



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:14 pm GMT

PDB ID : 4TS1  
Title : CRYSTAL STRUCTURE OF A DELETION MUTANT OF A TYROSYL-  
T/RNA SYNTHETASE COMPLEXED WITH TYROSINE  
Authors : Brick, P.; Blow, D.M.  
Deposited on : 1989-06-29  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

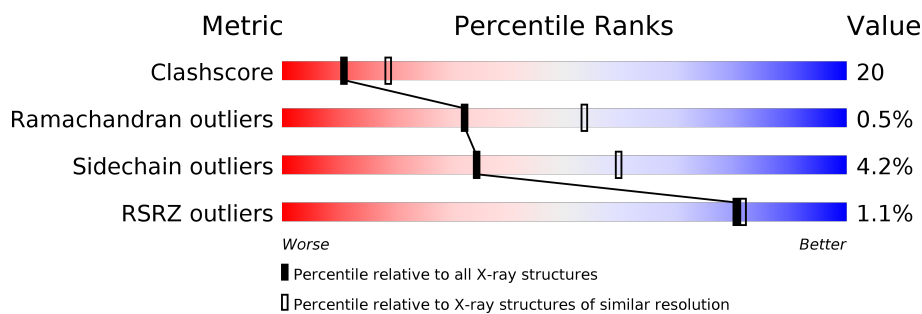
# 1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	319	
1	B	319	

## 2 Entry composition [i](#)

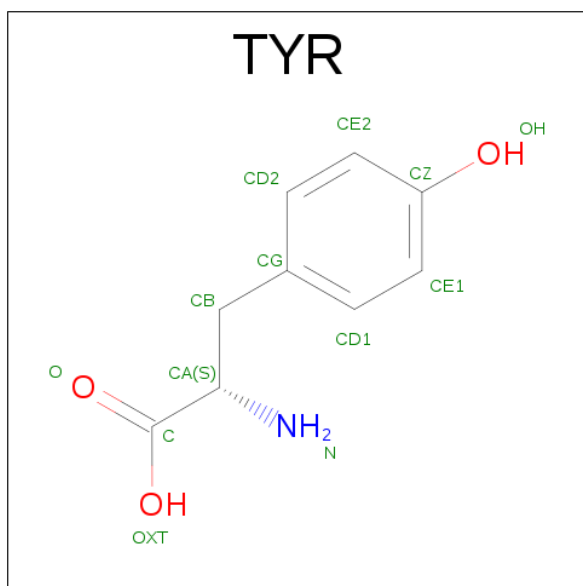
There are 3 unique types of molecules in this entry. The entry contains 4990 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2423	1551	409	456	7			
1	B	311	Total	C	N	O	S	0	0	0
			2397	1529	410	451	7			

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



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

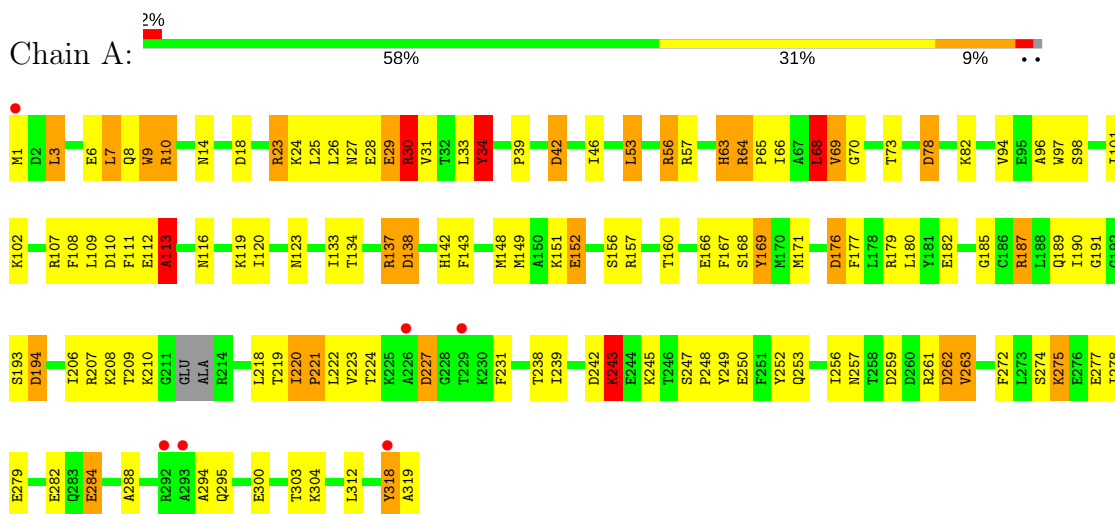
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total 72	O 72	0	0
3	B	72	Total 72	O 72	0	0

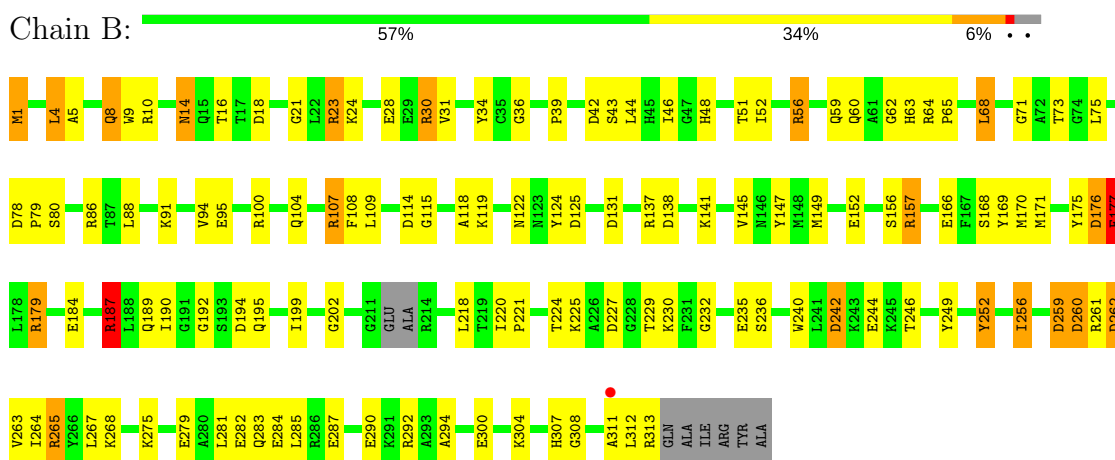
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

#### • Molecule 1: TYROSYL-tRNA SYNTHETASE



#### • Molecule 1: TYROSYL-tRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.46Å 67.06Å 61.37Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 29.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 96.6 (29.42-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.97 (at 2.51Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.187 , (Not available) (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 76.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.05	2/2472 (0.1%)	2.00	65/3349 (1.9%)
1	B	1.05	2/2445 (0.1%)	2.02	68/3312 (2.1%)
All	All	1.05	4/4917 (0.1%)	2.01	133/6661 (2.0%)

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	B	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	GLU	CB-CG	-6.38	1.40	1.52
1	A	193	SER	CB-OG	-5.90	1.34	1.42
1	A	166	GLU	CD-OE1	-5.65	1.19	1.25
1	B	1	MET	N-CA	5.18	1.56	1.46

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ARG	NE-CZ-NH1	-16.13	112.23	120.30
1	A	56	ARG	NE-CZ-NH2	-15.55	112.53	120.30
1	A	157	ARG	NE-CZ-NH1	-14.36	113.12	120.30
1	B	30	ARG	NE-CZ-NH2	13.71	127.16	120.30
1	B	179	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	B	242	ASP	CB-CG-OD2	-12.80	106.78	118.30
1	B	137	ARG	NE-CZ-NH1	-12.14	114.23	120.30
1	B	187	ARG	NE-CZ-NH1	-11.64	114.48	120.30
1	A	207	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	B	260	ASP	CB-CG-OD1	11.36	128.52	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	TYR	CB-CG-CD2	11.08	127.65	121.00
1	A	138	ASP	CB-CG-OD1	11.02	128.22	118.30
1	B	187	ARG	CD-NE-CZ	-10.86	108.39	123.60
1	B	137	ARG	CD-NE-CZ	10.70	138.58	123.60
1	B	259	ASP	CB-CG-OD2	10.26	127.53	118.30
1	A	207	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	10	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	B	138	ASP	CB-CG-OD1	9.80	127.12	118.30
1	B	194	ASP	CB-CG-OD2	9.70	127.03	118.30
1	B	244	GLU	OE1-CD-OE2	9.70	134.94	123.30
1	B	261	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	B	30	ARG	CD-NE-CZ	-9.51	110.28	123.60
1	B	131	ASP	CB-CG-OD1	9.45	126.81	118.30
1	A	169	TYR	CB-CG-CD1	-9.37	115.38	121.00
1	B	23	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	B	114	ASP	CB-CG-OD1	9.23	126.60	118.30
1	A	149	MET	CA-CB-CG	9.18	128.91	113.30
1	A	157	ARG	CD-NE-CZ	-9.01	110.99	123.60
1	A	57	ARG	CD-NE-CZ	8.92	136.08	123.60
1	A	18	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	A	194	ASP	CB-CG-OD1	8.69	126.12	118.30
1	B	265	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	A	107	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	B	137	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	B	262	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	69	VAL	C-N-CA	8.20	139.52	122.30
1	A	227	ASP	CB-CG-OD1	8.18	125.66	118.30
1	B	138	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	A	42	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	242	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	187	ARG	NH1-CZ-NH2	7.55	127.70	119.40
1	B	125	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	10	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	56	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	242	ASP	CB-CG-OD2	-7.29	111.73	118.30
1	B	177	PHE	CB-CG-CD2	7.28	125.89	120.80
1	A	152	GLU	CG-CD-OE1	7.14	132.58	118.30
1	B	107	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	260	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	A	157	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	34	TYR	CB-CG-CD2	7.02	125.21	121.00
1	B	179	ARG	NH1-CZ-NH2	7.02	127.12	119.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	TYR	CB-CG-CD1	6.96	125.18	121.00
1	B	157	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	B	4	LEU	CB-CA-C	6.68	122.89	110.20
1	B	292	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	68	LEU	CB-CG-CD2	-6.56	99.84	111.00
1	B	18	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	177	PHE	CB-CG-CD1	-6.40	116.32	120.80
1	B	14	ASN	OD1-CG-ND2	-6.37	107.25	121.90
1	A	64	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	261	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	166	GLU	N-CA-CB	-6.25	99.36	110.60
1	A	250	GLU	CB-CG-CD	6.22	131.00	114.20
1	A	78	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	157	ARG	CD-NE-CZ	-6.21	114.90	123.60
1	B	194	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	303	THR	O-C-N	6.17	132.57	122.70
1	A	111	PHE	CB-CG-CD1	-6.12	116.51	120.80
1	A	262	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	B	252	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	B	168	SER	CB-CA-C	-6.03	98.64	110.10
1	A	68	LEU	CB-CA-C	6.02	121.64	110.20
1	A	30	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	238	THR	CA-CB-CG2	6.00	120.79	112.40
1	B	236	SER	N-CA-CB	5.99	119.49	110.50
1	A	113	ALA	CA-C-O	5.99	132.68	120.10
1	A	23	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	A	29	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	B	265	ARG	CB-CA-C	5.94	122.28	110.40
1	A	123	ASN	CB-CA-C	5.90	122.19	110.40
1	A	3	LEU	CB-CA-C	5.88	121.37	110.20
1	A	96	ALA	N-CA-CB	5.88	118.33	110.10
1	A	53	LEU	CB-CA-C	5.83	121.28	110.20
1	B	14	ASN	CA-CB-CG	5.79	126.14	113.40
1	B	131	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	137	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	193	SER	CB-CA-C	-5.77	99.14	110.10
1	B	56	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	187	ARG	CD-NE-CZ	-5.75	115.54	123.60
1	B	166	GLU	O-C-N	-5.73	113.53	122.70
1	A	168	SER	CB-CA-C	-5.72	99.23	110.10
1	B	107	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	110	ASP	CB-CG-OD1	5.71	123.44	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	TYR	CA-CB-CG	-5.70	102.57	113.40
1	B	294	ALA	CB-CA-C	5.66	118.59	110.10
1	A	7	LEU	CB-CA-C	5.63	120.90	110.20
1	B	235	GLU	N-CA-CB	5.63	120.73	110.60
1	A	250	GLU	CG-CD-OE1	5.62	129.54	118.30
1	A	123	ASN	CA-C-N	5.62	129.56	117.20
1	B	42	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	A	34	TYR	CA-CB-CG	5.58	124.00	113.40
1	A	9	TRP	N-CA-CB	5.57	120.63	110.60
1	B	249	TYR	CB-CG-CD2	-5.51	117.70	121.00
1	A	123	ASN	O-C-N	-5.50	113.89	122.70
1	A	303	THR	N-CA-CB	5.49	120.73	110.30
1	A	63	HIS	O-C-N	-5.45	113.98	122.70
1	A	148	MET	CA-CB-CG	-5.45	104.04	113.30
1	B	292	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	42	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	189	GLN	CB-CG-CD	5.41	125.66	111.60
1	A	30	ARG	CA-CB-CG	5.40	125.28	113.40
1	B	242	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	42	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	114	ASP	OD1-CG-OD2	-5.37	113.11	123.30
1	B	290	GLU	O-C-N	5.34	131.25	122.70
1	B	56	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	60	GLN	CA-CB-CG	-5.32	101.69	113.40
1	B	246	THR	N-CA-CB	5.29	120.34	110.30
1	A	318	TYR	CA-CB-CG	-5.28	103.37	113.40
1	B	166	GLU	C-N-CA	5.28	134.90	121.70
1	A	151	LYS	CA-CB-CG	-5.28	101.79	113.40
1	A	176	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	147	TYR	O-C-N	5.19	131.01	122.70
1	B	14	ASN	CB-CG-OD1	5.18	131.97	121.60
1	B	202	GLY	C-N-CA	5.18	134.66	121.70
1	B	176	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	166	GLU	CG-CD-OE1	5.10	128.50	118.30
1	A	167	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	A	275	LYS	CA-C-N	-5.05	106.09	117.20
1	B	179	ARG	CD-NE-CZ	-5.05	116.53	123.60
1	A	23	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	263	VAL	N-CA-C	5.02	124.56	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	158	ILE	CB

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	2423	0	2309	103	1
1	B	2397	0	2300	90	0
2	A	13	0	8	1	0
2	B	13	0	8	2	0
3	A	72	0	0	5	0
3	B	72	0	0	9	0
All	All	4990	0	4625	191	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 20.

All (191) 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:46:ILE:HD11	1:B:232:GLY:HA2	1.36	1.01
1:B:30:ARG:HH12	1:B:115:GLY:HA3	1.28	0.97
1:B:24:LYS:HE2	1:B:28:GLU:OE1	1.64	0.97
1:A:31:VAL:H	1:A:63:HIS:HD2	0.96	0.96
1:B:31:VAL:H	1:B:63:HIS:HD2	1.00	0.91
1:B:30:ARG:HH12	1:B:115:GLY:CA	1.83	0.91
1:A:249:TYR:HE2	1:A:319:ALA:CB	1.84	0.90
1:A:23:ARG:O	1:A:27:ASN:OD1	1.91	0.89
1:A:31:VAL:H	1:A:63:HIS:CD2	1.89	0.84
1:A:46:ILE:HD13	1:A:239:ILE:HB	1.57	0.84
1:B:229:THR:HG22	1:B:230:LYS:N	1.93	0.84
1:A:249:TYR:CE2	1:A:319:ALA:HA	2.12	0.84
1:B:46:ILE:HD11	1:B:232:GLY:CA	2.08	0.83
1:B:229:THR:CG2	1:B:230:LYS:H	1.90	0.83
1:B:169:TYR:HH	2:B:320:TYR:N	1.77	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HD23	1:A:31:VAL:HG21	1.58	0.82
1:A:275:LYS:NZ	1:A:279:GLU:OE1	2.13	0.82
1:B:48:HIS:O	1:B:52:ILE:HG13	1.80	0.82
1:B:252:TYR:CE1	1:B:256:ILE:HD12	2.15	0.81
1:A:31:VAL:N	1:A:63:HIS:HD2	1.79	0.79
1:A:1:MET:N	1:A:23:ARG:HG3	1.99	0.78
1:B:1:MET:CA	1:B:23:ARG:HD3	2.15	0.76
1:A:249:TYR:HE2	1:A:319:ALA:CA	1.99	0.75
1:A:64:ARG:HH21	1:A:119:LYS:HE3	1.50	0.75
1:B:31:VAL:H	1:B:63:HIS:CD2	1.93	0.75
1:A:249:TYR:HE2	1:A:319:ALA:HB2	1.51	0.74
1:B:304:LYS:HG2	1:B:312:LEU:HD22	1.70	0.74
1:B:1:MET:CA	1:B:23:ARG:CD	2.66	0.74
1:A:24:LYS:O	1:A:28:GLU:HB2	1.88	0.74
1:A:249:TYR:CE2	1:A:319:ALA:HB2	2.23	0.72
1:B:104:GLN:O	1:B:107:ARG:HG3	1.90	0.72
1:B:229:THR:CG2	1:B:230:LYS:N	2.48	0.72
1:B:64:ARG:HH21	1:B:119:LYS:HE3	1.55	0.72
1:A:82:LYS:HE2	3:A:338:HOH:O	1.90	0.71
1:B:229:THR:HG22	1:B:230:LYS:H	1.53	0.71
1:A:263:VAL:HG11	1:A:294:ALA:HB1	1.71	0.71
1:A:69:VAL:HG21	1:A:102:LYS:HG2	1.71	0.71
1:A:208:LYS:NZ	3:A:388:HOH:O	2.23	0.70
1:B:187:ARG:HG3	3:B:323:HOH:O	1.90	0.70
1:B:152:GLU:O	1:B:156:SER:HB3	1.92	0.69
1:A:26:LEU:HD23	1:A:31:VAL:CG2	2.22	0.69
1:A:249:TYR:CE2	1:A:319:ALA:CA	2.75	0.69
1:B:21:GLY:O	3:B:337:HOH:O	2.10	0.69
1:B:260:ASP:O	1:B:263:VAL:HG12	1.93	0.69
1:A:142:HIS:O	1:A:208:LYS:NZ	2.18	0.69
1:B:44:LEU:H	1:B:104:GLN:HE22	1.41	0.68
1:A:31:VAL:O	1:A:63:HIS:HB3	1.94	0.67
1:A:274:SER:OG	1:A:277:GLU:HG3	1.94	0.67
1:A:152:GLU:O	1:A:156:SER:HB3	1.96	0.66
1:A:249:TYR:HE2	1:A:319:ALA:HA	1.53	0.66
1:B:31:VAL:N	1:B:63:HIS:HD2	1.85	0.66
1:A:187:ARG:HG3	3:A:321:HOH:O	1.95	0.66
1:A:1:MET:CA	1:A:27:ASN:HD21	2.09	0.66
1:A:263:VAL:HG21	1:A:295:GLN:NE2	2.12	0.65
1:B:43:SER:HB3	1:B:240:TRP:CE3	2.32	0.64
1:B:225:LYS:NZ	1:B:229:THR:HB	2.11	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD2	1:A:108:PHE:O	1.97	0.64
1:B:300:GLU:O	1:B:304:LYS:HG3	1.97	0.64
1:A:64:ARG:NH2	1:A:119:LYS:HE3	2.11	0.64
1:A:46:ILE:CD1	1:A:239:ILE:HB	2.28	0.64
1:B:30:ARG:HG3	1:B:62:GLY:O	1.98	0.63
1:B:30:ARG:NH1	1:B:115:GLY:CA	2.59	0.63
1:A:263:VAL:HG11	1:A:294:ALA:CB	2.29	0.62
1:A:9:TRP:HH2	1:A:278:ILE:HD12	1.65	0.62
1:B:64:ARG:NH2	1:B:184:GLU:OE2	2.25	0.62
1:A:263:VAL:CG1	1:A:294:ALA:HB1	2.30	0.61
1:A:187:ARG:CG	3:A:321:HOH:O	2.48	0.61
1:A:185:GLY:O	1:A:187:ARG:HG2	2.02	0.60
1:A:73:THR:HB	1:A:169:TYR:CE1	2.38	0.59
1:A:9:TRP:CH2	1:A:275:LYS:HA	2.37	0.59
1:B:64:ARG:NH2	1:B:119:LYS:HE3	2.18	0.59
1:A:30:ARG:NH2	1:A:64:ARG:HD3	2.18	0.58
1:B:86:ARG:CG	3:B:333:HOH:O	2.51	0.58
1:B:225:LYS:HZ3	1:B:229:THR:HB	1.69	0.58
1:A:116:ASN:N	1:A:116:ASN:OD1	2.37	0.58
1:A:249:TYR:CE2	1:A:319:ALA:CB	2.74	0.57
1:A:25:LEU:O	1:A:29:GLU:N	2.33	0.57
1:A:223:VAL:HG12	1:A:231:PHE:CG	2.39	0.57
1:A:182:GLU:OE1	1:A:210:LYS:NZ	2.30	0.57
1:B:91:LYS:O	1:B:95:GLU:HB2	2.05	0.57
1:A:256:ILE:HD12	1:A:257:ASN:N	2.20	0.56
1:A:9:TRP:CZ2	1:A:275:LYS:HA	2.41	0.56
1:B:141:LYS:NZ	3:B:321:HOH:O	2.39	0.56
1:A:6:GLU:O	1:A:10:ARG:HG3	2.06	0.55
1:A:194:ASP:OD2	1:A:194:ASP:N	2.39	0.55
1:A:263:VAL:CG2	1:A:295:GLN:NE2	2.68	0.55
1:B:39:PRO:HG2	1:B:94:VAL:HG13	1.89	0.55
1:B:304:LYS:HG2	1:B:312:LEU:CD2	2.36	0.55
1:A:253:GLN:NE2	1:A:319:ALA:HB1	2.22	0.55
1:B:285:LEU:HD12	1:B:285:LEU:O	2.07	0.54
1:B:30:ARG:NH1	1:B:115:GLY:C	2.61	0.54
1:B:56:ARG:HD2	1:B:108:PHE:O	2.08	0.54
1:A:1:MET:H2	1:A:23:ARG:HG3	1.71	0.54
1:A:34:TYR:HA	1:A:66:ILE:O	2.08	0.53
1:A:78:ASP:O	1:A:82:LYS:HD2	2.07	0.53
1:B:175:TYR:O	1:B:179:ARG:HG2	2.08	0.53
1:A:68:LEU:C	1:A:68:LEU:HD23	2.28	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLY:HA3	1:B:122:ASN:OD1	2.09	0.52
1:A:46:ILE:HD13	1:A:239:ILE:CB	2.35	0.52
1:B:78:ASP:HB2	1:B:169:TYR:CZ	2.44	0.52
1:B:68:LEU:HD23	1:B:68:LEU:C	2.29	0.52
1:A:143:PHE:CG	1:A:171:MET:HE1	2.45	0.52
1:B:78:ASP:OD2	1:B:80:SER:HB2	2.10	0.52
1:A:64:ARG:HH21	1:A:119:LYS:CE	2.23	0.52
1:B:229:THR:HG23	1:B:230:LYS:H	1.73	0.52
1:A:6:GLU:O	1:A:6:GLU:HG2	2.09	0.51
1:B:252:TYR:CZ	1:B:256:ILE:HD12	2.46	0.51
1:A:256:ILE:CD1	1:A:257:ASN:ND2	2.73	0.51
1:B:264:ILE:HD13	1:B:267:LEU:HD12	1.92	0.51
1:B:4:LEU:O	1:B:8:GLN:HB2	2.10	0.51
1:B:145:VAL:O	1:B:149:MET:HG2	2.11	0.51
1:A:14:ASN:HB2	1:A:221:PRO:HG3	1.93	0.51
1:A:56:ARG:HG2	1:A:272:PHE:CZ	2.46	0.51
1:A:65:PRO:CG	1:A:109:LEU:HD22	2.41	0.51
1:B:30:ARG:HH12	1:B:115:GLY:C	2.13	0.51
1:A:279:GLU:O	1:A:282:GLU:HB3	2.11	0.50
1:B:100:ARG:NH1	1:B:242:ASP:OD1	2.41	0.50
1:B:10:ARG:HD3	1:B:268:LYS:O	2.11	0.50
1:B:262:ASP:OD2	1:B:265:ARG:NH2	2.44	0.49
1:B:192:GLY:O	1:B:195:GLN:HB2	2.11	0.49
1:A:259:ASP:O	1:A:262:ASP:N	2.45	0.49
1:B:307:HIS:HB3	1:B:311:ALA:CB	2.43	0.48
1:A:143:PHE:CD1	1:A:171:MET:CE	2.96	0.48
1:A:227:ASP:C	1:A:227:ASP:OD2	2.52	0.48
1:A:256:ILE:HD12	1:A:257:ASN:ND2	2.29	0.48
1:A:78:ASP:HB2	1:A:169:TYR:CZ	2.49	0.47
1:A:275:LYS:O	1:A:279:GLU:HG3	2.14	0.47
1:A:42:ASP:OD1	1:A:245:LYS:NZ	2.45	0.47
1:A:220:ILE:N	1:A:220:ILE:CD1	2.77	0.47
1:A:112:GLU:O	1:A:113:ALA:O	2.33	0.47
1:A:1:MET:CA	1:A:23:ARG:HG3	2.45	0.47
1:A:134:THR:O	1:A:138:ASP:HB2	2.14	0.46
1:A:223:VAL:HG12	1:A:231:PHE:CD1	2.50	0.46
1:A:53:LEU:O	1:A:56:ARG:HB3	2.15	0.46
1:A:143:PHE:CE1	1:A:171:MET:HE2	2.50	0.46
1:B:109:LEU:HD13	1:B:118:ALA:HB1	1.98	0.46
1:B:16:THR:HG22	1:B:218:LEU:HG	1.97	0.46
1:A:190:ILE:HA	1:A:218:LEU:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:O	1:B:177:PHE:HD1	1.98	0.45
1:B:312:LEU:O	1:B:313:ARG:C	2.54	0.45
1:B:73:THR:HB	1:B:169:TYR:CE1	2.51	0.45
1:A:39:PRO:HB3	1:A:101:ILE:HD12	1.97	0.45
1:A:176:ASP:OD1	2:A:320:TYR:OH	2.27	0.45
1:A:209:THR:HG22	1:A:210:LYS:HG2	1.97	0.45
1:B:88:LEU:HA	3:B:332:HOH:O	2.16	0.45
1:A:191:GLY:O	1:A:219:THR:HA	2.17	0.45
1:B:30:ARG:HH11	1:B:30:ARG:HD3	1.18	0.45
1:A:284:GLU:O	1:A:288:ALA:N	2.50	0.45
1:B:195:GLN:O	1:B:199:ILE:HG13	2.18	0.44
1:B:9:TRP:CH2	1:B:275:LYS:HA	2.53	0.44
1:B:36:GLY:HA2	1:B:68:LEU:O	2.17	0.44
1:B:190:ILE:HD12	1:B:220:ILE:HD11	2.00	0.44
1:B:283:GLN:HE21	1:B:283:GLN:HB2	1.57	0.44
1:A:143:PHE:CD1	1:A:171:MET:HE2	2.53	0.43
1:B:176:ASP:OD1	2:B:320:TYR:OH	2.28	0.43
1:B:304:LYS:O	1:B:308:GLY:N	2.44	0.43
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.86	0.43
1:B:31:VAL:O	1:B:63:HIS:HB3	2.19	0.43
1:A:26:LEU:CD2	1:A:31:VAL:HG21	2.39	0.43
1:B:5:ALA:HA	1:B:8:GLN:HE21	1.83	0.43
1:A:222:LEU:CB	3:A:363:HOH:O	2.67	0.43
1:A:30:ARG:CZ	1:A:64:ARG:HD3	2.49	0.42
1:A:300:GLU:O	1:A:304:LYS:HG3	2.19	0.42
1:B:78:ASP:CG	1:B:80:SER:HB2	2.40	0.42
1:B:279:GLU:O	1:B:282:GLU:HB3	2.20	0.42
1:B:64:ARG:HH21	1:B:119:LYS:CE	2.29	0.42
1:A:94:VAL:O	1:A:97:TRP:HB2	2.20	0.42
1:A:247:SER:HA	1:A:248:PRO:HD3	1.69	0.42
1:B:259:ASP:HB3	3:B:368:HOH:O	2.20	0.42
1:A:65:PRO:HG3	1:A:109:LEU:HD22	2.03	0.41
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.68	0.41
1:B:51:THR:HB	3:B:329:HOH:O	2.21	0.41
1:A:137:ARG:NH2	1:B:75:LEU:O	2.53	0.41
1:A:304:LYS:HG2	1:A:312:LEU:HD22	2.02	0.41
1:A:189:GLN:HG2	1:A:190:ILE:N	2.35	0.41
1:B:170:MET:HG3	1:B:171:MET:HE3	2.01	0.41
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.90	0.41
1:A:98:SER:O	1:A:102:LYS:HG3	2.20	0.41
1:B:179:ARG:HA	1:B:179:ARG:HD2	1.85	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:HIS:O	1:B:51:THR:HG22	2.21	0.41
1:B:59:GLN:HB2	1:B:65:PRO:HG3	2.02	0.41
1:A:206:ILE:HD13	1:A:206:ILE:HG21	1.63	0.41
1:A:243:LYS:CG	1:A:243:LYS:O	2.68	0.41
1:B:14:ASN:HD22	1:B:221:PRO:HA	1.86	0.41
1:A:256:ILE:HD12	1:A:256:ILE:C	2.42	0.41
1:A:133:ILE:HD13	1:B:75:LEU:HD12	2.03	0.41
1:B:157:ARG:CG	3:B:357:HOH:O	2.69	0.40
1:B:227:ASP:C	1:B:227:ASP:OD1	2.60	0.40
1:A:120:ILE:HD13	1:A:120:ILE:HG21	1.91	0.40
1:B:4:LEU:HA	1:B:4:LEU:HD12	1.92	0.40
1:B:79:PRO:HA	3:B:372:HOH:O	2.20	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)
1:A:179:ARG:NH1	1:A:318:TYR:O[2_556]	2.10	0.10

## 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%)	294 (94%)	16 (5%)	3 (1%)	18	32
1	B	307/319 (96%)	301 (98%)	6 (2%)	0	100	100
All	All	620/638 (97%)	595 (96%)	22 (4%)	3 (0%)	32	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ALA

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	243	LYS
1	A	70	GLY

### 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	235/268 (88%)	222 (94%)	13 (6%)	25	46
1	B	237/268 (88%)	230 (97%)	7 (3%)	46	74
All	All	472/536 (88%)	452 (96%)	20 (4%)	34	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	8	GLN
1	A	30	ARG
1	A	33	LEU
1	A	34	TYR
1	A	68	LEU
1	A	160	THR
1	A	177	PHE
1	A	220	ILE
1	A	221	PRO
1	A	224	THR
1	A	243	LYS
1	A	284	GLU
1	B	8	GLN
1	B	34	TYR
1	B	177	PHE
1	B	187	ARG
1	B	224	THR
1	B	256	ILE
1	B	284	GLU

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

Mol	Chain	Res	Type
1	A	63	HIS
1	A	146	ASN
1	A	253	GLN
1	A	257	ASN
1	B	8	GLN
1	B	14	ASN
1	B	60	GLN
1	B	63	HIS
1	B	104	GLN
1	B	257	ASN
1	B	283	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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	A	320	-	9,13,13	1.18	1 (11%)	12,17,17	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TYR	B	320	-	9,13,13	1.11	1 (11%)	12,17,17	1.56	3 (25%)

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	A	320	-	-	0/4/8/8	0/1/1/1
2	TYR	B	320	-	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	320	TYR	CE2-CD2	2.01	1.42	1.38
2	A	320	TYR	CD1-CG	2.94	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	TYR	CD1-CE1-CZ	-2.68	116.83	119.88
2	B	320	TYR	CD2-CE2-CZ	2.38	122.57	119.88
2	B	320	TYR	CE1-CD1-CG	2.87	124.98	121.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/319 (99%)	-0.42	6 (1%) 67 69	5, 22, 61, 82	0
1	B	311/319 (97%)	-0.57	1 (0%) 93 94	3, 19, 52, 68	0
All	All	628/638 (98%)	-0.50	7 (1%) 80 81	3, 20, 56, 82	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	TYR	2.7
1	B	311	ALA	2.6
1	A	226	ALA	2.5
1	A	293	ALA	2.5
1	A	292	ARG	2.4
1	A	1	MET	2.2
1	A	229	THR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TYR	A	320	13/13	0.96	0.15	1.60	5,7,19,19	0
2	TYR	B	320	13/13	0.98	0.13	0.55	2,4,14,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.