



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:56 AM UTC

PDB ID : 1ASK / pdb_00001ask
Title : NUCLEAR TRANSPORT FACTOR 2 (NTF2) H66A MUTANT
Authors : Mccoy, A.J.; Stewart, M.J.
Deposited on : 1997-08-11
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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

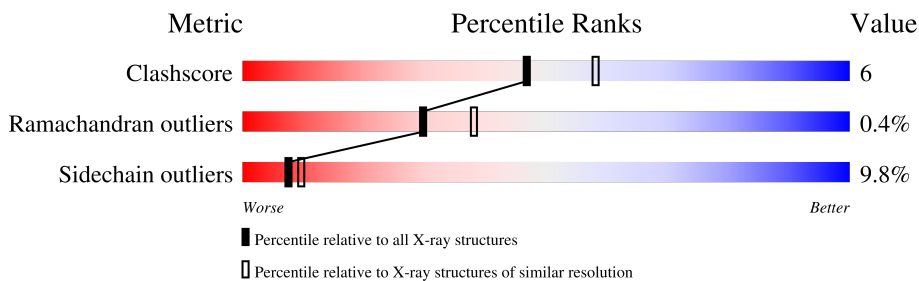
1 Overall quality at a glance

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	 53% 31% 8% 7%
1	B	127	 54% 29% 9% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2014 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 NUCLEAR TRANSPORT FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1000	640	166	187	7			
1	B	120	Total	C	N	O	S	0	0	0
			959	615	158	179	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	ALA	HIS	engineered mutation	UNP P61972
B	66	ALA	HIS	engineered mutation	UNP P61972

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		
2	B	31	Total	O	0	0
			31	31		

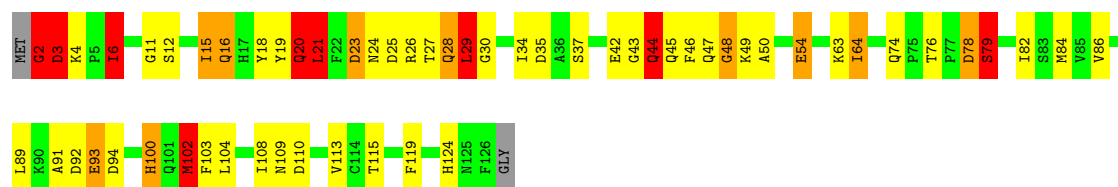
3 Residue-property plots [i](#)

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 was not executed.

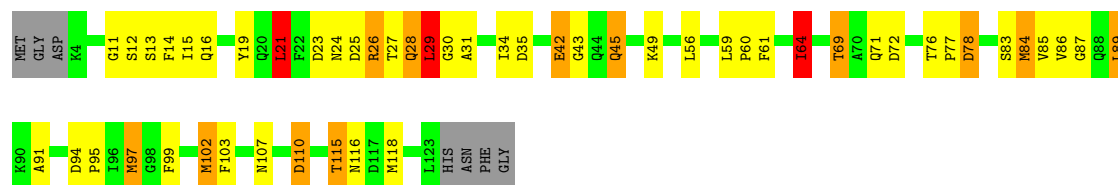
• Molecule 1: NUCLEAR TRANSPORT FACTOR 2

Chain A: 



• Molecule 1: NUCLEAR TRANSPORT FACTOR 2

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.00Å 57.46Å 87.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.2 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2014	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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	1.05	3/1025 (0.3%)	2.35	61/1389 (4.4%)
1	B	1.03	0/982	2.31	63/1331 (4.7%)
All	All	1.04	3/2007 (0.1%)	2.33	124/2720 (4.6%)

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	7
1	B	0	5
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	GLN	CD-OE1	10.10	1.42	1.23
1	A	44	GLN	CG-CD	6.95	1.69	1.52
1	A	44	GLN	CA-CB	6.17	1.62	1.53

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLN	OE1-CD-NE2	-14.48	108.12	122.60
1	A	44	GLN	OE1-CD-NE2	-13.05	109.55	122.60
1	A	23	ASP	O-C-N	-10.23	108.72	122.43
1	A	47	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	B	71	GLN	OE1-CD-NE2	-8.55	114.05	122.60
1	A	44	GLN	CB-CA-C	-8.45	95.94	109.80
1	B	76	THR	O-C-N	-8.40	115.09	121.14
1	A	21	LEU	O-C-N	-8.38	113.44	122.07
1	A	30	GLY	O-C-N	-8.32	113.42	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ASP	CA-CB-CG	-8.26	104.34	112.60
1	A	30	GLY	CA-C-N	8.13	131.99	120.28
1	A	30	GLY	C-N-CA	8.13	131.99	120.28
1	B	26	ARG	N-CA-C	7.90	122.59	113.19
1	B	45	GLN	O-C-N	-7.86	114.39	123.27
1	A	20	GLN	CB-CG-CD	7.86	125.96	112.60
1	B	97	MET	CA-C-N	7.70	128.37	120.60
1	B	97	MET	C-N-CA	7.70	128.37	120.60
1	B	116	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	A	110	ASP	O-C-N	-7.62	113.73	121.88
1	B	16	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	B	77	PRO	O-C-N	-7.43	112.20	122.30
1	B	34	ILE	CA-C-N	7.34	130.11	120.28
1	B	34	ILE	C-N-CA	7.34	130.11	120.28
1	B	11	GLY	CA-C-N	7.32	130.08	120.28
1	B	11	GLY	C-N-CA	7.32	130.08	120.28
1	B	107	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	A	26	ARG	N-CA-C	6.81	121.19	113.02
1	B	30	GLY	CA-C-N	6.78	129.66	120.38
1	B	30	GLY	C-N-CA	6.78	129.66	120.38
1	B	86	VAL	CG1-CB-CG2	-6.75	95.96	110.80
1	A	16	GLN	O-C-N	-6.74	115.13	122.07
1	A	27	THR	CA-C-N	6.66	134.56	121.58
1	A	27	THR	C-N-CA	6.66	134.56	121.58
1	B	19	TYR	CA-C-N	6.57	129.37	120.44
1	B	19	TYR	C-N-CA	6.57	129.37	120.44
1	A	28	GLN	O-C-N	-6.53	112.89	122.43
1	A	43	GLY	O-C-N	-6.52	113.87	122.28
1	B	78	ASP	CA-CB-CG	6.51	119.11	112.60
1	B	28	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	A	100	HIS	CA-CB-CG	6.45	120.25	113.80
1	A	29	LEU	CA-C-N	6.45	128.20	120.14
1	A	29	LEU	C-N-CA	6.45	128.20	120.14
1	B	30	GLY	O-C-N	-6.40	115.45	122.68
1	A	48	GLY	N-CA-C	6.36	120.18	112.48
1	B	12	SER	CB-CA-C	-6.33	100.28	110.79
1	A	29	LEU	O-C-N	-6.24	114.07	122.43
1	B	11	GLY	O-C-N	-6.23	116.20	122.18
1	B	19	TYR	O-C-N	-6.19	114.13	122.43
1	A	19	TYR	O-C-N	-6.18	114.67	122.27
1	A	64	ILE	CA-C-O	6.11	127.48	120.76
1	B	87	GLY	CA-C-O	6.09	128.52	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CA-C-O	6.05	128.74	118.94
1	A	76	THR	O-C-N	-6.03	116.80	121.14
1	A	24	ASN	CB-CG-ND2	6.01	125.42	116.40
1	B	69	THR	CA-CB-OG1	-6.01	100.59	109.60
1	B	102	MET	O-C-N	-6.01	116.03	123.36
1	A	78	ASP	O-C-N	-6.01	114.64	122.39
1	A	42	GLU	O-C-N	-5.98	115.14	122.55
1	B	85	VAL	CA-CB-CG1	5.97	120.55	110.40
1	B	64	ILE	CA-C-O	5.96	127.32	120.76
1	A	6	ILE	O-C-N	-5.96	115.86	121.87
1	B	27	THR	CA-C-N	5.96	133.16	122.38
1	B	27	THR	C-N-CA	5.96	133.16	122.38
1	A	104	LEU	N-CA-CB	5.93	119.90	110.65
1	B	64	ILE	CA-CB-CG2	5.87	120.49	110.50
1	B	103	PHE	CA-CB-CG	5.83	119.63	113.80
1	B	24	ASN	CB-CG-ND2	5.82	125.13	116.40
1	B	115	THR	O-C-N	-5.81	113.72	122.20
1	A	11	GLY	CA-C-N	5.80	128.33	120.38
1	A	11	GLY	C-N-CA	5.80	128.33	120.38
1	B	77	PRO	CA-C-N	5.76	131.71	122.83
1	B	77	PRO	C-N-CA	5.76	131.71	122.83
1	B	34	ILE	O-C-N	-5.75	115.38	122.57
1	B	110	ASP	N-CA-C	5.74	121.53	113.56
1	A	15	ILE	CB-CG1-CD1	5.72	125.82	113.80
1	B	60	PRO	N-CA-C	5.70	121.47	114.35
1	B	84	MET	CA-C-O	5.69	126.51	120.36
1	B	86	VAL	N-CA-CB	5.67	119.24	111.41
1	A	109	ASN	CA-CB-CG	5.61	118.21	112.60
1	B	31	ALA	O-C-N	-5.58	116.20	122.12
1	A	93	GLU	CB-CG-CD	5.52	121.98	112.60
1	B	19	TYR	N-CA-C	5.52	119.27	112.54
1	B	59	LEU	N-CA-CB	5.42	118.22	110.03
1	A	18	TYR	O-C-N	-5.41	116.46	122.09
1	A	4	LYS	CA-C-O	5.38	123.61	119.46
1	A	37	SER	CA-C-O	-5.38	115.70	121.56
1	A	12	SER	CB-CA-C	-5.37	101.56	110.68
1	A	44	GLN	CG-CD-OE1	5.34	131.47	120.80
1	A	21	LEU	CA-C-O	5.33	126.42	120.82
1	A	79	SER	CA-CB-OG	-5.30	100.51	111.10
1	A	3	ASP	CB-CA-C	5.29	120.95	110.42
1	B	99	PHE	CA-CB-CG	5.29	119.08	113.80
1	B	21	LEU	O-C-N	-5.28	116.39	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	76	THR	N-CA-C	-5.26	102.38	110.58
1	A	119	PHE	O-C-N	5.25	129.68	123.27
1	A	34	ILE	CA-C-O	5.23	127.31	120.78
1	A	76	THR	CA-C-N	5.22	124.83	119.56
1	A	76	THR	C-N-CA	5.22	124.83	119.56
1	B	49	LYS	CA-C-N	5.21	127.52	120.38
1	B	49	LYS	C-N-CA	5.21	127.52	120.38
1	B	13	SER	CB-CA-C	-5.20	102.01	110.85
1	A	86	VAL	N-CA-CB	5.20	118.58	111.41
1	B	42	GLU	CA-CB-CG	5.17	124.45	114.10
1	B	78	ASP	O-C-N	-5.17	115.52	122.19
1	A	2	GLY	N-CA-C	5.16	128.25	113.30
1	A	50	ALA	CA-C-N	5.14	127.58	120.29
1	A	50	ALA	C-N-CA	5.14	127.58	120.29
1	B	43	GLY	O-C-N	-5.14	115.82	122.34
1	A	94	ASP	CA-CB-CG	-5.11	107.50	112.60
1	A	21	LEU	CA-C-N	5.10	127.37	120.38
1	A	21	LEU	C-N-CA	5.10	127.37	120.38
1	A	54	GLU	CB-CG-CD	-5.08	103.97	112.60
1	B	59	LEU	CA-C-O	5.08	126.42	120.69
1	A	49	LYS	N-CA-C	5.06	117.18	111.11
1	A	102	MET	O-C-N	-5.06	117.10	123.27
1	B	76	THR	N-CA-C	-5.05	102.70	110.58
1	A	124	HIS	CA-CB-CG	5.04	118.84	113.80
1	B	107	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	42	GLU	O-C-N	-5.02	115.68	122.41
1	B	116	ASN	CB-CG-OD1	5.02	130.84	120.80
1	B	29	LEU	O-C-N	-5.01	115.55	122.46
1	B	14	PHE	CA-C-N	5.00	127.58	120.53
1	B	14	PHE	C-N-CA	5.00	127.58	120.53

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	THR	Mainchain
1	A	2	GLY	Mainchain
1	A	23	ASP	Mainchain
1	A	3	ASP	Mainchain
1	A	44	GLN	Sidechain
1	A	45	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	6	ILE	Mainchain
1	B	115	THR	Mainchain
1	B	23	ASP	Mainchain
1	B	26	ARG	Mainchain
1	B	45	GLN	Mainchain
1	B	72	ASP	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	1000	0	963	15	0
1	B	959	0	934	11	0
2	A	24	0	0	1	0
2	B	31	0	0	0	0
All	All	2014	0	1897	22	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 (22) 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:B:64:ILE:HD11	1:B:89:LEU:HG	1.68	0.75
1:B:21:LEU:HB3	1:B:29:LEU:HD13	1.72	0.70
1:A:84:MET:HB2	1:B:102:MET:HE3	1.79	0.64
1:A:2:GLY:O	1:A:3:ASP:HB2	1.99	0.60
1:A:82:ILE:HG13	1:A:102:MET:HE2	1.87	0.57
1:B:94:ASP:HB3	1:B:95:PRO:HD2	1.88	0.55
1:A:44:GLN:HB3	1:A:46:PHE:CE1	2.42	0.55
1:A:25:ASP:HB3	1:A:28:GLN:HE21	1.70	0.55
1:A:21:LEU:HB3	1:A:29:LEU:HD13	1.90	0.54
1:A:16:GLN:HG3	1:A:20:GLN:NE2	2.27	0.50
1:A:74:GLN:HG3	1:B:118:MET:HE2	1.94	0.49
1:A:35:ASP:O	1:A:48:GLY:HA2	2.14	0.46
1:B:64:ILE:HD12	1:B:91:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:HG3	2:A:137:HOH:O	2.16	0.46
1:B:15:ILE:HD11	1:B:83:SER:HB3	1.99	0.44
1:A:78:ASP:O	1:A:79:SER:HB2	2.18	0.44
1:B:29:LEU:HD23	1:B:56:LEU:HD13	2.00	0.43
1:A:84:MET:HB2	1:B:102:MET:CE	2.48	0.43
1:A:100:HIS:NE2	1:B:84:MET:HE3	2.34	0.41
1:B:25:ASP:HB3	1:B:28:GLN:OE1	2.19	0.41
1:A:91:ALA:O	1:A:92:ASP:C	2.63	0.41
1:A:108:ILE:HD12	1:A:113:VAL:HG21	2.03	0.41

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	123/127 (97%)	117 (95%)	5 (4%)	1 (1%)	16	20
1	B	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
All	All	241/254 (95%)	232 (96%)	8 (3%)	1 (0%)	30	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP

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	109/110 (99%)	98 (90%)	11 (10%)	7	9
1	B	105/110 (96%)	95 (90%)	10 (10%)	8	10
All	All	214/220 (97%)	193 (90%)	21 (10%)	7	10

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

Mol	Chain	Res	Type
1	A	6	ILE
1	A	15	ILE
1	A	20	GLN
1	A	21	LEU
1	A	29	LEU
1	A	54	GLU
1	A	63	LYS
1	A	64	ILE
1	A	79	SER
1	A	89	LEU
1	A	102	MET
1	B	21	LEU
1	B	29	LEU
1	B	42	GLU
1	B	61	PHE
1	B	64	ILE
1	B	69	THR
1	B	78	ASP
1	B	89	LEU
1	B	97	MET
1	B	110	ASP

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

Mol	Chain	Res	Type
1	A	28	GLN
1	A	45	GLN
1	A	47	GLN
1	A	107	ASN
1	B	45	GLN
1	B	47	GLN
1	B	71	GLN

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Mol	Chain	Res	Type
1	B	73	HIS
1	B	100	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.