



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:18 PM GMT

PDB ID : 1HMP  
Title : THE CRYSTAL STRUCTURE OF HUMAN HYPOXANTHINE-GUANINE  
PHOSPHORIBOSYLTRANSFERASE WITH BOUND GMP  
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Deposited on : 1994-06-03  
Resolution : 2.50 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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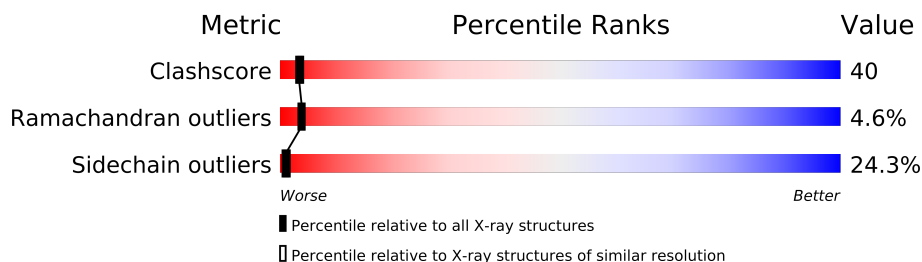
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	

## 2 Entry composition i

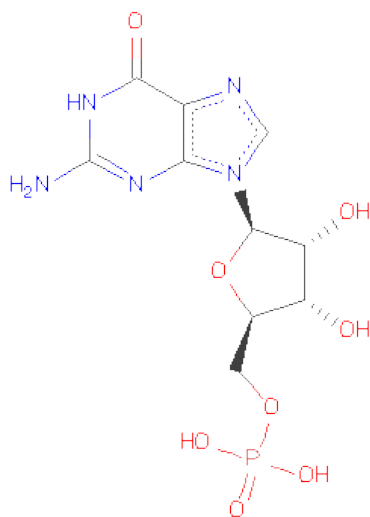
There are 3 unique types of molecules in this entry. The entry contains 3430 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HYPOXANTHINE GUANINE PHOSPHORIBOSYL-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1678	1072	284	312	10			
1	B	209	Total	C	N	O	S	0	0	0
			1619	1037	275	298	9			

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	38	Total 38	O 38	0	0

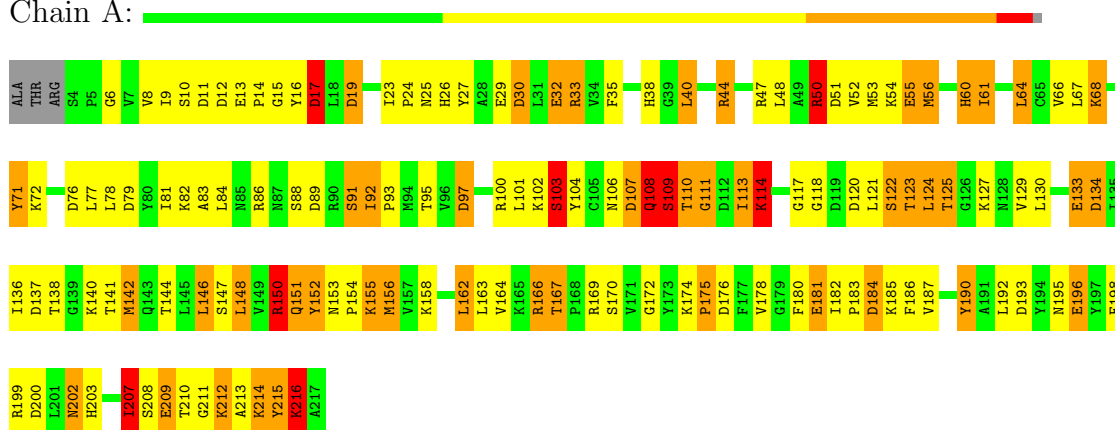
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

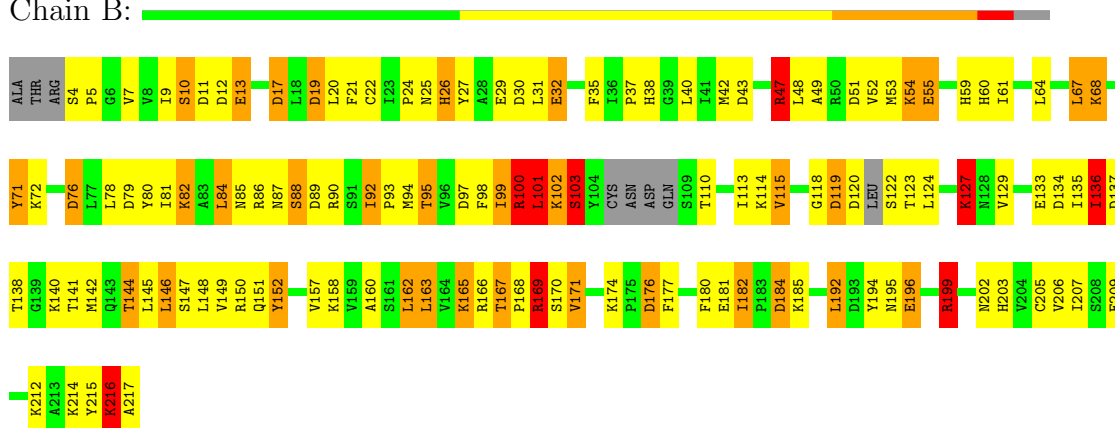
#### • Molecule 1: HYPOXANTHINE GUANINE PHOSPHORIBOSYL-TRANSFERASE

Chain A:



#### • Molecule 1: HYPOXANTHINE GUANINE PHOSPHORIBOSYL-TRANSFERASE

Chain B:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.50Å 66.45Å 52.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 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: 5GP

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	1.15	8/1711 (0.5%)	1.59	38/2311 (1.6%)
1	B	1.17	6/1650 (0.4%)	1.64	42/2230 (1.9%)
All	All	1.16	14/3361 (0.4%)	1.62	80/4541 (1.8%)

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	2	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	GLU	CD-OE1	7.98	1.34	1.25
1	A	181	GLU	CD-OE2	7.85	1.34	1.25
1	B	32	GLU	CD-OE2	7.76	1.34	1.25
1	B	196	GLU	CD-OE1	7.08	1.33	1.25
1	A	196	GLU	CD-OE2	6.90	1.33	1.25
1	A	32	GLU	CD-OE2	6.53	1.32	1.25
1	A	133	GLU	CD-OE1	6.37	1.32	1.25
1	A	55	GLU	CD-OE2	6.36	1.32	1.25
1	A	29	GLU	CD-OE1	6.07	1.32	1.25
1	B	181	GLU	CD-OE2	5.98	1.32	1.25
1	B	55	GLU	CD-OE2	5.87	1.32	1.25
1	B	209	GLU	CD-OE1	5.33	1.31	1.25
1	A	209	GLU	CD-OE2	5.24	1.31	1.25
1	A	196	GLU	CG-CD	-5.12	1.44	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	B	176	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	B	79	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	A	71	TYR	N-CA-CB	-8.48	95.33	110.60
1	A	50	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	B	17	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	A	109	SER	N-CA-CB	7.68	122.03	110.50
1	A	33	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	89	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	B	152	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	A	200	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	A	193	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	86	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	B	134	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	76	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	97	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	100	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	12	ASP	CB-CG-OD1	6.93	124.53	118.30
1	A	107	ASP	CB-CG-OD1	-6.85	112.13	118.30
1	A	71	TYR	CB-CG-CD1	6.84	125.10	121.00
1	A	134	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	B	12	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	166	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	19	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	B	12	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	B	43	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	19	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	71	TYR	CB-CG-CD1	-6.66	117.00	121.00
1	A	89	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	A	150	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	193	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	19	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	169	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	176	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	79	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	176	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	17	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	137	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	200	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	19	ASP	N-CA-CB	6.35	122.03	110.60
1	B	103	SER	N-CA-CB	6.23	119.84	110.50
1	B	170	SER	N-CA-CB	6.20	119.80	110.50
1	B	184	ASP	CB-CG-OD1	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	43	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	107	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	207	ILE	CB-CA-C	-5.96	99.69	111.60
1	B	134	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	50	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	110	THR	C-N-CA	5.87	134.64	122.30
1	A	12	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	76	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	86	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	47	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	152	TYR	CA-CB-CG	-5.54	102.87	113.40
1	B	119	ASP	C-N-CA	5.53	135.53	121.70
1	B	184	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	124	LEU	CB-CA-C	-5.51	99.74	110.20
1	A	76	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	11	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	30	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	A	79	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	136	ILE	CA-CB-CG2	5.35	121.59	110.90
1	B	19	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	127	LYS	CB-CA-C	-5.31	99.78	110.40
1	B	51	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	134	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	215	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	50	ARG	CD-NE-CZ	5.24	130.94	123.60
1	A	11	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	20	LEU	CB-CA-C	5.22	120.12	110.20
1	B	137	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	151	GLN	CB-CA-C	-5.21	99.99	110.40
1	B	100	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	51	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	A	216	LYS	N-CA-C	5.09	124.74	111.00
1	A	79	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	91	SER	N-CA-CB	5.08	118.12	110.50
1	A	110	THR	N-CA-C	5.04	124.61	111.00
1	B	166	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	19	ASP	CA

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Mol	Chain	Res	Type	Atom
1	B	136	ILE	CB

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1678	0	1675	139	0
1	B	1619	0	1597	132	0
2	A	24	0	12	3	0
2	B	24	0	11	2	0
3	A	47	0	0	6	0
3	B	38	0	0	2	0
All	All	3430	0	3295	266	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

All (266) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:LYS:HG3	1:A:55:GLU:HG2	1.46	0.97
1:A:56:MET:HB3	1:A:61:ILE:HD11	1.46	0.96
1:B:120:ASP:HA	1:B:124:LEU:HG	1.46	0.95
1:B:9:ILE:HG23	1:B:13:GLU:HG3	1.45	0.95
1:A:118:GLY:HA2	1:A:121:LEU:HG	1.52	0.91
1:A:54:LYS:CG	1:A:55:GLU:HG2	2.02	0.89
1:A:38:HIS:H	1:A:203:HIS:HD2	1.18	0.87
1:B:100:ARG:HG2	1:B:101:LEU:HD22	1.55	0.87
1:B:195:ASN:ND2	1:B:216:LYS:HA	1.90	0.86
1:A:68:LYS:HD3	2:A:300:5GP:O2'	1.78	0.84
1:A:121:LEU:HD12	1:A:152:TYR:CE1	2.14	0.82
1:B:38:HIS:H	1:B:203:HIS:HD2	1.29	0.81
1:B:135:ILE:HD11	1:B:165:LYS:HD2	1.62	0.80
1:A:167:THR:HG23	1:A:184:ASP:CG	2.02	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:THR:HG22	1:B:168:PRO:HD2	1.64	0.79
1:B:147:SER:O	1:B:150:ARG:HB3	1.84	0.78
1:B:85:ASN:O	1:B:88:SER:HB3	1.85	0.76
1:A:54:LYS:HG3	1:A:55:GLU:N	2.02	0.75
1:B:147:SER:HA	1:B:150:ARG:NH2	2.02	0.73
1:B:147:SER:HA	1:B:150:ARG:CZ	2.17	0.73
1:B:119:ASP:O	1:B:123:THR:HB	1.88	0.73
1:A:118:GLY:HA2	1:A:121:LEU:CG	2.17	0.73
1:B:199:ARG:HG2	1:B:199:ARG:HH11	1.53	0.73
1:B:67:LEU:HD23	1:B:98:PHE:CD2	2.24	0.72
1:A:51:ASP:O	1:A:54:LYS:HG2	1.89	0.72
1:B:167:THR:HG23	1:B:184:ASP:OD2	1.89	0.71
1:A:207:ILE:HD12	1:A:212:LYS:HG3	1.71	0.70
1:B:140:LYS:O	1:B:144:THR:HG23	1.92	0.70
1:A:121:LEU:HB2	1:A:152:TYR:CE2	2.28	0.69
1:A:14:PRO:O	1:A:33:ARG:HD3	1.92	0.69
1:B:118:GLY:C	1:B:120:ASP:H	1.93	0.69
1:A:202:ASN:OD1	1:A:202:ASN:N	2.26	0.69
1:A:196:GLU:OE2	1:B:95:THR:HB	1.92	0.69
1:B:38:HIS:H	1:B:203:HIS:CD2	2.11	0.69
1:B:160:ALA:HA	1:B:177:PHE:HB2	1.73	0.69
1:B:195:ASN:HD22	1:B:216:LYS:HA	1.57	0.68
1:B:199:ARG:HG2	1:B:199:ARG:NH1	2.05	0.68
1:B:113:ILE:CB	1:B:148:LEU:HD13	2.25	0.67
1:B:165:LYS:NZ	2:B:800:5GP:O6	2.28	0.67
1:A:17:ASP:HB2	1:A:19:ASP:OD2	1.95	0.67
1:A:118:GLY:HA2	1:A:121:LEU:HB2	1.76	0.66
1:A:151:GLN:O	1:A:153:ASN:N	2.28	0.66
1:B:118:GLY:O	1:B:122:SER:N	2.29	0.66
1:B:100:ARG:CG	1:B:101:LEU:HD22	2.26	0.66
1:A:183:PRO:O	1:A:185:LYS:N	2.29	0.66
1:A:209:GLU:OE2	1:A:212:LYS:NZ	2.29	0.65
1:A:120:ASP:O	1:A:123:THR:HB	1.97	0.65
1:A:148:LEU:O	1:A:151:GLN:HG2	1.96	0.65
1:A:153:ASN:N	1:A:154:PRO:HD3	2.11	0.65
1:A:164:VAL:O	1:A:182:ILE:N	2.29	0.65
3:A:913:HOH:O	1:B:92:ILE:HD13	1.95	0.65
1:B:129:VAL:HB	1:B:157:VAL:CG2	2.26	0.65
1:B:9:ILE:CG2	1:B:13:GLU:HG3	2.25	0.65
2:B:800:5GP:H5'2	3:B:876:HOH:O	1.97	0.64
1:A:138:THR:HG21	1:A:140:LYS:NZ	2.12	0.64
1:B:123:THR:O	1:B:127:LYS:HD3	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:GLY:HA2	1:A:44:ARG:HH21	1.63	0.64
1:A:138:THR:HG21	1:A:140:LYS:HZ1	1.63	0.63
1:B:142:MET:HE2	1:B:142:MET:HA	1.78	0.63
1:A:38:HIS:H	1:A:203:HIS:CD2	2.09	0.62
1:B:59:HIS:HB2	3:B:804:HOH:O	1.99	0.62
1:B:67:LEU:O	1:B:67:LEU:HD13	2.00	0.61
1:B:120:ASP:C	1:B:124:LEU:H	2.03	0.61
1:A:190:TYR:HB2	1:A:202:ASN:O	2.00	0.61
1:B:120:ASP:CB	1:B:124:LEU:HD12	2.30	0.61
1:B:118:GLY:HA2	1:B:152:TYR:CZ	2.34	0.61
1:B:47:ARG:HD3	1:B:47:ARG:O	2.01	0.61
1:A:66:VAL:HG21	1:A:142:MET:HE1	1.82	0.61
1:B:163:LEU:HG	1:B:182:ILE:CD1	2.31	0.60
1:A:48:LEU:O	1:A:52:VAL:HG23	2.00	0.60
1:A:6:GLY:HA2	1:A:44:ARG:NH2	2.17	0.60
1:B:31:LEU:HD22	1:B:205:CYS:HB2	1.83	0.60
1:B:9:ILE:HG23	1:B:13:GLU:CG	2.28	0.59
1:A:54:LYS:HE2	3:A:827:HOH:O	2.02	0.59
1:A:166:ARG:O	1:A:184:ASP:HB2	2.02	0.59
1:A:118:GLY:HA2	1:A:121:LEU:CB	2.32	0.59
1:B:13:GLU:HA	1:B:13:GLU:OE1	2.01	0.59
1:A:123:THR:HG22	1:A:124:LEU:N	2.16	0.59
1:B:4:SER:OG	1:B:5:PRO:HD2	2.03	0.59
1:A:136:ILE:HD12	1:A:175:PRO:HG3	1.84	0.59
1:B:100:ARG:O	1:B:101:LEU:HB2	2.03	0.58
1:A:164:VAL:O	1:A:181:GLU:HA	2.03	0.58
1:B:27:TYR:HA	1:B:30:ASP:OD2	2.04	0.58
1:A:142:MET:O	1:A:146:LEU:HD22	2.03	0.58
1:A:60:HIS:HE1	1:A:95:THR:OG1	1.86	0.58
1:B:133:GLU:OE1	1:B:142:MET:HE3	2.03	0.58
1:B:146:LEU:HA	1:B:149:VAL:HG12	1.87	0.57
1:A:121:LEU:HD12	1:A:152:TYR:CZ	2.38	0.57
1:A:125:THR:HA	1:A:153:ASN:O	2.03	0.57
1:A:30:ASP:O	1:A:207:ILE:HG22	2.05	0.57
1:A:210:THR:O	1:A:214:LYS:N	2.36	0.57
1:A:101:LEU:O	1:A:103:SER:N	2.38	0.56
1:A:118:GLY:HA3	1:A:152:TYR:OH	2.05	0.56
1:B:163:LEU:HG	1:B:182:ILE:HD11	1.87	0.56
1:A:196:GLU:O	1:B:93:PRO:HA	2.05	0.56
1:B:49:ALA:O	1:B:52:VAL:HB	2.04	0.56
1:B:129:VAL:HB	1:B:157:VAL:HG22	1.87	0.56
1:A:210:THR:O	1:A:214:LYS:HB3	2.05	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:202:ASN:N	1:B:202:ASN:OD1	2.33	0.55
1:B:199:ARG:CG	1:B:199:ARG:HH11	2.19	0.55
1:B:81:ILE:HG22	1:B:94:MET:CE	2.37	0.55
1:A:56:MET:CB	1:A:61:ILE:HD11	2.29	0.55
1:B:52:VAL:HG12	1:B:53:MET:N	2.17	0.55
1:A:155:LYS:HD2	1:A:155:LYS:O	2.07	0.55
1:B:10:SER:O	1:B:13:GLU:HB2	2.07	0.54
1:A:71:TYR:CD1	1:A:71:TYR:N	2.70	0.54
1:B:206:VAL:HG12	1:B:207:ILE:O	2.08	0.54
1:B:167:THR:HG21	1:B:169:ARG:HG2	1.90	0.54
1:B:115:VAL:O	1:B:118:GLY:N	2.38	0.54
1:A:208:SER:O	1:A:212:LYS:HB2	2.06	0.54
1:A:182:ILE:HB	1:A:183:PRO:CD	2.37	0.54
1:B:146:LEU:O	1:B:150:ARG:HB2	2.08	0.54
1:A:53:MET:SD	1:A:81:ILE:HG23	2.48	0.54
1:A:117:GLY:O	1:A:121:LEU:HG	2.07	0.54
1:B:194:TYR:CD2	1:B:215:TYR:HB2	2.43	0.54
1:A:30:ASP:HB3	1:A:211:GLY:HA3	1.89	0.54
1:A:129:VAL:HG12	1:A:130:LEU:N	2.24	0.53
1:A:163:LEU:HA	1:A:180:PHE:O	2.09	0.53
1:A:66:VAL:HG21	1:A:142:MET:CE	2.38	0.53
1:B:118:GLY:C	1:B:120:ASP:N	2.62	0.53
1:A:122:SER:O	1:A:125:THR:HG22	2.09	0.53
1:A:38:HIS:N	1:A:203:HIS:HD2	1.99	0.53
1:A:164:VAL:CG2	1:A:178:VAL:HG13	2.39	0.52
1:B:194:TYR:CE2	1:B:215:TYR:HB2	2.44	0.52
1:B:135:ILE:CD1	1:B:165:LYS:HD2	2.38	0.52
1:B:55:GLU:OE2	1:B:158:LYS:HE3	2.10	0.52
1:A:147:SER:HA	1:A:150:ARG:CD	2.40	0.52
1:A:50:ARG:C	1:A:50:ARG:HD3	2.30	0.52
1:A:71:TYR:CG	1:A:72:LYS:N	2.78	0.52
1:A:167:THR:HG21	1:A:169:ARG:HE	1.74	0.51
1:B:60:HIS:NE2	1:B:95:THR:CG2	2.73	0.51
1:A:187:VAL:HG23	1:A:192:LEU:HD12	1.92	0.51
1:B:120:ASP:HA	1:B:124:LEU:CG	2.31	0.51
1:B:171:VAL:O	1:B:171:VAL:HG13	2.10	0.51
1:A:118:GLY:CA	1:A:121:LEU:HB2	2.41	0.51
1:A:32:GLU:O	1:A:33:ARG:HG3	2.11	0.51
1:A:182:ILE:HB	1:A:183:PRO:HD2	1.93	0.51
1:B:167:THR:CG2	1:B:169:ARG:HG2	2.41	0.51
1:A:125:THR:HA	1:A:152:TYR:O	2.10	0.51
1:A:152:TYR:N	1:A:152:TYR:CD1	2.79	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:165:LYS:NZ	1:B:185:LYS:O	2.30	0.50
1:A:214:LYS:HG2	1:A:214:LYS:O	2.11	0.50
1:A:136:ILE:CD1	1:A:175:PRO:HG3	2.41	0.50
1:A:147:SER:HA	1:A:150:ARG:HD2	1.92	0.50
1:A:24:PRO:HD3	3:A:914:HOH:O	2.11	0.50
1:A:198:PHE:CZ	1:A:215:TYR:CE2	3.00	0.50
1:A:113:ILE:O	1:A:114:LYS:HB2	2.11	0.50
1:A:54:LYS:HE2	1:A:55:GLU:OE2	2.10	0.50
1:B:80:TYR:O	1:B:84:LEU:HD23	2.12	0.50
1:A:108:GLN:O	1:A:109:SER:HB2	2.11	0.50
1:B:7:VAL:HB	1:B:180:PHE:CD2	2.47	0.50
1:B:103:SER:CB	1:B:144:THR:HG21	2.41	0.49
1:B:81:ILE:HG22	1:B:94:MET:HE1	1.94	0.49
1:A:50:ARG:HD3	1:A:50:ARG:O	2.13	0.49
1:B:102:LYS:CB	1:B:141:THR:HG23	2.42	0.49
1:A:138:THR:HB	1:A:140:LYS:HZ3	1.77	0.49
1:B:157:VAL:O	1:B:157:VAL:HG12	2.11	0.49
1:A:83:ALA:HA	1:A:86:ARG:HG3	1.94	0.49
1:B:115:VAL:C	1:B:118:GLY:H	2.16	0.49
1:A:54:LYS:HG2	1:A:55:GLU:HG2	1.92	0.48
1:A:207:ILE:HD12	1:A:212:LYS:CG	2.40	0.48
1:B:129:VAL:HB	1:B:157:VAL:HG23	1.94	0.48
1:B:92:ILE:HA	1:B:93:PRO:HD3	1.72	0.48
1:A:60:HIS:CD2	1:A:127:LYS:NZ	2.81	0.48
1:A:10:SER:OG	1:A:10:SER:O	2.32	0.48
1:A:167:THR:HG21	1:A:169:ARG:HH21	1.79	0.48
1:A:133:GLU:HG2	1:A:134:ASP:H	1.78	0.48
1:B:135:ILE:HG13	1:B:136:ILE:N	2.29	0.48
1:B:146:LEU:N	1:B:146:LEU:HD13	2.29	0.48
2:A:300:5GP:H8	2:A:300:5GP:H5'1	1.95	0.48
1:B:72:LYS:NZ	1:B:76:ASP:OD1	2.44	0.47
1:A:54:LYS:CG	1:A:55:GLU:N	2.75	0.47
1:A:110:THR:CG2	1:A:111:GLY:N	2.77	0.47
1:A:151:GLN:C	1:A:153:ASN:H	2.17	0.47
1:A:26:HIS:HD2	1:B:88:SER:O	1.96	0.47
1:A:186:PHE:HD2	1:A:207:ILE:HD11	1.80	0.47
1:A:163:LEU:HD23	1:A:180:PHE:HB2	1.96	0.46
1:A:9:ILE:C	1:A:166:ARG:HH22	2.18	0.46
1:B:158:LYS:HG2	1:B:177:PHE:CE2	2.50	0.46
1:B:114:LYS:HA	1:B:152:TYR:OH	2.14	0.46
1:B:100:ARG:HD3	1:B:101:LEU:CD2	2.45	0.46
1:A:148:LEU:HD23	1:A:151:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138:THR:O	1:B:171:VAL:HG12	2.16	0.46
1:A:170:SER:C	1:A:172:GLY:H	2.17	0.46
1:B:54:LYS:HD2	1:B:54:LYS:HA	1.53	0.46
1:B:71:TYR:N	1:B:71:TYR:CD1	2.84	0.46
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.74	0.46
1:A:61:ILE:HG22	1:A:61:ILE:O	2.15	0.46
1:A:121:LEU:CB	1:A:152:TYR:CE2	2.98	0.46
1:A:16:TYR:CA	1:A:33:ARG:NH1	2.79	0.46
1:B:59:HIS:O	1:B:61:ILE:HG23	2.16	0.46
1:A:164:VAL:HG23	1:A:178:VAL:HG13	1.96	0.46
1:A:185:LYS:HE2	3:A:825:HOH:O	2.15	0.45
1:A:195:ASN:ND2	1:A:216:LYS:HA	2.31	0.45
1:B:162:LEU:O	1:B:162:LEU:HD22	2.16	0.45
1:B:22:CYS:O	1:B:203:HIS:HE1	1.99	0.45
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.76	0.45
1:A:8:VAL:CG1	1:A:9:ILE:N	2.78	0.45
1:B:163:LEU:HG	1:B:182:ILE:HD13	1.98	0.45
1:A:78:LEU:N	1:A:78:LEU:HD12	2.30	0.45
2:A:300:5GP:H5'2	3:A:893:HOH:O	2.16	0.45
1:B:38:HIS:NE2	1:B:42:MET:CE	2.80	0.45
1:B:47:ARG:HD3	1:B:47:ARG:C	2.37	0.45
1:A:147:SER:O	1:A:150:ARG:HD3	2.17	0.45
1:A:78:LEU:CD1	1:A:78:LEU:N	2.80	0.45
1:A:92:ILE:HD13	1:A:92:ILE:HA	1.83	0.45
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.68	0.45
1:B:142:MET:CE	1:B:142:MET:HA	2.46	0.44
1:B:92:ILE:N	1:B:92:ILE:HD13	2.32	0.44
1:A:141:THR:O	1:A:144:THR:OG1	2.31	0.44
1:B:195:ASN:O	1:B:196:GLU:HB2	2.16	0.44
1:A:211:GLY:HA2	1:A:214:LYS:HD2	1.99	0.44
1:B:199:ARG:CG	1:B:199:ARG:NH1	2.78	0.44
1:A:88:SER:O	1:B:26:HIS:HD2	2.01	0.44
1:B:113:ILE:O	1:B:152:TYR:OH	2.24	0.44
1:B:120:ASP:O	1:B:124:LEU:N	2.41	0.44
1:B:127:LYS:HD2	1:B:127:LYS:N	2.33	0.43
1:A:162:LEU:HD13	1:A:163:LEU:HG	2.00	0.43
1:A:209:GLU:O	1:A:213:ALA:N	2.36	0.43
1:A:17:ASP:N	1:A:17:ASP:OD1	2.51	0.43
1:B:195:ASN:HD22	1:B:216:LYS:CA	2.27	0.43
1:A:9:ILE:O	1:A:183:PRO:HG3	2.18	0.43
3:A:874:HOH:O	1:B:82:LYS:HE3	2.19	0.43
1:B:4:SER:HA	1:B:5:PRO:HD3	1.66	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:LEU:HB3	1:B:99:ILE:HD13	2.01	0.43
1:B:31:LEU:HD22	1:B:205:CYS:CB	2.46	0.42
1:A:138:THR:CG2	1:A:140:LYS:NZ	2.80	0.42
1:B:182:ILE:HG21	1:B:182:ILE:HD13	1.74	0.42
1:A:92:ILE:HA	1:A:93:PRO:HD3	1.95	0.42
1:B:38:HIS:NE2	1:B:42:MET:HE2	2.34	0.42
1:A:121:LEU:O	1:A:124:LEU:O	2.38	0.42
1:B:24:PRO:HG2	1:B:27:TYR:HD2	1.85	0.42
1:A:56:MET:HG2	1:A:61:ILE:HG12	2.02	0.42
1:B:138:THR:HG22	1:B:169:ARG:O	2.20	0.42
1:A:15:GLY:C	1:A:33:ARG:HH11	2.23	0.42
1:B:120:ASP:C	1:B:123:THR:N	2.68	0.42
1:B:101:LEU:HA	1:B:101:LEU:HD13	1.90	0.42
1:A:8:VAL:HG13	1:A:166:ARG:HH21	1.83	0.42
1:B:21:PHE:CD1	1:B:21:PHE:N	2.88	0.42
1:B:216:LYS:HB3	1:B:217:ALA:H	1.60	0.42
1:B:142:MET:HB2	1:B:142:MET:HE3	1.73	0.41
1:A:56:MET:HE2	1:A:158:LYS:HB2	2.01	0.41
1:B:113:ILE:O	1:B:118:GLY:N	2.53	0.41
1:B:192:LEU:N	1:B:192:LEU:CD1	2.84	0.41
1:A:212:LYS:HB3	1:A:212:LYS:HE2	1.14	0.41
1:A:16:TYR:N	1:A:33:ARG:HH11	2.18	0.41
1:A:129:VAL:N	1:A:156:MET:O	2.43	0.41
1:A:196:GLU:CD	1:B:95:THR:HB	2.40	0.41
1:A:186:PHE:CD2	1:A:207:ILE:HD11	2.56	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.79	0.41
1:B:37:PRO:HA	1:B:203:HIS:CD2	2.56	0.41
1:A:82:LYS:HD3	1:B:199:ARG:O	2.21	0.41
1:A:88:SER:O	1:B:26:HIS:CD2	2.74	0.41
1:B:147:SER:CA	1:B:150:ARG:NH2	2.80	0.41
1:A:27:TYR:HA	1:A:30:ASP:OD2	2.21	0.41
1:B:84:LEU:CD2	1:B:84:LEU:N	2.84	0.41
1:A:64:LEU:CD1	1:A:97:ASP:HB3	2.50	0.41
1:A:118:GLY:O	1:A:121:LEU:HB2	2.21	0.40
1:A:164:VAL:N	1:A:180:PHE:O	2.52	0.40
1:B:138:THR:CG2	1:B:169:ARG:HG3	2.51	0.40
1:B:138:THR:HG22	1:B:169:ARG:HG3	2.03	0.40
1:A:213:ALA:O	1:A:216:LYS:HD2	2.21	0.40
1:B:64:LEU:CD1	1:B:129:VAL:CG1	3.00	0.40
1:B:24:PRO:HG2	1:B:27:TYR:CD2	2.56	0.40
1:B:215:TYR:O	1:B:216:LYS:HG2	2.20	0.40
1:A:82:LYS:NZ	1:B:71:TYR:OH	2.26	0.40



There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/217 (98%)	172 (81%)	28 (13%)	12 (6%)	3	2
1	B	205/217 (94%)	182 (89%)	16 (8%)	7 (3%)	6	7
All	All	417/434 (96%)	354 (85%)	44 (11%)	19 (5%)	4	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	102	LYS
1	A	109	SER
1	A	111	GLY
1	A	114	LYS
1	A	125	THR
1	A	152	TYR
1	A	184	ASP
1	B	101	LEU
1	B	103	SER
1	A	108	GLN
1	B	216	LYS
1	A	103	SER
1	B	110	THR
1	A	190	TYR
1	B	68	LYS
1	A	175	PRO
1	B	102	LYS
1	B	115	VAL

### 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	183/191 (96%)	139 (76%)	44 (24%)	1	1
1	B	171/191 (90%)	129 (75%)	42 (25%)	1	1
All	All	354/382 (93%)	268 (76%)	86 (24%)	1	1

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	17	ASP
1	A	23	ILE
1	A	25	ASN
1	A	35	PHE
1	A	40	LEU
1	A	44	ARG
1	A	47	ARG
1	A	50	ARG
1	A	56	MET
1	A	60	HIS
1	A	61	ILE
1	A	64	LEU
1	A	67	LEU
1	A	77	LEU
1	A	91	SER
1	A	92	ILE
1	A	97	ASP
1	A	100	ARG
1	A	103	SER
1	A	104	TYR
1	A	106	ASN
1	A	107	ASP
1	A	108	GLN
1	A	113	ILE
1	A	114	LYS
1	A	122	SER
1	A	123	THR
1	A	142	MET

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Mol	Chain	Res	Type
1	A	146	LEU
1	A	148	LEU
1	A	150	ARG
1	A	151	GLN
1	A	155	LYS
1	A	156	MET
1	A	162	LEU
1	A	167	THR
1	A	174	LYS
1	A	199	ARG
1	A	202	ASN
1	A	207	ILE
1	A	212	LYS
1	A	214	LYS
1	A	216	LYS
1	B	10	SER
1	B	13	GLU
1	B	17	ASP
1	B	19	ASP
1	B	25	ASN
1	B	26	HIS
1	B	32	GLU
1	B	35	PHE
1	B	40	LEU
1	B	47	ARG
1	B	54	LYS
1	B	67	LEU
1	B	68	LYS
1	B	78	LEU
1	B	82	LYS
1	B	84	LEU
1	B	87	ASN
1	B	88	SER
1	B	90	ARG
1	B	92	ILE
1	B	95	THR
1	B	99	ILE
1	B	100	ARG
1	B	101	LEU
1	B	127	LYS
1	B	136	ILE
1	B	144	THR

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Mol	Chain	Res	Type
1	B	146	LEU
1	B	162	LEU
1	B	163	LEU
1	B	165	LYS
1	B	167	THR
1	B	169	ARG
1	B	171	VAL
1	B	174	LYS
1	B	176	ASP
1	B	182	ILE
1	B	192	LEU
1	B	199	ARG
1	B	212	LYS
1	B	214	LYS
1	B	216	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	60	HIS
1	A	108	GLN
1	A	128	ASN
1	A	153	ASN
1	A	203	HIS
1	B	26	HIS
1	B	195	ASN
1	B	203	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	5GP	A	300	-	26,26,26	1.10	2 (7%)	37,40,40	3.99	5 (13%)
2	5GP	B	800	-	26,26,26	1.04	1 (3%)	37,40,40	5.28	10 (27%)

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	5GP	A	300	-	-	0/10/26/26	0/1/3/3
2	5GP	B	800	-	-	0/10/26/26	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	5GP	O3'-C3'	-2.71	1.36	1.43
2	A	300	5GP	C8-N7	-2.16	1.30	1.34
2	A	300	5GP	C6-N1	2.03	1.40	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	5GP	C6-C5-N7	-29.59	130.16	134.14
2	A	300	5GP	C6-C5-N7	-22.90	131.06	134.14
2	B	800	5GP	C1'-N9-C4	-6.71	115.05	126.64
2	B	800	5GP	C8-N9-C1'	5.98	138.16	126.38
2	A	300	5GP	C1'-N9-C4	-3.68	120.27	126.64
2	B	800	5GP	N2-C2-N1	-3.66	113.83	117.86
2	A	300	5GP	C6-N1-C2	3.00	124.75	119.51
2	B	800	5GP	C6-N1-C2	2.77	124.36	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	5GP	P-O5'-C5'	-2.68	110.44	118.19
2	B	800	5GP	C2-N3-C4	-2.57	111.48	115.09
2	A	300	5GP	N2-C2-N1	-2.28	115.35	117.86
2	B	800	5GP	O5'-P-O1P	-2.15	100.40	106.71
2	A	300	5GP	C2'-C1'-N9	-2.12	107.83	113.27
2	B	800	5GP	N1-C2-N3	2.10	124.72	121.78
2	B	800	5GP	C4'-O4'-C1'	-2.08	107.49	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.