



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:18 PM UTC

PDB ID : 2TS1 / pdb_00002ts1
Title : STRUCTURE OF TYROSYL-T/RNA SYNTHETASE REFINED AT 2.3
ANGSTROMS RESOLUTION. INTERACTION OF THE ENZYME WITH
THE TYROSYL ADENYLATE INTERMEDIATE
Authors : Brick, P.; Bhat, T.N.; Blow, D.M.
Deposited on : 1989-06-29
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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

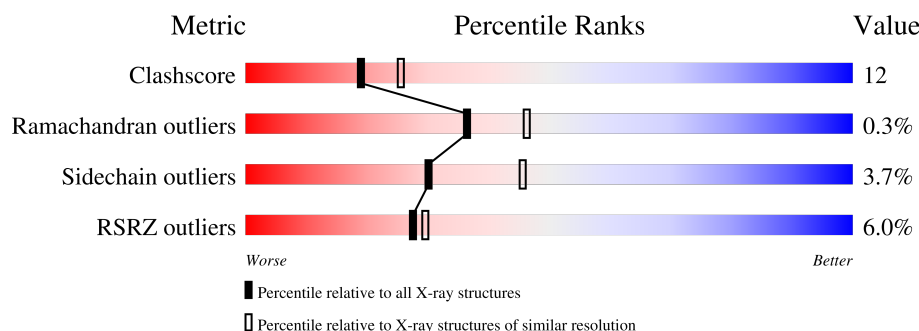
1 Overall quality at a glance

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)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	419	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2567 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
			2457	1568	425	457	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Chain A:

4 Data and refinement statistics

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) – 2.30 79.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 98.6 (79.20-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.10Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.228 , (Not available) 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2567	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.31	3/2505 (0.1%)	2.49	174/3389 (5.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ASN	C-N	-5.90	1.26	1.33
1	A	73	THR	C-O	5.76	1.31	1.24
1	A	193	SER	N-CA	-5.27	1.39	1.46

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	GLU	CA-C-O	-11.48	108.77	120.82
1	A	126	TRP	CA-C-O	-10.61	107.62	118.97
1	A	283	GLN	OE1-CD-NE2	-10.40	112.19	122.60
1	A	192	GLY	CA-C-N	10.34	134.54	120.38
1	A	192	GLY	C-N-CA	10.34	134.54	120.38
1	A	283	GLN	CB-CG-CD	10.17	129.89	112.60
1	A	58	PHE	CA-CB-CG	10.09	123.89	113.80
1	A	64	ARG	CD-NE-CZ	9.78	138.10	124.40
1	A	179	ARG	CA-C-N	9.30	133.50	120.29
1	A	179	ARG	C-N-CA	9.30	133.50	120.29
1	A	18	ASP	CA-CB-CG	9.23	121.83	112.60
1	A	264	ILE	CA-C-O	-9.06	111.25	120.85
1	A	157	ARG	N-CA-C	9.04	128.16	113.89
1	A	308	GLY	CA-C-N	8.90	132.55	120.54
1	A	308	GLY	C-N-CA	8.90	132.55	120.54
1	A	110	ASP	CA-C-O	8.42	129.37	120.36
1	A	137	ARG	CD-NE-CZ	8.38	136.14	124.40
1	A	237	GLY	N-CA-C	-8.36	99.80	111.76
1	A	101	ILE	CB-CA-C	8.22	123.24	112.14
1	A	202	GLY	CA-C-N	8.20	131.09	120.44
1	A	202	GLY	C-N-CA	8.20	131.09	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	PHE	CA-C-N	8.18	132.16	120.79
1	A	164	PHE	C-N-CA	8.18	132.16	120.79
1	A	120	ILE	N-CA-CB	8.15	122.66	111.41
1	A	134	THR	O-C-N	7.65	130.35	122.09
1	A	40	THR	CA-CB-OG1	-7.63	98.16	109.60
1	A	15	GLN	CG-CD-NE2	-7.59	105.02	116.40
1	A	28	GLU	CA-CB-CG	7.50	129.10	114.10
1	A	38	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	30	ARG	N-CA-CB	7.42	121.97	109.87
1	A	36	GLY	CA-C-O	-7.25	114.32	120.92
1	A	306	VAL	N-CA-C	7.17	117.27	110.53
1	A	193	SER	O-C-N	7.15	129.70	122.12
1	A	74	GLY	O-C-N	-7.14	114.56	122.84
1	A	126	TRP	O-C-N	7.09	131.06	122.48
1	A	313	ARG	CD-NE-CZ	7.08	134.32	124.40
1	A	142	HIS	CA-CB-CG	-7.08	106.72	113.80
1	A	261	ARG	CG-CD-NE	7.01	127.43	112.00
1	A	187	ARG	CD-NE-CZ	-6.98	114.63	124.40
1	A	270	PHE	CA-C-O	-6.92	111.26	119.15
1	A	23	ARG	CA-C-N	6.91	130.39	120.79
1	A	23	ARG	C-N-CA	6.91	130.39	120.79
1	A	74	GLY	CA-C-O	6.88	127.96	119.01
1	A	316	ILE	O-C-N	6.87	129.04	121.90
1	A	158	ILE	N-CA-C	6.85	121.63	112.04
1	A	120	ILE	N-CA-C	-6.84	98.53	108.11
1	A	87	THR	N-CA-CB	6.83	121.54	110.41
1	A	160	THR	N-CA-C	-6.81	103.86	111.28
1	A	30	ARG	N-CA-C	-6.75	98.92	109.25
1	A	137	ARG	NE-CZ-NH2	6.71	125.24	119.20
1	A	269	TYR	N-CA-C	6.71	118.39	111.14
1	A	2	ASP	CA-CB-CG	-6.70	105.90	112.60
1	A	89	ASN	CA-CB-CG	-6.67	105.93	112.60
1	A	157	ARG	NE-CZ-NH2	-6.65	113.21	119.20
1	A	56	ARG	NH1-CZ-NH2	6.65	127.94	119.30
1	A	234	THR	CA-CB-OG1	-6.63	99.66	109.60
1	A	198	ASN	CA-CB-CG	6.59	119.19	112.60
1	A	214	ARG	N-CA-CB	-6.55	99.37	110.50
1	A	292	ARG	N-CA-CB	-6.49	102.33	112.13
1	A	269	TYR	CB-CA-C	-6.48	100.66	110.90
1	A	90	ALA	CA-C-O	-6.47	114.09	121.72
1	A	103	GLU	O-C-N	6.43	128.69	122.07
1	A	222	LEU	CB-CA-C	6.39	120.33	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	CA-C-N	6.38	129.35	120.29
1	A	267	LEU	C-N-CA	6.38	129.35	120.29
1	A	309	GLU	N-CA-C	6.28	118.65	111.11
1	A	56	ARG	NE-CZ-NH2	-6.22	113.61	119.20
1	A	273	LEU	N-CA-CB	6.21	119.10	109.97
1	A	23	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	A	41	ALA	N-CA-CB	6.16	121.92	111.57
1	A	283	GLN	CB-CA-C	6.14	121.94	110.70
1	A	189	GLN	CA-C-O	-6.14	114.07	120.70
1	A	155	GLN	CA-C-N	6.14	133.26	121.54
1	A	155	GLN	C-N-CA	6.14	133.26	121.54
1	A	258	THR	CA-CB-OG1	-6.14	100.39	109.60
1	A	23	ARG	CA-C-O	6.12	127.25	120.82
1	A	2	ASP	N-CA-CB	6.12	119.38	110.26
1	A	93	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	85	GLU	CA-C-O	-6.12	114.46	121.19
1	A	245	LYS	N-CA-C	-6.08	105.88	113.55
1	A	201	ALA	CA-C-N	6.08	126.69	120.00
1	A	201	ALA	C-N-CA	6.08	126.69	120.00
1	A	7	LEU	CA-C-O	6.04	126.95	120.55
1	A	103	GLU	N-CA-CB	6.03	118.76	110.01
1	A	130	LEU	N-CA-CB	-6.03	100.61	109.95
1	A	197	GLY	CA-C-N	6.02	129.46	120.31
1	A	197	GLY	C-N-CA	6.02	129.46	120.31
1	A	14	ASN	CA-C-O	5.99	127.80	120.56
1	A	261	ARG	CD-NE-CZ	5.98	132.77	124.40
1	A	64	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	A	194	ASP	O-C-N	5.93	131.08	122.43
1	A	300	GLU	CA-C-N	5.91	128.45	120.65
1	A	300	GLU	C-N-CA	5.91	128.45	120.65
1	A	101	ILE	N-CA-C	-5.90	104.60	110.62
1	A	297	THR	N-CA-CB	5.90	118.79	110.12
1	A	181	TYR	CA-C-O	5.84	126.95	120.82
1	A	51	THR	CA-CB-OG1	-5.80	100.90	109.60
1	A	27	ASN	CA-C-O	-5.78	113.32	119.97
1	A	29	GLU	CB-CG-CD	5.76	122.40	112.60
1	A	76	ILE	O-C-N	5.74	126.40	121.98
1	A	287	GLU	CA-C-O	-5.72	113.04	119.79
1	A	58	PHE	N-CA-CB	5.71	118.35	110.07
1	A	190	ILE	CB-CG1-CD1	5.70	125.78	113.80
1	A	157	ARG	CA-C-O	-5.68	112.61	119.03
1	A	202	GLY	CA-C-O	5.67	126.67	120.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	PHE	CA-C-N	5.66	127.80	120.44
1	A	251	PHE	C-N-CA	5.66	127.80	120.44
1	A	274	SER	N-CA-CB	5.65	117.93	110.25
1	A	265	ARG	CA-CB-CG	5.62	125.35	114.10
1	A	132	VAL	CB-CA-C	5.60	119.14	111.97
1	A	77	GLY	CA-C-N	5.60	129.04	121.20
1	A	77	GLY	C-N-CA	5.60	129.04	121.20
1	A	174	ALA	CA-C-O	5.56	126.84	120.90
1	A	250	GLU	CA-CB-CG	5.54	125.18	114.10
1	A	81	GLY	CA-C-O	5.52	126.31	119.25
1	A	146	ASN	CA-C-N	5.48	127.89	120.44
1	A	146	ASN	C-N-CA	5.48	127.89	120.44
1	A	157	ARG	CB-CA-C	-5.47	100.34	109.75
1	A	129	PRO	N-CA-C	5.45	121.17	114.35
1	A	168	SER	CA-CB-OG	-5.44	100.22	111.10
1	A	304	LYS	CA-C-O	5.44	126.19	120.42
1	A	203	LEU	CA-C-O	-5.43	115.12	120.82
1	A	126	TRP	N-CA-C	-5.41	107.04	113.97
1	A	246	THR	CA-CB-OG1	-5.41	101.48	109.60
1	A	307	HIS	CA-CB-CG	5.39	119.19	113.80
1	A	251	PHE	N-CA-C	-5.38	105.31	111.07
1	A	44	LEU	N-CA-C	-5.35	103.63	110.53
1	A	314	GLN	O-C-N	5.35	127.86	122.09
1	A	55	MET	CA-C-N	5.32	127.40	120.28
1	A	55	MET	C-N-CA	5.32	127.40	120.28
1	A	84	SER	N-CA-C	5.31	117.89	109.50
1	A	8	GLN	N-CA-C	-5.30	105.41	111.14
1	A	73	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	16	THR	CB-CA-C	5.29	120.14	109.68
1	A	292	ARG	CA-C-N	5.28	127.36	120.28
1	A	292	ARG	C-N-CA	5.28	127.36	120.28
1	A	29	GLU	N-CA-CB	-5.26	103.24	111.56
1	A	181	TYR	N-CA-C	-5.25	105.45	111.07
1	A	2	ASP	N-CA-C	-5.25	105.16	112.45
1	A	58	PHE	N-CA-C	-5.25	105.47	111.14
1	A	128	GLY	O-C-N	5.24	127.01	121.77
1	A	171	MET	CA-CB-CG	5.22	124.54	114.10
1	A	302	VAL	CA-C-O	-5.21	115.33	120.85
1	A	253	GLN	CA-CB-CG	-5.21	103.69	114.10
1	A	317	ARG	CG-CD-NE	-5.20	100.56	112.00
1	A	282	GLU	CA-C-O	5.19	126.05	120.55
1	A	102	LYS	O-C-N	5.18	127.48	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	MET	CA-C-O	5.17	126.25	120.82
1	A	87	THR	O-C-N	5.17	128.85	123.06
1	A	121	LYS	CA-C-O	-5.16	115.57	121.40
1	A	148	MET	CA-C-N	5.15	128.14	120.31
1	A	148	MET	C-N-CA	5.15	128.14	120.31
1	A	111	PHE	O-C-N	5.13	128.67	122.35
1	A	223	VAL	CA-C-O	-5.12	114.76	120.95
1	A	303	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	57	ARG	N-CA-C	-5.10	105.72	111.28
1	A	17	THR	CA-C-O	-5.07	114.37	120.10
1	A	159	GLU	N-CA-C	-5.07	104.74	112.04
1	A	159	GLU	CA-C-O	5.07	126.64	120.31
1	A	167	PHE	CA-C-N	5.06	129.99	121.14
1	A	167	PHE	C-N-CA	5.06	129.99	121.14
1	A	135	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	132	VAL	CA-C-N	5.05	127.38	120.46
1	A	132	VAL	C-N-CA	5.05	127.38	120.46
1	A	179	ARG	N-CA-C	5.05	116.79	111.28
1	A	124	TYR	CA-CB-CG	-5.04	104.83	113.90
1	A	259	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	152	GLU	CA-C-O	-5.03	115.52	120.90
1	A	192	GLY	N-CA-C	-5.03	103.86	112.30
1	A	237	GLY	CA-C-N	5.02	127.83	120.71
1	A	237	GLY	C-N-CA	5.02	127.83	120.71
1	A	74	GLY	CA-C-N	5.02	131.46	122.38
1	A	74	GLY	C-N-CA	5.02	131.46	122.38
1	A	175	TYR	CA-C-O	-5.00	115.25	120.55

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	2457	0	2385	57	0
2	A	110	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2567	0	2385	57	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 12.

All (57) 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	1.17	0.88
1:A:234:THR:HG22	1:A:236:SER:H	1.47	0.79
1:A:45:HIS:H	1:A:48:HIS:CD2	2.06	0.70
1:A:283:GLN:HG3	1:A:286:ARG:NH1	2.12	0.64
1:A:222:LEU:HD23	2:A:493:HOH:O	1.97	0.64
1:A:72:ALA:O	1:A:75:LEU:HB2	1.98	0.63
1:A:292:ARG:NH1	1:A:295:GLN:HG2	2.13	0.63
1:A:148:MET:HE3	1:A:171:MET:HE3	1.82	0.62
1:A:145:VAL:O	1:A:149:MET:HG2	2.00	0.61
1:A:54:THR:HG21	1:A:220:ILE:HD11	1.81	0.61
1:A:31:VAL:O	1:A:63:HIS:HB3	2.00	0.60
1:A:48:HIS:O	1:A:52:ILE:HG13	2.00	0.60
1:A:100:ARG:NH2	1:A:242:ASP:OD1	2.32	0.60
1:A:253:GLN:HA	1:A:256:ILE:HG22	1.83	0.60
1:A:110:ASP:OD2	1:A:113:ALA:HB2	2.01	0.60
1:A:24:LYS:NZ	1:A:28:GLU:OE2	2.35	0.59
1:A:64:ARG:HD2	2:A:485:HOH:O	2.04	0.57
1:A:292:ARG:HH11	1:A:295:GLN:HG2	1.71	0.56
1:A:314:GLN:O	1:A:318:ILE:HG13	2.06	0.55
1:A:152:GLU:O	1:A:156:SER:HB2	2.07	0.55
1:A:157:ARG:O	1:A:161:GLY:N	2.39	0.54
1:A:33:LEU:HA	1:A:188:LEU:O	2.08	0.53
1:A:9:TRP:CZ2	1:A:275:LYS:HG3	2.43	0.53
1:A:239:ILE:HG23	1:A:246:THR:HG21	1.91	0.53
1:A:297:THR:O	1:A:301:GLU:HG2	2.09	0.53
1:A:178:LEU:HD11	1:A:210:LYS:HE2	1.90	0.53
1:A:256:ILE:O	1:A:292:ARG:NH1	2.42	0.53
1:A:234:THR:HG22	1:A:236:SER:N	2.19	0.53
1:A:75:LEU:HD21	1:A:91:LYS:HA	1.92	0.52
1:A:154:VAL:O	1:A:155:GLN:C	2.53	0.51
1:A:91:LYS:O	1:A:95:GLU:HB2	2.11	0.50
1:A:281:LEU:HD22	1:A:294:ALA:HA	1.94	0.50
1:A:73:THR:HB	1:A:169:TYR:CE1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:HB2	1:A:65:PRO:HG3	1.95	0.49
1:A:274:SER:N	1:A:277:GLU:OE2	2.23	0.49
1:A:53:LEU:O	1:A:56:ARG:HB3	2.15	0.47
1:A:56:ARG:O	1:A:60:GLN:HG3	2.15	0.47
1:A:1:MET:N	1:A:27:ASN:HD21	2.12	0.47
1:A:53:LEU:O	1:A:57:ARG:HG3	2.15	0.46
1:A:78:ASP:HB2	1:A:169:TYR:CZ	2.51	0.46
1:A:17:THR:HG21	1:A:203:LEU:CD1	2.46	0.45
1:A:102:LYS:HG3	1:A:120:ILE:HG21	1.98	0.45
1:A:44:LEU:HD13	1:A:52:ILE:HD11	1.98	0.45
1:A:190:ILE:HA	1:A:218:LEU:O	2.17	0.44
1:A:187:ARG:HG3	2:A:420:HOH:O	2.18	0.44
1:A:72:ALA:HB2	1:A:124:TYR:HA	2.01	0.43
1:A:298:LEU:O	1:A:302:VAL:HG23	2.19	0.43
1:A:171:MET:HA	1:A:171:MET:HE2	2.01	0.42
1:A:38:ASP:OD2	1:A:70:GLY:HA3	2.19	0.42
1:A:9:TRP:CH2	1:A:275:LYS:HA	2.55	0.42
1:A:304:LYS:HG3	1:A:312:LEU:HD22	2.02	0.42
1:A:250:GLU:HG2	2:A:525:HOH:O	2.20	0.41
1:A:168:SER:O	1:A:169:TYR:C	2.63	0.41
1:A:227:ASP:OD1	1:A:227:ASP:C	2.63	0.41
1:A:101:ILE:O	1:A:102:LYS:C	2.63	0.40
1:A:113:ALA:O	1:A:117:PRO:HB3	2.22	0.40
1:A:128:GLY:N	1:A:129:PRO:HD2	2.37	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	313/419 (75%)	304 (97%)	8 (3%)	1 (0%)	36 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	SER

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	244/349 (70%)	235 (96%)	9 (4%)	30	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	33	LEU
1	A	114	ASP
1	A	179	ARG
1	A	190	ILE
1	A	222	LEU
1	A	256	ILE
1	A	261	ARG
1	A	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	48	HIS
1	A	60	GLN
1	A	89	ASN
1	A	155	GLN
1	A	173	GLN
1	A	189	GLN
1	A	198	ASN
1	A	257	ASN
1	A	283	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	317/419 (75%)	0.07	19 (5%)	27 29	2, 13, 33, 48	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	SER	4.9
1	A	114	ASP	4.4
1	A	160	THR	4.0
1	A	309	GLU	3.3
1	A	211	GLY	3.2
1	A	158	ILE	3.1
1	A	146	ASN	2.6
1	A	313	ARG	2.5
1	A	317	ARG	2.5
1	A	222	LEU	2.5
1	A	159	GLU	2.4
1	A	156	SER	2.4
1	A	115	GLY	2.3
1	A	86	ARG	2.3
1	A	244	GLU	2.3
1	A	233	LYS	2.2
1	A	235	GLU	2.2
1	A	283	GLN	2.1
1	A	187	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.