



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:45 AM UTC

PDB ID : 1TYC / pdb_00001tyc
Title : STRUCTURAL ANALYSIS OF A SERIES OF MUTANTS OF TYROSYL-
TRNA SYNTHETASE: ENHANCEMENT OF CATALYSIS BY HY-
DROPHOBIC INTERACTIONS
Authors : Brown, K.A.; Brick, P.; De Meester, P.; Blow, D.M.
Deposited on : 1992-07-06
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

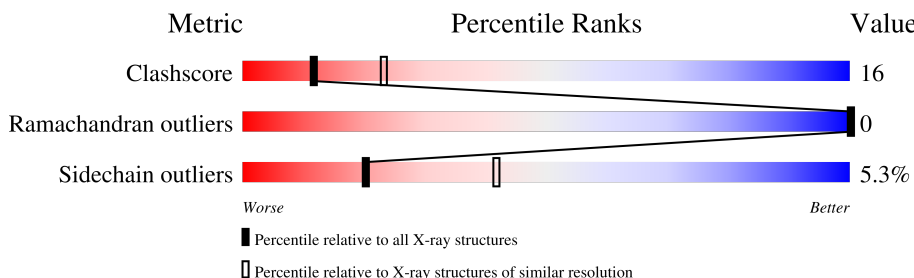
1 Overall quality at a glance

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	319	 49% 38% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2634 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 TYROSYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2463	1572	428	456	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	PRO	THR	conflict	UNP P00952

- Molecule 2 is water.

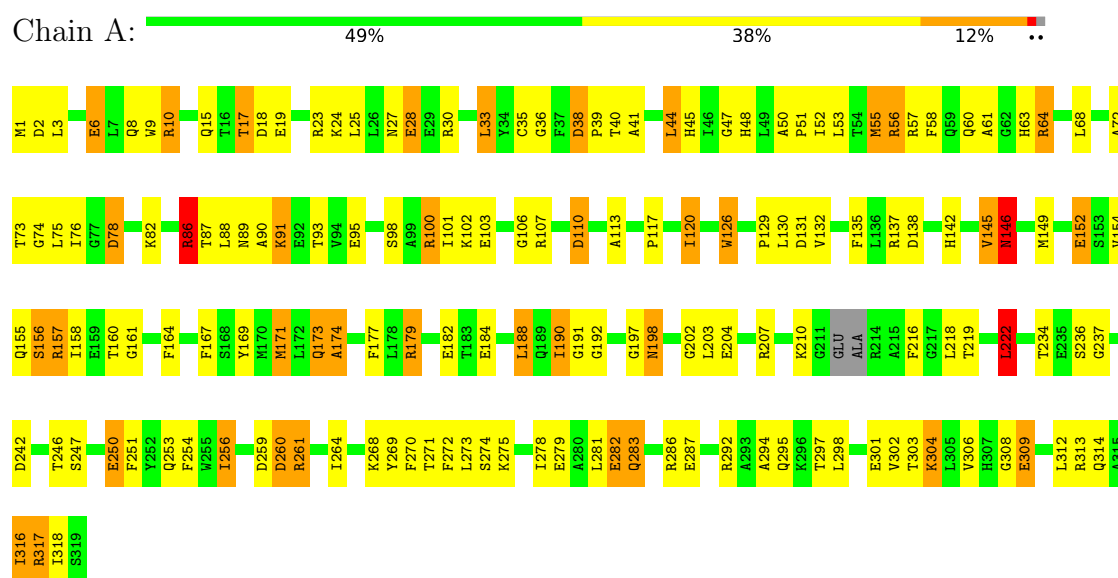
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	171	Total	O	0	0
			171	171		

3 Residue-property plots

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: TYROSYL-tRNA SYNTHETASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.46Å 64.46Å 237.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.219 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2634	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	0.98	0/2512	2.34	126/3398 (3.7%)

There are no bond length outliers.

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ARG	CD-NE-CZ	35.55	174.17	124.40
1	A	58	PHE	CA-CB-CG	10.23	124.03	113.80
1	A	308	GLY	CA-C-N	9.56	133.45	120.54
1	A	308	GLY	C-N-CA	9.56	133.45	120.54
1	A	157	ARG	N-CA-C	8.87	126.44	114.12
1	A	313	ARG	CD-NE-CZ	8.53	136.34	124.40
1	A	192	GLY	CA-C-N	8.11	131.48	120.38
1	A	192	GLY	C-N-CA	8.11	131.48	120.38
1	A	120	ILE	N-CA-CB	8.04	122.51	111.41
1	A	89	ASN	OD1-CG-ND2	8.03	130.63	122.60
1	A	28	GLU	CA-CB-CG	7.94	129.97	114.10
1	A	38	ASP	CA-CB-CG	7.85	120.45	112.60
1	A	164	PHE	CA-C-N	7.81	131.65	120.79
1	A	164	PHE	C-N-CA	7.81	131.65	120.79
1	A	179	ARG	CA-C-N	7.78	131.34	120.29
1	A	179	ARG	C-N-CA	7.78	131.34	120.29
1	A	86	ARG	NE-CZ-NH2	7.55	126.00	119.20
1	A	142	HIS	CA-CB-CG	-7.46	106.34	113.80
1	A	55	MET	CA-C-O	7.43	128.62	120.82
1	A	137	ARG	CD-NE-CZ	7.41	134.77	124.40
1	A	103	GLU	CA-C-O	-7.36	113.09	120.82
1	A	283	GLN	CB-CG-CD	7.28	124.97	112.60
1	A	317	ARG	N-CA-CB	7.14	121.35	110.28
1	A	30	ARG	N-CA-C	-6.99	98.56	109.25
1	A	132	VAL	CB-CA-C	6.92	120.74	111.88
1	A	145	VAL	CA-C-N	6.92	130.12	120.29
1	A	145	VAL	C-N-CA	6.92	130.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	192	GLY	N-CA-C	-6.91	101.94	112.51
1	A	237	GLY	N-CA-C	-6.89	103.08	112.52
1	A	30	ARG	N-CA-CB	6.81	120.97	109.87
1	A	55	MET	CA-C-N	6.76	129.67	120.54
1	A	55	MET	C-N-CA	6.76	129.67	120.54
1	A	40	THR	CA-CB-OG1	-6.67	99.59	109.60
1	A	100	ARG	CA-C-N	6.60	129.50	120.46
1	A	100	ARG	C-N-CA	6.60	129.50	120.46
1	A	35	CYS	CA-C-O	-6.59	112.69	120.60
1	A	126	TRP	CA-C-O	-6.58	111.46	118.77
1	A	138	ASP	CA-CB-CG	6.58	119.17	112.60
1	A	101	ILE	CB-CA-C	6.56	121.00	112.14
1	A	64	ARG	CD-NE-CZ	6.50	133.51	124.40
1	A	90	ALA	CA-C-O	-6.50	114.14	121.81
1	A	110	ASP	CA-C-O	6.32	127.13	120.36
1	A	174	ALA	CA-C-N	6.28	128.69	120.28
1	A	174	ALA	C-N-CA	6.28	128.69	120.28
1	A	126	TRP	O-C-N	6.24	129.21	122.34
1	A	78	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	316	ILE	O-C-N	6.17	128.31	121.90
1	A	41	ALA	N-CA-CB	6.14	121.89	111.57
1	A	197	GLY	CA-C-N	6.12	128.48	120.28
1	A	197	GLY	C-N-CA	6.12	128.48	120.28
1	A	158	ILE	N-CA-C	6.04	118.60	111.05
1	A	93	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	101	ILE	CA-CB-CG2	6.01	120.72	110.50
1	A	274	SER	N-CA-CB	5.97	118.37	110.25
1	A	237	GLY	CA-C-O	-5.97	116.34	122.25
1	A	190	ILE	CB-CG1-CD1	5.94	126.27	113.80
1	A	44	LEU	N-CA-C	-5.91	102.91	110.53
1	A	10	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	283	GLN	CB-CA-C	5.86	120.81	110.85
1	A	179	ARG	CD-NE-CZ	5.86	132.60	124.40
1	A	261	ARG	CD-NE-CZ	5.85	132.59	124.40
1	A	222	LEU	CB-CA-C	5.83	119.41	109.72
1	A	167	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	106	GLY	CA-C-N	5.80	128.52	120.29
1	A	106	GLY	C-N-CA	5.80	128.52	120.29
1	A	129	PRO	N-CA-C	5.78	120.69	114.68
1	A	246	THR	CA-CB-OG1	-5.77	100.95	109.60
1	A	107	ARG	CB-CA-C	-5.74	101.10	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLU	CB-CA-C	-5.73	101.11	110.85
1	A	146	ASN	CA-C-N	5.70	128.19	120.44
1	A	146	ASN	C-N-CA	5.70	128.19	120.44
1	A	184	GLU	CB-CG-CD	5.64	122.19	112.60
1	A	152	GLU	CA-C-O	-5.63	114.87	120.90
1	A	130	LEU	CB-CA-C	5.63	119.03	109.80
1	A	251	PHE	CA-C-N	5.58	128.07	120.54
1	A	251	PHE	C-N-CA	5.58	128.07	120.54
1	A	56	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	A	283	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	303	THR	CA-CB-OG1	-5.56	101.27	109.60
1	A	36	GLY	CA-C-O	-5.52	115.27	121.23
1	A	120	ILE	N-CA-C	-5.50	100.42	108.11
1	A	309	GLU	N-CA-C	5.48	117.69	111.11
1	A	88	LEU	O-C-N	5.46	129.42	123.04
1	A	287	GLU	CA-C-O	-5.46	113.35	119.79
1	A	179	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	A	160	THR	N-CA-C	-5.43	105.36	111.28
1	A	270	PHE	CA-C-O	-5.41	112.98	119.15
1	A	173	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	2	ASP	N-CA-CB	5.37	118.27	110.26
1	A	278	ILE	CA-C-O	-5.35	115.38	120.95
1	A	76	ILE	O-C-N	5.35	126.10	121.98
1	A	282	GLU	CA-C-O	5.35	126.09	120.42
1	A	316	ILE	CA-C-O	-5.34	115.12	121.05
1	A	87	THR	N-CA-CB	5.32	119.08	110.41
1	A	270	PHE	N-CA-C	5.32	119.92	113.38
1	A	202	GLY	CA-C-N	5.29	127.81	120.29
1	A	202	GLY	C-N-CA	5.29	127.81	120.29
1	A	250	GLU	CA-CB-CG	5.27	124.64	114.10
1	A	260	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	6	GLU	N-CA-CB	5.25	117.93	110.16
1	A	306	VAL	CA-C-O	-5.22	114.75	120.96
1	A	131	ASP	CB-CG-OD2	5.17	130.29	118.40
1	A	135	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	179	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	A	91	LYS	CB-CA-C	-5.14	102.25	110.79
1	A	188	LEU	O-C-N	5.14	129.43	123.41
1	A	17	THR	CA-C-O	-5.13	115.11	120.55
1	A	198	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	269	TYR	N-CA-C	5.13	116.68	111.14
1	A	40	THR	O-C-N	5.12	128.24	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	PHE	CB-CA-C	5.11	119.37	110.94
1	A	171	MET	CA-C-N	5.10	127.38	120.44
1	A	171	MET	C-N-CA	5.10	127.38	120.44
1	A	251	PHE	N-CA-C	-5.10	105.61	111.07
1	A	254	PHE	CA-C-O	-5.06	115.48	120.90
1	A	74	GLY	N-CA-C	-5.06	109.11	114.67
1	A	98	SER	CA-C-N	5.06	127.06	120.28
1	A	98	SER	C-N-CA	5.06	127.06	120.28
1	A	15	GLN	CG-CD-NE2	-5.06	108.82	116.40
1	A	177	PHE	CB-CA-C	5.05	118.80	110.88
1	A	63	HIS	O-C-N	5.04	128.73	123.03
1	A	2	ASP	CA-C-O	-5.04	113.86	120.00
1	A	317	ARG	CA-CB-CG	5.03	124.15	114.10
1	A	247	SER	CA-C-N	5.00	124.78	119.28
1	A	247	SER	C-N-CA	5.00	124.78	119.28

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	2463	0	2396	77	0
2	A	171	0	0	5	0
All	All	2634	0	2396	77	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 16.

All (77) 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:45:HIS:H	1:A:48:HIS:HD2	1.21	0.85
1:A:234:THR:HG22	1:A:236:SER:H	1.44	0.83
1:A:1:MET:N	1:A:27:ASN:HD21	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:O	1:A:156:SER:HB3	1.89	0.71
1:A:283:GLN:HG3	1:A:286:ARG:NH1	2.08	0.68
1:A:82:LYS:HD3	1:A:86:ARG:HH11	1.58	0.67
1:A:45:HIS:H	1:A:48:HIS:CD2	2.10	0.66
1:A:9:TRP:CZ2	1:A:275:LYS:HG3	2.31	0.66
1:A:50:ALA:HB3	1:A:51:PRO:HD3	1.78	0.66
1:A:72:ALA:O	1:A:75:LEU:HB2	2.02	0.60
1:A:100:ARG:NH2	1:A:242:ASP:OD2	2.33	0.59
1:A:75:LEU:HD21	1:A:91:LYS:HA	1.84	0.57
1:A:292:ARG:NH1	1:A:295:GLN:HG2	2.20	0.57
1:A:190:ILE:HA	1:A:218:LEU:O	2.05	0.56
1:A:110:ASP:OD2	1:A:113:ALA:HB2	2.06	0.56
1:A:48:HIS:O	1:A:52:ILE:HG13	2.06	0.55
1:A:82:LYS:CD	1:A:86:ARG:HH11	2.18	0.55
1:A:234:THR:HG22	1:A:236:SER:N	2.18	0.54
1:A:145:VAL:O	1:A:149:MET:HG2	2.07	0.54
1:A:146:ASN:HB2	2:A:378:HOH:O	2.08	0.54
1:A:44:LEU:HD13	1:A:52:ILE:HD11	1.89	0.54
1:A:24:LYS:NZ	1:A:28:GLU:OE2	2.41	0.53
1:A:171:MET:O	1:A:174:ALA:HB3	2.08	0.52
1:A:222:LEU:HD23	2:A:393:HOH:O	2.09	0.52
1:A:64:ARG:HD2	2:A:385:HOH:O	2.08	0.52
1:A:149:MET:O	1:A:155:GLN:HG2	2.10	0.52
1:A:171:MET:HA	1:A:171:MET:HE2	1.90	0.52
1:A:17:THR:HG21	1:A:203:LEU:CD1	2.40	0.51
1:A:283:GLN:HG3	1:A:286:ARG:HH12	1.74	0.51
1:A:157:ARG:O	1:A:161:GLY:N	2.41	0.50
1:A:314:GLN:O	1:A:318:ILE:HG13	2.11	0.50
1:A:273:LEU:HD11	1:A:297:THR:HG21	1.92	0.50
1:A:33:LEU:HA	1:A:188:LEU:O	2.11	0.50
1:A:91:LYS:O	1:A:95:GLU:HB2	2.12	0.50
1:A:182:GLU:OE2	1:A:210:LYS:NZ	2.36	0.49
1:A:264:ILE:O	1:A:268:LYS:HG3	2.13	0.49
1:A:3:LEU:HD22	1:A:61:ALA:HB3	1.95	0.48
1:A:253:GLN:HA	1:A:256:ILE:HG22	1.95	0.48
1:A:45:HIS:CE1	1:A:47:GLY:HA3	2.49	0.48
1:A:25:LEU:HD22	1:A:216:PHE:HE1	1.78	0.48
1:A:82:LYS:HD3	1:A:86:ARG:NH1	2.28	0.48
1:A:292:ARG:HH11	1:A:295:GLN:HG2	1.79	0.47
1:A:126:TRP:HB2	2:A:363:HOH:O	2.14	0.47
1:A:10:ARG:HD3	1:A:268:LYS:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:O	1:A:292:ARG:NH1	2.47	0.47
1:A:281:LEU:HD22	1:A:294:ALA:HA	1.97	0.47
1:A:297:THR:O	1:A:301:GLU:HG2	2.15	0.47
1:A:154:VAL:O	1:A:155:GLN:C	2.58	0.46
1:A:82:LYS:CG	1:A:86:ARG:HH11	2.28	0.45
1:A:304:LYS:HG3	1:A:312:LEU:CD2	2.46	0.45
1:A:113:ALA:O	1:A:117:PRO:HB3	2.17	0.45
1:A:259:ASP:OD1	1:A:260:ASP:N	2.50	0.45
1:A:78:ASP:HB2	1:A:169:TYR:CZ	2.52	0.44
1:A:173:GLN:CD	1:A:198:ASN:HB3	2.42	0.44
1:A:204:GLU:OE2	1:A:207:ARG:NH2	2.50	0.44
1:A:38:ASP:HA	1:A:39:PRO:HD3	1.84	0.44
1:A:1:MET:H3	1:A:27:ASN:HD21	1.62	0.43
1:A:73:THR:HB	1:A:169:TYR:CE2	2.54	0.43
1:A:53:LEU:O	1:A:56:ARG:HB3	2.19	0.43
1:A:309:GLU:OE1	1:A:312:LEU:HD23	2.18	0.43
1:A:53:LEU:O	1:A:57:ARG:HG3	2.19	0.42
1:A:9:TRP:CE2	1:A:275:LYS:HG3	2.54	0.42
1:A:56:ARG:O	1:A:60:GLN:HG3	2.20	0.42
1:A:279:GLU:O	1:A:282:GLU:HB3	2.19	0.42
1:A:19:GLU:OE2	1:A:23:ARG:NH1	2.47	0.42
1:A:3:LEU:HD22	1:A:61:ALA:CB	2.49	0.42
1:A:82:LYS:HG2	1:A:86:ARG:NH1	2.35	0.42
1:A:52:ILE:O	1:A:55:MET:HB2	2.21	0.41
1:A:1:MET:H1	1:A:27:ASN:HD21	1.64	0.41
1:A:191:GLY:O	1:A:219:THR:HA	2.20	0.41
1:A:283:GLN:HE21	1:A:286:ARG:HH12	1.68	0.41
1:A:6:GLU:O	1:A:10:ARG:HG3	2.19	0.41
1:A:250:GLU:HG2	2:A:472:HOH:O	2.20	0.41
1:A:312:LEU:O	1:A:316:ILE:HG13	2.20	0.41
1:A:102:LYS:HG3	1:A:120:ILE:HG21	2.02	0.41
1:A:298:LEU:O	1:A:302:VAL:HG23	2.21	0.40
1:A:82:LYS:CG	1:A:86:ARG:NH1	2.85	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	313/319 (98%)	305 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	245/269 (91%)	232 (95%)	13 (5%)	20	42

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	33	LEU
1	A	68	LEU
1	A	86	ARG
1	A	146	ASN
1	A	156	SER
1	A	179	ARG
1	A	222	LEU
1	A	256	ILE
1	A	261	ARG
1	A	271	THR
1	A	304	LYS
1	A	317	ARG

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	8	GLN
1	A	27	ASN
1	A	48	HIS
1	A	60	GLN
1	A	89	ASN
1	A	155	GLN
1	A	257	ASN
1	A	283	GLN
1	A	314	GLN

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.