



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:27 AM EDT

PDB ID : 2O2E / pdb_00002o2e
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 : 2006-11-29
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

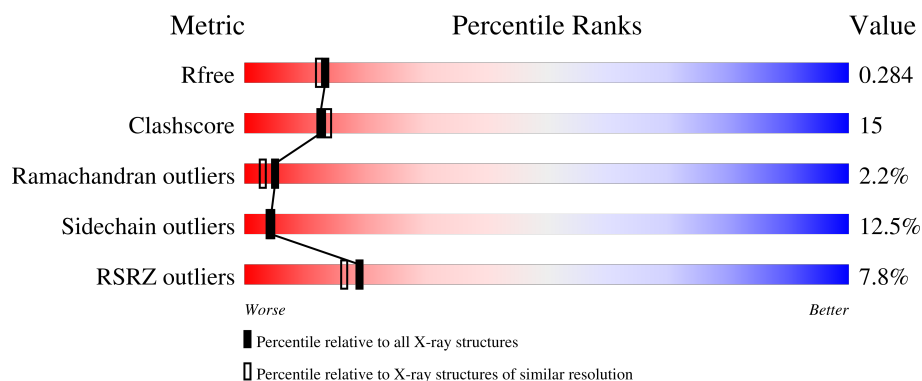
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	5% 39% 28% 7% 25%
1	B	422	7% 34% 28% 9% 25%

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			

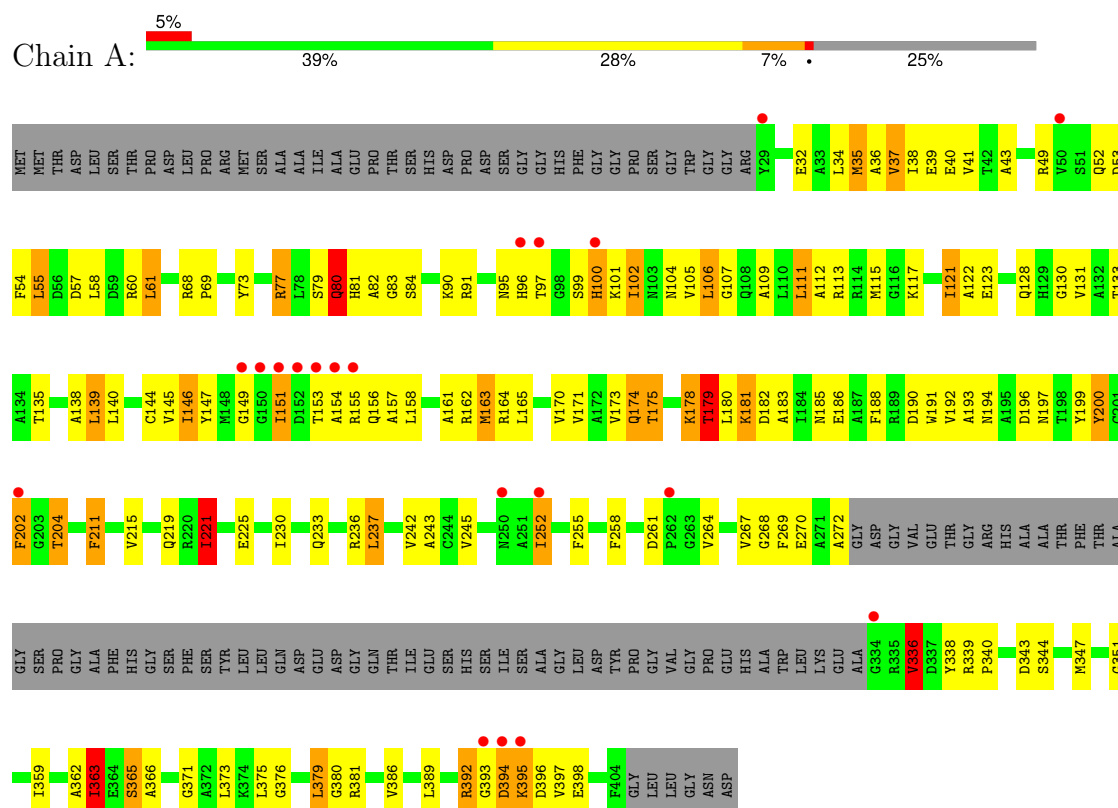
- Molecule 2 is water.

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

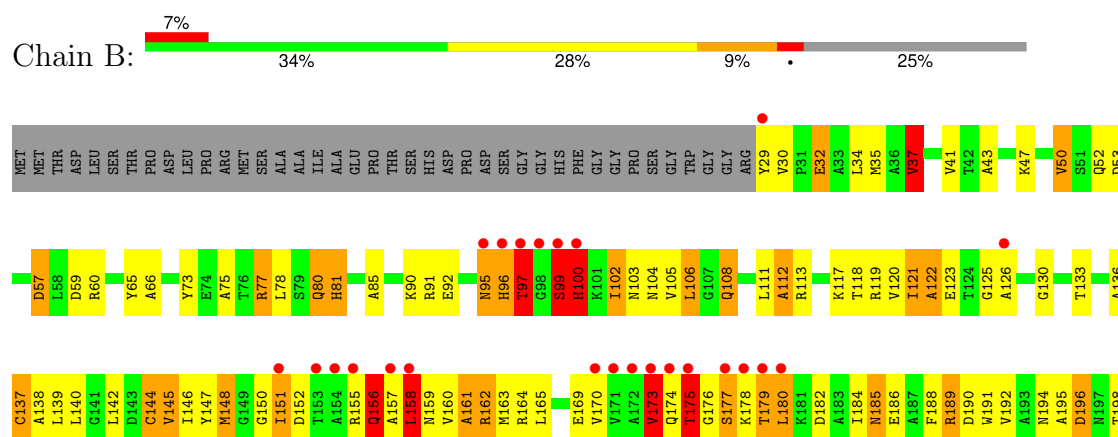
3 Residue-property plots

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



ASP	R335	V336	D337	Y338	R339	P340	I341	T342	D343	S344	E345	A346	M347	F350	G351	L352	I353	C354	R355	M356	I359	I360	E364	S365	A368	V369	A370	G371	V377	E378	L379	A383	V384	I385	L389	R392	G393	D394	K395	D396	T399	A400	A401	K402	W403	F404	GLY	LEU	LEU	LEU	GLY	ASN			
	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	LEU	GLN	ASP	GLU	ASP	GLY	GLN	THR	ILE	GLU	SER	HIS	SER	ILE	SER	ALA	GLY	LEU	ASP	TYR	PRO	GLU	HIS	ALA	TRP	LEU	LYS	GLU	ALA
	Y199	G203	G207	P208	T213	M214	V215	F218	I221	I222	E225	A226	R227	V228	Q229	I230	Q233	A234	G235	R236	L237	P238	V241	V242	V245	G246	G247	G248	S249	R250	A251	I252	G253	I254	F255	R256	A257	F258	D261	P262	G263	V264	V267	E270	A271	A272	G273	D274							

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.98Å 56.46Å 120.55Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.20 19.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.92-2.20) 99.4 (19.92-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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	2.25	81/2403 (3.4%)	1.83	46/3252 (1.4%)
1	B	2.27	84/2411 (3.5%)	1.79	53/3263 (1.6%)
All	All	2.26	165/4814 (3.4%)	1.81	99/6515 (1.5%)

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 (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	ALA	CA-CB	11.62	1.65	1.53
1	A	36	ALA	CA-CB	11.05	1.71	1.53
1	B	370	ALA	C-O	-10.76	1.11	1.24
1	B	97	THR	CA-CB	10.59	1.71	1.53
1	B	371	GLY	N-CA	10.41	1.59	1.45
1	B	78	LEU	N-CA	10.23	1.59	1.46
1	A	109	ALA	CA-CB	9.78	1.68	1.53
1	A	135	THR	C-O	-9.49	1.13	1.24
1	A	151	ILE	C-O	9.23	1.34	1.24
1	B	233	GLN	C-O	8.98	1.35	1.24
1	A	165	LEU	N-CA	8.92	1.57	1.46
1	B	118	THR	CA-CB	8.62	1.66	1.54
1	A	146	ILE	CA-C	8.48	1.63	1.52
1	A	171	VAL	CA-CB	8.46	1.64	1.53
1	B	173	VAL	CA-CB	8.37	1.64	1.54
1	B	238	PRO	CA-C	8.26	1.62	1.52
1	B	252	ILE	CG1-CD1	8.14	1.83	1.51
1	B	342	THR	N-CA	8.14	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	MET	C-O	-8.10	1.14	1.24
1	A	138	ALA	CA-CB	-8.05	1.40	1.53
1	B	213	THR	CA-CB	8.04	1.66	1.53
1	B	151	ILE	CA-CB	7.93	1.64	1.54
1	A	122	ALA	CA-CB	7.92	1.67	1.53
1	A	394	ASP	N-CA	7.86	1.54	1.46
1	A	55	LEU	C-O	-7.83	1.14	1.24
1	B	117	LYS	CA-C	7.62	1.63	1.53
1	B	215	VAL	CA-C	7.50	1.61	1.52
1	A	146	ILE	N-CA	-7.49	1.37	1.46
1	B	75	ALA	CA-CB	-7.43	1.43	1.52
1	A	191	TRP	N-CA	7.40	1.55	1.46
1	B	123	GLU	N-CA	-7.40	1.36	1.45
1	B	369	VAL	CA-CB	7.38	1.63	1.54
1	A	37	VAL	CA-CB	7.25	1.64	1.54
1	B	112	ALA	CA-CB	7.18	1.64	1.53
1	A	40	GLU	C-O	-7.18	1.15	1.24
1	B	264	VAL	C-O	-7.10	1.16	1.24
1	B	175	THR	CA-CB	7.10	1.65	1.53
1	A	255	PHE	N-CA	7.04	1.55	1.46
1	B	360	ILE	C-N	6.96	1.41	1.33
1	A	242	VAL	CA-CB	6.86	1.64	1.54
1	B	144	CYS	N-CA	-6.83	1.38	1.46
1	A	178	LYS	C-O	-6.81	1.15	1.23
1	A	121	ILE	N-CA	6.81	1.53	1.46
1	A	163	MET	CG-SD	6.76	1.97	1.80
1	A	192	VAL	C-O	-6.73	1.16	1.24
1	B	222	ILE	CA-C	-6.71	1.44	1.52
1	B	264	VAL	CB-CG1	6.70	1.74	1.52
1	A	97	THR	CA-CB	6.67	1.61	1.53
1	B	145	VAL	CA-CB	6.66	1.64	1.54
1	A	219	GLN	C-O	-6.65	1.15	1.24
1	B	237	LEU	CA-C	6.57	1.59	1.53
1	B	252	ILE	CA-CB	6.55	1.63	1.54
1	A	157	ALA	N-CA	-6.51	1.38	1.46
1	A	236	ARG	C-O	-6.50	1.17	1.23
1	B	126	ALA	CA-C	6.49	1.61	1.52
1	A	373	LEU	N-CA	6.48	1.54	1.46
1	A	395	LYS	N-CA	6.47	1.54	1.46
1	B	226	ALA	N-CA	6.47	1.54	1.46
1	A	61	LEU	CG-CD2	6.46	1.73	1.52
1	B	97	THR	N-CA	6.39	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	ILE	N-CA	6.39	1.51	1.46
1	A	366	ALA	C-O	6.37	1.32	1.24
1	A	131	VAL	CA-C	6.35	1.60	1.52
1	B	364	GLU	C-O	-6.32	1.16	1.24
1	A	196	ASP	CB-CG	6.30	1.67	1.52
1	B	236	ARG	N-CA	6.28	1.53	1.46
1	A	131	VAL	N-CA	6.20	1.53	1.46
1	A	113	ARG	CZ-NH1	6.20	1.41	1.32
1	B	50	VAL	CA-CB	6.16	1.62	1.54
1	B	30	VAL	CA-CB	6.13	1.62	1.54
1	B	60	ARG	CG-CD	6.11	1.70	1.52
1	B	340	PRO	CA-C	6.08	1.58	1.52
1	A	135	THR	N-CA	6.04	1.53	1.46
1	A	363	ILE	CA-CB	6.03	1.62	1.54
1	A	359	ILE	C-O	-6.01	1.17	1.24
1	B	394	ASP	N-CA	5.99	1.53	1.46
1	B	228	VAL	CA-CB	5.99	1.61	1.54
1	A	339	ARG	C-N	5.99	1.40	1.33
1	A	179	THR	CA-CB	5.98	1.63	1.53
1	B	80	GLN	CG-CD	5.98	1.67	1.52
1	B	228	VAL	C-O	-5.97	1.17	1.24
1	A	53	ASP	CA-CB	5.95	1.62	1.53
1	A	149	GLY	CA-C	5.91	1.60	1.51
1	A	144	CYS	N-CA	-5.90	1.38	1.46
1	B	126	ALA	CA-CB	5.88	1.63	1.53
1	A	183	ALA	N-CA	5.87	1.53	1.46
1	A	386	VAL	C-O	-5.85	1.17	1.24
1	B	399	THR	CA-CB	-5.79	1.44	1.53
1	B	360	ILE	CA-CB	5.79	1.59	1.53
1	A	230	ILE	CA-CB	5.78	1.62	1.54
1	B	385	ILE	C-O	5.75	1.29	1.24
1	B	230	ILE	CG1-CD1	5.73	1.74	1.51
1	B	85	ALA	CA-C	-5.72	1.45	1.53
1	B	383	ALA	CA-CB	-5.69	1.44	1.53
1	A	359	ILE	CA-CB	5.69	1.60	1.54
1	B	395	LYS	N-CA	5.68	1.53	1.46
1	A	95	ASN	N-CA	5.67	1.53	1.46
1	B	81	HIS	CA-CB	5.67	1.62	1.53
1	A	43	ALA	CA-CB	5.66	1.62	1.53
1	B	221	ILE	CA-C	5.65	1.59	1.52
1	A	179	THR	CA-C	5.62	1.60	1.52
1	A	200	TYR	N-CA	-5.61	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	TYR	CB-CG	-5.61	1.39	1.51
1	A	73	TYR	CA-C	5.61	1.59	1.52
1	A	164	ARG	CB-CG	5.59	1.69	1.52
1	B	226	ALA	CA-CB	-5.59	1.44	1.53
1	B	120	VAL	CA-CB	5.59	1.62	1.54
1	A	161	ALA	CA-CB	5.58	1.62	1.53
1	A	151	ILE	CA-C	5.54	1.59	1.52
1	B	377	VAL	CB-CG2	5.53	1.70	1.52
1	A	54	PHE	CA-C	5.53	1.59	1.52
1	A	175	THR	CA-C	5.48	1.60	1.53
1	B	108	GLN	CA-C	-5.47	1.46	1.52
1	B	359	ILE	CA-CB	5.47	1.60	1.54
1	A	336	VAL	CA-CB	5.47	1.60	1.54
1	A	233	GLN	CA-C	-5.45	1.45	1.52
1	A	39	GLU	CA-C	5.44	1.59	1.52
1	A	109	ALA	N-CA	5.43	1.52	1.46
1	B	34	LEU	N-CA	5.42	1.53	1.46
1	B	241	VAL	CA-CB	5.42	1.61	1.54
1	A	60	ARG	CG-CD	5.38	1.68	1.52
1	A	147	TYR	CG-CD2	5.35	1.50	1.39
1	B	368	ALA	N-CA	5.35	1.52	1.46
1	B	41	VAL	CA-CB	5.33	1.60	1.54
1	B	402	LYS	N-CA	5.31	1.53	1.46
1	B	345	GLU	N-CA	-5.29	1.40	1.46
1	A	188	PHE	C-O	5.29	1.30	1.24
1	B	354	CYS	CA-C	-5.27	1.46	1.52
1	A	173	VAL	CA-CB	-5.26	1.48	1.54
1	A	139	LEU	CG-CD1	5.25	1.69	1.52
1	A	243	ALA	CA-CB	5.25	1.62	1.53
1	A	52	GLN	CD-NE2	5.25	1.44	1.33
1	A	252	ILE	CG1-CD1	5.25	1.72	1.51
1	B	162	ARG	N-CA	5.25	1.52	1.46
1	A	194	ASN	N-CA	-5.23	1.40	1.46
1	B	122	ALA	C-O	-5.23	1.18	1.23
1	B	158	LEU	CG-CD2	5.23	1.69	1.52
1	B	236	ARG	C-O	-5.21	1.17	1.23
1	B	335	ARG	CD-NE	5.21	1.53	1.46
1	A	193	ALA	N-CA	-5.18	1.39	1.46
1	B	103	ASN	CB-CG	5.18	1.65	1.52
1	B	119	ARG	CA-C	5.18	1.58	1.52
1	B	198	THR	CA-C	5.17	1.59	1.52
1	A	268	GLY	CA-C	5.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	CG1-CD1	5.16	1.71	1.51
1	B	156	GLN	N-CA	5.16	1.52	1.46
1	B	122	ALA	CA-CB	-5.13	1.45	1.53
1	B	258	PHE	C-O	5.13	1.30	1.24
1	A	131	VAL	CA-CB	5.13	1.60	1.54
1	A	38	ILE	N-CA	5.12	1.52	1.46
1	A	196	ASP	CA-C	5.11	1.59	1.52
1	B	165	LEU	N-CA	5.10	1.52	1.46
1	B	251	ALA	CA-CB	-5.10	1.45	1.53
1	A	77	ARG	N-CA	5.08	1.52	1.46
1	A	162	ARG	CB-CG	5.08	1.67	1.52
1	B	73	TYR	CA-CB	5.07	1.62	1.53
1	B	378	GLU	N-CA	5.05	1.52	1.46
1	A	41	VAL	N-CA	5.04	1.52	1.46
1	A	186	GLU	N-CA	5.04	1.52	1.46
1	A	180	LEU	N-CA	5.03	1.52	1.46
1	B	100	HIS	CA-C	5.03	1.59	1.52
1	A	156	GLN	N-CA	5.02	1.52	1.46
1	B	75	ALA	CA-C	5.01	1.59	1.52
1	B	91	ARG	C-O	5.01	1.31	1.23
1	A	128	GLN	N-CA	5.01	1.52	1.46

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	GLY	CA-C-N	11.57	131.33	119.76
1	B	207	GLY	C-N-CA	11.57	131.33	119.76
1	B	370	ALA	N-CA-C	-10.44	99.90	111.07
1	B	77	ARG	NE-CZ-NH2	-9.35	110.79	119.20
1	A	83	GLY	N-CA-C	-8.88	102.52	115.30
1	A	175	THR	N-CA-CB	-8.74	97.17	110.45
1	A	190	ASP	N-CA-C	-8.03	102.61	111.36
1	A	237	LEU	CA-C-N	-8.00	109.84	119.84
1	A	237	LEU	C-N-CA	-8.00	109.84	119.84
1	B	37	VAL	CB-CA-C	7.80	122.98	112.22
1	A	57	ASP	CB-CA-C	7.79	124.10	110.85
1	B	215	VAL	N-CA-C	7.72	118.46	110.36
1	A	60	ARG	NE-CZ-NH1	-7.34	114.16	121.50
1	A	68	ARG	N-CA-C	-7.31	100.88	110.39
1	B	185	ASN	N-CA-C	7.18	119.19	111.36
1	A	146	ILE	CB-CG1-CD1	-7.11	98.86	113.80
1	B	354	CYS	N-CA-C	-7.07	103.50	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	THR	N-CA-CB	-7.04	99.57	110.56
1	B	261	ASP	CA-C-N	6.85	127.12	119.32
1	B	261	ASP	C-N-CA	6.85	127.12	119.32
1	B	137	CYS	N-CA-C	6.72	118.60	111.28
1	B	242	VAL	N-CA-CB	-6.71	100.44	111.45
1	B	343	ASP	N-CA-C	-6.65	104.12	111.36
1	A	211	PHE	N-CA-C	6.58	120.32	109.79
1	B	336	VAL	CB-CA-C	6.56	118.90	110.96
1	A	60	ARG	CB-CG-CD	6.48	126.21	111.30
1	A	394	ASP	N-CA-C	6.47	118.23	108.46
1	B	60	ARG	CB-CA-C	-6.41	100.81	110.88
1	A	49	ARG	CA-C-N	6.38	128.84	120.60
1	A	49	ARG	C-N-CA	6.38	128.84	120.60
1	A	215	VAL	CB-CA-C	-6.35	103.56	112.14
1	B	396	ASP	N-CA-C	-6.32	103.91	113.89
1	A	101	LYS	N-CA-C	-6.30	103.72	111.40
1	A	40	GLU	CB-CA-C	-6.22	101.11	110.88
1	B	218	PHE	N-CA-C	-6.19	104.53	111.28
1	B	151	ILE	CB-CA-C	6.14	120.04	110.95
1	A	151	ILE	N-CA-C	6.10	116.74	110.82
1	A	117	LYS	N-CA-C	-6.04	101.53	110.48
1	A	351	GLY	N-CA-C	-6.04	105.04	112.77
1	A	96	HIS	CB-CA-C	6.03	120.64	109.54
1	B	157	ALA	CA-C-N	5.91	128.47	120.44
1	B	157	ALA	C-N-CA	5.91	128.47	120.44
1	A	359	ILE	CA-C-N	-5.84	118.63	122.60
1	A	359	ILE	C-N-CA	-5.84	118.63	122.60
1	A	97	THR	N-CA-C	-5.82	99.66	108.67
1	A	154	ALA	N-CA-C	-5.80	104.32	111.40
1	A	140	LEU	CA-C-N	-5.75	112.77	121.51
1	A	140	LEU	C-N-CA	-5.75	112.77	121.51
1	A	135	THR	N-CA-C	-5.74	104.93	111.07
1	B	249	SER	N-CA-C	-5.64	100.05	109.24
1	A	365	SER	CA-CB-OG	-5.62	99.87	111.10
1	B	257	ALA	N-CA-C	5.60	119.22	112.38
1	A	202	PHE	N-CA-C	5.60	118.77	110.48
1	B	396	ASP	N-CA-CB	-5.58	102.91	110.95
1	B	221	ILE	CA-C-N	5.57	127.58	120.56
1	B	221	ILE	C-N-CA	5.57	127.58	120.56
1	A	264	VAL	CB-CA-C	-5.56	104.23	110.96
1	B	66	ALA	CA-C-N	-5.56	115.57	123.08
1	B	66	ALA	C-N-CA	-5.56	115.57	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	CG-CD-NE	-5.56	99.78	112.00
1	A	90	LYS	N-CA-C	-5.53	99.50	108.41
1	B	159	ASN	N-CA-C	-5.51	105.43	111.82
1	A	107	GLY	N-CA-C	-5.48	106.15	112.50
1	A	362	ALA	N-CA-C	-5.45	103.33	110.53
1	B	43	ALA	N-CA-C	-5.44	105.43	111.36
1	B	255	PHE	N-CA-C	5.43	119.07	112.23
1	B	225	GLU	N-CA-C	-5.38	105.49	111.36
1	A	60	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	A	221	ILE	CB-CG1-CD1	-5.38	102.50	113.80
1	B	213	THR	CA-CB-CG2	5.38	119.64	110.50
1	A	37	VAL	N-CA-C	-5.36	105.16	111.00
1	B	59	ASP	CA-C-N	5.34	127.38	120.44
1	B	59	ASP	C-N-CA	5.34	127.38	120.44
1	B	242	VAL	CG1-CB-CG2	5.33	122.53	110.80
1	A	91	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	B	360	ILE	O-C-N	5.31	125.81	120.92
1	A	80	GLN	N-CA-C	-5.31	104.91	111.33
1	B	161	ALA	N-CA-C	-5.30	105.40	111.07
1	A	151	ILE	CG1-CB-CG2	5.28	126.52	110.70
1	B	335	ARG	CB-CG-CD	5.26	123.41	111.30
1	B	377	VAL	N-CA-C	-5.26	104.52	111.09
1	A	163	MET	N-CA-C	5.24	117.39	111.11
1	B	173	VAL	N-CA-CB	5.19	117.28	111.21
1	B	235	GLY	N-CA-C	-5.18	108.17	115.32
1	A	102	ILE	CG1-CB-CG2	5.17	126.21	110.70
1	B	92	GLU	N-CA-C	-5.16	106.81	113.01
1	B	123	GLU	N-CA-C	-5.16	101.70	109.85
1	A	61	LEU	N-CA-C	5.14	117.28	111.11
1	B	263	GLY	N-CA-C	5.14	120.32	114.67
1	B	192	VAL	CB-CA-C	-5.13	105.41	111.97
1	B	242	VAL	CA-CB-CG1	5.12	119.11	110.40
1	A	37	VAL	CB-CA-C	5.10	119.07	112.24
1	B	164	ARG	CB-CG-CD	-5.08	99.62	111.30
1	B	60	ARG	CA-CB-CG	5.07	124.23	114.10
1	B	90	LYS	CA-C-N	-5.06	115.02	122.06
1	B	90	LYS	C-N-CA	-5.06	115.02	122.06
1	A	130	GLY	N-CA-C	-5.04	106.39	112.49
1	B	177	SER	N-CA-C	5.03	121.51	110.80
1	B	175	THR	N-CA-C	5.03	121.51	110.80

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	69	0
1	B	2373	0	2364	78	0
2	A	16	0	0	0	0
2	B	18	0	0	0	0
All	All	4772	0	4724	145	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 (145) 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:CG1	1:B:264:VAL:CB	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:B:125:GLY:O	1:B:148:MET:HE2	1.47	1.13
1:A:146:ILE:CD1	1:A:163:MET:HE3	1.87	1.05
1:A:146:ILE:HD13	1:A:163:MET:HE3	1.03	1.02
1:B:249:SER:O	1:B:250:ASN:CB	2.08	1.01
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:35:MET:HA	1:A:35:MET:HE2	1.50	0.93
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:A:146:ILE:CB	1:A:163:MET:HE1	2.02	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:MET:HE1	1:A:363:ILE:HG12	1.54	0.87
1:A:146:ILE:CD1	1:A:163:MET:CE	2.46	0.87
1:B:185:ASN:O	1:B:189:ARG:HG3	1.75	0.86
1:B:395:LYS:HA	1:B:395:LYS:NZ	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	1.57	0.84
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:394:ASP:O	1:B:395:LYS:HB2	1.84	0.77
1:A:146:ILE:HD13	1:A:163:MET:HE2	1.66	0.76
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:A:35:MET:HA	1:A:35:MET:CE	2.18	0.74
1:B:125:GLY:O	1:B:148:MET:CE	2.34	0.73
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: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:CD2	1:A:237:LEU:H	2.08	0.66
1:A:237:LEU:HD22	1:A:237:LEU:H	1.61	0.66
1:A:146:ILE:CG2	1:A:163:MET:HE1	2.25	0.66
1:A:146:ILE:HB	1:A:163:MET:CE	2.24	0.65
1:B:247:GLY:HA3	1:B:364:GLU:OE2	1.99	0.63
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:163:MET:HE2	1:A:170:VAL:HG22	1.83	0.60
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:363:ILE:HD12	1:A:396:ASP:CG	2.29	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:395:LYS:HZ2	1:B:395:LYS:C	2.13	0.55
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:146:ILE:HG21	1:A:163:MET:HE1	1.88	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:B:347:MET:HE1	1:B:400:ALA:HA	1.90	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: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: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
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:146:ILE:CG1	1:A:163:MET:HE3	2.40	0.48
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:163:MET:HE2	1:B:170:VAL:HG22	1.96	0.48
1:A:34:LEU:O	1:A:37:VAL:HG12	2.14	0.48
1:B:347:MET:CE	1:B:400:ALA:HA	2.44	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:A:82:ALA:C	1:A:84:SER:N	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:SER:O	1:B:102:ILE:HG12	2.14	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:A:69:PRO:HA	1:A:225:GLU:CD	2.41	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:146:ILE:CG1	1:A:163:MET:CE	2.94	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:32:GLU:O	1:B:35:MET:HG2	2.19	0.43
1:B:137:CYS:HB3	1:B:142:LEU:O	2.18	0.43
1:B:336:VAL:HG22	1:B:338:TYR:CZ	2.54	0.43
1:A:79:SER:O	1:A:84:SER:HA	2.18	0.42
1:A:202:PHE:CE2	1:A:211:PHE:CE1	3.07	0.42
1:B:158:LEU:H	1:B:158:LEU:CD2	2.32	0.42
1:B:179:THR:O	1:B:180:LEU:HB3	2.20	0.42
1:B:350:PHE:CD1	1:B:350:PHE:C	2.98	0.42
1:B:158:LEU:O	1:B:162:ARG:HG3	2.19	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:145:VAL:C	1:B:146:ILE:HG12	2.44	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:A:32:GLU:O	1:A:35:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:VAL:HG12	1:B:136:ALA:CB	2.50	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:B:395:LYS:NZ	1:B:395:LYS:C	2.79	0.40
1:B:121:ILE:HA	1:B:145:VAL:O	2.21	0.40
1:A:200:TYR:CD1	1:A:200:TYR:C	2.99	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%)	294 (94%)	15 (5%)	2 (1%)	21	23
1	B	312/422 (74%)	286 (92%)	14 (4%)	12 (4%)	2	1
All	All	623/844 (74%)	580 (93%)	29 (5%)	14 (2%)	5	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
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

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Mol	Chain	Res	Type
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%)	208 (88%)	28 (12%)	5	4
1	B	237/314 (76%)	206 (87%)	31 (13%)	4	3
All	All	473/628 (75%)	414 (88%)	59 (12%)	4	4

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	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	245	VAL
1	A	252	ILE
1	A	267	VAL
1	A	270	GLU

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Mol	Chain	Res	Type
1	A	336	VAL
1	A	343	ASP
1	A	344	SER
1	A	363	ILE
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	95	ASN
1	B	96	HIS
1	B	97	THR
1	B	100	HIS
1	B	102	ILE
1	B	106	LEU
1	B	111	LEU
1	B	121	ILE
1	B	148	MET
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
1	B	252	ILE
1	B	274	ASP
1	B	336	VAL
1	B	352	LEU
1	B	379	LEU
1	B	395	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	81	HIS
1	A	96	HIS
1	A	156	GLN
1	A	174	GLN
1	A	197	ASN
1	A	250	ASN
1	B	46	GLN
1	B	52	GLN
1	B	81	HIS
1	B	103	ASN
1	B	231	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/422 (74%)	0.12	20 (6%) 26 23	27, 42, 66, 82	0
1	B	316/422 (74%)	0.43	29 (9%) 14 12	22, 47, 88, 104	0
All	All	631/844 (74%)	0.28	49 (7%) 19 16	22, 43, 79, 104	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	VAL	5.6
1	B	99	SER	5.1
1	B	180	LEU	4.3
1	B	97	THR	4.0
1	B	158	LEU	3.9
1	B	95	ASN	3.7
1	B	172	ALA	3.6
1	A	100	HIS	3.6
1	B	175	THR	3.5
1	B	151	ILE	3.5
1	A	96	HIS	3.5
1	B	96	HIS	3.4
1	A	393	GLY	3.4
1	A	202	PHE	3.3
1	B	157	ALA	3.3
1	A	153	THR	3.3
1	A	149	GLY	3.3
1	B	98	GLY	3.2
1	A	151	ILE	3.2
1	A	262	PRO	3.1
1	B	179	THR	3.0
1	B	170	VAL	2.9
1	A	155	ARG	2.8
1	A	252	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	100	HIS	2.8
1	A	152	ASP	2.8
1	A	394	ASP	2.8
1	B	174	GLN	2.7
1	A	97	THR	2.7
1	B	171	VAL	2.7
1	A	334	GLY	2.6
1	B	126	ALA	2.5
1	A	154	ALA	2.4
1	B	177	SER	2.3
1	A	250	ASN	2.3
1	A	395	LYS	2.3
1	B	270	GLU	2.3
1	B	154	ALA	2.3
1	B	29	TYR	2.2
1	B	153	THR	2.2
1	A	29	TYR	2.2
1	B	248	GLY	2.2
1	B	252	ILE	2.1
1	B	392	ARG	2.1
1	A	50	VAL	2.1
1	B	155	ARG	2.1
1	A	150	GLY	2.1
1	B	178	LYS	2.1
1	B	272	ALA	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 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.