



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:21 PM UTC

PDB ID : 1CLQ / pdb_00001clq
Title : CRYSTAL STRUCTURE OF A REPLICATION FORK DNA POLYMERASE EDITING COMPLEX AT 2.7 Å 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

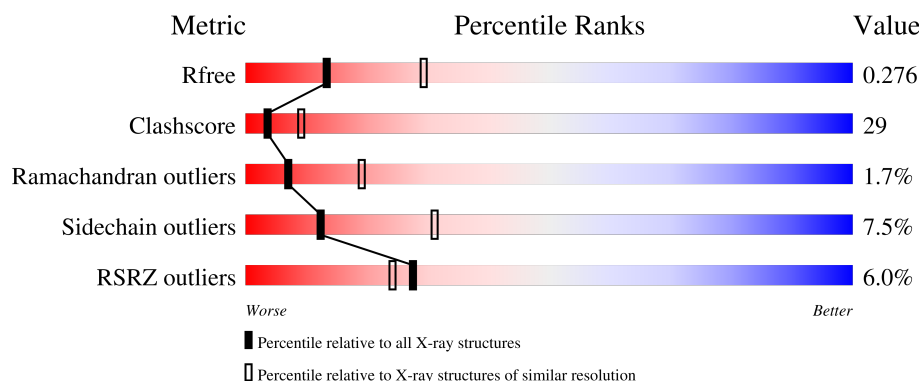
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	E	11	45% 82% 9% 9%
2	D	12	58% 67% 33%
3	A	903	5% 55% 39% 6%

2 Entry composition

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 (CCD ID: CA) (formula: Ca).

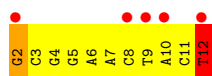
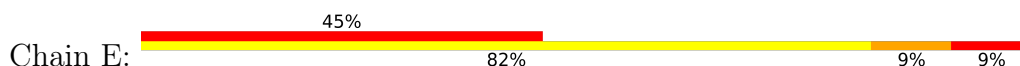
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ca	0	0
			1	1		
4	D	2	Total	Ca	0	0
			2	2		
4	A	6	Total	Ca	0	0
			6	6		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

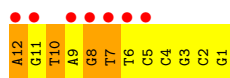
3 Residue-property plots

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.

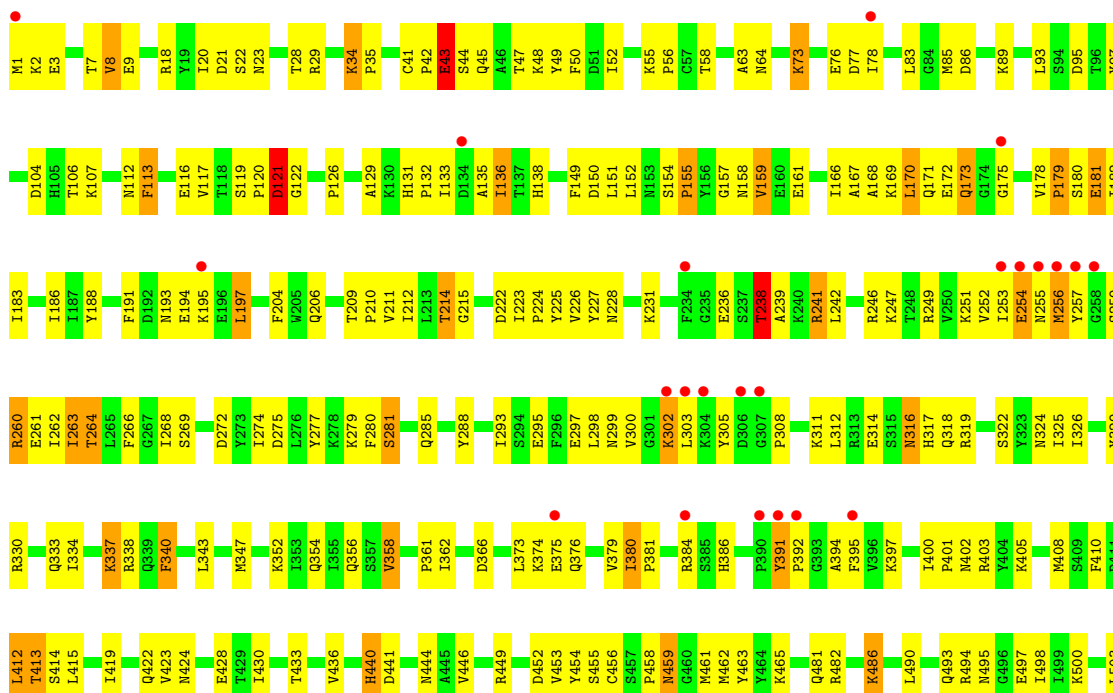
- Molecule 1: DNA (5'-D(*GP*CP*GP*GP*AP*AP*CP*TP*AP*CP*T)-3')

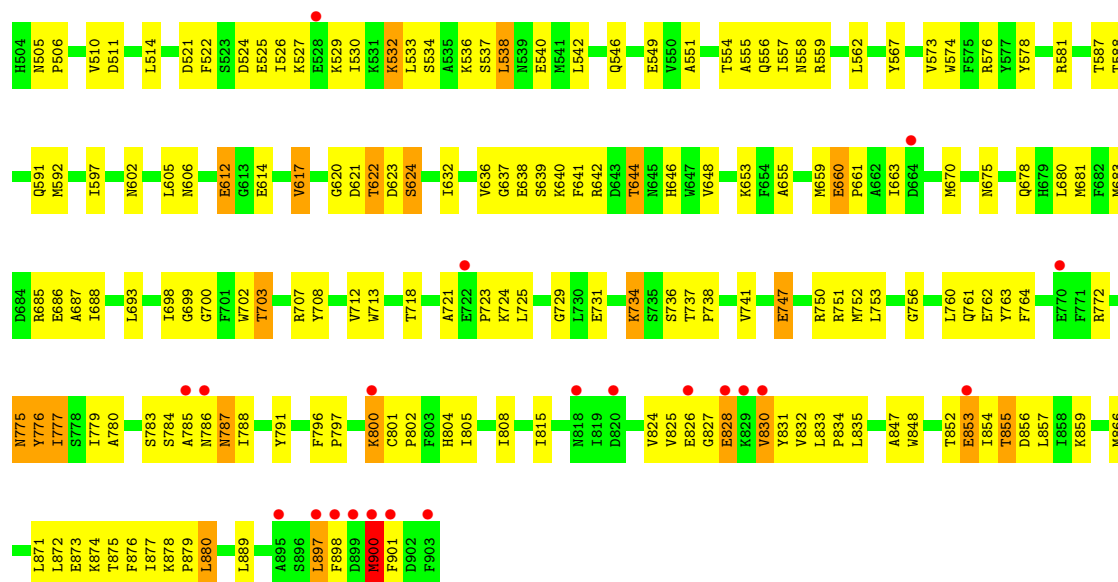


- Molecule 2: DNA (5'-D(*AP*GP*TP*AP*GP*TP*TP*CP*CP*GP*CP*G)-3')



- Molecule 3: PROTEIN (DNA POLYMERASE)





4 Data and refinement statistics

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 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (40.00-2.70) 97.2 (40.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.284 0.225 , 0.276	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 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.51	0/250	1.20	3/384 (0.8%)
2	D	0.52	0/273	1.55	8/420 (1.9%)
3	A	0.52	0/7562	1.03	38/10217 (0.4%)
All	All	0.52	0/8085	1.06	49/11021 (0.4%)

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

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	211	VAL	N-CA-C	-10.75	103.20	111.90
2	D	12	DA	C8-N9-C1'	10.03	142.09	127.05
2	D	12	DA	C4-N9-C1'	-10.03	112.01	127.05
3	A	712	VAL	N-CA-C	10.03	122.12	108.89
3	A	900	MET	N-CA-C	-9.80	101.89	114.04
2	D	12	DA	N9-C1'-C2'	9.63	127.94	113.50
1	E	12	DT	C2'-C3'-O3'	-8.82	98.28	111.50
3	A	239	ALA	N-CA-C	-8.71	103.17	113.88
3	A	456	CYS	N-CA-C	8.44	122.54	110.14
3	A	159	VAL	N-CA-C	8.00	118.29	108.53
3	A	756	GLY	N-CA-C	7.76	119.92	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	34	LYS	CA-C-N	7.57	127.47	120.21
3	A	34	LYS	C-N-CA	7.57	127.47	120.21
3	A	242	LEU	N-CA-C	-7.56	104.06	113.28
3	A	557	ILE	N-CA-C	-7.38	101.86	111.09
3	A	622	THR	N-CA-C	-7.29	104.53	113.50
3	A	354	GLN	N-CA-C	-7.23	99.58	110.28
3	A	436	VAL	N-CA-C	7.19	118.94	108.58
2	D	7	DT	C2'-C3'-O3'	7.18	122.27	111.50
3	A	486	LYS	N-CA-C	-6.88	103.48	110.97
3	A	901	PHE	N-CA-C	-6.24	99.71	109.25
3	A	856	ASP	N-CA-C	-6.12	105.66	113.01
1	E	2	DG	O5'-C5'-C4'	-6.08	101.68	110.80
3	A	413	THR	N-CA-C	6.01	119.06	110.10
1	E	12	DT	C4'-C3'-O3'	5.86	118.78	110.00
2	D	1	DG	C2'-C3'-O3'	-5.85	102.72	111.50
3	A	830	VAL	N-CA-C	5.80	117.07	108.65
3	A	260	ARG	N-CA-C	5.78	117.85	109.07
2	D	10	DT	C2'-C3'-O3'	5.59	119.88	111.50
3	A	238	THR	N-CA-C	-5.59	104.69	113.02
2	D	8	DG	C2'-C3'-O3'	5.53	119.79	111.50
3	A	703	THR	N-CA-C	-5.52	106.68	113.41
3	A	55	LYS	CA-C-N	5.48	125.42	119.78
3	A	55	LYS	C-N-CA	5.48	125.42	119.78
3	A	113	PHE	N-CA-C	5.33	117.29	109.24
3	A	412	LEU	CA-CB-CG	5.33	134.96	116.30
3	A	263	ILE	N-CA-C	5.30	115.25	107.15
3	A	324	ASN	N-CA-C	-5.26	104.99	111.40
3	A	340	PHE	N-CA-C	5.26	117.92	111.82
3	A	639	SER	N-CA-C	-5.24	105.56	112.94
3	A	763	TYR	N-CA-C	5.18	117.01	111.36
3	A	648	VAL	N-CA-C	-5.15	105.36	110.62
3	A	155	PRO	N-CA-C	-5.13	107.93	114.35
3	A	640	LYS	N-CA-C	-5.10	106.30	112.88
3	A	380	ILE	CA-C-N	5.08	125.36	119.92
3	A	380	ILE	C-N-CA	5.08	125.36	119.92
3	A	400	ILE	N-CA-C	-5.08	102.63	107.76
2	D	12	DA	O4'-C1'-C2'	5.05	113.98	106.40
3	A	405	LYS	N-CA-C	5.04	116.46	110.97

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	46	0
3	A	7381	0	7265	383	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	448	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 29.

All (448) 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
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:347:MET:HE2	3:A:358:VAL:HG22	1.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:8:DG:H2'	2:D:7:DT:H71	1.59	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
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:253:ILE:C	3:A:254:GLU:HG2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:A:316:ASN:C	3:A:316:ASN:HD22	2.04	0.66
3:A:171:GLN:C	3:A:173:GLN:H	2.03	0.65
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:104:ASP:CG	3:A:106:THR:HG22	2.24	0.63
3:A:542:LEU:HD23	3:A:542:LEU:C	2.23	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:663:ILE:HD13	3:A:683:MET:HE2	1.80	0.63
3:A:621:ASP:HB3	3:A:624:SER:H	1.64	0.62
3:A:157:GLY:C	3:A:158:ASN:HD22	2.07	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:316:ASN:ND2	3:A:316:ASN:C	2.58	0.61
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: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:298:LEU:O	3:A:300:VAL:HG23	2.00	0.61
3:A:197:LEU:C	3:A:197:LEU:HD13	2.26	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:HZ3	1.66	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:152:LEU:HD11	3:A:161:GLU:HG2	1.84	0.60
3:A:347:MET:HE2	3:A:358:VAL:CG2	2.24	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
2:D:7:DT:H3'	3:A:256:MET:HE1	1.83	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:800:LYS:HB2	3:A:800:LYS:HZ2	1.67	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: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: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: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: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:28:THR:HG22	3:A:29:ARG:N	2.19	0.57
3:A:510:VAL:HG23	3:A:510:VAL:O	2.05	0.57
3:A:724:LYS:HB3	3:A:724:LYS:HZ2	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:461:MET:HE1	3:A:581:ARG:HD2	1.88	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:493:GLN:HB2	3:A:549:GLU:CD	2.32	0.55
3:A:175:GLY:O	3:A:319:ARG:NH2	2.40	0.54
3:A:433:THR:O	3:A:462:MET:HE2	2.06	0.54
3:A:700:GLY:HA2	3:A:753:LEU:HD22	1.89	0.54
3:A:592:MET:HE2	3:A:670:MET:SD	2.47	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:408:MET:HE2	3:A:685:ARG:HG3	1.88	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: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:112:ASN:C	3:A:112:ASN:HD22	2.15	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:180:SER:C	3:A:182:ILE:H	2.17	0.52
3:A:249:ARG:O	3:A:264:THR:HG23	2.10	0.52
3:A:663:ILE:HG21	3:A:683:MET:HE2	1.91	0.52
3:A:700:GLY:HA2	3:A:753:LEU:CD2	2.40	0.52
1:E:2:DG:O5'	3:A:255:ASN:CG	2.53	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
3:A:786:ASN:HA	3:A:826:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:786:ASN:OD1	3:A:827:GLY:HA2	2.10	0.52
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:825:VAL:C	3:A:828:GLU:HG2	2.36	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: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:171:GLN:C	3:A:173:GLN:N	2.70	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
1:E:2:DG:HO5'	3:A:255:ASN:N	2.06	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: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
3:A:578:TYR:C	3:A:578:TYR:CD1	2.92	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: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
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:356:GLN:C	3:A:358:VAL:H	2.22	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:775:ASN:OD1	3:A:775:ASN:C	2.57	0.47
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
3:A:752:MET:HE3	3:A:889:LEU:HD12	1.97	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:699:GLY:C	3:A:753:LEU:HD22	2.41	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:9:GLU:HG2	3:A:266:PHE:HD2	1.81	0.46
3:A:494:ARG:NH1	3:A:521:ASP:CG	2.73	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: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
3:A:779:ILE:HD11	3:A:866:MET:HE1	1.98	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:97:TYR:O	3:A:352:LYS:NZ	2.46	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:193:ASN:OD1	3:A:193:ASN:C	2.61	0.44
3:A:461:MET:HE3	3:A:581:ARG:HD2	1.98	0.44
3:A:302:LYS:O	3:A:303:LEU:C	2.60	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:855:THR:C	3:A:857:LEU:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:A:644:THR:C	3:A:646:HIS:H	2.26	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: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:776:TYR:CG	3:A:777:ILE:N	2.86	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:391:TYR:O	3:A:392:PRO:C	2.61	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:317:HIS:O	3:A:318:GLN:C	2.62	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: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:855:THR:C	3:A:857:LEU:H	2.25	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
3:A:330:ARG:HH11	3:A:330:ARG:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:700:GLY:CA	3:A:753:LEU:HD22	2.49	0.42
3:A:252:VAL:C	3:A:253:ILE:HG13	2.45	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
3:A:551:ALA:O	3:A:554:THR:HG22	2.19	0.42
3:A:786:ASN:O	3:A:787:ASN:CG	2.62	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
3:A:775:ASN:CG	3:A:777:ILE:HG23	2.43	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: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:497:GLU:O	3:A:498:ILE:C	2.63	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:413:THR:O	3:A:414:SER:C	2.63	0.41
3:A:423:VAL:O	3:A:424:ASN:HB3	2.20	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:77:ASP:O	3:A:78:ILE:C	2.63	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:532:LYS:NZ	3:A:532:LYS:O	2.54	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:898:PHE:C	3:A:900:MET:H	2.28	0.41
3:A:49:TYR:C	3:A:50:PHE:CD1	2.99	0.41
3:A:412:LEU:HD23	3:A:623:ASP:O	2.20	0.41
3:A:42:PRO:C	3:A:44:SER:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	3:A:532:LYS:HE2	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
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:298:LEU:O	3:A:299:ASN:C	2.64	0.40
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:374:LYS:C	3:A:376:GLN:H	2.28	0.40
3:A:761:GLN:O	3:A:762:GLU:C	2.64	0.40
3:A:47:THR:CG2	3:A:48:LYS:H	2.23	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%)	7 19

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
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 ⓘ

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%)	12 31

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

Mol	Chain	Res	Type
3	A	8	VAL
3	A	43	GLU
3	A	64	ASN
3	A	73	LYS
3	A	86	ASP
3	A	107	LYS

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Mol	Chain	Res	Type
3	A	121	ASP
3	A	170	LEU
3	A	173	GLN
3	A	197	LEU
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	281	SER
3	A	295	GLU
3	A	314	GLU
3	A	316	ASN
3	A	337	LYS
3	A	343	LEU
3	A	358	VAL
3	A	362	ILE
3	A	373	LEU
3	A	375	GLU
3	A	391	TYR
3	A	440	HIS
3	A	441	ASP
3	A	446	VAL
3	A	459	ASN
3	A	532	LYS
3	A	536	LYS
3	A	538	LEU
3	A	556	GLN
3	A	562	LEU
3	A	612	GLU
3	A	617	VAL
3	A	624	SER
3	A	644	THR
3	A	653	LYS
3	A	660	GLU
3	A	718	THR
3	A	734	LYS
3	A	736	SER
3	A	747	GLU
3	A	760	LEU
3	A	772	ARG

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Mol	Chain	Res	Type
3	A	775	ASN
3	A	776	TYR
3	A	777	ILE
3	A	783	SER
3	A	800	LYS
3	A	832	VAL
3	A	835	LEU
3	A	853	GLU
3	A	855	THR
3	A	874	LYS
3	A	880	LEU
3	A	900	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	324	ASN
3	A	333	GLN
3	A	386	HIS
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 ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	-	29,30,30	2.98	15 (51%)	45,47,47	3.28	15 (33%)

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	-	-	7/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	GDP	PA-O3A	7.94	1.68	1.59
5	A	999	GDP	O6-C6	6.31	1.35	1.23
5	A	999	GDP	C8-N9	5.51	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	GDP	C2-N1	5.04	1.49	1.37
5	A	999	GDP	O4'-C1'	3.64	1.50	1.42
5	A	999	GDP	PB-O2B	-3.49	1.41	1.54
5	A	999	GDP	C5-C4	3.14	1.47	1.38
5	A	999	GDP	O4'-C4'	2.95	1.51	1.45
5	A	999	GDP	O3'-C3'	2.86	1.50	1.43
5	A	999	GDP	PB-O3B	2.84	1.65	1.54
5	A	999	GDP	C5-N7	-2.74	1.33	1.39
5	A	999	GDP	C8-N7	2.52	1.39	1.32
5	A	999	GDP	C5'-C4'	-2.37	1.44	1.51
5	A	999	GDP	C2-N3	-2.07	1.28	1.33
5	A	999	GDP	C6-N1	-2.04	1.35	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	999	GDP	N9-C8-N7	-9.88	95.09	113.40
5	A	999	GDP	C8-N7-C5	9.27	120.77	104.26
5	A	999	GDP	C6-C5-N7	8.27	145.35	130.29
5	A	999	GDP	C6-C5-C4	-5.48	110.58	118.83
5	A	999	GDP	N2-C2-N3	5.28	129.98	119.67
5	A	999	GDP	C8-N9-C4	5.09	115.57	106.03
5	A	999	GDP	C2-N3-C4	4.28	119.67	112.30
5	A	999	GDP	C4-C5-N7	-4.21	104.00	110.67
5	A	999	GDP	C5-C6-N1	4.13	123.77	113.25
5	A	999	GDP	C2-N1-C6	-3.71	118.38	125.11
5	A	999	GDP	N2-C2-N1	-3.58	109.21	116.76
5	A	999	GDP	O6-C6-C5	-3.44	117.44	126.53
5	A	999	GDP	C1'-N9-C8	-3.42	117.01	126.73
5	A	999	GDP	O2'-C2'-C3'	2.74	120.60	111.82
5	A	999	GDP	O5'-C5'-C4'	2.17	116.37	108.99

There are no chirality outliers.

All (7) 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	O4'-C1'-N9-C4
5	A	999	GDP	O4'-C1'-N9-C8
5	A	999	GDP	C5'-O5'-PA-O1A

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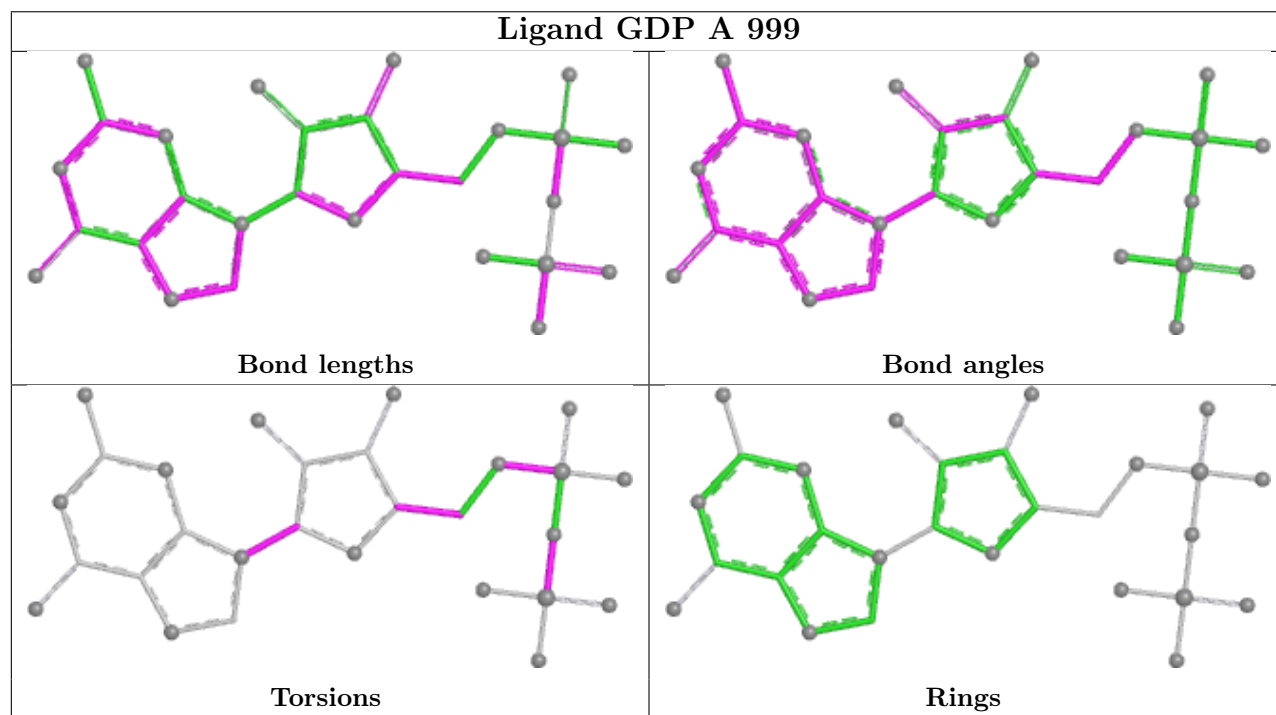
Mol	Chain	Res	Type	Atoms
5	A	999	GDP	PA-O3A-PB-O3B

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 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 ⓘ

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, 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	E	11/11 (100%)	2.12	5 (45%) 0 0	70, 104, 119, 122	0
2	D	12/12 (100%)	1.78	7 (58%) 0 0	49, 88, 122, 122	0
3	A	903/903 (100%)	0.26	44 (4%) 35 31	29, 53, 84, 119	0
All	All	926/926 (100%)	0.30	56 (6%) 27 24	29, 54, 86, 122	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	257	TYR	8.5
3	A	256	MET	5.3
3	A	901	PHE	4.5
1	E	12	DT	4.4
3	A	254	GLU	3.8
3	A	829	LYS	3.7
3	A	903	PHE	3.7
3	A	786	ASN	3.7
3	A	78	ILE	3.5
3	A	800	LYS	3.5
2	D	12	DA	3.5
3	A	255	ASN	3.4
3	A	392	PRO	3.4
3	A	1	MET	3.4
2	D	9	DA	3.3
3	A	391	TYR	3.2
1	E	10	DA	3.0
2	D	7	DT	2.9
3	A	390	PRO	2.8
3	A	134	ASP	2.8
3	A	303	LEU	2.7
3	A	304	LYS	2.7
3	A	722	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	306	ASP	2.7
1	E	2	DG	2.6
3	A	895	ALA	2.6
3	A	770	GLU	2.5
1	E	8	DC	2.5
2	D	11	DG	2.5
3	A	253	ILE	2.5
3	A	828	GLU	2.5
2	D	8	DG	2.5
3	A	175	GLY	2.5
3	A	818	ASN	2.4
3	A	785	ALA	2.4
3	A	528	GLU	2.3
3	A	830	VAL	2.3
3	A	384	ARG	2.3
3	A	234	PHE	2.3
3	A	307	GLY	2.2
3	A	898	PHE	2.2
2	D	6	DT	2.2
3	A	395	PHE	2.2
3	A	899	ASP	2.2
3	A	900	MET	2.2
3	A	375	GLU	2.1
3	A	302	LYS	2.1
1	E	9	DT	2.1
3	A	826	GLU	2.1
3	A	664	ASP	2.0
3	A	853	GLU	2.0
3	A	195	LYS	2.0
3	A	897	LEU	2.0
3	A	258	GLY	2.0
3	A	820	ASP	2.0
2	D	5	DC	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](#)

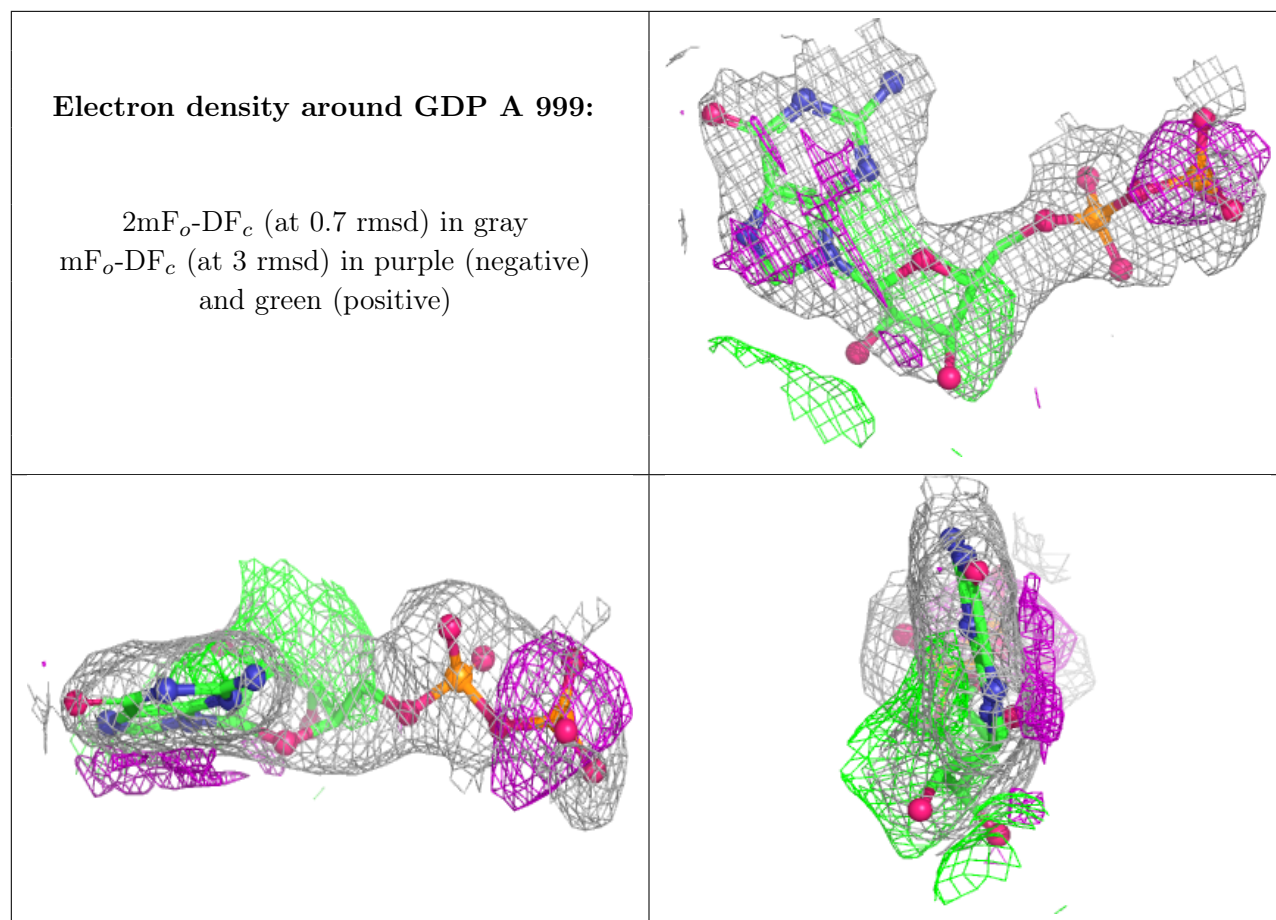
There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	1006	1/1	0.78	0.19	107,107,107,107	0
4	CA	A	1002	1/1	0.79	0.15	97,97,97,97	0
5	GDP	A	999	28/28	0.80	0.17	35,76,122,122	0
4	CA	A	1005	1/1	0.84	0.27	94,94,94,94	0
4	CA	E	1024	1/1	0.90	0.17	122,122,122,122	0
4	CA	A	1025	1/1	0.90	0.08	82,82,82,82	0
4	CA	D	1003	1/1	0.90	0.09	73,73,73,73	0
4	CA	D	1009	1/1	0.92	0.08	78,78,78,78	0
4	CA	A	1004	1/1	0.96	0.09	58,58,58,58	0
4	CA	A	1001	1/1	0.97	0.12	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.