Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 08:13 AM EDT

PDB ID	:	3N75
Title	:	X-ray Crystal Structure of the Escherichia coli Inducible Lysine Decarboxylase LdcI
Authors	:	Kanjee, U.; Alexopoulos, E.; Pai, E.F.; Houry, W.A.
Deposited on	:	2010-05-26
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

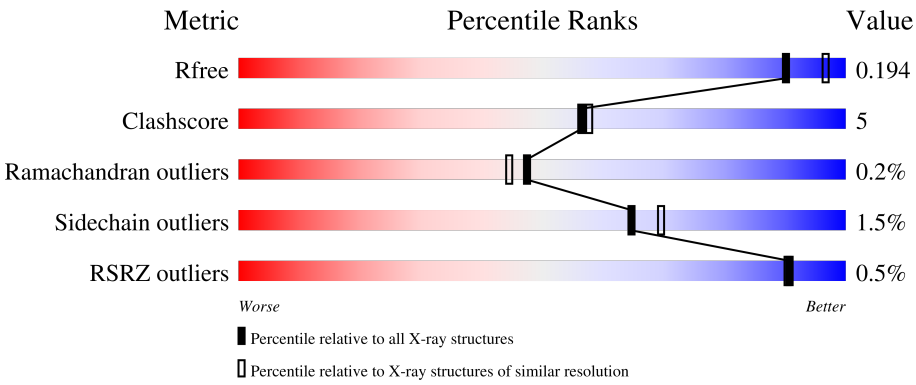
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	715	89% 9% ••
1	B	715	% 89% 10% •
1	C	715	88% 11% ••
1	D	715	89% 10% •
1	E	715	89% 10% ••

2 Entry composition (i)

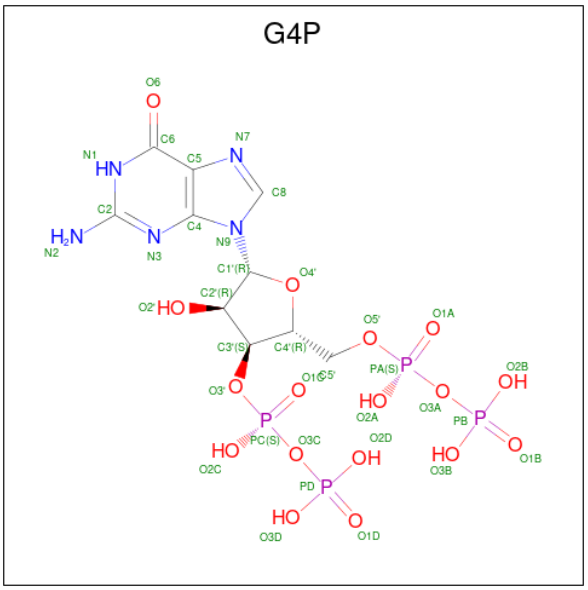
There are 5 unique types of molecules in this entry. The entry contains 32266 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine decarboxylase, inducible.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	711	5705	3650	953	1064	1	37	0	1	0
1	B	711	5705	3650	953	1064	1	37	0	1	0
1	C	711	5711	3654	953	1066	1	37	0	2	0
1	D	711	5711	3654	953	1066	1	37	0	2	0
1	E	711	5705	3650	953	1064	1	37	0	1	0

- Molecule 2 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	72	20	10	34	8	0	1

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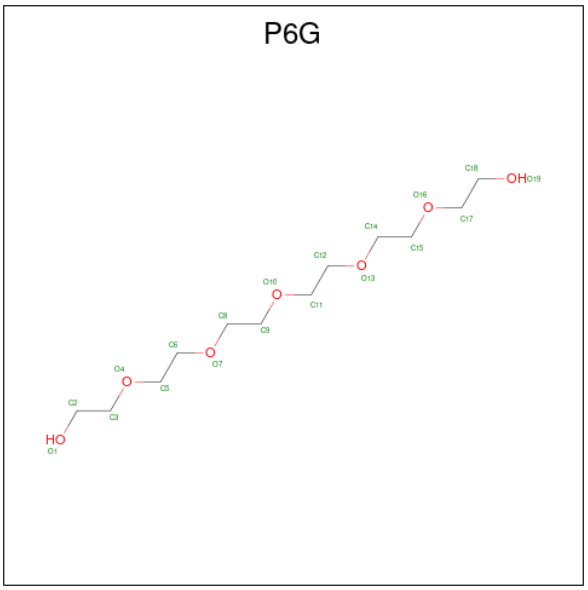
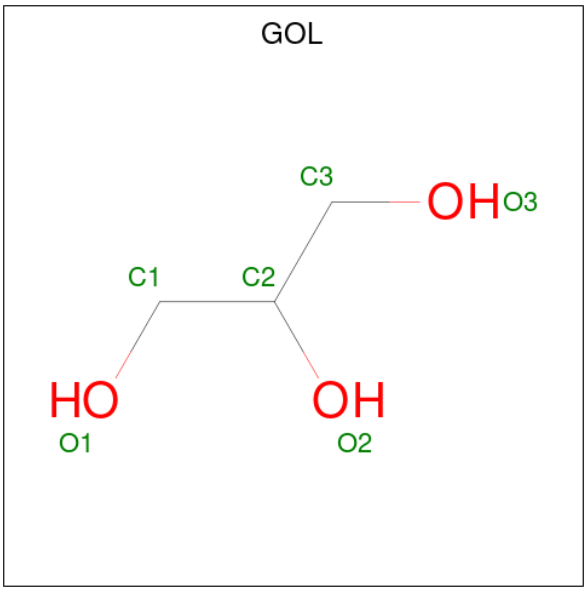
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	72	20	10	34	8	0	1
			Total	C	N	O	P		
2	C	1	72	20	10	34	8	0	1
			Total	C	N	O	P		
2	D	1	72	20	10	34	8	0	1
			Total	C	N	O	P		
2	E	1	36	10	5	17	4	0	0

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	19	12	7	0	0
			Total	C	O		
3	B	1	16	10	6	0	0
			Total	C	O		
3	C	1	16	10	6	0	0
			Total	C	O		
3	D	1	16	10	6	0	0
			Total	C	O		
3	E	1	16	10	6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	E	1	6	3	3	0	0

- Molecule 5 is water.

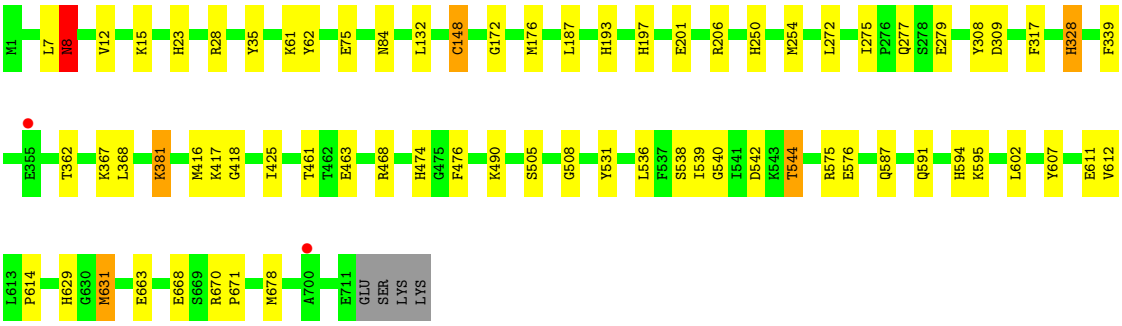
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	632	632	632	0	0
5	B	491	491	491	0	0
5	C	716	716	716	0	0
5	D	704	704	704	0	0
5	E	749	749	749	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

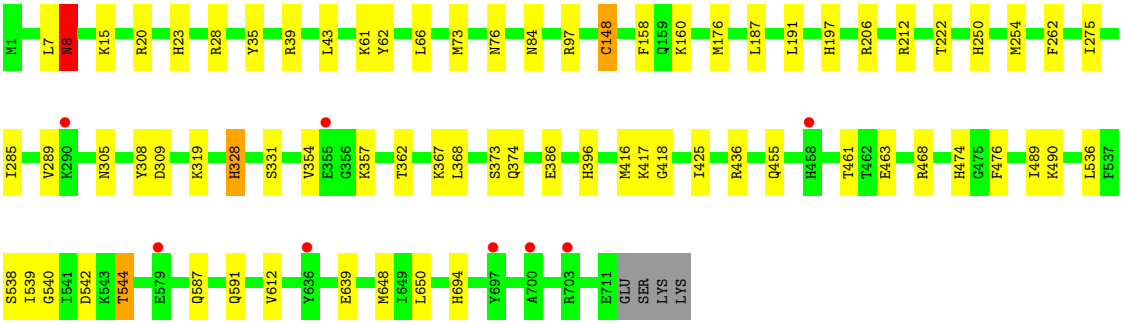
• Molecule 1: Lysine decarboxylase, inducible

Chain A:



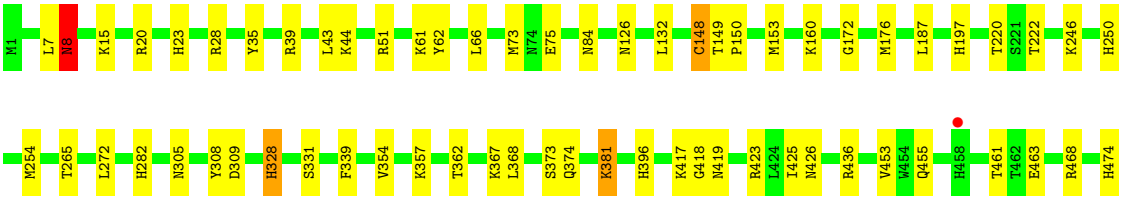
• Molecule 1: Lysine decarboxylase, inducible

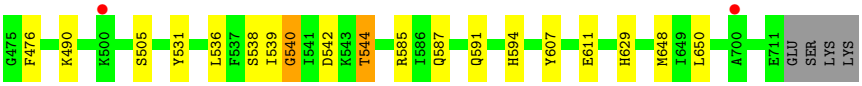
Chain B:



• Molecule 1: Lysine decarboxylase, inducible

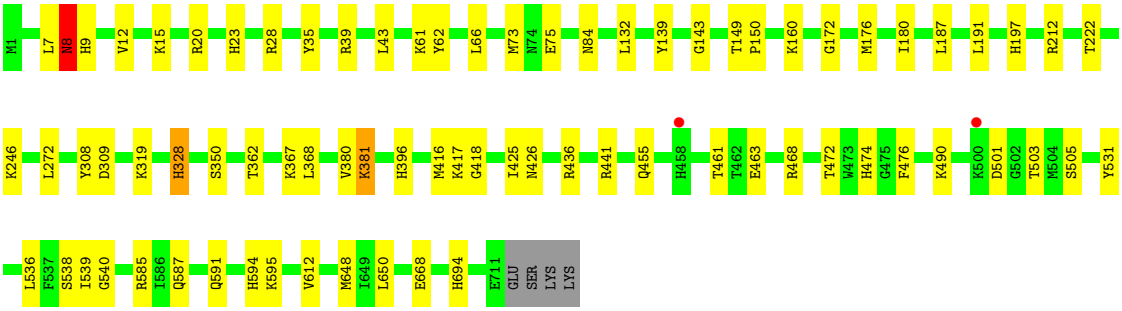
Chain C:





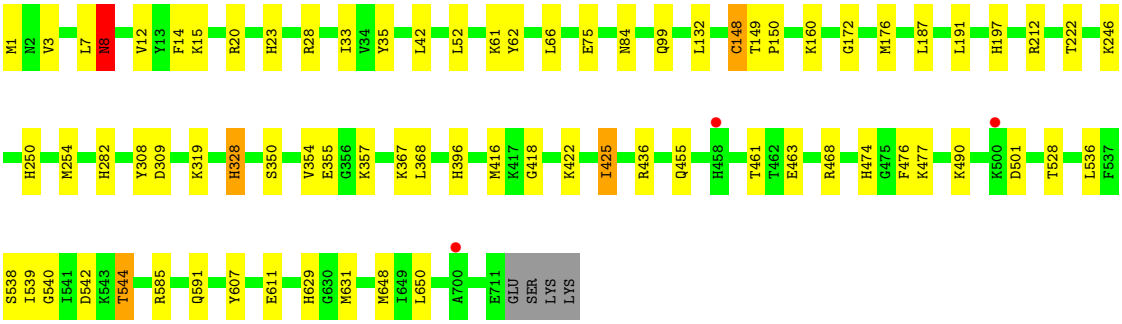
• Molecule 1: Lysine decarboxylase, inducible

Chain D:



• Molecule 1: Lysine decarboxylase, inducible

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.76Å 181.99Å 170.90Å 90.00° 125.41° 90.00°	Depositor
Resolution (Å)	49.89 – 2.00 49.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.89-2.00) 99.8 (49.89-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.168 , 0.194 0.169 , 0.194	Depositor DCC
R_{free} test set	22770 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32266	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, G4P, GOL, P6G

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	0.73	4/5824 (0.1%)	0.75	8/7893 (0.1%)
1	B	0.69	5/5824 (0.1%)	0.74	8/7893 (0.1%)
1	C	0.76	4/5833 (0.1%)	0.78	8/7905 (0.1%)
1	D	0.76	3/5833 (0.1%)	0.77	8/7905 (0.1%)
1	E	0.78	4/5824 (0.1%)	0.78	12/7893 (0.2%)
All	All	0.74	20/29138 (0.1%)	0.76	44/39489 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	10

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	ASN	CB-CG	-8.75	1.30	1.51
1	C	148	CYS	CB-SG	-8.56	1.67	1.82
1	A	8	ASN	CB-CG	-8.50	1.31	1.51
1	B	8	ASN	CB-CG	-8.44	1.31	1.51
1	C	8	ASN	CB-CG	-8.21	1.32	1.51
1	D	8	ASN	CB-CG	-8.13	1.32	1.51
1	B	148	CYS	CB-SG	-7.82	1.69	1.82
1	E	148	CYS	CB-SG	-7.37	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	CYS	CB-SG	-7.27	1.69	1.82
1	A	576	GLU	N-CA	6.91	1.60	1.46
1	D	8	ASN	CA-C	6.87	1.70	1.52
1	E	8	ASN	CA-C	6.61	1.70	1.52
1	D	8	ASN	N-CA	6.51	1.59	1.46
1	B	8	ASN	N-CA	6.45	1.59	1.46
1	B	8	ASN	CA-C	6.38	1.69	1.52
1	E	8	ASN	N-CA	6.37	1.59	1.46
1	A	8	ASN	CA-C	5.75	1.68	1.52
1	C	8	ASN	N-CA	5.62	1.57	1.46
1	B	540	GLY	N-CA	5.45	1.54	1.46
1	C	8	ASN	CA-C	5.28	1.66	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	8	ASN	N-CA-C	14.79	150.92	111.00
1	B	8	ASN	N-CA-C	14.60	150.41	111.00
1	A	8	ASN	N-CA-C	14.13	149.16	111.00
1	D	8	ASN	N-CA-C	14.09	149.03	111.00
1	C	8	ASN	N-CA-C	14.02	148.84	111.00
1	B	20	ARG	NE-CZ-NH2	-12.53	114.04	120.30
1	B	20	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	D	20	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	E	20	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	C	20	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	C	20	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	B	540	GLY	N-CA-C	8.16	133.49	113.10
1	E	540	GLY	N-CA-C	8.03	133.18	113.10
1	A	631	MET	CB-CG-SD	-7.75	89.14	112.40
1	C	540	GLY	N-CA-C	7.42	131.66	113.10
1	A	540	GLY	N-CA-C	7.42	131.65	113.10
1	D	540	GLY	N-CA-C	7.26	131.26	113.10
1	A	28	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	E	20	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	E	8	ASN	N-CA-CB	-6.68	98.57	110.60
1	C	28	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	E	28	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	D	20	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	D	28	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	576	GLU	N-CA-C	6.16	127.62	111.00
1	B	8	ASN	N-CA-CB	-5.99	99.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	425	ILE	CG1-CB-CG2	-5.95	98.31	111.40
1	E	631	MET	CB-CG-SD	-5.88	94.75	112.40
1	D	272	LEU	CA-CB-CG	-5.84	101.87	115.30
1	E	1	MET	CG-SD-CE	5.81	109.50	100.20
1	A	8	ASN	N-CA-CB	-5.80	100.16	110.60
1	C	28	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	28	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	28	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	8	ASN	CB-CA-C	-5.29	99.81	110.40
1	E	33	ILE	N-CA-C	-5.29	96.72	111.00
1	A	272	LEU	CA-CB-CG	-5.29	103.14	115.30
1	A	28	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	453	VAL	CB-CA-C	-5.14	101.63	111.40
1	B	76	ASN	N-CA-C	5.12	124.82	111.00
1	C	272	LEU	CA-CB-CG	-5.12	103.53	115.30
1	B	8	ASN	CB-CA-C	-5.05	100.30	110.40
1	B	28	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	441	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	ILE	Peptide
1	A	575	ARG	Peptide
1	A	75	GLU	Peptide
1	B	539	ILE	Peptide
1	C	539	ILE	Peptide
1	C	75	GLU	Peptide
1	D	539	ILE	Peptide
1	D	75	GLU	Peptide
1	E	539	ILE	Peptide
1	E	75	GLU	Peptide

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	A	5705	0	5622	48	0
1	B	5705	0	5622	58	0
1	C	5711	0	5628	63	0
1	D	5711	0	5628	60	0
1	E	5705	0	5622	54	0
2	A	72	0	22	6	0
2	B	72	0	22	10	0
2	C	72	0	22	3	0
2	D	72	0	22	4	0
2	E	36	0	11	2	0
3	A	19	0	26	1	0
3	B	16	0	21	1	0
3	C	16	0	21	1	0
3	D	16	0	21	1	0
3	E	16	0	21	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
4	E	6	0	8	2	0
5	A	632	0	0	6	0
5	B	491	0	0	6	0
5	C	716	0	0	11	0
5	D	704	0	0	10	0
5	E	749	0	0	12	0
All	All	32266	0	28371	286	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 5.

All (286) 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)
1:A:7:LEU:O	1:A:8:ASN:HB2	1.65	0.97
1:B:417:LYS:NZ	2:B:716[B]:G4P:O1D	2.01	0.93
1:E:7:LEU:O	1:E:8:ASN:HB2	1.68	0.91
1:D:417:LYS:HE2	2:D:716[B]:G4P:O2D	1.72	0.89
1:C:417:LYS:NZ	2:C:716[B]:G4P:O2D	2.07	0.88
1:A:417:LYS:NZ	2:A:716[B]:G4P:O2D	2.09	0.86
1:D:417:LYS:NZ	2:D:716[B]:G4P:O2D	2.08	0.85
1:B:542:ASP:OD1	1:B:544:THR:HB	1.76	0.85
1:B:7:LEU:O	1:B:8:ASN:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:O	1:C:8:ASN:HB2	1.74	0.84
1:D:417:LYS:CE	2:D:716[B]:G4P:O2D	2.24	0.84
1:D:7:LEU:O	1:D:8:ASN:HB2	1.77	0.83
1:A:8:ASN:OD1	1:A:61:LYS:NZ	2.11	0.81
1:E:8:ASN:OD1	1:E:61:LYS:NZ	2.12	0.81
1:C:461:THR:HG21	1:C:463:GLU:OE2	1.81	0.80
1:E:461:THR:HG21	1:E:463:GLU:OE2	1.83	0.79
1:D:436:ARG:HH11	1:D:455:GLN:HE21	1.32	0.78
1:D:8:ASN:OD1	1:D:61:LYS:NZ	2.16	0.78
1:C:8:ASN:OD1	1:C:61:LYS:NZ	2.15	0.77
1:B:544:THR:HG21	5:D:897:HOH:O	1.84	0.77
1:C:43:LEU:HD22	1:C:73:MET:CE	2.15	0.76
1:B:43:LEU:HD22	1:B:73:MET:CE	2.16	0.76
1:D:416:MET:SD	1:D:425:ILE:HD11	2.26	0.76
1:B:490:LYS:HD2	1:B:536:LEU:HD22	1.68	0.76
1:C:250:HIS:O	1:C:254:MET:HG3	1.88	0.74
1:B:328:HIS:HD2	5:B:793:HOH:O	1.70	0.73
1:D:461:THR:HG21	1:D:463:GLU:OE2	1.88	0.73
1:D:461:THR:HG23	1:D:463:GLU:HG2	1.71	0.72
1:C:461:THR:HG23	1:C:463:GLU:HG2	1.72	0.72
1:E:474:HIS:HD2	1:E:476:PHE:H	1.38	0.71
5:B:755:HOH:O	1:E:544:THR:HG21	1.90	0.71
1:C:474:HIS:HD2	1:C:476:PHE:H	1.38	0.70
1:A:544:THR:HG21	5:C:913:HOH:O	1.91	0.70
1:C:544:THR:HG21	5:E:825:HOH:O	1.92	0.70
1:C:436:ARG:HH11	1:C:455:GLN:HE21	1.36	0.70
1:D:474:HIS:HD2	1:D:476:PHE:H	1.39	0.70
1:E:461:THR:HG22	5:E:1916:HOH:O	1.92	0.69
1:B:436:ARG:HH11	1:B:455:GLN:HE21	1.38	0.68
1:E:542:ASP:OD1	1:E:544:THR:HB	1.93	0.68
1:B:417:LYS:CE	2:B:716[B]:G4P:O1D	2.42	0.68
1:C:39:ARG:HG2	1:C:66:LEU:HD23	1.76	0.68
1:E:436:ARG:HH11	1:E:455:GLN:HE21	1.40	0.68
1:E:591:GLN:HG3	5:E:1830:HOH:O	1.93	0.68
1:A:416:MET:SD	1:A:425:ILE:HD11	2.34	0.67
1:E:422:LYS:HE3	5:E:2268:HOH:O	1.95	0.66
1:B:461:THR:HG21	1:B:463:GLU:OE2	1.94	0.66
1:D:531:TYR:OH	1:D:594:HIS:HD2	1.78	0.66
1:A:461:THR:HG21	1:A:463:GLU:OE2	1.95	0.66
1:D:15:LYS:NZ	1:D:84:ASN:HD21	1.94	0.66
1:C:39:ARG:HG2	1:C:66:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:VAL:HG11	1:B:357:LYS:HD2	1.78	0.65
1:B:461:THR:HG23	1:B:463:GLU:HG2	1.77	0.65
1:C:542:ASP:OD1	1:C:544:THR:HB	1.96	0.65
1:A:328:HIS:HD2	5:A:737:HOH:O	1.80	0.65
1:B:368:LEU:HD23	1:B:538:SER:HB3	1.80	0.64
1:A:587:GLN:O	1:A:591:GLN:HG3	1.96	0.64
1:A:490:LYS:HD2	1:A:536:LEU:HD22	1.78	0.64
1:D:23:HIS:HD2	1:D:35:TYR:OH	1.80	0.64
1:D:490:LYS:HD2	1:D:536:LEU:HD22	1.80	0.63
1:B:8:ASN:OD1	1:B:61:LYS:NZ	2.20	0.63
1:C:43:LEU:HD22	1:C:73:MET:HE2	1.80	0.63
1:E:528:THR:HG21	5:E:2688:HOH:O	1.98	0.62
1:B:461:THR:HG22	5:B:2223:HOH:O	1.98	0.62
1:C:461:THR:HG22	5:C:1933:HOH:O	1.99	0.62
1:A:15:LYS:NZ	1:A:84:ASN:HD21	1.98	0.61
1:C:436:ARG:HB3	1:C:455:GLN:HE22	1.64	0.61
1:C:531:TYR:OH	1:C:594:HIS:HD2	1.83	0.61
1:C:368:LEU:HD23	1:C:538:SER:HB3	1.83	0.61
1:A:461:THR:HG22	5:A:2044:HOH:O	2.00	0.61
1:C:15:LYS:NZ	1:C:84:ASN:HD21	1.98	0.61
1:D:591:GLN:HG3	5:D:1809:HOH:O	2.00	0.61
1:D:418:GLY:N	2:D:716[A]:G4P:O3D	2.34	0.61
1:A:418:GLY:N	2:A:716[A]:G4P:O3D	2.33	0.60
1:B:474:HIS:HD2	1:B:476:PHE:H	1.48	0.60
1:E:328:HIS:HD2	5:E:732:HOH:O	1.83	0.60
1:E:416:MET:SD	1:E:425:ILE:HD11	2.42	0.60
1:B:15:LYS:NZ	1:B:84:ASN:HD21	1.98	0.60
1:B:212[B]:ARG:NH2	1:B:386:GLU:CD	2.54	0.60
1:A:474:HIS:HD2	1:A:476:PHE:H	1.49	0.60
1:B:416:MET:SD	1:B:425:ILE:HD11	2.41	0.60
1:D:436:ARG:HH11	1:D:455:GLN:NE2	1.98	0.60
1:B:418:GLY:N	2:B:716[A]:G4P:O3D	2.35	0.59
1:B:39:ARG:HG2	1:B:66:LEU:HD23	1.85	0.59
1:B:206:ARG:NH2	2:B:716[A]:G4P:O1B	2.34	0.59
1:B:206:ARG:NH2	2:B:716[B]:G4P:O1B	2.35	0.59
1:D:461:THR:HG22	5:D:1937:HOH:O	2.03	0.58
1:E:461:THR:HG23	1:E:463:GLU:HG2	1.85	0.58
1:B:43:LEU:HD22	1:B:73:MET:HE2	1.83	0.58
1:D:246:LYS:HD3	1:D:648:MET:CE	2.34	0.58
1:D:23:HIS:CD2	1:D:35:TYR:OH	2.57	0.58
1:E:23:HIS:HD2	1:E:35:TYR:OH	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212[B]:ARG:HH21	1:B:386:GLU:CD	2.07	0.57
1:B:39:ARG:HG2	1:B:66:LEU:CD2	2.34	0.57
1:C:591:GLN:HG3	5:C:936:HOH:O	2.04	0.57
1:D:368:LEU:HD23	1:D:538:SER:HB3	1.87	0.57
1:C:436:ARG:HH11	1:C:455:GLN:NE2	2.02	0.56
1:A:531:TYR:OH	1:A:594:HIS:HD2	1.88	0.56
1:B:43:LEU:HD22	1:B:73:MET:HE1	1.87	0.56
1:A:542:ASP:OD1	1:A:544:THR:HB	2.06	0.56
1:B:436:ARG:HH11	1:B:455:GLN:NE2	2.03	0.55
1:E:368:LEU:HD23	1:E:538:SER:HB3	1.89	0.55
1:A:368:LEU:HD23	1:A:538:SER:HB3	1.89	0.55
1:E:15:LYS:NZ	1:E:84:ASN:HD21	2.05	0.55
1:E:418:GLY:N	2:E:716:G4P:O3D	2.34	0.55
1:C:328:HIS:HD2	5:C:763:HOH:O	1.90	0.55
1:D:436:ARG:HB3	1:D:455:GLN:HE22	1.72	0.54
1:B:319:LYS:O	1:B:357:LYS:NZ	2.37	0.54
1:C:339:PHE:HB2	1:C:425:ILE:HG13	1.90	0.54
1:E:490:LYS:HD2	1:E:536:LEU:HD22	1.90	0.54
1:B:418:GLY:CA	2:B:716[A]:G4P:O3D	2.56	0.53
1:C:468:ARG:O	1:C:474:HIS:HE1	1.91	0.53
1:B:436:ARG:HB3	1:B:455:GLN:HE22	1.73	0.53
1:E:282:HIS:HE2	4:E:718:GOL:HO2	1.54	0.53
1:B:639:GLU:HG3	5:B:3242:HOH:O	2.08	0.53
1:C:474:HIS:CD2	1:C:476:PHE:H	2.23	0.53
1:D:187:LEU:O	1:D:197:HIS:HD2	1.91	0.53
1:D:612:VAL:HG11	1:D:668:GLU:HG2	1.90	0.53
1:E:436:ARG:HH11	1:E:455:GLN:NE2	2.07	0.53
1:C:43:LEU:HD22	1:C:73:MET:HE1	1.88	0.53
1:D:474:HIS:CD2	1:D:476:PHE:H	2.25	0.53
1:B:648:MET:HE3	1:B:650:LEU:HD22	1.91	0.52
1:E:436:ARG:HB3	1:E:455:GLN:HE22	1.75	0.52
1:E:23:HIS:CD2	1:E:35:TYR:OH	2.63	0.52
1:B:250:HIS:O	1:B:254:MET:HG3	2.10	0.52
1:E:354:VAL:HG11	1:E:357:LYS:HD2	1.91	0.52
1:D:246:LYS:HD3	1:D:648:MET:HE2	1.92	0.51
1:D:531:TYR:OH	1:D:594:HIS:CD2	2.60	0.51
1:E:319:LYS:NZ	1:E:350:SER:O	2.43	0.51
3:A:717:P6G:H61	5:A:1358:HOH:O	2.09	0.51
1:A:8:ASN:ND2	1:A:62:TYR:OH	2.43	0.51
1:E:8:ASN:ND2	1:E:62:TYR:OH	2.42	0.51
1:B:490:LYS:CD	1:B:536:LEU:HD22	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:TYR:OH	1:A:594:HIS:CD2	2.63	0.51
1:C:15:LYS:HZ1	1:C:84:ASN:HD21	1.59	0.51
1:D:212[B]:ARG:HG2	1:D:380:VAL:HB	1.93	0.51
1:E:648:MET:HE3	1:E:650:LEU:HB2	1.93	0.51
1:E:474:HIS:CD2	1:E:476:PHE:H	2.25	0.50
1:C:607:TYR:CE1	1:C:611[A]:GLU:HG3	2.46	0.50
1:C:187:LEU:O	1:C:197:HIS:HD2	1.94	0.50
1:C:490:LYS:HD2	1:C:536:LEU:HD22	1.93	0.50
1:B:187:LEU:O	1:B:197:HIS:HD2	1.95	0.50
1:B:8:ASN:ND2	1:B:62:TYR:OH	2.43	0.50
1:E:629:HIS:HE1	5:E:875:HOH:O	1.93	0.50
2:A:716[A]:G4P:O2B	1:D:585:ARG:NH2	2.43	0.50
2:A:716[B]:G4P:O2B	1:D:585:ARG:NH2	2.43	0.50
1:C:126:ASN:HB3	5:C:2579:HOH:O	2.10	0.50
1:C:418:GLY:N	2:C:716[A]:G4P:O3D	2.43	0.49
1:D:505:SER:O	1:D:594:HIS:HE1	1.95	0.49
1:A:668:GLU:HB2	5:A:880:HOH:O	2.12	0.49
1:A:629:HIS:HE1	5:A:848:HOH:O	1.96	0.49
1:C:648:MET:HE3	1:C:650:LEU:HB2	1.94	0.49
1:E:416:MET:SD	1:E:425:ILE:CD1	3.01	0.49
1:C:246:LYS:HD3	1:C:648:MET:CE	2.43	0.49
1:D:472:THR:HA	5:D:2596:HOH:O	2.11	0.49
1:B:417:LYS:HE2	2:B:716[B]:G4P:O1D	2.13	0.49
1:E:607:TYR:O	1:E:611:GLU:HG2	2.13	0.48
1:E:436:ARG:HD3	1:E:455:GLN:NE2	2.29	0.48
1:C:354:VAL:HG11	1:C:357:LYS:HD2	1.94	0.48
1:C:585:ARG:NH2	2:E:716:G4P:O2B	2.45	0.48
1:D:468:ARG:O	1:D:474:HIS:HE1	1.95	0.48
1:E:477:LYS:HE3	5:E:2726:HOH:O	2.13	0.48
1:A:132:LEU:HD23	1:A:132:LEU:C	2.34	0.48
1:D:416:MET:SD	1:D:425:ILE:CD1	2.98	0.48
1:A:187:LEU:O	1:A:197:HIS:HD2	1.96	0.48
1:C:531:TYR:OH	1:C:594:HIS:CD2	2.65	0.48
1:C:505:SER:O	1:C:594:HIS:HE1	1.97	0.47
1:D:212[B]:ARG:HD2	5:D:1466:HOH:O	2.14	0.47
1:C:417:LYS:CE	2:C:716[B]:G4P:O2D	2.61	0.47
1:D:650:LEU:HB3	1:D:694:HIS:HB2	1.97	0.47
1:E:250:HIS:O	1:E:254:MET:HG3	2.15	0.47
1:D:328:HIS:HD2	5:D:756:HOH:O	1.98	0.47
1:A:23:HIS:HD2	1:A:35:TYR:OH	1.98	0.47
1:A:368:LEU:CD2	1:A:538:SER:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:LEU:O	1:E:197:HIS:HD2	1.97	0.47
1:D:490:LYS:CD	1:D:536:LEU:HD22	2.45	0.46
1:D:587:GLN:O	1:D:591:GLN:HG3	2.15	0.46
1:C:629:HIS:HE1	5:C:839:HOH:O	1.97	0.46
1:D:319:LYS:NZ	1:D:350:SER:O	2.48	0.46
1:B:206:ARG:HH21	2:B:716[A]:G4P:PB	2.38	0.46
1:B:328:HIS:HE1	1:B:362:THR:OG1	1.98	0.46
1:B:416:MET:SD	1:B:425:ILE:CD1	3.03	0.46
1:A:339:PHE:CB	1:A:425:ILE:HD13	2.44	0.46
1:A:505:SER:O	1:A:594:HIS:HE1	1.99	0.46
1:A:595:LYS:HA	1:A:595:LYS:HD3	1.58	0.46
1:B:474:HIS:CD2	1:B:476:PHE:H	2.30	0.46
1:D:39:ARG:HG2	1:D:66:LEU:CD2	2.46	0.46
1:B:158:PHE:CE1	1:B:176:MET:HE1	2.50	0.46
1:B:587:GLN:O	1:B:591:GLN:HG3	2.15	0.45
1:D:39:ARG:HG2	1:D:66:LEU:HD23	1.98	0.45
1:D:43:LEU:HD22	1:D:73:MET:CE	2.47	0.45
1:A:339:PHE:HB2	1:A:425:ILE:HD13	1.99	0.45
1:A:461:THR:HG23	1:A:463:GLU:HG2	1.99	0.45
1:A:468:ARG:O	1:A:474:HIS:HE1	1.98	0.45
1:B:212[B]:ARG:NH2	1:B:386:GLU:OE1	2.49	0.45
1:A:15:LYS:HZ1	1:A:84:ASN:HD21	1.63	0.45
1:A:206:ARG:NH2	2:A:716[A]:G4P:O1B	2.31	0.45
1:A:206:ARG:NH2	2:A:716[B]:G4P:O1B	2.31	0.45
1:B:468:ARG:O	1:B:474:HIS:HE1	2.00	0.45
1:E:222:THR:HG23	1:E:396:HIS:HB3	1.98	0.45
1:B:354:VAL:CG1	1:B:357:LYS:HD2	2.44	0.45
1:D:149:THR:HA	1:D:150:PRO:C	2.37	0.45
1:A:250:HIS:O	1:A:254:MET:HG3	2.17	0.45
1:C:587:GLN:O	1:C:591:GLN:HG3	2.17	0.45
1:C:220:THR:HG23	1:C:362:THR:HB	1.99	0.45
3:C:717:P6G:H62	5:C:1874:HOH:O	2.17	0.45
1:D:595:LYS:HA	1:D:595:LYS:HD3	1.75	0.45
1:E:172:GLY:O	1:E:176:MET:HG2	2.17	0.45
1:C:8:ASN:ND2	1:C:62:TYR:OH	2.50	0.44
1:C:23:HIS:HD2	1:C:35:TYR:OH	2.00	0.44
1:C:172:GLY:O	1:C:176:MET:HG2	2.16	0.44
1:C:265:THR:HG22	5:C:3167:HOH:O	2.15	0.44
1:B:43:LEU:CD2	1:B:73:MET:HE1	2.48	0.44
1:A:614:PRO:HB2	1:A:663:GLU:HB3	1.98	0.44
1:D:8:ASN:ND2	1:D:62:TYR:OH	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:HIS:HE1	5:D:2027:HOH:O	1.99	0.44
1:C:282:HIS:NE2	4:C:718:GOL:H2	2.32	0.44
1:D:180:ILE:HD11	1:D:187:LEU:HD22	2.00	0.44
1:E:282:HIS:NE2	4:E:718:GOL:O2	2.38	0.44
1:C:23:HIS:CD2	1:C:35:TYR:OH	2.71	0.44
1:D:328:HIS:HE1	1:D:362:THR:OG1	2.01	0.44
1:A:23:HIS:CD2	1:A:35:TYR:OH	2.71	0.44
1:A:172:GLY:O	1:A:176:MET:HG2	2.18	0.44
1:A:602:LEU:HG	1:A:678:MET:HE1	1.98	0.44
1:D:436:ARG:NH1	1:D:455:GLN:HE21	2.07	0.44
1:A:381:LYS:HE3	1:A:381:LYS:HB2	1.85	0.43
1:D:9:HIS:HD2	5:D:1877:HOH:O	2.01	0.43
1:D:222:THR:HG23	1:D:396:HIS:HB3	2.00	0.43
1:A:591:GLN:HG3	5:A:1420:HOH:O	2.18	0.43
1:A:193:HIS:ND1	1:A:201:GLU:OE2	2.52	0.43
1:B:15:LYS:HZ1	1:B:84:ASN:HD21	1.64	0.43
1:C:222:THR:HG23	1:C:396:HIS:HB3	2.00	0.43
1:E:99:GLN:NE2	5:E:2436:HOH:O	2.49	0.43
1:E:416:MET:HE3	5:E:856:HOH:O	2.18	0.43
1:C:419:ASN:O	1:C:423:ARG:HG3	2.18	0.43
1:D:381:LYS:HB2	1:D:381:LYS:HE3	1.62	0.43
1:B:591:GLN:HG3	5:B:2642:HOH:O	2.18	0.43
1:E:468:ARG:O	1:E:474:HIS:HE1	2.01	0.43
1:D:43:LEU:HD22	1:D:73:MET:HE1	2.00	0.43
1:E:436:ARG:HD3	1:E:455:GLN:HE22	1.84	0.43
1:C:44:LYS:HG3	1:E:14:PHE:CE1	2.54	0.42
1:C:305:ASN:O	1:C:331:SER:HA	2.19	0.42
1:C:328:HIS:HE1	1:C:362:THR:OG1	2.02	0.42
1:E:355:GLU:HG2	5:E:1604:HOH:O	2.18	0.42
1:A:275:ILE:HG22	1:A:279:GLU:HB2	2.01	0.42
1:C:132:LEU:HD23	1:C:132:LEU:C	2.39	0.42
1:A:508:GLY:HA3	1:A:594:HIS:CD2	2.54	0.42
1:E:461:THR:CG2	1:E:463:GLU:OE2	2.61	0.42
3:B:717:P6G:H111	5:B:1872:HOH:O	2.19	0.42
1:E:42:LEU:HD23	1:E:66:LEU:HD21	2.02	0.42
1:A:277:GLN:HB3	1:A:317:PHE:CZ	2.54	0.42
1:B:650:LEU:HB3	1:B:694:HIS:HB2	2.01	0.42
1:C:436:ARG:NH1	1:C:455:GLN:HE21	2.11	0.42
1:D:212[A]:ARG:HG3	1:D:212[A]:ARG:HH11	1.84	0.42
1:A:607:TYR:O	1:A:611:GLU:HG2	2.19	0.42
1:E:212[A]:ARG:HH11	1:E:212[A]:ARG:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LYS:CD	1:A:536:LEU:HD22	2.49	0.42
1:C:197:HIS:HE1	5:C:738:HOH:O	2.02	0.42
1:C:246:LYS:HG3	1:C:250:HIS:CE1	2.54	0.42
1:E:197:HIS:HE1	5:E:2716:HOH:O	2.03	0.42
1:D:501:ASP:HB3	1:D:503:THR:HG23	2.02	0.41
1:C:373:SER:O	1:C:374:GLN:HB2	2.20	0.41
1:C:381:LYS:HE3	1:C:381:LYS:HB2	1.84	0.41
1:B:222:THR:HG23	1:B:396:HIS:HB3	2.01	0.41
1:B:373:SER:O	1:B:374:GLN:HB2	2.19	0.41
1:E:246:LYS:HD3	1:E:648:MET:CE	2.51	0.41
1:B:23:HIS:HD2	1:B:35:TYR:OH	2.03	0.41
1:D:139:TYR:CE1	1:D:143:GLY:HA3	2.55	0.41
1:D:426:ASN:ND2	5:D:1092:HOH:O	2.53	0.41
1:A:670:ARG:N	1:A:671:PRO:CD	2.84	0.41
3:D:717:P6G:H21	5:D:2225:HOH:O	2.19	0.41
1:B:262:PHE:HB3	1:B:275:ILE:HD13	2.03	0.41
1:D:132:LEU:C	1:D:132:LEU:HD23	2.42	0.41
1:E:3:VAL:HB	1:E:52:LEU:HA	2.03	0.41
2:B:716[B]:G4P:O2B	1:E:585:ARG:NH2	2.45	0.40
1:C:490:LYS:CD	1:C:536:LEU:HD22	2.51	0.40
1:B:305:ASN:O	1:B:331:SER:HA	2.20	0.40
1:E:132:LEU:C	1:E:132:LEU:HD23	2.41	0.40
1:B:97:ARG:HD2	2:B:716[A]:G4P:C8	2.52	0.40
1:C:51:ARG:HD3	5:C:1023:HOH:O	2.22	0.40
1:D:172:GLY:O	1:D:176:MET:HG2	2.21	0.40
1:C:149:THR:HA	1:C:150:PRO:C	2.41	0.40
1:C:426:ASN:ND2	5:C:1213:HOH:O	2.54	0.40
1:A:328:HIS:HE1	1:A:362:THR:OG1	2.05	0.40
1:B:285:ILE:O	1:B:289:VAL:HG23	2.21	0.40
1:E:149:THR:HA	1:E:150:PRO:C	2.42	0.40
1:E:368:LEU:CD2	1:E:538:SER:HB3	2.51	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	
1	A	709/715 (99%)	692 (98%)	16 (2%)	1 (0%)	51	49
1	B	709/715 (99%)	693 (98%)	15 (2%)	1 (0%)	51	49
1	C	710/715 (99%)	691 (97%)	17 (2%)	2 (0%)	41	37
1	D	710/715 (99%)	693 (98%)	16 (2%)	1 (0%)	51	49
1	E	709/715 (99%)	693 (98%)	15 (2%)	1 (0%)	51	49
All	All	3547/3575 (99%)	3462 (98%)	79 (2%)	6 (0%)	47	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	B	8	ASN
1	C	8	ASN
1	D	8	ASN
1	E	8	ASN
1	C	540	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	621/624 (100%)	611 (98%)	10 (2%)	62	67
1	B	621/624 (100%)	611 (98%)	10 (2%)	62	67
1	C	622/624 (100%)	613 (99%)	9 (1%)	67	72
1	D	622/624 (100%)	614 (99%)	8 (1%)	69	74
1	E	621/624 (100%)	611 (98%)	10 (2%)	62	67
All	All	3107/3120 (100%)	3060 (98%)	47 (2%)	65	69

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	VAL
1	A	148	CYS
1	A	308	TYR
1	A	309	ASP
1	A	328	HIS
1	A	381	LYS
1	A	544	THR
1	A	612	VAL
1	A	631	MET
1	B	8	ASN
1	B	148	CYS
1	B	160	LYS
1	B	191	LEU
1	B	308	TYR
1	B	309	ASP
1	B	328	HIS
1	B	489	ILE
1	B	544	THR
1	B	612	VAL
1	C	8	ASN
1	C	148	CYS
1	C	153	MET
1	C	160	LYS
1	C	308	TYR
1	C	309	ASP
1	C	328	HIS
1	C	381	LYS
1	C	544	THR
1	D	8	ASN
1	D	12	VAL
1	D	160	LYS
1	D	191	LEU
1	D	308	TYR
1	D	309	ASP
1	D	328	HIS
1	D	381	LYS
1	E	8	ASN
1	E	12	VAL
1	E	148	CYS
1	E	160	LYS
1	E	191	LEU
1	E	308	TYR

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Mol	Chain	Res	Type
1	E	309	ASP
1	E	328	HIS
1	E	501	ASP
1	E	544	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	37	ASN
1	A	84	ASN
1	A	115	ASN
1	A	174	ASN
1	A	197	HIS
1	A	224	ASN
1	A	328	HIS
1	A	474	HIS
1	A	587	GLN
1	A	594	HIS
1	A	629	HIS
1	B	9	HIS
1	B	23	HIS
1	B	37	ASN
1	B	84	ASN
1	B	115	ASN
1	B	174	ASN
1	B	197	HIS
1	B	224	ASN
1	B	328	HIS
1	B	374	GLN
1	B	426	ASN
1	B	455	GLN
1	B	474	HIS
1	C	9	HIS
1	C	23	HIS
1	C	37	ASN
1	C	84	ASN
1	C	115	ASN
1	C	174	ASN
1	C	197	HIS
1	C	224	ASN
1	C	328	HIS

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Mol	Chain	Res	Type
1	C	374	GLN
1	C	426	ASN
1	C	455	GLN
1	C	474	HIS
1	C	478	ASN
1	C	594	HIS
1	C	629	HIS
1	C	699	GLN
1	D	9	HIS
1	D	23	HIS
1	D	37	ASN
1	D	84	ASN
1	D	115	ASN
1	D	174	ASN
1	D	197	HIS
1	D	224	ASN
1	D	328	HIS
1	D	374	GLN
1	D	426	ASN
1	D	455	GLN
1	D	474	HIS
1	D	594	HIS
1	E	9	HIS
1	E	23	HIS
1	E	37	ASN
1	E	84	ASN
1	E	115	ASN
1	E	174	ASN
1	E	197	HIS
1	E	224	ASN
1	E	328	HIS
1	E	374	GLN
1	E	426	ASN
1	E	455	GLN
1	E	474	HIS
1	E	521	HIS
1	E	587	GLN
1	E	629	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	B	367	1	23,24,25	1.74	3 (13%)	25,32,34	1.68	7 (28%)
1	LLP	D	367	1	23,24,25	1.85	5 (21%)	25,32,34	1.79	5 (20%)
1	LLP	E	367	1	23,24,25	1.80	5 (21%)	25,32,34	1.87	5 (20%)
1	LLP	C	367	1	23,24,25	1.83	5 (21%)	25,32,34	1.95	5 (20%)
1	LLP	A	367	1	23,24,25	1.82	4 (17%)	25,32,34	1.65	6 (24%)

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
1	LLP	B	367	1	-	3/16/17/19	0/1/1/1
1	LLP	D	367	1	-	3/16/17/19	0/1/1/1
1	LLP	E	367	1	-	3/16/17/19	0/1/1/1
1	LLP	C	367	1	-	3/16/17/19	0/1/1/1
1	LLP	A	367	1	-	3/16/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	LLP	O3-C3	-5.92	1.23	1.37
1	D	367	LLP	O3-C3	-5.68	1.23	1.37
1	E	367	LLP	O3-C3	-5.64	1.23	1.37
1	A	367	LLP	O3-C3	-5.48	1.24	1.37
1	C	367	LLP	O3-C3	-5.31	1.24	1.37
1	C	367	LLP	C4-C4'	3.44	1.53	1.46
1	A	367	LLP	C4-C4'	3.33	1.53	1.46
1	B	367	LLP	C4-C4'	3.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	367	LLP	C4-C4'	2.86	1.52	1.46
1	E	367	LLP	C4-C4'	2.81	1.52	1.46
1	D	367	LLP	C2-N1	2.78	1.39	1.33
1	C	367	LLP	C4'-NZ	2.77	1.36	1.27
1	D	367	LLP	C4'-NZ	2.63	1.36	1.27
1	A	367	LLP	C4'-NZ	2.61	1.36	1.27
1	B	367	LLP	C4'-NZ	2.54	1.35	1.27
1	E	367	LLP	C4'-NZ	2.46	1.35	1.27
1	C	367	LLP	C6-N1	2.42	1.39	1.34
1	A	367	LLP	C2-N1	2.42	1.38	1.33
1	E	367	LLP	C2-N1	2.35	1.38	1.33
1	D	367	LLP	C6-N1	2.31	1.39	1.34
1	C	367	LLP	C2-N1	2.14	1.37	1.33
1	E	367	LLP	C4-C5	-2.03	1.39	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	367	LLP	OP4-C5'-C5	5.38	119.61	109.35
1	E	367	LLP	OP4-C5'-C5	4.59	118.11	109.35
1	C	367	LLP	OP4-P-OP1	-4.23	94.61	106.47
1	A	367	LLP	OP4-C5'-C5	4.20	117.35	109.35
1	D	367	LLP	OP4-C5'-C5	3.93	116.84	109.35
1	E	367	LLP	OP4-P-OP1	-3.76	95.92	106.47
1	D	367	LLP	OP4-P-OP1	-3.60	96.38	106.47
1	B	367	LLP	OP4-C5'-C5	3.38	115.79	109.35
1	E	367	LLP	C4-C4'-NZ	-3.29	109.21	124.31
1	D	367	LLP	CE-NZ-C4'	-3.17	109.16	118.90
1	B	367	LLP	C4-C4'-NZ	-3.15	109.84	124.31
1	C	367	LLP	C4-C4'-NZ	-3.14	109.89	124.31
1	B	367	LLP	OP4-P-OP1	-3.11	97.76	106.47
1	A	367	LLP	OP4-P-OP1	-3.09	97.79	106.47
1	A	367	LLP	C4-C4'-NZ	-3.00	110.52	124.31
1	E	367	LLP	OP3-P-OP1	2.51	120.50	110.68
1	B	367	LLP	CE-NZ-C4'	-2.50	111.24	118.90
1	D	367	LLP	C4-C4'-NZ	-2.38	113.37	124.31
1	B	367	LLP	OP2-P-OP4	-2.37	100.42	106.73
1	C	367	LLP	CE-NZ-C4'	-2.29	111.85	118.90
1	A	367	LLP	CE-NZ-C4'	-2.28	111.89	118.90
1	C	367	LLP	OP3-P-OP2	2.25	116.23	107.64
1	B	367	LLP	C5-C6-N1	-2.25	120.08	123.82
1	A	367	LLP	OP3-P-OP1	2.20	119.31	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	367	LLP	C3-C2-N1	-2.13	118.02	120.77
1	B	367	LLP	OP3-P-OP2	2.12	115.75	107.64
1	A	367	LLP	C5-C6-N1	-2.03	120.43	123.82
1	D	367	LLP	C5-C6-N1	-2.02	120.45	123.82

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	367	LLP	C4-C4'-NZ-CE
1	B	367	LLP	C4-C4'-NZ-CE
1	D	367	LLP	C4-C4'-NZ-CE
1	E	367	LLP	C4-C4'-NZ-CE
1	C	367	LLP	C4-C4'-NZ-CE
1	A	367	LLP	CD-CE-NZ-C4'
1	E	367	LLP	CD-CE-NZ-C4'
1	B	367	LLP	CD-CE-NZ-C4'
1	D	367	LLP	CD-CE-NZ-C4'
1	A	367	LLP	C3-C4-C4'-NZ
1	B	367	LLP	C3-C4-C4'-NZ
1	C	367	LLP	C3-C4-C4'-NZ
1	E	367	LLP	C3-C4-C4'-NZ
1	C	367	LLP	CD-CE-NZ-C4'
1	D	367	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	716[B]	-	30,38,38	0.98	1 (3%)	42,61,61	1.54	8 (19%)
2	G4P	C	716[B]	-	30,38,38	1.00	1 (3%)	42,61,61	1.42	6 (14%)
3	P6G	A	717	-	18,18,18	0.56	0	17,17,17	0.52	0
4	GOL	E	718	-	5,5,5	0.39	0	5,5,5	0.75	0
3	P6G	D	717	-	15,15,18	0.46	0	14,14,17	0.33	0
2	G4P	E	716	-	30,38,38	0.98	2 (6%)	42,61,61	1.34	6 (14%)
3	P6G	B	717	-	15,15,18	0.51	0	14,14,17	0.47	0
2	G4P	A	716[B]	-	30,38,38	1.11	1 (3%)	42,61,61	1.34	6 (14%)
3	P6G	C	717	-	15,15,18	0.43	0	14,14,17	0.39	0
2	G4P	B	716[B]	-	30,38,38	1.07	1 (3%)	42,61,61	1.51	6 (14%)
4	GOL	A	718	-	5,5,5	0.34	0	5,5,5	0.55	0
2	G4P	D	716[A]	-	30,38,38	0.98	1 (3%)	42,61,61	1.36	5 (11%)
2	G4P	C	716[A]	-	30,38,38	1.01	1 (3%)	42,61,61	1.37	6 (14%)
4	GOL	D	718	-	5,5,5	0.50	0	5,5,5	0.63	0
4	GOL	C	718	-	5,5,5	0.28	0	5,5,5	0.26	0
2	G4P	A	716[A]	-	30,38,38	1.12	1 (3%)	42,61,61	1.30	5 (11%)
4	GOL	B	718	-	5,5,5	0.38	0	5,5,5	0.31	0
3	P6G	E	717	-	15,15,18	0.50	0	14,14,17	0.37	0
2	G4P	B	716[A]	-	30,38,38	1.07	1 (3%)	42,61,61	1.38	5 (11%)

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	716[B]	-	-	2/23/43/43	0/3/3/3
2	G4P	C	716[B]	-	-	3/23/43/43	0/3/3/3
3	P6G	A	717	-	-	9/16/16/16	-
4	GOL	E	718	-	-	2/4/4/4	-
3	P6G	D	717	-	-	8/13/13/16	-
2	G4P	E	716	-	-	3/23/43/43	0/3/3/3
3	P6G	B	717	-	-	11/13/13/16	-
2	G4P	A	716[B]	-	-	3/23/43/43	0/3/3/3
3	P6G	C	717	-	-	8/13/13/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G4P	B	716[B]	-	-	2/23/43/43	0/3/3/3
4	GOL	A	718	-	-	2/4/4/4	-
2	G4P	D	716[A]	-	-	3/23/43/43	0/3/3/3
2	G4P	C	716[A]	-	-	3/23/43/43	0/3/3/3
4	GOL	D	718	-	-	0/4/4/4	-
4	GOL	C	718	-	-	1/4/4/4	-
2	G4P	A	716[A]	-	-	5/23/43/43	0/3/3/3
4	GOL	B	718	-	-	2/4/4/4	-
3	P6G	E	717	-	-	8/13/13/16	-
2	G4P	B	716[A]	-	-	4/23/43/43	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	716[A]	G4P	C5-C6	-4.39	1.38	1.47
2	A	716[B]	G4P	C5-C6	-4.36	1.38	1.47
2	B	716[B]	G4P	C5-C6	-3.92	1.39	1.47
2	B	716[A]	G4P	C5-C6	-3.92	1.39	1.47
2	D	716[A]	G4P	C5-C6	-3.83	1.39	1.47
2	E	716	G4P	C5-C6	-3.80	1.39	1.47
2	D	716[B]	G4P	C5-C6	-3.78	1.39	1.47
2	C	716[B]	G4P	C5-C6	-3.64	1.40	1.47
2	C	716[A]	G4P	C5-C6	-3.63	1.40	1.47
2	E	716	G4P	O4'-C1'	2.06	1.44	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	716[B]	G4P	PC-O3C-PD	-3.53	120.70	132.83
2	E	716	G4P	C5-C6-N1	3.51	120.14	113.95
2	B	716[B]	G4P	PC-O3C-PD	-3.48	120.89	132.83
2	A	716[A]	G4P	C5-C6-N1	3.27	119.73	113.95
2	A	716[B]	G4P	C5-C6-N1	3.27	119.73	113.95
2	D	716[A]	G4P	C5-C6-N1	3.16	119.53	113.95
2	D	716[B]	G4P	C5-C6-N1	3.15	119.51	113.95
2	C	716[B]	G4P	C3'-C2'-C1'	2.94	106.41	99.89
2	C	716[B]	G4P	C5-C6-N1	2.90	119.07	113.95
2	D	716[B]	G4P	C2-N1-C6	-2.89	119.78	125.10
2	C	716[A]	G4P	C5-C6-N1	2.89	119.05	113.95
2	D	716[A]	G4P	C2-N1-C6	-2.88	119.80	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	716[A]	G4P	C3'-C2'-C1'	2.86	106.23	99.89
2	B	716[B]	G4P	C5-C6-N1	2.85	118.98	113.95
2	B	716[B]	G4P	C2-N1-C6	-2.84	119.87	125.10
2	C	716[B]	G4P	PC-O3C-PD	-2.83	123.12	132.83
2	B	716[A]	G4P	C2-N1-C6	-2.82	119.91	125.10
2	B	716[A]	G4P	C5-C6-N1	2.80	118.89	113.95
2	D	716[A]	G4P	C3'-C2'-C1'	2.74	105.95	99.89
2	D	716[B]	G4P	C3'-C2'-C1'	2.72	105.91	99.89
2	E	716	G4P	C2-N1-C6	-2.72	120.09	125.10
2	B	716[B]	G4P	C8-N7-C5	2.70	108.13	102.99
2	C	716[B]	G4P	C2-N1-C6	-2.69	120.14	125.10
2	B	716[A]	G4P	C8-N7-C5	2.68	108.09	102.99
2	A	716[B]	G4P	C2-N1-C6	-2.64	120.23	125.10
2	C	716[A]	G4P	C2-N1-C6	-2.64	120.24	125.10
2	B	716[B]	G4P	C3'-C2'-C1'	2.64	105.73	99.89
2	C	716[A]	G4P	C8-N7-C5	2.62	107.98	102.99
2	A	716[A]	G4P	C2-N1-C6	-2.60	120.30	125.10
2	D	716[B]	G4P	O3C-PC-O3'	-2.60	97.24	102.48
2	C	716[B]	G4P	C8-N7-C5	2.60	107.94	102.99
2	B	716[A]	G4P	C3'-C2'-C1'	2.53	105.50	99.89
2	D	716[A]	G4P	C8-N7-C5	2.53	107.81	102.99
2	D	716[B]	G4P	C8-N7-C5	2.52	107.79	102.99
2	A	716[A]	G4P	C3'-C2'-C1'	2.50	105.42	99.89
2	B	716[B]	G4P	O5'-C5'-C4'	-2.43	100.61	108.99
2	A	716[B]	G4P	C3'-C2'-C1'	2.42	105.24	99.89
2	C	716[B]	G4P	O5'-C5'-C4'	-2.40	100.73	108.99
2	E	716	G4P	C3'-C2'-C1'	2.38	105.17	99.89
2	A	716[B]	G4P	PC-O3C-PD	-2.27	125.03	132.83
2	C	716[A]	G4P	O5'-C5'-C4'	-2.26	101.22	108.99
2	E	716	G4P	C8-N7-C5	2.20	107.18	102.99
2	B	716[A]	G4P	O5'-C5'-C4'	-2.19	101.46	108.99
2	A	716[B]	G4P	C8-N7-C5	2.18	107.13	102.99
2	D	716[B]	G4P	O5'-C5'-C4'	-2.17	101.52	108.99
2	A	716[A]	G4P	C8-N7-C5	2.17	107.12	102.99
2	E	716	G4P	O2A-PA-O1A	2.14	122.82	112.24
2	A	716[A]	G4P	O6-C6-C5	-2.07	120.32	124.37
2	A	716[B]	G4P	O6-C6-C5	-2.07	120.33	124.37
2	C	716[A]	G4P	O3C-PC-O3'	2.07	106.65	102.48
2	E	716	G4P	O6-C6-C5	-2.05	120.36	124.37
2	D	716[A]	G4P	O6-C6-C5	-2.03	120.41	124.37
2	D	716[B]	G4P	O6-C6-C5	-2.03	120.41	124.37

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	716[A]	G4P	PD-O3C-PC-O3'
2	A	716[B]	G4P	C3'-O3'-PC-O3C
2	B	716[A]	G4P	PD-O3C-PC-O3'
2	B	716[B]	G4P	C3'-O3'-PC-O3C
2	C	716[B]	G4P	C3'-O3'-PC-O3C
2	D	716[B]	G4P	C3'-O3'-PC-O1C
2	D	716[B]	G4P	C3'-O3'-PC-O3C
3	C	717	P6G	O10-C11-C12-O13
3	A	717	P6G	O16-C17-C18-O19
3	D	717	P6G	O7-C8-C9-O10
2	A	716[A]	G4P	C3'-O3'-PC-O3C
2	B	716[A]	G4P	C3'-O3'-PC-O3C
2	C	716[A]	G4P	C3'-O3'-PC-O3C
2	E	716	G4P	C3'-O3'-PC-O3C
3	E	717	P6G	O4-C5-C6-O7
3	B	717	P6G	C8-C9-O10-C11
3	B	717	P6G	O13-C14-C15-O16
3	C	717	P6G	O13-C14-C15-O16
3	D	717	P6G	O1-C2-C3-O4
3	E	717	P6G	O1-C2-C3-O4
3	A	717	P6G	O10-C11-C12-O13
3	B	717	P6G	O7-C8-C9-O10
3	D	717	P6G	O13-C14-C15-O16
2	D	716[A]	G4P	C3'-O3'-PC-O3C
3	E	717	P6G	O13-C14-C15-O16
3	B	717	P6G	O4-C5-C6-O7
2	A	716[A]	G4P	C3'-O3'-PC-O2C
2	A	716[B]	G4P	C3'-O3'-PC-O1C
2	B	716[B]	G4P	C3'-O3'-PC-O1C
2	C	716[B]	G4P	C3'-O3'-PC-O1C
2	E	716	G4P	C3'-O3'-PC-O2C
4	A	718	GOL	O2-C2-C3-O3
4	E	718	GOL	O2-C2-C3-O3
2	C	716[A]	G4P	PD-O3C-PC-O3'
2	D	716[A]	G4P	PD-O3C-PC-O3'
2	E	716	G4P	PD-O3C-PC-O3'
3	C	717	P6G	C15-C14-O13-C12
3	E	717	P6G	C12-C11-O10-C9
3	D	717	P6G	C12-C11-O10-C9
3	A	717	P6G	C6-C5-O4-C3
3	A	717	P6G	C9-C8-O7-C6
3	A	717	P6G	C11-C12-O13-C14

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Mol	Chain	Res	Type	Atoms
3	A	717	P6G	C14-C15-O16-C17
3	E	717	P6G	C8-C9-O10-C11
3	B	717	P6G	C11-C12-O13-C14
3	E	717	P6G	C9-C8-O7-C6
3	B	717	P6G	C6-C5-O4-C3
4	B	718	GOL	O2-C2-C3-O3
4	C	718	GOL	O1-C1-C2-O2
3	D	717	P6G	C15-C14-O13-C12
3	A	717	P6G	O13-C14-C15-O16
3	C	717	P6G	C9-C8-O7-C6
3	B	717	P6G	C2-C3-O4-C5
3	C	717	P6G	C5-C6-O7-C8
3	D	717	P6G	C5-C6-O7-C8
3	D	717	P6G	C8-C9-O10-C11
2	A	716[B]	G4P	PD-O3C-PC-O1C
3	E	717	P6G	C15-C14-O13-C12
3	C	717	P6G	O1-C2-C3-O4
3	B	717	P6G	C5-C6-O7-C8
3	B	717	P6G	C12-C11-O10-C9
3	C	717	P6G	C6-C5-O4-C3
3	A	717	P6G	C5-C6-O7-C8
2	B	716[A]	G4P	C3'-O3'-PC-O2C
2	C	716[A]	G4P	C3'-O3'-PC-O2C
2	D	716[A]	G4P	C3'-O3'-PC-O2C
2	C	716[B]	G4P	PD-O3C-PC-O1C
3	E	717	P6G	O7-C8-C9-O10
4	A	718	GOL	C1-C2-C3-O3
4	B	718	GOL	C1-C2-C3-O3
3	B	717	P6G	O10-C11-C12-O13
3	C	717	P6G	C12-C11-O10-C9
2	A	716[A]	G4P	PD-O3C-PC-O1C
2	A	716[A]	G4P	PD-O3C-PC-O2C
2	B	716[A]	G4P	PD-O3C-PC-O1C
4	E	718	GOL	C1-C2-C3-O3
3	D	717	P6G	C11-C12-O13-C14
3	B	717	P6G	C9-C8-O7-C6
3	A	717	P6G	C18-C17-O16-C15

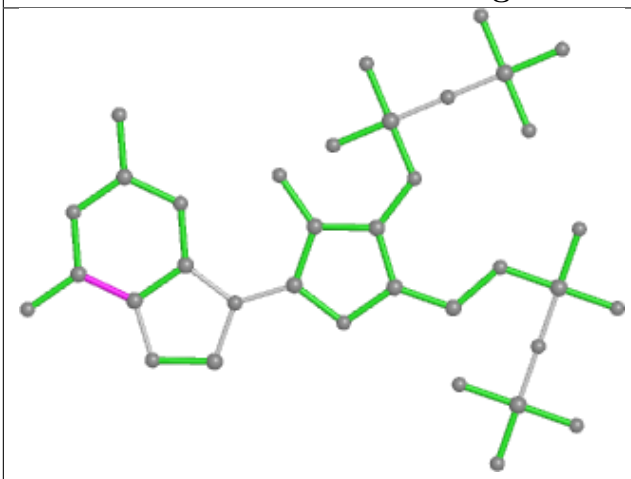
There are no ring outliers.

15 monomers are involved in 32 short contacts:

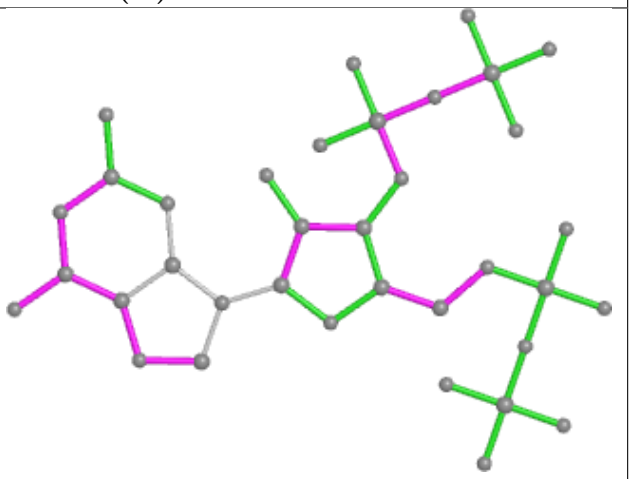
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	716[B]	G4P	3	0
2	C	716[B]	G4P	2	0
3	A	717	P6G	1	0
4	E	718	GOL	2	0
3	D	717	P6G	1	0
2	E	716	G4P	2	0
3	B	717	P6G	1	0
2	A	716[B]	G4P	3	0
3	C	717	P6G	1	0
2	B	716[B]	G4P	5	0
2	D	716[A]	G4P	1	0
2	C	716[A]	G4P	1	0
4	C	718	GOL	1	0
2	A	716[A]	G4P	3	0
2	B	716[A]	G4P	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

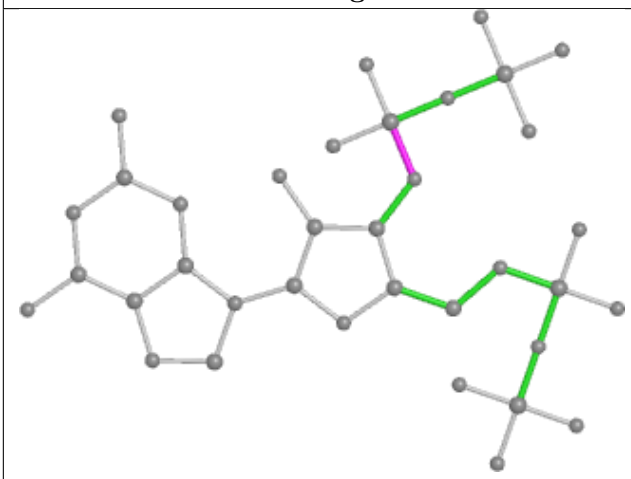
Ligand G4P D 716 (B)



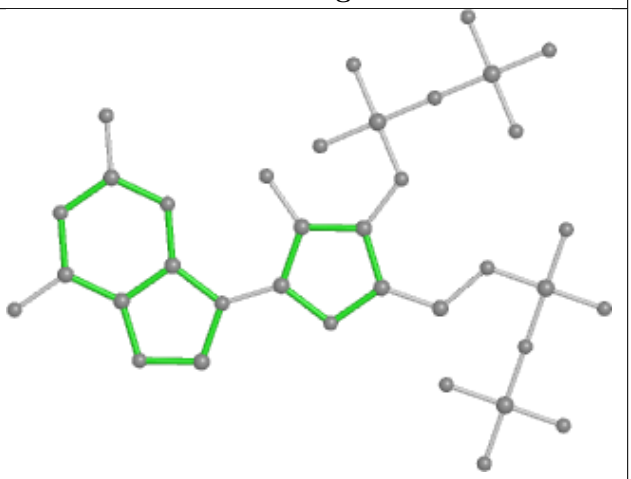
Bond lengths



Bond angles

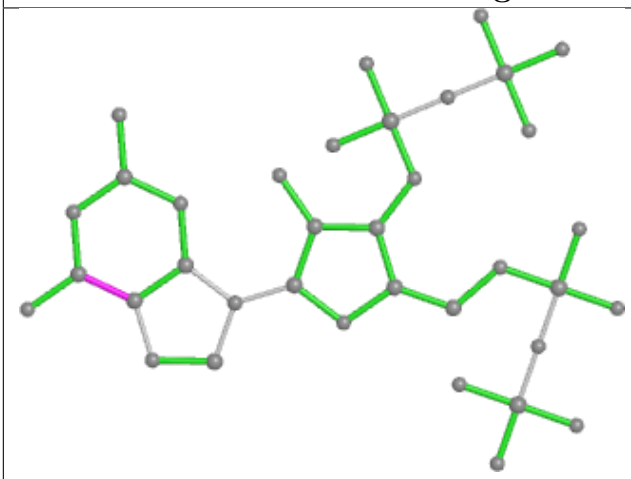


Torsions



Rings

Ligand G4P C 716 (B)



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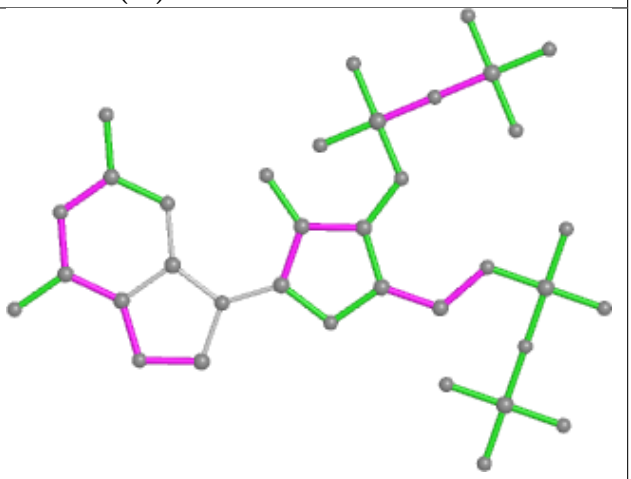
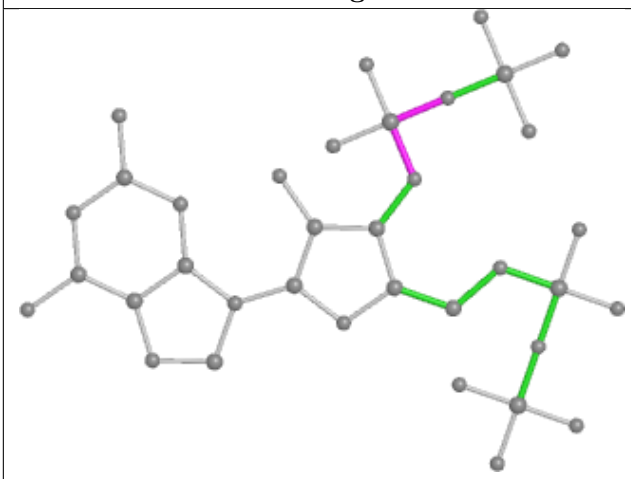


Bond angles



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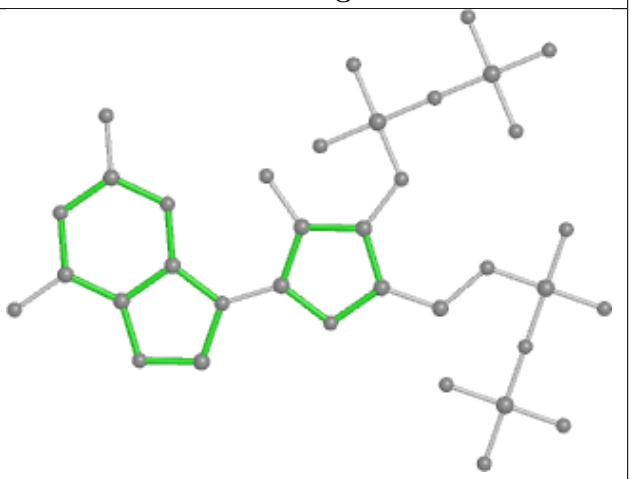
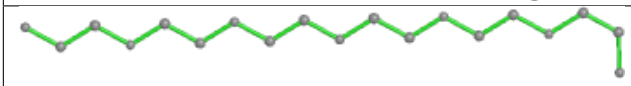


Rings

Ligand P6G A 717



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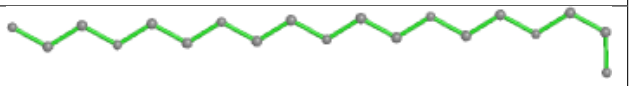
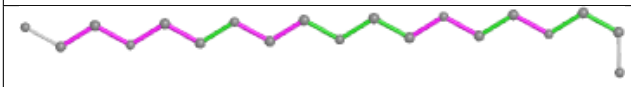


Bond angles



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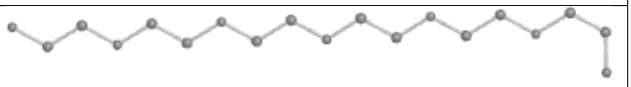
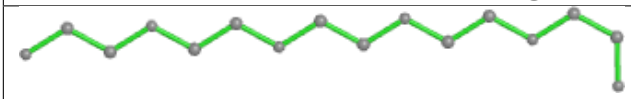
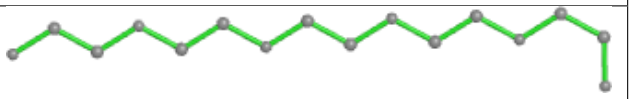


Rings

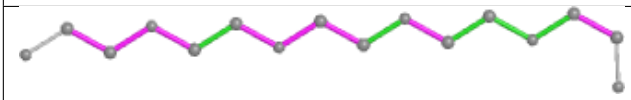
Ligand P6G D 717



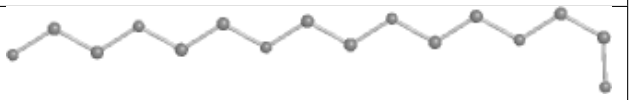
Bond lengths



Bond angles

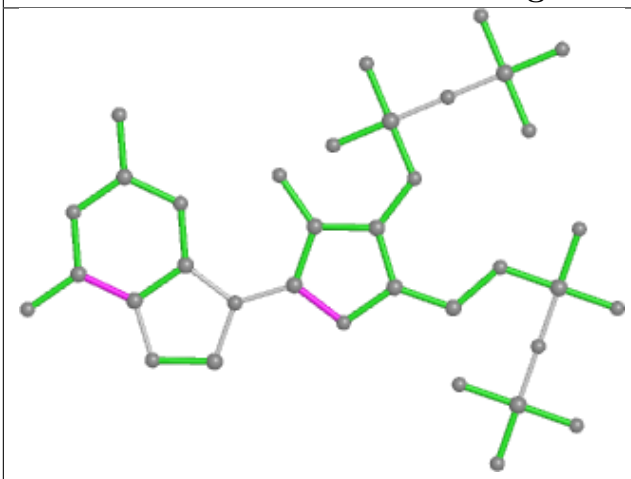


Torsions



Rings

Ligand G4P E 716



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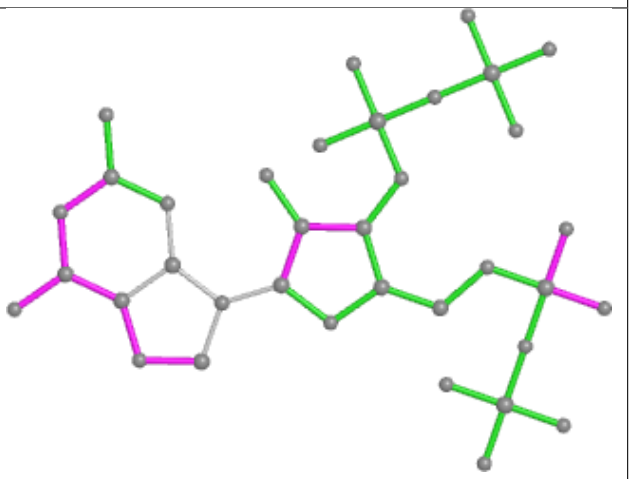

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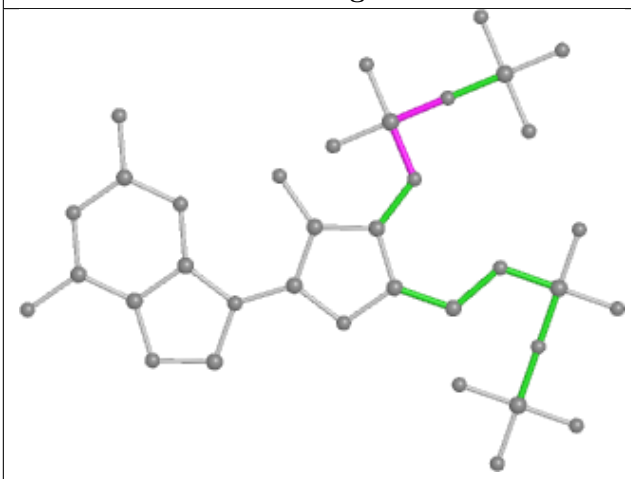

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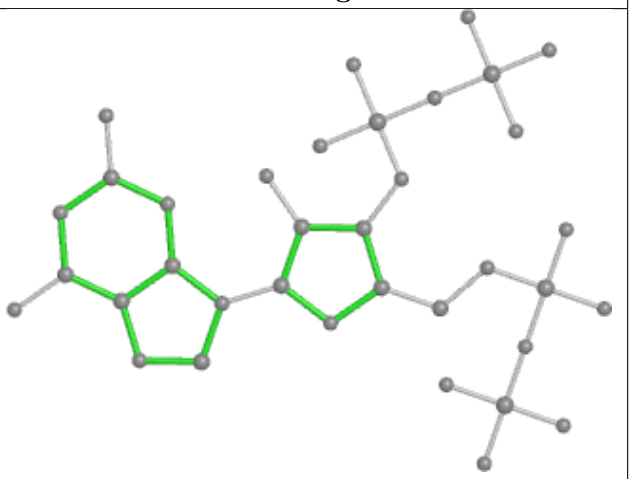
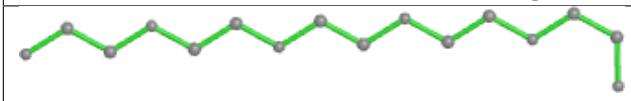


Rings

Ligand P6G B 717



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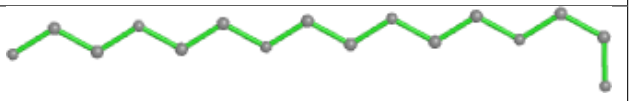
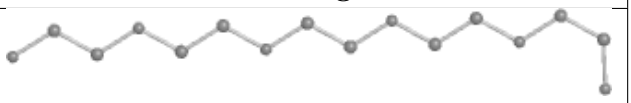


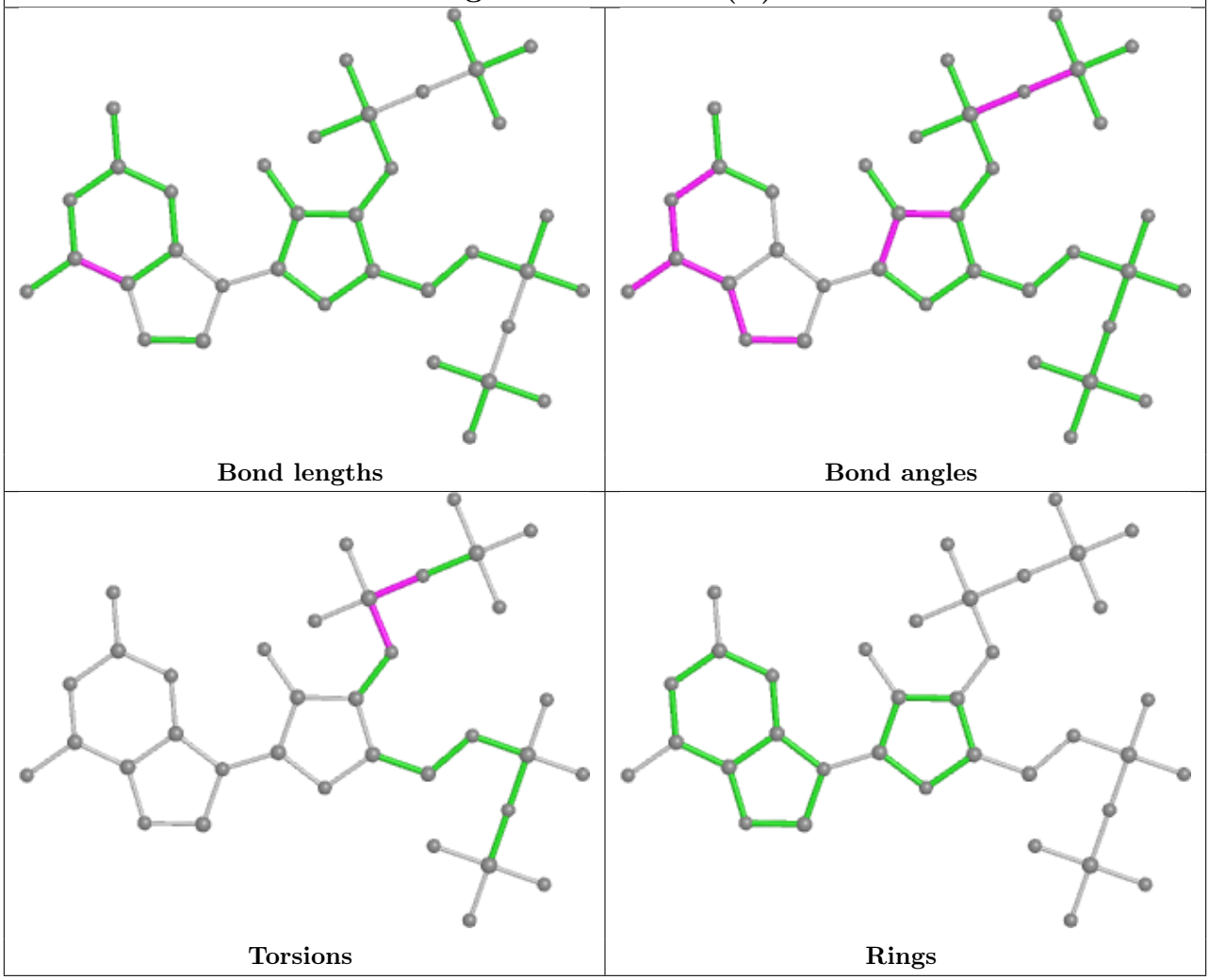
Bond angles

Torsions

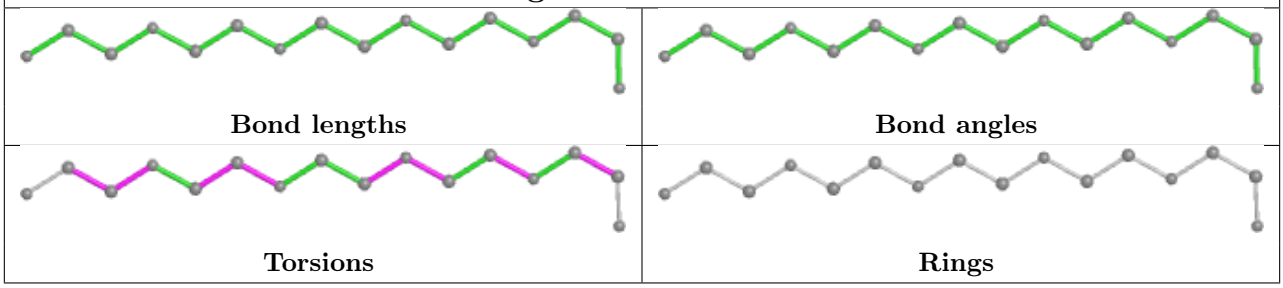


Rings

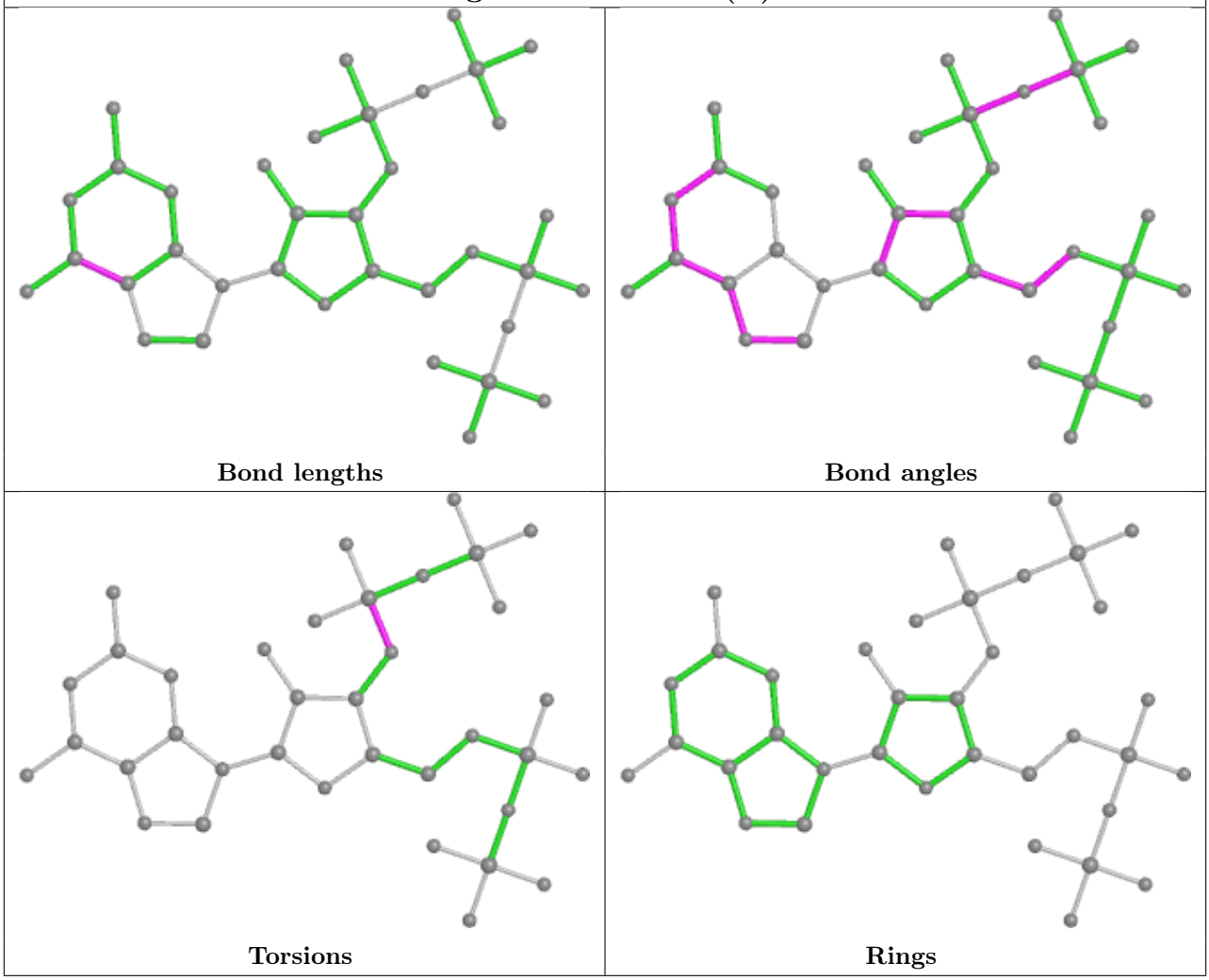
Ligand G4P A 716 (B)



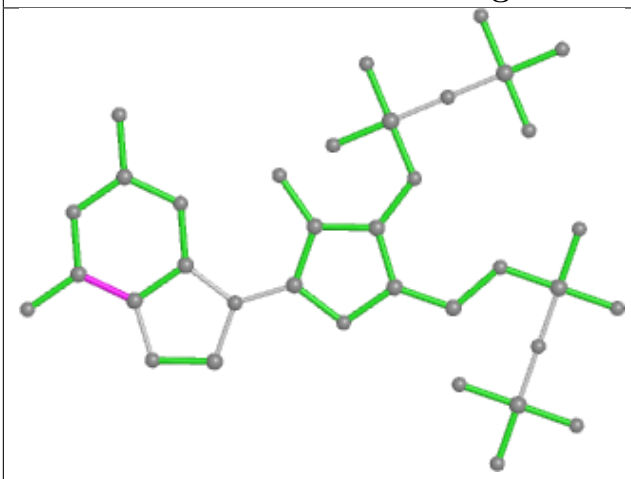
Ligand P6G C 717



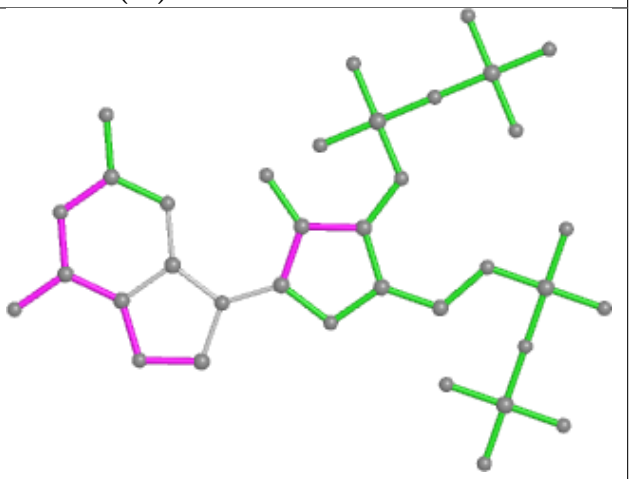
Ligand G4P B 716 (B)



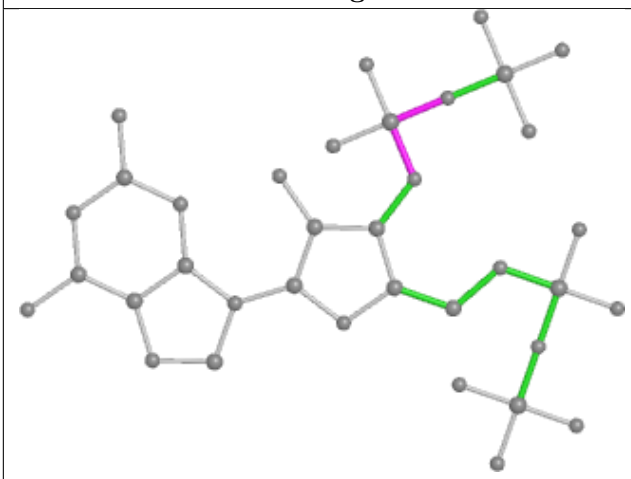
Ligand G4P D 716 (A)



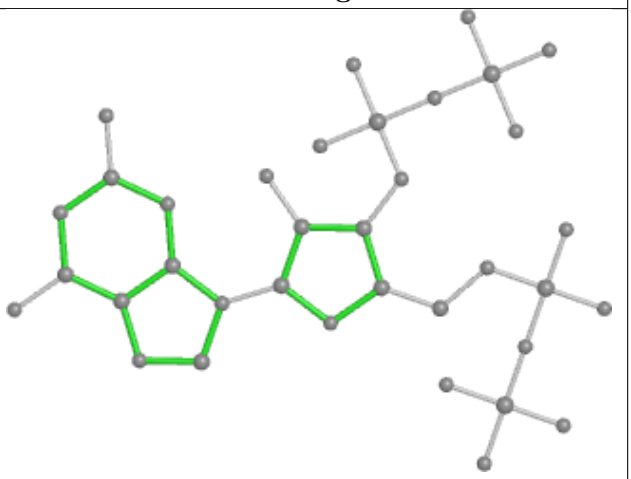
Bond lengths



Bond angles

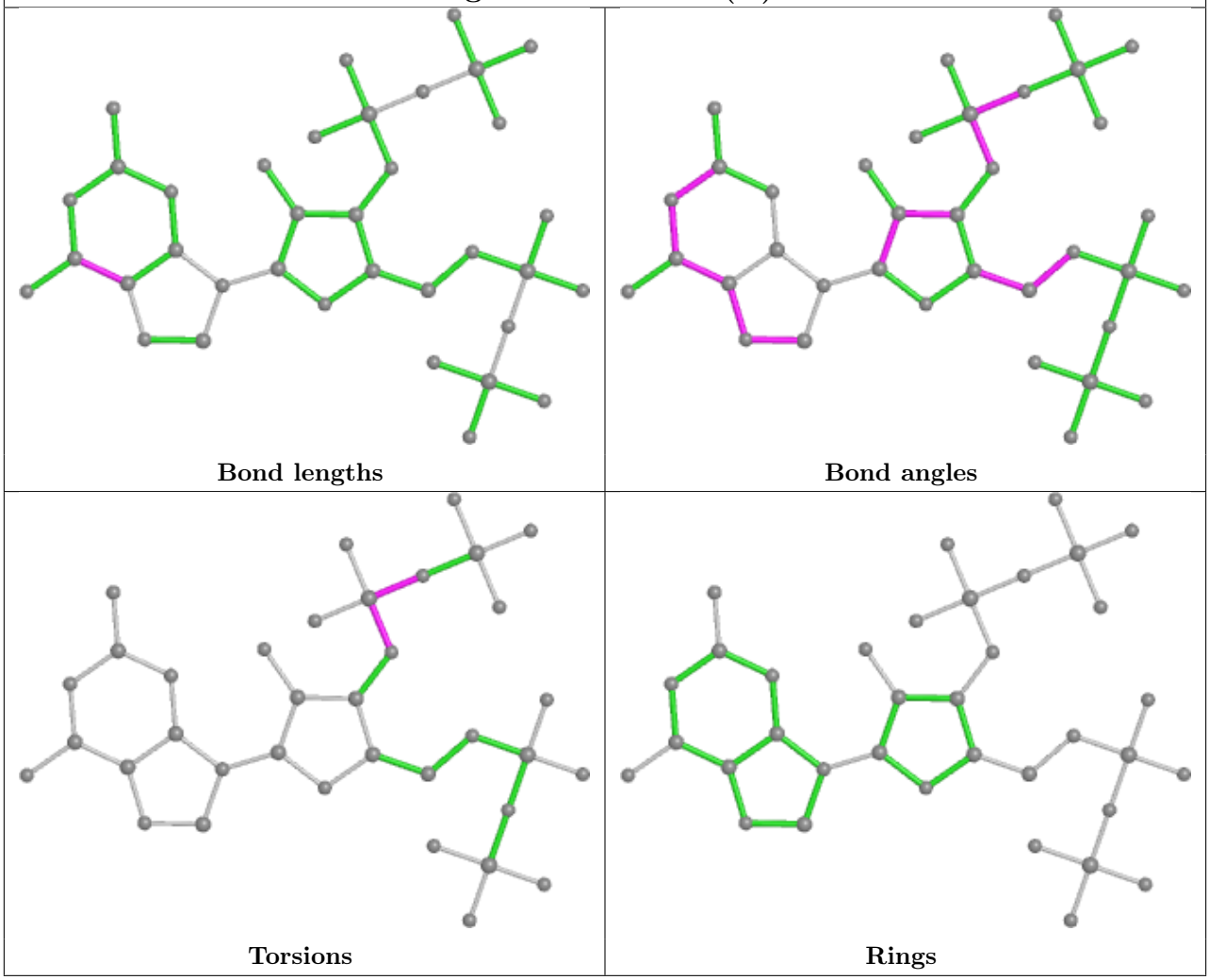


Torsions

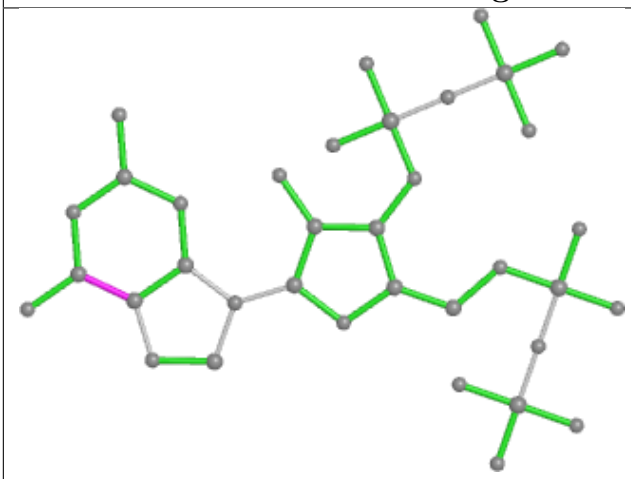


Rings

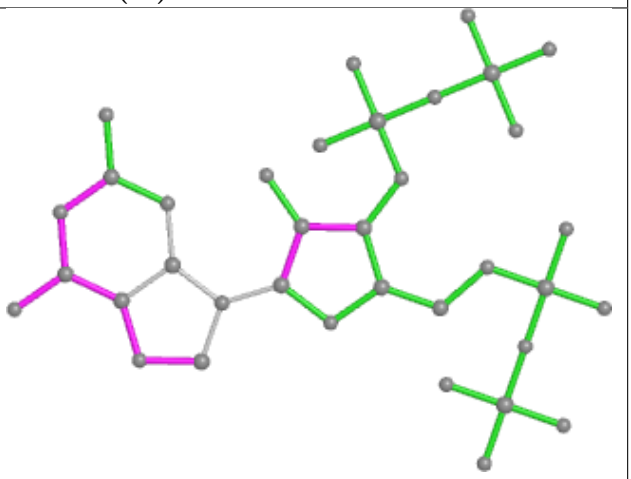
Ligand G4P C 716 (A)



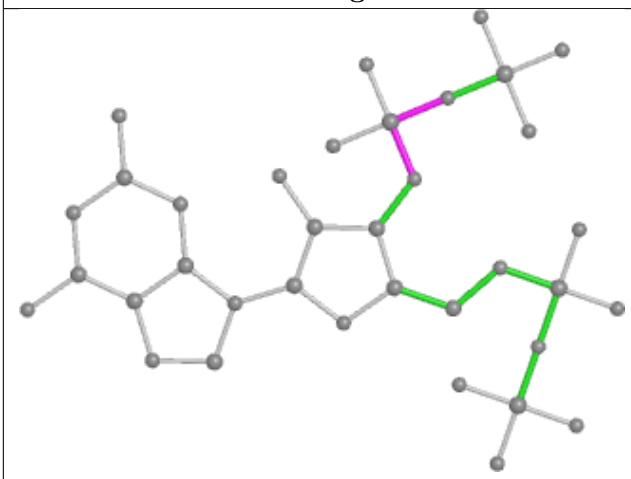
Ligand G4P A 716 (A)



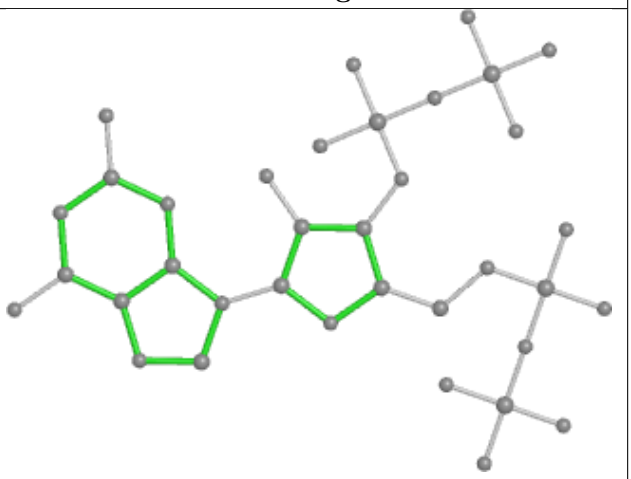
Bond lengths



Bond angles

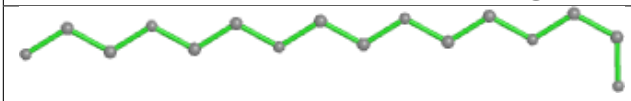


Torsions

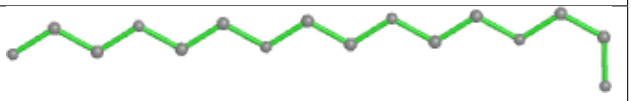


Rings

Ligand P6G E 717

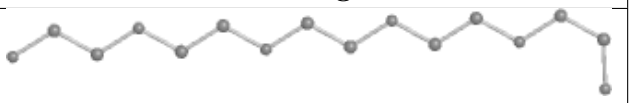


Bond lengths



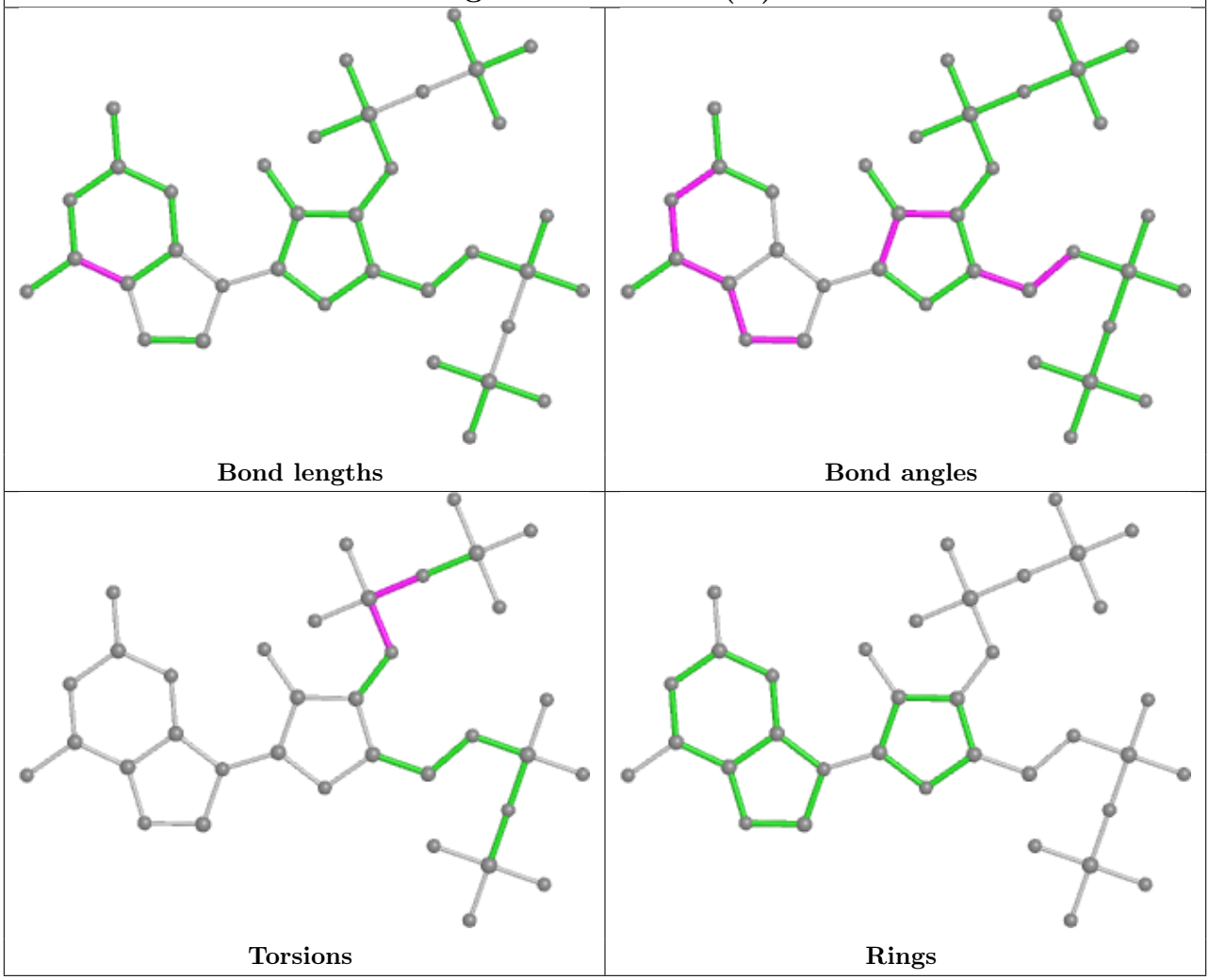
Bond angles

Torsions



Rings

Ligand G4P B 716 (A)



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	710/715 (99%)	-0.62	2 (0%)	94	93	16, 26, 42, 56	0
1	B	710/715 (99%)	-0.48	8 (1%)	80	79	16, 32, 49, 60	0
1	C	710/715 (99%)	-0.71	3 (0%)	92	92	15, 23, 37, 54	0
1	D	710/715 (99%)	-0.70	2 (0%)	94	93	15, 22, 37, 57	0
1	E	710/715 (99%)	-0.66	3 (0%)	92	92	15, 23, 37, 60	0
All	All	3550/3575 (99%)	-0.63	18 (0%)	91	90	15, 25, 42, 60	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	700	ALA	3.2
1	E	500	LYS	2.8
1	B	355	GLU	2.7
1	D	500	LYS	2.7
1	A	700	ALA	2.6
1	B	458	HIS	2.5
1	B	697	TYR	2.3
1	E	700	ALA	2.3
1	C	458	HIS	2.2
1	B	636	TYR	2.2
1	B	703	ARG	2.2
1	A	355	GLU	2.1
1	B	290	LYS	2.1
1	B	579	GLU	2.1
1	C	500	LYS	2.1
1	D	458	HIS	2.1
1	E	458	HIS	2.0
1	C	700	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	LLP	A	367	24/25	0.98	0.12	20,23,27,30	0
1	LLP	B	367	24/25	0.98	0.10	25,30,33,35	0
1	LLP	C	367	24/25	0.98	0.13	19,22,26,28	0
1	LLP	D	367	24/25	0.98	0.13	17,20,24,25	0
1	LLP	E	367	24/25	0.98	0.12	18,21,25,27	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	C	718	6/6	0.63	0.20	58,59,60,62	0
4	GOL	E	718	6/6	0.74	0.20	56,57,58,61	0
4	GOL	A	718	6/6	0.75	0.20	54,55,55,59	0
4	GOL	B	718	6/6	0.76	0.23	57,61,62,63	0
4	GOL	D	718	6/6	0.80	0.18	62,65,65,65	0
3	P6G	B	717	16/19	0.86	0.16	53,55,58,59	0
3	P6G	A	717	19/19	0.86	0.16	53,56,59,59	0
3	P6G	D	717	16/19	0.89	0.17	50,57,62,63	0
3	P6G	E	717	16/19	0.90	0.16	49,52,57,57	0
2	G4P	B	716[A]	36/36	0.91	0.15	37,46,61,61	36
2	G4P	B	716[B]	36/36	0.91	0.15	37,46,62,62	36
3	P6G	C	717	16/19	0.91	0.15	50,52,57,58	0
2	G4P	D	716[A]	36/36	0.91	0.14	37,45,51,52	36
2	G4P	D	716[B]	36/36	0.91	0.14	38,45,55,56	36
2	G4P	A	716[A]	36/36	0.92	0.14	30,40,48,49	36
2	G4P	A	716[B]	36/36	0.92	0.14	30,40,51,52	36
2	G4P	C	716[A]	36/36	0.93	0.13	37,41,48,49	36

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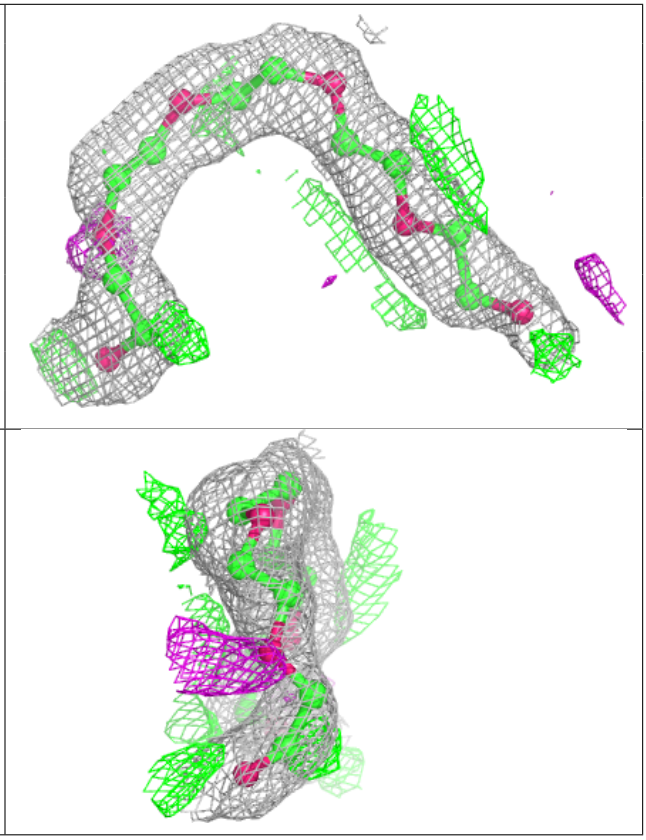
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G4P	C	716[B]	36/36	0.93	0.13	37,41,53,54	36
2	G4P	E	716	36/36	0.97	0.10	26,33,41,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

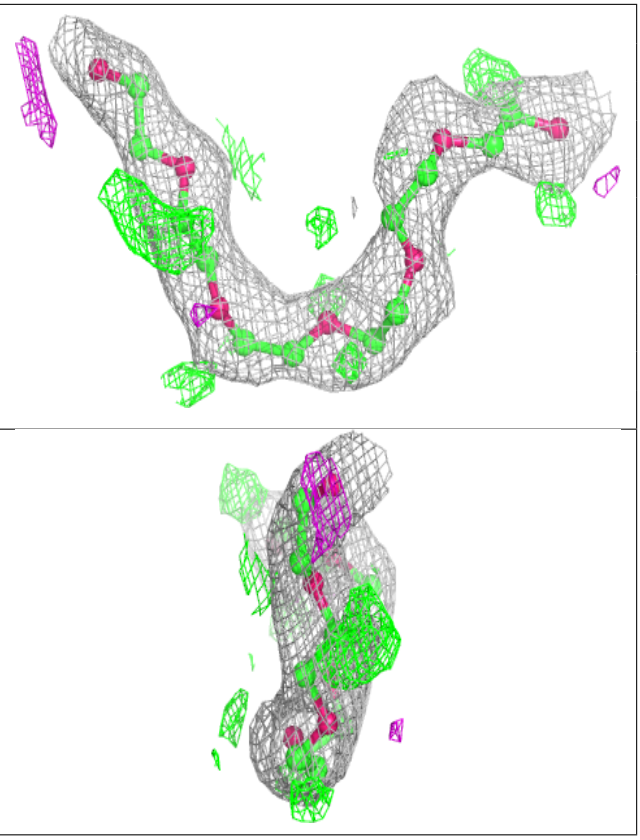
Electron density around P6G B 717:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



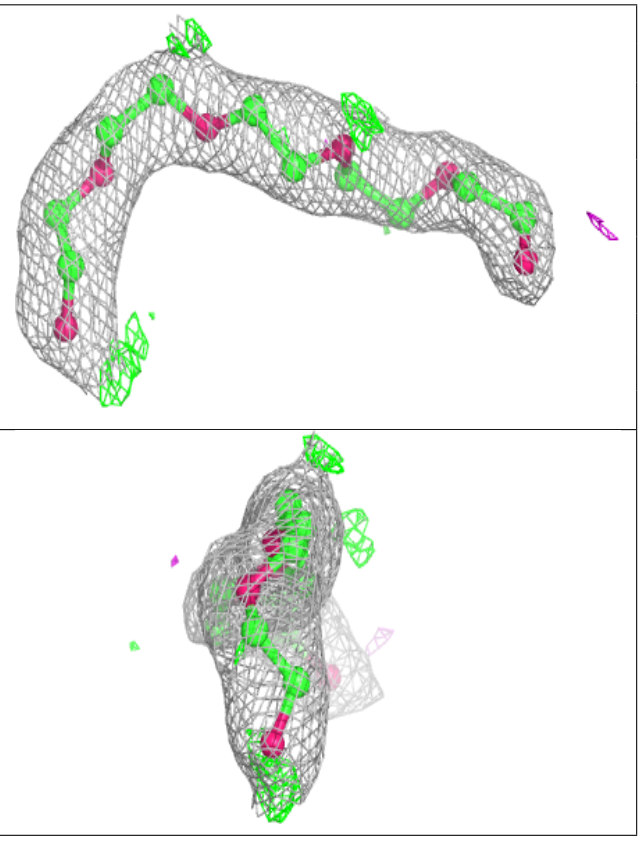
Electron density around P6G A 717:

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



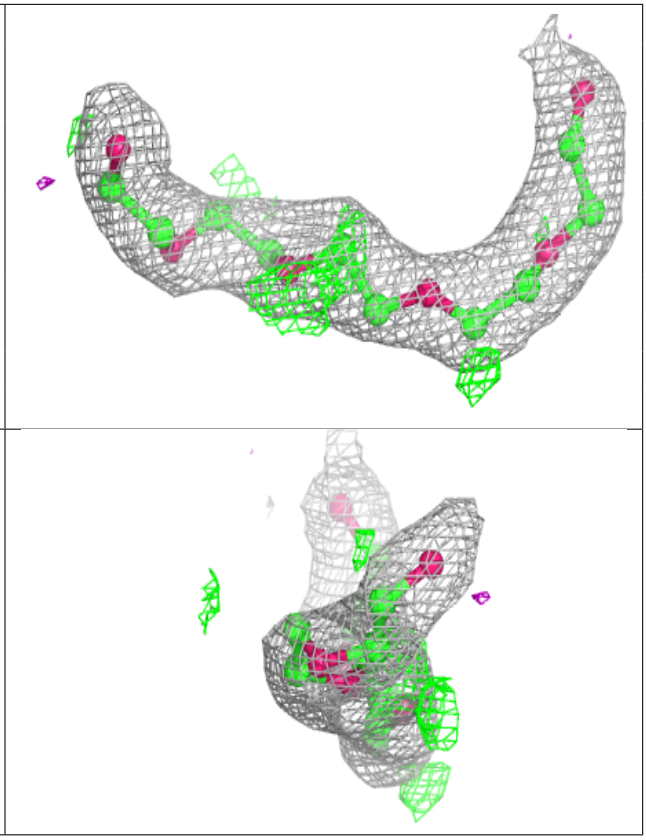
Electron density around P6G D 717:

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



Electron density around P6G E 717:

$2mF_o$-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 B 716 (A):

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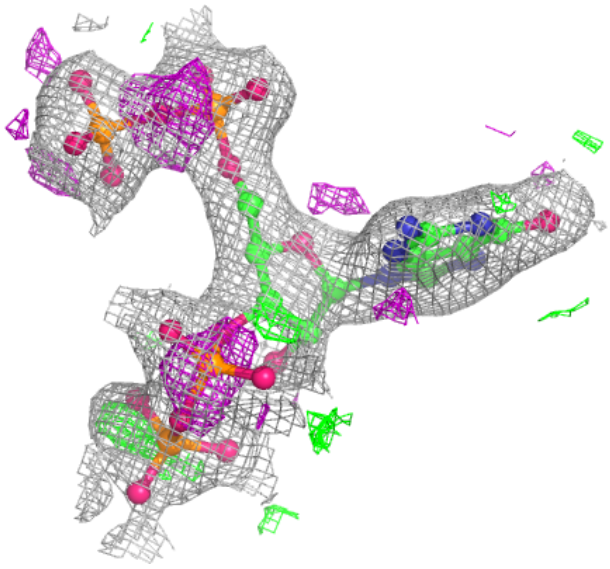
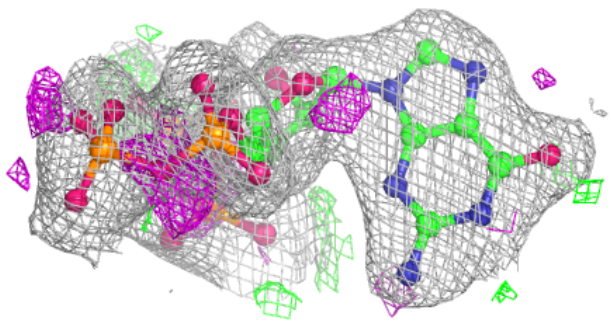
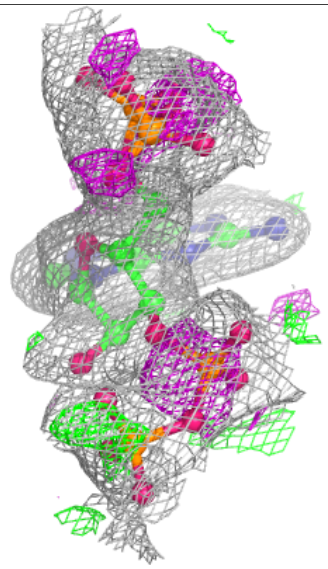
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

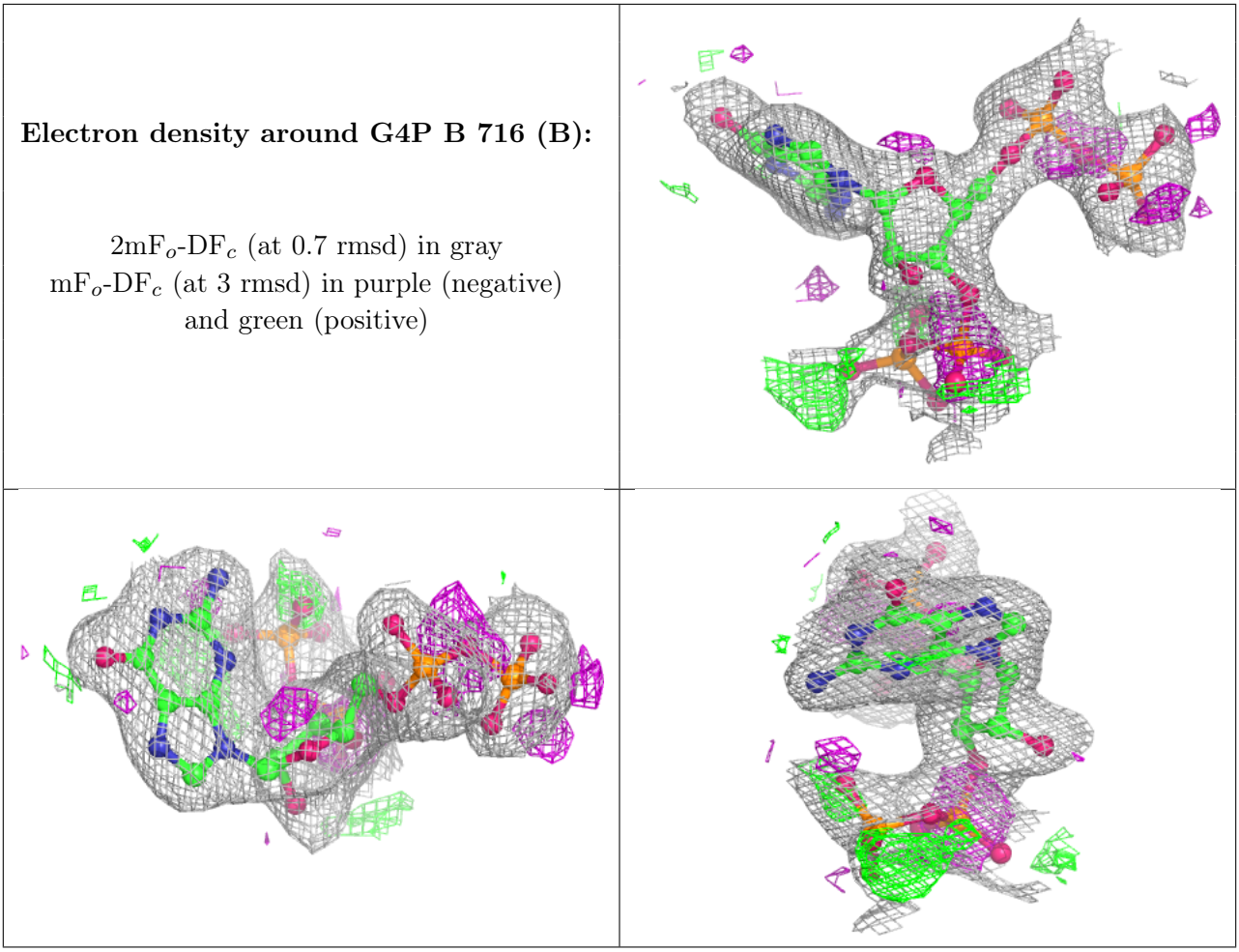






Electron density around G4P B 716 (B):

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



Electron density around P6G C 717:

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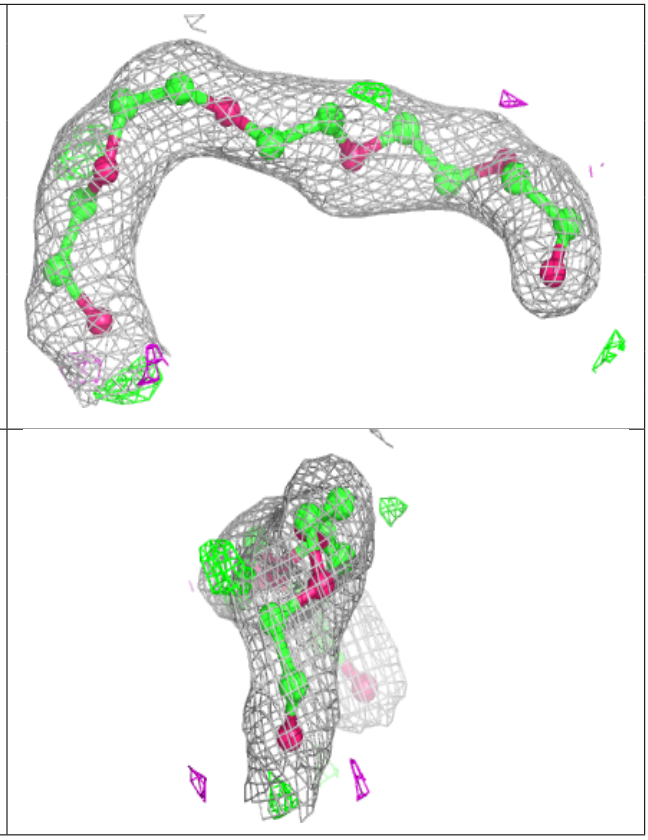
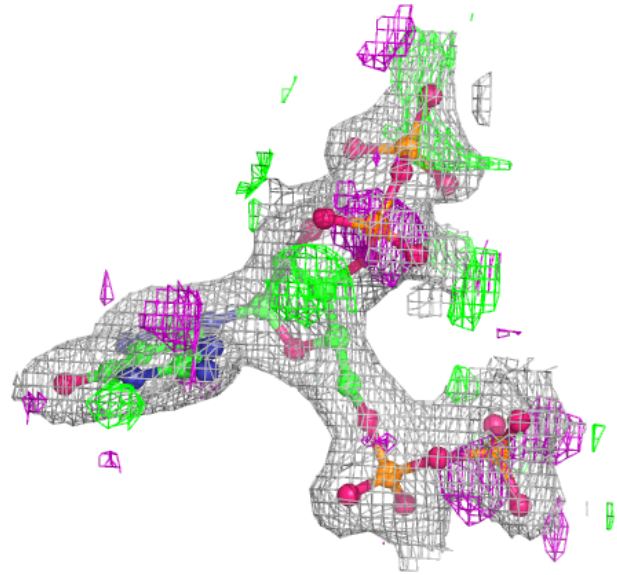
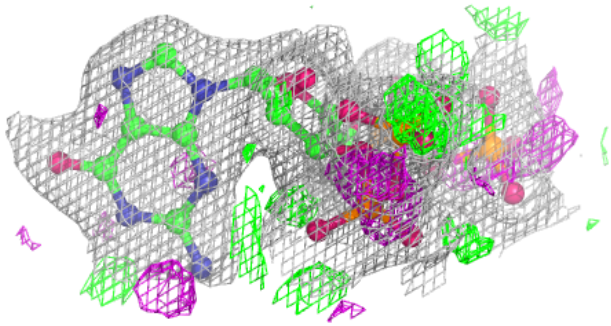
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

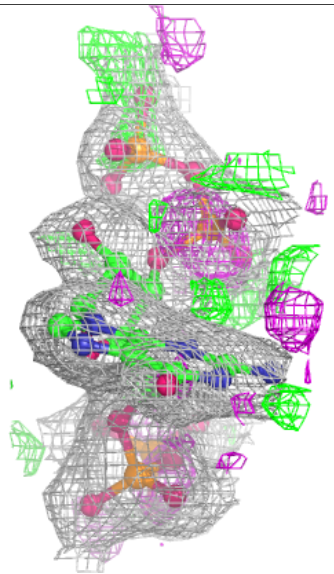


Electron density around G4P D 716 (A):

$2mF_o$-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 716 (B):

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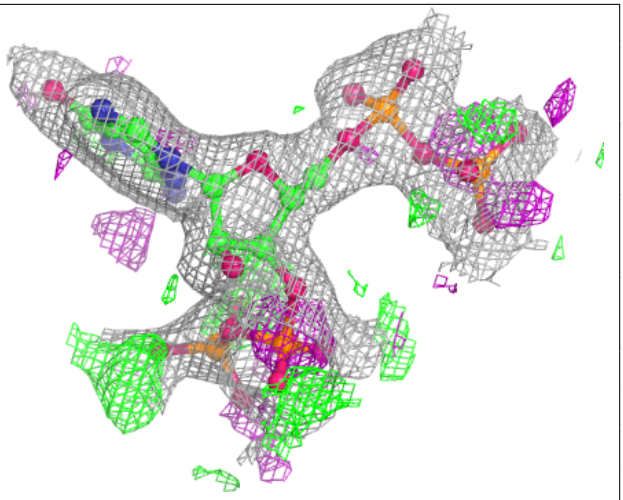
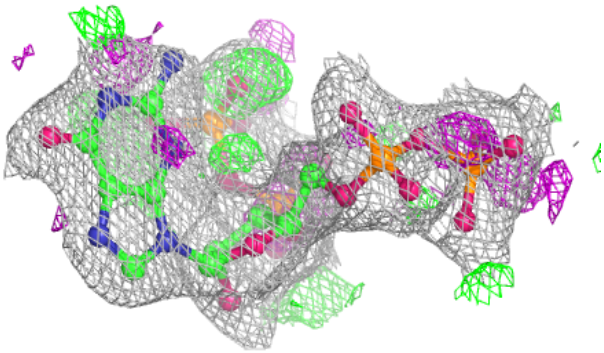
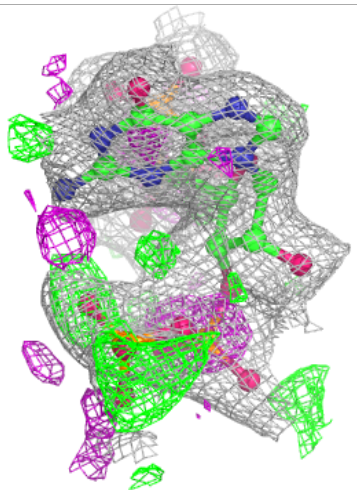
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

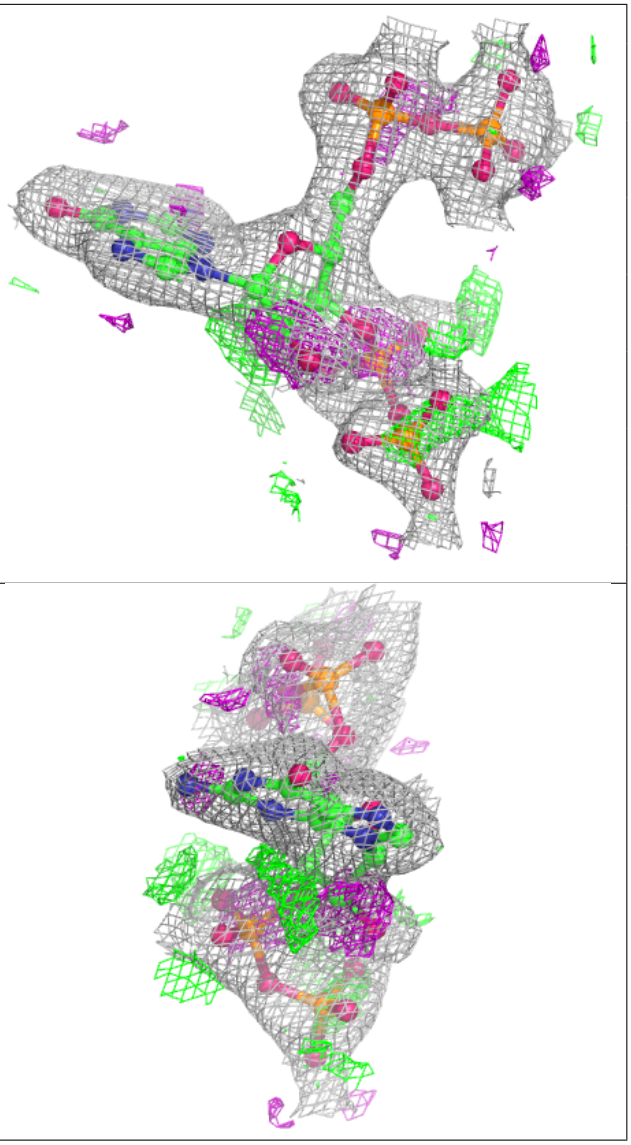






Electron density around G4P A 716 (A):

$2mF_o$-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 716 (B):

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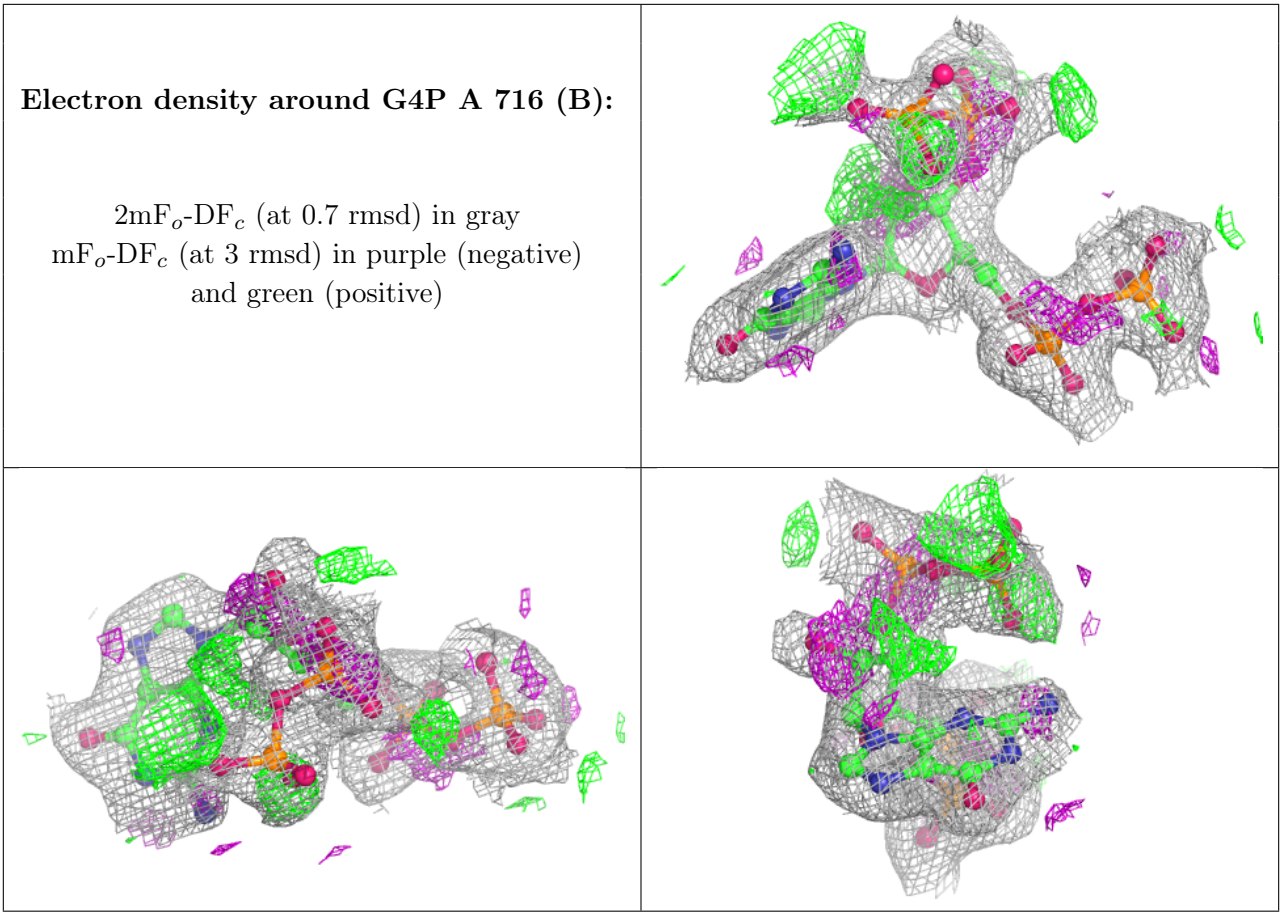
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G4P C 716 (A):

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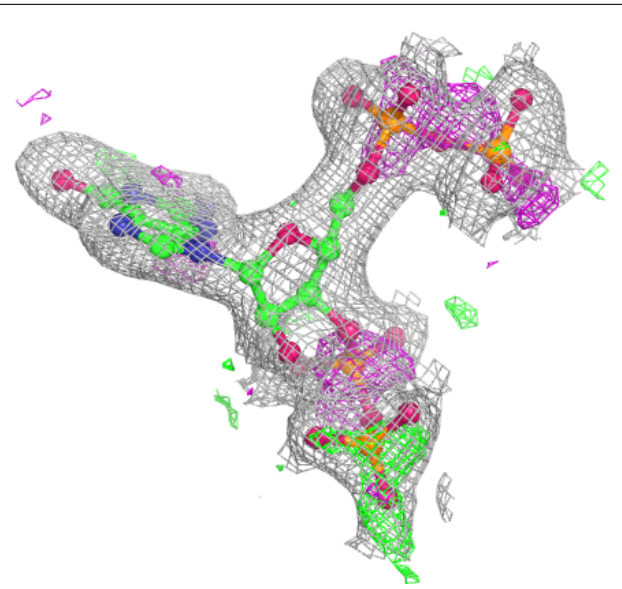
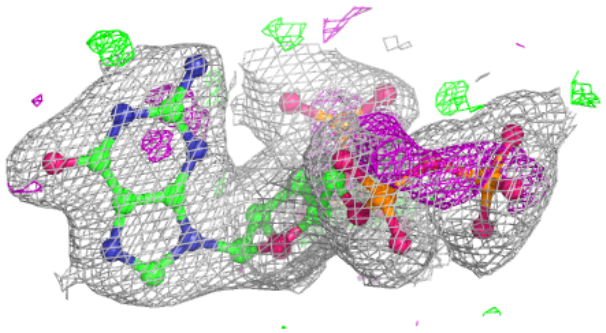
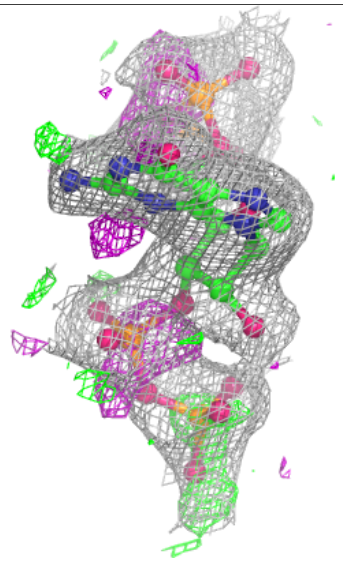
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around G4P C 716 (B):

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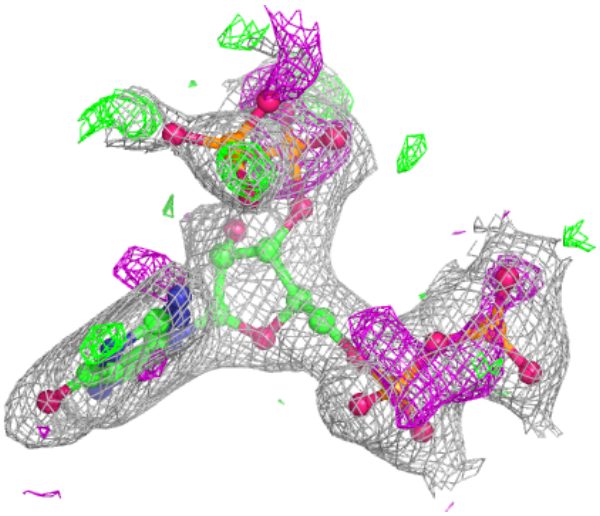
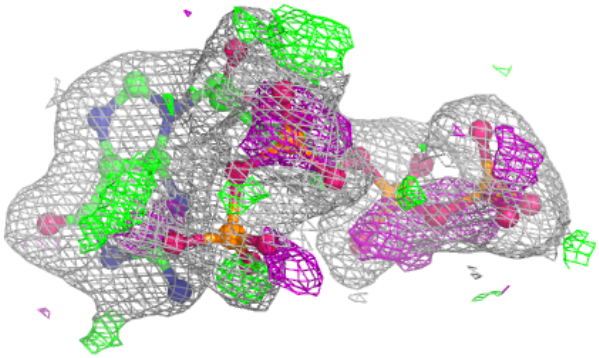
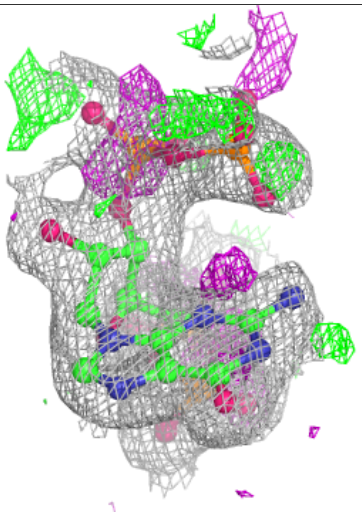
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

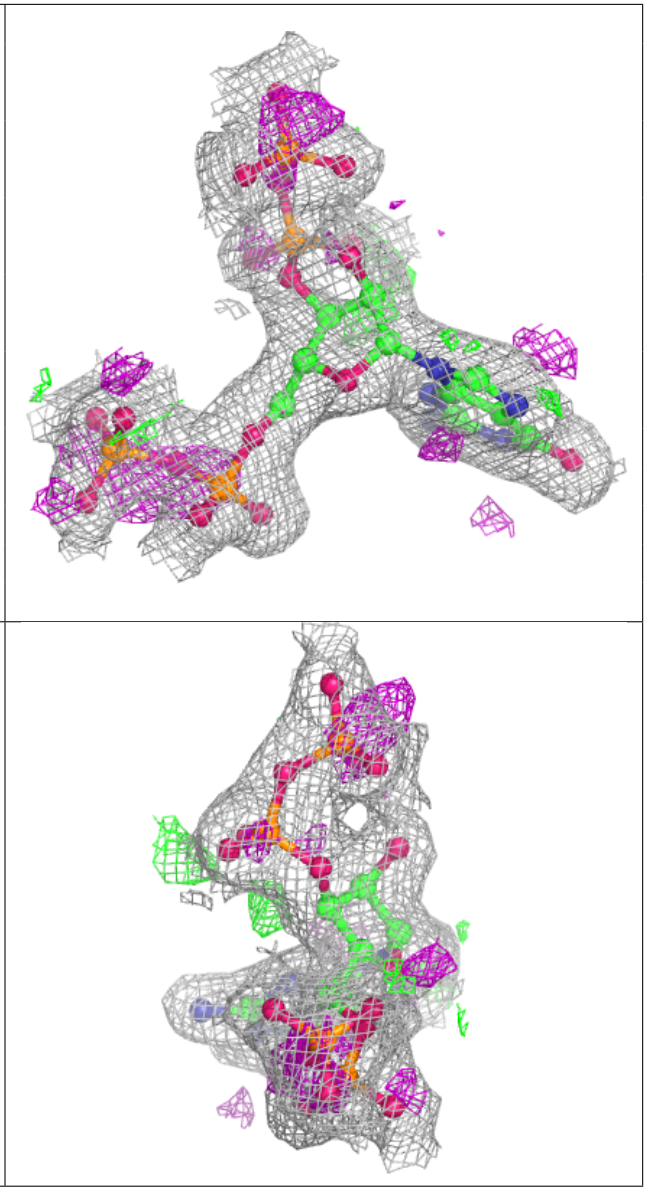






Electron density around G4P E 716:

$2mF_o$-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.