



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 12:39 AM EDT

PDB ID : 1NXH
Title : X-RAY STRUCTURE: NORTHEAST STRUCTURAL GENOMICS CON-
SORTIUM TARGET TT87
Authors : Khayat, R.; Savchenko, A.; Edwards, A.; Arowsmith, C.; Tong, L.; Northeast
Structural Genomics Consortium (NESG)
Deposited on : unknown
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

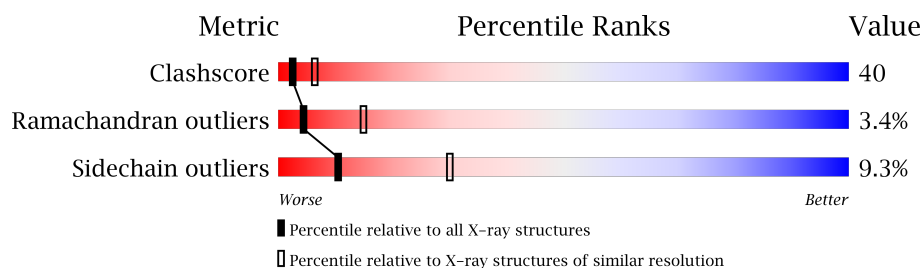
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	126	
1	B	126	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2012 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 MTH396 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	Se	0	0	0
			1029	641	182	199	2	5			
1	B	118	Total	C	N	O	S	Se	0	0	0
			983	613	176	187	2	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MSE	MET	MODIFIED RESIDUE	UNP O26496
A	10	MSE	MET	MODIFIED RESIDUE	UNP O26496
A	44	MSE	MET	MODIFIED RESIDUE	UNP O26496
A	49	MSE	MET	MODIFIED RESIDUE	UNP O26496
A	84	MSE	MET	MODIFIED RESIDUE	UNP O26496
B	207	MSE	MET	MODIFIED RESIDUE	GB 15678424
B	210	MSE	MET	MODIFIED RESIDUE	GB 15678424
B	244	MSE	MET	MODIFIED RESIDUE	GB 15678424
B	249	MSE	MET	MODIFIED RESIDUE	GB 15678424
B	284	MSE	MET	MODIFIED RESIDUE	GB 15678424

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Note EDS was not executed.

- Chain A:
-
- 39% 48% 10%
- MET ASP E3 G4 E5 R8 L9 M10 K11 R12 R13 I14 L15 E16 S17 Q21 Y22 V25 R26 P27 L28 S29 R30 E31 L32 E33 R34 D35 V36 E37 E38 F39 D40 D41 L42 L43 D44 D45 L46 L47 D48 M49 S50 S51 A54 L55 H56 P57 A62 R63 P64 R65 G66 L67 R68

- Chain B:
-
- 38% 51% 5% 6%
- MET ASP GLU GLY E205 R208 L209 M210 K211 R212 R213 I214 L215 E216 S217 Y218 R219 G220 Q221 E222 D223 D224 V225 P227 L228 S229 R230 E231 L232 GLU R318 R319 I320 ASP V236 E237 E238 P239 Q240 D241 I242 L243 E244 D248 M249 S250 S251 L252 E253 A254 L255 E256 P257 R258 P259 R263 D264

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.22Å 80.22Å 106.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.80	Depositor
% Data completeness (in resolution range)	91.2 (19.90-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2012	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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	0.47	0/1037	0.68	0/1382
1	B	0.44	0/990	0.61	0/1317
All	All	0.46	0/2027	0.65	0/2699

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1029	0	1031	95	0
1	B	983	0	989	85	0
All	All	2012	0	2020	163	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 40.

All (163) 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:29:SER:HA	1:A:33:GLU:HB2	1.27	1.13
1:B:211:LYS:HD3	1:B:244:MSE:HE2	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:CA	1:A:33:GLU:HB2	2.00	0.92
1:A:30:ARG:HE	1:A:30:ARG:HA	1.36	0.86
1:B:321:HIS:O	1:B:325:ARG:HG2	1.77	0.85
1:B:307:ARG:HG2	1:B:312:ALA:HB2	1.56	0.85
1:A:26:LYS:HB3	1:A:27:PRO:HD3	1.58	0.84
1:A:29:SER:HA	1:A:33:GLU:CB	2.08	0.82
1:A:63:ARG:HA	1:B:279:TRP:HH2	1.50	0.77
1:B:319:ARG:O	1:B:323:ILE:HG13	1.84	0.76
1:A:12:ARG:NH1	1:A:44:MSE:HG3	2.01	0.75
1:B:248:ASP:O	1:B:252:LEU:HD23	1.87	0.74
1:B:284:MSE:HE2	1:B:286:ILE:HD11	1.70	0.73
1:A:31:GLU:C	1:A:33:GLU:N	2.36	0.73
1:A:33:GLU:O	1:A:33:GLU:HG3	1.88	0.73
1:B:205:GLU:OE1	1:B:208:ARG:HD2	1.89	0.72
1:A:84:MSE:HE1	1:B:228:LEU:HD11	1.73	0.70
1:A:31:GLU:C	1:A:33:GLU:H	1.91	0.70
1:B:256:HIS:O	1:B:259:PHE:HB2	1.92	0.69
1:A:33:GLU:C	1:A:34:ILE:HD12	2.13	0.68
1:A:79:TRP:HB3	1:A:84:MSE:HE2	1.74	0.68
1:A:32:LEU:HG	1:B:317:ARG:CD	2.25	0.67
1:B:307:ARG:CG	1:B:312:ALA:HB2	2.25	0.66
1:B:213:ARG:NH2	1:B:216:GLU:HB3	2.10	0.66
1:A:11:LYS:HG3	1:A:44:MSE:SE	2.45	0.66
1:A:63:ARG:O	1:A:67:ILE:HG13	1.96	0.66
1:B:205:GLU:HA	1:B:208:ARG:CZ	2.26	0.66
1:A:63:ARG:N	1:A:64:PRO:HD2	2.10	0.65
1:A:21:GLN:HA	1:A:25:VAL:HG23	1.77	0.65
1:A:33:GLU:O	1:A:34:ILE:C	2.34	0.64
1:A:32:LEU:O	1:A:34:ILE:N	2.31	0.63
1:A:100:THR:HG22	1:A:104:LEU:HD22	1.80	0.63
1:B:213:ARG:HH21	1:B:216:GLU:HB3	1.64	0.62
1:A:84:MSE:HG2	1:B:259:PHE:CE2	2.34	0.61
1:A:99:ILE:O	1:A:103:VAL:HG12	2.00	0.61
1:A:10:MSE:HE3	1:A:49:MSE:CE	2.31	0.61
1:B:221:GLN:O	1:B:226:LYS:HB2	2.01	0.61
1:B:211:LYS:CD	1:B:244:MSE:HE2	2.23	0.60
1:A:33:GLU:O	1:A:34:ILE:HD12	2.02	0.60
1:B:255:LEU:HB3	1:B:259:PHE:CZ	2.37	0.60
1:A:84:MSE:HE1	1:B:228:LEU:CD1	2.31	0.60
1:A:30:ARG:HE	1:A:30:ARG:CA	2.10	0.59
1:B:223:ASP:C	1:B:227:PRO:HG2	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:HIS:HA	1:A:77:LEU:HD12	1.84	0.58
1:A:32:LEU:HG	1:B:317:ARG:HD3	1.86	0.58
1:B:227:PRO:O	1:B:229:SER:N	2.33	0.58
1:B:225:VAL:HG11	1:B:240:GLN:HE21	1.69	0.58
1:B:215:LEU:HB3	1:B:240:GLN:HE22	1.69	0.58
1:B:284:MSE:CE	1:B:286:ILE:HD11	2.35	0.57
1:A:74:ASP:HB3	1:A:113:LEU:HD11	1.87	0.57
1:A:80:LEU:HD12	1:A:84:MSE:HE3	1.87	0.57
1:A:84:MSE:HG2	1:B:259:PHE:CZ	2.40	0.57
1:A:33:GLU:O	1:A:35:ASP:N	2.38	0.56
1:A:100:THR:CG2	1:A:104:LEU:HD22	2.36	0.56
1:A:56:HIS:HB3	1:A:57:PRO:HD3	1.87	0.56
1:A:84:MSE:O	1:A:85:GLU:HB2	2.06	0.56
1:A:10:MSE:O	1:A:13:ARG:HB2	2.04	0.56
1:B:237:GLU:O	1:B:240:GLN:HB2	2.05	0.56
1:A:10:MSE:HE3	1:A:49:MSE:HE2	1.88	0.55
1:B:263:ARG:O	1:B:267:ILE:HG13	2.06	0.55
1:A:3:GLU:C	1:A:5:GLU:H	2.10	0.55
1:B:222:GLU:HA	1:B:222:GLU:OE1	2.06	0.55
1:A:8:ARG:O	1:A:12:ARG:HB2	2.07	0.55
1:B:224:VAL:HG21	1:B:259:PHE:CD1	2.41	0.55
1:A:95:LEU:O	1:A:99:ILE:HG12	2.07	0.55
1:B:215:LEU:HB3	1:B:240:GLN:NE2	2.23	0.54
1:B:205:GLU:HA	1:B:208:ARG:NH1	2.23	0.54
1:B:205:GLU:CA	1:B:208:ARG:CZ	2.87	0.53
1:B:208:ARG:O	1:B:212:ARG:HB2	2.08	0.53
1:B:219:ARG:HB3	1:B:256:HIS:NE2	2.24	0.53
1:A:32:LEU:HG	1:B:317:ARG:HD2	1.92	0.52
1:B:219:ARG:O	1:B:223:ASP:HB3	2.10	0.52
1:A:98:GLU:OE2	1:A:119:ARG:HD2	2.09	0.52
1:A:31:GLU:HB3	1:B:321:HIS:CE1	2.45	0.52
1:A:63:ARG:HA	1:B:279:TRP:CH2	2.38	0.52
1:B:317:ARG:HG2	1:B:321:HIS:CE1	2.45	0.52
1:A:83:VAL:O	1:B:258:ARG:NH1	2.41	0.51
1:A:30:ARG:NE	1:A:30:ARG:HA	2.15	0.51
1:A:48:ASP:OD1	1:A:51:SER:OG	2.24	0.51
1:A:62:ALA:C	1:A:64:PRO:HD2	2.31	0.51
1:B:224:VAL:C	1:B:227:PRO:HD2	2.32	0.50
1:B:205:GLU:N	1:B:208:ARG:NH2	2.59	0.50
1:B:295:LEU:O	1:B:299:ILE:HG12	2.12	0.50
1:B:225:VAL:HG11	1:B:240:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:HA	1:A:25:VAL:CG2	2.41	0.49
1:B:238:GLU:O	1:B:241:ASP:N	2.45	0.49
1:B:294:ALA:O	1:B:297:ASP:HB2	2.12	0.49
1:B:226:LYS:N	1:B:227:PRO:CD	2.75	0.49
1:A:99:ILE:HD11	1:A:116:GLY:HA2	1.95	0.48
1:B:210:MSE:HB2	1:B:249:MSE:HE1	1.95	0.48
1:A:115:GLU:HG2	1:A:118:ARG:NH2	2.28	0.48
1:A:29:SER:HA	1:A:33:GLU:CD	2.34	0.48
1:A:36:VAL:O	1:A:37:GLU:C	2.51	0.48
1:A:63:ARG:N	1:A:64:PRO:CD	2.77	0.48
1:B:251:SER:O	1:B:255:LEU:HG	2.14	0.48
1:B:274:ASP:HB3	1:B:313:LEU:HD21	1.96	0.47
1:A:31:GLU:O	1:A:32:LEU:HB2	2.14	0.47
1:A:115:GLU:HG2	1:A:118:ARG:HH21	1.79	0.47
1:B:228:LEU:HD12	1:B:239:PHE:CZ	2.50	0.47
1:A:35:ASP:O	1:A:36:VAL:C	2.52	0.47
1:B:214:ILE:O	1:B:217:SER:CB	2.63	0.47
1:A:34:ILE:O	1:A:35:ASP:O	2.33	0.47
1:B:238:GLU:O	1:B:242:ILE:HG12	2.15	0.47
1:A:94:ALA:O	1:A:98:GLU:HG2	2.15	0.47
1:A:84:MSE:CE	1:B:228:LEU:HD11	2.42	0.47
1:B:325:ARG:HG3	1:B:325:ARG:NH1	2.30	0.47
1:A:29:SER:HA	1:A:33:GLU:CG	2.45	0.46
1:B:308:GLU:O	1:B:309:TYR:C	2.54	0.46
1:A:46:LYS:HG3	1:B:286:ILE:CG2	2.46	0.46
1:B:247:LEU:HD22	1:B:255:LEU:HD11	1.97	0.46
1:B:215:LEU:HD22	1:B:244:MSE:CE	2.45	0.46
1:B:298:GLU:OE2	1:B:319:ARG:NH1	2.45	0.46
1:A:26:LYS:HB3	1:A:27:PRO:CD	2.37	0.46
1:A:108:GLU:O	1:A:109:TYR:C	2.53	0.45
1:A:46:LYS:HG3	1:B:286:ILE:HG23	1.98	0.45
1:A:82:ASP:N	1:A:82:ASP:OD2	2.50	0.45
1:B:211:LYS:C	1:B:213:ARG:N	2.66	0.45
1:A:14:ILE:O	1:A:17:SER:HB3	2.16	0.45
1:B:263:ARG:N	1:B:264:PRO:CD	2.80	0.45
1:A:27:PRO:O	1:A:29:SER:N	2.43	0.45
1:A:38:GLU:O	1:A:41:ASP:N	2.50	0.45
1:B:284:MSE:O	1:B:285:GLU:HB2	2.16	0.45
1:B:270:LYS:HG2	1:B:309:TYR:CZ	2.53	0.44
1:B:219:ARG:C	1:B:256:HIS:HE1	2.21	0.44
1:B:238:GLU:O	1:B:239:PHE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ILE:HD13	1:B:324:LEU:HB3	1.98	0.44
1:A:27:PRO:C	1:A:29:SER:H	2.21	0.44
1:A:64:PRO:HG2	1:A:65:ARG:H	1.81	0.44
1:A:68:ARG:NH2	1:A:93:GLU:OE2	2.51	0.44
1:B:255:LEU:HB3	1:B:259:PHE:CE2	2.52	0.44
1:B:244:MSE:CE	1:B:244:MSE:HA	2.48	0.43
1:A:9:LEU:O	1:A:13:ARG:HG3	2.18	0.43
1:A:3:GLU:O	1:A:5:GLU:N	2.46	0.43
1:A:107:ARG:HH11	1:A:107:ARG:HG2	1.82	0.43
1:A:38:GLU:O	1:A:39:PHE:C	2.57	0.43
1:A:125:ARG:NE	1:B:238:GLU:OE2	2.52	0.42
1:A:100:THR:HA	1:A:103:VAL:CG1	2.49	0.42
1:A:94:ALA:O	1:A:97:ASP:HB2	2.19	0.42
1:B:236:VAL:O	1:B:237:GLU:C	2.57	0.42
1:A:31:GLU:O	1:A:33:GLU:N	2.52	0.42
1:B:221:GLN:HB3	1:B:221:GLN:HE21	1.65	0.42
1:B:239:PHE:HA	1:B:242:ILE:HG12	2.00	0.42
1:A:21:GLN:CA	1:A:25:VAL:HG23	2.48	0.42
1:B:242:ILE:HD13	1:B:242:ILE:N	2.35	0.42
1:A:56:HIS:O	1:A:57:PRO:C	2.58	0.42
1:A:109:TYR:O	1:A:110:SER:C	2.58	0.42
1:A:14:ILE:O	1:A:17:SER:CB	2.67	0.42
1:A:47:LEU:HD13	1:A:55:LEU:HD11	2.02	0.41
1:B:238:GLU:HG2	1:B:242:ILE:HD11	2.02	0.41
1:A:98:GLU:CD	1:A:119:ARG:NH1	2.74	0.41
1:A:32:LEU:C	1:A:34:ILE:H	2.24	0.41
1:A:15:LEU:CD1	1:A:44:MSE:HG2	2.51	0.41
1:B:214:ILE:O	1:B:217:SER:HB3	2.19	0.41
1:B:239:PHE:CA	1:B:242:ILE:HG12	2.51	0.41
1:A:21:GLN:O	1:A:26:LYS:CB	2.69	0.40
1:A:26:LYS:O	1:A:29:SER:OG	2.34	0.40
1:B:229:SER:C	1:B:231:GLU:H	2.25	0.40
1:B:308:GLU:HB2	1:B:311:GLU:HG3	2.03	0.40
1:A:117:ARG:O	1:A:120:LEU:HB3	2.21	0.40
1:A:34:ILE:CG2	1:B:321:HIS:HD2	2.35	0.40
1:B:271:LEU:O	1:B:272:HIS:C	2.59	0.40
1:A:3:GLU:C	1:A:5:GLU:N	2.74	0.40
1:B:284:MSE:SE	1:B:286:ILE:HD11	2.72	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	122/126 (97%)	94 (77%)	23 (19%)	5 (4%)	3	11
1	B	114/126 (90%)	95 (83%)	16 (14%)	3 (3%)	6	21
All	All	236/252 (94%)	189 (80%)	39 (16%)	8 (3%)	4	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	34	ILE
1	A	35	ASP
1	B	254	ALA
1	A	54	ALA
1	B	228	LEU
1	A	36	VAL
1	B	230	ARG

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	115/112 (103%)	101 (88%)	14 (12%)	6	17
1	B	110/112 (98%)	103 (94%)	7 (6%)	20	50
All	All	225/224 (100%)	204 (91%)	21 (9%)	10	30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	GLU
1	A	16	GLU
1	A	25	VAL
1	A	30	ARG
1	A	34	ILE
1	A	35	ASP
1	A	80	LEU
1	A	82	ASP
1	A	103	VAL
1	A	104	LEU
1	A	107	ARG
1	A	110	SER
1	A	113	LEU
1	B	205	GLU
1	B	209	LEU
1	B	216	GLU
1	B	244	MSE
1	B	248	ASP
1	B	296	LYS
1	B	307	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	72	HIS
1	A	121	HIS
1	B	221	GLN
1	B	240	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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](#)

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 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.