3:A:48:LYS:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:440:HIS:CD2	3:A:444:ASN:HD22	2.34	0.46
3:A:461:MET:HE3	3:A:581:ARG:HD2	1.97	0.46
3:A:775:ASN:HD21	3:A:777:ILE:HG23	1.79	0.46
3:A:776:TYR:CE2	3:A:854:ILE:HD13	2.51	0.46
3:A:178:VAL:HG22	3:A:326:ILE:HD11	1.98	0.45
3:A:391:TYR:CD1	3:A:391:TYR:N	2.85	0.45
3:A:34:LYS:HA	3:A:35:PRO:HD2	1.84	0.45
3:A:120:PRO:HD2	3:A:131:HIS:NE2	2.31	0.45
3:A:170:LEU:H	3:A:170:LEU:CD2	2.28	0.45
3:A:481:GLN:HE21	3:A:559:ARG:HD2	1.82	0.45
2:D:3:DG:OP1	3:A:288:TYR:N	2.44	0.45
3:A:119:SER:HA	3:A:131:HIS:HD2	1.81	0.45
3:A:151:LEU:HG	3:A:152:LEU:N	2.31	0.45
3:A:191:PHE:CD2	3:A:197:LEU:HA	2.51	0.45
3:A:193:ASN:OD1	3:A:195:LYS:N	2.50	0.45
3:A:280:PHE:HB2	3:A:340:PHE:CE1	2.52	0.45
3:A:529:LYS:O	3:A:533:LEU:CD2	2.64	0.45
3:A:638:GLU:HA	3:A:641:PHE:HD2	1.82	0.45
3:A:3:GLU:HB2	3:A:20:ILE:O	2.17	0.45
3:A:262:ILE:HG13	3:A:262:ILE:O	2.17	0.45
3:A:703:THR:OG1	3:A:707:ARG:HB3	2.16	0.45
1:E:3:DC:O2	1:E:4:DG:C5	2.70	0.45
1:E:8:DC:H42	2:D:8:DG:H1	0.60	0.45
3:A:121:ASP:HB2	3:A:122:GLY:H	1.62	0.45
3:A:415:LEU:O	3:A:419:ILE:HG13	2.17	0.45
3:A:784:SER:HB2	3:A:828:GLU:O	2.17	0.45
3:A:7:THR:OG1	3:A:18:ARG:HD3	2.18	0.44
3:A:28:THR:HG22	3:A:29:ARG:H	1.80	0.44
3:A:605:LEU:HD22	3:A:632:ILE:HD11	1.99	0.44
3:A:170:LEU:HD22	3:A:170:LEU:H	1.81	0.44
3:A:308:PRO:HG3	3:A:311:LYS:HE3	1.99	0.44
3:A:43:GLU:OE2	3:A:56:PRO:CD	2.66	0.44
3:A:47:THR:HG22	3:A:48:LYS:HG2	2.00	0.44
3:A:227:TYR:CB	3:A:263:ILE:HD13	2.48	0.44
3:A:459:ASN:H	3:A:459:ASN:ND2	2.15	0.44
3:A:764:PHE:CD1	3:A:876:PHE:HE2	2.36	0.44
3:A:500:LYS:O	3:A:503:LEU:HB2	2.17	0.44
1:E:3:DC:C2'	1:E:4:DG:C8	3.01	0.44
3:A:526:ILE:O	3:A:530:ILE:HG12	2.17	0.44
3:A:573:VAL:HG23	3:A:574:TRP:CD1	2.53	0.44
3:A:833:LEU:HD13	3:A:866:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:511:ASP:OD2	3:A:534:SER:N	2.51	0.44
3:A:136:ILE:HG22	3:A:149:PHE:HB2	1.97	0.43
3:A:186:ILE:HD13	3:A:325:ILE:HD13	2.00	0.43
2:D:9:DA:H2"	2:D:8:DG:H8	1.83	0.43
3:A:395:PHE:HB2	3:A:591:GLN:HG2	2.00	0.43
3:A:52:ILE:O	3:A:428:GLU:HG3	2.18	0.43
3:A:112:ASN:HD22	3:A:113:PHE:N	2.16	0.43
3:A:227:TYR:CG	3:A:263:ILE:HD13	2.53	0.43
3:A:775:ASN:ND2	3:A:777:ILE:HG23	2.34	0.43
3:A:800:LYS:HB2	3:A:800:LYS:HZ2	1.83	0.43
3:A:257:TYR:CE1	3:A:787:ASN:ND2	2.84	0.43
3:A:330:ARG:O	3:A:334:ILE:HG13	2.18	0.43
3:A:660:GLU:CB	3:A:661:PRO:HD3	2.49	0.43
3:A:725:LEU:HD11	3:A:750:ARG:HB2	2.00	0.43
3:A:308:PRO:CG	3:A:311:LYS:HE3	2.49	0.43
3:A:578:TYR:CD1	3:A:578:TYR:C	2.92	0.43
3:A:776:TYR:CG	3:A:777:ILE:N	2.86	0.43
3:A:800:LYS:HB2	3:A:800:LYS:HZ3	1.84	0.43
3:A:815:ILE:O	3:A:815:ILE:HG23	2.18	0.43
2:D:8:DG:C2'	2:D:7:DT:OP1	2.63	0.43
3:A:41:CYS:HB2	3:A:42:PRO:HD2	2.01	0.43
3:A:422:GLN:NE2	3:A:681:MET:HG2	2.32	0.43
3:A:505:ASN:N	3:A:506:PRO:HD3	2.33	0.43
3:A:486:LYS:HG2	6:A:1130:HOH:O	2.18	0.43
3:A:260:ARG:HD3	3:A:260:ARG:HA	1.87	0.43
3:A:481:GLN:NE2	3:A:559:ARG:NH1	2.63	0.43
3:A:779:ILE:HD11	3:A:866:MET:HE1	2.01	0.43
3:A:379:VAL:HA	5:A:999:GDP:HN1	1.84	0.43
3:A:786:ASN:O	3:A:787:ASN:ND2	2.51	0.43
3:A:117:VAL:HG22	3:A:133:ILE:HA	2.00	0.42
3:A:808:ILE:CG2	3:A:824:VAL:HG11	2.45	0.42
3:A:834:PRO:HG3	3:A:871:LEU:HG	2.00	0.42
3:A:274:ILE:CG2	3:A:275:ASP:N	2.82	0.42
3:A:482:ARG:HG2	3:A:559:ARG:HB2	2.00	0.42
3:A:824:VAL:O	3:A:824:VAL:HG13	2.18	0.42
2:D:8:DG:C4	2:D:7:DT:H72	2.54	0.42
3:A:330:ARG:HH11	3:A:330:ARG:CG	2.32	0.42
3:A:356:GLN:C	3:A:358:VAL:H	2.22	0.42
3:A:700:GLY:CA	3:A:753:LEU:HD22	2.49	0.42
3:A:397:LYS:HB3	3:A:620:GLY:H	1.85	0.42
3:A:529:LYS:O	3:A:533:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:551:ALA:O	3:A:554:THR:HG22	2.19	0.42
3:A:621:ASP:HB3	3:A:624:SER:N	2.33	0.42
3:A:34:LYS:HG2	3:A:63:ALA:O	2.20	0.42
3:A:169:LYS:HA	3:A:169:LYS:HD3	1.80	0.42
3:A:305:TYR:CE1	3:A:312:LEU:HD22	2.55	0.42
3:A:503:LEU:HD21	3:A:538:LEU:HB3	2.02	0.42
1:E:8:DC:N4	2:D:8:DG:C6	2.82	0.42
3:A:430:ILE:HD13	3:A:463:TYR:CE2	2.55	0.42
3:A:459:ASN:N	3:A:459:ASN:ND2	2.67	0.42
3:A:775:ASN:OD1	3:A:775:ASN:C	2.57	0.42
3:A:43:GLU:OE2	3:A:56:PRO:HD2	2.20	0.42
3:A:384:ARG:HG3	3:A:384:ARG:NH1	2.35	0.42
3:A:8:VAL:HG21	3:A:93:LEU:CD1	2.43	0.42
3:A:285:GLN:HA	3:A:285:GLN:OE1	2.20	0.41
3:A:872:LEU:CD2	3:A:877:ILE:HD11	2.49	0.41
1:E:7:DA:C4	1:E:8:DC:C5	3.08	0.41
3:A:238:THR:O	3:A:238:THR:OG1	2.37	0.41
3:A:254:GLU:HB3	3:A:259:SER:HB2	2.02	0.41
3:A:423:VAL:O	3:A:424:ASN:HB3	2.20	0.41
3:A:699:GLY:C	3:A:753:LEU:HD22	2.41	0.41
3:A:149:PHE:CD1	3:A:149:PHE:N	2.88	0.41
3:A:257:TYR:CZ	3:A:787:ASN:OD1	2.73	0.41
3:A:384:ARG:O	3:A:386:HIS:CE1	2.73	0.41
3:A:804:HIS:O	3:A:808:ILE:HG13	2.20	0.41
3:A:453:VAL:HG23	3:A:454:TYR:CE2	2.54	0.41
3:A:494:ARG:NH1	3:A:521:ASP:CG	2.73	0.41
3:A:638:GLU:HA	3:A:641:PHE:CD2	2.55	0.41
3:A:776:TYR:OH	3:A:854:ILE:HD11	2.20	0.41
3:A:412:LEU:HD23	3:A:623:ASP:O	2.20	0.41
3:A:455:SER:HB2	3:A:465:LYS:HG2	2.03	0.41
3:A:494:ARG:NH1	3:A:521:ASP:OD2	2.53	0.41
2:D:11:DG:C2'	2:D:10:DT:O5'	2.58	0.41
3:A:253:ILE:HG22	3:A:254:GLU:N	2.36	0.41
3:A:329:TYR:CD2	3:A:333:GLN:NE2	2.89	0.41
3:A:449:ARG:NH1	3:A:452:ASP:OD1	2.51	0.41
3:A:532:LYS:HE2	3:A:532:LYS:O	2.20	0.41
3:A:542:LEU:O	3:A:546:GLN:HB2	2.21	0.41
3:A:41:CYS:HB3	3:A:58:THR:HG23	2.03	0.41
3:A:152:LEU:HD22	3:A:159:VAL:O	2.21	0.41
3:A:180:SER:O	3:A:182:ILE:N	2.54	0.41
3:A:486:LYS:HE2	3:A:486:LYS:HB2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:638:GLU:O	3:A:638:GLU:HG2	2.21	0.41
3:A:801:CYS:HA	3:A:802:PRO:HD3	1.85	0.41
3:A:380:ILE:HA	3:A:381:PRO:HD3	1.88	0.40
3:A:533:LEU:CB	3:A:538:LEU:HD13	2.50	0.40
3:A:737:THR:HA	3:A:738:PRO:HD3	1.97	0.40
3:A:95:ASP:OD1	3:A:374:LYS:HE3	2.21	0.40
3:A:209:THR:HA	3:A:210:PRO:HD3	1.93	0.40
3:A:524:ASP:OD1	3:A:525:GLU:N	2.54	0.40
3:A:796:PHE:HB3	3:A:797:PRO:HD2	2.03	0.40
1:E:3:DC:H5"	3:A:253:ILE:HD13	2.03	0.40
3:A:179:PRO:O	3:A:183:ILE:HG13	2.22	0.40
3:A:47:THR:CG2	3:A:48:LYS:H	2.23	0.40
3:A:724:LYS:HB3	3:A:724:LYS:HZ2	1.83	0.40
3:A:791:TYR:CE2	3:A:802:PRO:CD	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	901/903 (100%)	820 (91%)	66 (7%)	15 (2%)	9 23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	167	ALA
3	A	256	MET
3	A	642	ARG
3	A	787	ASN
3	A	172	GLU
3	A	181	GLU
3	A	637	GLY

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Mol	Chain	Res	Type
3	A	897	LEU
3	A	43	GLU
3	A	121	ASP
3	A	136	ILE
3	A	179	PRO
3	A	302	LYS
3	A	780	ALA
3	A	828	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	802/802 (100%)	742 (92%)	60 (8%)	13 31

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	43	GLU
3	A	64	ASN
3	A	73	LYS
3	A	86	ASP
3	A	107	LYS
3	A	112	ASN
3	A	121	ASP
3	A	214	THR
3	A	238	THR
3	A	241	ARG
3	A	254	GLU
3	A	264	THR
3	A	268	ILE
3	A	273	TYR
3	A	275	ASP
3	A	281	SER
3	A	284	ASN
3	A	295	GLU

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Mol	Chain	Res	Type
3	A	314	GLU
3	A	316	ASN
3	A	327	ASP
3	A	337	LYS
3	A	343	LEU
3	A	358	VAL
3	A	373	LEU
3	A	375	GLU
3	A	391	TYR
3	A	402	ASN
3	A	440	HIS
3	A	441	ASP
3	A	459	ASN
3	A	493	GLN
3	A	519	ARG
3	A	532	LYS
3	A	536	LYS
3	A	556	GLN
3	A	612	GLU
3	A	624	SER
3	A	644	THR
3	A	649	ASP
3	A	653	LYS
3	A	660	GLU
3	A	685	ARG
3	A	718	THR
3	A	734	LYS
3	A	736	SER
3	A	747	GLU
3	A	760	LEU
3	A	772	ARG
3	A	775	ASN
3	A	776	TYR
3	A	777	ILE
3	A	783	SER
3	A	812	ASN
3	A	832	VAL
3	A	835	LEU
3	A	843	ASP
3	A	855	THR
3	A	880	LEU
3	A	900	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS
3	A	64	ASN
3	A	112	ASN
3	A	158	ASN
3	A	173	GLN
3	A	206	GLN
3	A	232	ASN
3	A	284	ASN
3	A	299	ASN
3	A	316	ASN
3	A	333	GLN
3	A	402	ASN
3	A	422	GLN
3	A	424	ASN
3	A	440	HIS
3	A	459	ASN
3	A	480	ASN
3	A	481	GLN
3	A	485	HIS
3	A	645	ASN
3	A	678	GLN
3	A	773	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are 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	$\#\|Z\| > 2$
5	GDP	A	999	-	24,30,30	2.73	10 (41%)	30,47,47	2.76	9 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	A	999	-	-	5/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	GDP	O4'-C1'	6.69	1.50	1.41
5	A	999	GDP	O6-C6	6.02	1.35	1.23
5	A	999	GDP	C2-N1	4.93	1.49	1.37
5	A	999	GDP	PB-O2B	-3.38	1.41	1.54
5	A	999	GDP	O3'-C3'	3.00	1.50	1.43
5	A	999	GDP	O4'-C4'	2.93	1.51	1.45
5	A	999	GDP	PB-O3B	2.72	1.65	1.54
5	A	999	GDP	C8-N7	2.70	1.39	1.35
5	A	999	GDP	C5'-C4'	-2.29	1.44	1.51
5	A	999	GDP	C2-N3	-2.03	1.28	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	999	GDP	C8-N7-C5	9.33	120.77	102.99
5	A	999	GDP	C5-C6-N1	5.56	123.77	113.95
5	A	999	GDP	N2-C2-N3	5.26	129.98	119.74
5	A	999	GDP	C2-N1-C6	-3.65	118.38	125.10
5	A	999	GDP	O6-C6-C5	-3.55	117.44	124.37
5	A	999	GDP	N2-C2-N1	-3.52	109.21	116.71
5	A	999	GDP	O4'-C1'-C2'	-2.73	102.94	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	999	GDP	O2'-C2'-C3'	2.71	120.60	111.82
5	A	999	GDP	O5'-C5'-C4'	2.14	116.37	108.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	999	GDP	PA-O3A-PB-O2B
5	A	999	GDP	C3'-C4'-C5'-O5'
5	A	999	GDP	O4'-C4'-C5'-O5'
5	A	999	GDP	PA-O3A-PB-O3B
5	A	999	GDP	C5'-O5'-PA-O1A

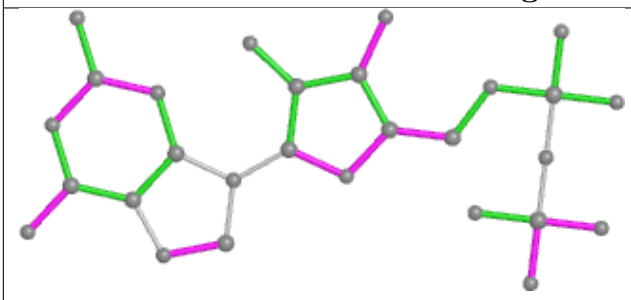
There are no ring outliers.

1 monomer is involved in 3 short contacts:

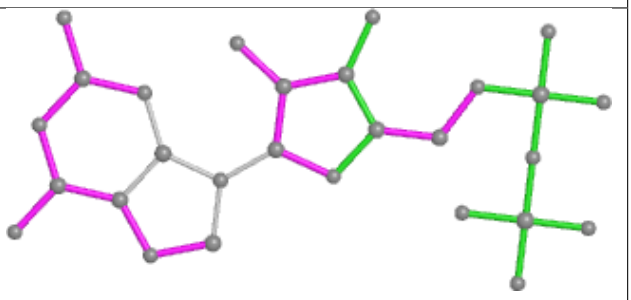
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	999	GDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

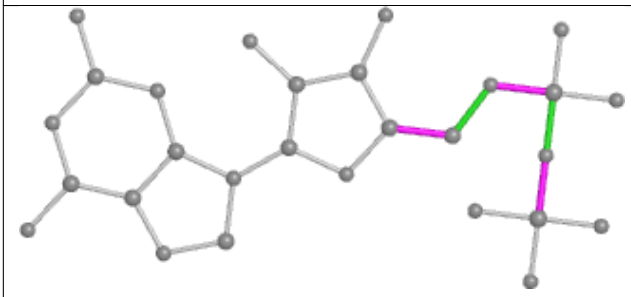
Ligand GDP A 999



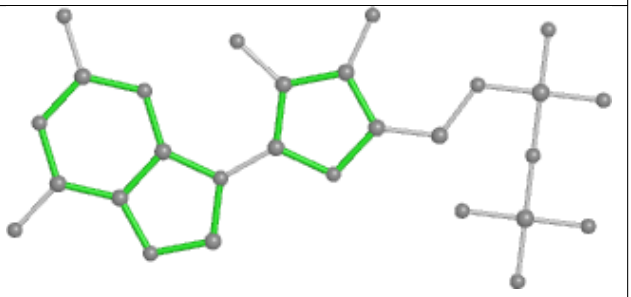
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	E	11/11 (100%)	1.10	2 (18%)	1	1	70, 104, 119, 122	0
2	D	12/12 (100%)	1.56	4 (33%)	0	0	49, 88, 122, 122	0
3	A	903/903 (100%)	-0.11	17 (1%)	66	69	29, 53, 84, 119	0
All	All	926/926 (100%)	-0.08	23 (2%)	57	59	29, 54, 86, 122	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	257	TYR	11.9
2	D	11	DG	5.2
3	A	903	PHE	4.5
1	E	12	DT	4.0
3	A	256	MET	4.0
2	D	12	DA	3.8
3	A	900	MET	3.7
2	D	10	DT	3.7
2	D	9	DA	3.6
3	A	722	GLU	3.5
3	A	254	GLU	3.5
3	A	895	ALA	3.2
3	A	175	GLY	3.1
3	A	901	PHE	2.8
3	A	819	ILE	2.5
1	E	10	DA	2.5
3	A	857	LEU	2.4
3	A	183	ILE	2.4
3	A	508	LEU	2.4
3	A	897	LEU	2.4
3	A	786	ASN	2.4
3	A	255	ASN	2.1
3	A	391	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)

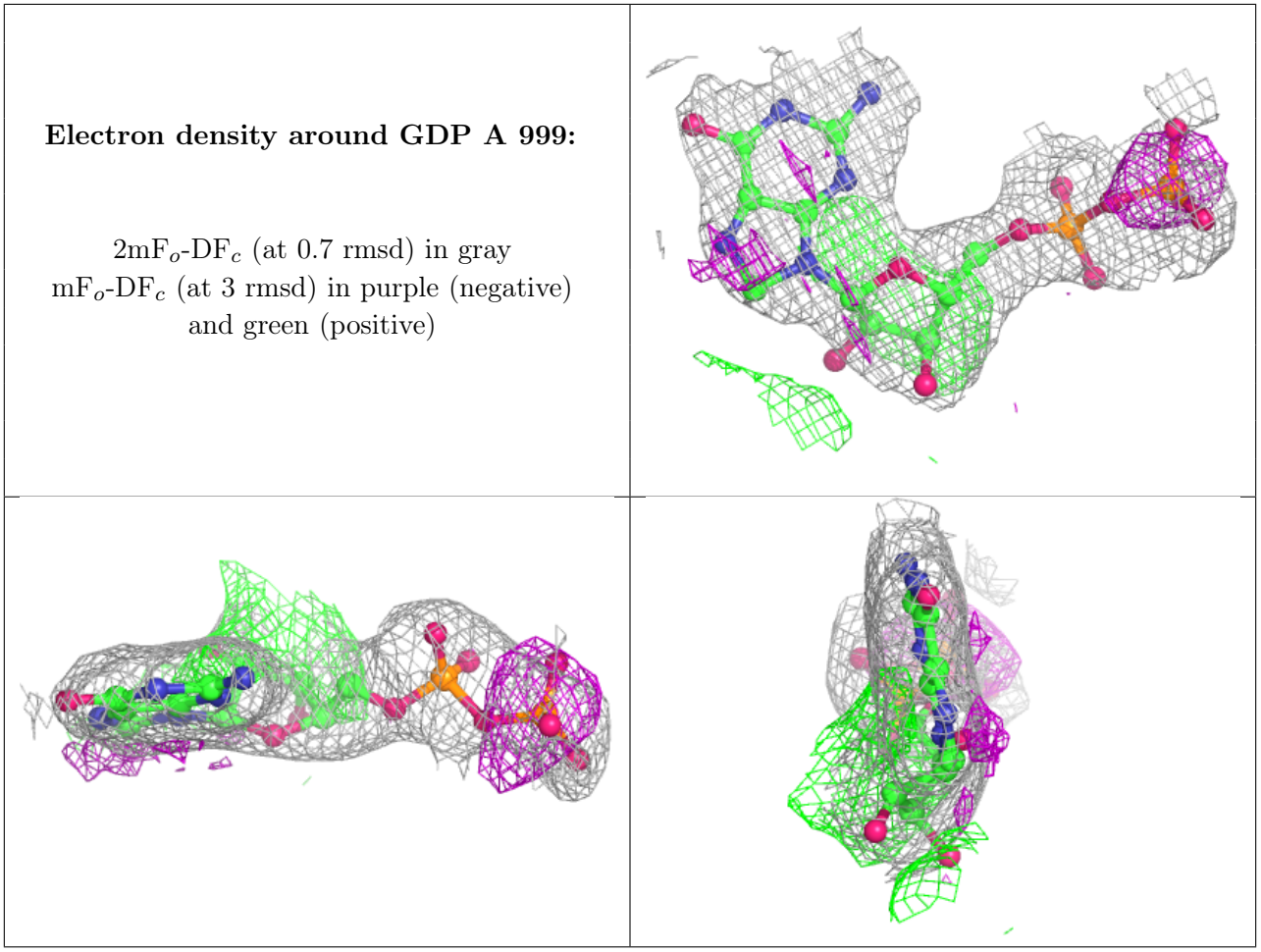
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	1025	1/1	0.60	0.14	82,82,82,82	0
4	CA	A	1002	1/1	0.71	0.25	97,97,97,97	0
4	CA	A	1005	1/1	0.75	0.26	94,94,94,94	0
5	GDP	A	999	28/28	0.82	0.24	35,76,122,122	0
4	CA	D	1003	1/1	0.85	0.22	73,73,73,73	0
4	CA	A	1006	1/1	0.85	0.24	107,107,107,107	0
4	CA	D	1009	1/1	0.90	0.09	78,78,78,78	0
4	CA	A	1004	1/1	0.92	0.19	58,58,58,58	0
4	CA	E	1024	1/1	0.93	0.35	122,122,122,122	0
4	CA	A	1001	1/1	0.99	0.19	63,63,63,63	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 GDP A 999:

$2mF_o$-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.