



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:04 PM UTC

PDB ID : 1TYA / pdb_00001tya
Title : STRUCTURAL ANALYSIS OF A SERIES OF MUTANTS OF TYROSYL-
TRNA SYNTHETASE: ENHANCEMENT OF CATALYSIS BY HY-
DROPHOBIC INTERACTIONS
Authors : Brown, K.A.; De Meester, P.; Blow, D.M.
Deposited on : 1992-07-06
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

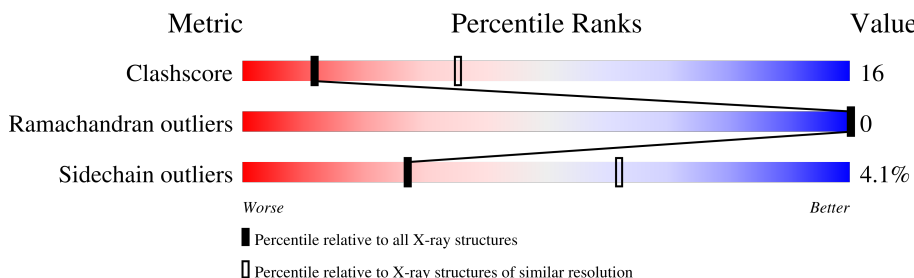
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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	E	319	 45% 44% 11% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2636 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.

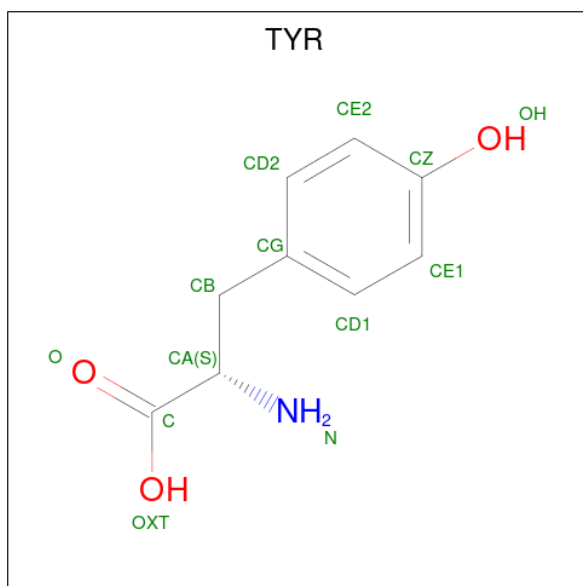
- Molecule 1 is a protein called TYROSYL-tRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	317	Total	C	N	O	S	0	0	0
			2461	1570	428	456	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	51	ALA	THR	conflict	UNP P00952

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	162	Total 162	O 162	0	0

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) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.205 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2636	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	E	1.17	1/2509 (0.0%)	2.38	151/3393 (4.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	86	ARG	NE-CZ	-5.58	1.26	1.33

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	86	ARG	CD-NE-CZ	39.53	179.74	124.40
1	E	58	PHE	CA-CB-CG	10.94	124.74	113.80
1	E	179	ARG	CD-NE-CZ	10.15	138.62	124.40
1	E	38	ASP	CA-CB-CG	9.97	122.57	112.60
1	E	313	ARG	CD-NE-CZ	9.71	138.00	124.40
1	E	173	GLN	OE1-CD-NE2	-9.21	113.39	122.60
1	E	40	THR	CA-CB-OG1	-8.79	96.41	109.60
1	E	308	GLY	CA-C-N	8.46	131.97	120.38
1	E	308	GLY	C-N-CA	8.46	131.97	120.38
1	E	171	MET	CA-C-N	8.40	131.36	120.44
1	E	171	MET	C-N-CA	8.40	131.36	120.44
1	E	237	GLY	N-CA-C	-8.32	99.86	111.76
1	E	78	ASP	CA-CB-CG	8.30	120.90	112.60
1	E	120	ILE	N-CA-CB	8.24	122.78	111.41
1	E	35	CYS	CA-C-O	-7.75	111.29	120.60
1	E	179	ARG	CA-C-N	7.75	131.30	120.29
1	E	179	ARG	C-N-CA	7.75	131.30	120.29
1	E	261	ARG	CG-CD-NE	7.73	129.00	112.00
1	E	157	ARG	CA-C-O	-7.47	110.59	119.03
1	E	164	PHE	CA-C-N	7.40	131.07	120.79
1	E	164	PHE	C-N-CA	7.40	131.07	120.79
1	E	49	LEU	N-CA-C	7.37	118.96	111.07
1	E	87	THR	O-C-N	7.35	131.26	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	GLY	CA-C-N	7.33	130.42	120.38
1	E	192	GLY	C-N-CA	7.33	130.42	120.38
1	E	64	ARG	CD-NE-CZ	7.24	134.54	124.40
1	E	101	ILE	CB-CA-C	7.18	121.83	112.14
1	E	189	GLN	CA-C-O	-7.14	112.45	120.66
1	E	30	ARG	N-CA-C	-7.09	98.39	109.25
1	E	177	PHE	CA-CB-CG	7.09	120.89	113.80
1	E	160	THR	N-CA-C	-6.97	103.68	111.28
1	E	21	GLY	O-C-N	6.94	128.84	122.18
1	E	46	ILE	CA-C-N	6.87	128.95	120.22
1	E	46	ILE	C-N-CA	6.87	128.95	120.22
1	E	101	ILE	CA-CB-CG2	6.87	122.17	110.50
1	E	142	HIS	CA-CB-CG	-6.78	107.02	113.80
1	E	183	THR	N-CA-C	6.76	121.27	112.89
1	E	157	ARG	N-CA-C	6.75	124.56	113.89
1	E	30	ARG	N-CA-CB	6.73	120.84	109.87
1	E	93	THR	CA-CB-OG1	-6.72	99.52	109.60
1	E	103	GLU	CA-C-O	-6.63	114.03	121.00
1	E	63	HIS	CG-CD2-NE2	-6.54	100.66	107.20
1	E	309	GLU	N-CA-C	6.54	119.24	111.33
1	E	36	GLY	O-C-N	-6.53	116.69	123.48
1	E	98	SER	CA-C-N	6.51	129.00	120.28
1	E	98	SER	C-N-CA	6.51	129.00	120.28
1	E	188	LEU	CA-C-O	-6.48	112.57	120.54
1	E	106	GLY	CA-C-N	6.46	128.93	120.28
1	E	106	GLY	C-N-CA	6.46	128.93	120.28
1	E	36	GLY	CA-C-N	6.45	131.94	122.39
1	E	36	GLY	C-N-CA	6.45	131.94	122.39
1	E	173	GLN	CG-CD-OE1	6.35	133.50	120.80
1	E	158	ILE	N-CA-C	6.35	120.93	112.04
1	E	270	PHE	CA-C-O	-6.33	111.94	119.35
1	E	102	LYS	N-CA-C	-6.28	104.44	111.28
1	E	167	PHE	CA-CB-CG	6.24	120.04	113.80
1	E	58	PHE	CA-C-O	-6.06	114.00	120.42
1	E	219	THR	CA-CB-CG2	6.03	120.76	110.50
1	E	55	MET	CA-C-O	6.00	127.12	120.82
1	E	58	PHE	N-CA-C	-5.95	104.88	111.36
1	E	101	ILE	CA-CB-CG1	-5.91	100.34	110.40
1	E	237	GLY	CA-C-O	-5.88	115.89	122.24
1	E	33	LEU	CA-C-O	-5.84	114.61	121.44
1	E	18	ASP	CA-CB-CG	5.82	118.42	112.60
1	E	189	GLN	N-CA-CB	5.80	121.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	259	ASP	CA-CB-CG	5.79	118.39	112.60
1	E	9	TRP	CA-C-N	5.79	129.11	120.31
1	E	9	TRP	C-N-CA	5.79	129.11	120.31
1	E	159	GLU	N-CA-C	-5.75	104.46	112.45
1	E	182	GLU	CG-CD-OE2	5.73	131.59	118.40
1	E	63	HIS	CA-CB-CG	-5.72	108.08	113.80
1	E	283	GLN	CB-CG-CD	5.71	122.31	112.60
1	E	29	GLU	CB-CG-CD	5.69	122.28	112.60
1	E	261	ARG	CD-NE-CZ	5.69	132.37	124.40
1	E	16	THR	CB-CA-C	5.66	120.89	109.68
1	E	119	LYS	N-CA-C	-5.65	100.47	109.23
1	E	242	ASP	CA-CB-CG	5.63	118.23	112.60
1	E	149	MET	CA-C-N	5.62	130.11	120.72
1	E	149	MET	C-N-CA	5.62	130.11	120.72
1	E	149	MET	CA-CB-CG	5.62	125.34	114.10
1	E	63	HIS	CE1-NE2-CD2	5.61	114.61	109.00
1	E	2	ASP	CA-CB-CG	-5.58	107.02	112.60
1	E	119	LYS	CA-C-O	-5.57	114.60	121.06
1	E	107	ARG	CB-CA-C	-5.55	101.57	110.79
1	E	40	THR	N-CA-C	-5.55	105.28	113.61
1	E	180	LEU	CA-C-O	5.51	126.26	120.42
1	E	58	PHE	N-CA-CB	5.50	118.30	110.16
1	E	287	GLU	CA-C-O	-5.45	113.36	119.79
1	E	132	VAL	CB-CA-C	5.44	118.85	111.88
1	E	138	ASP	CA-CB-CG	5.44	118.04	112.60
1	E	74	GLY	CA-C-N	5.42	132.14	122.06
1	E	74	GLY	C-N-CA	5.42	132.14	122.06
1	E	251	PHE	CA-C-N	5.41	127.48	120.44
1	E	251	PHE	C-N-CA	5.41	127.48	120.44
1	E	269	TYR	CB-CA-C	-5.41	102.36	110.90
1	E	250	GLU	CA-CB-CG	5.41	124.91	114.10
1	E	2	ASP	N-CA-CB	5.40	118.25	110.20
1	E	6	GLU	CB-CG-CD	5.39	121.77	112.60
1	E	15	GLN	CG-CD-NE2	-5.39	108.32	116.40
1	E	200	THR	CA-CB-OG1	-5.38	101.53	109.60
1	E	66	ILE	CA-C-O	-5.37	114.81	120.39
1	E	251	PHE	N-CA-C	-5.37	105.33	111.07
1	E	15	GLN	OE1-CD-NE2	5.36	127.95	122.60
1	E	144	SER	CA-C-N	5.36	128.93	120.47
1	E	144	SER	C-N-CA	5.36	128.93	120.47
1	E	144	SER	O-C-N	-5.34	116.96	123.16
1	E	89	ASN	N-CA-C	-5.33	102.63	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	ILE	N-CA-C	-5.33	100.64	108.11
1	E	204	GLU	CG-CD-OE1	5.33	130.66	118.40
1	E	137	ARG	CD-NE-CZ	5.32	131.85	124.40
1	E	316	ILE	O-C-N	5.32	127.43	121.90
1	E	77	GLY	CA-C-N	5.31	128.63	121.20
1	E	77	GLY	C-N-CA	5.31	128.63	121.20
1	E	146	ASN	CA-C-N	5.31	127.83	120.29
1	E	146	ASN	C-N-CA	5.31	127.83	120.29
1	E	3	LEU	O-C-N	5.28	127.51	122.07
1	E	189	GLN	N-CA-C	-5.25	100.47	109.24
1	E	59	GLN	CA-C-N	5.25	127.84	120.28
1	E	59	GLN	C-N-CA	5.25	127.84	120.28
1	E	283	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	E	300	GLU	CA-C-N	5.24	127.25	120.44
1	E	300	GLU	C-N-CA	5.24	127.25	120.44
1	E	27	ASN	CA-C-O	-5.23	113.96	119.97
1	E	192	GLY	N-CA-C	-5.20	104.55	112.51
1	E	140	GLY	N-CA-C	5.20	119.17	112.83
1	E	125	ASP	CA-C-O	-5.19	115.05	120.55
1	E	44	LEU	N-CA-C	-5.18	103.20	110.35
1	E	260	ASP	CA-C-N	5.18	127.75	120.28
1	E	260	ASP	C-N-CA	5.18	127.75	120.28
1	E	234	THR	CA-CB-OG1	-5.18	101.83	109.60
1	E	292	ARG	N-CA-CB	-5.17	104.34	112.46
1	E	21	GLY	CA-C-O	-5.15	115.44	121.00
1	E	159	GLU	CA-C-O	5.14	126.27	120.00
1	E	35	CYS	O-C-N	5.14	129.54	123.33
1	E	87	THR	N-CA-CB	5.14	118.10	110.29
1	E	166	GLU	CB-CG-CD	5.14	121.33	112.60
1	E	130	LEU	CB-CA-C	5.13	118.21	109.80
1	E	161	GLY	O-C-N	5.11	126.93	122.64
1	E	202	GLY	CA-C-N	5.09	127.52	120.29
1	E	202	GLY	C-N-CA	5.09	127.52	120.29
1	E	238	THR	N-CA-C	5.09	117.42	110.24
1	E	67	ALA	N-CA-C	-5.08	100.45	108.73
1	E	269	TYR	N-CA-C	5.07	116.62	111.14
1	E	231	PHE	N-CA-CB	5.05	117.42	109.69
1	E	126	TRP	CA-C-O	-5.05	113.56	118.97
1	E	304	LYS	CA-C-N	5.05	127.31	120.65
1	E	304	LYS	C-N-CA	5.05	127.31	120.65
1	E	179	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	E	120	ILE	CA-C-O	-5.01	115.12	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	97	TRP	CA-C-O	-5.01	115.11	120.42
1	E	173	GLN	N-CA-C	-5.00	105.90	111.36

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	E	2461	0	2394	77	0
2	E	13	0	8	1	0
3	E	162	0	0	3	1
All	All	2636	0	2402	77	1

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:E:45:HIS:H	1:E:48:HIS:HD2	1.21	0.86
1:E:82:LYS:HD3	1:E:86:ARG:HH11	1.45	0.80
1:E:110:ASP:OD2	1:E:113:ALA:HB2	1.91	0.71
1:E:45:HIS:H	1:E:48:HIS:CD2	2.07	0.69
1:E:36:GLY:HA3	2:E:320:TYR:CD1	2.31	0.66
1:E:82:LYS:CD	1:E:86:ARG:HH11	2.11	0.64
1:E:234:THR:HG22	1:E:236:SER:H	1.63	0.64
1:E:292:ARG:NH1	1:E:295:GLN:HG2	2.15	0.61
1:E:253:GLN:HA	1:E:256:ILE:HG22	1.83	0.60
1:E:291:LYS:O	1:E:292:ARG:HB2	2.01	0.59
1:E:292:ARG:HH11	1:E:295:GLN:HG2	1.67	0.59
1:E:72:ALA:O	1:E:75:LEU:HB2	2.03	0.59
1:E:148:MET:HE3	1:E:171:MET:HE3	1.86	0.58
1:E:314:GLN:O	1:E:318:ILE:HG13	2.02	0.58
1:E:44:LEU:HD13	1:E:52:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:N	1:E:27:ASN:HD21	2.01	0.57
1:E:9:TRP:CZ2	1:E:275:LYS:HG3	2.39	0.57
1:E:146:ASN:HB2	3:E:377:HOH:O	2.04	0.57
1:E:102:LYS:HG3	1:E:120:ILE:HG21	1.86	0.56
1:E:187:ARG:HD3	1:E:214:ARG:O	2.06	0.56
1:E:196:TRP:HE3	1:E:219:THR:HG23	1.69	0.56
1:E:3:LEU:HD22	1:E:61:ALA:HB3	1.88	0.55
1:E:82:LYS:CG	1:E:86:ARG:HH11	2.19	0.55
1:E:54:THR:HG21	1:E:220:ILE:HD11	1.87	0.55
1:E:82:LYS:HD3	1:E:86:ARG:NH1	2.20	0.55
1:E:149:MET:O	1:E:155:GLN:HG2	2.08	0.54
1:E:48:HIS:O	1:E:52:ILE:HG13	2.09	0.53
1:E:3:LEU:HD22	1:E:61:ALA:CB	2.38	0.53
1:E:195:GLN:O	1:E:199:ILE:HG13	2.09	0.53
1:E:145:VAL:O	1:E:149:MET:HG2	2.09	0.52
1:E:275:LYS:NZ	1:E:279:GLU:OE2	2.35	0.52
1:E:310:GLU:O	1:E:314:GLN:HG3	2.10	0.52
1:E:45:HIS:CE1	1:E:47:GLY:HA3	2.45	0.51
1:E:264:ILE:O	1:E:268:LYS:HG3	2.10	0.51
1:E:194:ASP:OD1	1:E:195:GLN:HG2	2.10	0.51
1:E:100:ARG:NH2	1:E:242:ASP:OD2	2.40	0.51
1:E:171:MET:HA	1:E:171:MET:HE2	1.93	0.50
1:E:187:ARG:HG3	3:E:321:HOH:O	2.11	0.50
1:E:17:THR:HG21	1:E:203:LEU:CD1	2.42	0.49
1:E:256:ILE:O	1:E:292:ARG:NH1	2.45	0.49
1:E:283:GLN:HG3	1:E:286:ARG:NH1	2.28	0.48
1:E:154:VAL:O	1:E:155:GLN:C	2.56	0.47
1:E:157:ARG:O	1:E:161:GLY:N	2.44	0.47
1:E:312:LEU:O	1:E:316:ILE:HG13	2.15	0.46
1:E:46:ILE:HD11	1:E:232:GLY:HA2	1.98	0.46
1:E:126:TRP:HB2	3:E:364:HOH:O	2.16	0.46
1:E:264:ILE:HG22	1:E:268:LYS:HE3	1.98	0.46
1:E:53:LEU:O	1:E:57:ARG:HG3	2.17	0.45
1:E:27:ASN:HD22	1:E:27:ASN:N	2.15	0.44
1:E:12:LEU:O	1:E:220:ILE:HD13	2.17	0.44
1:E:24:LYS:NZ	1:E:28:GLU:OE2	2.50	0.44
1:E:191:GLY:O	1:E:219:THR:HA	2.17	0.44
1:E:297:THR:O	1:E:301:GLU:HG2	2.18	0.44
1:E:9:TRP:CH2	1:E:275:LYS:HA	2.53	0.44
1:E:52:ILE:O	1:E:55:MET:HB2	2.18	0.43
1:E:189:GLN:HG2	1:E:190:ILE:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:ASP:OD1	1:E:260:ASP:N	2.52	0.43
1:E:193:SER:HG	1:E:221:PRO:HA	1.83	0.43
1:E:38:ASP:HA	1:E:39:PRO:HD3	1.84	0.43
1:E:26:LEU:HD23	1:E:31:VAL:HG21	2.01	0.43
1:E:281:LEU:HD22	1:E:294:ALA:HA	2.01	0.43
1:E:143:PHE:CG	1:E:171:MET:HE1	2.54	0.42
1:E:190:ILE:HA	1:E:218:LEU:O	2.19	0.42
1:E:91:LYS:O	1:E:95:GLU:HB2	2.19	0.42
1:E:282:GLU:HB3	1:E:283:GLN:NE2	2.35	0.42
1:E:56:ARG:O	1:E:60:GLN:HG3	2.20	0.41
1:E:72:ALA:HB2	1:E:124:TYR:HA	2.02	0.41
1:E:196:TRP:O	1:E:200:THR:HG23	2.20	0.41
1:E:105:LEU:HD23	1:E:105:LEU:HA	1.93	0.41
1:E:42:ASP:HB3	1:E:97:TRP:CD1	2.56	0.41
1:E:182:GLU:OE2	1:E:210:LYS:NZ	2.42	0.41
1:E:113:ALA:O	1:E:117:PRO:HB3	2.21	0.41
1:E:73:THR:HB	1:E:169:TYR:CE2	2.57	0.40
1:E:22:LEU:O	1:E:26:LEU:HG	2.21	0.40
1:E:134:THR:O	1:E:138:ASP:HB2	2.21	0.40
1:E:126:TRP:NE1	1:E:176:ASP:OD1	2.51	0.40
1:E:204:GLU:OE2	1:E:207:ARG:NH2	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:379:HOH:O	3:E:414:HOH:O[5_664]	1.74	0.46

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	E	313/319 (98%)	303 (97%)	10 (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	E	244/268 (91%)	234 (96%)	10 (4%)	27	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	8	GLN
1	E	33	LEU
1	E	68	LEU
1	E	114	ASP
1	E	149	MET
1	E	179	ARG
1	E	222	LEU
1	E	256	ILE
1	E	261	ARG
1	E	304	LYS

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

Mol	Chain	Res	Type
1	E	14	ASN
1	E	27	ASN
1	E	48	HIS
1	E	60	GLN
1	E	146	ASN
1	E	155	GLN
1	E	257	ASN
1	E	283	GLN

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Mol	Chain	Res	Type
1	E	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TYR	E	320	-	12,13,13	0.86	1 (8%)	13,17,17	1.03	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYR	E	320	-	-	2/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	320	TYR	OXT-C	-2.04	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	320	TYR	CG-CB-CA	2.96	120.19	114.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	320	TYR	CA-CB-CG-CD1
2	E	320	TYR	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	320	TYR	1	0

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.