



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 2O2J / pdb_00002o2j
Title : Mycobacterium tuberculosis tryptophan synthase beta chain dimer (apoform)
Authors : Burenkov, G.P.; Kachalova, G.S.; Bartunik, H.D.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on : 2006-11-29
Resolution : 2.56 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

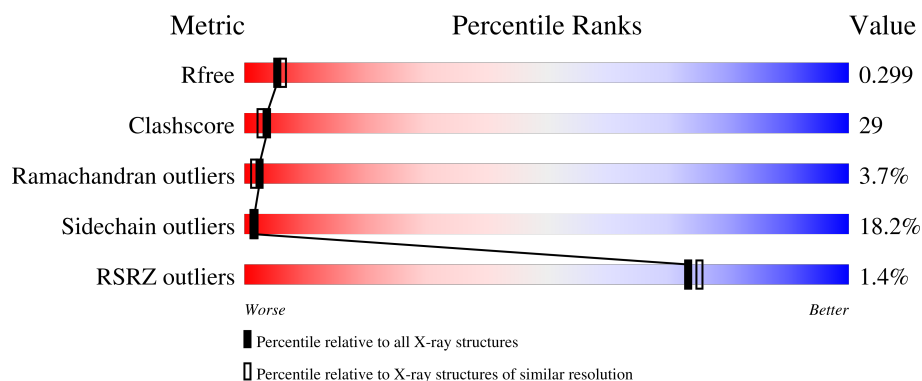
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	422	
1	B	422	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4758 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			

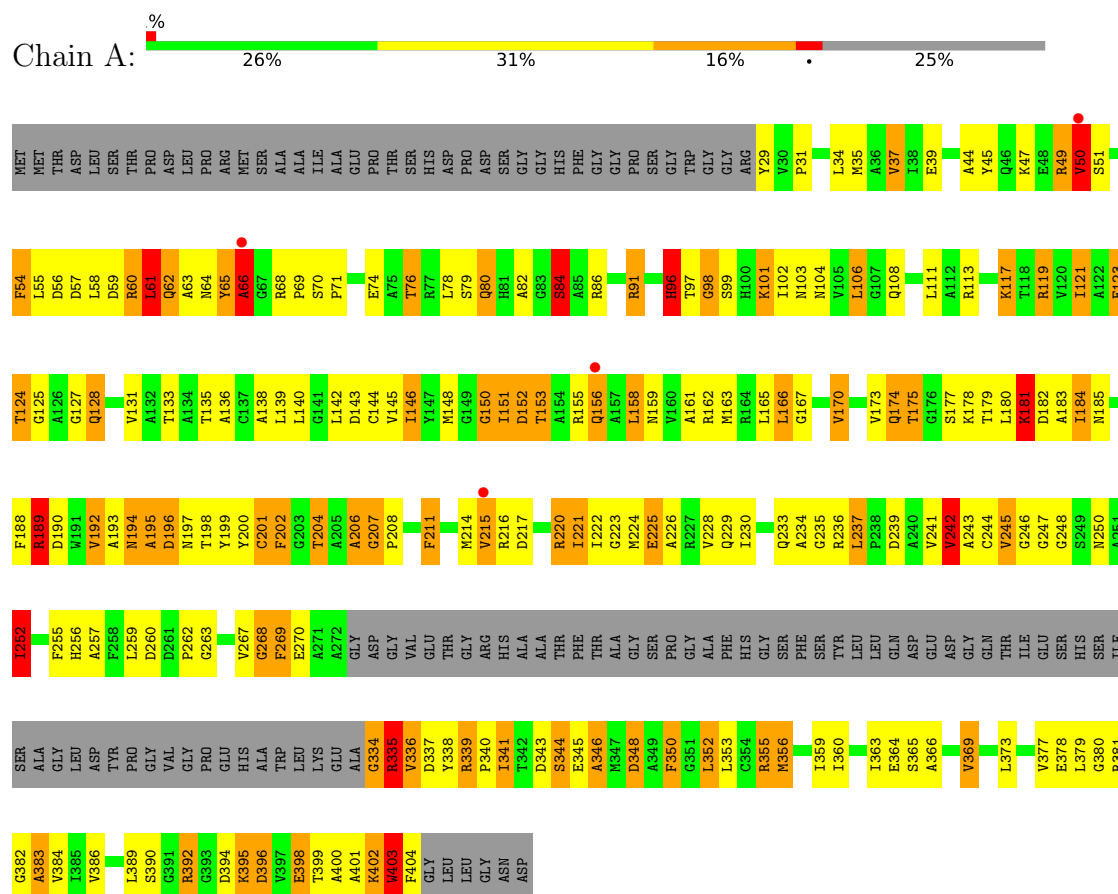
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	12	Total	O	0	0
			12	12		

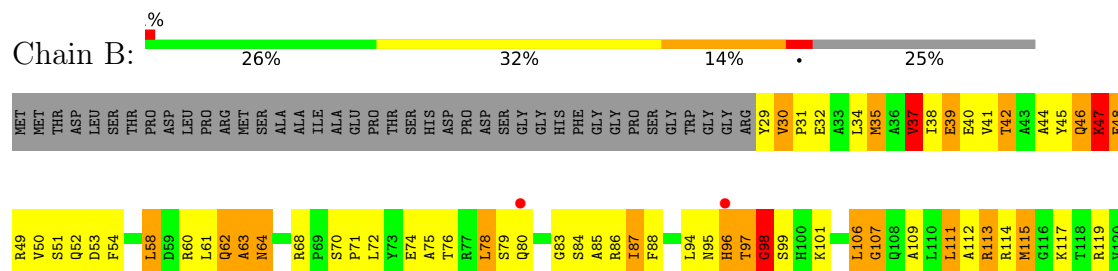
3 Residue-property plots

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



V386	V387	N388	L389	S390	G391	R392	G393	D394	K395	D396	V397	E398	T399	A400	A401	K402	M403	F404	GLY	LEU	LEU	GLY	ASN	ASP																																			
V192	A193	N194	A195	D196	N197	T198	Y199	Y200	C201	F202	G203		G207	P208	H209	P210	F211	F212	T213	M214	V215	R216	D217	F218	Q219	R220	I221	I222		E225	A226	R227	V228	Q229	I230	Q231	G232	Q233	A234		R236	L237	P238	D239	A240	V241	V242		V245	G246	G247	G248	S249	N250	A251	I252	G253	I254	F255
H256	A257	F258	L259	D260	R263	L266	V267		E270	A271	A272	G273	D274	GLY	VAL	GLU	THR	GLY	ARG	HIS	ALA	ALA	THR	PHE	THR	ALA	GLY	SER	PRO	GLY	ALA	PHE	HIS	GLY	SER	PHE	SER	TYR	LEU	GLN	ASP	GLU	ASP	GLY	GLN	THR	ILE	GLU	SER	HIS	SER	ILE	SER	ALA	GLY	LEU	ASP		
TYR	PRO	GLY	VAL	PRO	GLU	HIS	ALA	TRP	LEU	LYS	GLU	ALA	GLY	R335	V336	D337	Y338	R339	P340	T341	T342	D343	S344	E345	A346	R347	D348	A349	F350	G351	L352	L353	C354	R355	M356	E357	G358	I359	P361	A362	I363	E364	S365	A366		V369	A370		L373	K374	L375	G376	V377	E378	L379		I385		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.82Å 114.97Å 159.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.56 10.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.00-2.56) 95.0 (10.00-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.304 0.214 , 0.299	Depositor DCC
R_{free} test set	1239 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4758	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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	2.15	82/2403 (3.4%)	1.93	72/3252 (2.2%)
1	B	2.14	76/2411 (3.2%)	1.93	71/3263 (2.2%)
All	All	2.15	158/4814 (3.3%)	1.93	143/6515 (2.2%)

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	A	0	7
1	B	0	6
All	All	0	13

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	TYR	C-O	15.32	1.43	1.24
1	B	63	ALA	CA-CB	10.76	1.70	1.53
1	B	192	VAL	CA-CB	-10.08	1.41	1.54
1	A	131	VAL	CA-CB	-9.70	1.43	1.54
1	A	383	ALA	CA-CB	-9.09	1.38	1.53
1	A	236	ARG	C-O	-8.81	1.14	1.23
1	A	146	ILE	N-CA	-8.67	1.36	1.46
1	B	109	ALA	CA-CB	-8.51	1.39	1.53
1	B	227	ARG	C-O	8.41	1.34	1.24
1	A	222	ILE	CA-CB	-8.33	1.45	1.54
1	A	222	ILE	CA-C	8.27	1.62	1.52
1	A	215	VAL	CA-CB	8.19	1.66	1.54
1	A	229	GLN	N-CA	8.15	1.56	1.46
1	B	154	ALA	CA-CB	8.11	1.67	1.53
1	A	348	ASP	CA-C	8.07	1.63	1.52
1	B	184	ILE	CA-CB	8.07	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ASN	CB-CG	7.94	1.72	1.52
1	B	53	ASP	CA-C	-7.89	1.42	1.52
1	B	234	ALA	CA-CB	-7.89	1.41	1.53
1	A	97	THR	N-CA	7.82	1.55	1.46
1	A	96	HIS	CA-C	7.68	1.63	1.52
1	A	138	ALA	CA-CB	-7.61	1.41	1.53
1	B	111	LEU	CA-C	7.45	1.62	1.52
1	B	226	ALA	CA-C	7.44	1.62	1.52
1	B	112	ALA	CA-CB	-7.42	1.41	1.53
1	A	146	ILE	CA-CB	-7.39	1.45	1.54
1	A	395	LYS	N-CA	7.30	1.55	1.46
1	A	133	THR	CA-CB	7.23	1.64	1.53
1	A	360	ILE	CA-C	-7.15	1.47	1.53
1	A	51	SER	N-CA	7.15	1.54	1.46
1	A	143	ASP	C-O	-7.07	1.14	1.23
1	B	234	ALA	C-O	-7.06	1.15	1.24
1	B	228	VAL	CA-CB	7.04	1.63	1.54
1	B	39	GLU	CB-CG	6.96	1.73	1.52
1	A	144	CYS	N-CA	-6.86	1.37	1.46
1	A	142	LEU	N-CA	6.84	1.54	1.46
1	A	234	ALA	CA-CB	-6.84	1.43	1.53
1	B	193	ALA	CA-CB	-6.79	1.41	1.53
1	B	242	VAL	CA-CB	-6.76	1.45	1.54
1	A	346	ALA	CA-CB	-6.75	1.43	1.53
1	B	106	LEU	C-O	-6.71	1.16	1.24
1	A	226	ALA	N-CA	6.65	1.54	1.46
1	B	154	ALA	N-CA	6.62	1.54	1.46
1	B	38	ILE	CA-CB	-6.59	1.45	1.54
1	B	58	LEU	C-O	6.56	1.31	1.24
1	A	121	ILE	C-O	6.55	1.30	1.23
1	B	96	HIS	CA-CB	6.53	1.64	1.53
1	A	220	ARG	N-CA	-6.52	1.38	1.46
1	A	170	VAL	CA-CB	-6.47	1.46	1.54
1	B	256	HIS	C-O	-6.46	1.16	1.24
1	B	97	THR	CA-CB	6.45	1.63	1.53
1	B	366	ALA	CA-C	6.45	1.61	1.52
1	A	59	ASP	C-O	-6.43	1.16	1.24
1	B	115	MET	CB-CG	-6.42	1.33	1.52
1	A	344	SER	N-CA	-6.41	1.38	1.46
1	B	44	ALA	CA-CB	-6.40	1.43	1.53
1	B	122	ALA	C-O	-6.37	1.16	1.23
1	A	257	ALA	CA-CB	6.36	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	TRP	C-O	6.33	1.32	1.24
1	A	360	ILE	CA-CB	6.33	1.60	1.53
1	B	107	GLY	C-O	6.27	1.31	1.23
1	A	99	SER	CA-C	6.23	1.61	1.52
1	A	50	VAL	CA-CB	6.22	1.62	1.54
1	B	341	ILE	CA-CB	6.22	1.62	1.54
1	B	343	ASP	CA-C	6.22	1.61	1.52
1	B	163	MET	N-CA	-6.22	1.38	1.46
1	B	254	ILE	C-O	6.21	1.32	1.24
1	A	189	ARG	N-CA	6.17	1.54	1.46
1	A	335	ARG	CA-C	6.12	1.61	1.52
1	A	233	GLN	CA-C	-6.03	1.44	1.52
1	B	151	ILE	CA-CB	6.00	1.62	1.54
1	A	386	VAL	C-O	5.98	1.30	1.24
1	A	54	PHE	CA-C	-5.97	1.45	1.52
1	B	398	GLU	C-N	-5.95	1.25	1.33
1	A	201	CYS	N-CA	-5.94	1.38	1.46
1	A	252	ILE	C-O	-5.94	1.16	1.24
1	B	68	ARG	N-CA	5.92	1.54	1.46
1	A	252	ILE	CG1-CD1	5.92	1.74	1.51
1	A	80	GLN	CA-C	5.91	1.60	1.52
1	B	122	ALA	CA-CB	-5.91	1.43	1.53
1	A	101	LYS	CD-CE	5.90	1.70	1.52
1	B	40	GLU	CG-CD	5.89	1.66	1.52
1	B	39	GLU	N-CA	5.89	1.53	1.46
1	B	273	GLY	N-CA	5.89	1.53	1.45
1	A	348	ASP	CB-CG	5.87	1.66	1.52
1	A	352	LEU	N-CA	-5.87	1.39	1.46
1	A	250	ASN	CA-C	5.86	1.60	1.52
1	A	166	LEU	CG-CD2	5.84	1.71	1.52
1	A	211	PHE	C-O	-5.83	1.17	1.24
1	A	44	ALA	CA-CB	-5.81	1.44	1.53
1	A	350	PHE	C-O	5.78	1.30	1.24
1	A	390	SER	CA-C	-5.78	1.45	1.52
1	B	128	GLN	CG-CD	5.77	1.66	1.52
1	B	220	ARG	CA-C	-5.76	1.44	1.52
1	B	214	MET	CA-C	-5.76	1.45	1.52
1	B	135	THR	N-CA	5.75	1.52	1.46
1	B	40	GLU	CB-CG	5.71	1.69	1.52
1	A	146	ILE	CG1-CD1	-5.71	1.29	1.51
1	A	403	TRP	CA-C	5.70	1.60	1.52
1	B	42	THR	CA-CB	-5.68	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	ILE	CA-CB	-5.63	1.47	1.54
1	B	48	GLU	CA-C	-5.63	1.45	1.53
1	A	66	ALA	CA-CB	5.58	1.65	1.53
1	A	341	ILE	CA-CB	5.57	1.61	1.54
1	A	140	LEU	C-O	5.56	1.31	1.24
1	A	179	THR	CA-C	5.53	1.59	1.52
1	B	254	ILE	CA-CB	5.51	1.62	1.54
1	B	360	ILE	CA-C	5.50	1.57	1.53
1	A	58	LEU	N-CA	-5.50	1.39	1.46
1	B	386	VAL	C-O	5.49	1.30	1.24
1	A	104	ASN	CA-CB	5.48	1.61	1.53
1	B	388	ASN	C-O	-5.47	1.17	1.24
1	A	86	ARG	C-O	5.46	1.30	1.24
1	B	185	ASN	C-O	5.43	1.30	1.24
1	B	249	SER	N-CA	5.41	1.53	1.46
1	A	355	ARG	CG-CD	5.40	1.68	1.52
1	A	139	LEU	N-CA	-5.40	1.39	1.46
1	B	113	ARG	N-CA	5.39	1.52	1.46
1	A	184	ILE	CA-C	5.38	1.60	1.52
1	A	206	ALA	CA-C	5.36	1.57	1.52
1	B	225	GLU	N-CA	-5.34	1.39	1.46
1	A	153	THR	CA-CB	5.34	1.61	1.53
1	B	232	GLY	N-CA	5.34	1.53	1.45
1	B	136	ALA	C-O	5.33	1.30	1.24
1	B	252	ILE	CG1-CD1	5.30	1.72	1.51
1	A	395	LYS	CA-C	5.30	1.59	1.52
1	A	76	THR	N-CA	5.28	1.53	1.46
1	A	348	ASP	CA-CB	5.28	1.61	1.53
1	A	384	VAL	CB-CG1	5.27	1.70	1.52
1	B	365	SER	CA-C	-5.27	1.45	1.52
1	B	39	GLU	CG-CD	5.26	1.65	1.52
1	B	343	ASP	CB-CG	5.26	1.65	1.52
1	B	30	VAL	CA-C	5.25	1.58	1.52
1	A	119	ARG	CA-C	-5.23	1.46	1.52
1	B	161	ALA	CA-C	5.21	1.59	1.52
1	B	345	GLU	CA-C	5.20	1.59	1.52
1	A	151	ILE	CA-CB	5.17	1.61	1.54
1	A	54	PHE	N-CA	-5.16	1.40	1.46
1	B	130	GLY	C-O	5.15	1.30	1.23
1	B	390	SER	CA-C	-5.15	1.46	1.52
1	B	400	ALA	CA-CB	-5.15	1.45	1.53
1	B	216	ARG	NE-CZ	5.15	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	VAL	CA-CB	-5.14	1.48	1.54
1	B	87	ILE	C-O	-5.13	1.18	1.24
1	B	123	GLU	C-O	-5.12	1.17	1.23
1	B	252	ILE	CA-CB	5.11	1.62	1.54
1	B	135	THR	CA-C	5.10	1.59	1.52
1	A	194	ASN	C-O	5.09	1.30	1.24
1	A	226	ALA	CA-CB	-5.08	1.45	1.53
1	B	61	LEU	C-O	-5.08	1.17	1.24
1	A	344	SER	CA-C	-5.05	1.46	1.52
1	B	200	TYR	N-CA	-5.05	1.39	1.46
1	A	401	ALA	CA-CB	-5.04	1.45	1.53
1	A	236	ARG	N-CA	5.03	1.52	1.46
1	A	50	VAL	CA-C	5.03	1.59	1.52
1	A	244	CYS	C-O	-5.02	1.18	1.24
1	A	44	ALA	CA-C	-5.02	1.46	1.52
1	B	138	ALA	CA-CB	5.00	1.61	1.53

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	GLY	N-CA-C	11.61	126.38	112.33
1	A	396	ASP	N-CA-C	-10.61	100.35	113.18
1	B	95	ASN	CB-CA-C	-10.50	93.52	109.90
1	A	51	SER	N-CA-C	9.86	124.52	110.23
1	B	351	GLY	N-CA-C	-8.64	101.71	112.77
1	B	167	GLY	CA-C-N	-8.52	105.92	122.02
1	B	167	GLY	C-N-CA	-8.52	105.92	122.02
1	A	236	ARG	N-CA-C	8.24	119.50	108.38
1	B	347	MET	CA-C-N	-8.21	109.27	120.28
1	B	347	MET	C-N-CA	-8.21	109.27	120.28
1	A	170	VAL	CB-CA-C	-8.09	99.89	110.98
1	A	66	ALA	N-CA-C	-7.84	95.55	108.49
1	A	228	VAL	N-CA-C	-7.79	102.85	110.72
1	B	339	ARG	CB-CG-CD	-7.70	93.59	111.30
1	A	61	LEU	CA-C-N	-7.68	108.48	122.38
1	A	61	LEU	C-N-CA	-7.68	108.48	122.38
1	B	222	ILE	CA-C-N	7.66	128.44	119.94
1	B	222	ILE	C-N-CA	7.66	128.44	119.94
1	B	207	GLY	CA-C-N	7.65	127.66	119.78
1	B	207	GLY	C-N-CA	7.65	127.66	119.78
1	B	265	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	A	360	ILE	N-CA-C	-7.53	99.54	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	SER	N-CA-C	-7.47	103.22	111.36
1	B	192	VAL	CB-CA-C	-7.37	102.19	112.14
1	B	37	VAL	CB-CA-C	7.36	123.36	111.29
1	B	360	ILE	N-CA-C	7.34	114.81	107.55
1	A	58	LEU	N-CA-C	-7.24	102.39	112.45
1	A	91	ARG	N-CA-C	7.16	120.63	110.68
1	A	211	PHE	CA-C-N	-7.14	110.91	119.84
1	A	211	PHE	C-N-CA	-7.14	110.91	119.84
1	B	175	THR	CB-CA-C	-7.01	96.48	110.42
1	B	337	ASP	N-CA-CB	6.95	120.21	109.85
1	A	233	GLN	CA-C-N	-6.89	111.55	122.29
1	A	233	GLN	C-N-CA	-6.89	111.55	122.29
1	A	124	THR	N-CA-C	6.84	119.25	108.79
1	B	64	ASN	N-CA-CB	-6.71	103.79	113.65
1	A	241	VAL	CA-C-N	-6.56	113.82	122.94
1	A	241	VAL	C-N-CA	-6.56	113.82	122.94
1	B	52	GLN	N-CA-C	6.51	120.68	112.87
1	B	237	LEU	CA-C-N	-6.51	113.59	120.03
1	B	237	LEU	C-N-CA	-6.51	113.59	120.03
1	A	102	ILE	N-CA-CB	6.47	119.34	110.54
1	A	381	ARG	N-CA-C	-6.44	100.64	110.30
1	B	98	GLY	N-CA-C	6.39	128.31	113.18
1	A	66	ALA	N-CA-CB	-6.30	101.59	111.23
1	A	225	GLU	N-CA-C	-6.30	104.49	111.36
1	B	78	LEU	N-CA-C	-6.30	105.72	113.41
1	B	359	ILE	N-CA-C	-6.29	99.36	108.17
1	A	50	VAL	CA-C-N	6.20	129.51	120.71
1	A	50	VAL	C-N-CA	6.20	129.51	120.71
1	A	229	GLN	N-CA-C	6.17	118.97	111.82
1	A	179	THR	N-CA-C	6.15	117.23	108.74
1	A	62	GLN	CB-CA-C	6.12	121.04	110.01
1	B	71	PRO	CB-CA-C	-6.11	102.98	110.98
1	B	186	GLU	N-CA-C	-6.08	104.65	111.28
1	B	169	GLU	N-CA-C	-6.04	99.39	109.24
1	B	143	ASP	N-CA-CB	6.03	118.88	110.26
1	A	356	MET	CA-CB-CG	5.99	126.09	114.10
1	B	94	LEU	N-CA-C	-5.97	106.04	113.38
1	A	216	ARG	CB-CG-CD	5.94	124.96	111.30
1	A	269	PHE	CA-C-N	-5.94	113.31	122.87
1	A	269	PHE	C-N-CA	-5.94	113.31	122.87
1	B	163	MET	CG-SD-CE	-5.92	87.87	100.90
1	B	70	SER	CA-C-N	5.90	125.81	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	SER	C-N-CA	5.90	125.81	119.85
1	A	235	GLY	N-CA-C	-5.86	107.59	115.21
1	B	48	GLU	CA-C-N	5.86	130.06	120.63
1	B	48	GLU	C-N-CA	5.86	130.06	120.63
1	A	181	LYS	N-CA-C	-5.85	104.59	110.97
1	A	68	ARG	N-CA-C	-5.84	102.25	110.31
1	B	72	LEU	N-CA-C	-5.83	97.81	108.02
1	A	131	VAL	CB-CA-C	-5.83	104.52	111.81
1	A	377	VAL	CB-CA-C	-5.75	104.53	111.88
1	A	384	VAL	CB-CA-C	-5.71	102.62	110.96
1	A	199	TYR	CB-CA-C	5.69	119.24	109.51
1	B	168	ALA	N-CA-C	5.66	119.13	110.36
1	A	206	ALA	N-CA-C	5.59	119.79	112.13
1	B	389	LEU	CA-C-N	-5.55	115.39	122.77
1	B	389	LEU	C-N-CA	-5.55	115.39	122.77
1	A	97	THR	N-CA-CB	5.53	118.10	109.97
1	A	352	LEU	N-CA-CB	-5.53	102.05	110.07
1	B	97	THR	CB-CA-C	5.53	118.12	110.16
1	B	95	ASN	CA-C-N	-5.51	113.14	122.67
1	B	95	ASN	C-N-CA	-5.51	113.14	122.67
1	A	243	ALA	N-CA-C	5.50	117.43	109.07
1	A	344	SER	CA-C-N	5.49	127.58	120.44
1	A	344	SER	C-N-CA	5.49	127.58	120.44
1	B	387	VAL	N-CA-C	5.49	115.79	108.11
1	B	379	LEU	N-CA-C	-5.48	107.24	114.04
1	A	56	ASP	N-CA-C	-5.47	105.73	112.90
1	B	140	LEU	N-CA-CB	-5.45	102.60	110.56
1	B	229	GLN	N-CA-C	-5.45	104.88	112.45
1	A	181	LYS	CA-C-N	5.44	127.83	120.38
1	A	181	LYS	C-N-CA	5.44	127.83	120.38
1	A	389	LEU	CB-CA-C	-5.43	102.56	111.68
1	B	96	HIS	N-CA-CB	5.41	118.85	110.46
1	A	113	ARG	N-CA-C	-5.41	105.46	111.36
1	A	189	ARG	CB-CA-C	-5.40	100.82	110.70
1	A	167	GLY	CA-C-N	-5.39	114.19	122.87
1	A	167	GLY	C-N-CA	-5.39	114.19	122.87
1	A	131	VAL	N-CA-CB	5.39	116.49	110.62
1	B	135	THR	N-CA-C	5.38	117.58	111.02
1	B	353	LEU	N-CA-C	5.37	117.13	111.28
1	B	193	ALA	N-CA-C	-5.36	106.74	113.28
1	B	191	TRP	N-CA-C	-5.36	105.48	112.23
1	A	268	GLY	N-CA-C	-5.36	100.78	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	PRO	CA-C-N	-5.33	116.16	123.14
1	A	340	PRO	C-N-CA	-5.33	116.16	123.14
1	B	175	THR	N-CA-C	5.33	122.15	110.80
1	A	44	ALA	CA-C-N	-5.32	112.22	120.31
1	A	44	ALA	C-N-CA	-5.32	112.22	120.31
1	B	85	ALA	CA-C-N	-5.31	115.57	123.11
1	B	85	ALA	C-N-CA	-5.31	115.57	123.11
1	A	82	ALA	N-CA-C	5.30	117.24	110.61
1	A	39	GLU	N-CA-C	5.29	117.73	111.33
1	B	96	HIS	CB-CA-C	5.27	119.57	110.45
1	B	185	ASN	N-CA-C	5.26	117.09	111.36
1	A	184	ILE	N-CA-C	5.25	117.62	111.05
1	B	220	ARG	N-CA-C	-5.24	106.15	112.54
1	A	142	LEU	CA-C-N	-5.24	112.72	120.94
1	A	142	LEU	C-N-CA	-5.24	112.72	120.94
1	A	252	ILE	N-CA-C	5.23	119.42	111.89
1	A	104	ASN	N-CA-CB	5.22	117.80	110.12
1	B	76	THR	OG1-CB-CG2	-5.21	98.87	109.30
1	B	378	GLU	N-CA-CB	-5.21	102.28	110.46
1	B	210	PRO	N-CA-C	5.20	120.44	114.20
1	B	51	SER	CA-C-N	5.19	130.64	120.99
1	B	51	SER	C-N-CA	5.19	130.64	120.99
1	B	106	LEU	CB-CG-CD1	5.16	126.19	110.70
1	B	214	MET	CB-CG-SD	-5.15	97.25	112.70
1	A	400	ALA	N-CA-C	-5.14	105.13	111.40
1	B	336	VAL	CA-C-N	-5.14	113.75	120.95
1	B	336	VAL	C-N-CA	-5.14	113.75	120.95
1	B	369	VAL	N-CA-C	-5.14	104.67	111.09
1	B	189	ARG	N-CA-C	-5.08	105.75	111.28
1	A	341	ILE	N-CA-C	5.08	115.22	108.11
1	A	236	ARG	O-C-N	-5.07	117.57	122.99
1	B	231	GLN	N-CA-C	-5.06	105.89	111.71
1	A	242	VAL	N-CA-CB	-5.03	103.19	111.44
1	A	267	VAL	N-CA-C	5.03	115.09	107.75
1	B	53	ASP	CA-C-N	-5.02	113.92	120.44
1	B	53	ASP	C-N-CA	-5.02	113.92	120.44
1	A	230	ILE	N-CA-C	-5.01	105.54	112.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	GLN	Peptide
1	A	263	GLY	Peptide
1	A	334	GLY	Peptide
1	A	65	TYR	Mainchain
1	A	66	ALA	Peptide
1	A	84	SER	Peptide
1	A	98	GLY	Peptide
1	B	361	PRO	Peptide
1	B	390	SER	Peptide
1	B	391	GLY	Peptide
1	B	395	LYS	Peptide
1	B	397	VAL	Peptide
1	B	98	GLY	Peptide

5.2 Too-close contacts [i](#)

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	137	0
1	B	2373	0	2364	143	0
2	A	8	0	0	6	0
2	B	12	0	0	1	0
All	All	4758	0	4724	273	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 29.

All (273) 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:252:ILE:CD1	1:A:252:ILE:CG1	1.74	1.61
1:B:265:ARG:HH11	1:B:265:ARG:CG	1.50	1.23
1:B:179:THR:CG2	1:B:180:LEU:H	1.58	1.16
1:B:98:GLY:HA2	1:B:101:LYS:H	1.01	1.14
1:A:335:ARG:HA	2:A:414:HOH:O	1.49	1.13
1:B:265:ARG:NH1	1:B:265:ARG:HG3	1.32	1.11
1:B:395:LYS:HA	1:B:397:VAL:H	0.99	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:HG22	1:B:180:LEU:N	1.61	1.09
1:B:395:LYS:N	1:B:397:VAL:HG23	1.73	1.03
1:B:179:THR:HG22	1:B:180:LEU:H	0.88	1.02
1:B:395:LYS:H	1:B:397:VAL:HG23	1.26	1.00
1:B:395:LYS:CA	1:B:397:VAL:HG23	1.93	0.99
1:B:395:LYS:HA	1:B:397:VAL:HG23	1.47	0.96
1:B:395:LYS:HA	1:B:397:VAL:N	1.80	0.96
1:A:335:ARG:HG2	1:A:335:ARG:HH11	1.31	0.95
1:B:395:LYS:CA	1:B:397:VAL:H	1.79	0.95
1:A:158:LEU:HD23	1:A:158:LEU:H	1.34	0.93
1:B:98:GLY:HA2	1:B:101:LYS:N	1.86	0.90
1:A:158:LEU:HD11	1:B:395:LYS:HE2	1.54	0.90
1:A:202:PHE:HZ	1:A:211:PHE:CE1	1.91	0.89
1:B:265:ARG:CG	1:B:265:ARG:NH1	2.20	0.85
1:A:335:ARG:CA	2:A:414:HOH:O	2.14	0.85
1:B:175:THR:HG22	1:B:176:GLY:H	1.39	0.85
1:A:158:LEU:HD11	1:B:395:LYS:CE	2.07	0.84
1:B:265:ARG:HH11	1:B:265:ARG:HG3	0.69	0.84
1:B:395:LYS:H	1:B:397:VAL:CG2	1.91	0.83
1:A:202:PHE:CZ	1:A:211:PHE:CD1	2.67	0.82
1:A:335:ARG:HG2	1:A:335:ARG:NH1	1.92	0.81
1:B:216:ARG:HD3	2:B:415:HOH:O	1.81	0.81
1:B:30:VAL:HG12	1:B:35:MET:HE1	1.64	0.80
1:B:219:GLN:HG3	1:B:250:ASN:HD22	1.45	0.80
1:A:151:ILE:HG12	1:A:178:LYS:O	1.82	0.80
1:A:334:GLY:N	1:A:336:VAL:H	1.81	0.78
1:A:335:ARG:C	2:A:414:HOH:O	2.25	0.78
1:B:156:GLN:OE1	1:B:156:GLN:HA	1.83	0.78
1:A:74:GLU:HG2	1:A:76:THR:HG22	1.66	0.77
1:B:63:ALA:O	1:B:64:ASN:HB2	1.83	0.77
1:A:117:LYS:NZ	1:A:195:ALA:O	2.17	0.77
1:B:29:TYR:O	1:B:30:VAL:HG23	1.84	0.76
1:A:202:PHE:CZ	1:A:211:PHE:CE1	2.75	0.74
1:B:185:ASN:ND2	1:B:185:ASN:H	1.85	0.74
1:A:188:PHE:HZ	1:A:208:PRO:HG2	1.51	0.74
1:A:181:LYS:O	1:A:185:ASN:ND2	2.21	0.73
1:A:158:LEU:O	1:A:162:ARG:N	2.20	0.73
1:A:188:PHE:HZ	1:A:208:PRO:CG	2.01	0.73
1:B:151:ILE:HG22	1:B:155:ARG:NH2	2.04	0.73
1:A:175:THR:O	1:A:175:THR:HG22	1.86	0.72
1:A:150:GLY:O	1:A:153:THR:HB	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:SER:O	1:B:250:ASN:HB3	1.89	0.71
1:A:123:GLU:OE1	1:A:200:TYR:OH	2.08	0.71
1:A:355:ARG:HD3	2:A:413:HOH:O	1.90	0.71
1:A:202:PHE:CZ	1:A:211:PHE:HD1	2.09	0.71
1:B:45:TYR:O	1:B:48:GLU:HB2	1.90	0.71
1:A:202:PHE:HZ	1:A:211:PHE:CD1	2.05	0.70
1:B:197:ASN:ND2	1:B:198:THR:OG1	2.24	0.70
1:B:151:ILE:CG2	1:B:155:ARG:NH2	2.55	0.69
1:B:179:THR:CG2	1:B:180:LEU:N	2.30	0.69
1:A:184:ILE:CG2	1:A:188:PHE:CE2	2.76	0.69
1:A:66:ALA:O	1:A:103:ASN:ND2	2.24	0.69
1:A:402:LYS:O	1:A:404:PHE:N	2.25	0.69
2:A:415:HOH:O	1:B:96:HIS:HB2	1.92	0.69
1:B:32:GLU:O	1:B:35:MET:HB2	1.93	0.68
1:A:163:MET:HE2	1:A:170:VAL:HG22	1.76	0.68
1:A:49:ARG:HG3	1:A:217:ASP:OD2	1.93	0.67
1:A:158:LEU:CD1	1:B:395:LYS:HE2	2.25	0.67
1:A:335:ARG:HH11	1:A:335:ARG:CG	2.02	0.66
1:B:402:LYS:O	1:B:404:PHE:N	2.29	0.66
1:A:158:LEU:O	1:A:161:ALA:N	2.28	0.66
1:B:395:LYS:HA	1:B:397:VAL:CG2	2.24	0.66
1:B:245:VAL:O	1:B:247:GLY:N	2.28	0.66
1:B:402:LYS:O	1:B:403:TRP:C	2.40	0.65
1:A:163:MET:CE	1:A:170:VAL:HG22	2.27	0.65
1:B:163:MET:CE	1:B:170:VAL:HG22	2.26	0.65
1:A:252:ILE:CD1	1:A:252:ILE:CB	2.72	0.65
1:B:113:ARG:HD3	1:B:142:LEU:HD21	1.80	0.64
1:B:80:GLN:OE1	1:B:80:GLN:N	2.31	0.63
1:A:217:ASP:O	1:A:220:ARG:HB2	1.99	0.63
1:A:245:VAL:O	1:A:247:GLY:N	2.30	0.63
1:B:249:SER:O	1:B:250:ASN:CB	2.46	0.62
1:B:179:THR:O	1:B:182:ASP:HB2	1.99	0.62
1:B:156:GLN:OE1	1:B:156:GLN:CA	2.48	0.62
1:B:219:GLN:O	1:B:222:ILE:HG13	2.01	0.61
1:A:188:PHE:CZ	1:A:208:PRO:HG2	2.33	0.61
1:A:155:ARG:O	1:A:156:GLN:HG2	1.99	0.61
1:B:370:ALA:O	1:B:373:LEU:HB2	2.02	0.60
1:B:348:ASP:O	1:B:352:LEU:HB2	2.02	0.60
1:B:239:ASP:O	1:B:265:ARG:NH1	2.34	0.60
1:A:121:ILE:HA	1:A:145:VAL:O	2.02	0.60
1:B:375:LEU:HD12	1:B:379:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:PHE:CD1	1:B:202:PHE:C	2.80	0.59
1:B:30:VAL:CG1	1:B:35:MET:HE1	2.32	0.59
1:B:219:GLN:HG3	1:B:250:ASN:ND2	2.14	0.59
1:A:223:GLY:O	1:A:224:MET:C	2.44	0.59
1:A:355:ARG:C	1:A:356:MET:HE2	2.28	0.59
1:A:158:LEU:H	1:A:158:LEU:CD2	2.12	0.58
1:B:45:TYR:CE2	1:B:49:ARG:HG3	2.38	0.58
1:A:382:GLY:O	1:A:383:ALA:C	2.44	0.58
1:B:180:LEU:HD13	1:B:184:ILE:CD1	2.33	0.58
1:A:152:ASP:N	1:A:152:ASP:OD1	2.35	0.58
1:A:175:THR:O	1:A:175:THR:CG2	2.51	0.58
1:B:192:VAL:O	1:B:192:VAL:HG12	1.99	0.58
1:B:335:ARG:HD2	1:B:335:ARG:O	2.03	0.58
1:B:356:MET:HE2	1:B:356:MET:CA	2.34	0.57
1:A:158:LEU:HD23	1:A:158:LEU:N	2.11	0.57
1:A:339:ARG:NH2	1:A:378:GLU:OE1	2.38	0.57
1:A:96:HIS:ND1	1:A:96:HIS:N	2.53	0.56
1:A:392:ARG:HD3	1:A:392:ARG:H	1.70	0.56
1:B:356:MET:HE2	1:B:356:MET:N	2.20	0.56
1:B:30:VAL:HG12	1:B:35:MET:CE	2.35	0.56
1:B:347:MET:HG2	1:B:403:TRP:CD2	2.40	0.56
1:A:45:TYR:CD2	1:A:214:MET:HE2	2.41	0.56
1:B:185:ASN:ND2	1:B:185:ASN:N	2.54	0.56
1:B:356:MET:HE2	1:B:356:MET:HA	1.88	0.56
1:A:239:ASP:OD2	1:A:383:ALA:HA	2.07	0.55
1:A:202:PHE:HZ	1:A:211:PHE:HE1	1.45	0.55
1:A:124:THR:OG1	1:A:127:GLY:HA2	2.06	0.55
1:A:194:ASN:O	1:A:195:ALA:C	2.49	0.55
1:B:115:MET:HE2	1:B:117:LYS:HE2	1.89	0.55
1:B:180:LEU:HD13	1:B:184:ILE:HD11	1.88	0.54
1:A:200:TYR:HE1	1:A:202:PHE:CD1	2.25	0.54
1:A:74:GLU:HG2	1:A:76:THR:CG2	2.36	0.54
1:A:402:LYS:O	1:A:403:TRP:C	2.50	0.54
1:A:402:LYS:O	1:A:404:PHE:C	2.51	0.54
1:B:181:LYS:O	1:B:185:ASN:ND2	2.41	0.53
1:B:218:PHE:O	1:B:221:ILE:HB	2.08	0.53
1:B:342:THR:O	1:B:343:ASP:C	2.52	0.53
1:B:230:ILE:HG21	1:B:238:PRO:HD3	1.91	0.52
1:A:260:ASP:O	1:A:262:PRO:HD3	2.10	0.52
1:A:369:VAL:O	1:A:373:LEU:HG	2.09	0.52
1:B:163:MET:HE2	1:B:170:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG22	1:B:155:ARG:CZ	2.40	0.51
1:A:200:TYR:HE1	1:A:202:PHE:HD1	1.58	0.51
1:A:34:LEU:HD23	1:A:192:VAL:HG23	1.93	0.51
1:A:350:PHE:CD1	1:A:350:PHE:C	2.89	0.51
1:A:45:TYR:CG	1:A:214:MET:HE2	2.46	0.51
1:A:155:ARG:C	1:A:156:GLN:HG2	2.36	0.50
1:B:45:TYR:O	1:B:48:GLU:N	2.31	0.50
1:A:79:SER:OG	1:A:84:SER:HA	2.11	0.50
1:B:175:THR:CG2	1:B:176:GLY:H	2.16	0.50
1:B:188:PHE:CZ	1:B:208:PRO:HG2	2.46	0.50
1:B:34:LEU:HD11	1:B:188:PHE:CG	2.46	0.50
1:B:144:CYS:O	1:B:168:ALA:HB1	2.12	0.50
1:A:57:ASP:O	1:A:61:LEU:HB2	2.12	0.50
1:B:98:GLY:CA	1:B:101:LYS:H	1.95	0.50
1:A:189:ARG:O	1:A:193:ALA:CB	2.59	0.50
1:A:345:GLU:O	1:A:346:ALA:C	2.55	0.50
1:B:352:LEU:CD2	1:B:356:MET:HG2	2.41	0.50
1:A:108:GLN:OE1	1:A:202:PHE:CE2	2.65	0.50
1:A:363:ILE:HD12	1:A:396:ASP:OD1	2.11	0.50
1:B:46:GLN:O	1:B:48:GLU:N	2.45	0.50
1:A:188:PHE:HZ	1:A:208:PRO:HG3	1.75	0.49
1:B:202:PHE:CD1	1:B:202:PHE:O	2.66	0.49
1:A:382:GLY:C	1:A:383:ALA:O	2.55	0.49
1:B:236:ARG:HH12	1:B:239:ASP:CG	2.21	0.49
1:A:184:ILE:HG22	1:A:188:PHE:CE2	2.48	0.49
1:A:363:ILE:HD12	1:A:396:ASP:CG	2.37	0.49
1:B:133:THR:O	1:B:134:ALA:C	2.52	0.49
1:B:151:ILE:CG2	1:B:155:ARG:HH21	2.26	0.49
1:A:34:LEU:O	1:A:37:VAL:HG12	2.12	0.49
1:A:158:LEU:CD2	1:A:158:LEU:N	2.73	0.49
1:B:137:CYS:HB3	1:B:144:CYS:HB2	1.95	0.49
1:B:41:VAL:HB	1:B:211:PHE:CZ	2.48	0.48
1:B:363:ILE:O	1:B:364:GLU:C	2.54	0.48
1:A:62:GLN:HE22	1:A:221:ILE:HG12	1.78	0.48
1:B:34:LEU:HD11	1:B:188:PHE:CD1	2.48	0.48
1:A:101:LYS:NZ	1:A:128:GLN:HG2	2.29	0.48
1:A:255:PHE:O	1:A:256:HIS:C	2.54	0.48
1:B:345:GLU:OE2	1:B:374:LYS:NZ	2.44	0.48
1:A:60:ARG:HB3	1:A:60:ARG:CZ	2.43	0.48
1:A:135:THR:HG23	1:B:358:GLY:O	2.14	0.48
1:B:31:PRO:O	1:B:34:LEU:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:C	1:A:161:ALA:H	2.20	0.48
1:A:242:VAL:HG22	1:A:269:PHE:HE2	1.79	0.48
1:A:29:TYR:O	1:A:31:PRO:HD3	2.14	0.47
1:B:200:TYR:HE2	1:B:202:PHE:HB3	1.79	0.47
1:B:345:GLU:CD	1:B:374:LYS:NZ	2.72	0.47
1:B:395:LYS:C	1:B:397:VAL:H	2.22	0.47
1:A:98:GLY:HA2	1:A:101:LYS:HD2	1.96	0.47
1:A:200:TYR:CE1	1:A:202:PHE:CD1	3.02	0.47
1:B:211:PHE:N	1:B:212:PRO:HD3	2.29	0.47
1:A:152:ASP:HA	1:A:155:ARG:HG2	1.95	0.47
1:B:175:THR:HG22	1:B:176:GLY:N	2.19	0.47
1:B:58:LEU:O	1:B:62:GLN:HG2	2.15	0.47
1:B:137:CYS:CB	1:B:144:CYS:HB2	2.45	0.47
1:A:382:GLY:O	1:A:383:ALA:O	2.32	0.47
1:A:106:LEU:HD12	1:A:136:ALA:CB	2.44	0.47
1:A:163:MET:HE2	1:A:170:VAL:CG2	2.43	0.47
1:A:69:PRO:HA	1:A:225:GLU:CD	2.40	0.46
1:B:37:VAL:HG21	1:B:195:ALA:HB2	1.96	0.46
1:B:363:ILE:HG13	1:B:396:ASP:HB3	1.96	0.46
1:A:96:HIS:CE1	2:A:415:HOH:O	2.68	0.46
1:B:98:GLY:HA3	1:B:101:LYS:HD2	1.96	0.46
1:A:190:ASP:OD1	1:A:194:ASN:ND2	2.49	0.46
1:A:206:ALA:O	1:A:207:GLY:O	2.34	0.46
1:B:220:ARG:O	1:B:221:ILE:C	2.58	0.46
1:A:392:ARG:HH12	1:A:395:LYS:CE	2.29	0.46
1:A:202:PHE:CD2	1:A:202:PHE:N	2.68	0.45
1:A:356:MET:HE2	1:A:356:MET:HA	1.98	0.45
1:B:270:GLU:OE2	1:B:338:TYR:HB3	2.16	0.45
1:B:355:ARG:C	1:B:356:MET:HE2	2.40	0.45
1:B:162:ARG:O	1:B:163:MET:C	2.58	0.45
1:A:356:MET:HE2	1:A:356:MET:CA	2.47	0.45
1:B:202:PHE:CE2	1:B:211:PHE:HD2	2.35	0.45
1:A:214:MET:HB2	1:A:214:MET:HE3	1.59	0.45
1:B:163:MET:HE2	1:B:170:VAL:HG21	1.99	0.45
1:A:398:GLU:HB3	1:A:399:THR:H	1.52	0.44
1:A:63:ALA:O	1:A:64:ASN:HB2	2.16	0.44
1:A:125:GLY:O	1:A:148:MET:HE3	2.18	0.44
1:B:192:VAL:O	1:B:192:VAL:CG1	2.55	0.44
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.67	0.44
1:B:395:LYS:HA	1:B:397:VAL:CB	2.48	0.44
1:A:78:LEU:O	1:A:79:SER:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD22	1:B:358:GLY:HA2	1.99	0.44
1:A:180:LEU:HA	1:A:183:ALA:HB3	2.00	0.44
1:B:392:ARG:C	1:B:394:ASP:H	2.26	0.44
1:B:180:LEU:CD1	1:B:184:ILE:HD11	2.48	0.43
1:A:119:ARG:O	1:A:198:THR:HA	2.17	0.43
1:A:194:ASN:O	1:A:196:ASP:N	2.52	0.43
1:B:350:PHE:CD1	1:B:350:PHE:C	2.96	0.43
1:B:230:ILE:HD12	1:B:230:ILE:HA	1.75	0.43
1:B:236:ARG:NH2	1:B:239:ASP:OD2	2.46	0.43
1:A:91:ARG:CZ	1:A:359:ILE:HD13	2.49	0.43
1:B:180:LEU:HD13	1:B:184:ILE:HD12	1.99	0.43
1:B:83:GLY:O	1:B:84:SER:HB2	2.19	0.43
1:A:54:PHE:HD2	1:A:55:LEU:HD23	1.84	0.42
1:A:119:ARG:NH1	1:A:198:THR:OG1	2.50	0.42
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.82	0.42
1:B:151:ILE:HG21	1:B:155:ARG:NH2	2.34	0.42
1:B:241:VAL:C	1:B:242:VAL:HG23	2.43	0.42
1:A:348:ASP:O	1:A:352:LEU:HB2	2.18	0.42
1:A:403:TRP:C	1:A:403:TRP:CD1	2.97	0.42
1:B:156:GLN:C	1:B:158:LEU:H	2.27	0.42
1:B:241:VAL:HG21	1:B:258:PHE:CD2	2.54	0.42
1:A:158:LEU:HD11	1:B:395:LYS:NZ	2.33	0.42
1:A:392:ARG:HH12	1:A:395:LYS:HE3	1.84	0.42
1:A:270:GLU:O	1:A:341:ILE:N	2.43	0.42
1:A:338:TYR:O	1:A:339:ARG:HG2	2.19	0.42
1:B:60:ARG:CZ	1:B:60:ARG:HB3	2.49	0.42
1:B:58:LEU:HD13	1:B:107:GLY:HA2	2.02	0.42
1:B:87:ILE:N	1:B:87:ILE:HD13	2.35	0.42
1:B:219:GLN:CG	1:B:250:ASN:HD22	2.24	0.42
1:A:162:ARG:HG2	1:B:360:ILE:CD1	2.50	0.41
1:B:37:VAL:HG13	1:B:191:TRP:CE2	2.56	0.41
1:B:54:PHE:CD2	1:B:54:PHE:C	2.98	0.41
1:B:74:GLU:HB2	1:B:88:PHE:CE2	2.55	0.41
1:B:121:ILE:HD11	1:B:191:TRP:HB2	2.02	0.41
1:A:54:PHE:CD2	1:A:55:LEU:HD23	2.56	0.41
1:B:75:ALA:HB1	1:B:357:GLU:OE2	2.19	0.41
1:A:121:ILE:HD13	1:A:121:ILE:HG21	1.82	0.41
1:A:121:ILE:HG23	1:A:198:THR:HG23	2.02	0.41
1:B:45:TYR:O	1:B:46:GLN:C	2.62	0.41
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.65	0.41
1:B:149:GLY:O	1:B:152:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:CE	1:B:170:VAL:CG2	2.95	0.41
1:B:365:SER:O	1:B:366:ALA:C	2.62	0.41
1:A:159:ASN:HA	1:A:162:ARG:HB2	2.02	0.41
1:A:245:VAL:CG2	1:A:268:GLY:HA3	2.51	0.41
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.82	0.41
1:A:364:GLU:HG3	1:A:365:SER:N	2.35	0.41
1:A:188:PHE:CZ	1:A:208:PRO:CG	2.92	0.41
1:B:62:GLN:O	1:B:63:ALA:C	2.62	0.41
1:A:392:ARG:C	1:A:394:ASP:H	2.28	0.41
1:B:267:VAL:HG21	1:B:375:LEU:HD21	2.03	0.41
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.85	0.41
1:A:70:SER:HA	1:A:71:PRO:HD3	1.64	0.41
1:A:174:GLN:HA	1:A:178:LYS:HG2	2.03	0.41
1:B:117:LYS:HB3	1:B:197:ASN:O	2.21	0.41
1:A:363:ILE:O	1:A:366:ALA:HB3	2.21	0.40
1:B:336:VAL:HG13	1:B:338:TYR:CZ	2.56	0.40
1:A:69:PRO:HA	1:A:225:GLU:OE2	2.21	0.40
1:A:200:TYR:CD1	1:A:200:TYR:C	2.99	0.40
1:B:46:GLN:O	1:B:47:LYS:C	2.64	0.40
1:B:123:GLU:OE1	1:B:200:TYR:OH	2.25	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	311/422 (74%)	266 (86%)	32 (10%)	13 (4%)	2	1
1	B	312/422 (74%)	274 (88%)	28 (9%)	10 (3%)	3	2
All	All	623/844 (74%)	540 (87%)	60 (10%)	23 (4%)	2	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	403	TRP
1	B	47	LYS
1	B	246	GLY
1	B	272	ALA
1	A	207	GLY
1	A	246	GLY
1	A	248	GLY
1	A	49	ARG
1	A	195	ALA
1	A	204	THR
1	A	343	ASP
1	B	79	SER
1	B	396	ASP
1	B	398	GLU
1	B	403	TRP
1	B	343	ASP
1	A	177	SER
1	A	245	VAL
1	A	402	LYS
1	B	176	GLY
1	B	203	GLY
1	A	150	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%)	194 (82%)	42 (18%)	2	1
1	B	237/314 (76%)	193 (81%)	44 (19%)	1	1
All	All	473/628 (75%)	387 (82%)	86 (18%)	2	1

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET

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Mol	Chain	Res	Type
1	A	37	VAL
1	A	47	LYS
1	A	50	VAL
1	A	60	ARG
1	A	61	LEU
1	A	80	GLN
1	A	84	SER
1	A	96	HIS
1	A	106	LEU
1	A	111	LEU
1	A	117	LYS
1	A	123	GLU
1	A	128	GLN
1	A	146	ILE
1	A	152	ASP
1	A	158	LEU
1	A	173	VAL
1	A	174	GLN
1	A	175	THR
1	A	181	LYS
1	A	182	ASP
1	A	189	ARG
1	A	192	VAL
1	A	196	ASP
1	A	197	ASN
1	A	201	CYS
1	A	202	PHE
1	A	204	THR
1	A	215	VAL
1	A	221	ILE
1	A	237	LEU
1	A	242	VAL
1	A	252	ILE
1	A	335	ARG
1	A	336	VAL
1	A	337	ASP
1	A	339	ARG
1	A	344	SER
1	A	379	LEU
1	A	392	ARG
1	A	398	GLU
1	B	35	MET

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Mol	Chain	Res	Type
1	B	37	VAL
1	B	39	GLU
1	B	42	THR
1	B	46	GLN
1	B	47	LYS
1	B	50	VAL
1	B	62	GLN
1	B	86	ARG
1	B	97	THR
1	B	106	LEU
1	B	111	LEU
1	B	114	ARG
1	B	119	ARG
1	B	121	ILE
1	B	128	GLN
1	B	155	ARG
1	B	156	GLN
1	B	173	VAL
1	B	175	THR
1	B	178	LYS
1	B	180	LEU
1	B	185	ASN
1	B	186	GLU
1	B	216	ARG
1	B	221	ILE
1	B	222	ILE
1	B	236	ARG
1	B	237	LEU
1	B	252	ILE
1	B	260	ASP
1	B	265	ARG
1	B	267	VAL
1	B	270	GLU
1	B	335	ARG
1	B	336	VAL
1	B	337	ASP
1	B	347	MET
1	B	352	LEU
1	B	375	LEU
1	B	377	VAL
1	B	385	ILE
1	B	392	ARG

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Mol	Chain	Res	Type
1	B	396	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	80	GLN
1	A	174	GLN
1	A	185	ASN
1	A	197	ASN
1	A	233	GLN
1	A	256	HIS
1	B	62	GLN
1	B	185	ASN
1	B	197	ASN
1	B	231	GLN
1	B	233	GLN
1	B	250	ASN
1	B	367	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 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 [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, 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	315/422 (74%)	-0.42	4 (1%) 75 76	21, 44, 78, 86	0
1	B	316/422 (74%)	-0.49	5 (1%) 70 72	21, 42, 66, 84	0
All	All	631/844 (74%)	-0.46	9 (1%) 73 75	21, 43, 76, 86	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	LYS	6.0
1	A	156	GLN	5.9
1	B	80	GLN	2.8
1	B	273	GLY	2.7
1	A	50	VAL	2.3
1	B	393	GLY	2.2
1	B	96	HIS	2.2
1	A	215	VAL	2.2
1	A	66	ALA	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 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.