Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 04:51 PM EDT

PDB ID	:	3FLM
Title	:	Crystal structure of menD from E.coli
Authors	:	Priyadarshi, A.; Hwang, K.Y.
Deposited on	:	2008-12-19
Resolution	:	2.70 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:

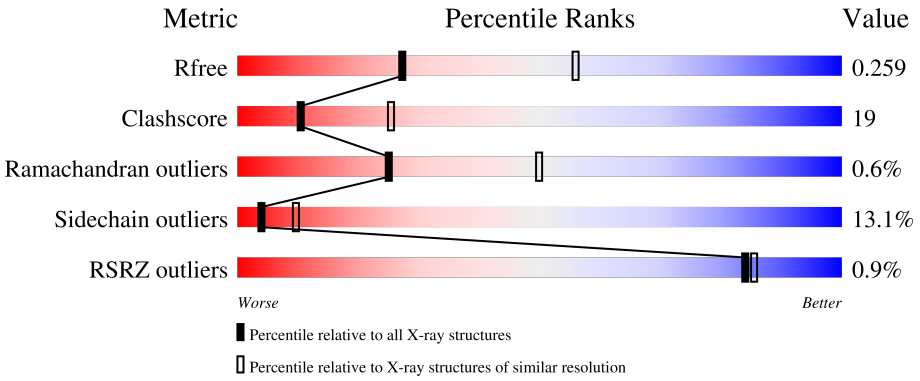
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

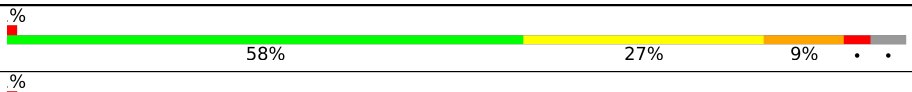
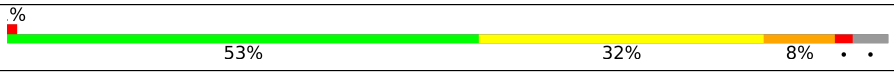
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	556	
1	B	556	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8317 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxyl ate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4158	2636	752	756	14			
1	B	531	Total	C	N	O	S	0	0	0
			4127	2614	747	752	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	PRO	engineered mutation	UNP P17109
B	36	LEU	PRO	engineered mutation	UNP P17109

- Molecule 2 is water.

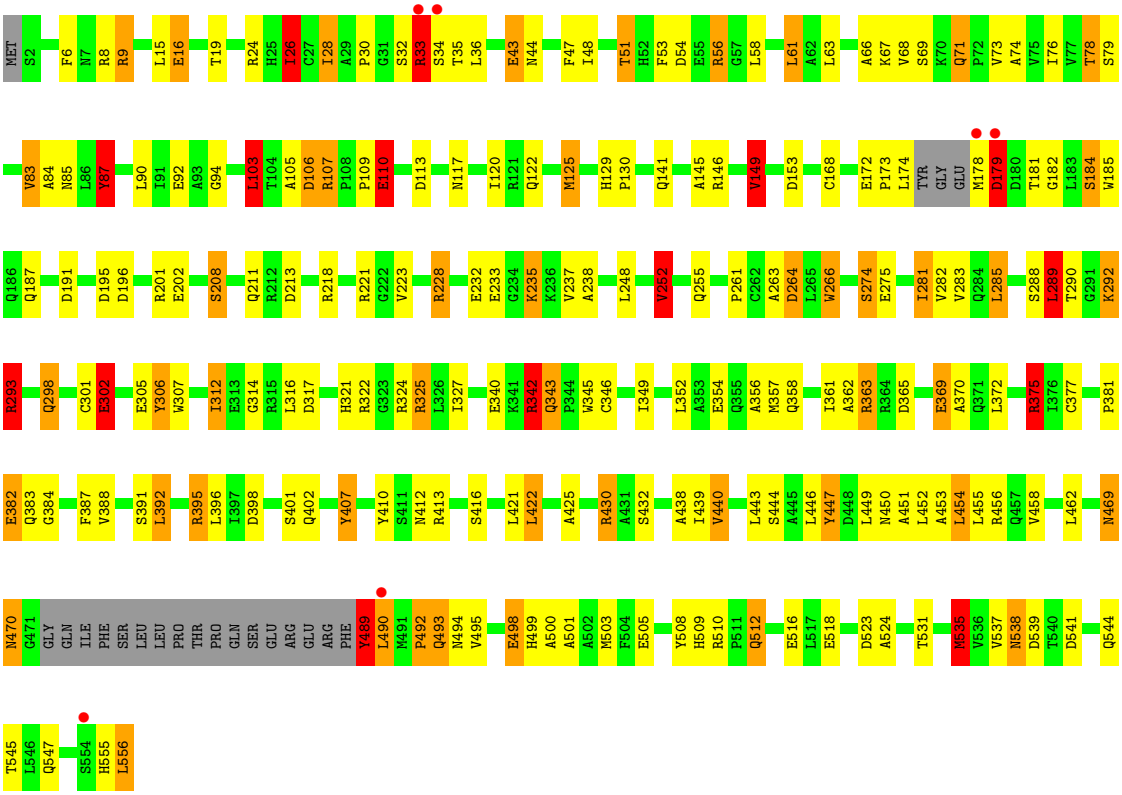
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	18	Total	O	0	0
			18	18		

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.

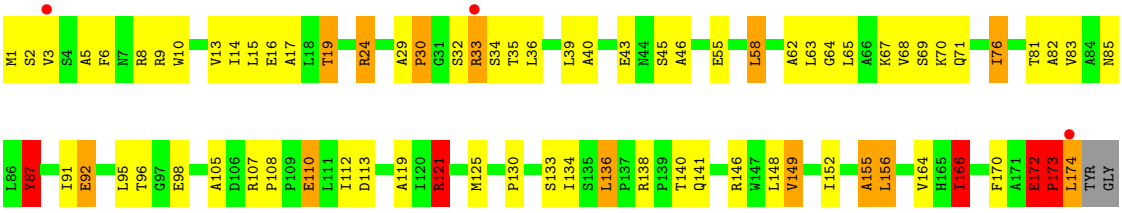
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

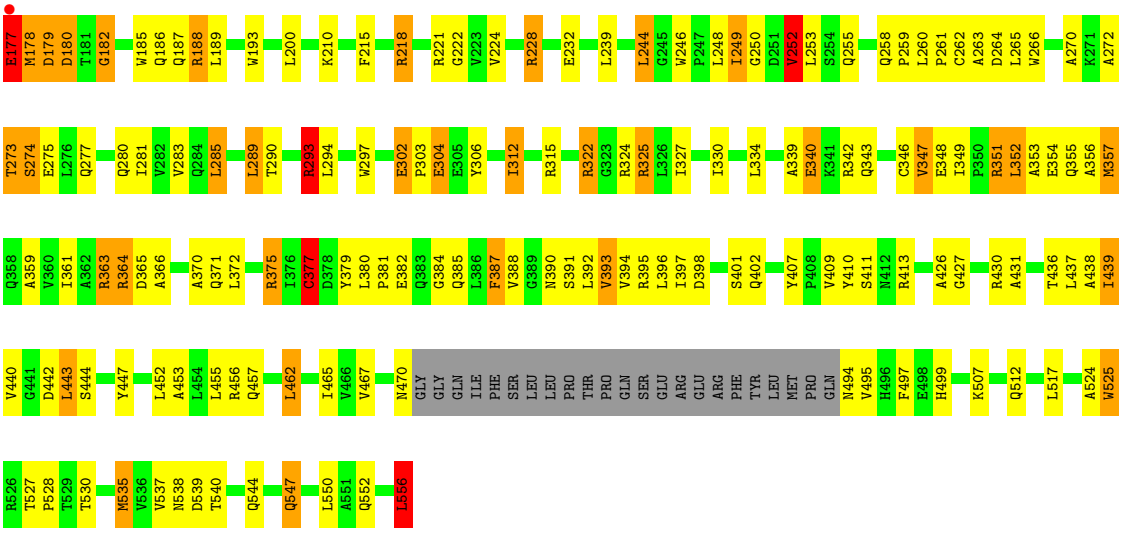
Chain A:



• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain B:




E177 M178 D179 D180 T181 G182 W185 Q186 Q187 R188 L189 W193 L200 K210 F215 R218 R221 G222 V223 V224 R228 E232 L239 L244 G245 W246 P247 L248 I249 G250 D251 V252 L253 S254 Q255 Q258 P259 L260 P261 C262 A263 D264 L265 W266 A270 K271 A272
T273 S274 E275 L276 Q277 Q280 I281 V282 V283 Q284 L285 L289 T290 R293 L294 W297 E302 P303 E304 E305 Y306 I312 R315 R322 G323 R324 R325 L326 I327 I330 L334 A339 E340 K341 R342 Q343 C346 V347 E348 I349 P350 R351 L352 A353 E354 Q355 A356 M357
Q358 A359 V360 I361 A362 R363 R364 D365 A366 A370 Q371 L372 R375 I376 C377 D378 Y379 L380 P381 E382 Q383 G384 Q385 L386 F387 V388 G389 N390 S391 L392 V393 V394 R395 L396 I397 D398 S401 Q402 Y407 P408 V409 Y410 S411 N412 R413 A426 G427 R430 A431 T436 L437 A438 I439
V440 G441 D442 L443 S444 Y447 L452 A453 L454 L455 R456 Q457 L462 I465 V466 V467 N470 GLY GLY GLN ILE PHE SER LEU LEU PRO THR PRO GLN SER GLU ARG GLU ARG PHE TYR LEU MET PRO GLN N494 V496 H496 F497 E498 H499 K507 Q512 L517 A524 W525
R526 T527 P528 T529 T530 M535 V536 V537 N538 D539 T540 Q544 Q547 L550 A551 Q552 L556

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.07Å 118.07Å 176.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 41.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.70) 98.3 (41.74-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.270 0.178 , 0.259	Depositor DCC
R_{free} test set	1725 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8317	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 (i)

5.1 Standard geometry (i)

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	1.57	41/4258 (1.0%)	1.42	64/5806 (1.1%)
1	B	1.51	33/4225 (0.8%)	1.39	44/5760 (0.8%)
All	All	1.54	74/8483 (0.9%)	1.41	108/11566 (0.9%)

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	3	5
1	B	0	6
All	All	3	11

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	GLU	CG-CD	10.85	1.68	1.51
1	A	110	GLU	CB-CG	-10.21	1.32	1.52
1	B	105	ALA	CA-CB	-9.62	1.32	1.52
1	A	518	GLU	CG-CD	8.62	1.64	1.51
1	A	105	ALA	CA-CB	-8.26	1.35	1.52
1	B	92	GLU	CD-OE2	8.03	1.34	1.25
1	A	149	VAL	CB-CG2	-7.81	1.36	1.52
1	B	193	TRP	CB-CG	-7.79	1.36	1.50
1	B	525	TRP	CB-CG	7.47	1.63	1.50
1	A	149	VAL	CB-CG1	-7.20	1.37	1.52
1	B	155	ALA	CA-CB	-7.17	1.37	1.52
1	B	340	GLU	CG-CD	7.12	1.62	1.51
1	B	92	GLU	CD-OE1	6.72	1.33	1.25
1	B	232	GLU	CG-CD	6.66	1.61	1.51
1	B	62	ALA	CA-CB	-6.60	1.38	1.52
1	B	351	ARG	CG-CD	6.53	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	TYR	CE1-CZ	6.45	1.47	1.38
1	B	377	CYS	CB-SG	-6.38	1.71	1.82
1	A	505	GLU	CD-OE1	6.38	1.32	1.25
1	A	505	GLU	CG-CD	6.30	1.61	1.51
1	B	30	PRO	CA-C	6.29	1.65	1.52
1	B	306	TYR	CD1-CE1	-6.27	1.29	1.39
1	A	365	ASP	CB-CG	6.26	1.65	1.51
1	A	547	GLN	CG-CD	6.26	1.65	1.51
1	A	16	GLU	CD-OE2	6.24	1.32	1.25
1	A	440	VAL	CB-CG2	-6.21	1.39	1.52
1	B	30	PRO	N-CA	6.18	1.57	1.47
1	A	388	VAL	CB-CG1	-6.18	1.39	1.52
1	B	224	VAL	CA-CB	-6.11	1.42	1.54
1	A	73	VAL	CB-CG1	-6.04	1.40	1.52
1	A	407	TYR	CD2-CE2	-6.01	1.30	1.39
1	B	55	GLU	CD-OE2	-5.96	1.19	1.25
1	B	388	VAL	CB-CG2	-5.96	1.40	1.52
1	B	302	GLU	CG-CD	5.95	1.60	1.51
1	B	497	PHE	CE2-CZ	5.93	1.48	1.37
1	B	3	VAL	CA-CB	5.90	1.67	1.54
1	A	356	ALA	CA-CB	-5.85	1.40	1.52
1	B	121	ARG	CG-CD	5.81	1.66	1.51
1	A	202	GLU	CG-CD	5.76	1.60	1.51
1	B	387	PHE	CE2-CZ	5.72	1.48	1.37
1	B	354	GLU	CG-CD	5.70	1.60	1.51
1	A	523	ASP	CB-CG	5.69	1.63	1.51
1	A	83	VAL	CA-CB	-5.64	1.43	1.54
1	A	94	GLY	C-O	-5.64	1.14	1.23
1	A	16	GLU	CG-CD	5.62	1.60	1.51
1	A	6	PHE	CB-CG	-5.59	1.41	1.51
1	B	87	TYR	CB-CG	5.56	1.59	1.51
1	A	252	VAL	CB-CG1	-5.52	1.41	1.52
1	A	141	GLN	CD-NE2	5.51	1.46	1.32
1	A	518	GLU	CB-CG	5.49	1.62	1.52
1	A	266	TRP	CB-CG	5.49	1.60	1.50
1	B	83	VAL	CA-CB	-5.46	1.43	1.54
1	A	545	THR	CA-CB	-5.43	1.39	1.53
1	A	354	GLU	CG-CD	5.40	1.60	1.51
1	A	92	GLU	CD-OE2	5.35	1.31	1.25
1	A	43	GLU	CB-CG	5.32	1.62	1.52
1	B	119	ALA	CA-CB	5.31	1.63	1.52
1	A	66	ALA	CA-CB	-5.30	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	PHE	CB-CG	-5.30	1.42	1.51
1	B	547	GLN	CG-CD	5.28	1.63	1.51
1	A	87	TYR	CE1-CZ	5.28	1.45	1.38
1	B	45	SER	CB-OG	-5.27	1.35	1.42
1	A	342	ARG	CG-CD	5.26	1.65	1.51
1	A	382	GLU	CD-OE1	5.24	1.31	1.25
1	A	292	LYS	CD-CE	5.21	1.64	1.51
1	A	232	GLU	CD-OE1	5.14	1.31	1.25
1	B	170	PHE	CD1-CE1	-5.13	1.28	1.39
1	A	518	GLU	CD-OE2	5.12	1.31	1.25
1	A	141	GLN	CG-CD	5.11	1.62	1.51
1	B	149	VAL	CB-CG1	-5.08	1.42	1.52
1	B	537	VAL	CB-CG2	-5.08	1.42	1.52
1	A	425	ALA	CA-CB	-5.08	1.41	1.52
1	A	85	ASN	C-O	-5.06	1.13	1.23
1	B	444	SER	N-CA	-5.03	1.36	1.46

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	430	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	107	ARG	NE-CZ-NH1	-11.03	114.79	120.30
1	B	218	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	B	228	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	61	LEU	CB-CG-CD1	-9.77	94.39	111.00
1	B	228	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	33	ARG	CB-CA-C	-9.57	91.25	110.40
1	A	196	ASP	CB-CA-C	-9.45	91.50	110.40
1	B	315	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	A	289	LEU	CB-CG-CD2	-8.95	95.79	111.00
1	B	138	ARG	NE-CZ-NH1	-8.89	115.85	120.30
1	A	510	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	324	ARG	NE-CZ-NH1	-8.47	116.07	120.30
1	B	252	VAL	CB-CA-C	-8.34	95.55	111.40
1	A	443	LEU	CB-CG-CD1	-8.11	97.21	111.00
1	A	264	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	179	ASP	CB-CA-C	-7.68	95.03	110.40
1	B	375	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	156	LEU	CB-CG-CD1	-7.60	98.09	111.00
1	A	106	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	195	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	228	ARG	NE-CZ-NH2	-7.07	116.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ASP	CB-CG-OD1	-7.05	111.96	118.30
1	A	503	MET	CG-SD-CE	7.01	111.41	100.20
1	A	181	THR	C-N-CA	-7.00	107.60	122.30
1	B	285	LEU	CA-CB-CG	6.98	131.35	115.30
1	A	58	LEU	CB-CG-CD2	-6.89	99.28	111.00
1	A	90	LEU	CB-CG-CD2	-6.87	99.33	111.00
1	A	556	LEU	CA-CB-CG	6.85	131.04	115.30
1	B	221	ARG	NE-CZ-NH1	-6.79	116.90	120.30
1	B	293	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	538	ASN	CB-CA-C	-6.60	97.20	110.40
1	B	172	GLU	C-N-CD	-6.58	106.12	120.60
1	B	556	LEU	CA-CB-CG	6.53	130.31	115.30
1	B	136	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	A	248	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	A	196	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	351	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	113	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	218	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	33	ARG	N-CA-C	6.34	128.12	111.00
1	A	264	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	34	SER	CB-CA-C	-6.23	98.27	110.10
1	B	352	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	106	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	B	325	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	375	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	110	GLU	CB-CA-C	-6.07	98.27	110.40
1	A	15	LEU	CA-CB-CG	-6.03	101.42	115.30
1	A	213	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	125	MET	CB-CA-C	-6.03	98.35	110.40
1	A	146	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	442	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	244	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	110	GLU	CB-CA-C	-5.92	98.55	110.40
1	B	58	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	213	ASP	CB-CG-OD1	5.88	123.60	118.30
1	B	76	ILE	CG1-CB-CG2	-5.85	98.53	111.40
1	A	352	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	392	LEU	CB-CG-CD2	5.83	120.92	111.00
1	A	153	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	223	VAL	CB-CA-C	-5.70	100.57	111.40
1	B	377	CYS	N-CA-CB	5.70	120.85	110.60
1	B	200	LEU	CB-CG-CD2	-5.69	101.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	ARG	CB-CG-CD	5.64	126.27	111.60
1	B	365	ASP	N-CA-C	5.64	126.22	111.00
1	A	293	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	364	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	A	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	334	LEU	CA-CB-CG	-5.55	102.53	115.30
1	A	87	TYR	CG-CD2-CE2	5.53	125.72	121.30
1	A	375	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	510	ARG	N-CA-C	-5.52	96.11	111.00
1	B	427	GLY	N-CA-C	-5.51	99.32	113.10
1	A	555	HIS	CB-CA-C	-5.51	99.38	110.40
1	B	352	LEU	CB-CG-CD1	-5.43	101.76	111.00
1	A	103	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	B	110	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	B	166	ILE	CG1-CB-CG2	-5.42	99.49	111.40
1	A	325	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	264	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	125	MET	CG-SD-CE	-5.35	91.65	100.20
1	A	179	ASP	C-N-CA	5.34	135.05	121.70
1	A	430	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	26	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	A	9	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	324	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	A	454	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	B	352	LEU	CB-CG-CD2	5.30	120.01	111.00
1	A	391	SER	N-CA-CB	-5.25	102.63	110.50
1	A	509	HIS	CB-CA-C	-5.24	99.93	110.40
1	B	439	ILE	CB-CA-C	-5.22	101.16	111.60
1	A	274	SER	CB-CA-C	5.20	119.97	110.10
1	A	535	MET	CB-CA-C	-5.19	100.02	110.40
1	B	107	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	B	297	TRP	CA-CB-CG	-5.17	103.88	113.70
1	A	343	GLN	CB-CA-C	5.16	120.73	110.40
1	A	538	ASN	CB-CA-C	-5.13	100.14	110.40
1	A	443	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	146	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	322	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	168	CYS	CA-CB-SG	-5.05	104.90	114.00
1	B	462	LEU	CB-CG-CD1	5.05	119.59	111.00
1	A	325	ARG	CA-CB-CG	5.04	124.49	113.40
1	B	293	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	201	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	153	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	35	THR	CB
1	A	302	GLU	CA
1	A	493	GLN	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	ASP	Peptide
1	A	302	GLU	Peptide
1	A	469	ASN	Peptide
1	A	489	TYR	Peptide
1	A	492	PRO	Peptide
1	B	172	GLU	Peptide
1	B	173	PRO	Peptide
1	B	177	GLU	Peptide
1	B	179	ASP	Peptide
1	B	182	GLY	Peptide
1	B	390	ASN	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	4158	0	4131	152	0
1	B	4127	0	4102	160	0
2	A	14	0	0	0	0
2	B	18	0	0	0	0
All	All	8317	0	8233	304	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 19.

All (304) 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:33:ARG:NH2	1:B:174:LEU:HD21	1.51	1.25
1:A:493:GLN:HG2	1:A:494:ASN:N	1.60	1.16
1:B:33:ARG:HH22	1:B:174:LEU:HD21	1.00	1.14
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.03	1.13
1:B:363:ARG:HB3	1:B:363:ARG:HH11	1.16	1.10
1:B:252:VAL:HG22	1:B:398:ASP:HB2	1.44	0.97
1:B:293:ARG:HH11	1:B:293:ARG:HG2	1.29	0.93
1:A:372:LEU:HD22	1:A:535:MET:HE2	1.52	0.92
1:A:281:ILE:HD12	1:A:282:VAL:N	1.84	0.91
1:A:33:ARG:O	1:A:33:ARG:HG3	1.66	0.91
1:A:489:TYR:O	1:A:489:TYR:CD1	2.23	0.90
1:A:493:GLN:CG	1:A:494:ASN:N	2.30	0.90
1:A:179:ASP:OD2	1:A:179:ASP:C	2.10	0.90
1:A:372:LEU:HD22	1:A:535:MET:CE	2.02	0.90
1:A:16:GLU:O	1:A:19:THR:HB	1.72	0.89
1:A:358:GLN:O	1:A:361:ILE:HG12	1.74	0.88
1:B:174:LEU:N	1:B:174:LEU:HD23	1.88	0.87
1:A:538:ASN:HB2	1:A:541:ASP:OD2	1.74	0.86
1:B:33:ARG:HH22	1:B:174:LEU:CD2	1.87	0.86
1:B:372:LEU:HD22	1:B:535:MET:CE	2.05	0.86
1:A:493:GLN:CG	1:A:494:ASN:H	1.88	0.86
1:B:363:ARG:HB3	1:B:363:ARG:NH1	1.92	0.85
1:A:489:TYR:O	1:A:489:TYR:CG	2.29	0.83
1:B:179:ASP:C	1:B:179:ASP:OD1	2.13	0.83
1:A:381:PRO:HG2	1:A:384:GLY:HA3	1.61	0.82
1:A:122:GLN:O	1:A:125:MET:HB2	1.81	0.81
1:A:293:ARG:HH11	1:A:293:ARG:CG	1.89	0.81
1:B:372:LEU:HD22	1:B:535:MET:HE2	1.61	0.81
1:A:264:ASP:O	1:A:293:ARG:HG3	1.80	0.81
1:A:301:CYS:O	1:A:302:GLU:HB3	1.81	0.81
1:B:33:ARG:O	1:B:33:ARG:CD	2.30	0.80
1:B:177:GLU:CA	1:B:177:GLU:OE2	2.30	0.79
1:A:375:ARG:HG2	1:A:375:ARG:HH11	1.47	0.79
1:A:361:ILE:HG13	1:A:362:ALA:N	1.99	0.78
1:B:293:ARG:HG2	1:B:293:ARG:NH1	1.87	0.78
1:B:381:PRO:HG2	1:B:384:GLY:HA3	1.66	0.77
1:A:9:ARG:HG3	1:A:182:GLY:HA3	1.67	0.77
1:A:281:ILE:HD12	1:A:282:VAL:H	1.49	0.77
1:A:422:LEU:N	1:A:422:LEU:HD23	2.00	0.77
1:B:177:GLU:OE2	1:B:177:GLU:HA	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ARG:HG2	1:A:293:ARG:NH1	1.77	0.76
1:A:498:GLU:HG3	1:A:508:TYR:CE2	2.21	0.74
1:B:363:ARG:HH11	1:B:363:ARG:CB	1.98	0.74
1:B:24:ARG:HD3	1:B:46:ALA:O	1.87	0.74
1:B:357:MET:O	1:B:361:ILE:HG13	1.88	0.74
1:B:24:ARG:CD	1:B:46:ALA:O	2.37	0.73
1:A:178:MET:O	1:A:178:MET:HG3	1.87	0.72
1:B:174:LEU:N	1:B:174:LEU:CD2	2.49	0.72
1:A:28:ILE:O	1:A:51:THR:HA	1.89	0.72
1:A:173:PRO:HD2	1:A:173:PRO:O	1.91	0.71
1:A:68:VAL:HG22	1:A:410:TYR:CZ	2.26	0.70
1:A:84:ALA:HB1	1:B:87:TYR:HB3	1.74	0.70
1:A:252:VAL:HG22	1:A:398:ASP:HB2	1.73	0.70
1:A:34:SER:OG	1:A:78:THR:CA	2.40	0.70
1:B:33:ARG:O	1:B:33:ARG:CG	2.40	0.69
1:B:173:PRO:C	1:B:174:LEU:HD23	2.14	0.69
1:B:409:VAL:HG12	1:B:410:TYR:N	2.07	0.68
1:B:33:ARG:O	1:B:33:ARG:HD3	1.93	0.68
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.59	0.68
1:B:121:ARG:NH2	1:B:121:ARG:HG3	2.09	0.68
1:A:261:PRO:HG3	1:A:402:GLN:NE2	2.08	0.68
1:B:164:VAL:HG12	1:B:166:ILE:HD12	1.76	0.68
1:A:129:HIS:N	1:A:130:PRO:CD	2.57	0.67
1:A:305:GLU:HG2	1:A:307:TRP:HE1	1.60	0.67
1:A:489:TYR:N	1:A:490:LEU:HA	2.09	0.67
1:A:470:ASN:OD1	1:A:470:ASN:N	2.28	0.67
1:A:275:GLU:OE1	1:A:349:ILE:HG12	1.96	0.66
1:A:421:LEU:HD12	1:A:444:SER:HB3	1.77	0.66
1:B:69:SER:OG	1:B:71:GLN:HG2	1.95	0.66
1:B:177:GLU:OE2	1:B:177:GLU:N	2.29	0.66
1:B:372:LEU:HD22	1:B:535:MET:HE3	1.76	0.65
1:B:179:ASP:OD1	1:B:180:ASP:N	2.30	0.64
1:A:179:ASP:OD2	1:A:179:ASP:O	2.16	0.64
1:A:342:ARG:HB3	1:A:342:ARG:NH1	2.13	0.64
1:B:293:ARG:HH11	1:B:293:ARG:CG	2.07	0.64
1:A:76:ILE:HG12	1:A:103:LEU:HD12	1.78	0.64
1:A:512:GLN:HB2	1:A:516:GLU:OE1	1.97	0.64
1:A:34:SER:O	1:A:36:LEU:N	2.32	0.63
1:A:34:SER:OG	1:A:78:THR:N	2.32	0.61
1:A:342:ARG:CB	1:A:342:ARG:HH11	2.14	0.61
1:A:173:PRO:O	1:A:173:PRO:CD	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:HG12	1:B:166:ILE:CD1	2.32	0.60
1:B:263:ALA:HA	1:B:266:TRP:CE2	2.37	0.60
1:B:393:VAL:HG21	1:B:467:VAL:HG21	1.84	0.59
1:B:355:GLN:NE2	1:B:556:LEU:HG	2.18	0.59
1:B:33:ARG:HE	1:B:33:ARG:HA	1.67	0.59
1:B:381:PRO:HD2	1:B:407:TYR:OH	2.02	0.59
1:B:259:PRO:C	1:B:261:PRO:HD3	2.22	0.59
1:A:342:ARG:NH1	1:A:342:ARG:CB	2.65	0.59
1:B:121:ARG:CG	1:B:121:ARG:HH21	2.16	0.59
1:B:252:VAL:CG2	1:B:398:ASP:HB2	2.25	0.59
1:A:538:ASN:CB	1:A:541:ASP:OD2	2.50	0.58
1:B:327:ILE:HD12	1:B:327:ILE:N	2.18	0.58
1:A:499:HIS:HB3	1:B:499:HIS:HB3	1.85	0.58
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.38	0.58
1:B:263:ALA:HA	1:B:266:TRP:NE1	2.19	0.58
1:A:26:ILE:HG12	1:A:74:ALA:HB3	1.86	0.57
1:A:375:ARG:HG2	1:A:375:ARG:NH1	2.11	0.57
1:A:290:THR:OG1	1:A:413:ARG:NH1	2.35	0.57
1:B:15:LEU:HD12	1:B:40:ALA:HB3	1.85	0.57
1:B:8:ARG:HD3	1:B:36:LEU:CD2	2.35	0.57
1:B:121:ARG:HG3	1:B:121:ARG:HH21	1.69	0.57
1:A:301:CYS:O	1:A:302:GLU:CB	2.52	0.57
1:A:33:ARG:NH1	1:A:106:ASP:O	2.38	0.56
1:A:372:LEU:HD22	1:A:535:MET:HE3	1.82	0.56
1:A:228:ARG:NH2	1:A:288:SER:OG	2.38	0.56
1:B:283:VAL:HG12	1:B:285:LEU:HD22	1.87	0.56
1:B:290:THR:HA	1:B:413:ARG:NH1	2.21	0.56
1:A:490:LEU:H	1:B:457:GLN:NE2	2.02	0.56
1:B:394:VAL:HA	1:B:397:ILE:HD12	1.86	0.56
1:A:34:SER:OG	1:A:78:THR:HA	2.05	0.56
1:B:244:LEU:HG	1:B:339:ALA:HB1	1.88	0.56
1:B:272:ALA:HB1	1:B:349:ILE:HD13	1.87	0.56
1:B:9:ARG:HB3	1:B:186:GLN:NE2	2.21	0.56
1:A:191:ASP:OD1	1:A:191:ASP:C	2.45	0.55
1:A:489:TYR:HA	1:A:490:LEU:HD13	1.87	0.55
1:B:430:ARG:NH2	1:B:457:GLN:HB2	2.22	0.55
1:A:422:LEU:HB2	1:A:451:ALA:HB3	1.89	0.55
1:B:24:ARG:HD2	1:B:46:ALA:O	2.05	0.55
1:A:84:ALA:O	1:A:87:TYR:HB2	2.07	0.54
1:B:182:GLY:O	1:B:185:TRP:HB3	2.06	0.54
1:B:108:PRO:HB2	1:B:110:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:PRO:O	1:B:261:PRO:CD	2.56	0.54
1:B:33:ARG:O	1:B:33:ARG:HG3	2.07	0.53
1:B:249:ILE:N	1:B:249:ILE:HD12	2.24	0.53
1:A:129:HIS:H	1:A:130:PRO:CD	2.22	0.53
1:B:259:PRO:O	1:B:261:PRO:HD2	2.09	0.53
1:A:469:ASN:C	1:A:469:ASN:OD1	2.43	0.53
1:B:262:CYS:O	1:B:263:ALA:C	2.48	0.53
1:A:490:LEU:H	1:B:457:GLN:HE22	1.57	0.52
1:B:409:VAL:CG1	1:B:410:TYR:N	2.72	0.52
1:A:361:ILE:C	1:A:363:ARG:H	2.11	0.52
1:B:16:GLU:O	1:B:19:THR:HB	2.10	0.52
1:B:15:LEU:CD1	1:B:40:ALA:HB3	2.40	0.52
1:B:112:ILE:O	1:B:113:ASP:HB2	2.09	0.51
1:A:208:SER:HB2	1:A:327:ILE:H	1.75	0.51
1:B:17:ALA:HB2	1:B:149:VAL:HG23	1.91	0.51
1:A:382:GLU:O	1:A:383:GLN:HB2	2.10	0.51
1:B:262:CYS:O	1:B:265:LEU:N	2.33	0.51
1:B:285:LEU:HD12	1:B:330:ILE:HG23	1.91	0.51
1:A:489:TYR:CD1	1:A:489:TYR:C	2.84	0.51
1:B:455:LEU:HD22	1:B:462:LEU:HD13	1.93	0.51
1:A:145:ALA:O	1:A:149:VAL:HG12	2.11	0.50
1:A:107:ARG:NH1	1:A:117:ASN:O	2.44	0.50
1:B:426:ALA:O	1:B:430:ARG:HG3	2.10	0.50
1:B:437:LEU:HD11	1:B:465:ILE:HG13	1.92	0.50
1:B:8:ARG:HD3	1:B:36:LEU:HD21	1.93	0.50
1:B:215:PHE:HA	1:B:218:ARG:HE	1.77	0.50
1:B:409:VAL:HG12	1:B:410:TYR:H	1.75	0.50
1:A:469:ASN:OD1	1:A:469:ASN:O	2.30	0.50
1:B:258:GLN:O	1:B:261:PRO:HD3	2.12	0.50
1:B:187:GLN:C	1:B:189:LEU:N	2.64	0.49
1:A:361:ILE:O	1:A:363:ARG:N	2.46	0.49
1:A:358:GLN:O	1:A:361:ILE:CG1	2.56	0.49
1:B:259:PRO:C	1:B:261:PRO:CD	2.80	0.49
1:B:379:TYR:CZ	1:B:517:LEU:HD23	2.47	0.49
1:B:33:ARG:HE	1:B:33:ARG:CA	2.23	0.49
1:B:363:ARG:NH1	1:B:363:ARG:CB	2.67	0.49
1:B:387:PHE:O	1:B:438:ALA:HA	2.11	0.49
1:B:274:SER:HA	1:B:277:GLN:HE21	1.76	0.49
1:B:430:ARG:HH21	1:B:457:GLN:HB2	1.77	0.49
1:A:33:ARG:NH2	1:A:172:GLU:OE2	2.46	0.49
1:A:221:ARG:HD2	1:A:345:TRP:CE3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LEU:HD23	1:A:455:LEU:HD12	1.95	0.49
1:B:218:ARG:NH2	1:B:340:GLU:HB2	2.27	0.49
1:A:34:SER:HG	1:A:78:THR:N	2.10	0.48
1:A:34:SER:O	1:A:35:THR:C	2.50	0.48
1:A:524:ALA:HB2	1:A:531:THR:HG21	1.96	0.48
1:B:372:LEU:CD2	1:B:535:MET:CE	2.85	0.48
1:B:17:ALA:CB	1:B:149:VAL:HG23	2.44	0.48
1:B:249:ILE:N	1:B:249:ILE:CD1	2.77	0.48
1:A:211:GLN:OE1	1:A:324:ARG:NH2	2.44	0.48
1:A:469:ASN:O	1:A:469:ASN:CG	2.50	0.48
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.68	0.47
1:B:9:ARG:O	1:B:13:VAL:HG23	2.14	0.47
1:B:67:LYS:O	1:B:70:LYS:HE2	2.15	0.47
1:B:270:ALA:HA	1:B:273:THR:OG1	2.15	0.47
1:A:446:LEU:HD21	1:A:495:VAL:HG11	1.97	0.47
1:A:252:VAL:HG13	1:A:398:ASP:HA	1.97	0.47
1:A:375:ARG:HH11	1:A:375:ARG:CG	2.22	0.47
1:B:67:LYS:HE2	1:B:98:GLU:OE2	2.14	0.47
1:A:44:ASN:HB3	1:A:47:PHE:CE2	2.50	0.47
1:A:538:ASN:ND2	1:A:541:ASP:OD2	2.47	0.47
1:B:280:GLN:O	1:B:304:GLU:N	2.46	0.47
1:A:412:ASN:O	1:A:416:SER:HA	2.15	0.47
1:A:469:ASN:HA	1:A:537:VAL:O	2.15	0.46
1:B:63:LEU:HD21	1:B:92:GLU:HG2	1.97	0.46
1:A:48:ILE:N	1:A:48:ILE:HD13	2.30	0.46
1:A:387:PHE:O	1:A:438:ALA:HA	2.15	0.46
1:B:69:SER:O	1:B:70:LYS:HB2	2.15	0.46
1:B:401:SER:OG	1:B:402:GLN:N	2.48	0.46
1:B:8:ARG:NH2	1:B:43:GLU:OE2	2.47	0.46
1:B:366:ALA:O	1:B:371:GLN:HG2	2.16	0.46
1:B:81:THR:O	1:B:82:ALA:C	2.53	0.46
1:B:275:GLU:OE1	1:B:349:ILE:HG12	2.16	0.46
1:B:35:THR:O	1:B:39:LEU:HG	2.16	0.46
1:B:130:PRO:HG2	1:B:133:SER:OG	2.16	0.46
1:B:244:LEU:HG	1:B:339:ALA:CB	2.45	0.46
1:B:452:LEU:O	1:B:453:ALA:C	2.53	0.46
1:B:353:ALA:O	1:B:356:ALA:HB3	2.15	0.45
1:B:381:PRO:HB3	1:B:525:TRP:CZ2	2.51	0.45
1:A:69:SER:CB	1:A:71:GLN:HG3	2.47	0.45
1:A:283:VAL:HG12	1:A:285:LEU:HD22	1.97	0.45
1:A:395:ARG:HG3	1:A:395:ARG:NH1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:HIS:HB3	1:B:499:HIS:O	2.17	0.45
1:B:134:ILE:HD11	1:B:155:ALA:HB2	1.98	0.45
1:B:289:LEU:HG	1:B:294:LEU:HD21	1.98	0.45
1:B:392:LEU:HD12	1:B:395:ARG:NH1	2.32	0.45
1:A:33:ARG:HB3	1:A:78:THR:OG1	2.17	0.45
1:A:263:ALA:HA	1:A:266:TRP:CD1	2.52	0.45
1:A:298:GLN:HG3	1:A:306:TYR:OH	2.16	0.45
1:B:527:THR:HB	1:B:528:PRO:CD	2.46	0.45
1:A:305:GLU:HG2	1:A:307:TRP:NE1	2.30	0.45
1:B:187:GLN:O	1:B:188:ARG:C	2.53	0.45
1:B:361:ILE:O	1:B:364:ARG:HB3	2.16	0.45
1:B:5:ALA:O	1:B:8:ARG:HB2	2.17	0.44
1:B:260:LEU:HA	1:B:261:PRO:HD2	1.67	0.44
1:A:33:ARG:HD2	1:A:79:SER:HB3	1.99	0.44
1:A:53:PHE:CD1	1:A:54:ASP:N	2.85	0.44
1:A:453:ALA:O	1:A:456:ARG:HG3	2.18	0.44
1:A:493:GLN:HG3	1:A:494:ASN:H	1.78	0.44
1:A:462:LEU:C	1:A:462:LEU:HD23	2.38	0.44
1:B:312:ILE:HD13	1:B:312:ILE:HG21	1.64	0.44
1:B:356:ALA:O	1:B:359:ALA:HB3	2.17	0.44
1:B:370:ALA:HA	1:B:396:LEU:HD13	1.99	0.44
1:B:372:LEU:CD2	1:B:535:MET:HE3	2.45	0.44
1:B:347:VAL:HG12	1:B:348:GLU:HG2	2.00	0.44
1:A:56:ARG:NH1	1:A:447:TYR:HE1	2.16	0.43
1:A:500:ALA:O	1:A:501:ALA:C	2.54	0.43
1:B:76:ILE:HD13	1:B:76:ILE:HG21	1.82	0.43
1:B:259:PRO:O	1:B:261:PRO:HD3	2.16	0.43
1:B:462:LEU:HD23	1:B:462:LEU:C	2.38	0.43
1:A:184:SER:HA	1:A:187:GLN:HB2	1.99	0.43
1:A:261:PRO:HG3	1:A:402:GLN:HE21	1.80	0.43
1:A:120:ILE:HG22	1:B:95:LEU:HD11	2.00	0.43
1:A:489:TYR:N	1:A:490:LEU:HD12	2.33	0.43
1:B:452:LEU:HD23	1:B:455:LEU:HD12	2.00	0.43
1:A:33:ARG:CG	1:A:34:SER:N	2.72	0.43
1:B:156:LEU:HA	1:B:156:LEU:HD13	1.65	0.43
1:A:314:GLY:O	1:A:325:ARG:HD3	2.19	0.43
1:B:178:MET:HE2	1:B:178:MET:HB3	1.91	0.43
1:B:397:ILE:O	1:B:401:SER:HB3	2.18	0.43
1:A:281:ILE:HD12	1:A:281:ILE:C	2.37	0.43
1:A:456:ARG:HE	1:A:456:ARG:HB3	1.66	0.43
1:B:1:MET:O	1:B:2:SER:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HG22	1:B:228:ARG:NH2	2.34	0.43
1:B:272:ALA:HB2	1:B:352:LEU:CD1	2.49	0.43
1:B:462:LEU:O	1:B:530:THR:HA	2.18	0.43
1:A:33:ARG:C	1:A:35:THR:H	2.21	0.43
1:A:235:LYS:O	1:A:238:ALA:HB3	2.19	0.43
1:A:69:SER:HB2	1:A:71:GLN:HG3	2.00	0.42
1:B:8:ARG:CD	1:B:36:LEU:CD2	2.96	0.42
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.43	0.42
1:A:361:ILE:C	1:A:363:ARG:N	2.72	0.42
1:B:222:GLY:HA3	1:B:246:TRP:CD2	2.54	0.42
1:A:361:ILE:CG1	1:A:362:ALA:N	2.76	0.42
1:B:377:CYS:HA	1:B:380:LEU:HG	2.02	0.42
1:B:507:LYS:NZ	1:B:524:ALA:HA	2.34	0.42
1:B:272:ALA:CB	1:B:349:ILE:HD13	2.49	0.42
1:A:33:ARG:NH1	1:A:107:ARG:HA	2.35	0.42
1:A:450:ASN:C	1:A:450:ASN:OD1	2.58	0.42
1:B:302:GLU:N	1:B:303:PRO:CD	2.82	0.42
1:A:63:LEU:O	1:A:67:LYS:HB2	2.20	0.42
1:A:317:ASP:OD1	1:A:317:ASP:C	2.58	0.42
1:B:385:GLN:HG3	1:B:436:THR:HG23	2.00	0.42
1:B:552:GLN:O	1:B:556:LEU:HD13	2.19	0.42
1:A:33:ARG:C	1:A:35:THR:N	2.73	0.42
1:A:252:VAL:CG2	1:A:398:ASP:HB2	2.46	0.42
1:A:317:ASP:OD2	1:A:321:HIS:ND1	2.45	0.42
1:A:372:LEU:CD2	1:A:535:MET:CE	2.88	0.42
1:A:107:ARG:HH11	1:A:107:ARG:HD3	1.62	0.42
1:A:182:GLY:O	1:A:185:TRP:HB3	2.20	0.42
1:B:136:LEU:HD22	1:B:148:LEU:CD1	2.50	0.42
1:A:83:VAL:O	1:A:84:ALA:C	2.58	0.41
1:A:109:PRO:O	1:A:110:GLU:C	2.53	0.41
1:B:250:GLY:O	1:B:258:GLN:HG2	2.20	0.41
1:B:443:LEU:HD23	1:B:443:LEU:HA	1.63	0.41
1:A:34:SER:OG	1:A:78:THR:CB	2.68	0.41
1:A:68:VAL:HG11	1:A:432:SER:HB3	2.02	0.41
1:A:449:LEU:HD12	1:A:449:LEU:HA	1.79	0.41
1:A:8:ARG:NH1	1:A:43:GLU:OE2	2.53	0.41
1:A:56:ARG:HD3	1:B:85:ASN:OD1	2.20	0.41
1:A:218:ARG:O	1:A:218:ARG:HG3	2.21	0.41
1:A:369:GLU:HG2	1:A:396:LEU:CD1	2.50	0.41
1:A:407:TYR:CD1	1:A:407:TYR:C	2.94	0.41
1:B:391:SER:O	1:B:392:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HG13	1:A:316:LEU:HD11	2.02	0.41
1:A:370:ALA:HA	1:A:396:LEU:HD13	2.03	0.41
1:B:91:ILE:O	1:B:92:GLU:C	2.59	0.41
1:A:61:LEU:HA	1:A:61:LEU:HD12	1.88	0.41
1:A:129:HIS:H	1:A:130:PRO:HD3	1.86	0.41
1:B:409:VAL:CG1	1:B:410:TYR:H	2.32	0.41
1:A:233:GLU:O	1:A:237:VAL:HG23	2.21	0.41
1:A:493:GLN:HB3	1:B:456:ARG:CZ	2.52	0.40
1:B:10:TRP:O	1:B:14:ILE:HG13	2.20	0.40
1:B:14:ILE:HG23	1:B:152:ILE:HD11	2.03	0.40
1:B:65:LEU:HA	1:B:431:ALA:HB2	2.02	0.40
1:B:29:ALA:HB2	1:B:58:LEU:HD22	2.03	0.40
1:B:68:VAL:HG22	1:B:410:TYR:CZ	2.56	0.40
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.86	0.40
1:A:34:SER:C	1:A:36:LEU:N	2.74	0.40
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.89	0.40
1:B:527:THR:HB	1:B:528:PRO:HD2	2.02	0.40
1:B:9:ARG:HH11	1:B:9:ARG:HD3	1.76	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	529/556 (95%)	489 (92%)	37 (7%)	3 (1%)	25	50
1	B	525/556 (94%)	487 (93%)	35 (7%)	3 (1%)	25	50
All	All	1054/1112 (95%)	976 (93%)	72 (7%)	6 (1%)	25	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	PRO
1	A	492	PRO
1	A	30	PRO
1	B	64	GLY
1	A	302	GLU
1	B	30	PRO

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	433/452 (96%)	378 (87%)	55 (13%)	4 10
1	B	430/452 (95%)	372 (86%)	58 (14%)	4 9
All	All	863/904 (96%)	750 (87%)	113 (13%)	4 10

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	26	ILE
1	A	28	ILE
1	A	32	SER
1	A	33	ARG
1	A	51	THR
1	A	71	GLN
1	A	78	THR
1	A	87	TYR
1	A	103	LEU
1	A	110	GLU
1	A	149	VAL
1	A	174	LEU
1	A	184	SER
1	A	208	SER
1	A	235	LYS
1	A	252	VAL
1	A	255	GLN

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Mol	Chain	Res	Type
1	A	274	SER
1	A	281	ILE
1	A	285	LEU
1	A	289	LEU
1	A	292	LYS
1	A	293	ARG
1	A	298	GLN
1	A	302	GLU
1	A	312	ILE
1	A	340	GLU
1	A	342	ARG
1	A	343	GLN
1	A	346	CYS
1	A	357	MET
1	A	363	ARG
1	A	369	GLU
1	A	375	ARG
1	A	377	CYS
1	A	392	LEU
1	A	395	ARG
1	A	401	SER
1	A	422	LEU
1	A	430	ARG
1	A	439	ILE
1	A	440	VAL
1	A	447	TYR
1	A	458	VAL
1	A	470	ASN
1	A	489	TYR
1	A	490	LEU
1	A	493	GLN
1	A	498	GLU
1	A	512	GLN
1	A	535	MET
1	A	539	ASP
1	A	544	GLN
1	A	556	LEU
1	B	19	THR
1	B	24	ARG
1	B	32	SER
1	B	33	ARG
1	B	87	TYR

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Mol	Chain	Res	Type
1	B	121	ARG
1	B	140	THR
1	B	146	ARG
1	B	166	ILE
1	B	172	GLU
1	B	174	LEU
1	B	177	GLU
1	B	178	MET
1	B	180	ASP
1	B	188	ARG
1	B	210	LYS
1	B	239	LEU
1	B	248	LEU
1	B	249	ILE
1	B	252	VAL
1	B	253	LEU
1	B	255	GLN
1	B	273	THR
1	B	274	SER
1	B	281	ILE
1	B	289	LEU
1	B	293	ARG
1	B	304	GLU
1	B	312	ILE
1	B	322	ARG
1	B	325	ARG
1	B	342	ARG
1	B	343	GLN
1	B	346	CYS
1	B	347	VAL
1	B	351	ARG
1	B	357	MET
1	B	363	ARG
1	B	375	ARG
1	B	377	CYS
1	B	382	GLU
1	B	393	VAL
1	B	411	SER
1	B	439	ILE
1	B	440	VAL
1	B	443	LEU
1	B	447	TYR

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Mol	Chain	Res	Type
1	B	470	ASN
1	B	494	ASN
1	B	495	VAL
1	B	512	GLN
1	B	535	MET
1	B	539	ASP
1	B	540	THR
1	B	544	GLN
1	B	547	GLN
1	B	550	LEU
1	B	556	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	343	GLN
1	A	402	GLN
1	B	71	GLN
1	B	117	ASN
1	B	141	GLN
1	B	277	GLN
1	B	355	GLN
1	B	457	GLN
1	B	538	ASN

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	535/556 (96%)	-0.51	6 (1%) 80 82	13, 25, 49, 80	10 (1%)
1	B	531/556 (95%)	-0.42	4 (0%) 86 87	13, 28, 52, 87	11 (2%)
All	All	1066/1112 (95%)	-0.47	10 (0%) 84 85	13, 26, 50, 87	21 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	SER	4.1
1	B	177	GLU	3.4
1	B	33	ARG	3.1
1	A	33	ARG	3.0
1	A	178	MET	2.4
1	A	490	LEU	2.4
1	A	179	ASP	2.4
1	B	3	VAL	2.4
1	B	174	LEU	2.2
1	A	554	SER	2.2

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.