



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:00 PM UTC

PDB ID : 1QMA / pdb_00001qma
Title : Nuclear Transport Factor 2 (NTF2) W7A mutant
Authors : Bayliss, R.; Ribbeck, K.; Akin, D.; Kent, H.M.; Feldherr, C.M.; Gorlich, D.; Stewart, M.J.
Deposited on : 1999-09-23
Resolution : 2.50 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

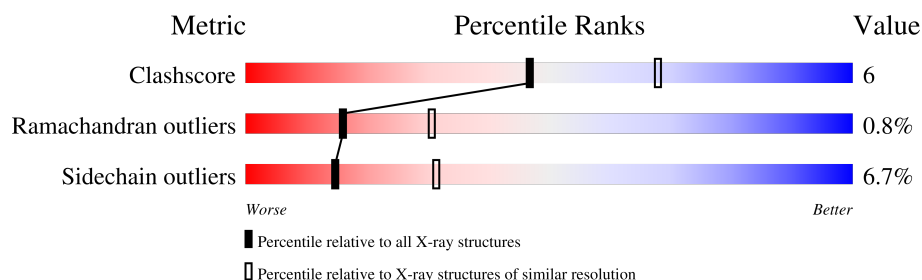
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	126	 55% 31% 11% .
1	B	126	 61% 26% 11% .
1	C	126	 56% 30% 11% .
1	D	126	 63% 25% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4054 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	126	Total	C	N	O	S	66	0	0
			997	636	167	187	7			
1	B	124	Total	C	N	O	S	39	0	0
			988	631	166	184	7			
1	C	126	Total	C	N	O	S	63	0	0
			997	636	167	187	7			
1	D	124	Total	C	N	O	S	38	0	0
			988	631	166	184	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	TRP	engineered mutation	UNP P13662
B	7	ALA	TRP	engineered mutation	UNP P13662
C	7	ALA	TRP	engineered mutation	UNP P13662
D	7	ALA	TRP	engineered mutation	UNP P13662

- Molecule 2 is water.

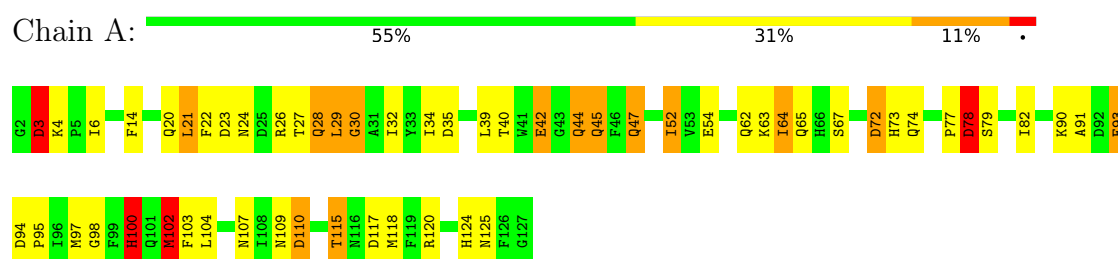
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		
2	B	21	Total	O	0	0
			21	21		
2	C	19	Total	O	0	0
			19	19		
2	D	20	Total	O	0	0
			20	20		

3 Residue-property plots [i](#)

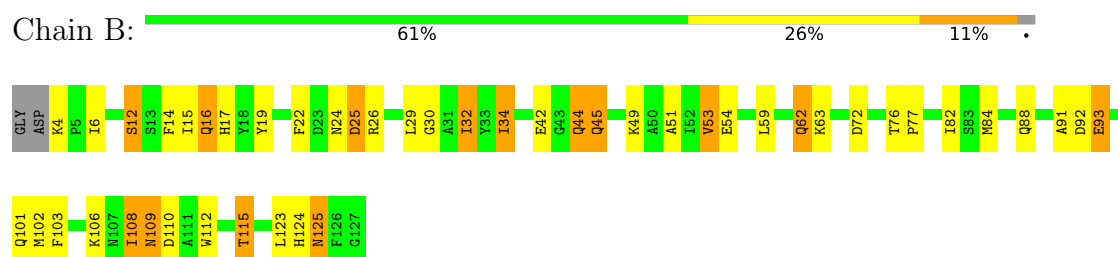
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

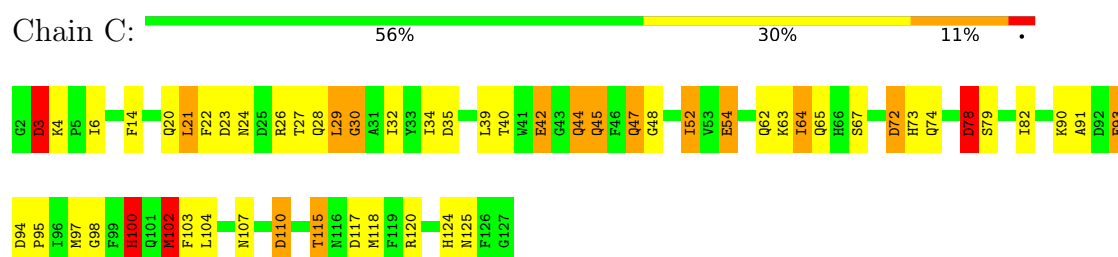
• Molecule 1: NUCLEAR TRANSPORT FACTOR 2



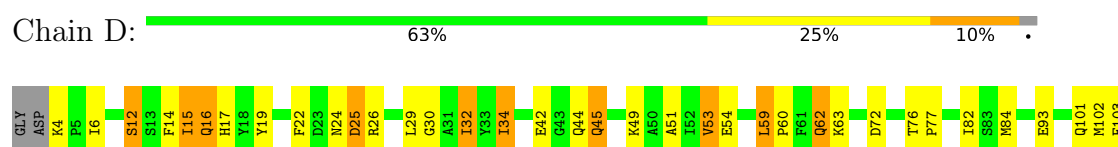
• Molecule 1: NUCLEAR TRANSPORT FACTOR 2

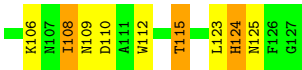


• Molecule 1: NUCLEAR TRANSPORT FACTOR 2



• Molecule 1: NUCLEAR TRANSPORT FACTOR 2





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.65Å 75.41Å 64.54Å 90.00° 115.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	100.0 (6.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4054	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	2.78	18/1021 (1.8%)	2.73	51/1382 (3.7%)
1	B	1.37	8/1012 (0.8%)	2.50	45/1370 (3.3%)
1	C	3.06	21/1021 (2.1%)	2.83	55/1382 (4.0%)
1	D	1.95	12/1012 (1.2%)	2.54	47/1370 (3.4%)
All	All	2.39	59/4066 (1.5%)	2.65	198/5504 (3.6%)

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	13
1	B	0	11
1	C	0	12
1	D	0	10
All	All	0	46

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	ASN	CB-CG	56.00	2.92	1.52
1	D	63	LYS	CE-NZ	44.93	2.84	1.49
1	A	93	GLU	CD-OE1	42.03	2.05	1.25
1	C	93	GLU	CD-OE1	39.81	2.00	1.25
1	A	125	ASN	CB-CG	38.22	2.47	1.52
1	C	90	LYS	CG-CD	-28.05	0.68	1.52
1	A	90	LYS	CG-CD	-25.90	0.74	1.52
1	A	78	ASP	CG-OD2	25.62	1.74	1.25
1	C	78	ASP	CG-OD2	25.47	1.73	1.25
1	C	28	GLN	CG-CD	24.16	2.12	1.52
1	A	62	GLN	CG-CD	23.75	2.11	1.52
1	A	65	GLN	CG-CD	-23.61	0.93	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	65	GLN	CG-CD	-22.63	0.95	1.52
1	C	62	GLN	CG-CD	21.64	2.06	1.52
1	D	16	GLN	CD-OE1	20.63	1.62	1.23
1	A	4	LYS	C-N	19.41	1.57	1.33
1	B	16	GLN	CD-OE1	18.57	1.58	1.23
1	B	63	LYS	CE-NZ	18.20	2.04	1.49
1	C	23	ASP	CG-OD1	-16.37	0.94	1.25
1	B	12	SER	CB-OG	-15.59	1.10	1.42
1	A	93	GLU	CD-OE2	-14.86	0.97	1.25
1	C	4	LYS	C-N	13.79	1.50	1.33
1	A	23	ASP	CG-OD1	-13.52	0.99	1.25
1	D	12	SER	CB-OG	-13.03	1.16	1.42
1	D	25	ASP	CB-CG	-12.64	1.20	1.52
1	A	20	GLN	CG-CD	11.89	1.81	1.52
1	B	25	ASP	CB-CG	-11.23	1.24	1.52
1	A	28	GLN	CG-CD	10.31	1.77	1.52
1	A	47	GLN	CD-OE1	9.66	1.42	1.23
1	A	63	LYS	CG-CD	9.62	1.81	1.52
1	C	63	LYS	CG-CD	9.40	1.80	1.52
1	D	124	HIS	CB-CG	-9.00	1.37	1.50
1	C	93	GLU	CD-OE2	-8.98	1.08	1.25
1	C	47	GLN	CD-OE1	8.88	1.40	1.23
1	B	93	GLU	CG-CD	-8.51	1.30	1.52
1	D	54	GLU	CG-CD	-8.30	1.31	1.52
1	D	93	GLU	CG-CD	-8.26	1.31	1.52
1	C	54	GLU	CD-OE2	7.92	1.40	1.25
1	C	20	GLN	CG-CD	7.78	1.71	1.52
1	C	4	LYS	CA-C	7.71	1.62	1.52
1	D	4	LYS	CG-CD	-7.50	1.29	1.52
1	C	44	GLN	CD-NE2	-7.34	1.17	1.33
1	A	44	GLN	CD-NE2	-7.18	1.18	1.33
1	C	3	ASP	C-N	7.09	1.48	1.33
1	A	3	ASP	C-N	7.05	1.48	1.33
1	B	88	GLN	CD-NE2	-7.02	1.18	1.33
1	A	109	ASN	CB-CG	6.67	1.68	1.52
1	B	4	LYS	CG-CD	-6.51	1.32	1.52
1	B	62	GLN	CB-CG	-6.40	1.33	1.52
1	C	110	ASP	CB-CG	6.38	1.68	1.52
1	C	24	ASN	CG-OD1	-6.10	1.11	1.23
1	A	4	LYS	CA-C	5.89	1.60	1.52
1	A	47	GLN	CD-NE2	5.70	1.45	1.33
1	D	44	GLN	CG-CD	5.63	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	44	GLN	CD-OE1	-5.52	1.13	1.23
1	D	62	GLN	CB-CG	-5.51	1.35	1.52
1	D	49	LYS	CE-NZ	5.50	1.65	1.49
1	C	47	GLN	CD-NE2	5.41	1.44	1.33
1	C	54	GLU	CB-CG	-5.14	1.37	1.52

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	ASN	CA-CB-CG	-35.13	77.47	112.60
1	D	25	ASP	CA-CB-CG	31.68	144.28	112.60
1	B	25	ASP	CA-CB-CG	30.77	143.37	112.60
1	C	78	ASP	OD1-CG-OD2	-29.39	52.37	122.90
1	D	16	GLN	OE1-CD-NE2	-29.28	93.32	122.60
1	A	78	ASP	OD1-CG-OD2	-28.93	53.47	122.90
1	B	16	GLN	OE1-CD-NE2	-28.10	94.50	122.60
1	A	125	ASN	CA-CB-CG	-26.30	86.30	112.60
1	C	65	GLN	CB-CG-CD	25.17	155.39	112.60
1	A	65	GLN	CB-CG-CD	23.64	152.79	112.60
1	A	47	GLN	OE1-CD-NE2	-21.71	100.89	122.60
1	C	47	GLN	OE1-CD-NE2	-20.64	101.96	122.60
1	D	109	ASN	CA-CB-CG	18.25	130.85	112.60
1	A	44	GLN	CG-CD-NE2	-17.68	89.87	116.40
1	C	110	ASP	CA-CB-CG	-16.91	95.69	112.60
1	A	93	GLU	CG-CD-OE2	16.48	156.31	118.40
1	C	93	GLU	CG-CD-OE2	16.41	156.15	118.40
1	C	65	GLN	CG-CD-NE2	16.38	140.97	116.40
1	B	125	ASN	CB-CG-ND2	15.96	140.33	116.40
1	A	110	ASP	CA-CB-CG	-15.83	96.77	112.60
1	C	44	GLN	CG-CD-NE2	-15.79	92.72	116.40
1	C	44	GLN	OE1-CD-NE2	-15.65	106.95	122.60
1	C	93	GLU	OE1-CD-OE2	-14.81	87.35	122.90
1	A	93	GLU	OE1-CD-OE2	-14.54	88.00	122.90
1	C	28	GLN	CG-CD-NE2	14.37	137.95	116.40
1	A	65	GLN	CG-CD-NE2	14.23	137.74	116.40
1	B	109	ASN	CA-CB-CG	13.91	126.52	112.60
1	A	109	ASN	CA-CB-CG	-13.91	98.69	112.60
1	C	28	GLN	CB-CG-CD	-13.43	89.78	112.60
1	D	44	GLN	OE1-CD-NE2	13.09	135.69	122.60
1	D	4	LYS	CB-CG-CD	12.35	139.71	111.30
1	B	125	ASN	CB-CG-OD1	-12.11	96.58	120.80
1	A	44	GLN	OE1-CD-NE2	-11.98	110.62	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	GLN	CB-CG-CD	-11.74	92.64	112.60
1	C	65	GLN	CG-CD-OE1	-11.40	98.00	120.80
1	D	124	HIS	CA-CB-CG	11.13	124.93	113.80
1	A	62	GLN	CB-CG-CD	-10.96	93.97	112.60
1	A	78	ASP	CB-CG-OD2	-10.94	93.23	118.40
1	B	26	ARG	CA-C-N	10.74	139.84	122.65
1	B	26	ARG	C-N-CA	10.74	139.84	122.65
1	D	26	ARG	CA-C-N	10.71	139.79	122.65
1	D	26	ARG	C-N-CA	10.71	139.79	122.65
1	D	4	LYS	CG-CD-CE	10.54	135.54	111.30
1	D	45	GLN	CB-CG-CD	-10.13	95.37	112.60
1	B	93	GLU	CB-CG-CD	10.08	129.74	112.60
1	A	65	GLN	CG-CD-OE1	-9.99	100.81	120.80
1	B	4	LYS	CB-CG-CD	9.73	133.68	111.30
1	C	100	HIS	CA-CB-CG	9.68	123.48	113.80
1	A	100	HIS	CA-CB-CG	9.59	123.39	113.80
1	B	125	ASN	CA-CB-CG	9.57	122.17	112.60
1	C	78	ASP	CB-CG-OD2	-9.39	96.81	118.40
1	C	102	MET	CA-CB-CG	9.36	132.83	114.10
1	A	4	LYS	CA-C-N	9.36	130.06	120.14
1	A	4	LYS	C-N-CA	9.36	130.06	120.14
1	D	16	GLN	CG-CD-NE2	9.35	130.42	116.40
1	D	54	GLU	CB-CG-CD	-9.30	96.78	112.60
1	A	102	MET	CA-CB-CG	9.30	132.70	114.10
1	C	28	GLN	CG-CD-OE1	-9.27	102.26	120.80
1	D	12	SER	CA-CB-OG	9.22	129.55	111.10
1	B	54	GLU	CB-CG-CD	-9.02	97.27	112.60
1	D	59	LEU	CA-C-O	8.88	128.09	119.75
1	B	59	LEU	CA-C-O	8.67	127.90	119.75
1	A	20	GLN	CB-CG-CD	-8.66	97.88	112.60
1	D	125	ASN	CA-CB-CG	-8.65	103.95	112.60
1	B	4	LYS	CG-CD-CE	8.51	130.88	111.30
1	C	23	ASP	CB-CG-OD1	8.45	137.84	118.40
1	B	16	GLN	CG-CD-NE2	8.41	129.01	116.40
1	A	24	ASN	OD1-CG-ND2	8.31	130.91	122.60
1	B	63	LYS	CD-CE-NZ	-8.28	85.41	111.90
1	C	45	GLN	O-C-N	-8.22	113.57	123.27
1	D	93	GLU	CB-CG-CD	8.10	126.36	112.60
1	A	45	GLN	O-C-N	-7.90	113.94	123.27
1	D	51	ALA	CA-C-N	7.85	130.44	120.56
1	D	51	ALA	C-N-CA	7.85	130.44	120.56
1	B	12	SER	CA-CB-OG	7.80	126.69	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ALA	CA-C-N	7.78	130.37	120.56
1	B	51	ALA	C-N-CA	7.78	130.37	120.56
1	A	103	PHE	CA-CB-CG	7.65	121.45	113.80
1	B	30	GLY	O-C-N	-7.57	114.82	122.17
1	C	21	LEU	O-C-N	-7.51	114.33	122.07
1	C	103	PHE	CA-CB-CG	7.48	121.28	113.80
1	A	21	LEU	O-C-N	-7.45	114.39	122.07
1	A	23	ASP	CB-CG-OD1	7.45	135.53	118.40
1	A	93	GLU	CG-CD-OE1	-7.43	101.31	118.40
1	D	30	GLY	O-C-N	-7.17	115.21	122.17
1	A	72	ASP	O-C-N	-7.16	114.78	123.30
1	C	26	ARG	CA-C-N	7.10	135.42	121.58
1	C	26	ARG	C-N-CA	7.10	135.42	121.58
1	C	3	ASP	CA-C-N	-7.04	104.62	121.80
1	C	3	ASP	C-N-CA	-7.04	104.62	121.80
1	A	3	ASP	CA-C-N	-7.02	104.66	121.80
1	A	3	ASP	C-N-CA	-7.02	104.66	121.80
1	A	26	ARG	CA-C-N	7.00	135.22	121.58
1	A	26	ARG	C-N-CA	7.00	135.22	121.58
1	B	44	GLN	OE1-CD-NE2	6.94	129.54	122.60
1	C	72	ASP	O-C-N	-6.86	115.13	123.30
1	B	77	PRO	O-C-N	-6.79	113.10	122.27
1	A	28	GLN	CB-CG-CD	-6.71	101.19	112.60
1	D	54	GLU	CG-CD-OE1	6.70	133.80	118.40
1	D	77	PRO	O-C-N	-6.62	113.33	122.27
1	D	109	ASN	CB-CG-ND2	-6.56	106.56	116.40
1	B	49	LYS	CA-C-N	6.49	129.31	120.54
1	B	49	LYS	C-N-CA	6.49	129.31	120.54
1	C	110	ASP	CB-CG-OD1	6.49	133.32	118.40
1	B	25	ASP	CB-CG-OD2	6.44	133.21	118.40
1	C	93	GLU	CG-CD-OE1	-6.41	103.66	118.40
1	C	4	LYS	CA-C-N	6.41	126.93	120.14
1	C	4	LYS	C-N-CA	6.41	126.93	120.14
1	D	44	GLN	CG-CD-NE2	-6.25	107.02	116.40
1	D	25	ASP	CB-CG-OD2	6.25	132.78	118.40
1	A	124	HIS	CA-CB-CG	-6.21	107.58	113.80
1	C	124	HIS	CA-CB-CG	-6.20	107.60	113.80
1	D	42	GLU	O-C-N	-6.07	115.02	122.55
1	D	25	ASP	CB-CG-OD1	-6.05	104.48	118.40
1	B	24	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	D	49	LYS	CA-C-N	6.02	128.67	120.54
1	D	49	LYS	C-N-CA	6.02	128.67	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	GLN	CB-CG-CD	-6.01	102.38	112.60
1	A	115	THR	O-C-N	-6.00	113.45	122.28
1	B	25	ASP	CB-CG-OD1	-5.99	104.62	118.40
1	A	52	ILE	CA-C-N	5.95	128.86	120.42
1	A	52	ILE	C-N-CA	5.95	128.86	120.42
1	B	110	ASP	N-CA-C	5.94	119.82	112.58
1	B	54	GLU	CG-CD-OE1	5.93	132.04	118.40
1	C	117	ASP	CA-CB-CG	5.89	118.50	112.60
1	C	42	GLU	O-C-N	-5.86	114.55	122.41
1	D	110	ASP	N-CA-C	5.86	119.73	112.58
1	B	29	LEU	CA-C-N	5.80	126.53	120.03
1	B	29	LEU	C-N-CA	5.80	126.53	120.03
1	D	29	LEU	CA-C-N	5.80	126.52	120.03
1	D	29	LEU	C-N-CA	5.80	126.52	120.03
1	A	42	GLU	O-C-N	-5.79	114.66	122.41
1	C	52	ILE	CA-C-N	5.76	128.60	120.42
1	C	52	ILE	C-N-CA	5.76	128.60	120.42
1	B	77	PRO	CA-C-O	5.74	127.78	119.34
1	D	103	PHE	CA-CB-CG	5.71	119.51	113.80
1	B	103	PHE	CA-CB-CG	5.71	119.51	113.80
1	C	115	THR	O-C-N	-5.69	113.91	122.28
1	B	109	ASN	CB-CG-ND2	-5.68	107.88	116.40
1	B	19	TYR	N-CA-C	5.67	118.40	111.82
1	C	14	PHE	CA-C-N	5.67	127.91	120.60
1	C	14	PHE	C-N-CA	5.67	127.91	120.60
1	D	19	TYR	N-CA-C	5.62	118.34	111.82
1	C	54	GLU	CB-CG-CD	-5.62	103.05	112.60
1	C	29	LEU	CA-C-N	5.60	127.14	120.14
1	C	29	LEU	C-N-CA	5.60	127.14	120.14
1	A	117	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	108	ILE	CA-C-N	5.58	130.06	122.19
1	D	108	ILE	C-N-CA	5.58	130.06	122.19
1	D	22	PHE	CA-C-N	5.57	127.74	120.28
1	D	22	PHE	C-N-CA	5.57	127.74	120.28
1	D	77	PRO	CA-C-O	5.56	127.52	119.34
1	D	24	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	98	GLY	N-CA-C	-5.53	105.01	112.14
1	A	29	LEU	CA-C-N	5.53	127.05	120.14
1	A	29	LEU	C-N-CA	5.53	127.05	120.14
1	D	17	HIS	CA-CB-CG	5.53	119.33	113.80
1	A	14	PHE	CA-C-N	5.53	128.01	120.77
1	A	14	PHE	C-N-CA	5.53	128.01	120.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD1	5.52	131.10	118.40
1	C	98	GLY	N-CA-C	-5.51	105.03	112.14
1	B	22	PHE	CA-C-N	5.50	127.64	120.28
1	B	22	PHE	C-N-CA	5.50	127.64	120.28
1	A	90	LYS	CB-CG-CD	5.47	123.89	111.30
1	B	17	HIS	CA-CB-CG	5.38	119.17	113.80
1	B	42	GLU	O-C-N	-5.36	115.90	122.55
1	D	54	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	C	90	LYS	CB-CG-CD	5.35	123.60	111.30
1	C	35	ASP	CB-CG-OD2	5.35	130.70	118.40
1	C	47	GLN	CG-CD-NE2	5.34	124.40	116.40
1	C	47	GLN	CG-CD-OE1	-5.32	110.16	120.80
1	C	23	ASP	OD1-CG-OD2	-5.30	110.18	122.90
1	A	30	GLY	CA-C-N	5.29	128.11	120.38
1	A	30	GLY	C-N-CA	5.29	128.11	120.38
1	B	12	SER	O-C-N	-5.29	116.51	122.12
1	A	35	ASP	CB-CG-OD2	5.26	130.49	118.40
1	A	73	HIS	CA-CB-CG	-5.25	108.55	113.80
1	B	30	GLY	CA-C-N	5.24	128.98	120.60
1	B	30	GLY	C-N-CA	5.24	128.98	120.60
1	D	30	GLY	CA-C-N	5.22	128.96	120.60
1	D	30	GLY	C-N-CA	5.22	128.96	120.60
1	C	20	GLN	CB-CG-CD	-5.17	103.81	112.60
1	B	53	VAL	O-C-N	-5.17	116.86	121.87
1	C	110	ASP	CB-CG-OD2	-5.16	106.54	118.40
1	D	12	SER	O-C-N	-5.16	116.66	122.12
1	A	47	GLN	CG-CD-NE2	5.13	124.09	116.40
1	B	108	ILE	CA-C-N	5.13	129.42	122.19
1	B	108	ILE	C-N-CA	5.13	129.42	122.19
1	C	74	GLN	CA-CB-CG	5.10	124.31	114.10
1	A	77	PRO	O-C-N	-5.09	115.40	122.27
1	D	15	ILE	CA-C-O	-5.08	114.98	120.47
1	C	30	GLY	CA-C-N	5.08	127.79	120.38
1	C	30	GLY	C-N-CA	5.08	127.79	120.38
1	D	53	VAL	O-C-N	-5.07	116.95	121.87
1	D	109	ASN	CB-CG-OD1	5.07	130.94	120.80
1	C	48	GLY	CA-C-O	5.03	126.61	122.24
1	A	74	GLN	CA-CB-CG	5.02	124.14	114.10
1	C	73	HIS	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	THR	Mainchain
1	A	27	THR	Mainchain
1	A	28	GLN	Sidechain
1	A	3	ASP	Mainchain
1	A	30	GLY	Mainchain
1	A	34	ILE	Mainchain
1	A	42	GLU	Mainchain
1	A	44	GLN	Sidechain
1	A	45	GLN	Mainchain
1	A	47	GLN	Sidechain
1	A	72	ASP	Mainchain
1	A	78	ASP	Sidechain
1	A	93	GLU	Sidechain
1	B	101	GLN	Mainchain
1	B	112	TRP	Mainchain
1	B	115	THR	Mainchain
1	B	15	ILE	Mainchain
1	B	16	GLN	Sidechain
1	B	34	ILE	Mainchain
1	B	44	GLN	Sidechain
1	B	45	GLN	Sidechain
1	B	53	VAL	Mainchain
1	B	72	ASP	Mainchain
1	B	76	THR	Mainchain
1	C	115	THR	Mainchain
1	C	27	THR	Mainchain
1	C	3	ASP	Mainchain
1	C	30	GLY	Mainchain
1	C	34	ILE	Mainchain
1	C	42	GLU	Mainchain
1	C	44	GLN	Sidechain
1	C	45	GLN	Mainchain
1	C	47	GLN	Sidechain
1	C	72	ASP	Mainchain
1	C	78	ASP	Sidechain
1	C	93	GLU	Sidechain
1	D	101	GLN	Mainchain
1	D	112	TRP	Mainchain
1	D	115	THR	Mainchain
1	D	15	ILE	Mainchain
1	D	16	GLN	Sidechain
1	D	34	ILE	Mainchain
1	D	45	GLN	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	53	VAL	Mainchain
1	D	72	ASP	Mainchain
1	D	76	THR	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	997	0	959	16	0
1	B	988	0	956	10	0
1	C	997	0	959	16	0
1	D	988	0	956	10	0
2	A	24	0	0	0	0
2	B	21	0	0	0	0
2	C	19	0	0	0	0
2	D	20	0	0	0	0
All	All	4054	0	3830	42	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 (42) 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:102:MET:HG2	1:B:102:MET:HE2	1.71	0.73
1:C:102:MET:HG2	1:D:102:MET:HE2	1.72	0.71
1:C:102:MET:HE3	1:D:82:ILE:HG21	1.81	0.62
1:A:102:MET:HE3	1:B:82:ILE:HG21	1.82	0.61
1:A:107:ASN:HD21	1:A:110:ASP:HA	1.67	0.60
1:C:107:ASN:HD21	1:C:110:ASP:HA	1.66	0.59
1:A:94:ASP:HB3	1:A:95:PRO:HD2	1.86	0.58
1:C:94:ASP:HB3	1:C:95:PRO:HD2	1.85	0.57
1:C:82:ILE:HG12	1:D:102:MET:HE1	1.87	0.56
1:C:78:ASP:O	1:C:79:SER:HB2	2.08	0.54
1:A:78:ASP:O	1:A:79:SER:HB2	2.08	0.54
1:C:64:ILE:HD12	1:C:91:ALA:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HG12	1:B:102:MET:HE1	1.90	0.53
1:D:34:ILE:HD11	1:D:115:THR:HG22	1.93	0.50
1:A:64:ILE:HD12	1:A:91:ALA:HB2	1.93	0.50
1:C:104:LEU:HD22	1:D:82:ILE:HD11	1.94	0.49
1:A:104:LEU:HD22	1:B:82:ILE:HD11	1.95	0.49
1:B:106:LYS:HD3	1:B:108:ILE:HD11	1.95	0.48
1:C:82:ILE:HD12	1:C:104:LEU:HD13	1.96	0.48
1:B:14:PHE:HZ	1:B:32:ILE:HD13	1.79	0.47
1:B:34:ILE:HD11	1:B:115:THR:HG22	1.97	0.47
1:C:39:LEU:HD22	1:C:52:ILE:HG23	1.98	0.46
1:C:21:LEU:O	1:C:22:PHE:C	2.59	0.46
1:D:14:PHE:HZ	1:D:32:ILE:HD13	1.81	0.45
1:A:100:HIS:CD2	1:A:120:ARG:HB3	2.51	0.45
1:A:100:HIS:NE2	1:B:84:MET:HE3	2.32	0.45
1:C:100:HIS:CD2	1:C:120:ARG:HB3	2.51	0.45
1:D:106:LYS:HD3	1:D:108:ILE:HD11	1.99	0.45
1:A:21:LEU:O	1:A:22:PHE:C	2.59	0.45
1:C:100:HIS:NE2	1:D:84:MET:HE3	2.32	0.45
1:A:82:ILE:HD12	1:A:104:LEU:HD13	1.98	0.44
1:A:39:LEU:HD22	1:A:52:ILE:HG23	2.00	0.44
1:A:40:THR:HB	1:A:118:MET:HG2	2.00	0.44
1:C:29:LEU:O	1:C:32:ILE:HG12	2.19	0.43
1:C:40:THR:HB	1:C:118:MET:HG2	2.01	0.43
1:A:29:LEU:O	1:A:32:ILE:HG12	2.19	0.43
1:D:59:LEU:HA	1:D:60:PRO:HD3	1.87	0.42
1:B:106:LYS:HG2	1:B:108:ILE:HG13	2.02	0.42
1:C:102:MET:HE1	1:C:104:LEU:HB2	2.00	0.42
1:A:102:MET:HE1	1:A:104:LEU:HB2	2.00	0.42
1:D:106:LYS:HG2	1:D:108:ILE:HG13	2.02	0.41
1:B:91:ALA:O	1:B:92:ASP:C	2.64	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	124/126 (98%)	116 (94%)	7 (6%)	1 (1%)	16	31
1	B	122/126 (97%)	114 (93%)	7 (6%)	1 (1%)	16	31
1	C	124/126 (98%)	116 (94%)	7 (6%)	1 (1%)	16	31
1	D	122/126 (97%)	114 (93%)	7 (6%)	1 (1%)	16	31
All	All	492/504 (98%)	460 (94%)	28 (6%)	4 (1%)	16	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	C	3	ASP
1	B	124	HIS
1	D	124	HIS

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	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	B	108/109 (99%)	99 (92%)	9 (8%)	10	22
1	C	108/109 (99%)	101 (94%)	7 (6%)	15	32
1	D	108/109 (99%)	102 (94%)	6 (6%)	19	39
All	All	432/436 (99%)	403 (93%)	29 (7%)	15	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	54	GLU
1	A	64	ILE
1	A	67	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	MET
1	A	100	HIS
1	A	102	MET
1	B	6	ILE
1	B	12	SER
1	B	25	ASP
1	B	32	ILE
1	B	62	GLN
1	B	93	GLU
1	B	109	ASN
1	B	123	LEU
1	B	125	ASN
1	C	6	ILE
1	C	54	GLU
1	C	64	ILE
1	C	67	SER
1	C	97	MET
1	C	100	HIS
1	C	102	MET
1	D	6	ILE
1	D	12	SER
1	D	25	ASP
1	D	32	ILE
1	D	62	GLN
1	D	123	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	B	17	HIS
1	B	71	GLN
1	B	73	HIS
1	B	100	HIS
1	B	116	ASN
1	C	107	ASN
1	D	44	GLN
1	D	71	GLN
1	D	73	HIS
1	D	100	HIS
1	D	116	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 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.