Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 05:12 PM EDT

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 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:

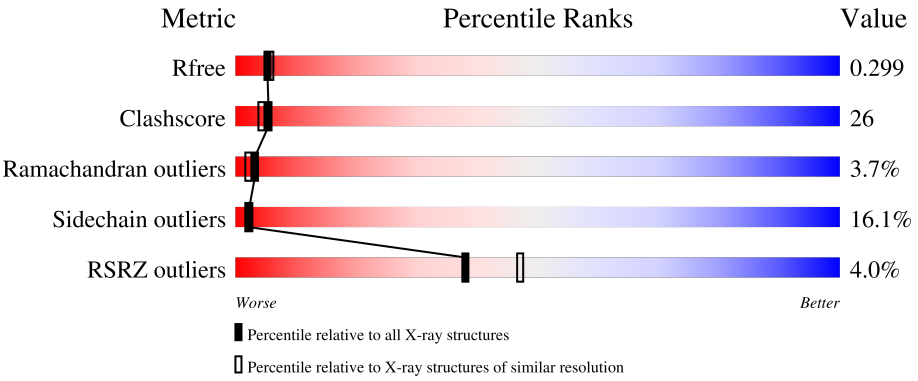
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 <=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	4% 33% 26% 13% · 25%
1	B	422	2% 37% 26% 9% · 25%

2 Entry composition (i)

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			

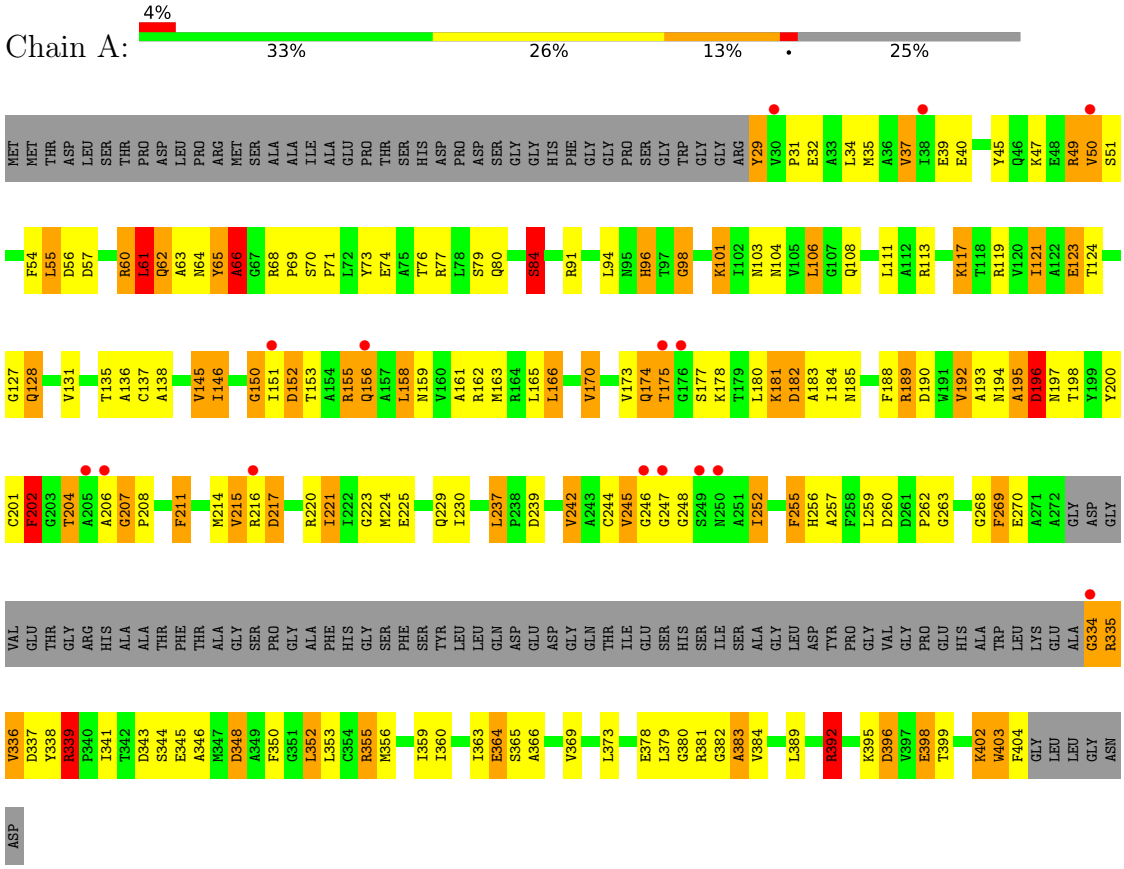
- Molecule 2 is water.

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

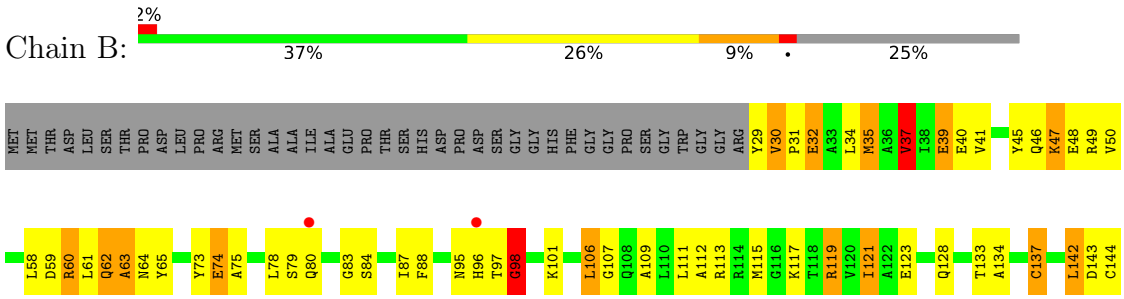
3 Residue-property plots (i)

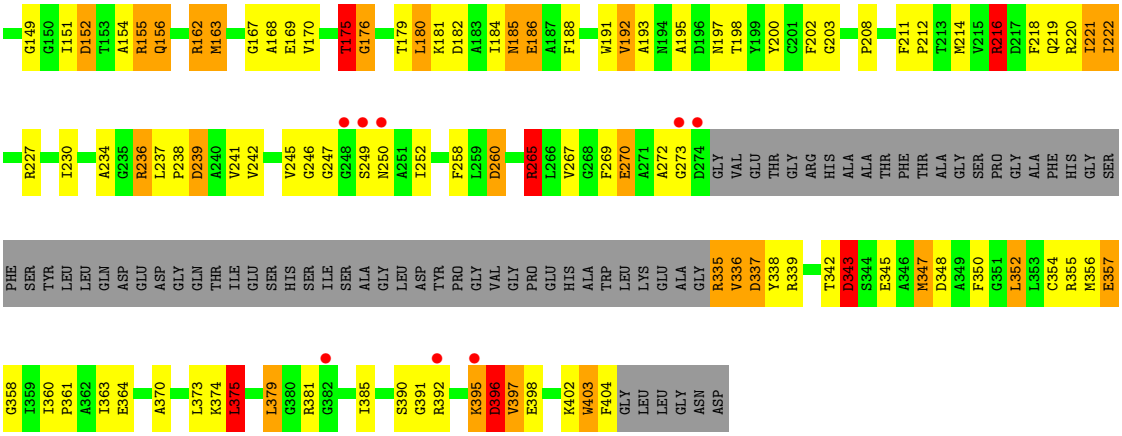
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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




G149 G150 I151 D152 T153 A154 R155 Q156 R162 M163 G167 A168 E169 V170 T175 G176 T179 L180 K181 D182 A183 I184 N185 E186 A187 F188 W191 V192 A193 N194 A195 D196 N197 T198 Y199 Y200 C201 F202 G203 P208 F211 P212 T213 M214 V215 R216 D217 F218 Q219 R220 I221 I222
R227 I230 A234 G235 R236 L237 P238 D239 A240 V241 V242 V245 G246 G247 G248 S249 N250 A251 I252 F258 L259 D260 R265 L266 V267 G268 F269 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 LEU GLN GLN ASP GLU ASP GLY GLN THR ILE GLU SER HIS SER ILE SER ALA GLY LEU ASP TYR PRO GLY VAL GLY PRO GLU HIS ALA TRP LEU LYS GLU ALA GLY R335 V336 D337 Y338 R339 T342 D343 S344 E345 A346 M347 D348 A349 F350 G351 L352 L353 C354 R355 M356 E357
G358 I359 I360 P361 A362 I363 E364 A370 L373 K374 L376 L379 G380 R381 G382 I385 S390 G391 R392 K396 D396 V397 E398 K402 W403 F404 GLY LEU LEU GLY ASN ASP

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.12%)	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)	0.33 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.72	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

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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

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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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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 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	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

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 26.

All (247) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:402:LYS:O	1:B:403:TRP:C	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:180:LEU:HD13	1:B:184:ILE:CD1	2.33	0.58
1:A:175:THR:O	1:A:175:THR:CG2	2.51	0.58
1:B:192:VAL:HG12	1:B:192:VAL:O	1.99	0.58
1:B:335:ARG:HD2	1:B:335:ARG:O	2.03	0.58
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:30:VAL:HG12	1:B:35:MET:CE	2.35	0.56
1:B:163:MET:HE2	1:B:170:VAL:CG2	2.36	0.56
1:B:347:MET:HG2	1:B:403:TRP:CD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:A:402:LYS:O	1:A:404:PHE:C	2.51	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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:CD2	1:A:202:PHE:N	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:63:ALA:O	1:A:64:ASN:HB2	2.16	0.45
1:A:345:GLU:O	1:A:346:ALA:C	2.55	0.45
1:A:363:ILE:HD12	1:A:396:ASP:CG	2.37	0.45
1:B:202:PHE:CE2	1:B:211:PHE:HD2	2.35	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:A:353:LEU:HD12	1:A:353:LEU:HA	1.67	0.44
1:B:363:ILE:O	1:B:364:GLU:C	2.54	0.44
1:B:395:LYS:HA	1:B:397:VAL:CB	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG21	1:B:155:ARG:NH2	2.34	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
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: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:B:356:MET:CE	1:B:356:MET:HA	2.51	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: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
1:A:69:PRO:HA	1:A:225:GLU:CD	2.40	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:B:220:ARG:O	1:B:221:ILE:C	2.58	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: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: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 (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%)	3	1
1	B	312/422 (74%)	274 (88%)	28 (9%)	10 (3%)	4	3
All	All	623/844 (74%)	540 (87%)	60 (10%)	23 (4%)	3	2

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

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Mol	Chain	Res	Type
1	A	150	GLY

5.3.2 Protein sidechains (i)

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%)	203 (86%)	34 (14%)	3 3
All	All	473/628 (75%)	397 (84%)	76 (16%)	2 2

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

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Mol	Chain	Res	Type
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
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

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

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	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 (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 monosaccharides 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, 95^{th} 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%)	0.11	15 (4%)	30	39	21, 44, 78, 86	0
1	B	316/422 (74%)	-0.02	10 (3%)	47	57	21, 42, 66, 84	0
All	All	631/844 (74%)	0.05	25 (3%)	38	47	21, 43, 76, 86	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	VAL	5.6
1	B	273	GLY	5.5
1	B	249	SER	5.2
1	B	274	ASP	5.2
1	A	205	ALA	5.1
1	A	250	ASN	4.9
1	A	156	GLN	4.4
1	B	395	LYS	3.7
1	B	96	HIS	3.3
1	B	248	GLY	3.2
1	B	392	ARG	3.1
1	A	247	GLY	2.7
1	A	175	THR	2.7
1	B	80	GLN	2.7
1	B	250	ASN	2.6
1	A	176	GLY	2.6
1	B	382	GLY	2.5
1	A	206	ALA	2.5
1	A	246	GLY	2.4
1	A	334	GLY	2.4
1	A	38	ILE	2.3
1	A	249	SER	2.1
1	A	151	ILE	2.1
1	A	216	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	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 monosaccharides 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.