Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 12:54 PM EDT

PDB ID	:	1LL6
Title	:	STRUCTURE OF THE D169N MUTANT OF C. IMMITIS CHITINASE 1
Authors	:	Bortone, K.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on	:	2002-04-26
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

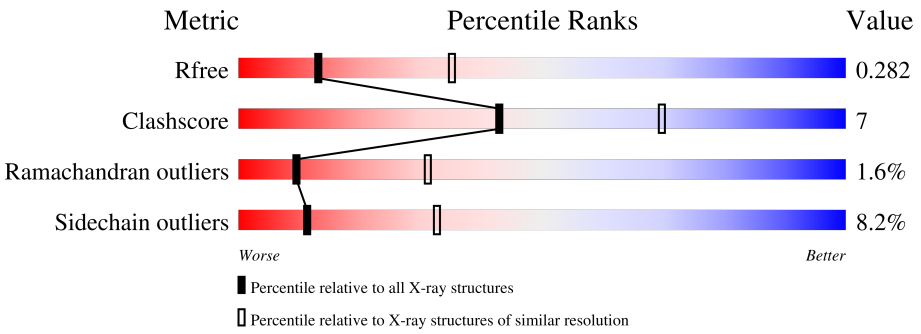
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Mol	Chain	Length	Quality of chain
1	A	392	72% 24% •
1	B	392	72% 23% •
1	C	392	71% 25% 5%
1	D	392	71% 23% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12375 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 CHITINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3083	1963	511	597	12	0	0	0
1	B	392	3083	1963	511	597	12	0	0	0
1	C	392	3083	1963	511	597	12	0	0	0
1	D	392	3083	1963	511	597	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ASN	ASP	engineered mutation	UNP P54196
B	169	ASN	ASP	engineered mutation	UNP P54196
C	169	ASN	ASP	engineered mutation	UNP P54196
D	169	ASN	ASP	engineered mutation	UNP P54196

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	12	12	12	0	0
2	B	12	12	12	0	0
2	C	7	7	7	0	0
2	D	12	12	12	0	0

3 Residue-property plots (i)

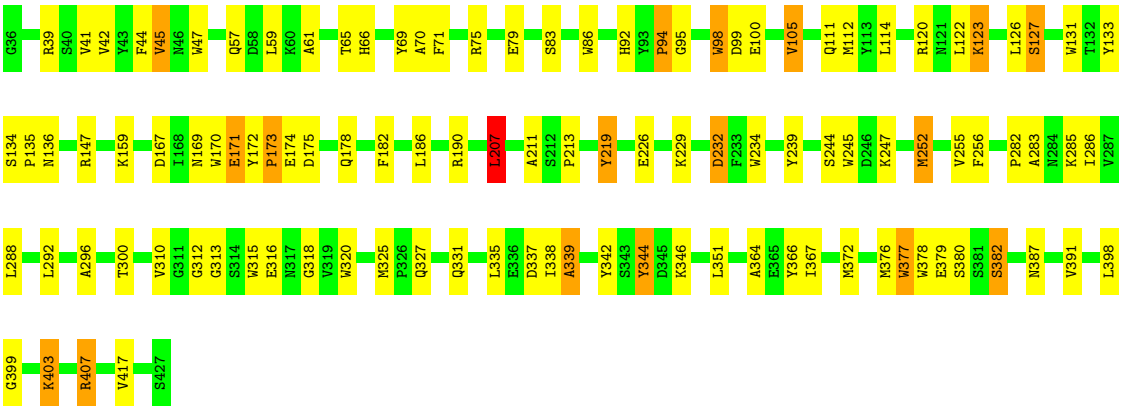
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: CHITINASE 1

Chain A:

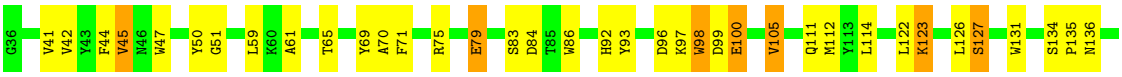
• Molecule 1: CHITINASE 1

Chain B:



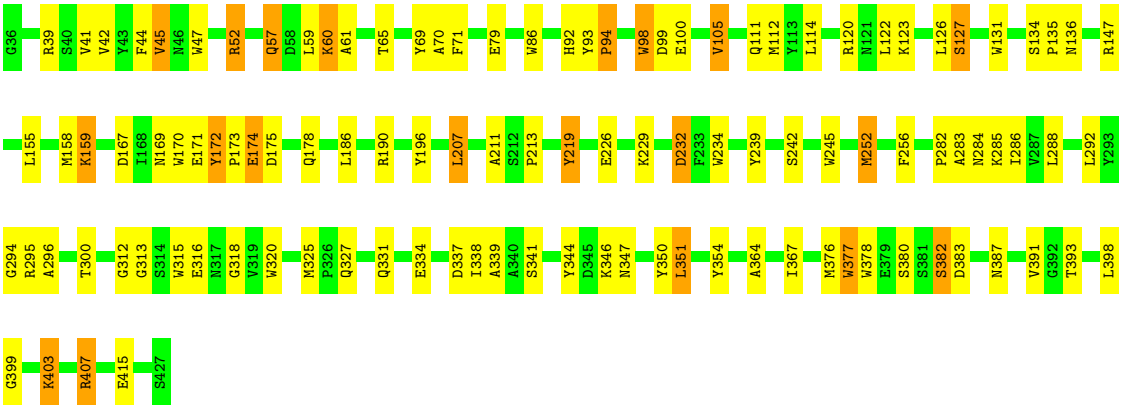
• Molecule 1: CHITINASE 1

Chain C:



- Molecule 1: CHITINASE 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.89Å 78.18Å 88.43Å 80.51° 82.13° 66.99°	Depositor
Resolution (Å)	5.00 – 2.80 19.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.80) 89.5 (19.97-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.79Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.182 , 0.256 0.237 , 0.282	Depositor DCC
R_{free} test set	1609 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 55.4	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	0.85	EDS
Total number of atoms	12375	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.83	0/3165	1.53	52/4282 (1.2%)
1	B	0.84	0/3165	1.56	58/4282 (1.4%)
1	C	0.84	0/3165	1.56	61/4282 (1.4%)
1	D	0.85	1/3165 (0.0%)	1.53	54/4282 (1.3%)
All	All	0.84	1/12660 (0.0%)	1.55	225/17128 (1.3%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	378	TRP	CD1-NE1	-5.03	1.29	1.38

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	B	407	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	A	407	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	C	407	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	252	MET	CG-SD-CE	-10.54	83.34	100.20
1	B	377	TRP	CD1-CG-CD2	10.22	114.48	106.30
1	A	377	TRP	CD1-CG-CD2	9.97	114.28	106.30
1	D	320	TRP	CD1-CG-CD2	9.92	114.23	106.30
1	C	377	TRP	CD1-CG-CD2	9.58	113.96	106.30
1	B	47	TRP	CD1-CG-CD2	9.43	113.84	106.30
1	B	320	TRP	CD1-CG-CD2	9.37	113.80	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	234	TRP	CD1-CG-CD2	9.32	113.76	106.30
1	B	377	TRP	CE2-CD2-CG	-9.27	99.88	107.30
1	C	75	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	A	315	TRP	CD1-CG-CD2	9.10	113.58	106.30
1	B	315	TRP	CD1-CG-CD2	9.03	113.52	106.30
1	A	315	TRP	CE2-CD2-CG	-9.01	100.09	107.30
1	A	245	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	D	47	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	B	245	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	A	320	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	A	47	TRP	CD1-CG-CD2	8.78	113.33	106.30
1	B	47	TRP	CE2-CD2-CG	-8.78	100.28	107.30
1	D	377	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	A	377	TRP	CE2-CD2-CG	-8.62	100.41	107.30
1	C	377	TRP	CE2-CD2-CG	-8.61	100.41	107.30
1	C	315	TRP	CD1-CG-CD2	8.59	113.17	106.30
1	C	190	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C	245	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	D	98	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	C	252	MET	CG-SD-CE	-8.46	86.66	100.20
1	D	407	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	D	315	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	C	320	TRP	CD1-CG-CD2	8.38	113.00	106.30
1	C	234	TRP	CD1-CG-CD2	8.33	112.97	106.30
1	C	407	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	D	407	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	B	245	TRP	CE2-CD2-CG	-8.29	100.66	107.30
1	B	315	TRP	CE2-CD2-CG	-8.26	100.69	107.30
1	D	252	MET	CG-SD-CE	-8.24	87.01	100.20
1	A	245	TRP	CE2-CD2-CG	-8.23	100.72	107.30
1	B	407	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	C	47	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	D	377	TRP	CE2-CD2-CG	-8.17	100.77	107.30
1	B	98	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	D	320	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	C	131	TRP	CD1-CG-CD2	8.11	112.78	106.30
1	C	147	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	378	TRP	CE2-CD2-CG	-8.05	100.86	107.30
1	C	131	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	D	315	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	C	245	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	86	TRP	CE2-CD2-CG	-7.86	101.02	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	234	TRP	CD1-CG-CD2	7.84	112.58	106.30
1	B	320	TRP	CE2-CD2-CG	-7.83	101.03	107.30
1	D	219	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	A	47	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	C	234	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	D	245	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	320	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	131	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	B	86	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	D	86	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	C	47	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	D	47	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	C	86	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	B	131	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	A	234	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	D	245	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	C	190	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	D	98	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	A	98	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	D	131	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	219	TYR	CB-CG-CD1	-7.54	116.48	121.00
1	B	98	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	C	315	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	A	170	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	C	86	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	B	190	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	D	234	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	378	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	D	86	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	D	378	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	252	MET	CG-SD-CE	-7.30	88.52	100.20
1	A	190	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	D	147	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	131	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	C	98	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	86	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	C	147	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	170	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	B	86	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	C	98	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	98	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	B	170	TRP	CE2-CD2-CG	-7.05	101.66	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	219	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	C	320	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	D	131	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	131	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	75	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	234	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	407	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	C	344	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	A	147	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	378	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	A	234	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	B	378	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	D	170	TRP	CE2-CD2-CG	-6.79	101.86	107.30
1	C	378	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	B	245	TRP	CG-CD2-CE3	6.76	139.98	133.90
1	C	170	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	C	245	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	B	245	TRP	CB-CG-CD1	-6.65	118.35	127.00
1	A	190	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	245	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	A	378	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	C	378	TRP	CD1-CG-CD2	6.52	111.51	106.30
1	B	147	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	170	TRP	CD1-CG-CD2	6.47	111.47	106.30
1	A	105	VAL	CB-CA-C	-6.37	99.31	111.40
1	D	170	TRP	CD1-CG-CD2	6.27	111.31	106.30
1	D	170	TRP	CG-CD2-CE3	6.24	139.51	133.90
1	A	172	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	245	TRP	CB-CG-CD1	-6.20	118.94	127.00
1	D	320	TRP	CG-CD1-NE1	-6.15	103.95	110.10
1	C	170	TRP	CG-CD2-CE3	6.15	139.43	133.90
1	B	170	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	A	171	GLU	CA-CB-CG	6.11	126.85	113.40
1	D	105	VAL	CB-CA-C	-6.11	99.78	111.40
1	C	105	VAL	CB-CA-C	-6.10	99.81	111.40
1	A	377	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	B	171	GLU	CA-CB-CG	6.06	126.74	113.40
1	B	342	TYR	CB-CG-CD1	-6.01	117.40	121.00
1	D	383	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	234	TRP	CG-CD1-NE1	-5.99	104.11	110.10
1	A	170	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	D	171	GLU	CA-CB-CG	5.87	126.31	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	245	TRP	CB-CG-CD1	-5.86	119.38	127.00
1	C	320	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	C	315	TRP	CG-CD2-CE3	5.85	139.16	133.90
1	D	120	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	47	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	C	171	GLU	CA-CB-CG	5.81	126.18	113.40
1	A	170	TRP	CD1-CG-CD2	5.80	110.94	106.30
1	C	45	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	D	288	LEU	CA-CB-CG	5.74	128.49	115.30
1	D	245	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	A	295	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	320	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	B	377	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	A	120	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	315	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	C	288	LEU	CA-CB-CG	5.63	128.24	115.30
1	D	45	VAL	CA-CB-CG2	-5.62	102.47	110.90
1	D	378	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	D	158	MET	CG-SD-CE	-5.61	91.22	100.20
1	C	377	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	B	378	TRP	CG-CD2-CE3	5.58	138.92	133.90
1	A	419	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	47	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	B	47	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	D	207	LEU	CA-CB-CG	5.54	128.05	115.30
1	B	245	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	C	324	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	315	TRP	CB-CG-CD1	-5.50	119.84	127.00
1	C	84	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	377	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	C	246	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	315	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	A	315	TRP	CG-CD2-CE3	5.45	138.80	133.90
1	C	377	TRP	CG-CD2-CE3	5.44	138.79	133.90
1	A	207	LEU	CA-CB-CG	5.42	127.78	115.30
1	B	47	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	C	315	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	B	105	VAL	CB-CA-C	-5.40	101.15	111.40
1	D	315	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	B	45	VAL	CA-CB-CG2	-5.38	102.84	110.90
1	A	377	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	A	344	TYR	CB-CG-CD2	-5.36	117.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	44	PHE	N-CA-C	-5.36	96.53	111.00
1	B	75	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	86	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	C	207	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	247	LYS	CA-CB-CG	-5.35	101.64	113.40
1	C	245	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	A	245	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	B	288	LEU	CA-CB-CG	5.30	127.49	115.30
1	D	351	LEU	CA-CB-CG	5.30	127.49	115.30
1	C	377	TRP	CB-CG-CD1	-5.30	120.11	127.00
1	B	219	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	D	315	TRP	CB-CG-CD1	-5.28	120.14	127.00
1	C	248	VAL	CA-CB-CG2	-5.28	102.99	110.90
1	A	147	ARG	CB-CG-CD	-5.27	97.91	111.60
1	C	86	TRP	CG-CD2-CE3	5.26	138.63	133.90
1	B	39	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	378	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	C	131	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	D	44	PHE	N-CA-C	-5.21	96.93	111.00
1	B	207	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	120	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	47	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	D	52	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	315	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	C	93	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	D	147	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	417	VAL	CG1-CB-CG2	5.12	119.10	110.90
1	C	98	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	A	234	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	D	377	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	B	234	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	C	172	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	C	96	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	190	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	172	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	288	LEU	CA-CB-CG	5.05	126.91	115.30
1	D	377	TRP	CG-CD2-CE3	5.05	138.44	133.90
1	A	98	TRP	CG-CD2-CE3	5.04	138.43	133.90
1	A	315	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	B	344	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	44	PHE	N-CA-C	-5.02	97.44	111.00
1	A	182	PHE	CB-CG-CD2	-5.00	117.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	ASP	CB-CG-OD1	5.00	122.80	118.30
1	B	44	PHE	N-CA-C	-5.00	97.49	111.00
1	C	320	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	D	47	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	350	TYR	Sidechain

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	3083	0	2963	44	0
1	B	3083	0	2963	45	0
1	C	3083	0	2963	46	0
1	D	3083	0	2963	42	0
2	A	12	0	0	1	0
2	B	12	0	0	0	0
2	C	7	0	0	1	0
2	D	12	0	0	0	0
All	All	12375	0	11852	165	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 7.

All (165) 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:95:GLY:H	1:C:51:GLY:HA2	1.33	0.92
1:A:347:ASN:HA	1:D:94:PRO:HG2	1.63	0.80
1:D:282:PRO:HG2	1:D:285:LYS:HD3	1.75	0.68
1:D:169:ASN:ND2	1:D:211:ALA:HB3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PRO:HG2	1:A:285:LYS:HD3	1.75	0.66
1:A:169:ASN:ND2	1:A:211:ALA:HB3	2.10	0.66
1:A:328:GLN:HE21	1:D:60:LYS:N	1.94	0.65
1:C:282:PRO:HG2	1:C:285:LYS:HD3	1.78	0.64
1:B:282:PRO:HG2	1:B:285:LYS:HD3	1.80	0.63
1:C:169:ASN:ND2	1:C:211:ALA:HB3	2.14	0.62
1:B:95:GLY:HA2	1:C:51:GLY:O	1.99	0.62
1:A:75:ARG:NH2	1:B:244:SER:O	2.34	0.61
1:B:95:GLY:N	1:C:51:GLY:HA2	2.11	0.61
1:D:226:GLU:HA	1:D:229:LYS:HZ2	1.67	0.60
1:D:42:VAL:HG23	1:D:377:TRP:HB2	1.84	0.59
1:A:172:TYR:CE2	1:A:213:PRO:HB3	2.39	0.58
1:B:169:ASN:ND2	1:B:211:ALA:HB3	2.18	0.58
1:B:42:VAL:HG23	1:B:377:TRP:HB2	1.86	0.57
1:C:172:TYR:CE2	1:C:213:PRO:HB3	2.40	0.57
1:D:69:TYR:CD1	1:D:112:MET:SD	2.98	0.56
1:D:283:ALA:HA	1:D:286:ILE:HD12	1.87	0.56
1:A:42:VAL:HG23	1:A:377:TRP:HB2	1.87	0.56
1:A:92:HIS:NE2	1:A:98:TRP:HA	2.20	0.56
1:D:172:TYR:CE2	1:D:213:PRO:HB3	2.42	0.55
1:C:256:PHE:HB2	1:C:338:ILE:HA	1.88	0.55
1:C:313:GLY:HA3	1:C:316:GLU:O	2.07	0.55
1:B:292:LEU:O	1:B:382:SER:HB2	2.07	0.55
1:A:111:GLN:HA	1:A:114:LEU:HD12	1.88	0.54
1:A:313:GLY:HA3	1:A:316:GLU:O	2.08	0.54
1:B:226:GLU:HA	1:B:229:LYS:HZ2	1.73	0.54
1:A:347:ASN:OD1	1:D:93:TYR:HD2	1.90	0.54
1:D:292:LEU:O	1:D:382:SER:HB2	2.08	0.54
1:B:172:TYR:CE2	1:B:213:PRO:HB3	2.43	0.54
1:A:256:PHE:HB2	1:A:338:ILE:HA	1.89	0.53
1:B:95:GLY:CA	1:C:51:GLY:O	2.56	0.53
1:D:70:ALA:HB1	1:D:71:PHE:CD2	2.43	0.53
1:C:42:VAL:HG23	1:C:377:TRP:HB2	1.89	0.53
1:A:174:GLU:HG2	1:A:178:GLN:NE2	2.23	0.53
1:A:328:GLN:HE21	1:D:60:LYS:H	1.56	0.52
1:B:283:ALA:HA	1:B:286:ILE:HD12	1.92	0.52
1:C:283:ALA:HA	1:C:286:ILE:HD12	1.90	0.52
1:B:256:PHE:HB2	1:B:338:ILE:HA	1.89	0.52
1:C:92:HIS:NE2	1:C:98:TRP:HA	2.25	0.52
1:A:69:TYR:CD1	1:A:112:MET:SD	3.03	0.52
1:C:292:LEU:O	1:C:382:SER:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:O	1:A:382:SER:HB2	2.10	0.52
1:B:313:GLY:HA3	1:B:316:GLU:O	2.10	0.52
1:A:283:ALA:HA	1:A:286:ILE:HD12	1.91	0.51
1:C:111:GLN:HA	1:C:114:LEU:HD12	1.91	0.51
1:D:92:HIS:NE2	1:D:98:TRP:HA	2.25	0.51
1:A:83:SER:HG	1:A:133:TYR:HE1	1.58	0.51
1:B:174:GLU:HG2	1:B:178:GLN:NE2	2.26	0.51
1:D:111:GLN:HA	1:D:114:LEU:HD12	1.92	0.51
1:B:377:TRP:CE2	1:B:391:VAL:HG22	2.46	0.51
1:B:70:ALA:HB1	1:B:71:PHE:CD2	2.46	0.51
1:D:213:PRO:O	1:D:219:TYR:HD1	1.94	0.51
1:D:256:PHE:HB2	1:D:338:ILE:HA	1.92	0.51
1:D:313:GLY:HA3	1:D:316:GLU:O	2.11	0.51
1:D:296:ALA:HA	1:D:351:LEU:O	2.11	0.50
1:A:65:THR:O	1:A:123:LYS:HE3	2.11	0.50
1:A:377:TRP:CE2	1:A:391:VAL:HG22	2.45	0.50
1:C:377:TRP:CE2	1:C:391:VAL:HG22	2.46	0.50
1:A:213:PRO:O	1:A:219:TYR:HD1	1.95	0.50
1:C:226:GLU:HA	1:C:229:LYS:HZ2	1.76	0.50
1:B:65:THR:O	1:B:123:LYS:HE3	2.12	0.49
1:C:213:PRO:O	1:C:219:TYR:HD1	1.95	0.49
1:D:377:TRP:CE2	1:D:391:VAL:HG22	2.47	0.49
1:B:174:GLU:HG2	1:B:178:GLN:CD	2.32	0.49
1:C:174:GLU:HG2	1:C:178:GLN:NE2	2.27	0.49
1:B:213:PRO:O	1:B:219:TYR:HD1	1.96	0.49
1:A:344:TYR:HE2	1:A:346:LYS:HD2	1.78	0.49
1:D:174:GLU:HG2	1:D:178:GLN:NE2	2.28	0.49
1:C:70:ALA:HB1	1:C:71:PHE:CD2	2.47	0.48
1:A:296:ALA:HA	1:A:351:LEU:O	2.13	0.48
1:B:69:TYR:CD1	1:B:112:MET:SD	3.06	0.48
1:A:134:SER:N	1:A:135:PRO:HD2	2.28	0.48
1:A:41:VAL:O	1:A:376:MET:HA	2.13	0.48
1:B:92:HIS:NE2	1:B:98:TRP:HA	2.27	0.48
1:B:296:ALA:HA	1:B:351:LEU:O	2.13	0.48
1:C:296:ALA:HA	1:C:351:LEU:O	2.13	0.47
1:D:41:VAL:O	1:D:376:MET:HA	2.14	0.47
1:B:95:GLY:H	1:C:51:GLY:CA	2.15	0.47
1:C:312:GLY:O	1:C:318:GLY:N	2.47	0.47
1:D:174:GLU:HG2	1:D:178:GLN:CD	2.34	0.47
1:C:344:TYR:HE2	1:C:346:LYS:HD2	1.80	0.47
1:B:41:VAL:O	1:B:376:MET:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:HD3	1:C:100:GLU:HG3	1.97	0.47
1:A:328:GLN:NE2	2:A:434:HOH:O	2.47	0.47
1:C:399:GLY:O	1:C:403:LYS:HD3	2.14	0.47
1:A:70:ALA:HB1	1:A:71:PHE:CD2	2.48	0.47
1:A:174:GLU:HG2	1:A:178:GLN:CD	2.35	0.47
1:A:207:LEU:HD12	1:A:232:ASP:OD2	2.14	0.47
1:A:399:GLY:O	1:A:403:LYS:HD3	2.15	0.47
1:B:134:SER:N	1:B:135:PRO:HD2	2.30	0.47
1:B:344:TYR:HE2	1:B:346:LYS:HD2	1.79	0.47
1:C:70:ALA:HA	1:C:71:PHE:HA	1.66	0.46
1:C:127:SER:HA	1:C:167:ASP:O	2.15	0.46
1:C:341:SER:OG	1:C:359:ILE:HG13	2.15	0.46
1:A:226:GLU:HA	1:A:229:LYS:HZ2	1.80	0.46
1:B:61:ALA:HB1	1:B:122:LEU:HD22	1.97	0.46
1:A:312:GLY:O	1:A:318:GLY:N	2.49	0.46
1:C:41:VAL:O	1:C:376:MET:HA	2.16	0.45
1:B:364:ALA:O	1:B:367:ILE:HB	2.16	0.45
1:B:111:GLN:HA	1:B:114:LEU:HD12	1.96	0.45
1:D:325:MET:HE2	1:D:327:GLN:HG3	1.99	0.45
1:B:399:GLY:O	1:B:403:LYS:HD3	2.16	0.45
1:A:364:ALA:O	1:A:367:ILE:HB	2.16	0.45
1:C:174:GLU:HG2	1:C:178:GLN:CD	2.37	0.45
1:A:127:SER:HA	1:A:167:ASP:O	2.17	0.45
1:B:83:SER:HG	1:B:133:TYR:HE1	1.62	0.45
1:A:97:LYS:HD3	1:A:100:GLU:HG3	2.00	0.44
1:B:244:SER:HB3	1:B:310:VAL:HG11	1.99	0.44
1:B:312:GLY:O	1:B:318:GLY:N	2.49	0.44
1:B:325:MET:HE2	1:B:327:GLN:HG3	1.99	0.44
1:C:364:ALA:O	1:C:367:ILE:HB	2.16	0.44
1:C:65:THR:O	1:C:123:LYS:HE3	2.18	0.44
1:D:39:ARG:NH2	1:D:284:ASN:O	2.50	0.44
1:D:312:GLY:O	1:D:318:GLY:N	2.50	0.44
1:A:70:ALA:HA	1:A:71:PHE:HA	1.67	0.44
1:C:69:TYR:CD1	1:C:112:MET:SD	3.11	0.44
1:D:61:ALA:HB1	1:D:122:LEU:HD22	2.00	0.44
1:C:187:LYS:O	1:C:191:GLU:HG3	2.17	0.43
1:D:242:SER:O	1:D:295:ARG:HD2	2.19	0.43
1:B:127:SER:HA	1:B:167:ASP:O	2.18	0.43
1:A:61:ALA:HB1	1:A:122:LEU:HD22	2.00	0.43
1:D:127:SER:HA	1:D:167:ASP:O	2.19	0.43
1:A:92:HIS:CD2	1:A:98:TRP:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLU:HG2	1:B:178:GLN:OE1	2.19	0.42
1:C:159:LYS:HD3	1:C:415:GLU:HB2	2.00	0.42
1:D:159:LYS:HD3	1:D:415:GLU:HB2	2.00	0.42
1:D:65:THR:O	1:D:123:LYS:HE3	2.19	0.42
1:C:61:ALA:HB1	1:C:122:LEU:HD22	2.01	0.42
1:A:334:GLU:HA	1:A:341:SER:HB3	2.01	0.42
1:A:341:SER:OG	1:A:359:ILE:HG13	2.19	0.42
1:B:41:VAL:HG22	1:B:66:HIS:HB2	2.02	0.42
1:C:226:GLU:HA	1:C:229:LYS:NZ	2.34	0.42
1:C:92:HIS:CD2	1:C:98:TRP:HA	2.54	0.42
1:A:244:SER:HB3	1:A:310:VAL:HG11	2.02	0.42
1:D:344:TYR:HE2	1:D:346:LYS:HD2	1.84	0.42
1:B:255:VAL:CG2	1:B:339:ALA:HB3	2.50	0.42
1:B:366:TYR:CE2	1:B:372:MET:SD	3.13	0.42
1:D:92:HIS:CD2	1:D:98:TRP:HA	2.55	0.42
1:B:92:HIS:CD2	1:B:98:TRP:HA	2.55	0.42
1:D:399:GLY:O	1:D:403:LYS:HD3	2.19	0.42
1:C:153:THR:O	1:C:157:LEU:HB2	2.20	0.41
1:D:39:ARG:HH11	1:D:39:ARG:HD3	1.65	0.41
1:A:347:ASN:OD1	1:D:57:GLN:NE2	2.53	0.41
1:C:294:GLY:HA3	1:C:354:TYR:HB3	2.02	0.41
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.85	0.41
1:C:180:ASN:HB3	2:C:434:HOH:O	2.20	0.41
1:B:94:PRO:HB3	1:C:50:TYR:C	2.40	0.41
1:B:207:LEU:HD12	1:B:232:ASP:OD2	2.21	0.41
1:D:134:SER:N	1:D:135:PRO:HD2	2.36	0.41
1:D:364:ALA:O	1:D:367:ILE:HB	2.20	0.41
1:A:294:GLY:HA3	1:A:354:TYR:HB3	2.03	0.41
1:B:171:GLU:HA	1:B:172:TYR:CD2	2.55	0.41
1:A:187:LYS:O	1:A:191:GLU:HG3	2.20	0.41
1:B:173:PRO:HG2	1:B:182:PHE:CD2	2.56	0.41
1:C:134:SER:N	1:C:135:PRO:HD2	2.36	0.41
1:C:307:PHE:HD1	1:C:309:GLY:O	2.04	0.41
1:D:155:LEU:HD21	1:D:196:TYR:HB2	2.03	0.41
1:C:334:GLU:HA	1:C:341:SER:HB3	2.02	0.40
1:D:294:GLY:HA3	1:D:354:TYR:HB3	2.03	0.40
1:D:334:GLU:HA	1:D:341:SER:HB3	2.04	0.40
1:C:79:GLU:HG2	1:C:153:THR:HG21	2.04	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	390/392 (100%)	367 (94%)	16 (4%)	7 (2%)	8 28
1	B	390/392 (100%)	369 (95%)	16 (4%)	5 (1%)	12 36
1	C	390/392 (100%)	368 (94%)	15 (4%)	7 (2%)	8 28
1	D	390/392 (100%)	367 (94%)	17 (4%)	6 (2%)	10 33
All	All	1560/1568 (100%)	1471 (94%)	64 (4%)	25 (2%)	9 31

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	B	99	ASP
1	C	99	ASP
1	D	99	ASP
1	A	83	SER
1	A	380	SER
1	C	380	SER
1	D	380	SER
1	A	100	GLU
1	A	173	PRO
1	A	174	GLU
1	A	339	ALA
1	B	100	GLU
1	B	380	SER
1	C	100	GLU
1	D	100	GLU
1	D	339	ALA
1	B	173	PRO
1	B	339	ALA
1	C	83	SER
1	C	173	PRO
1	C	174	GLU

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Mol	Chain	Res	Type
1	C	339	ALA
1	D	173	PRO
1	D	174	GLU

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	326/326 (100%)	299 (92%)	27 (8%)	11 32
1	B	326/326 (100%)	299 (92%)	27 (8%)	11 32
1	C	326/326 (100%)	300 (92%)	26 (8%)	12 34
1	D	326/326 (100%)	299 (92%)	27 (8%)	11 32
All	All	1304/1304 (100%)	1197 (92%)	107 (8%)	11 33

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	57	GLN
1	A	59	LEU
1	A	79	GLU
1	A	105	VAL
1	A	126	LEU
1	A	127	SER
1	A	136	ASN
1	A	159	LYS
1	A	175	ASP
1	A	186	LEU
1	A	207	LEU
1	A	232	ASP
1	A	239	TYR
1	A	252	MET
1	A	300	THR
1	A	331	GLN
1	A	335	LEU

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Mol	Chain	Res	Type
1	A	337	ASP
1	A	347	ASN
1	A	379	GLU
1	A	382	SER
1	A	387	ASN
1	A	398	LEU
1	A	403	LYS
1	A	407	ARG
1	A	417	VAL
1	B	45	VAL
1	B	57	GLN
1	B	59	LEU
1	B	79	GLU
1	B	94	PRO
1	B	105	VAL
1	B	123	LYS
1	B	126	LEU
1	B	127	SER
1	B	136	ASN
1	B	159	LYS
1	B	175	ASP
1	B	186	LEU
1	B	207	LEU
1	B	232	ASP
1	B	239	TYR
1	B	252	MET
1	B	300	THR
1	B	331	GLN
1	B	335	LEU
1	B	337	ASP
1	B	379	GLU
1	B	382	SER
1	B	387	ASN
1	B	398	LEU
1	B	403	LYS
1	B	407	ARG
1	C	45	VAL
1	C	59	LEU
1	C	79	GLU
1	C	105	VAL
1	C	123	LYS
1	C	126	LEU

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Mol	Chain	Res	Type
1	C	127	SER
1	C	136	ASN
1	C	139	THR
1	C	159	LYS
1	C	186	LEU
1	C	207	LEU
1	C	239	TYR
1	C	252	MET
1	C	300	THR
1	C	331	GLN
1	C	335	LEU
1	C	337	ASP
1	C	347	ASN
1	C	379	GLU
1	C	382	SER
1	C	387	ASN
1	C	393	THR
1	C	398	LEU
1	C	403	LYS
1	C	407	ARG
1	D	45	VAL
1	D	57	GLN
1	D	59	LEU
1	D	60	LYS
1	D	79	GLU
1	D	94	PRO
1	D	105	VAL
1	D	126	LEU
1	D	127	SER
1	D	136	ASN
1	D	159	LYS
1	D	175	ASP
1	D	186	LEU
1	D	207	LEU
1	D	232	ASP
1	D	239	TYR
1	D	252	MET
1	D	300	THR
1	D	331	GLN
1	D	337	ASP
1	D	347	ASN
1	D	382	SER

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Mol	Chain	Res	Type
1	D	387	ASN
1	D	393	THR
1	D	398	LEU
1	D	403	LYS
1	D	407	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	119	ASN
1	A	169	ASN
1	A	327	GLN
1	A	328	GLN
1	B	66	HIS
1	B	111	GLN
1	B	119	ASN
1	B	169	ASN
1	B	327	GLN
1	B	347	ASN
1	C	66	HIS
1	C	119	ASN
1	C	169	ASN
1	C	327	GLN
1	D	66	HIS
1	D	119	ASN
1	D	169	ASN
1	D	327	GLN
1	D	347	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 (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.