



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:01 PM UTC

PDB ID : 9HS2 / pdb_00009hs2
Title : Crystal structure of the Escherichia coli nucleosidase PpnN (ppGpp form)
Authors : Baerentsen, R.L.; Brodersen, D.E.
Deposited on : 2024-12-18
Resolution : 3.40 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

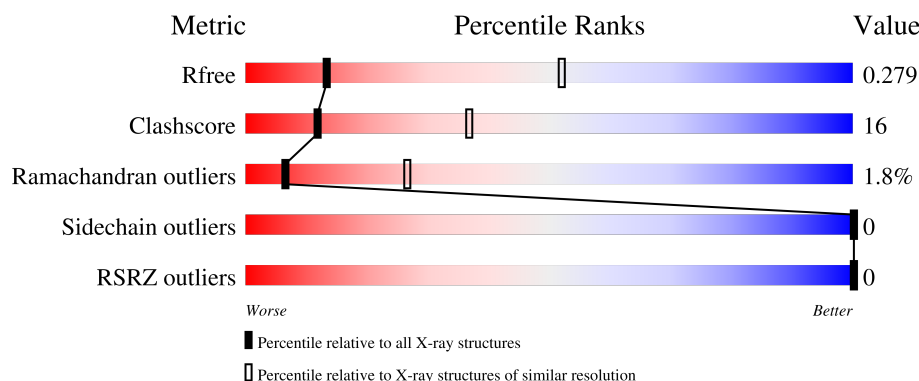
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	 66% 29% 5%
1	B	460	 62% 32% 5%
1	C	460	 64% 32% 2%
1	D	460	 63% 32% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14063 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3470	2197	620	632	21			
1	B	435	Total	C	N	O	S	0	0	0
			3427	2168	610	628	21			
1	C	444	Total	C	N	O	S	0	0	0
			3502	2217	624	640	21			
1	D	441	Total	C	N	O	S	0	0	0
			3472	2196	619	636	21			

There are 28 discrepancies between the modelled and reference sequences:

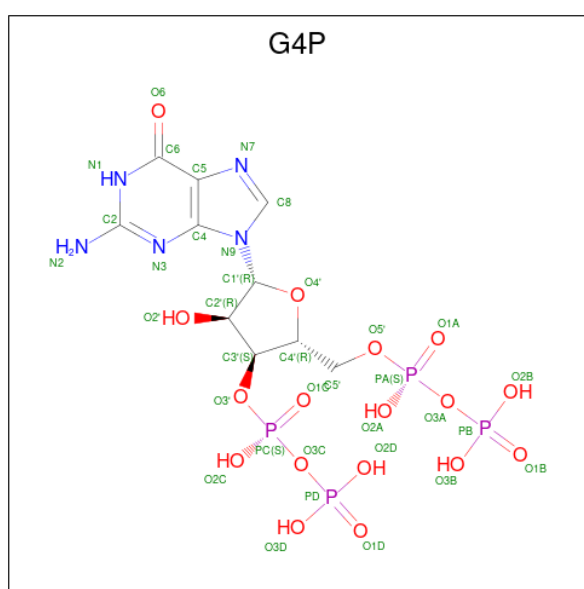
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	THR	-	expression tag	UNP P0ADR8
A	-4	ASP	-	expression tag	UNP P0ADR8
A	-3	PRO	-	expression tag	UNP P0ADR8
A	-2	ALA	-	expression tag	UNP P0ADR8
A	-1	LEU	-	expression tag	UNP P0ADR8
A	0	ARG	-	expression tag	UNP P0ADR8
A	1	ALA	-	expression tag	UNP P0ADR8
B	-5	THR	-	expression tag	UNP P0ADR8
B	-4	ASP	-	expression tag	UNP P0ADR8
B	-3	PRO	-	expression tag	UNP P0ADR8
B	-2	ALA	-	expression tag	UNP P0ADR8
B	-1	LEU	-	expression tag	UNP P0ADR8
B	0	ARG	-	expression tag	UNP P0ADR8
B	1	ALA	-	expression tag	UNP P0ADR8
C	-5	THR	-	expression tag	UNP P0ADR8
C	-4	ASP	-	expression tag	UNP P0ADR8
C	-3	PRO	-	expression tag	UNP P0ADR8
C	-2	ALA	-	expression tag	UNP P0ADR8
C	-1	LEU	-	expression tag	UNP P0ADR8
C	0	ARG	-	expression tag	UNP P0ADR8
C	1	ALA	-	expression tag	UNP P0ADR8

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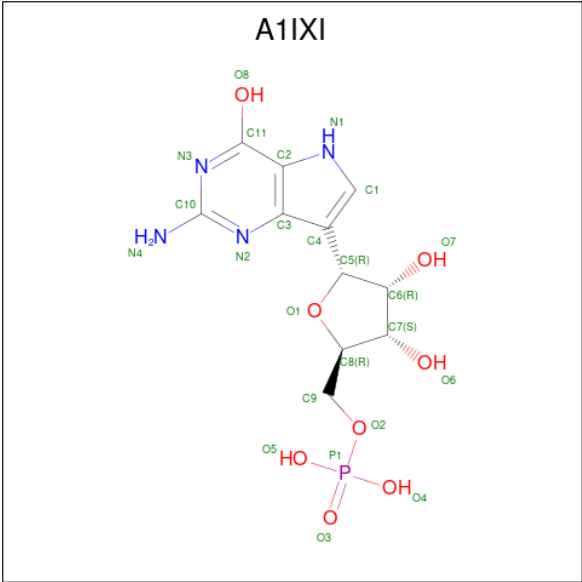
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	THR	-	expression tag	UNP P0ADR8
D	-4	ASP	-	expression tag	UNP P0ADR8
D	-3	PRO	-	expression tag	UNP P0ADR8
D	-2	ALA	-	expression tag	UNP P0ADR8
D	-1	LEU	-	expression tag	UNP P0ADR8
D	0	ARG	-	expression tag	UNP P0ADR8
D	1	ALA	-	expression tag	UNP P0ADR8

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	B	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	C	1	Total 36	C 10	N 5	O 17	P 4	0	0
2	D	1	Total 36	C 10	N 5	O 17	P 4	0	0

- Molecule 3 is 9-deazaguanosine-5'-monophosphate (CCD ID: A1IXI) (formula: $C_{11}H_{15}N_4O_8P$) (labeled as "Ligand of Interest" by depositor).

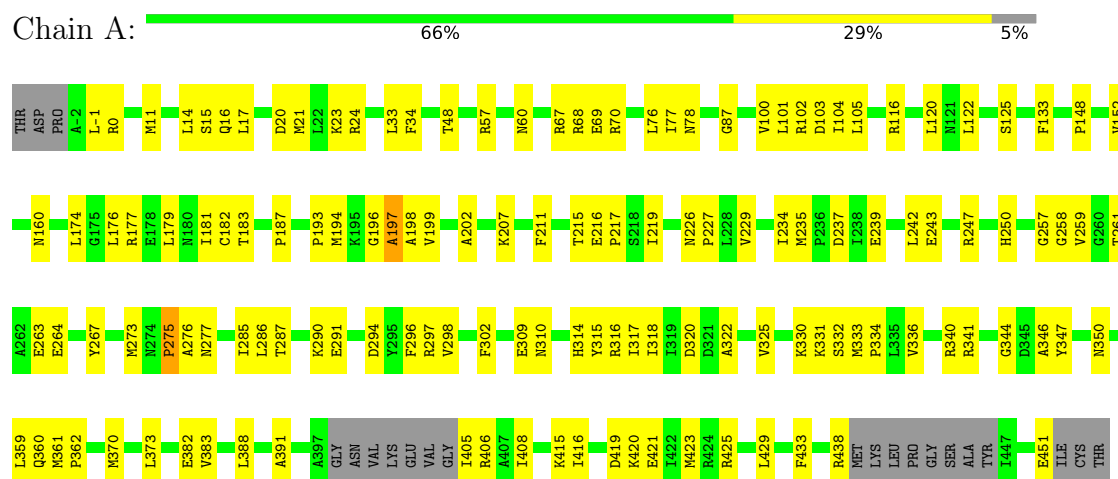


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	11	4	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	11	4	8	1		

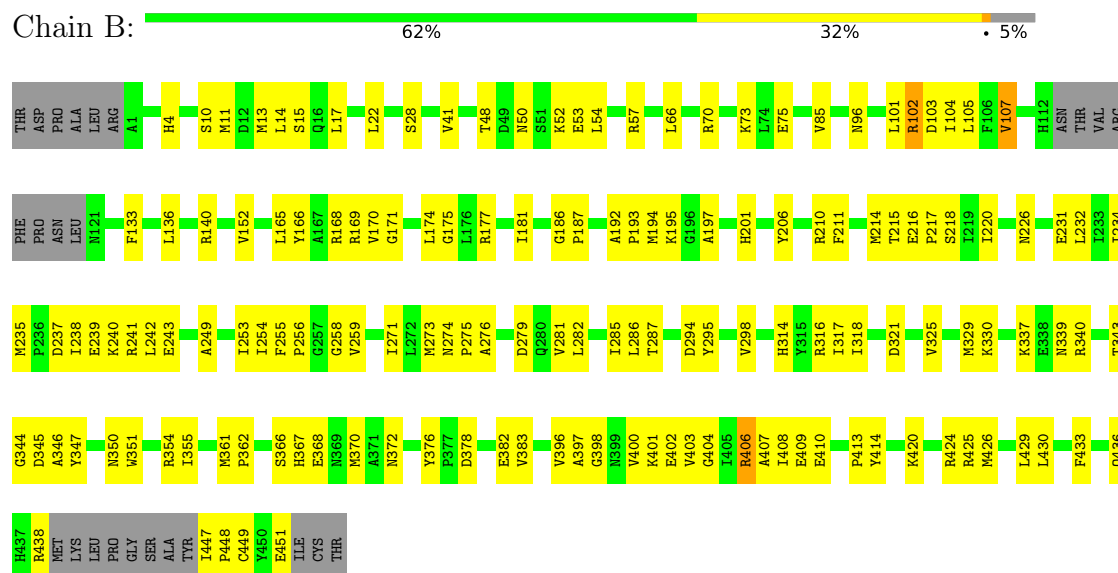
3 Residue-property plots

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: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase

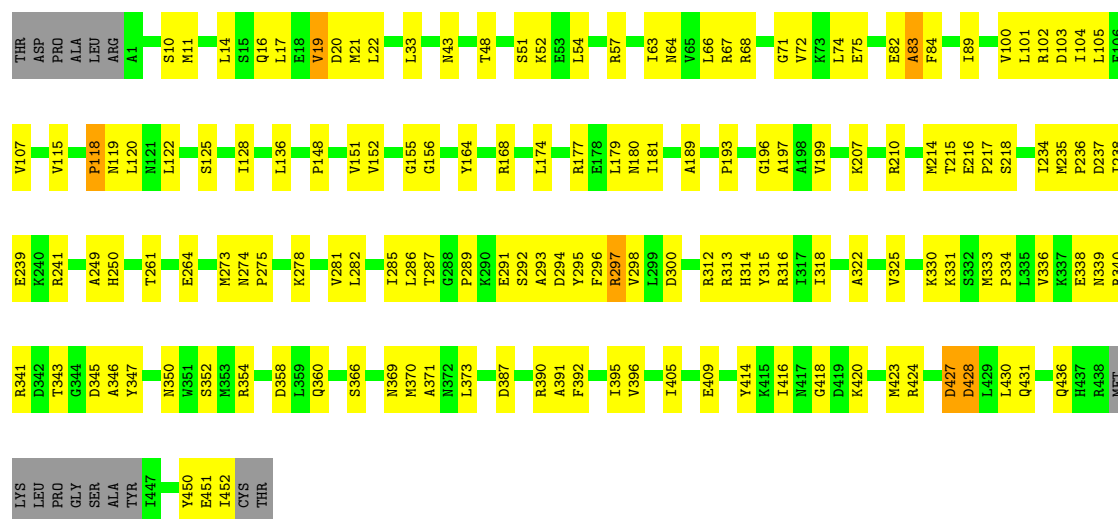


- Molecule 1: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase



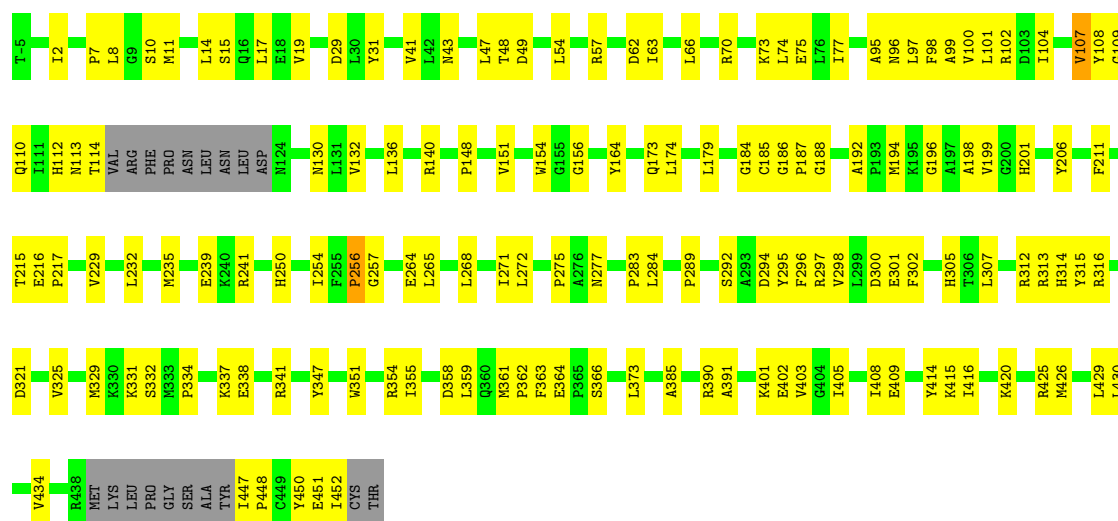
- Molecule 1: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase

Chain C:  64% 32% ..



● Molecule 1: Pyrimidine/purine nucleotide 5'-monophosphate nucleosidase

Chain D:  63% 32% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.12Å 155.12Å 226.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.11 – 3.40 53.11 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (53.11-3.40) 99.3 (53.11-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.283 0.221 , 0.279	Depositor DCC
R_{free} test set	1927 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	121.4	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 123.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14063	wwPDB-VP
Average B, all atoms (Å ²)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: A1IXI, G4P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/3536	0.79	2/4783 (0.0%)
1	B	0.46	0/3491	0.72	0/4720
1	C	0.54	0/3569	0.83	0/4829
1	D	0.54	0/3537	0.79	0/4784
All	All	0.51	0/14133	0.78	2/19116 (0.0%)

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	B	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ILE	CA-C-N	5.06	128.29	122.83
1	A	77	ILE	C-N-CA	5.06	128.29	122.83

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	ARG	Sidechain
1	C	19	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	C	297	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3470	0	3494	110	1
1	B	3427	0	3446	110	1
1	C	3502	0	3526	124	1
1	D	3472	0	3496	107	0
2	A	36	0	11	0	0
2	B	36	0	11	2	0
2	C	36	0	11	4	0
2	D	36	0	11	5	0
3	A	24	0	0	1	0
3	D	24	0	0	1	0
All	All	14063	0	14006	442	2

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 16.

All (442) 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:502:G4P:O4'	2:D:502:G4P:C1'	1.64	1.18
2:B:501:G4P:O4'	2:B:501:G4P:C1'	1.63	1.13
1:A:23:LYS:HZ1	1:A:67:ARG:NH2	1.48	1.08
1:B:194:MET:HE2	1:B:211:PHE:HB3	1.49	0.94
1:D:194:MET:HE2	1:D:211:PHE:HB3	1.49	0.93
1:A:23:LYS:HZ1	1:A:67:ARG:HH21	1.14	0.92
1:C:48:THR:HG21	1:C:57:ARG:HH12	1.38	0.87
1:B:368:GLU:OE2	1:B:372:ASN:ND2	2.08	0.87
1:D:48:THR:HG21	1:D:57:ARG:HH12	1.40	0.85
1:A:11:MET:HE3	1:A:102:ARG:HG3	1.59	0.84
1:A:67:ARG:O	1:A:68:ARG:HD3	1.80	0.82
1:B:343:THR:HG23	1:B:345:ASP:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLY:HA2	1:B:404:GLY:HA3	1.60	0.80
1:B:400:VAL:HG23	1:B:401:LYS:HD2	1.63	0.79
1:B:237:ASP:OD2	1:B:240:LYS:NZ	2.17	0.78
1:A:290:LYS:HB3	1:A:291:GLU:OE2	1.85	0.76
1:D:305:HIS:HB3	1:D:425:ARG:NH1	2.00	0.75
1:A:23:LYS:HZ1	1:A:67:ARG:CZ	1.99	0.75
1:C:343:THR:HG23	1:C:345:ASP:HB2	1.68	0.75
1:A:23:LYS:NZ	1:A:67:ARG:NH2	2.32	0.75
1:C:297:ARG:NH2	1:C:298:VAL:HB	2.01	0.75
1:C:331:LYS:O	1:C:334:PRO:HD2	1.87	0.74
1:D:48:THR:HG21	1:D:57:ARG:NH1	2.03	0.74
1:C:216:GLU:OE2	1:C:218:SER:OG	2.03	0.74
1:C:285:ILE:HG21	1:C:325:VAL:HG13	1.70	0.74
1:C:66:LEU:HD11	1:C:75:GLU:HB2	1.69	0.73
1:C:423:MET:HE3	1:C:452:ILE:HG23	1.70	0.73
1:A:298:VAL:HG22	1:A:429:LEU:HD12	1.71	0.72
1:D:307:LEU:HD21	1:D:385:ALA:HB2	1.71	0.72
1:A:20:ASP:OD1	1:A:67:ARG:NH1	2.23	0.71
1:C:100:VAL:HG13	1:C:104:ILE:HG13	1.72	0.71
1:D:271:ILE:HG21	1:D:355:ILE:HG12	1.72	0.71
1:B:271:ILE:HD13	1:B:355:ILE:HG12	1.71	0.70
1:D:337:LYS:NZ	1:D:347:TYR:CZ	2.60	0.70
1:D:447:ILE:HG21	1:D:452:ILE:HG23	1.73	0.69
1:A:344:GLY:HA2	1:B:70:ARG:HH21	1.56	0.69
1:B:286:LEU:HB2	1:B:317:ILE:HD12	1.75	0.68
1:A:177:ARG:HB3	1:A:330:LYS:HD3	1.75	0.68
1:C:341:ARG:HH21	2:C:501:G4P:H5'	1.60	0.67
1:C:286:LEU:HD23	1:C:296:PHE:HE1	1.60	0.67
1:C:216:GLU:OE1	1:C:238:ILE:HG23	1.94	0.66
1:C:420:LYS:H	1:C:420:LYS:HD2	1.60	0.66
1:C:103:ASP:HA	1:C:107:VAL:HB	1.77	0.66
1:D:41:VAL:HG21	1:D:100:VAL:HG21	1.77	0.66
1:D:294:ASP:N	1:D:294:ASP:OD1	2.26	0.65
1:D:8:LEU:HD23	1:D:95:ALA:HB2	1.78	0.65
1:B:168:ARG:HH11	1:B:195:LYS:HD3	1.61	0.65
1:B:11:MET:HE3	1:B:102:ARG:HG3	1.78	0.65
1:B:424:ARG:HH21	1:B:425:ARG:HD3	1.60	0.65
1:A:194:MET:SD	1:A:211:PHE:HB3	2.37	0.64
1:B:165:LEU:O	1:B:169:ARG:HG2	1.98	0.64
1:A:286:LEU:HB3	1:A:296:PHE:CE1	2.33	0.63
1:A:416:ILE:HB	1:A:423:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:O	1:A:277:ASN:N	2.32	0.63
1:D:148:PRO:HB3	1:D:250:HIS:CG	2.34	0.63
1:C:366:SER:OG	1:C:369:ASN:HB2	1.99	0.63
1:D:132:VAL:O	1:D:136:LEU:HD12	1.99	0.62
1:D:312:ARG:NH1	1:D:312:ARG:O	2.32	0.62
1:B:239:GLU:HG3	1:B:362:PRO:HG3	1.81	0.62
1:B:50:ASN:HD21	1:B:57:ARG:NH2	1.97	0.62
1:B:274:ASN:ND2	1:B:275:PRO:HD2	2.15	0.62
1:C:286:LEU:HB3	1:C:296:PHE:CE1	2.34	0.62
1:A:285:ILE:HG21	1:A:325:VAL:HG13	1.80	0.62
1:A:316:ARG:O	1:A:317:ILE:HG13	1.99	0.62
1:A:333:MET:HB2	1:A:334:PRO:HD3	1.82	0.62
1:D:29:ASP:N	1:D:29:ASP:OD1	2.28	0.62
1:A:340:ARG:HH21	1:A:350:ASN:HB2	1.65	0.61
1:B:52:LYS:HD3	1:B:53:GLU:N	2.15	0.61
1:B:370:MET:HE1	1:B:414:TYR:CE1	2.36	0.61
1:A:331:LYS:O	1:A:334:PRO:HD2	2.01	0.60
1:C:291:GLU:CD	1:C:291:GLU:H	2.10	0.60
1:C:431:GLN:OE1	1:C:431:GLN:N	2.35	0.60
1:D:11:MET:HG3	1:D:101:LEU:HD23	1.83	0.60
1:A:23:LYS:NZ	1:A:67:ARG:HH21	1.92	0.59
1:B:397:ALA:HB1	1:B:401:LYS:HD3	1.83	0.59
1:B:298:VAL:HG22	1:B:429:LEU:HD12	1.83	0.59
2:D:502:G4P:O1D	2:D:502:G4P:O2'	2.18	0.59
1:A:226:ASN:HB2	1:A:227:PRO:HD2	1.85	0.59
1:C:136:LEU:HD21	1:C:214:MET:CE	2.33	0.59
1:B:361:MET:HE3	1:B:362:PRO:HD2	1.85	0.59
1:A:199:VAL:O	1:A:202:ALA:HB3	2.02	0.59
1:B:10:SER:HA	1:B:140:ARG:NH1	2.18	0.59
1:C:341:ARG:NH2	2:C:501:G4P:H5'	2.17	0.59
1:D:373:LEU:HD21	1:D:391:ALA:HB2	1.84	0.59
1:C:289:PRO:HD2	1:C:292:SER:HB3	1.84	0.58
1:C:333:MET:HB2	1:C:334:PRO:HD3	1.83	0.58
1:D:331:LYS:O	1:D:334:PRO:HD2	2.03	0.58
1:B:295:TYR:HA	1:B:436:GLN:NE2	2.17	0.58
1:C:100:VAL:O	1:C:104:ILE:HB	2.04	0.58
1:B:279:ASP:OD1	1:B:279:ASP:N	2.37	0.58
1:D:338:GLU:O	1:D:341:ARG:N	2.36	0.58
1:C:338:GLU:O	1:C:341:ARG:N	2.35	0.58
1:A:275:PRO:C	1:A:277:ASN:H	2.12	0.57
1:C:64:ASN:HB2	1:C:75:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ARG:O	1:D:301:GLU:HG2	2.03	0.57
1:A:332:SER:O	1:A:336:VAL:HG23	2.05	0.57
1:C:11:MET:HE3	1:C:14:LEU:HD11	1.87	0.57
1:D:271:ILE:HG12	1:D:359:LEU:HD13	1.87	0.57
1:D:420:LYS:NZ	1:D:452:ILE:HA	2.20	0.56
1:B:52:LYS:NZ	1:B:53:GLU:OE2	2.32	0.56
1:B:168:ARG:NH1	1:B:195:LYS:HD3	2.20	0.56
1:B:235:MET:HG3	1:B:241:ARG:HA	1.88	0.56
1:B:253:ILE:HG13	1:B:329:MET:HE3	1.87	0.56
1:D:420:LYS:HZ2	1:D:452:ILE:HA	1.70	0.56
1:D:426:MET:HB3	1:D:430:LEU:HD23	1.87	0.56
1:A:370:MET:HE1	1:A:391:ALA:HA	1.87	0.56
1:D:312:ARG:O	1:D:312:ARG:HG2	2.06	0.55
1:A:316:ARG:C	1:A:317:ILE:HG13	2.31	0.55
1:A:382:GLU:HG2	1:A:383:VAL:N	2.20	0.55
1:C:19:VAL:HG13	1:C:72:VAL:HB	1.88	0.55
1:C:48:THR:HG21	1:C:57:ARG:NH1	2.17	0.55
1:A:16:GLN:HG3	1:B:351:TRP:CE3	2.42	0.55
1:A:239:GLU:HG3	1:A:362:PRO:HG3	1.87	0.55
1:C:101:LEU:HD12	1:C:105:LEU:HD12	1.89	0.55
1:C:405:ILE:O	1:C:409:GLU:HG3	2.07	0.55
1:A:273:MET:HG2	1:A:314:HIS:CD2	2.40	0.55
1:D:151:VAL:HG21	1:D:179:LEU:HD23	1.88	0.55
1:A:261:THR:O	1:A:264:GLU:HB2	2.07	0.55
1:B:50:ASN:ND2	1:B:53:GLU:HB2	2.22	0.54
1:B:216:GLU:OE1	1:B:238:ILE:HG23	2.08	0.54
1:C:68:ARG:NH1	2:D:502:G4P:O1B	2.38	0.54
1:D:96:ASN:O	1:D:99:ALA:HB3	2.07	0.54
1:C:10:SER:HB3	1:C:102:ARG:NH1	2.22	0.54
1:C:340:ARG:NH2	1:C:350:ASN:HD22	2.06	0.54
1:C:19:VAL:O	1:C:22:LEU:HB2	2.08	0.54
1:D:254:ILE:HD12	1:D:265:LEU:HD13	1.89	0.54
1:D:132:VAL:HG22	1:D:235:MET:CE	2.38	0.54
1:B:216:GLU:HG2	1:B:218:SER:H	1.73	0.53
1:D:312:ARG:HH22	1:D:313:ARG:NH2	2.06	0.53
1:D:100:VAL:HG13	1:D:104:ILE:HG13	1.91	0.53
1:C:181:ILE:HD11	1:C:197:ALA:HB2	1.88	0.53
1:A:67:ARG:C	1:A:68:ARG:HD3	2.33	0.53
1:A:318:ILE:HD12	1:A:325:VAL:HG22	1.90	0.53
1:A:101:LEU:O	1:A:101:LEU:HG	2.08	0.53
1:A:258:GLY:HA2	1:A:438:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:HB3	1:C:330:LYS:HD3	1.91	0.53
1:D:97:LEU:O	1:D:100:VAL:N	2.40	0.53
1:D:414:TYR:O	1:D:416:ILE:HG12	2.09	0.53
1:D:7:PRO:HA	1:D:98:PHE:CE1	2.43	0.53
1:A:294:ASP:HA	1:A:297:ARG:HB2	1.91	0.53
1:C:424:ARG:HD3	1:C:428:ASP:OD2	2.08	0.53
1:A:120:LEU:HG	1:A:122:LEU:HG	1.91	0.52
1:A:340:ARG:NH2	1:A:350:ASN:HB2	2.24	0.52
1:B:237:ASP:OD1	1:B:240:LYS:N	2.33	0.52
1:B:413:PRO:HB2	1:B:451:GLU:CD	2.33	0.52
1:C:10:SER:HB3	1:C:102:ARG:HH11	1.73	0.52
1:D:358:ASP:O	1:D:390:ARG:NH1	2.42	0.52
1:A:148:PRO:HB3	1:A:250:HIS:CG	2.45	0.52
1:C:392:PHE:O	1:C:396:VAL:HB	2.10	0.52
1:B:181:ILE:N	1:B:181:ILE:HD12	2.24	0.52
1:C:333:MET:O	1:C:336:VAL:N	2.43	0.52
1:A:100:VAL:HG13	1:A:104:ILE:HG13	1.92	0.52
1:A:291:GLU:H	1:A:291:GLU:CD	2.17	0.52
1:A:405:ILE:HG12	1:A:408:ILE:HG23	1.90	0.52
1:B:258:GLY:HA2	1:B:438:ARG:HD2	1.91	0.52
1:B:294:ASP:OD1	1:B:295:TYR:N	2.42	0.52
1:C:358:ASP:N	1:C:358:ASP:OD1	2.41	0.52
1:A:243:GLU:OE2	1:A:247:ARG:NH2	2.39	0.51
1:C:16:GLN:HG3	1:D:351:TRP:CD2	2.45	0.51
1:D:215:THR:HA	1:D:241:ARG:HE	1.75	0.51
1:D:268:LEU:HD13	1:D:284:LEU:HD22	1.92	0.51
1:D:447:ILE:HG22	1:D:450:TYR:HE1	1.76	0.51
1:B:217:PRO:HD3	1:B:235:MET:O	2.10	0.51
1:D:154:TRP:CE3	1:D:264:GLU:HB3	2.45	0.51
1:A:181:ILE:HD13	1:A:193:PRO:HB2	1.92	0.51
1:B:210:ARG:NH1	1:B:231:GLU:OE1	2.43	0.51
1:C:216:GLU:HG2	1:C:217:PRO:HD2	1.93	0.51
1:D:401:LYS:HB3	1:D:403:VAL:HG23	1.92	0.51
1:D:10:SER:HA	1:D:140:ARG:NH1	2.26	0.51
1:D:373:LEU:CD2	1:D:391:ALA:HB2	2.41	0.51
1:B:370:MET:HE1	1:B:414:TYR:CZ	2.46	0.51
1:C:181:ILE:HD13	1:C:193:PRO:HB2	1.93	0.51
1:C:118:PRO:O	1:C:120:LEU:N	2.43	0.50
1:D:15:SER:O	1:D:19:VAL:HG23	2.10	0.50
1:D:41:VAL:HG21	1:D:100:VAL:CG2	2.40	0.50
1:B:186:GLY:O	1:B:226:ASN:ND2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:HIS:CE1	1:B:414:TYR:HE1	2.29	0.50
1:A:196:GLY:O	1:A:199:VAL:N	2.45	0.50
1:C:312:ARG:HD3	1:C:315:TYR:CZ	2.46	0.50
1:C:115:VAL:HG12	1:C:118:PRO:HA	1.94	0.50
1:B:402:GLU:HB3	1:B:406:ARG:HG2	1.93	0.50
1:C:297:ARG:O	1:C:300:ASP:N	2.45	0.50
1:A:152:VAL:HA	1:A:182:CYS:O	2.12	0.49
1:A:419:ASP:O	1:A:423:MET:HG2	2.11	0.49
1:C:297:ARG:HH21	1:C:298:VAL:HB	1.76	0.49
1:C:180:ASN:HB3	1:C:210:ARG:O	2.12	0.49
1:A:310:ASN:OD1	1:A:310:ASN:N	2.46	0.49
1:A:340:ARG:HG2	1:A:346:ALA:O	2.13	0.49
1:A:406:ARG:NH1	1:A:406:ARG:HG2	2.27	0.49
1:A:415:LYS:HG2	1:A:451:GLU:HB3	1.93	0.49
1:B:166:TYR:O	1:B:170:VAL:HG23	2.12	0.49
1:C:156:GLY:H	1:C:189:ALA:CB	2.24	0.49
1:C:67:ARG:O	1:C:68:ARG:HD3	2.12	0.49
1:A:302:PHE:HZ	1:A:388:LEU:HD22	1.77	0.49
1:D:132:VAL:HG22	1:D:235:MET:HE1	1.94	0.49
1:A:34:PHE:CD2	1:A:105:LEU:HD11	2.48	0.49
1:B:403:VAL:O	1:B:407:ALA:HB3	2.11	0.49
1:C:136:LEU:HD21	1:C:214:MET:HE1	1.95	0.49
1:D:102:ARG:NH2	1:D:232:LEU:O	2.46	0.49
1:D:49:ASP:OD1	1:D:49:ASP:N	2.39	0.49
1:D:275:PRO:O	1:D:277:ASN:N	2.46	0.49
1:B:273:MET:HG2	1:B:314:HIS:CD2	2.48	0.49
1:C:52:LYS:HD3	1:C:52:LYS:H	1.78	0.49
1:C:216:GLU:HG2	1:C:217:PRO:CD	2.43	0.49
1:A:259:VAL:HG23	1:A:433:PHE:CD2	2.48	0.48
1:B:177:ARG:HB3	1:B:330:LYS:HD3	1.95	0.48
1:B:376:TYR:HB2	1:B:378:ASP:OD1	2.13	0.48
1:C:287:THR:HA	1:C:318:ILE:O	2.12	0.48
1:A:273:MET:HG2	1:A:314:HIS:NE2	2.28	0.48
1:B:316:ARG:C	1:B:317:ILE:HD13	2.39	0.48
1:B:408:ILE:HD13	1:B:449:CYS:HA	1.95	0.48
1:A:69:GLU:HB2	1:B:344:GLY:O	2.14	0.48
1:A:309:GLU:HG3	1:A:309:GLU:O	2.14	0.48
1:C:352:SER:O	1:C:354:ARG:NH1	2.46	0.48
1:A:250:HIS:NE2	1:A:347:TYR:O	2.45	0.48
1:B:321:ASP:O	1:B:325:VAL:HG23	2.14	0.48
1:B:340:ARG:NH2	1:B:350:ASN:HD22	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:TYR:CE1	1:D:192:ALA:HB2	2.49	0.48
1:A:340:ARG:NH2	1:A:350:ASN:HD22	2.10	0.48
1:D:70:ARG:NH2	1:D:73:LYS:HD2	2.29	0.48
1:D:154:TRP:CZ3	1:D:264:GLU:HB3	2.48	0.48
1:C:52:LYS:HD3	1:C:52:LYS:N	2.29	0.48
1:D:156:GLY:HA3	1:D:257:GLY:HA2	1.95	0.48
1:C:43:ASN:HB3	1:C:54:LEU:HD21	1.95	0.48
1:C:427:ASP:O	1:C:430:LEU:N	2.42	0.48
1:D:321:ASP:O	1:D:325:VAL:HG23	2.14	0.48
1:A:-1:LEU:HB3	1:A:87:GLY:HA2	1.95	0.48
1:B:210:ARG:HD2	1:B:231:GLU:OE2	2.14	0.48
1:B:259:VAL:HG21	1:B:396:VAL:HG11	1.94	0.47
1:A:116:ARG:HA	1:A:116:ARG:HD2	1.77	0.47
1:C:17:LEU:HB2	1:D:130:ASN:CG	2.39	0.47
1:D:283:PRO:HG2	1:D:332:SER:HB3	1.97	0.47
1:B:433:PHE:HA	1:B:436:GLN:OE1	2.14	0.47
1:C:346:ALA:N	1:D:70:ARG:HB3	2.30	0.47
1:D:256:PRO:HA	1:D:295:TYR:CE2	2.49	0.47
1:D:402:GLU:HA	1:D:405:ILE:HG23	1.96	0.47
1:B:201:HIS:CE1	1:B:206:TYR:CD2	3.02	0.47
1:B:237:ASP:CG	1:B:240:LYS:HZ2	2.22	0.47
1:C:151:VAL:CG2	1:C:179:LEU:HD23	2.44	0.47
1:A:181:ILE:HD12	1:A:197:ALA:HB2	1.96	0.47
1:A:287:THR:O	1:A:296:PHE:HZ	1.98	0.47
1:B:408:ILE:HB	1:B:413:PRO:HA	1.96	0.47
1:C:370:MET:HG3	1:C:414:TYR:CE1	2.49	0.47
1:D:447:ILE:HG22	1:D:450:TYR:CE1	2.49	0.47
1:D:447:ILE:HA	1:D:450:TYR:CE1	2.50	0.47
1:A:33:LEU:HA	1:A:33:LEU:HD12	1.61	0.46
1:A:287:THR:O	1:A:296:PHE:CZ	2.68	0.46
1:B:170:VAL:HG21	1:B:255:PHE:CE1	2.50	0.46
1:B:170:VAL:HG21	1:B:255:PHE:HE1	1.78	0.46
1:C:125:SER:HA	1:C:128:ILE:HD12	1.97	0.46
1:D:17:LEU:HD12	1:D:17:LEU:HA	1.68	0.46
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.67	0.46
1:C:340:ARG:HA	1:C:343:THR:HG22	1.97	0.46
1:B:237:ASP:OD1	1:B:239:GLU:N	2.48	0.46
1:B:339:ASN:O	1:B:343:THR:HG22	2.16	0.46
1:D:430:LEU:O	1:D:434:VAL:HG23	2.16	0.46
1:A:15:SER:HB3	1:B:133:PHE:CD2	2.50	0.46
1:A:235:MET:HE3	1:A:235:MET:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:VAL:HG12	1:C:336:VAL:HG22	1.97	0.46
1:C:281:VAL:O	1:C:282:LEU:HD22	2.15	0.46
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.72	0.46
1:B:271:ILE:HG23	1:B:354:ARG:O	2.15	0.46
1:C:156:GLY:H	1:C:189:ALA:HB3	1.81	0.46
1:D:198:ALA:HB1	3:D:501:A1IXI:C11	2.45	0.46
1:C:155:GLY:HA3	1:C:189:ALA:HB1	1.97	0.46
1:A:183:THR:HG23	1:A:194:MET:HE2	1.98	0.46
1:A:198:ALA:HB1	3:A:502:A1IXI:C3	2.45	0.46
1:B:274:ASN:CG	1:B:275:PRO:HD2	2.40	0.46
1:C:278:LYS:HD2	1:C:278:LYS:C	2.41	0.46
1:A:216:GLU:HG2	1:A:217:PRO:HD2	1.97	0.46
1:C:51:SER:HB3	1:C:52:LYS:HD3	1.98	0.46
1:D:216:GLU:HG2	1:D:217:PRO:HD2	1.98	0.46
1:A:48:THR:HG21	1:A:57:ARG:HH12	1.81	0.46
1:B:48:THR:OG1	1:B:54:LEU:HD13	2.15	0.46
1:B:420:LYS:HD2	1:B:420:LYS:HA	1.82	0.46
1:A:60:ASN:HB2	1:A:78:ASN:ND2	2.32	0.45
1:A:406:ARG:HG2	1:A:406:ARG:HH11	1.82	0.45
1:C:273:MET:HG2	1:C:314:HIS:NE2	2.31	0.45
1:A:320:ASP:O	1:A:320:ASP:OD1	2.33	0.45
1:B:215:THR:HA	1:B:241:ARG:HE	1.81	0.45
1:C:347:TYR:CZ	2:C:501:G4P:C5	2.99	0.45
1:B:343:THR:CG2	1:B:345:ASP:HB2	2.39	0.45
1:D:272:LEU:O	1:D:314:HIS:CE1	2.69	0.45
1:D:363:PHE:CD1	1:D:390:ARG:HB3	2.51	0.45
1:B:426:MET:O	1:B:430:LEU:HG	2.17	0.45
1:C:83:ALA:O	1:C:89:ILE:HD12	2.15	0.45
1:A:21:MET:HA	1:A:24:ARG:HH11	1.81	0.45
1:C:82:GLU:C	1:C:84:PHE:H	2.24	0.45
1:A:174:LEU:O	1:A:179:LEU:HB2	2.17	0.45
1:B:194:MET:CE	1:B:211:PHE:HB3	2.35	0.45
1:D:66:LEU:HD21	1:D:75:GLU:HB2	1.99	0.45
1:D:363:PHE:HD1	1:D:390:ARG:HD2	1.81	0.45
1:A:100:VAL:HG22	1:A:234:ILE:HD11	1.98	0.45
1:A:275:PRO:C	1:A:277:ASN:N	2.75	0.45
1:C:181:ILE:HG21	1:C:193:PRO:HB2	1.99	0.45
1:A:242:LEU:HB3	1:A:267:TYR:CE2	2.51	0.45
1:A:370:MET:O	1:A:373:LEU:HB2	2.17	0.45
1:B:337:LYS:NZ	1:B:347:TYR:CZ	2.85	0.45
1:B:152:VAL:CG2	1:B:249:ALA:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:MET:HG3	1:C:101:LEU:HD23	1.99	0.45
1:C:68:ARG:NH1	2:D:502:G4P:O3B	2.50	0.45
1:A:-1:LEU:HD12	1:A:0:ARG:O	2.16	0.44
1:A:267:TYR:HE1	1:A:359:LEU:HB3	1.81	0.44
1:A:336:VAL:CG1	1:A:340:ARG:NH1	2.80	0.44
1:C:316:ARG:HE	1:C:316:ARG:HB3	1.58	0.44
1:B:287:THR:HA	1:B:318:ILE:O	2.17	0.44
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.77	0.44
1:D:2:ILE:HG22	1:D:77:ILE:HG13	1.99	0.44
1:C:215:THR:HG23	1:C:234:ILE:HG23	2.00	0.44
1:D:110:GLN:O	1:D:114:THR:HB	2.17	0.44
1:A:382:GLU:HG2	1:A:383:VAL:H	1.82	0.44
1:C:63:ILE:HD11	1:C:74:LEU:HD13	1.99	0.44
1:C:339:ASN:O	1:C:343:THR:HG22	2.18	0.44
1:D:283:PRO:HG2	1:D:332:SER:CB	2.48	0.44
1:D:283:PRO:O	1:D:329:MET:HE1	2.18	0.44
1:B:136:LEU:HD21	1:B:214:MET:CE	2.48	0.44
1:C:125:SER:OG	1:C:360:GLN:CD	2.61	0.44
1:C:427:ASP:O	1:C:428:ASP:C	2.61	0.44
1:D:113:ASN:OD1	1:D:113:ASN:O	2.36	0.44
1:A:70:ARG:HB3	1:B:346:ALA:N	2.32	0.44
1:A:237:ASP:OD2	1:A:239:GLU:HB2	2.18	0.44
1:B:103:ASP:O	1:B:107:VAL:HB	2.18	0.44
1:C:273:MET:HG2	1:C:314:HIS:CD2	2.52	0.44
1:B:256:PRO:HD3	1:B:287:THR:O	2.18	0.44
1:C:450:TYR:O	1:C:451:GLU:OE2	2.36	0.44
1:B:382:GLU:HG2	1:B:383:VAL:N	2.32	0.44
1:C:148:PRO:HA	1:C:250:HIS:CE1	2.53	0.44
1:C:151:VAL:HG21	1:C:174:LEU:HD22	1.99	0.44
1:C:164:TYR:HE2	1:C:168:ARG:HH21	1.66	0.44
1:D:47:LEU:H	1:D:47:LEU:HD12	1.82	0.44
1:D:201:HIS:CE1	1:D:206:TYR:CD2	3.06	0.44
1:A:336:VAL:HG13	1:A:340:ARG:NH1	2.32	0.43
1:C:52:LYS:H	1:C:52:LYS:CD	2.31	0.43
1:B:165:LEU:HD23	1:B:165:LEU:HA	1.78	0.43
1:D:108:TYR:O	1:D:112:HIS:HB2	2.18	0.43
1:C:274:ASN:ND2	1:C:275:PRO:HD2	2.33	0.43
1:D:43:ASN:HB3	1:D:54:LEU:HD21	2.00	0.43
1:D:420:LYS:HE3	1:D:452:ILE:HB	2.00	0.43
1:A:33:LEU:HD21	1:A:217:PRO:HB3	2.00	0.43
1:A:421:GLU:O	1:A:425:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD21	1:B:214:MET:HE2	2.00	0.43
1:B:447:ILE:HG12	1:B:451:GLU:HG2	2.01	0.43
1:D:302:PHE:HB2	1:D:429:LEU:HD11	1.99	0.43
1:D:361:MET:HA	1:D:362:PRO:HD3	1.87	0.43
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.72	0.43
1:A:133:PHE:HZ	1:B:13:MET:HG3	1.84	0.43
1:A:382:GLU:HG2	1:A:383:VAL:HG23	2.01	0.43
1:B:192:ALA:N	1:B:193:PRO:HD2	2.33	0.43
1:A:263:GLU:HG2	1:A:264:GLU:N	2.33	0.43
1:A:361:MET:HA	1:A:362:PRO:HD3	1.83	0.43
1:C:74:LEU:HD23	1:C:74:LEU:HA	1.69	0.43
1:D:184:GLY:C	1:D:186:GLY:H	2.27	0.43
1:C:103:ASP:O	1:C:107:VAL:HB	2.18	0.43
1:C:347:TYR:CE2	2:C:501:G4P:N7	2.86	0.43
1:C:152:VAL:CG2	1:C:249:ALA:HB2	2.49	0.42
1:C:371:ALA:HA	1:C:416:ILE:HA	2.02	0.42
1:D:148:PRO:HA	1:D:250:HIS:CE1	2.54	0.42
1:D:300:ASP:OD1	1:D:315:TYR:OH	2.27	0.42
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.81	0.42
1:C:19:VAL:HG11	1:C:71:GLY:O	2.19	0.42
1:A:125:SER:OG	1:A:360:GLN:NE2	2.47	0.42
1:A:215:THR:HG23	1:A:234:ILE:HG23	2.01	0.42
1:A:315:TYR:HE1	1:A:317:ILE:HD11	1.85	0.42
1:B:4:HIS:HB3	1:B:73:LYS:HE2	2.01	0.42
1:B:11:MET:HE3	1:B:102:ARG:CG	2.49	0.42
1:C:14:LEU:HD23	1:C:14:LEU:HA	1.37	0.42
1:B:253:ILE:HD11	1:B:329:MET:HG3	2.02	0.42
1:B:254:ILE:HB	1:B:286:LEU:HG	2.01	0.42
1:D:2:ILE:HG22	1:D:77:ILE:CG1	2.49	0.42
1:A:207:LYS:HE3	1:A:207:LYS:HA	2.01	0.42
1:A:336:VAL:HG13	1:A:340:ARG:HH11	1.85	0.42
1:B:366:SER:C	1:B:370:MET:HE2	2.44	0.42
1:C:179:LEU:HD11	1:C:330:LYS:HD2	2.01	0.42
1:C:313:ARG:HE	1:C:313:ARG:HB2	1.61	0.42
1:A:420:LYS:HD2	1:A:420:LYS:HA	1.83	0.42
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.61	0.42
1:D:363:PHE:CD1	1:D:390:ARG:HD2	2.54	0.42
1:D:364:GLU:C	1:D:366:SER:H	2.27	0.42
1:D:415:LYS:HA	1:D:451:GLU:HB3	2.01	0.42
1:B:22:LEU:HD12	1:B:101:LEU:HD11	2.02	0.42
1:B:85:VAL:HG13	1:B:85:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:HD11	1:B:234:ILE:HG21	2.01	0.42
1:B:409:GLU:HG3	1:B:410:GLU:N	2.35	0.42
1:C:21:MET:O	1:C:21:MET:HG2	2.19	0.42
1:C:120:LEU:HD12	1:C:120:LEU:HA	1.77	0.42
1:D:268:LEU:HD23	1:D:268:LEU:HA	1.73	0.42
1:C:148:PRO:HB3	1:C:250:HIS:CG	2.55	0.41
1:C:286:LEU:HD23	1:C:296:PHE:CE1	2.48	0.41
1:D:31:TYR:OH	1:D:62:ASP:OD1	2.11	0.41
1:D:239:GLU:H	1:D:239:GLU:HG2	1.54	0.41
1:D:277:ASN:CG	1:D:354:ARG:H	2.28	0.41
1:D:408:ILE:HG12	1:D:409:GLU:OE1	2.20	0.41
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.61	0.41
1:C:294:ASP:HB2	1:C:436:GLN:OE1	2.20	0.41
1:C:373:LEU:HD22	1:C:387:ASP:OD1	2.20	0.41
1:B:242:LEU:O	1:B:243:GLU:C	2.64	0.41
1:C:312:ARG:HD3	1:C:315:TYR:OH	2.20	0.41
1:D:426:MET:HA	1:D:429:LEU:HB2	2.01	0.41
1:B:281:VAL:O	1:B:282:LEU:HD22	2.20	0.41
1:D:196:GLY:O	1:D:199:VAL:N	2.53	0.41
1:A:70:ARG:HD2	2:B:501:G4P:C2	2.50	0.41
1:A:261:THR:HG22	1:A:264:GLU:OE1	2.20	0.41
1:B:41:VAL:CG1	1:B:96:ASN:HB2	2.50	0.41
1:C:215:THR:HA	1:C:241:ARG:HE	1.86	0.41
1:C:237:ASP:OD1	1:C:239:GLU:HB2	2.20	0.41
1:C:261:THR:HG22	1:C:264:GLU:OE1	2.19	0.41
1:B:102:ARG:NH2	1:B:232:LEU:O	2.53	0.41
1:D:289:PRO:HD2	1:D:292:SER:HB3	2.02	0.41
1:A:216:GLU:OE1	1:A:219:ILE:HG13	2.21	0.41
1:D:173:GLN:O	1:D:174:LEU:C	2.64	0.41
1:A:17:LEU:HD12	1:A:17:LEU:HA	1.81	0.41
1:C:207:LYS:NZ	1:C:207:LYS:HB2	2.35	0.41
1:C:291:GLU:CD	1:C:291:GLU:N	2.78	0.41
1:C:391:ALA:O	1:C:395:ILE:HG12	2.21	0.41
1:D:298:VAL:HA	1:D:301:GLU:HG2	2.03	0.41
1:D:347:TYR:CZ	2:D:502:G4P:C5	3.03	0.41
1:A:102:ARG:HE	1:A:103:ASP:CG	2.29	0.41
1:A:257:GLY:HA3	1:A:261:THR:HG23	2.02	0.41
1:B:17:LEU:HD23	1:B:17:LEU:O	2.21	0.41
1:B:171:GLY:O	1:B:175:GLY:N	2.37	0.41
1:B:400:VAL:HG23	1:B:401:LYS:N	2.36	0.41
1:C:82:GLU:O	1:C:84:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:MET:HA	1:C:236:PRO:HD3	1.85	0.41
1:C:261:THR:OG1	1:C:295:TYR:OH	2.22	0.41
1:C:336:VAL:O	1:C:340:ARG:HG2	2.21	0.41
1:D:107:VAL:O	1:D:109:GLY:N	2.54	0.41
1:A:16:GLN:HG3	1:B:351:TRP:CZ3	2.56	0.41
1:A:133:PHE:CD2	1:B:15:SER:HB3	2.57	0.40
1:B:253:ILE:HA	1:B:285:ILE:O	2.20	0.40
1:B:433:PHE:HA	1:B:433:PHE:HD1	1.78	0.40
1:C:120:LEU:HG	1:C:122:LEU:HG	2.03	0.40
1:C:196:GLY:O	1:C:199:VAL:N	2.54	0.40
1:C:345:ASP:C	1:D:70:ARG:HB3	2.45	0.40
1:C:358:ASP:O	1:C:390:ARG:NH1	2.55	0.40
1:D:29:ASP:C	1:D:31:TYR:H	2.29	0.40
1:D:156:GLY:HA3	1:D:257:GLY:CA	2.51	0.40
1:D:312:ARG:HH22	1:D:313:ARG:HH21	1.68	0.40
1:B:66:LEU:HD21	1:B:75:GLU:HB2	2.03	0.40
1:B:220:ILE:HG21	1:B:234:ILE:HD13	2.03	0.40
1:D:63:ILE:HD11	1:D:74:LEU:HD22	2.03	0.40
1:D:296:PHE:O	1:D:297:ARG:C	2.65	0.40
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:NZ	1:C:118:PRO:O[6_435]	1.96	0.24
1:A:0:ARG:NH1	1:A:341:ARG:NH1[3_444]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/460 (94%)	380 (88%)	45 (10%)	8 (2%)	6	26
1	B	429/460 (93%)	396 (92%)	26 (6%)	7 (2%)	7	29
1	C	440/460 (96%)	387 (88%)	44 (10%)	9 (2%)	6	25
1	D	435/460 (95%)	387 (89%)	40 (9%)	8 (2%)	6	26
All	All	1737/1840 (94%)	1550 (89%)	155 (9%)	32 (2%)	6	26

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	20	ASP
1	C	119	ASN
1	D	256	PRO
1	A	160	ASN
1	A	276	ALA
1	B	102	ARG
1	D	107	VAL
1	D	188	GLY
1	D	316	ARG
1	A	197	ALA
1	A	275	PRO
1	B	28	SER
1	B	187	PRO
1	B	197	ALA
1	C	83	ALA
1	C	293	ALA
1	C	322	ALA
1	C	428	ASP
1	D	185	CYS
1	D	448	PRO
1	B	448	PRO
1	A	176	LEU
1	B	107	VAL
1	B	276	ALA
1	C	118	PRO
1	C	427	ASP
1	A	229	VAL
1	A	322	ALA
1	C	418	GLY
1	D	187	PRO
1	D	229	VAL
1	A	187	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/391 (96%)	374 (100%)	0	100	100
1	B	369/391 (94%)	369 (100%)	0	100	100
1	C	378/391 (97%)	378 (100%)	0	100	100
1	D	374/391 (96%)	374 (100%)	0	100	100
All	All	1495/1564 (96%)	1495 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	203	GLN
1	A	230	ASN
1	A	280	GLN
1	A	350	ASN
1	A	360	GLN
1	B	50	ASN
1	B	203	GLN
1	B	274	ASN
1	B	305	HIS
1	B	314	HIS
1	B	350	ASN
1	B	399	ASN
1	C	16	GLN
1	C	127	HIS
1	C	157	HIS
1	C	339	ASN
1	C	350	ASN
1	D	32	GLN
1	D	203	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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	G4P	D	502	-	36,38,38	3.52	12 (33%)	56,61,61	1.97	15 (26%)
3	A1IXI	A	502	-	24,26,26	4.11	12 (50%)	31,40,40	2.27	11 (35%)
2	G4P	B	501	-	36,38,38	3.77	14 (38%)	56,61,61	1.96	19 (33%)
3	A1IXI	D	501	-	24,26,26	4.14	13 (54%)	31,40,40	2.09	12 (38%)
2	G4P	A	501	-	36,38,38	3.45	11 (30%)	56,61,61	1.90	15 (26%)
2	G4P	C	501	-	36,38,38	3.45	12 (33%)	56,61,61	1.60	12 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G4P	D	502	-	-	6/27/43/43	0/3/3/3
3	A1IXI	A	502	-	-	9/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G4P	B	501	-	-	6/27/43/43	0/3/3/3
3	A1IXI	D	501	-	-	5/10/26/26	0/3/3/3
2	G4P	A	501	-	-	5/27/43/43	0/3/3/3
2	G4P	C	501	-	-	8/27/43/43	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	G4P	O6-C6	11.16	1.44	1.23
2	A	501	G4P	O6-C6	11.15	1.44	1.23
2	C	501	G4P	O6-C6	10.63	1.43	1.23
2	D	502	G4P	O6-C6	10.46	1.43	1.23
3	D	501	A1IXI	C7-C6	-10.33	1.25	1.53
3	A	502	A1IXI	C7-C6	-10.16	1.25	1.53
2	D	502	G4P	O4'-C1'	9.64	1.64	1.42
2	B	501	G4P	O4'-C1'	9.29	1.63	1.42
2	C	501	G4P	O4'-C1'	9.15	1.63	1.42
2	A	501	G4P	O4'-C1'	9.07	1.63	1.42
2	B	501	G4P	PC-O3C	8.91	1.69	1.59
2	B	501	G4P	PA-O3A	8.45	1.68	1.59
3	A	502	A1IXI	C5-C4	-7.98	1.39	1.50
2	C	501	G4P	PC-O3C	7.61	1.67	1.59
3	A	502	A1IXI	C7-C8	7.58	1.72	1.53
3	D	501	A1IXI	C5-C4	-7.15	1.40	1.50
2	B	501	G4P	C2'-C1'	-7.10	1.31	1.53
2	A	501	G4P	C2'-C1'	-7.06	1.31	1.53
3	D	501	A1IXI	C7-C8	6.97	1.70	1.53
2	D	502	G4P	C2'-C1'	-6.94	1.31	1.53
3	A	502	A1IXI	O1-C5	6.86	1.53	1.43
3	D	501	A1IXI	O1-C8	-6.69	1.30	1.45
2	A	501	G4P	PA-O3A	6.63	1.66	1.59
2	D	502	G4P	PC-O3C	6.58	1.66	1.59
2	D	502	G4P	PA-O3A	6.55	1.66	1.59
2	C	501	G4P	C2'-C1'	-6.49	1.33	1.53
3	A	502	A1IXI	O1-C8	-6.23	1.31	1.45
3	D	501	A1IXI	C6-C5	6.13	1.62	1.53
3	D	501	A1IXI	O1-C5	6.06	1.52	1.43
2	C	501	G4P	O4'-C4'	-5.86	1.32	1.45
3	A	502	A1IXI	C10-N4	5.78	1.45	1.33
2	C	501	G4P	PA-O3A	5.31	1.65	1.59
2	A	501	G4P	PC-O3C	5.28	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	A1IXI	C10-N4	5.28	1.44	1.33
2	A	501	G4P	O4'-C4'	-4.95	1.34	1.45
2	D	502	G4P	C2-N2	4.91	1.45	1.34
2	B	501	G4P	O4'-C4'	-4.76	1.34	1.45
2	C	501	G4P	C2-N2	4.54	1.44	1.34
2	D	502	G4P	O4'-C4'	-4.52	1.35	1.45
3	D	501	A1IXI	O7-C6	4.42	1.53	1.43
3	A	502	A1IXI	O7-C6	4.11	1.53	1.43
2	A	501	G4P	C2-N2	4.10	1.43	1.34
2	B	501	G4P	C2-N2	3.75	1.43	1.34
2	D	502	G4P	O3'-C3'	-3.42	1.32	1.44
2	C	501	G4P	C6-N1	-3.19	1.32	1.38
2	A	501	G4P	O3'-C3'	-3.08	1.33	1.44
2	B	501	G4P	O3'-C3'	-3.03	1.33	1.44
2	A	501	G4P	C6-N1	-3.01	1.33	1.38
3	A	502	A1IXI	O6-C7	2.99	1.50	1.43
2	D	502	G4P	C5-N7	-2.95	1.33	1.39
2	B	501	G4P	C6-N1	-2.88	1.33	1.38
2	D	502	G4P	C6-N1	-2.76	1.33	1.38
3	A	502	A1IXI	C1-N1	-2.70	1.32	1.37
3	D	501	A1IXI	O6-C7	2.68	1.49	1.43
3	D	501	A1IXI	C2-N1	-2.62	1.33	1.37
3	A	502	A1IXI	C6-C5	2.62	1.57	1.53
3	A	502	A1IXI	C2-N1	-2.54	1.33	1.37
2	B	501	G4P	C5-N7	-2.51	1.34	1.39
2	C	501	G4P	O3'-C3'	-2.50	1.35	1.44
2	C	501	G4P	C2-N1	-2.47	1.31	1.37
3	A	502	A1IXI	O8-C11	2.47	1.41	1.29
3	D	501	A1IXI	C1-N1	-2.42	1.33	1.37
2	A	501	G4P	C5-N7	-2.36	1.34	1.39
2	B	501	G4P	C2-N1	-2.34	1.31	1.37
2	A	501	G4P	C2-N1	-2.28	1.32	1.37
3	D	501	A1IXI	O8-C11	2.27	1.40	1.29
2	D	502	G4P	C8-N9	-2.26	1.32	1.37
2	C	501	G4P	O2'-C2'	2.23	1.48	1.43
2	D	502	G4P	C5'-C4'	2.22	1.58	1.51
2	C	501	G4P	C5-N7	-2.20	1.34	1.39
2	B	501	G4P	O2'-C2'	2.10	1.48	1.43
2	B	501	G4P	C4-N9	-2.10	1.32	1.38
3	D	501	A1IXI	C10-N2	-2.07	1.31	1.35
2	B	501	G4P	C8-N9	-2.06	1.32	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	G4P	C5-C4-N3	-6.16	118.59	128.39
3	A	502	A1IXI	C8-O1-C5	-6.05	93.29	108.44
2	A	501	G4P	C5-C4-N3	-6.03	118.80	128.39
2	B	501	G4P	C5-C4-N3	-5.90	119.00	128.39
2	C	501	G4P	C5-C4-N3	-5.26	120.02	128.39
2	D	502	G4P	N9-C4-N3	4.95	135.85	125.95
2	D	502	G4P	C2-N3-C4	4.85	120.66	112.30
2	A	501	G4P	C2-N3-C4	4.70	120.40	112.30
3	A	502	A1IXI	C7-C6-C5	-4.67	96.17	101.69
3	D	501	A1IXI	C3-C2-N1	4.65	109.39	105.81
2	C	501	G4P	C2-N3-C4	4.36	119.80	112.30
2	B	501	G4P	N9-C4-N3	4.24	134.42	125.95
2	A	501	G4P	N9-C4-N3	4.20	134.34	125.95
2	A	501	G4P	O4'-C1'-N9	4.18	117.82	108.36
3	D	501	A1IXI	O1-C8-C7	4.12	113.33	105.15
3	D	501	A1IXI	O7-C6-C5	4.04	120.79	111.21
3	A	502	A1IXI	C3-C2-N1	3.93	108.83	105.81
2	B	501	G4P	C4'-O4'-C1'	-3.89	100.89	109.47
3	A	502	A1IXI	N4-C10-N2	3.85	123.00	117.22
2	B	501	G4P	C2-N3-C4	3.82	118.89	112.30
2	C	501	G4P	N9-C4-N3	3.68	133.32	125.95
2	B	501	G4P	C2-N1-C6	-3.56	118.66	125.11
2	D	502	G4P	O4'-C4'-C5'	3.39	120.19	109.33
2	D	502	G4P	O6-C6-C5	-3.36	117.66	126.53
2	B	501	G4P	O4'-C1'-N9	3.33	115.90	108.36
3	A	502	A1IXI	C3-N2-C10	3.20	120.80	116.80
2	A	501	G4P	C2-N1-C6	-3.20	119.31	125.11
2	D	502	G4P	C2-N1-C6	-3.17	119.35	125.11
2	D	502	G4P	O3B-PB-O3A	3.12	115.09	104.64
3	D	501	A1IXI	C8-O1-C5	-3.10	100.68	108.44
3	A	502	A1IXI	N3-C10-N2	-2.97	120.93	125.48
2	B	501	G4P	O2'-C2'-C3'	2.96	119.46	111.19
2	D	502	G4P	C2'-C3'-C4'	2.92	108.34	103.24
2	B	501	G4P	O4'-C4'-C5'	2.86	118.50	109.33
3	D	501	A1IXI	C10-N3-C11	2.86	122.46	116.31
3	D	501	A1IXI	O8-C11-C2	-2.85	117.92	126.02
3	A	502	A1IXI	C10-N3-C11	2.78	122.30	116.31
3	D	501	A1IXI	N3-C10-N2	-2.78	121.22	125.48
3	D	501	A1IXI	O1-C5-C6	2.77	108.98	105.15
2	A	501	G4P	O2B-PB-O3A	2.76	113.88	104.64
2	B	501	G4P	O2C-PC-O3C	2.72	114.64	107.27
2	D	502	G4P	C8-N7-C5	2.71	109.09	104.26
2	D	502	G4P	N9-C8-N7	-2.70	108.39	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1IXI	O2-P1-O3	2.67	113.65	106.44
2	A	501	G4P	C4-C5-N7	-2.64	106.48	110.67
2	D	502	G4P	C5-C6-N1	2.64	119.98	113.25
2	C	501	G4P	PA-O5'-C5'	-2.63	106.31	121.35
2	B	501	G4P	C4-C5-N7	-2.61	106.53	110.67
2	A	501	G4P	C8-N7-C5	2.59	108.87	104.26
2	A	501	G4P	C4'-O4'-C1'	-2.58	103.77	109.47
2	C	501	G4P	O2D-PD-O3C	2.57	113.25	104.64
3	A	502	A1IXI	O1-C8-C7	2.54	110.20	105.15
2	B	501	G4P	O3'-C3'-C4'	-2.53	101.13	110.03
2	B	501	G4P	C8-N7-C5	2.52	108.74	104.26
3	D	501	A1IXI	C3-N2-C10	2.48	119.89	116.80
3	D	501	A1IXI	O8-C11-N3	2.48	123.72	117.24
3	D	501	A1IXI	O1-C8-C9	-2.47	101.41	109.33
2	D	502	G4P	O3'-C3'-C4'	-2.44	101.45	110.03
2	A	501	G4P	O3D-PD-O3C	2.40	112.69	104.64
2	A	501	G4P	C6-C5-N7	2.35	134.57	130.29
2	C	501	G4P	C5'-C4'-C3'	-2.34	106.60	114.38
2	D	502	G4P	O5'-C5'-C4'	2.29	116.80	108.99
2	C	501	G4P	O4'-C1'-N9	2.29	113.55	108.36
2	A	501	G4P	C2'-C3'-C4'	2.27	107.21	103.24
2	A	501	G4P	C5-C6-N1	2.26	119.00	113.25
2	A	501	G4P	O4'-C4'-C5'	2.26	116.56	109.33
2	C	501	G4P	C2-N1-C6	-2.23	121.06	125.11
2	C	501	G4P	O6-C6-C5	-2.22	120.67	126.53
3	A	502	A1IXI	O6-C7-C6	2.21	118.91	111.82
3	A	502	A1IXI	C2-C11-N3	-2.20	118.36	123.91
3	D	501	A1IXI	C2-C11-N3	-2.20	118.36	123.91
2	A	501	G4P	N9-C8-N7	-2.19	109.34	113.40
2	C	501	G4P	C5-C6-N1	2.16	118.76	113.25
2	B	501	G4P	N9-C8-N7	-2.12	109.47	113.40
2	C	501	G4P	C6-C5-N7	2.11	134.13	130.29
2	B	501	G4P	C5'-C4'-C3'	-2.09	107.41	114.38
2	D	502	G4P	C4'-O4'-C1'	-2.09	104.86	109.47
2	C	501	G4P	C8-N7-C5	2.08	107.97	104.26
2	B	501	G4P	C1'-N9-C8	-2.03	120.96	126.73
2	B	501	G4P	O2B-PB-O3A	2.03	111.45	104.64
2	B	501	G4P	O2D-PD-O3C	2.02	111.40	104.64
2	D	502	G4P	C4-C5-N7	-2.02	107.47	110.67
2	B	501	G4P	O3D-PD-O3C	2.01	111.37	104.64
2	B	501	G4P	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	G4P	C5'-O5'-PA-O3A
2	A	501	G4P	C5'-O5'-PA-O2A
2	B	501	G4P	PC-O3C-PD-O3D
2	D	502	G4P	PA-O3A-PB-O3B
2	D	502	G4P	C3'-O3'-PC-O2C
2	D	502	G4P	C3'-O3'-PC-O3C
3	A	502	A1IXI	O1-C8-C9-O2
3	A	502	A1IXI	C1-C4-C5-O1
3	A	502	A1IXI	C9-O2-P1-O3
3	A	502	A1IXI	C9-O2-P1-O4
3	A	502	A1IXI	C9-O2-P1-O5
3	D	501	A1IXI	C1-C4-C5-C6
3	D	501	A1IXI	C9-O2-P1-O5
2	C	501	G4P	C3'-C4'-C5'-O5'
3	A	502	A1IXI	C7-C8-C9-O2
2	B	501	G4P	O4'-C4'-C5'-O5'
2	B	501	G4P	C3'-C4'-C5'-O5'
2	C	501	G4P	O4'-C4'-C5'-O5'
2	D	502	G4P	O4'-C4'-C5'-O5'
2	D	502	G4P	C3'-C4'-C5'-O5'
2	C	501	G4P	O4'-C1'-N9-C4
2	C	501	G4P	C4'-C3'-O3'-PC
2	C	501	G4P	C2'-C3'-O3'-PC
2	A	501	G4P	C3'-C4'-C5'-O5'
3	D	501	A1IXI	C7-C8-C9-O2
3	D	501	A1IXI	O1-C8-C9-O2
2	C	501	G4P	O4'-C1'-N9-C8
2	A	501	G4P	O4'-C4'-C5'-O5'
2	B	501	G4P	PD-O3C-PC-O3'
2	D	502	G4P	C3'-O3'-PC-O1C
3	D	501	A1IXI	C3-C4-C5-C6
3	A	502	A1IXI	C1-C4-C5-C6
2	C	501	G4P	C5'-O5'-PA-O3A
3	A	502	A1IXI	C8-C9-O2-P1
2	A	501	G4P	C4'-C5'-O5'-PA
2	B	501	G4P	PC-O3C-PD-O1D
2	B	501	G4P	PC-O3C-PD-O2D
2	C	501	G4P	C3'-O3'-PC-O1C
3	A	502	A1IXI	C3-C4-C5-C6

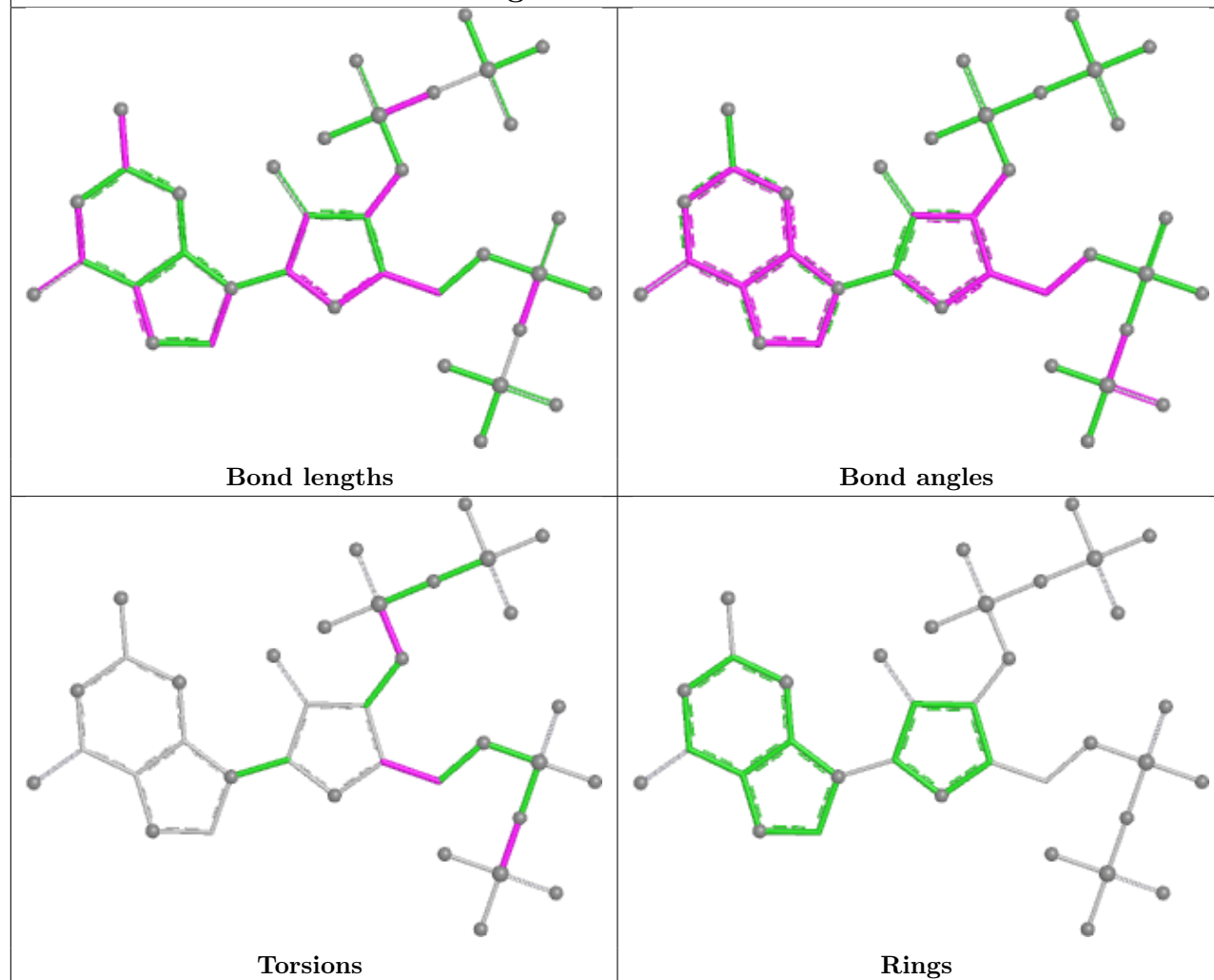
There are no ring outliers.

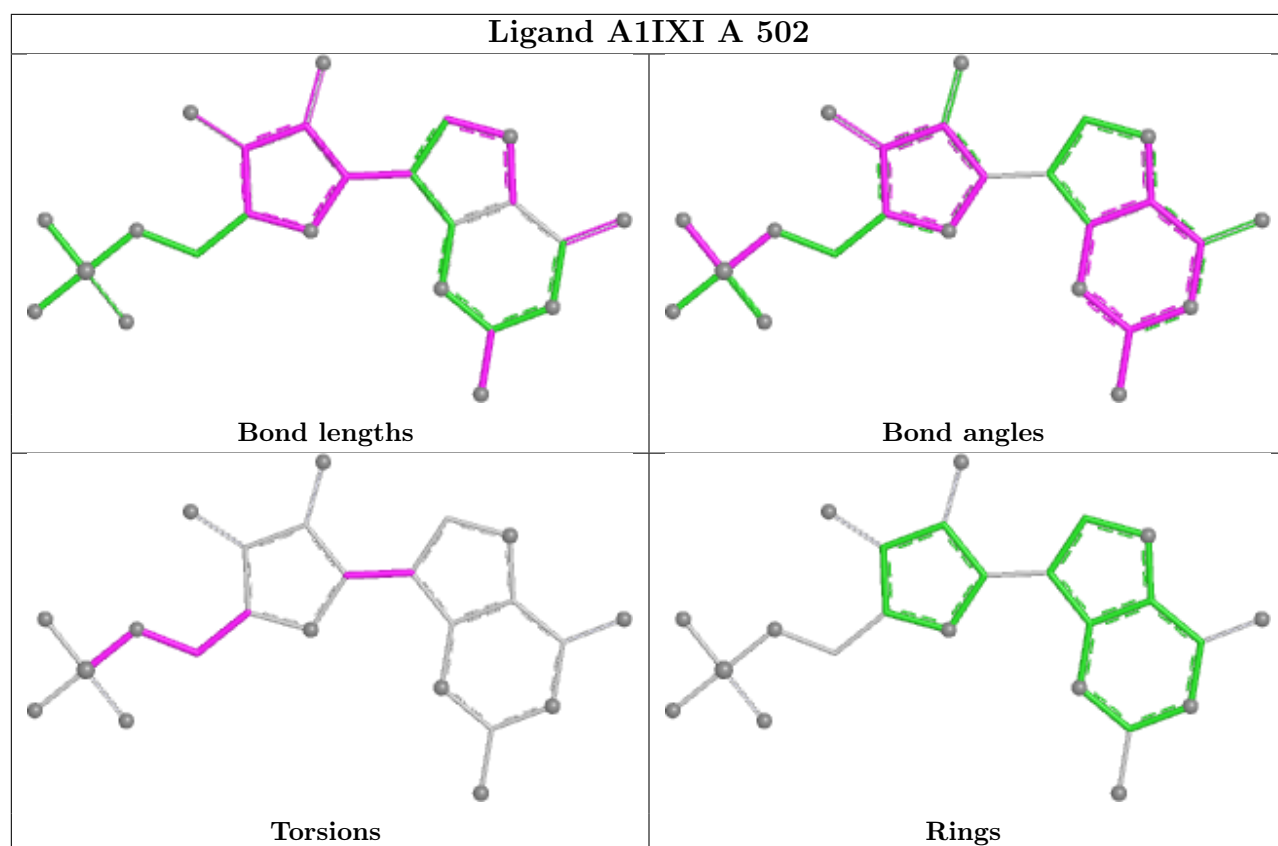
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	G4P	5	0
3	A	502	A1IXI	1	0
2	B	501	G4P	2	0
3	D	501	A1IXI	1	0
2	C	501	G4P	4	0

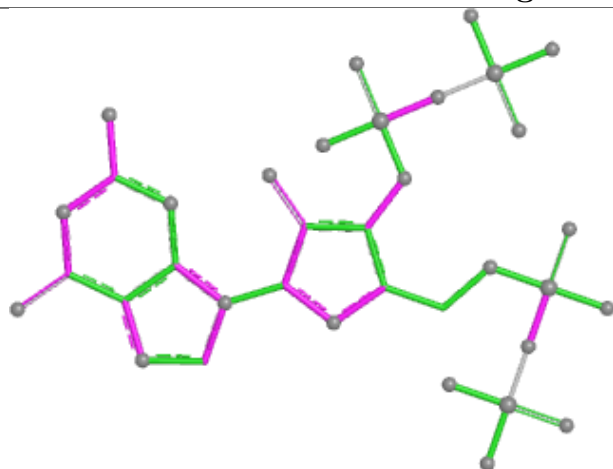
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand G4P D 502

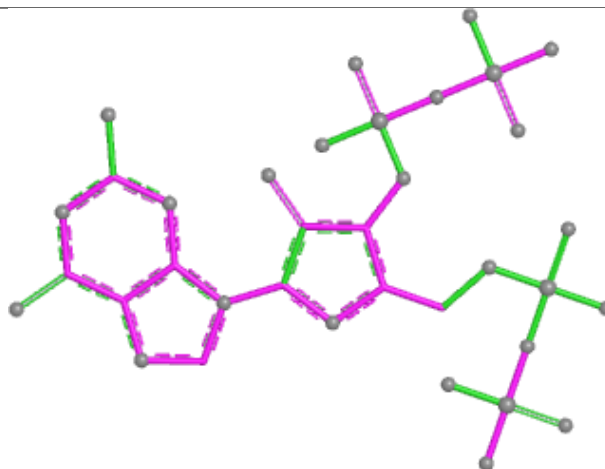




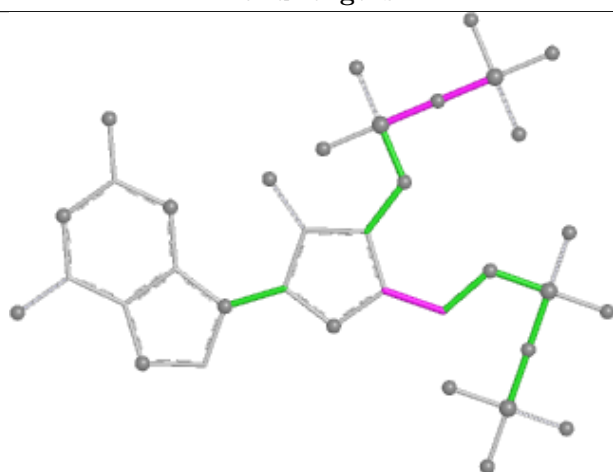
Ligand G4P B 501



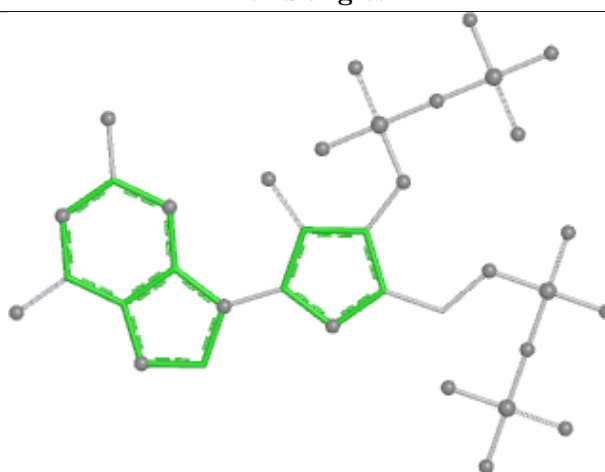
Bond lengths



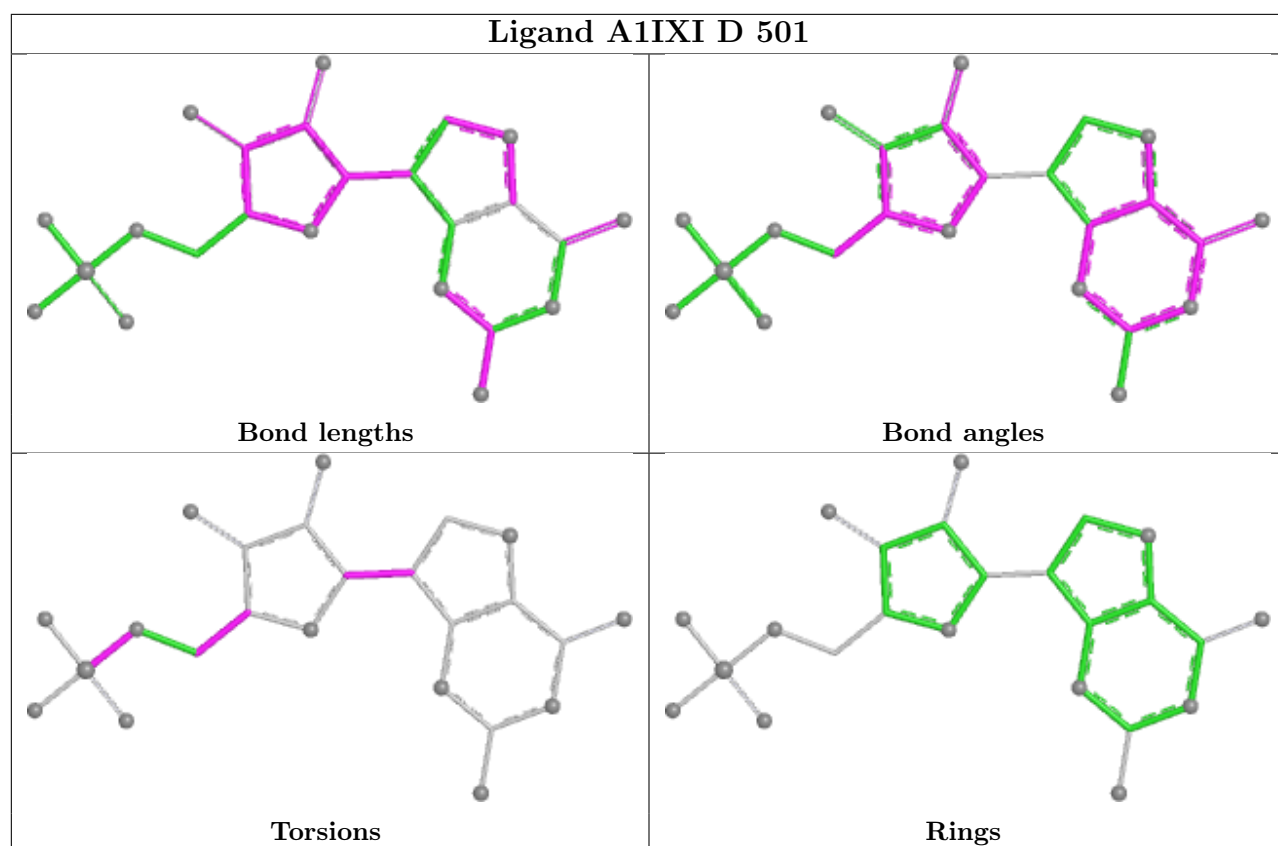
Bond angles



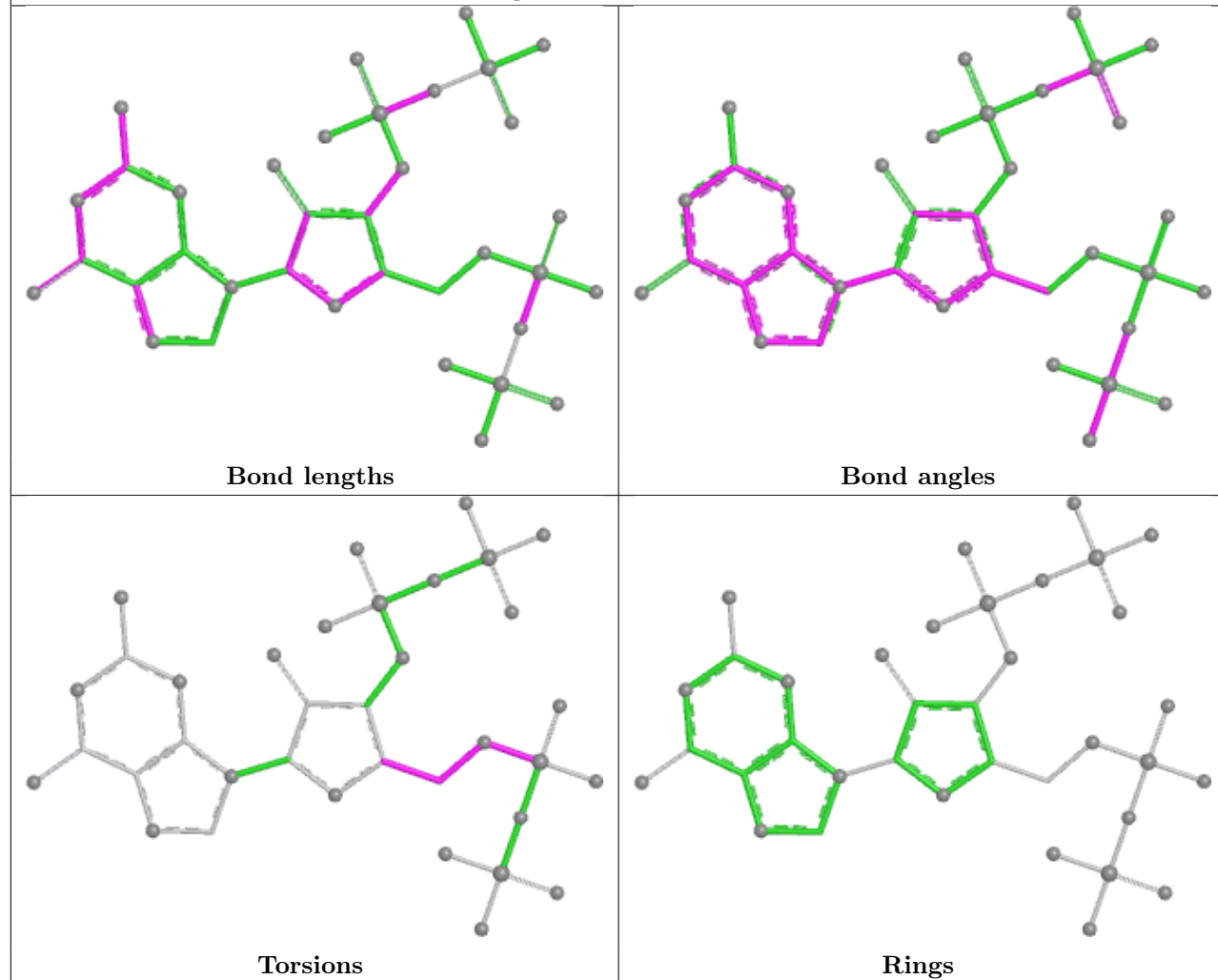
Torsions

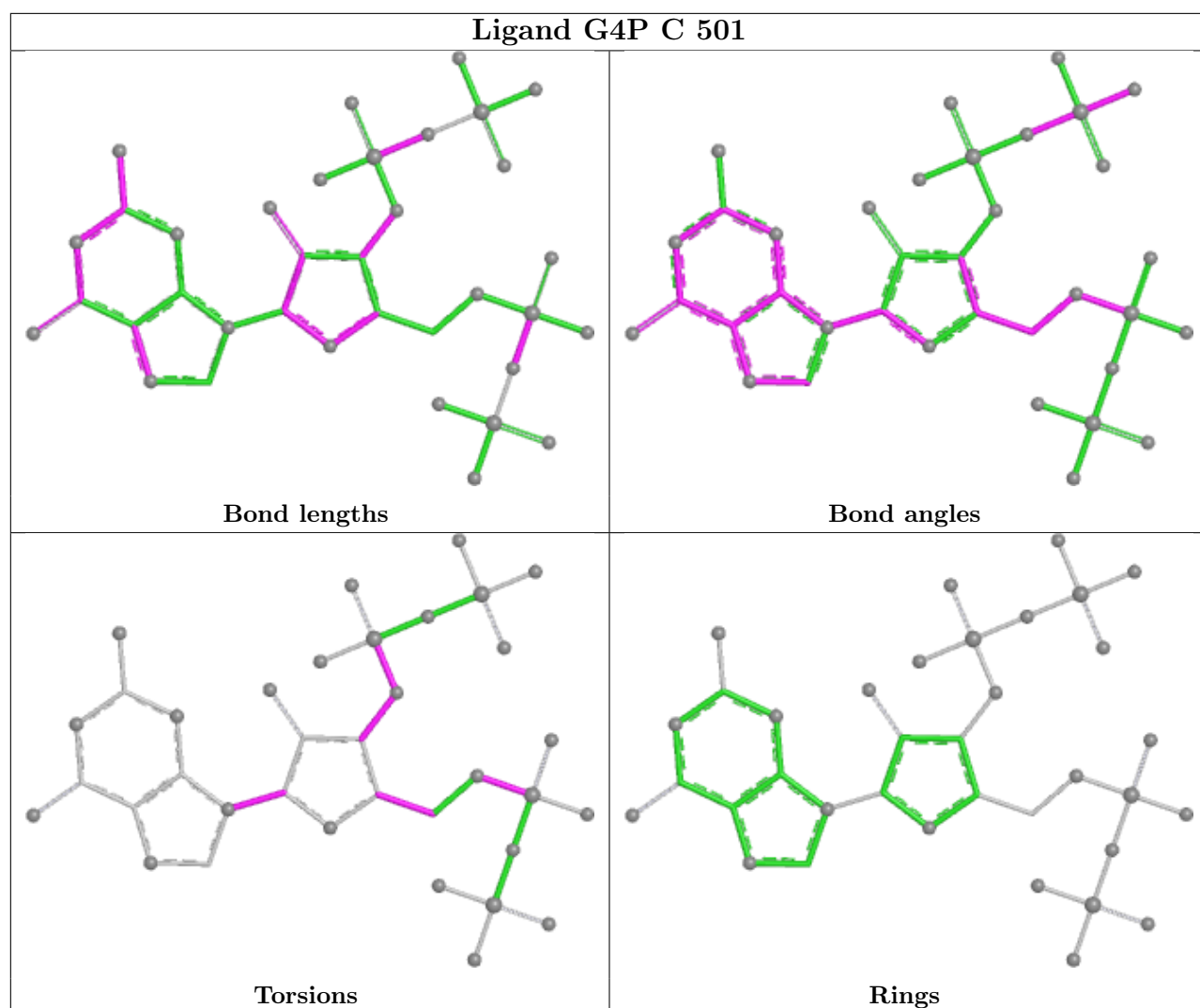


Rings



Ligand G4P A 501





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/460 (95%)	-0.41	0 100 100	84, 121, 253, 354	0
1	B	435/460 (94%)	-0.41	0 100 100	88, 138, 282, 421	0
1	C	444/460 (96%)	-0.48	0 100 100	80, 122, 256, 355	0
1	D	441/460 (95%)	-0.38	0 100 100	88, 122, 266, 416	0
All	All	1759/1840 (95%)	-0.42	0 100 100	80, 126, 266, 421	0

There are no RSRZ outliers to report.

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	G4P	B	501	36/36	0.69	0.10	122,169,219,242	0
2	G4P	D	502	36/36	0.73	0.10	111,151,205,224	36
3	A1IXI	A	502	24/24	0.79	0.16	120,136,150,165	24
2	G4P	C	501	36/36	0.82	0.09	112,132,177,195	36

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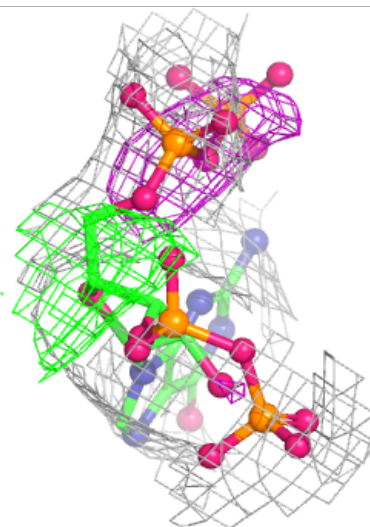
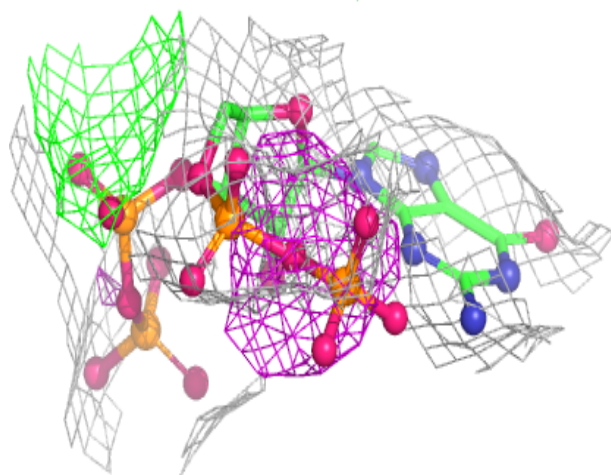
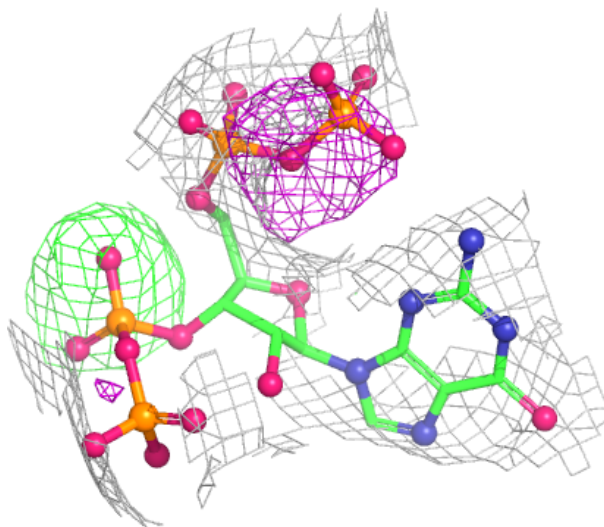
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1IXI	D	501	24/24	0.85	0.12	127,136,151,156	24
2	G4P	A	501	36/36	0.87	0.07	137,161,180,200	36

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.

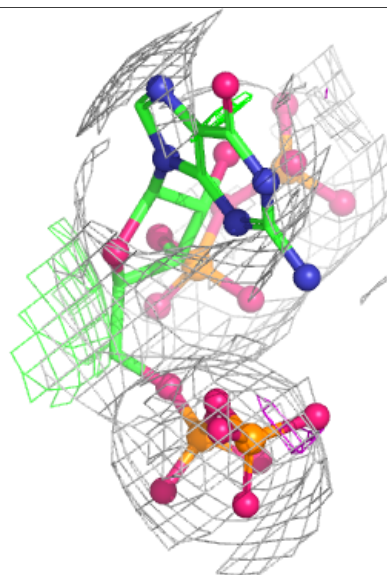
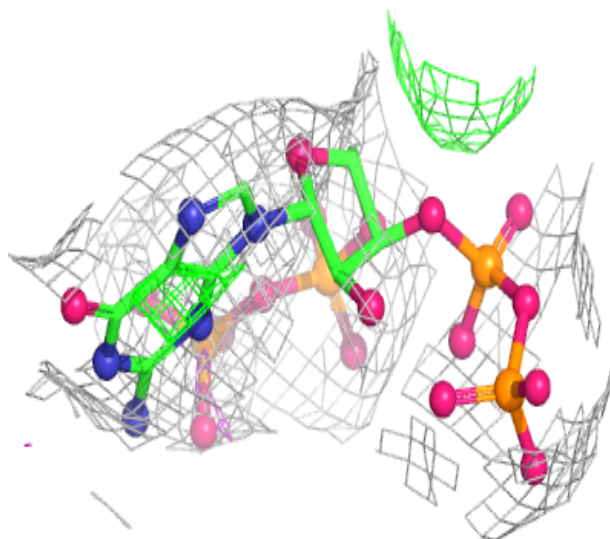
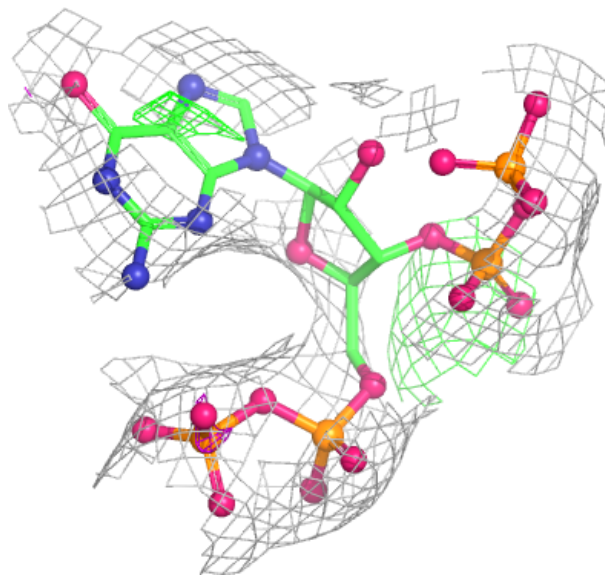
Electron density around G4P B 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



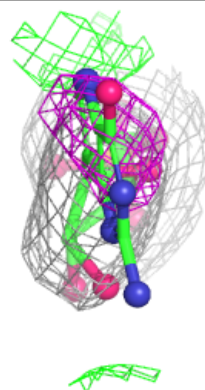
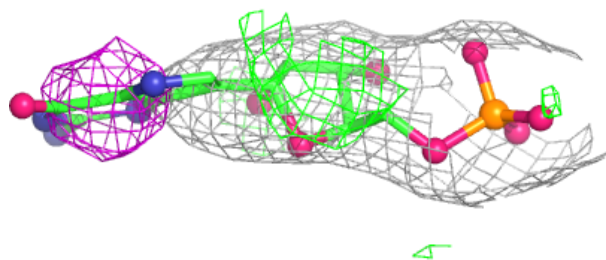
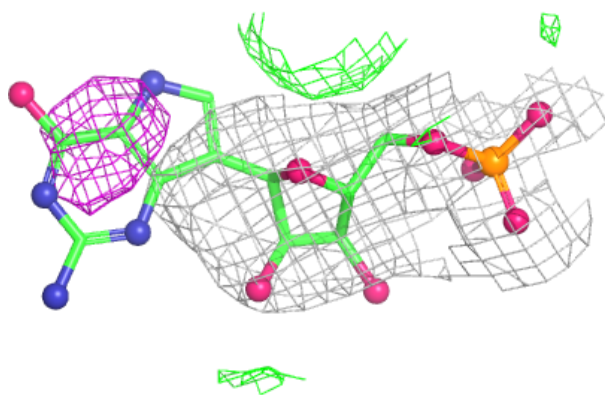
Electron density around G4P D 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



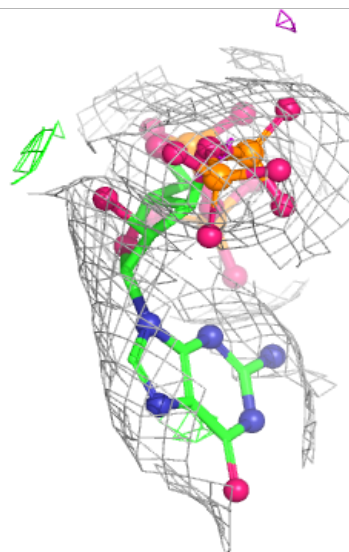
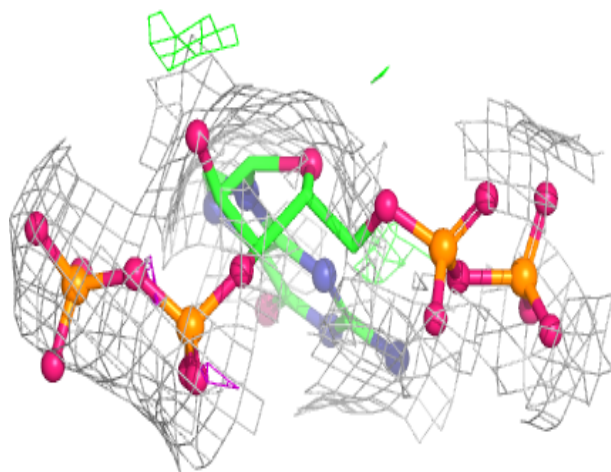
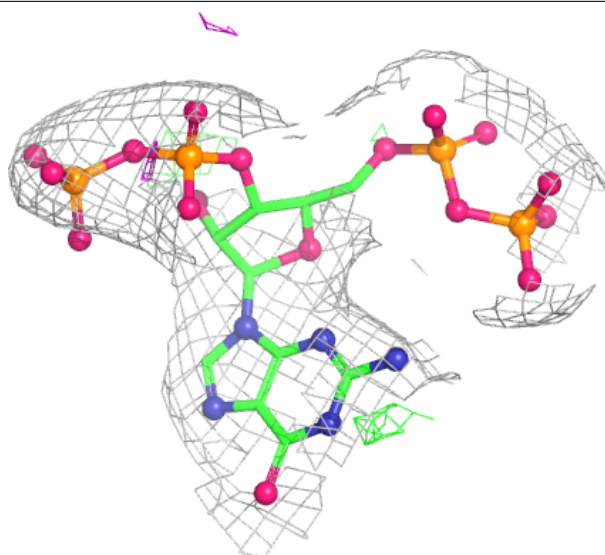
Electron density around A1IXI A 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



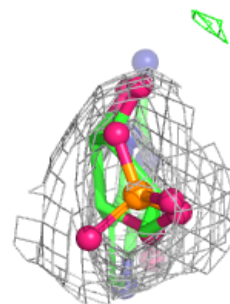
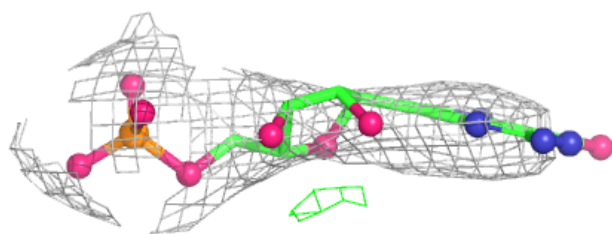
Electron density around G4P C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



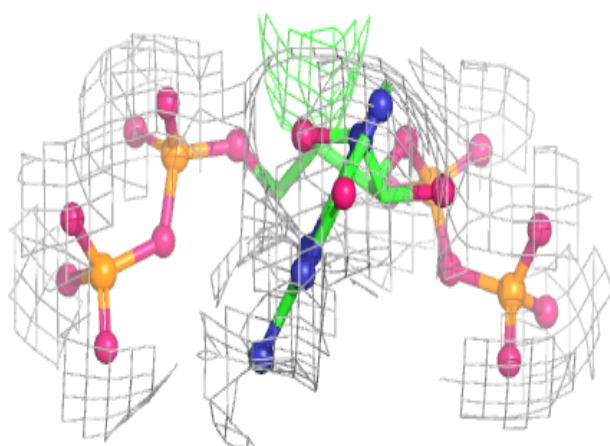
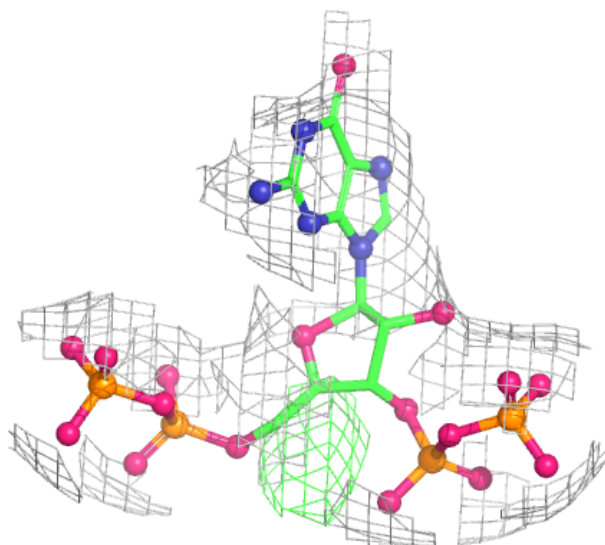
Electron density around A1IXI D 501:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G4P A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.