



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:57 pm BST

PDB ID : 2PGI
Title : THE CRYSTAL STRUCTURE OF PHOSPHOGLUCOSE ISOMERASE-AN ENZYME WITH AUTOCRINE MOTILITY FACTOR ACTIVITY IN TUMOR CELLS
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Deposited on : 1998-10-27
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **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) : 2.11

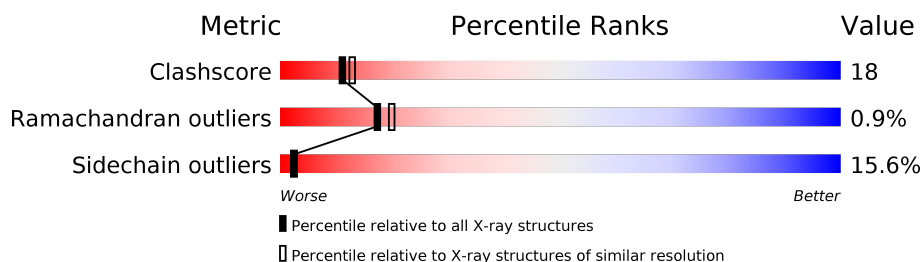
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3698 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 PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3514	2243	594	665	12			

- Molecule 2 is water.

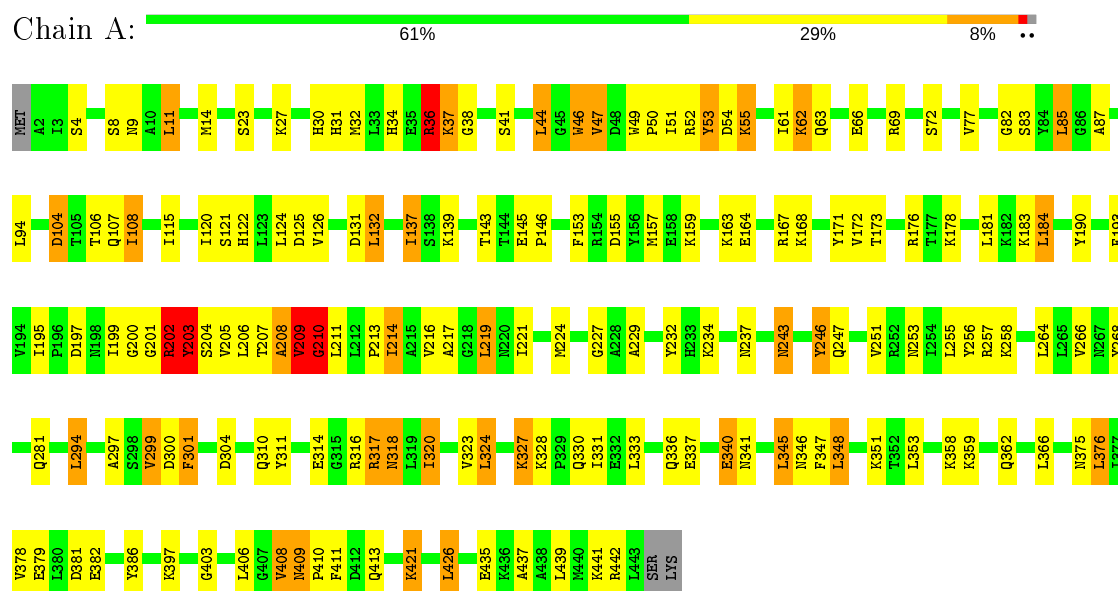
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total	O	0	0
			184	184		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 was not executed.

• Molecule 1: PHOSPHOGLUCOSE ISOMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	75.10 Å 93.73 Å 171.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.9 (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.185 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3698	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.80	5/3592 (0.1%)	0.74	3/4853 (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	15

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	LYS	C-N	-19.38	0.98	1.33
1	A	36	ARG	C-N	17.62	1.74	1.34
1	A	46	TRP	C-N	16.64	1.72	1.34
1	A	55	LYS	C-N	8.73	1.54	1.34
1	A	53	TYR	C-N	5.74	1.47	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	LYS	O-C-N	-14.03	100.25	122.70
1	A	46	TRP	C-N-CA	-9.66	97.55	121.70
1	A	47	VAL	O-C-N	-6.14	112.88	122.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ASP	Peptide
1	A	153	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	202	ARG	Mainchain,Peptide
1	A	203	TYR	Mainchain
1	A	208	ALA	Mainchain,Peptide
1	A	209	VAL	Peptide
1	A	210	GLY	Peptide
1	A	246	TYR	Sidechain
1	A	301	PHE	Mainchain,Peptide
1	A	311	TYR	Sidechain
1	A	317	ARG	Sidechain
1	A	55	LYS	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3514	0	3448	125	0
2	A	184	0	0	13	0
All	All	3698	0	3448	125	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 18.

All (125) 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:46:TRP:C	1:A:47:VAL:N	1.72	1.41
1:A:36:ARG:C	1:A:37:LYS:N	1.74	1.38
1:A:46:TRP:C	1:A:47:VAL:CA	2.40	0.89
1:A:256:TYR:HD1	1:A:294:LEU:HD13	1.43	0.81
1:A:61:ILE:HD11	1:A:207:THR:OG1	1.84	0.78
1:A:224:MET:HG2	2:A:579:HOH:O	1.84	0.78
1:A:87:ALA:HB2	1:A:209:VAL:HB	1.64	0.77
1:A:409:ASN:HD22	1:A:411:PHE:H	1.33	0.77
1:A:83:SER:HB3	1:A:137:ILE:HG12	1.66	0.77
1:A:41:SER:HA	1:A:44:LEU:HD22	1.66	0.77
1:A:32:MET:HG2	1:A:37:LYS:CD	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:HB3	2:A:484:HOH:O	1.88	0.73
1:A:202:ARG:NH1	1:A:281:GLN:HG2	2.03	0.73
1:A:200:GLY:HA3	2:A:547:HOH:O	1.92	0.69
1:A:204:SER:O	1:A:210:GLY:HA3	1.93	0.69
1:A:202:ARG:HH11	1:A:281:GLN:HG2	1.58	0.69
1:A:32:MET:HG2	1:A:37:LYS:HD3	1.75	0.67
1:A:253:ASN:O	1:A:257:ARG:HD3	1.96	0.66
1:A:210:GLY:O	1:A:214:ILE:HG23	1.96	0.66
1:A:8:SER:HA	1:A:11:LEU:HD22	1.77	0.66
1:A:54:ASP:HA	2:A:526:HOH:O	1.93	0.66
1:A:256:TYR:CD1	1:A:294:LEU:HD13	2.28	0.65
1:A:32:MET:HG2	1:A:37:LYS:HD2	1.78	0.65
1:A:30:HIS:HD2	1:A:246:TYR:OH	1.82	0.62
1:A:69:ARG:HD2	1:A:216:VAL:HA	1.81	0.61
1:A:208:ALA:O	1:A:209:VAL:HG22	2.00	0.61
1:A:37:LYS:HG2	1:A:38:GLY:N	2.15	0.61
1:A:409:ASN:ND2	1:A:411:PHE:H	1.99	0.60
1:A:132:LEU:HD13	1:A:157:MET:SD	2.41	0.60
1:A:317:ARG:N	1:A:317:ARG:HD2	2.17	0.59
1:A:203:TYR:H	1:A:203:TYR:HD1	1.51	0.59
1:A:202:ARG:HG2	1:A:203:TYR:CD1	2.38	0.58
1:A:155:ASP:O	1:A:159:LYS:HD3	2.04	0.57
1:A:203:TYR:HA	2:A:504:HOH:O	2.05	0.57
1:A:51:ILE:HG13	1:A:52:ARG:HG3	1.87	0.56
1:A:176:ARG:CZ	1:A:176:ARG:HB2	2.36	0.56
1:A:266:VAL:HB	1:A:299:VAL:HG12	1.89	0.55
1:A:85:LEU:HD23	1:A:281:GLN:HE21	1.72	0.54
1:A:408:VAL:O	1:A:410:PRO:HD3	2.08	0.54
1:A:264:LEU:HD23	1:A:297:ALA:HB3	1.90	0.53
1:A:247:GLN:O	1:A:251:VAL:HG13	2.08	0.53
1:A:347:PHE:CE1	1:A:348:LEU:HD13	2.43	0.53
1:A:163:LYS:O	1:A:167:ARG:HG3	2.09	0.53
1:A:327:LYS:HE2	1:A:381:ASP:HA	1.90	0.53
1:A:328:LYS:HZ2	1:A:382:GLU:CD	2.11	0.53
1:A:229:ALA:O	1:A:232:TYR:HB3	2.09	0.52
1:A:46:TRP:C	1:A:47:VAL:HA	2.30	0.52
1:A:214:ILE:HD12	1:A:219:LEU:CB	2.40	0.52
1:A:203:TYR:CD1	1:A:203:TYR:N	2.77	0.51
1:A:193:PHE:CB	1:A:207:THR:HG21	2.41	0.51
1:A:202:ARG:HG2	1:A:203:TYR:CE1	2.46	0.51
1:A:409:ASN:C	1:A:409:ASN:HD22	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:CG	1:A:203:TYR:CD1	2.93	0.51
1:A:145:GLU:HB2	1:A:146:PRO:HD3	1.92	0.51
1:A:441:LYS:HG3	2:A:494:HOH:O	2.09	0.50
1:A:122:HIS:O	1:A:125:ASP:HB2	2.10	0.50
1:A:69:ARG:HG2	1:A:106:THR:OG1	2.11	0.49
1:A:318:ASN:H	1:A:318:ASN:HD22	1.60	0.48
1:A:243:ASN:C	1:A:243:ASN:HD22	2.16	0.48
1:A:37:LYS:HG2	2:A:566:HOH:O	2.14	0.47
1:A:348:LEU:O	1:A:351:LYS:HB2	2.14	0.47
1:A:421:LYS:HD3	1:A:435:GLU:HG2	1.96	0.47
1:A:83:SER:HB3	1:A:137:ILE:CG1	2.39	0.47
1:A:137:ILE:HB	1:A:173:THR:HB	1.97	0.47
1:A:358:LYS:O	1:A:362:GLN:HG3	2.15	0.47
1:A:164:GLU:HA	1:A:167:ARG:HH11	1.80	0.47
1:A:210:GLY:O	1:A:213:PRO:HD2	2.15	0.47
1:A:227:GLY:HA3	1:A:386:TYR:O	2.15	0.47
1:A:172:VAL:HG13	1:A:181:LEU:HG	1.96	0.47
1:A:44:LEU:O	1:A:47:VAL:HG13	2.15	0.47
1:A:327:LYS:HZ3	1:A:379:GLU:HG2	1.80	0.46
1:A:203:TYR:HD1	1:A:203:TYR:N	2.11	0.46
1:A:82:GLY:HA3	1:A:202:ARG:HA	1.98	0.46
1:A:184:LEU:HD13	1:A:190:TYR:HE2	1.80	0.46
1:A:333:LEU:HB2	1:A:353:LEU:HD12	1.97	0.46
1:A:328:LYS:NZ	1:A:382:GLU:CD	2.69	0.46
1:A:437:ALA:O	1:A:441:LYS:HE2	2.15	0.45
1:A:205:VAL:HG11	2:A:579:HOH:O	2.15	0.45
1:A:320:ILE:HD12	1:A:376:LEU:HD22	1.98	0.45
1:A:299:VAL:HG22	1:A:304:ASP:CB	2.46	0.45
1:A:62:LYS:HD2	1:A:221:ILE:HD11	1.99	0.45
1:A:310:GLN:HB3	2:A:587:HOH:O	2.17	0.45
1:A:36:ARG:C	1:A:37:LYS:CA	2.78	0.45
1:A:199:ILE:CD1	1:A:206:LEU:HD11	2.46	0.45
1:A:426:LEU:HD13	1:A:439:LEU:HD23	1.99	0.44
1:A:4:SER:HB3	2:A:571:HOH:O	2.18	0.44
1:A:137:ILE:HG21	1:A:209:VAL:HG13	2.00	0.44
1:A:27:LYS:O	1:A:31:HIS:HD2	2.00	0.44
1:A:202:ARG:HB2	2:A:504:HOH:O	2.16	0.43
1:A:217:ALA:HB3	1:A:219:LEU:HD22	2.00	0.43
1:A:299:VAL:HG22	1:A:304:ASP:HB3	2.00	0.43
1:A:37:LYS:CG	1:A:38:GLY:N	2.81	0.43
1:A:49:TRP:HB3	1:A:50:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HE3	1:A:163:LYS:HB3	1.83	0.43
1:A:439:LEU:O	1:A:442:ARG:HB2	2.18	0.43
1:A:46:TRP:CA	1:A:47:VAL:N	2.72	0.43
1:A:202:ARG:NH2	2:A:533:HOH:O	2.51	0.43
1:A:268:TYR:HA	1:A:301:PHE:O	2.18	0.43
1:A:201:GLY:O	1:A:202:ARG:HD3	2.18	0.43
1:A:14:MET:HB2	1:A:258:LYS:HE3	2.01	0.43
1:A:348:LEU:HA	1:A:351:LYS:HD2	2.00	0.43
1:A:310:GLN:HE21	1:A:314:GLU:HB2	1.84	0.43
1:A:53:TYR:O	1:A:54:ASP:CB	2.67	0.43
1:A:107:GLN:C	1:A:108:ILE:HG12	2.38	0.42
1:A:53:TYR:O	1:A:54:ASP:HB3	2.19	0.42
1:A:214:ILE:HD12	1:A:219:LEU:HB3	2.01	0.42
1:A:9:ASN:HB2	1:A:375:ASN:O	2.18	0.42
1:A:403:GLY:HA3	1:A:410:PRO:HG3	2.00	0.42
1:A:300:ASP:HB3	2:A:462:HOH:O	2.19	0.41
1:A:324:LEU:HA	1:A:324:LEU:HD23	1.82	0.41
1:A:201:GLY:O	1:A:202:ARG:CD	2.68	0.41
1:A:316:ARG:C	1:A:317:ARG:HD2	2.40	0.41
1:A:435:GLU:OE1	1:A:435:GLU:N	2.50	0.41
1:A:115:ILE:O	1:A:115:ILE:HG22	2.19	0.41
1:A:266:VAL:HG22	1:A:323:VAL:HG13	2.03	0.41
1:A:143:THR:O	1:A:146:PRO:HD2	2.20	0.41
1:A:83:SER:O	1:A:209:VAL:HG11	2.21	0.41
1:A:34:HIS:HE1	1:A:397:LYS:NZ	2.19	0.41
1:A:201:GLY:O	1:A:202:ARG:CG	2.68	0.41
1:A:171:TYR:CD1	1:A:171:TYR:N	2.89	0.40
1:A:195:ILE:HG12	1:A:208:ALA:HB2	2.02	0.40
1:A:200:GLY:O	1:A:202:ARG:N	2.51	0.40
1:A:340:GLU:HG3	1:A:340:GLU:H	1.58	0.40
1:A:341:ASN:HB2	1:A:346:ASN:ND2	2.36	0.40
1:A:345:LEU:O	1:A:348:LEU:HB2	2.22	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	440/445 (99%)	418 (95%)	18 (4%)	4 (1%)	17 20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	VAL
1	A	202	ARG
1	A	36	ARG
1	A	210	GLY

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	371/374 (99%)	313 (84%)	58 (16%)	2 2

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	23	SER
1	A	36	ARG
1	A	44	LEU
1	A	62	LYS
1	A	63	GLN
1	A	66	GLU
1	A	72	SER
1	A	77	VAL
1	A	85	LEU
1	A	94	LEU
1	A	104	ASP
1	A	108	ILE

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Mol	Chain	Res	Type
1	A	120	ILE
1	A	121	SER
1	A	124	LEU
1	A	126	VAL
1	A	131	ASP
1	A	132	LEU
1	A	137	ILE
1	A	139	LYS
1	A	168	LYS
1	A	178	LYS
1	A	183	LYS
1	A	184	LEU
1	A	197	ASP
1	A	202	ARG
1	A	203	TYR
1	A	211	LEU
1	A	214	ILE
1	A	219	LEU
1	A	234	LYS
1	A	237	ASN
1	A	243	ASN
1	A	255	LEU
1	A	294	LEU
1	A	299	VAL
1	A	318	ASN
1	A	320	ILE
1	A	324	LEU
1	A	327	LYS
1	A	330	GLN
1	A	331	ILE
1	A	336	GLN
1	A	337	GLU
1	A	340	GLU
1	A	345	LEU
1	A	348	LEU
1	A	359	LYS
1	A	366	LEU
1	A	376	LEU
1	A	378	VAL
1	A	406	LEU
1	A	408	VAL
1	A	409	ASN

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Mol	Chain	Res	Type
1	A	413	GLN
1	A	421	LYS
1	A	426	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	31	HIS
1	A	34	HIS
1	A	233	HIS
1	A	237	ASN
1	A	243	ASN
1	A	281	GLN
1	A	310	GLN
1	A	318	ASN
1	A	336	GLN
1	A	357	ASN
1	A	409	ASN
1	A	413	GLN
1	A	422	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:ARG	C	37:LYS	N	1.74
1	A	46:TRP	C	47:VAL	N	1.72
1	A	37:LYS	C	38:GLY	N	0.98

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.