Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 05:04 am GMT

PDB ID	:	1QK5
Title	:	TOXOPLASMA GONDII HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE WITH XMP, PYROPHOSPHATE AND TWO MG2+ IONS
Authors	:	Heroux, A.; White, E.L.; Ross, L.J.; Davis, R.L.; Borhani, D.W.
Deposited on	:	1999-07-09
Resolution	:	1.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

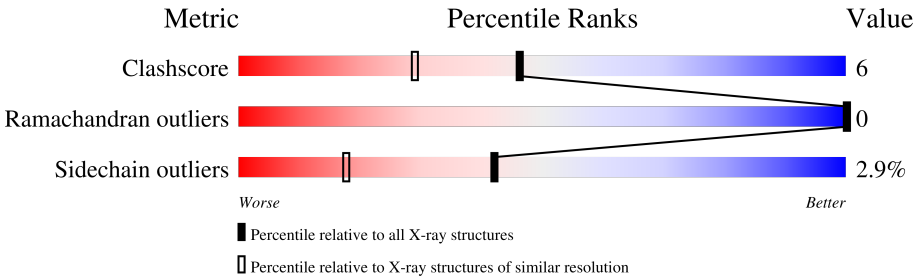
MolProbity	:	4.02b-467
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	233	72% 18% • 8%
1	B	233	75% 16% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3724 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.

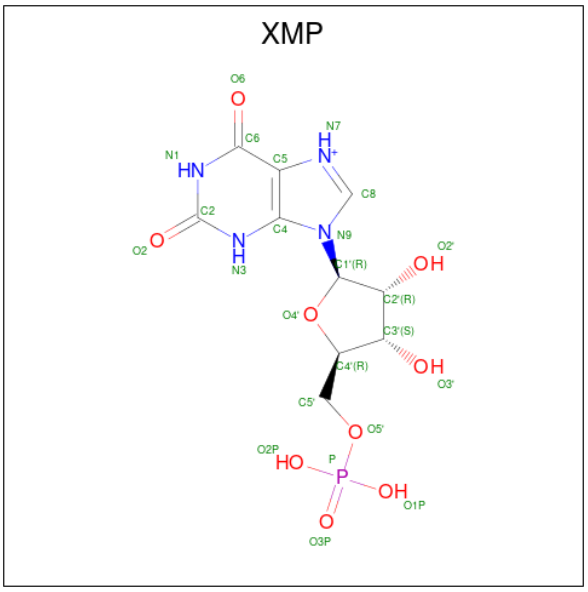
- Molecule 1 is a protein called HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1730	1124	285	313	8			
1	B	217	Total	C	N	O	S	0	0	0
			1742	1133	288	314	7			

There are 8 discrepancies between the modelled and reference sequences:

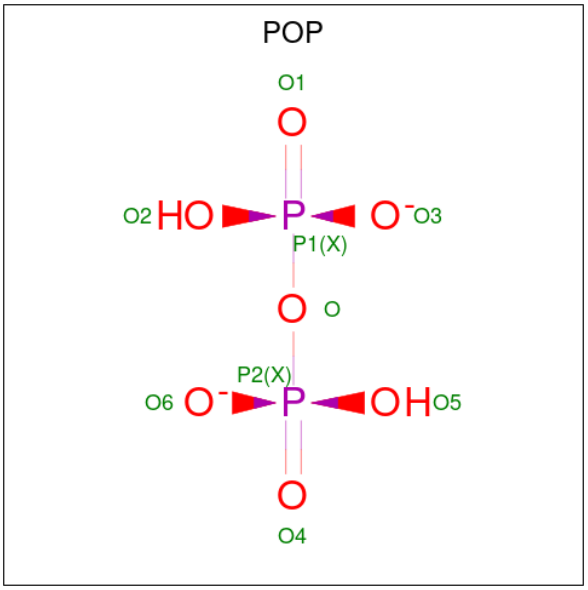
Chain	Residue	Modelled	Actual	Comment	Reference
A	0A	GLY	-	cloning artifact	UNP Q26997
A	0B	SER	-	cloning artifact	UNP Q26997
A	0C	HIS	-	cloning artifact	UNP Q26997
B	0A	GLY	-	cloning artifact	UNP Q26997
B	0B	SER	-	cloning artifact	UNP Q26997
B	0C	HIS	-	cloning artifact	UNP Q26997
A	150	ALA	ASP	engineered mutation	UNP Q26997
B	150	ALA	ASP	engineered mutation	UNP Q26997

- Molecule 2 is XANTHOSINE-5'-MONOPHOSPHATE (three-letter code: XMP) (formula: $C_{10}H_{14}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	4	9	1		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	P		0	0
			9	7	2			
3	B	1	Total	O	P		0	0
			9	7	2			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0
5	B	80	Total O 80 80	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. 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. 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.

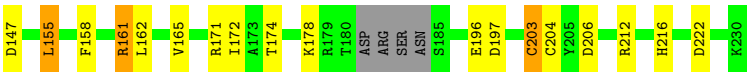
Note EDS failed to run properly.

• Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

Chain A:

• Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	55.21Å 112.25Å 144.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 1.60	Depositor
% Data completeness (in resolution range)	98.0 (13.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.261	Depositor
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.337	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3724	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POP, XMP, MG

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	0.76	0/1771	1.59	30/2388 (1.3%)
1	B	0.77	0/1783	1.90	38/2405 (1.6%)
All	All	0.76	0/3554	1.76	68/4793 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	212	ARG	NE-CZ-NH1	26.82	133.71	120.30
1	B	82	ARG	CD-NE-CZ	26.21	160.30	123.60
1	B	171	ARG	NE-CZ-NH1	18.86	129.73	120.30
1	B	82	ARG	NE-CZ-NH2	13.59	127.09	120.30
1	B	212	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	B	101	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	23	ASP	CB-CG-OD1	10.02	127.32	118.30
1	B	101	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	B	82	ARG	CG-CD-NE	9.82	132.42	111.80
1	A	133	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	B	55	ARG	CD-NE-CZ	9.21	136.50	123.60
1	A	171	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	B	32	PHE	CB-CG-CD1	8.54	126.78	120.80
1	B	171	ARG	CD-NE-CZ	8.51	135.51	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	114	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	B	9	TYR	CB-CG-CD2	8.12	125.88	121.00
1	A	171	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	55	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	171	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	23	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	55	ARG	CG-CD-NE	-7.84	95.33	111.80
1	A	55	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	147	ASP	CB-CG-OD1	7.66	125.20	118.30
1	B	82	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	B	222	ASP	CB-CG-OD1	7.46	125.02	118.30
1	B	65	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	9	TYR	CB-CG-CD1	-7.24	116.65	121.00
1	A	101	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	43	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	161	ARG	CD-NE-CZ	6.99	133.38	123.60
1	A	139	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	A	206	ASP	CB-CG-OD2	6.68	124.32	118.30
1	B	212	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
1	B	147	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	161	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	55	ARG	CD-NE-CZ	6.51	132.72	123.60
1	B	114	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	B	138	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	B	161	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	B	45	ILE	O-C-N	-6.19	112.79	122.70
1	A	171	ARG	O-C-N	6.17	132.58	122.70
1	A	185	SER	CA-C-O	6.17	133.05	120.10
1	B	114	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	197	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	206	ASP	O-C-N	6.09	132.45	122.70
1	A	43	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	98	TYR	CB-CG-CD2	5.91	124.55	121.00
1	B	32	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	A	61	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	A	61	TYR	CG-CD1-CE1	-5.69	116.75	121.30
1	B	128	THR	O-C-N	5.67	131.77	122.70
1	A	185	SER	O-C-N	-5.64	113.67	122.70
1	A	67	TYR	CG-CD1-CE1	5.62	125.79	121.30
1	A	215	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	67	TYR	CB-CG-CD1	5.39	124.23	121.00
1	B	222	ASP	CB-CG-OD2	-5.38	113.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	52	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	B	147	ASP	OD1-CG-OD2	-5.25	113.33	123.30
1	B	63	ILE	O-C-N	-5.20	114.38	122.70
1	B	196	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	101	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	219	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	B	15	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	54	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	23	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	139	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	102	GLU	OE1-CD-OE2	-5.05	117.24	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ILE	Mainchain

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	1730	0	1716	23	0
1	B	1742	0	1734	16	0
2	A	24	0	12	5	0
2	B	24	0	12	3	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	102	0	0	4	0
5	B	80	0	0	0	0
All	All	3724	0	3474	44	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 6.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:300:XMP:H8	2:A:300:XMP:H5'2	1.35	1.06
2:B:300:XMP:H5'2	2:B:300:XMP:H8	1.28	1.05
1:A:49:GLY:H	1:A:216:HIS:HD2	1.18	0.91
1:B:49:GLY:H	1:B:216:HIS:HD2	1.17	0.90
2:A:300:XMP:H8	2:A:300:XMP:C5'	2.04	0.87
2:A:300:XMP:H5'2	2:A:300:XMP:C8	2.07	0.85
1:B:49:GLY:H	1:B:216:HIS:CD2	2.01	0.78
2:B:300:XMP:H5'2	2:B:300:XMP:C8	2.12	0.76
1:A:49:GLY:H	1:A:216:HIS:CD2	2.03	0.75
1:A:112:TYR:OH	1:B:82:ARG:HD3	1.94	0.66
1:A:161:ARG:HG3	1:A:161:ARG:HH11	1.63	0.64
1:A:96:GLN:HG2	5:A:2048:HOH:O	2.02	0.59
1:B:178:LYS:HE3	2:B:300:XMP:H7	1.70	0.57
1:A:41:TYR:OH	1:A:227:LYS:HD3	2.06	0.56
1:B:127:LEU:O	1:B:161:ARG:NH2	2.39	0.56
1:A:26:PHE:CE2	1:A:219:VAL:HG11	2.42	0.54
2:A:300:XMP:H5'1	5:A:2100:HOH:O	2.06	0.54
1:A:82:ARG:HG3	1:B:112:TYR:OH	2.08	0.53
1:A:116:LYS:C	5:A:2101:HOH:O	2.48	0.52
1:B:203:CYS:O	1:B:204:CYS:HB2	2.09	0.51
1:A:5:PRO:HG2	1:A:8:ASP:OD2	2.11	0.50
1:A:8:ASP:HA	1:A:11:LYS:HD2	1.95	0.49
1:B:162:LEU:O	1:B:165:VAL:HG22	2.14	0.48
1:B:146:GLU:O	1:B:174:THR:HA	2.15	0.47
1:A:9:TYR:HA	5:A:2070:HOH:O	2.14	0.47
1:A:44:LYS:HB2	1:A:219:VAL:HG22	1.96	0.47
1:A:229:GLU:O	1:A:230:LYS:C	2.53	0.47
2:A:300:XMP:C5'	2:A:300:XMP:C8	2.81	0.46
1:A:26:PHE:CE2	1:A:219:VAL:CG1	2.98	0.45
1:B:49:GLY:N	1:B:216:HIS:HD2	1.99	0.45
1:B:113:VAL:HG22	1:B:131:SER:HB2	1.98	0.44
1:A:35:PRO:HA	1:A:36:PRO:HD3	1.87	0.44
1:A:142:VAL:HG11	1:A:162:LEU:HD21	2.00	0.44
1:B:155:LEU:HD23	1:B:172:ILE:HD13	2.00	0.44
1:B:127:LEU:HD21	1:B:158:PHE:HB2	1.99	0.44
1:A:161:ARG:HH11	1:A:161:ARG:CG	2.29	0.44
1:A:180:THR:HG22	1:A:197:ASP:CG	2.39	0.43
1:A:147:ASP:HB2	1:A:205:TYR:CE2	2.54	0.42
1:B:142:VAL:HG11	1:B:162:LEU:HD21	2.01	0.42
1:A:72:LEU:HD21	1:A:74:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG23	1:A:106:PRO:HD2	2.03	0.41
1:B:114:ARG:HB3	1:B:130:LEU:HB3	2.03	0.41
1:A:72:LEU:CD2	1:A:74:ILE:HD11	2.51	0.41
1:B:155:LEU:HD12	1:B:155:LEU:HA	1.87	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	209/233 (90%)	206 (99%)	3 (1%)	0	100	100
1	B	211/233 (91%)	205 (97%)	6 (3%)	0	100	100
All	All	420/466 (90%)	411 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/206 (91%)	183 (98%)	4 (2%)	53	29
1	B	188/206 (91%)	181 (96%)	7 (4%)	34	11
All	All	375/412 (91%)	364 (97%)	11 (3%)	42	18

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	102	GLU
1	A	114	ARG
1	A	161	ARG
1	B	4	LYS
1	B	23	ASP
1	B	30	ASP
1	B	51	LEU
1	B	114	ARG
1	B	155	LEU
1	B	203	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	96	GLN
1	A	216	HIS
1	B	37	HIS
1	B	86	ASN
1	B	96	GLN
1	B	216	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)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.