



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 06:52 PM EDT

PDB ID : 2O2E  
Title : Mycobacterium tuberculosis tryptophan synthase beta subunit dimer (apo-form)  
Authors : Burenkov, G.P.; Kachalova, G.S.; Bartunik, H.D.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)  
Deposited on : unknown  
Resolution : 2.20 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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)	:	rb-20030345

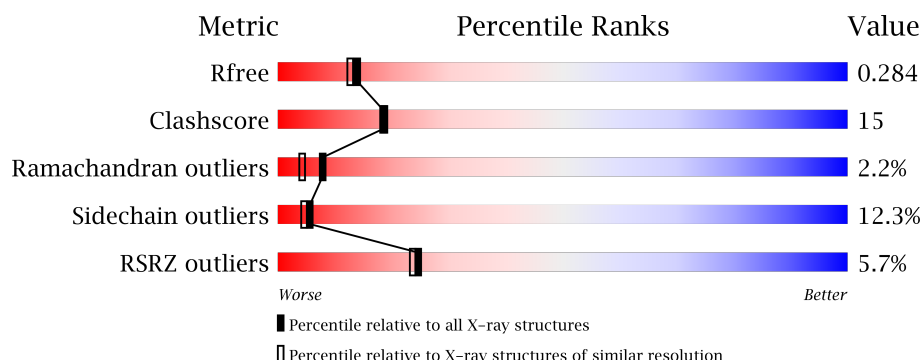
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	422	<div> <div>3%</div> <div>46%</div> <div>21%</div> <div>6%</div> <div>25%</div> </div>
1	B	422	<div> <div>6%</div> <div>43%</div> <div>22%</div> <div>7%</div> <div>25%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4772 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 Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2365	1481	431	440	13			
1	B	316	Total	C	N	O	S	0	0	0
			2373	1485	432	443	13			

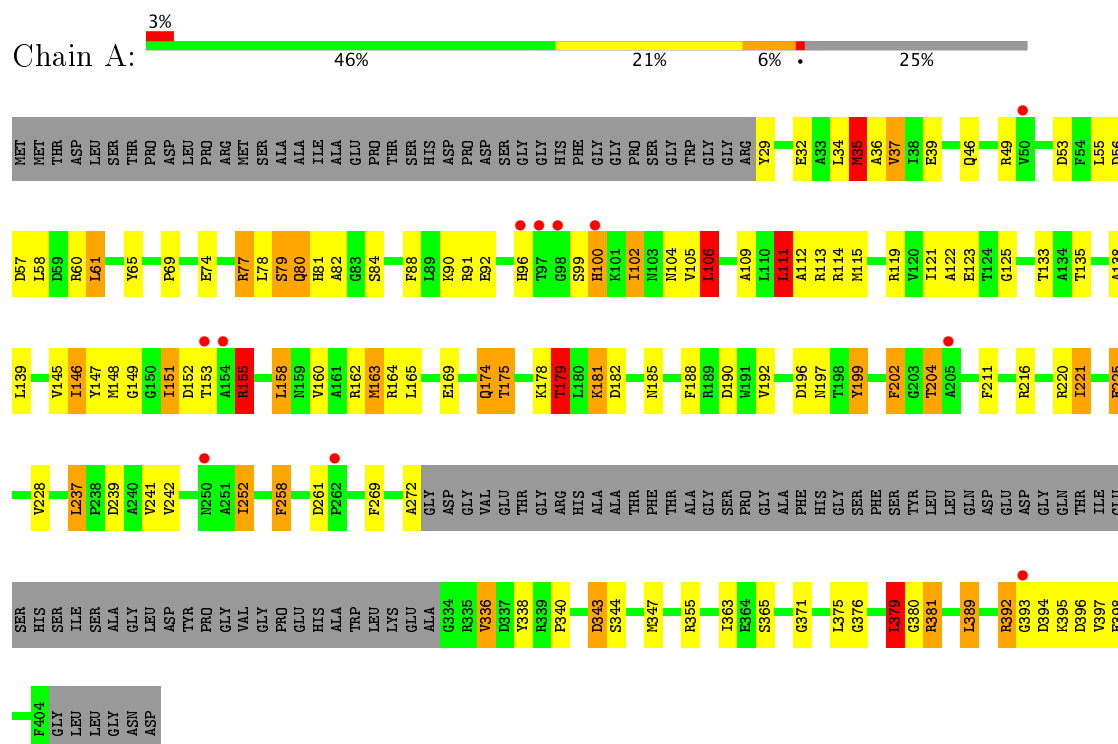
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	18	Total	O	0	0
			18	18		

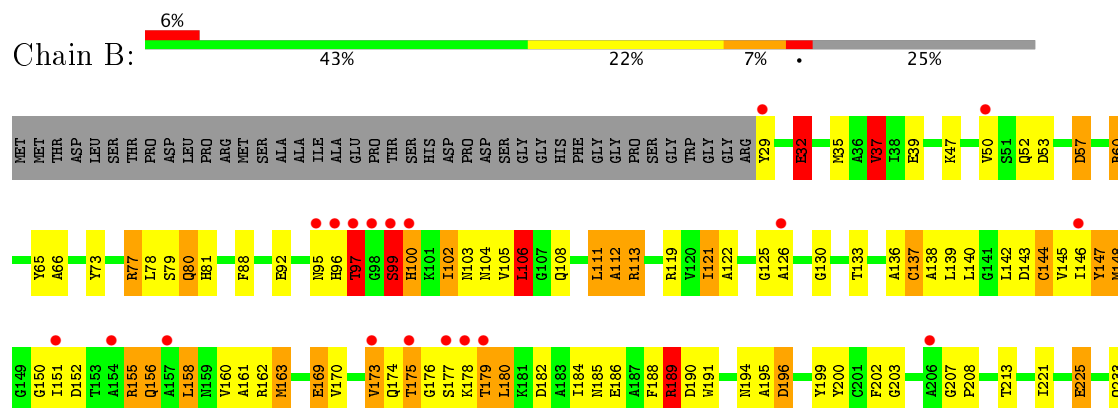
### 3 Residue-property plots [i](#)

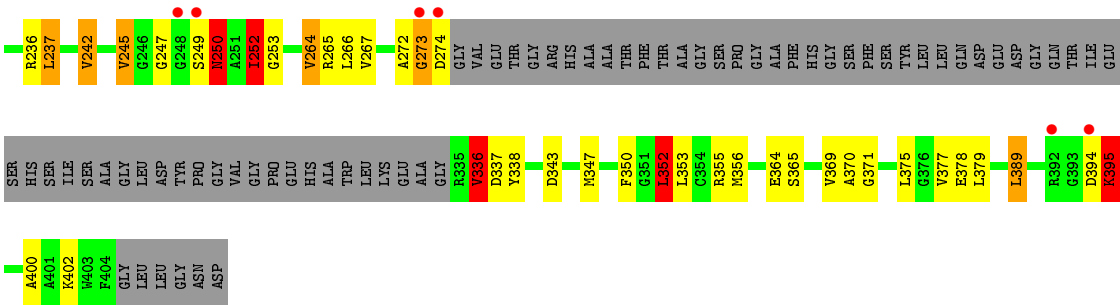
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Tryptophan synthase beta chain



#### • Molecule 1: Tryptophan synthase beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.98Å 56.46Å 120.55Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.92-2.20) 99.6 (19.90-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.211 , 0.281 0.215 , 0.284	Depositor DCC
$R_{free}$ test set	1926 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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	1.88	50/2403 (2.1%)	1.53	39/3252 (1.2%)
1	B	1.83	36/2411 (1.5%)	1.45	29/3263 (0.9%)
All	All	1.85	86/4814 (1.8%)	1.49	68/6515 (1.0%)

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	0	2

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	VAL	CB-CG1	10.38	1.74	1.52
1	B	371	GLY	N-CA	9.06	1.59	1.46
1	A	36	ALA	CA-CB	9.05	1.71	1.52
1	A	147	TYR	CG-CD2	8.80	1.50	1.39
1	B	377	VAL	CB-CG2	8.55	1.70	1.52
1	B	88	PHE	CE2-CZ	8.26	1.53	1.37
1	B	65	TYR	CB-CG	-8.23	1.39	1.51
1	B	169	GLU	CG-CD	7.78	1.63	1.51
1	A	109	ALA	CA-CB	7.67	1.68	1.52
1	A	196	ASP	CB-CG	7.64	1.67	1.51
1	A	160	VAL	CB-CG2	7.59	1.68	1.52
1	B	60	ARG	CG-CD	7.53	1.70	1.51
1	A	74	GLU	CB-CG	7.50	1.66	1.52
1	A	147	TYR	CE1-CZ	7.50	1.48	1.38
1	A	258	PHE	CE1-CZ	7.38	1.51	1.37
1	A	169	GLU	CD-OE2	7.35	1.33	1.25
1	A	147	TYR	CD2-CE2	7.19	1.50	1.39
1	A	37	VAL	CB-CG2	-6.96	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLN	CG-CD	6.93	1.67	1.51
1	B	97	THR	CA-CB	6.93	1.71	1.53
1	A	122	ALA	CA-CB	6.92	1.67	1.52
1	B	39	GLU	CG-CD	6.83	1.62	1.51
1	B	65	TYR	CD2-CE2	6.69	1.49	1.39
1	A	60	ARG	CG-CD	6.65	1.68	1.51
1	A	192	VAL	CB-CG2	6.55	1.66	1.52
1	B	78	LEU	N-CA	6.53	1.59	1.46
1	B	233	GLN	C-O	6.47	1.35	1.23
1	A	65	TYR	CE1-CZ	6.47	1.47	1.38
1	A	113	ARG	CZ-NH1	6.44	1.41	1.33
1	A	163	MET	CG-SD	6.35	1.97	1.81
1	A	88	PHE	CD2-CE2	6.26	1.51	1.39
1	A	65	TYR	CD2-CE2	6.26	1.48	1.39
1	A	164	ARG	CB-CG	6.18	1.69	1.52
1	A	155	ARG	CG-CD	6.17	1.67	1.51
1	B	370	ALA	C-O	-6.12	1.11	1.23
1	B	103	ASN	CB-CG	6.06	1.65	1.51
1	B	66	ALA	CA-CB	6.06	1.65	1.52
1	A	202	PHE	CE1-CZ	6.05	1.48	1.37
1	B	225	GLU	CD-OE2	-6.04	1.19	1.25
1	A	61	LEU	CG-CD2	5.95	1.73	1.51
1	B	88	PHE	CD2-CE2	5.93	1.51	1.39
1	A	88	PHE	CE2-CZ	5.92	1.48	1.37
1	A	241	VAL	CB-CG1	-5.92	1.40	1.52
1	B	169	GLU	CB-CG	5.88	1.63	1.52
1	B	92	GLU	CB-CG	5.87	1.63	1.52
1	B	112	ALA	CA-CB	5.85	1.64	1.52
1	A	216	ARG	CG-CD	5.80	1.66	1.51
1	A	199	TYR	CD1-CE1	5.76	1.48	1.39
1	B	77	ARG	CG-CD	5.74	1.66	1.51
1	A	151	ILE	C-O	5.73	1.34	1.23
1	A	225	GLU	CB-CG	5.68	1.62	1.52
1	A	147	TYR	CE2-CZ	5.67	1.46	1.38
1	B	189	ARG	CG-CD	5.66	1.66	1.51
1	B	137	CYS	CB-SG	5.64	1.91	1.82
1	B	202	PHE	CE1-CZ	5.64	1.48	1.37
1	A	138	ALA	CA-CB	-5.64	1.40	1.52
1	B	32	GLU	CG-CD	5.63	1.60	1.51
1	A	258	PHE	CD2-CE2	5.62	1.50	1.39
1	A	162	ARG	CB-CG	5.60	1.67	1.52
1	B	369	VAL	CB-CG1	5.56	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	LEU	N-CA	5.48	1.57	1.46
1	B	378	GLU	CB-CG	-5.43	1.41	1.52
1	A	242	VAL	CB-CG1	-5.39	1.41	1.52
1	A	135	THR	C-O	-5.35	1.13	1.23
1	B	79	SER	CB-OG	5.34	1.49	1.42
1	A	79	SER	CB-OG	-5.34	1.35	1.42
1	A	188	PHE	CE1-CZ	5.34	1.47	1.37
1	B	402	LYS	CE-NZ	5.31	1.62	1.49
1	A	53	ASP	CB-CG	5.31	1.62	1.51
1	A	336	VAL	CB-CG2	-5.30	1.41	1.52
1	B	73	TYR	CD1-CE1	5.24	1.47	1.39
1	A	149	GLY	CA-C	5.22	1.60	1.51
1	A	147	TYR	CG-CD1	5.20	1.46	1.39
1	B	126	ALA	CA-CB	5.19	1.63	1.52
1	A	77	ARG	CG-CD	5.19	1.65	1.51
1	A	39	GLU	CD-OE1	5.16	1.31	1.25
1	A	202	PHE	CE2-CZ	5.15	1.47	1.37
1	A	46	GLN	CB-CG	-5.15	1.38	1.52
1	B	200	TYR	CE1-CZ	5.15	1.45	1.38
1	A	381	ARG	CG-CD	5.14	1.64	1.51
1	B	147	TYR	CD2-CE2	5.14	1.47	1.39
1	A	92	GLU	CD-OE2	5.12	1.31	1.25
1	B	213	THR	CA-CB	5.11	1.66	1.53
1	A	228	VAL	CB-CG2	5.10	1.63	1.52
1	A	90	LYS	CD-CE	5.06	1.64	1.51
1	B	119	ARG	CG-CD	5.05	1.64	1.51

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH2	-19.03	110.79	120.30
1	A	91	ARG	NE-CZ-NH1	13.06	126.83	120.30
1	A	60	ARG	NE-CZ-NH1	-12.29	114.16	120.30
1	B	77	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	A	239	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	190	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	119	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	353	LEU	CB-CG-CD2	7.88	124.39	111.00
1	A	158	LEU	CA-CB-CG	7.40	132.32	115.30
1	A	389	LEU	CB-CG-CD1	-7.34	98.53	111.00
1	A	237	LEU	CB-CG-CD2	-7.31	98.58	111.00
1	B	242	VAL	CG1-CB-CG2	7.27	122.53	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	162	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	175	THR	N-CA-CB	-6.91	97.17	110.30
1	A	151	ILE	CG1-CB-CG2	6.88	126.52	111.40
1	A	239	ASP	CB-CG-OD1	-6.86	112.12	118.30
1	A	106	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	57	ASP	CB-CA-C	6.85	124.10	110.40
1	A	190	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	237	LEU	CB-CG-CD1	6.81	122.58	111.00
1	B	111	LEU	CB-CG-CD2	6.79	122.53	111.00
1	B	355	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	78	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	A	102	ILE	CG1-CB-CG2	6.73	126.21	111.40
1	A	343	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	B	236	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	196	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	114	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	B	143	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	A	162	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	375	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	B	389	LEU	CB-CG-CD2	6.24	121.60	111.00
1	B	37	VAL	CB-CA-C	6.10	122.98	111.40
1	B	336	VAL	CG1-CB-CG2	6.03	120.54	110.90
1	A	35	MET	CG-SD-CE	6.00	109.80	100.20
1	A	343	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	265	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	352	LEU	CB-CG-CD2	5.90	121.03	111.00
1	A	379	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	60	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	A	56	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	119	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	77	ARG	CG-CD-NE	-5.72	99.78	111.80
1	A	119	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	179	THR	N-CA-CB	-5.64	99.57	110.30
1	A	60	ARG	CB-CG-CD	5.62	126.21	111.60
1	B	242	VAL	CA-CB-CG1	5.47	119.11	110.90
1	A	158	LEU	CB-CG-CD2	5.44	120.25	111.00
1	B	163	MET	CG-SD-CE	-5.44	91.49	100.20
1	B	252	ILE	CG1-CB-CG2	5.43	123.36	111.40
1	A	355	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	146	ILE	CB-CG1-CD1	-5.37	98.86	113.90
1	A	220	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LEU	CB-CG-CD2	5.29	120.00	111.00
1	B	343	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	65	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
1	B	266	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	B	213	THR	CA-CB-CG2	5.17	119.64	112.40
1	B	236	ARG	CG-CD-NE	5.16	122.64	111.80
1	A	252	ILE	CG1-CB-CG2	5.15	122.73	111.40
1	B	265	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	152	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	96	HIS	CB-CA-C	5.12	120.64	110.40
1	B	106	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	355	ARG	CG-CD-NE	-5.08	101.14	111.80
1	A	49	ARG	CB-CA-C	-5.06	100.27	110.40
1	B	242	VAL	N-CA-CB	-5.03	100.44	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	ASN	Peptide
1	B	99	SER	Peptide

## 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	2365	0	2360	67	0
1	B	2373	0	2364	76	0
2	A	16	0	0	0	0
2	B	18	0	0	0	0
All	All	4772	0	4724	141	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 15.

All (141) 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:264:VAL:CB	1:B:264:VAL:CG1	1.74	1.64
1:B:252:ILE:CD1	1:B:252:ILE:CG1	1.83	1.55
1:A:146:ILE:HD13	1:A:163:MET:CE	1.55	1.35
1:A:146:ILE:HD13	1:A:163:MET:HE3	1.24	1.12
1:A:146:ILE:HD13	1:A:163:MET:HE2	1.39	1.02
1:B:249:SER:O	1:B:250:ASN:CB	2.08	1.01
1:A:146:ILE:CD1	1:A:163:MET:HE3	1.96	0.94
1:A:99:SER:O	1:A:100:HIS:HB2	1.64	0.94
1:B:173:VAL:HG11	1:B:186:GLU:HG3	1.50	0.94
1:A:146:ILE:CD1	1:A:163:MET:CE	2.46	0.94
1:A:392:ARG:HD3	1:A:392:ARG:H	1.31	0.92
1:B:395:LYS:HZ3	1:B:395:LYS:HA	1.36	0.90
1:A:237:LEU:N	1:A:237:LEU:HD22	1.86	0.90
1:B:188:PHE:HZ	1:B:208:PRO:HG2	1.37	0.88
1:B:249:SER:O	1:B:250:ASN:HB3	1.73	0.88
1:B:185:ASN:O	1:B:189:ARG:HG3	1.75	0.86
1:B:395:LYS:NZ	1:B:395:LYS:HA	1.90	0.86
1:A:139:LEU:O	1:B:77:ARG:HD2	1.75	0.84
1:A:146:ILE:HB	1:A:163:MET:HE1	1.62	0.82
1:B:174:GLN:O	1:B:178:LYS:HD3	1.80	0.81
1:A:77:ARG:NH1	1:B:138:ALA:O	2.15	0.80
1:B:147:TYR:OH	1:B:190:ASP:OD2	2.00	0.79
1:A:179:THR:CG2	1:A:181:LYS:HB2	2.12	0.78
1:B:125:GLY:O	1:B:148:MET:HE1	1.82	0.77
1:B:394:ASP:O	1:B:395:LYS:HB2	1.84	0.77
1:B:130:GLY:HA2	1:B:146:ILE:HD12	1.67	0.76
1:B:156:GLN:O	1:B:160:VAL:HG23	1.85	0.76
1:B:77:ARG:HD3	1:B:356:MET:O	1.85	0.76
1:B:125:GLY:O	1:B:148:MET:CE	2.34	0.76
1:A:35:MET:HA	1:A:35:MET:CE	2.18	0.74
1:A:146:ILE:CG1	1:A:163:MET:HE3	2.20	0.72
1:B:188:PHE:CZ	1:B:208:PRO:HG2	2.25	0.69
1:A:237:LEU:N	1:A:237:LEU:CD2	2.55	0.68
1:B:249:SER:O	1:B:250:ASN:HB2	1.92	0.68
1:A:146:ILE:CB	1:A:163:MET:CE	2.73	0.67
1:A:146:ILE:HB	1:A:163:MET:CE	2.24	0.67
1:B:264:VAL:CG1	1:B:264:VAL:CG2	2.71	0.67
1:A:111:LEU:O	1:A:115:MET:HG3	1.95	0.66
1:A:237:LEU:H	1:A:237:LEU:CD2	2.08	0.66
1:A:237:LEU:H	1:A:237:LEU:HD22	1.61	0.66
1:A:35:MET:HE2	1:A:35:MET:HA	1.79	0.64
1:B:247:GLY:HA3	1:B:364:GLU:OE2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:CB	1:A:163:MET:HE1	2.27	0.62
1:A:123:GLU:OE2	1:A:204:THR:HG21	2.00	0.62
1:B:176:GLY:O	1:B:178:LYS:N	2.33	0.62
1:A:392:ARG:NH2	1:A:395:LYS:HB2	2.17	0.60
1:B:151:ILE:HG22	1:B:155:ARG:HH21	1.68	0.59
1:B:188:PHE:HZ	1:B:208:PRO:CG	2.13	0.59
1:A:179:THR:HG22	1:A:182:ASP:H	1.68	0.58
1:B:250:ASN:H	1:B:253:GLY:H	1.52	0.58
1:A:179:THR:HG21	1:A:181:LYS:HB2	1.86	0.57
1:A:202:PHE:HE2	1:A:211:PHE:HE1	1.53	0.56
1:A:174:GLN:HG3	1:A:178:LYS:HE2	1.87	0.56
1:B:47:LYS:O	1:B:50:VAL:HG12	2.05	0.56
1:B:106:LEU:HD11	1:B:139:LEU:HD23	1.87	0.56
1:B:151:ILE:O	1:B:155:ARG:HG2	2.05	0.56
1:A:99:SER:O	1:A:100:HIS:CB	2.44	0.55
1:B:121:ILE:HD11	1:B:191:TRP:HB2	1.89	0.55
1:B:174:GLN:OE1	1:B:178:LYS:HE3	2.06	0.55
1:B:395:LYS:NZ	1:B:395:LYS:CA	2.65	0.54
1:A:202:PHE:CE2	1:A:211:PHE:HE1	2.26	0.54
1:A:392:ARG:HD3	1:A:392:ARG:N	2.10	0.54
1:B:112:ALA:HB2	1:B:199:TYR:CG	2.42	0.54
1:A:146:ILE:CB	1:A:163:MET:HE3	2.38	0.54
1:A:363:ILE:HD12	1:A:396:ASP:CG	2.29	0.54
1:A:151:ILE:O	1:A:155:ARG:HG2	2.08	0.53
1:A:392:ARG:O	1:A:394:ASP:N	2.42	0.53
1:B:185:ASN:O	1:B:189:ARG:CG	2.53	0.53
1:B:125:GLY:O	1:B:148:MET:HE2	2.08	0.53
1:B:264:VAL:CG1	1:B:264:VAL:CA	2.77	0.52
1:A:394:ASP:HA	1:A:397:VAL:HG23	1.89	0.52
1:B:113:ARG:NH2	1:B:140:LEU:O	2.43	0.52
1:B:182:ASP:O	1:B:186:GLU:HG2	2.09	0.51
1:A:123:GLU:OE2	1:A:204:THR:CG2	2.57	0.51
1:A:363:ILE:HD12	1:A:396:ASP:HB3	1.93	0.51
1:A:363:ILE:HD12	1:A:396:ASP:CB	2.40	0.51
1:B:53:ASP:O	1:B:57:ASP:HB2	2.10	0.51
1:B:37:VAL:HG13	1:B:191:TRP:CZ2	2.46	0.51
1:B:395:LYS:HZ2	1:B:395:LYS:C	2.13	0.51
1:A:258:PHE:HA	1:A:261:ASP:OD2	2.11	0.50
1:B:221:ILE:O	1:B:225:GLU:HG3	2.11	0.50
1:B:95:ASN:O	1:B:96:HIS:ND1	2.46	0.49
1:A:58:LEU:HD23	1:A:221:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLN:HB3	1:A:81:HIS:CD2	2.47	0.49
1:B:158:LEU:O	1:B:161:ALA:HB3	2.13	0.49
1:B:264:VAL:CG1	1:B:264:VAL:HB	2.19	0.49
1:A:105:VAL:HG11	1:A:133:THR:HA	1.94	0.48
1:B:395:LYS:HA	1:B:395:LYS:CE	2.44	0.48
1:B:194:ASN:O	1:B:196:ASP:N	2.46	0.48
1:B:347:MET:CE	1:B:400:ALA:HA	2.44	0.48
1:A:34:LEU:O	1:A:37:VAL:HG12	2.14	0.48
1:B:122:ALA:HB3	1:B:146:ILE:HD13	1.96	0.47
1:A:375:LEU:HG	1:A:379:LEU:HD22	1.97	0.47
1:B:99:SER:O	1:B:102:ILE:HG12	2.14	0.47
1:A:347:MET:CE	1:A:363:ILE:HG12	2.45	0.47
1:A:106:LEU:HD11	1:A:139:LEU:HD23	1.97	0.46
1:A:179:THR:HG22	1:A:181:LYS:HB2	1.96	0.46
1:A:392:ARG:HH22	1:A:395:LYS:HB2	1.78	0.46
1:A:336:VAL:HG22	1:A:338:TYR:CZ	2.51	0.46
1:B:163:MET:HE2	1:B:170:VAL:HG22	1.98	0.46
1:A:272:ALA:HB2	1:A:340:PRO:HB2	1.97	0.46
1:B:158:LEU:HD23	1:B:158:LEU:H	1.81	0.46
1:B:272:ALA:O	1:B:273:GLY:O	2.33	0.46
1:B:365:SER:HB3	1:B:389:LEU:HD22	1.97	0.45
1:B:150:GLY:HA3	1:B:178:LYS:HD2	1.98	0.45
1:A:121:ILE:HA	1:A:145:VAL:O	2.15	0.45
1:A:269:PHE:CZ	1:A:371:GLY:HA3	2.52	0.45
1:A:121:ILE:HG22	1:A:145:VAL:HB	2.00	0.44
1:B:152:ASP:OD1	1:B:155:ARG:NH1	2.51	0.44
1:A:112:ALA:HB2	1:A:199:TYR:CG	2.53	0.44
1:A:376:GLY:O	1:A:380:GLY:N	2.46	0.44
1:B:245:VAL:O	1:B:245:VAL:HG13	2.17	0.44
1:A:82:ALA:C	1:A:84:SER:N	2.70	0.43
1:A:395:LYS:HA	1:A:398:GLU:OE1	2.18	0.43
1:B:80:GLN:HG3	1:B:81:HIS:CD2	2.54	0.43
1:A:151:ILE:HG22	1:A:155:ARG:HE	1.84	0.43
1:B:104:ASN:OD1	1:B:108:GLN:NE2	2.49	0.43
1:B:207:GLY:HA2	1:B:208:PRO:HD3	1.82	0.43
1:B:137:CYS:HB3	1:B:142:LEU:O	2.18	0.43
1:B:32:GLU:O	1:B:35:MET:HG2	2.19	0.43
1:A:125:GLY:O	1:A:148:MET:HE2	2.19	0.43
1:B:336:VAL:HG22	1:B:338:TYR:CZ	2.54	0.43
1:A:202:PHE:CE2	1:A:211:PHE:CE1	3.07	0.42
1:A:79:SER:O	1:A:84:SER:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:CD2	1:B:158:LEU:H	2.32	0.42
1:B:179:THR:O	1:B:180:LEU:HB3	2.20	0.42
1:B:158:LEU:O	1:B:162:ARG:HG3	2.19	0.42
1:A:69:PRO:HA	1:A:225:GLU:CD	2.41	0.42
1:B:137:CYS:SG	1:B:144:CYS:HB2	2.60	0.42
1:B:185:ASN:O	1:B:189:ARG:N	2.48	0.42
1:A:365:SER:HB3	1:A:389:LEU:HD22	2.02	0.41
1:B:352:LEU:HD22	1:B:356:MET:HG2	2.02	0.41
1:B:267:VAL:HA	1:B:337:ASP:O	2.20	0.41
1:B:347:MET:O	1:B:350:PHE:HB3	2.20	0.41
1:B:105:VAL:HG12	1:B:136:ALA:CB	2.50	0.41
1:A:32:GLU:O	1:A:35:MET:HG2	2.21	0.41
1:B:163:MET:HB2	1:B:163:MET:HE2	1.95	0.41
1:A:55:LEU:HD22	1:A:221:ILE:CD1	2.52	0.40
1:B:105:VAL:HG11	1:B:133:THR:HA	2.04	0.40
1:A:35:MET:HA	1:A:35:MET:HE3	2.00	0.40
1:B:121:ILE:HA	1:B:145:VAL:O	2.21	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	311/422 (74%)	294 (94%)	15 (5%)	2 (1%)	28	29
1	B	312/422 (74%)	286 (92%)	14 (4%)	12 (4%)	4	1
All	All	623/844 (74%)	580 (93%)	29 (5%)	14 (2%)	8	4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	HIS

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Mol	Chain	Res	Type
1	B	97	THR
1	B	177	SER
1	B	273	GLY
1	B	99	SER
1	B	100	HIS
1	B	175	THR
1	B	180	LEU
1	B	195	ALA
1	B	250	ASN
1	B	395	LYS
1	A	393	GLY
1	B	184	ILE
1	B	203	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	236/314 (75%)	211 (89%)	25 (11%)	8	7
1	B	237/314 (76%)	204 (86%)	33 (14%)	4	3
All	All	473/628 (75%)	415 (88%)	58 (12%)	5	4

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	A	35	MET
1	A	61	LEU
1	A	80	GLN
1	A	102	ILE
1	A	104	ASN
1	A	106	LEU
1	A	111	LEU
1	A	153	THR
1	A	155	ARG

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Mol	Chain	Res	Type
1	A	158	LEU
1	A	174	GLN
1	A	175	THR
1	A	179	THR
1	A	181	LYS
1	A	185	ASN
1	A	197	ASN
1	A	204	THR
1	A	221	ILE
1	A	252	ILE
1	A	343	ASP
1	A	344	SER
1	A	379	LEU
1	A	381	ARG
1	A	392	ARG
1	B	29	TYR
1	B	32	GLU
1	B	37	VAL
1	B	52	GLN
1	B	57	ASP
1	B	60	ARG
1	B	97	THR
1	B	100	HIS
1	B	102	ILE
1	B	106	LEU
1	B	111	LEU
1	B	113	ARG
1	B	121	ILE
1	B	144	CYS
1	B	148	MET
1	B	155	ARG
1	B	156	GLN
1	B	158	LEU
1	B	169	GLU
1	B	173	VAL
1	B	175	THR
1	B	179	THR
1	B	189	ARG
1	B	196	ASP
1	B	237	LEU
1	B	242	VAL
1	B	245	VAL

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Mol	Chain	Res	Type
1	B	252	ILE
1	B	274	ASP
1	B	336	VAL
1	B	352	LEU
1	B	379	LEU
1	B	395	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	174	GLN
1	A	197	ASN
1	B	52	GLN
1	B	209	HIS

### 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](#)

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

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, 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	315/422 (74%)	-0.10	11 (3%) 44 42	27, 42, 66, 82	0
1	B	316/422 (74%)	0.14	25 (7%) 13 12	22, 47, 88, 104	0
All	All	631/844 (74%)	0.02	36 (5%) 24 24	22, 43, 79, 104	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	THR	6.1
1	B	99	SER	5.8
1	B	98	GLY	5.7
1	A	97	THR	5.0
1	A	98	GLY	4.4
1	B	96	HIS	4.2
1	B	50	VAL	3.9
1	B	173	VAL	3.7
1	A	96	HIS	3.6
1	B	154	ALA	3.5
1	A	50	VAL	3.5
1	B	157	ALA	3.4
1	B	394	ASP	3.4
1	A	154	ALA	3.4
1	A	100	HIS	3.2
1	B	274	ASP	3.1
1	B	100	HIS	3.1
1	B	248	GLY	3.0
1	A	262	PRO	3.0
1	B	175	THR	3.0
1	B	29	TYR	2.9
1	B	95	ASN	2.9
1	B	206	ALA	2.9
1	B	179	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	393	GLY	2.8
1	B	177	SER	2.7
1	B	178	LYS	2.7
1	A	153	THR	2.7
1	B	151	ILE	2.7
1	A	205	ALA	2.6
1	B	392	ARG	2.6
1	B	273	GLY	2.5
1	A	250	ASN	2.3
1	B	126	ALA	2.1
1	B	249	SER	2.1
1	B	146	ILE	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.