



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:03 PM GMT

PDB ID : 2O2J
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

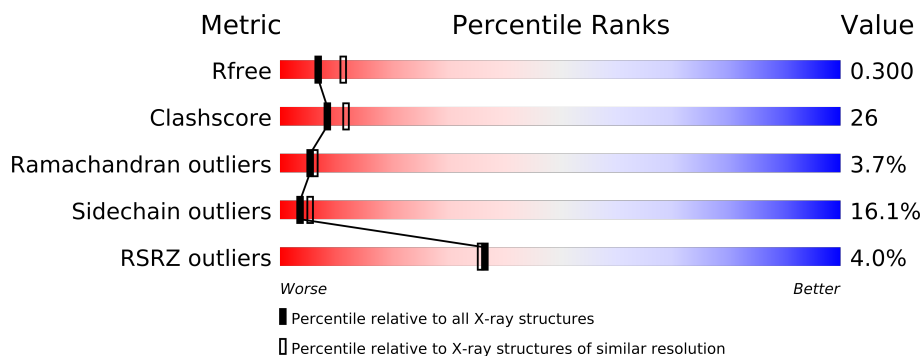
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2347 (2.60-2.52)
Clashscore	79885	2876 (2.60-2.52)
Ramachandran outliers	78287	2826 (2.60-2.52)
Sidechain outliers	78261	2826 (2.60-2.52)
RSRZ outliers	66119	2347 (2.60-2.52)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

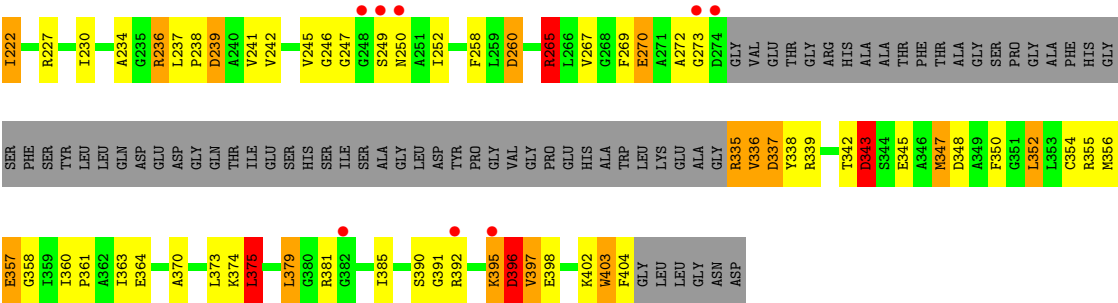
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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		



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 20.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.00-2.56) 96.8 (20.00-2.56)	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 0.216 , 0.300	Depositor DCC
R_{free} test set	1239 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 24208 reflections (0.004%)	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.

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	1.72	35/2403 (1.5%)	1.52	32/3252 (1.0%)
1	B	1.76	34/2411 (1.4%)	1.57	39/3263 (1.2%)
All	All	1.74	69/4814 (1.4%)	1.54	71/6515 (1.1%)

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 (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	39	GLU	CB-CG	11.15	1.73	1.52
1	A	65	TYR	C-O	10.49	1.43	1.23
1	B	40	GLU	CG-CD	9.89	1.66	1.51
1	B	40	GLU	CB-CG	9.17	1.69	1.52
1	A	104	ASN	CB-CG	9.07	1.72	1.51
1	B	39	GLU	CG-CD	8.84	1.65	1.51
1	A	73	TYR	CD2-CE2	8.39	1.51	1.39
1	B	63	ALA	CA-CB	8.32	1.70	1.52
1	A	384	VAL	CB-CG1	8.14	1.70	1.52
1	B	354	CYS	CB-SG	-8.02	1.68	1.82
1	A	101	LYS	CD-CE	7.56	1.70	1.51
1	A	348	ASP	CB-CG	7.13	1.66	1.51
1	B	270	GLU	CG-CD	7.04	1.62	1.51
1	A	170	VAL	CB-CG2	-6.98	1.38	1.52
1	B	154	ALA	CA-CB	6.98	1.67	1.52
1	A	383	ALA	CA-CB	-6.83	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLN	CG-CD	6.71	1.66	1.51
1	A	355	ARG	CG-CD	6.68	1.68	1.51
1	B	32	GLU	CB-CG	6.67	1.64	1.52
1	A	40	GLU	CD-OE1	6.56	1.32	1.25
1	B	74	GLU	CB-CG	6.54	1.64	1.52
1	A	137	CYS	CB-SG	6.49	1.93	1.82
1	B	343	ASP	CB-CG	6.40	1.65	1.51
1	A	40	GLU	CG-CD	6.38	1.61	1.51
1	A	66	ALA	CA-CB	6.33	1.65	1.52
1	B	109	ALA	CA-CB	-6.32	1.39	1.52
1	A	202	PHE	CE2-CZ	6.32	1.49	1.37
1	A	39	GLU	CG-CD	6.21	1.61	1.51
1	B	265	ARG	CG-CD	6.17	1.67	1.51
1	B	74	GLU	CD-OE2	6.13	1.32	1.25
1	B	192	VAL	CA-CB	-6.13	1.41	1.54
1	A	145	VAL	CB-CG2	6.11	1.65	1.52
1	B	270	GLU	CD-OE2	6.08	1.32	1.25
1	B	169	GLU	CB-CG	5.99	1.63	1.52
1	A	257	ALA	CA-CB	5.83	1.64	1.52
1	A	29	TYR	CD2-CE2	5.80	1.48	1.39
1	A	101	LYS	CE-NZ	5.72	1.63	1.49
1	B	115	MET	CB-CG	-5.68	1.33	1.51
1	B	350	PHE	CE2-CZ	5.65	1.48	1.37
1	B	227	ARG	C-O	5.62	1.34	1.23
1	A	215	VAL	CA-CB	5.59	1.66	1.54
1	B	73	TYR	CD2-CE2	5.58	1.47	1.39
1	A	29	TYR	CE2-CZ	5.50	1.45	1.38
1	B	357	GLU	CD-OE2	5.49	1.31	1.25
1	A	62	GLN	CB-CG	-5.46	1.37	1.52
1	A	364	GLU	CG-CD	5.43	1.60	1.51
1	B	269	PHE	CD2-CE2	5.41	1.50	1.39
1	B	270	GLU	CD-OE1	5.41	1.31	1.25
1	A	166	LEU	CG-CD2	5.40	1.71	1.51
1	B	169	GLU	CG-CD	5.37	1.60	1.51
1	A	211	PHE	CE2-CZ	5.37	1.47	1.37
1	A	202	PHE	CB-CG	-5.34	1.42	1.51
1	A	131	VAL	CA-CB	-5.32	1.43	1.54
1	B	234	ALA	CA-CB	-5.29	1.41	1.52
1	A	269	PHE	CE1-CZ	5.27	1.47	1.37
1	A	32	GLU	CB-CG	5.25	1.62	1.52
1	B	273	GLY	N-CA	5.24	1.53	1.46
1	B	242	VAL	CB-CG2	-5.21	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ALA	CA-CB	-5.20	1.41	1.52
1	B	193	ALA	CA-CB	-5.20	1.41	1.52
1	A	229	GLN	N-CA	5.20	1.56	1.46
1	A	381	ARG	CG-CD	5.18	1.65	1.51
1	B	65	TYR	CB-CG	-5.16	1.44	1.51
1	A	146	ILE	N-CA	-5.11	1.36	1.46
1	B	112	ALA	CA-CB	-5.05	1.41	1.52
1	B	186	GLU	CD-OE1	5.05	1.31	1.25
1	A	255	PHE	CB-CG	5.03	1.59	1.51
1	B	355	ARG	CG-CD	5.02	1.64	1.51
1	A	215	VAL	CB-CG1	5.02	1.63	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ARG	NE-CZ-NH2	11.47	126.04	120.30
1	B	60	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	B	260	ASP	CB-CG-OD1	-10.04	109.26	118.30
1	B	60	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	68	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	106	LEU	CB-CG-CD1	8.94	126.19	111.00
1	B	355	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	B	95	ASN	CB-CA-C	-8.44	93.52	110.40
1	A	392	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	55	LEU	CB-CG-CD2	8.03	124.64	111.00
1	A	352	LEU	CB-CG-CD1	-7.95	97.48	111.00
1	B	216	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	163	MET	CG-SD-CE	-7.71	87.87	100.20
1	B	106	LEU	CA-CB-CG	7.63	132.84	115.30
1	A	356	MET	CA-CB-CG	7.52	126.09	113.30
1	B	143	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	375	LEU	CB-CG-CD2	-7.42	98.38	111.00
1	B	119	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	343	ASP	CB-CG-OD2	7.13	124.71	118.30
1	A	396	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	106	LEU	CB-CG-CD2	-7.05	99.02	111.00
1	B	239	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	196	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	B	339	ARG	CB-CG-CD	-6.93	93.59	111.60
1	A	389	LEU	CB-CG-CD1	-6.91	99.26	111.00
1	A	113	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	379	LEU	CA-CB-CG	6.56	130.39	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ILE	CG1-CB-CG2	-6.54	97.02	111.40
1	A	77	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	59	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	B	167	GLY	C-N-CA	-6.31	105.92	121.70
1	B	37	VAL	CB-CA-C	6.29	123.36	111.40
1	A	339	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	106	LEU	CB-CG-CD2	-6.20	100.47	111.00
1	B	98	GLY	N-CA-C	6.09	128.31	113.10
1	B	143	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	66	ALA	N-CA-CB	-6.08	101.59	110.10
1	B	137	CYS	CA-CB-SG	-6.06	103.09	114.00
1	A	170	VAL	CB-CA-C	-6.06	99.89	111.40
1	A	61	LEU	CB-CG-CD1	-5.86	101.05	111.00
1	B	30	VAL	CG1-CB-CG2	-5.80	101.61	110.90
1	B	381	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	66	ALA	N-CA-C	-5.72	95.55	111.00
1	A	56	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	239	ASP	CB-CG-OD1	-5.71	113.17	118.30
1	B	214	MET	CG-SD-CE	-5.64	91.17	100.20
1	A	381	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	175	THR	CB-CA-C	-5.60	96.48	111.60
1	B	142	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	182	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	152	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	121	ILE	CG1-CB-CG2	-5.37	99.58	111.40
1	B	61	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	B	337	ASP	N-CA-CB	5.34	120.21	110.60
1	A	196	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	62	GLN	CB-CA-C	5.32	121.04	110.40
1	A	380	GLY	N-CA-C	5.31	126.38	113.10
1	A	61	LEU	C-N-CA	-5.29	108.48	121.70
1	A	94	LEU	CB-CG-CD2	5.23	119.89	111.00
1	B	375	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	217	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	162	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	381	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	216	ARG	CB-CG-CD	5.14	124.96	111.60
1	B	216	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	244	CYS	CA-CB-SG	-5.11	104.81	114.00
1	A	106	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	230	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	B	214	MET	CB-CG-SD	-5.05	97.25	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	51	SER	N-CA-C	5.01	124.52	111.00

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2365	0	2360	127	0
1	B	2373	0	2364	127	0
2	A	8	0	0	6	0
2	B	12	0	0	1	0
All	All	4758	0	4724	247	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (247) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:ILE:CG1	1:A:252:ILE:CD1	1.74	1.61
1:B:265:ARG:CG	1:B:265:ARG:HH11	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
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:H	1:A:158:LEU:HD23	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:NH1	1:B:265:ARG:CG	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:151:ILE:HG22	1:B:155:ARG:NH2	2.04	0.73
1:A:175:THR:HG22	1:A:175:THR:O	1.86	0.72
1:A:150:GLY:O	1:A:153:THR:HB	1.89	0.72
1:B:249:SER:O	1:B:250:ASN:HB3	1.89	0.72
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:335:ARG:C	2:A:414:HOH:O	2.25	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:179:THR:CG2	1:B:180:LEU:N	2.30	0.69
1:B:151:ILE:CG2	1:B:155:ARG:NH2	2.55	0.69
1:A:184:ILE:CG2	1:A:188:PHE:CE2	2.76	0.69
1:A:402:LYS:O	1:A:404:PHE:N	2.25	0.69
1:A:66:ALA:O	1:A:103:ASN:ND2	2.24	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: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:CG	1:A:335:ARG:HH11	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: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:CB	1:A:252:ILE:CD1	2.72	0.65
1:B:113:ARG:HD3	1:B:142:LEU:HD21	1.80	0.64
1:B:80:GLN:N	1:B:80:GLN:OE1	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:402:LYS:O	1:B:403:TRP:C	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:ILE:HA	1:A:145:VAL:O	2.02	0.60
1:A:152:ASP:N	1:A:152:ASP:OD1	2.35	0.59
1:B:375:LEU:HD12	1:B:379:LEU:HD13	1.83	0.59
1:B:219:GLN:HG3	1:B:250:ASN:ND2	2.14	0.59
1:A:158:LEU:CD2	1:A:158:LEU:H	2.12	0.58
1:B:45:TYR:CE2	1:B:49:ARG:HG3	2.38	0.58
1:B:180:LEU:HD13	1:B:184:ILE:CD1	2.33	0.58
1:A:175:THR:CG2	1:A:175:THR:O	2.51	0.58
1:B:192:VAL:O	1:B:192:VAL:HG12	1.99	0.58
1:B:335:ARG:O	1:B:335:ARG:HD2	2.03	0.58
1:A:158:LEU:N	1:A:158:LEU:HD23	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: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:B:163:MET:HE2	1:B:170:VAL:CG2	2.36	0.56
1:B:185:ASN:ND2	1:B:185:ASN:N	2.54	0.56
1:A:163:MET:HE2	1:A:170:VAL:HG22	1.86	0.55
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:B:202:PHE:CD1	1:B:202:PHE:C	2.80	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:223:GLY:O	1:A:224:MET:C	2.44	0.54
1:A:382:GLY:O	1:A:383:ALA:C	2.44	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:192:VAL:O	1:B:192:VAL:CG1	2.55	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:B:30:VAL:HG12	1:B:35:MET:HE3	1.92	0.52
1:A:369:VAL:O	1:A:373:LEU:HG	2.09	0.52
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:B:45:TYR:O	1:B:48:GLU:N	2.31	0.50
1:B:175:THR:CG2	1:B:176:GLY:H	2.16	0.50
1:A:79:SER:OG	1:A:84:SER:HA	2.11	0.50
1:B:188:PHE:CZ	1:B:208:PRO:HG2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:ASN:O	1:A:195:ALA:C	2.49	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:B:98:GLY:CA	1:B:101:LYS:H	1.95	0.50
1:A:57:ASP:O	1:A:61:LEU:HB2	2.12	0.50
1:B:352:LEU:CD2	1:B:356:MET:HG2	2.41	0.50
1:A:189:ARG:O	1:A:193:ALA:CB	2.59	0.50
1:A:108:GLN:OE1	1:A:202:PHE:CE2	2.65	0.50
1:B:46:GLN:O	1:B:48:GLU:N	2.45	0.50
1:A:363:ILE:HD12	1:A:396:ASP:OD1	2.11	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:402:LYS:O	1:A:403:TRP:C	2.50	0.49
1:A:184:ILE:HG22	1:A:188:PHE:CE2	2.48	0.49
1:B:151:ILE:CG2	1:B:155:ARG:HH21	2.26	0.49
1:A:402:LYS:O	1:A:404:PHE:C	2.51	0.49
1:A:158:LEU:CD2	1:A:158:LEU:N	2.73	0.49
1:A:34:LEU:O	1:A:37:VAL:HG12	2.12	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:34:LEU:HD11	1:B:188:PHE:CD1	2.48	0.48
1:A:62:GLN:HE22	1:A:221:ILE:HG12	1.78	0.48
1:A:101:LYS:NZ	1:A:128:GLN:HG2	2.29	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
1:B:342:THR:O	1:B:343:ASP:C	2.52	0.48
1:A:242:VAL:HG22	1:A:269:PHE:HE2	1.79	0.48
1:B:200:TYR:HE2	1:B:202:PHE:HB3	1.79	0.47
1:A:29:TYR:O	1:A:31:PRO:HD3	2.14	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:98:GLY:HA2	1:A:101:LYS:HD2	1.96	0.47
1:B:175:THR:HG22	1:B:176:GLY:N	2.19	0.47
1:A:152:ASP:HA	1:A:155:ARG:HG2	1.95	0.47
1:B:163:MET:HE2	1:B:170:VAL:HG22	1.97	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:B:163:MET:HE2	1:B:170:VAL:HG21	1.97	0.47
1:B:37:VAL:HG21	1:B:195:ALA:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:133:THR:O	1:B:134:ALA:C	2.52	0.46
1:A:45:TYR:CD2	1:A:214:MET:HE2	2.50	0.46
1:A:350:PHE:CD1	1:A:350:PHE:C	2.89	0.46
1:B:363:ILE:HG13	1:B:396:ASP:HB3	1.96	0.46
1:B:98:GLY:HA3	1:B:101:LYS:HD2	1.96	0.46
1:A:96:HIS:CE1	2:A:415:HOH:O	2.68	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:A:155:ARG:C	1:A:156:GLN:HG2	2.36	0.46
1:A:392:ARG:HH12	1:A:395:LYS:CE	2.29	0.46
1:A:202:PHE:N	1:A:202:PHE:CD2	2.68	0.45
1:A:255:PHE:O	1:A:256:HIS:C	2.54	0.45
1:B:270:GLU:OE2	1:B:338:TYR:HB3	2.16	0.45
1:A:345:GLU:O	1:A:346:ALA:C	2.55	0.45
1:A:63:ALA:O	1:A:64:ASN:HB2	2.16	0.45
1:B:202:PHE:CE2	1:B:211:PHE:HD2	2.35	0.45
1:A:363:ILE:HD12	1:A:396:ASP:CG	2.37	0.45
1:A:382:GLY:C	1:A:383:ALA:O	2.55	0.44
1:A:398:GLU:HB3	1:A:399:THR:H	1.52	0.44
1:B:236:ARG:HH12	1:B:239:ASP:CG	2.21	0.44
1:B:395:LYS:HA	1:B:397:VAL:CB	2.48	0.44
1:B:363:ILE:O	1:B:364:GLU:C	2.54	0.44
1:A:353:LEU:HA	1:A:353:LEU:HD12	1.67	0.44
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: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:158:LEU:C	1:A:161:ALA:H	2.20	0.43
1:A:194:ASN:O	1:A:196:ASP:N	2.52	0.43
1:B:236:ARG:NH2	1:B:239:ASP:OD2	2.46	0.43
1:B:230:ILE:HD12	1:B:230:ILE:HA	1.75	0.43
1:B:180:LEU:HD13	1:B:184:ILE:HD12	1.99	0.43
1:A:91:ARG:CZ	1:A:359:ILE:HD13	2.49	0.43
1:B:83:GLY:O	1:B:84:SER:HB2	2.19	0.43
1:B:151:ILE:HG21	1:B:155:ARG:NH2	2.34	0.42
1:A:119:ARG:NH1	1:A:198:THR:OG1	2.50	0.42
1:A:54:PHE:HD2	1:A:55:LEU:HD23	1.84	0.42
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.82	0.42
1:B:123:GLU:OE1	1:B:200:TYR:OH	2.25	0.42
1:A:348:ASP:O	1:A:352:LEU:HB2	2.18	0.42
1:B:241:VAL:HG21	1:B:258:PHE:CD2	2.54	0.42
1:B:345:GLU:CD	1:B:374:LYS:NZ	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:338:TYR:O	1:A:339:ARG:HG2	2.19	0.42
1:A:270:GLU:O	1:A:341:ILE:N	2.43	0.42
1:B:60:ARG:CZ	1:B:60:ARG:HB3	2.49	0.42
1:B:219:GLN:CG	1:B:250:ASN:HD22	2.24	0.42
1:B:58:LEU:HD13	1:B:107:GLY:HA2	2.02	0.42
1:B:87:ILE:HD13	1:B:87:ILE:N	2.35	0.42
1:A:162:ARG:HG2	1:B:360:ILE:CD1	2.50	0.41
1:B:121:ILE:HD11	1:B:191:TRP:HB2	2.02	0.41
1:B:37:VAL:HG13	1:B:191:TRP:CE2	2.56	0.41
1:B:74:GLU:HB2	1:B:88:PHE:CE2	2.55	0.41
1:B:356:MET:CE	1:B:356:MET:HA	2.51	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:149:GLY:O	1:B:152:ASP:N	2.53	0.41
1:B:78:LEU:HD23	1:B:78:LEU:HA	1.65	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:B:220:ARG:O	1:B:221:ILE:C	2.58	0.41
1:A:69:PRO:HA	1:A:225:GLU:CD	2.40	0.41
1:A:364:GLU:HG3	1:A:365:SER:N	2.35	0.41
1:A:259:LEU:HA	1:A:259:LEU:HD23	1.82	0.41
1:A:188:PHE:CZ	1:A:208:PRO:CG	2.92	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: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:70:SER:HA	1:A:71:PRO:HD3	1.64	0.41
1:A:163:MET:HE2	1:A:170:VAL:CG2	2.49	0.40
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:B:162:ARG:O	1:B:163:MET:C	2.58	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%)	266 (86%)	32 (10%)	13 (4%)	4	5
1	B	312/422 (74%)	274 (88%)	28 (9%)	10 (3%)	6	8
All	All	623/844 (74%)	540 (87%)	60 (10%)	23 (4%)	5	6

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	4
1	B	237/314 (76%)	203 (86%)	34 (14%)	5	7
All	All	473/628 (75%)	397 (84%)	76 (16%)	3	5

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
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	111	LEU
1	A	117	LYS
1	A	123	GLU
1	A	128	GLN
1	A	146	ILE
1	A	152	ASP
1	A	155	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	B	37	VAL
1	B	39	GLU
1	B	47	LYS
1	B	50	VAL
1	B	62	GLN
1	B	97	THR
1	B	106	LEU
1	B	111	LEU
1	B	119	ARG
1	B	121	ILE
1	B	155	ARG
1	B	156	GLN
1	B	175	THR
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	335	ARG
1	B	336	VAL
1	B	337	ASP
1	B	347	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	352	LEU
1	B	375	LEU
1	B	385	ILE
1	B	392	ARG
1	B	396	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	B	100	HIS
1	B	185	ASN
1	B	197	ASN
1	B	233	GLN
1	B	250	ASN
1	B	367	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.14	14 (4%) 33 32	21, 44, 78, 86	0
1	B	316/422 (74%)	0.02	11 (3%) 42 41	21, 42, 66, 84	0
All	All	631/844 (74%)	0.08	25 (3%) 36 36	21, 43, 76, 86	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ASN	5.8
1	A	50	VAL	5.1
1	B	273	GLY	5.0
1	B	274	ASP	4.7
1	B	249	SER	4.6
1	A	156	GLN	4.6
1	A	205	ALA	4.2
1	B	395	LYS	3.3
1	B	250	ASN	3.2
1	B	392	ARG	3.2
1	B	96	HIS	3.0
1	A	175	THR	2.6
1	A	246	GLY	2.6
1	A	206	ALA	2.6
1	A	247	GLY	2.5
1	A	249	SER	2.4
1	B	80	GLN	2.4
1	B	382	GLY	2.4
1	A	176	GLY	2.3
1	B	248	GLY	2.3
1	A	334	GLY	2.3
1	B	177	SER	2.2
1	A	151	ILE	2.2
1	A	38	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.