



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 01:27 PM EDT

PDB ID : 1YG8
Title : The structure of a V6A variant of ClpP.
Authors : Bewley, M.C.; Graziano, V.; Griffin, K.; Flanagan, J.M.
Deposited on : 2005-01-04
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

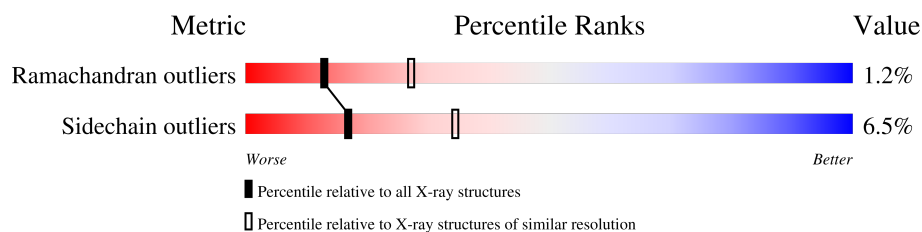
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)














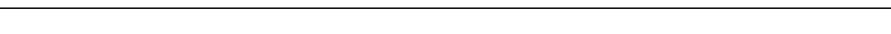





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	193	
1	B	193	
1	C	193	
1	D	193	
1	E	193	
1	F	193	
1	G	193	
1	H	193	
1	I	193	

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Mol	Chain	Length	Quality of chain
1	J	193	 82% 10% 7%
1	K	193	 86% 6% 7%
1	L	193	 88% • 7%
1	M	193	 87% 6% 7%
1	N	193	 88% 5% 7%
1	O	193	 81% 10% 7%
1	P	193	 87% 5% 7%
1	Q	193	 88% 5% 7%
1	R	193	 86% 6% 7%
1	S	193	 85% 7% 7%
1	T	193	 88% • 7%
1	U	193	 88% • 7%
1	V	193	 86% 7% 7%
1	W	193	 84% 8% 7%
1	X	193	 86% 6% 7%
1	Y	193	 87% 5% 7%
1	Z	193	 82% 10% 7%
1	a	193	 86% 7% 7%
1	b	193	 86% 6% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39312 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	B	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	C	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	D	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	E	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	F	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	G	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	H	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	I	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	J	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	K	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	L	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	M	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	N	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	O	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	P	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	R	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	S	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	T	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	U	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	V	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	W	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	X	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	Y	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	Z	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	a	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			
1	b	179	Total	C	N	O	S	0	0	0
			1404	885	244	264	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	VAL	engineered mutation	UNP P19245
B	3	ALA	VAL	engineered mutation	UNP P19245
C	3	ALA	VAL	engineered mutation	UNP P19245
D	3	ALA	VAL	engineered mutation	UNP P19245
E	3	ALA	VAL	engineered mutation	UNP P19245
F	3	ALA	VAL	engineered mutation	UNP P19245
G	3	ALA	VAL	engineered mutation	UNP P19245
H	3	ALA	VAL	engineered mutation	UNP P19245
I	3	ALA	VAL	engineered mutation	UNP P19245
J	3	ALA	VAL	engineered mutation	UNP P19245
K	3	ALA	VAL	engineered mutation	UNP P19245
L	3	ALA	VAL	engineered mutation	UNP P19245
M	3	ALA	VAL	engineered mutation	UNP P19245
N	3	ALA	VAL	engineered mutation	UNP P19245
O	3	ALA	VAL	engineered mutation	UNP P19245

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Chain	Residue	Modelled	Actual	Comment	Reference
P	3	ALA	VAL	engineered mutation	UNP P19245
Q	3	ALA	VAL	engineered mutation	UNP P19245
R	3	ALA	VAL	engineered mutation	UNP P19245
S	3	ALA	VAL	engineered mutation	UNP P19245
T	3	ALA	VAL	engineered mutation	UNP P19245
U	3	ALA	VAL	engineered mutation	UNP P19245
V	3	ALA	VAL	engineered mutation	UNP P19245
W	3	ALA	VAL	engineered mutation	UNP P19245
X	3	ALA	VAL	engineered mutation	UNP P19245
Y	3	ALA	VAL	engineered mutation	UNP P19245
Z	3	ALA	VAL	engineered mutation	UNP P19245
a	3	ALA	VAL	engineered mutation	UNP P19245
b	3	ALA	VAL	engineered mutation	UNP P19245

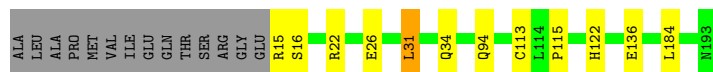
3 Residue-property plots [i](#)

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.


Note EDS was not executed.

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:  87% 6% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:  88% 5% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:  87% 5% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:  88% 5% 7%




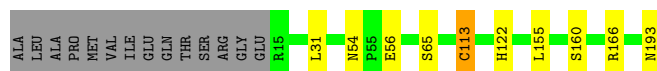
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:  88% 5% 7%




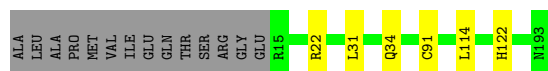
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:  88% 5% • 7%




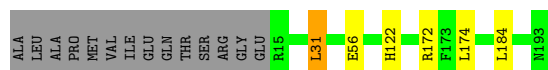
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:  90% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:  90% • • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:  87% 6% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:  82% 10% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:  86% 6% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:  88% • • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:  87% 6% 7%




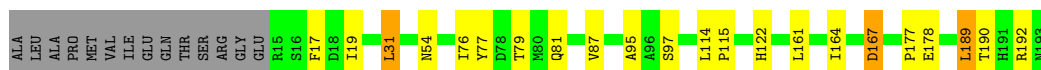
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:  88% 5% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:  81% 10% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:  87% 5% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:  88% 5% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R:  86% 6% 7%




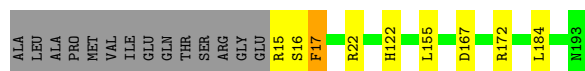
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S:  85% 7% 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:  88% • • 7%



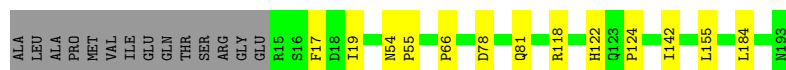
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U:  88% • • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:  86% 7% 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:  84% 8% • 7%




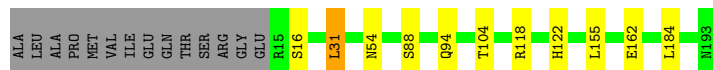
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:  86% 6% • 7%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:  87% 5% • 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:  82% 10% • 7%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:

86%

7%

7%



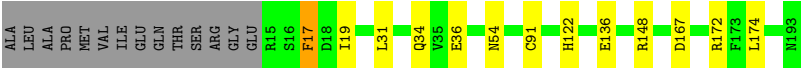
● Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:

86%

6%

7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.80Å 161.00Å 186.60Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	39312	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	0.59	0/1427	0.81	1/1921 (0.1%)
1	B	0.60	0/1427	0.81	1/1921 (0.1%)
1	C	0.59	0/1427	0.80	1/1921 (0.1%)
1	D	0.60	0/1427	0.77	0/1921
1	E	0.57	0/1427	0.82	0/1921
1	F	0.58	0/1427	0.79	0/1921
1	G	0.56	0/1427	0.80	0/1921
1	H	0.60	0/1427	0.78	1/1921 (0.1%)
1	I	0.59	0/1427	0.82	1/1921 (0.1%)
1	J	0.62	1/1427 (0.1%)	0.82	0/1921
1	K	0.62	0/1427	0.83	0/1921
1	L	0.58	0/1427	0.78	1/1921 (0.1%)
1	M	0.58	0/1427	0.80	0/1921
1	N	0.60	0/1427	0.81	0/1921
1	O	0.62	0/1427	0.79	1/1921 (0.1%)
1	P	0.62	0/1427	0.85	1/1921 (0.1%)
1	Q	0.59	0/1427	0.79	0/1921
1	R	0.57	0/1427	0.77	1/1921 (0.1%)
1	S	0.61	0/1427	0.82	0/1921
1	T	0.59	0/1427	0.82	1/1921 (0.1%)
1	U	0.61	0/1427	0.85	1/1921 (0.1%)
1	V	0.62	0/1427	0.85	2/1921 (0.1%)
1	W	0.59	0/1427	0.84	3/1921 (0.2%)
1	X	0.56	0/1427	0.81	1/1921 (0.1%)
1	Y	0.58	0/1427	0.83	1/1921 (0.1%)
1	Z	0.59	0/1427	0.78	0/1921
1	a	0.58	0/1427	0.79	0/1921
1	b	0.57	0/1427	0.81	1/1921 (0.1%)
All	All	0.59	1/39956 (0.0%)	0.81	19/53788 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	S	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	91	CYS	CB-SG	-5.19	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	78	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	U	31	LEU	CA-CB-CG	6.66	130.62	115.30
1	A	31	LEU	CA-CB-CG	6.23	129.62	115.30
1	X	31	LEU	CA-CB-CG	6.20	129.56	115.30
1	V	78	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	31	LEU	CA-CB-CG	5.86	128.77	115.30
1	Y	31	LEU	CA-CB-CG	5.75	128.53	115.30
1	L	31	LEU	CA-CB-CG	5.75	128.51	115.30
1	T	155	LEU	CA-CB-CG	5.69	128.38	115.30
1	W	114	LEU	CA-CB-CG	-5.31	103.09	115.30
1	R	31	LEU	CA-CB-CG	5.30	127.49	115.30
1	W	31	LEU	CA-CB-CG	5.29	127.47	115.30
1	W	93	GLY	N-CA-C	-5.25	99.97	113.10
1	O	31	LEU	N-CA-C	-5.23	96.88	111.00
1	P	31	LEU	N-CA-C	-5.19	96.98	111.00
1	H	31	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	17	PHE	N-CA-C	-5.11	97.21	111.00
1	I	37	ASP	N-CA-C	5.06	124.66	111.00
1	b	174	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	60	TYR	Sidechain
1	S	60	TYR	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	177/193 (92%)	167 (94%)	8 (4%)	2 (1%)	14	30
1	B	177/193 (92%)	166 (94%)	10 (6%)	1 (1%)	25	47
1	C	177/193 (92%)	162 (92%)	14 (8%)	1 (1%)	25	47
1	D	177/193 (92%)	165 (93%)	11 (6%)	1 (1%)	25	47
1	E	177/193 (92%)	165 (93%)	10 (6%)	2 (1%)	14	30
1	F	177/193 (92%)	163 (92%)	12 (7%)	2 (1%)	14	30
1	G	177/193 (92%)	161 (91%)	16 (9%)	0	100	100
1	H	177/193 (92%)	170 (96%)	7 (4%)	0	100	100
1	I	177/193 (92%)	162 (92%)	14 (8%)	1 (1%)	25	47
1	J	177/193 (92%)	162 (92%)	12 (7%)	3 (2%)	9	18
1	K	177/193 (92%)	156 (88%)	18 (10%)	3 (2%)	9	18
1	L	177/193 (92%)	160 (90%)	16 (9%)	1 (1%)	25	47
1	M	177/193 (92%)	167 (94%)	10 (6%)	0	100	100
1	N	177/193 (92%)	163 (92%)	14 (8%)	0	100	100
1	O	177/193 (92%)	144 (81%)	22 (12%)	11 (6%)	1	1
1	P	177/193 (92%)	154 (87%)	20 (11%)	3 (2%)	9	18
1	Q	177/193 (92%)	166 (94%)	10 (6%)	1 (1%)	25	47
1	R	177/193 (92%)	171 (97%)	6 (3%)	0	100	100
1	S	177/193 (92%)	158 (89%)	16 (9%)	3 (2%)	9	18
1	T	177/193 (92%)	162 (92%)	13 (7%)	2 (1%)	14	30
1	U	177/193 (92%)	157 (89%)	18 (10%)	2 (1%)	14	30
1	V	177/193 (92%)	154 (87%)	19 (11%)	4 (2%)	6	11
1	W	177/193 (92%)	157 (89%)	16 (9%)	4 (2%)	6	11
1	X	177/193 (92%)	162 (92%)	14 (8%)	1 (1%)	25	47
1	Y	177/193 (92%)	161 (91%)	14 (8%)	2 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	177/193 (92%)	164 (93%)	10 (6%)	3 (2%)	9	18
1	a	177/193 (92%)	168 (95%)	5 (3%)	4 (2%)	6	11
1	b	177/193 (92%)	161 (91%)	13 (7%)	3 (2%)	9	18
All	All	4956/5404 (92%)	4528 (91%)	368 (7%)	60 (1%)	13	27

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	B	54	ASN
1	J	16	SER
1	J	155	LEU
1	O	54	ASN
1	O	189	LEU
1	O	190	THR
1	P	122	HIS
1	Q	16	SER
1	S	191	HIS
1	V	124	PRO
1	W	155	LEU
1	W	156	HIS
1	b	17	PHE
1	b	54	ASN
1	C	16	SER
1	D	16	SER
1	E	19	ILE
1	F	113	CYS
1	J	156	HIS
1	K	155	LEU
1	L	175	SER
1	O	161	LEU
1	O	167	ASP
1	O	192	ARG
1	S	162	GLU
1	T	16	SER
1	T	17	PHE
1	X	17	PHE
1	a	16	SER
1	a	83	ILE
1	K	34	GLN
1	K	159	GLN

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Mol	Chain	Res	Type
1	U	54	ASN
1	Y	54	ASN
1	a	82	PHE
1	b	167	ASP
1	O	77	TYR
1	O	178	GLU
1	P	192	ARG
1	U	192	ARG
1	A	115	PRO
1	E	54	ASN
1	S	98	MET
1	Y	16	SER
1	Z	54	ASN
1	F	54	ASN
1	I	137	ILE
1	O	95	ALA
1	O	97	SER
1	V	54	ASN
1	W	70	ILE
1	Z	122	HIS
1	V	55	PRO
1	Z	115	PRO
1	O	76	ILE
1	V	66	PRO
1	a	54	ASN
1	P	19	ILE
1	W	177	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/162 (93%)	141 (93%)	10 (7%)	16	33
1	B	151/162 (93%)	143 (95%)	8 (5%)	22	45
1	C	151/162 (93%)	141 (93%)	10 (7%)	16	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	151/162 (93%)	143 (95%)	8 (5%)	22	45
1	E	151/162 (93%)	144 (95%)	7 (5%)	27	51
1	F	151/162 (93%)	142 (94%)	9 (6%)	19	39
1	G	151/162 (93%)	145 (96%)	6 (4%)	31	57
1	H	151/162 (93%)	145 (96%)	6 (4%)	31	57
1	I	151/162 (93%)	141 (93%)	10 (7%)	16	33
1	J	151/162 (93%)	135 (89%)	16 (11%)	6	12
1	K	151/162 (93%)	140 (93%)	11 (7%)	14	28
1	L	151/162 (93%)	143 (95%)	8 (5%)	22	45
1	M	151/162 (93%)	139 (92%)	12 (8%)	12	24
1	N	151/162 (93%)	142 (94%)	9 (6%)	19	39
1	O	151/162 (93%)	138 (91%)	13 (9%)	10	20
1	P	151/162 (93%)	141 (93%)	10 (7%)	16	33
1	Q	151/162 (93%)	142 (94%)	9 (6%)	19	39
1	R	151/162 (93%)	138 (91%)	13 (9%)	10	20
1	S	151/162 (93%)	141 (93%)	10 (7%)	16	33
1	T	151/162 (93%)	144 (95%)	7 (5%)	27	51
1	U	151/162 (93%)	144 (95%)	7 (5%)	27	51
1	V	151/162 (93%)	143 (95%)	8 (5%)	22	45
1	W	151/162 (93%)	141 (93%)	10 (7%)	16	33
1	X	151/162 (93%)	138 (91%)	13 (9%)	10	20
1	Y	151/162 (93%)	142 (94%)	9 (6%)	19	39
1	Z	151/162 (93%)	133 (88%)	18 (12%)	5	9
1	a	151/162 (93%)	142 (94%)	9 (6%)	19	39
1	b	151/162 (93%)	141 (93%)	10 (7%)	16	33
All	All	4228/4536 (93%)	3952 (94%)	276 (6%)	17	34

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	22	ARG
1	A	26	GLU

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Mol	Chain	Res	Type
1	A	31	LEU
1	A	34	GLN
1	A	94	GLN
1	A	113	CYS
1	A	122	HIS
1	A	136	GLU
1	A	184	LEU
1	B	15	ARG
1	B	22	ARG
1	B	31	LEU
1	B	113	CYS
1	B	122	HIS
1	B	148	ARG
1	B	155	LEU
1	B	184	LEU
1	C	17	PHE
1	C	22	ARG
1	C	25	LYS
1	C	31	LEU
1	C	113	CYS
1	C	118	ARG
1	C	122	HIS
1	C	142	ILE
1	C	172	ARG
1	C	184	LEU
1	D	19	ILE
1	D	31	LEU
1	D	34	GLN
1	D	56	GLU
1	D	122	HIS
1	D	142	ILE
1	D	172	ARG
1	D	189	LEU
1	E	16	SER
1	E	56	GLU
1	E	86	ASP
1	E	113	CYS
1	E	122	HIS
1	E	123	GLN
1	E	174	LEU
1	F	31	LEU
1	F	56	GLU

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Mol	Chain	Res	Type
1	F	65	SER
1	F	113	CYS
1	F	122	HIS
1	F	155	LEU
1	F	160	SER
1	F	166	ARG
1	F	193	ASN
1	G	22	ARG
1	G	31	LEU
1	G	34	GLN
1	G	91	CYS
1	G	114	LEU
1	G	122	HIS
1	H	31	LEU
1	H	56	GLU
1	H	122	HIS
1	H	172	ARG
1	H	174	LEU
1	H	184	LEU
1	I	17	PHE
1	I	19	ILE
1	I	21	SER
1	I	23	LEU
1	I	31	LEU
1	I	56	GLU
1	I	113	CYS
1	I	122	HIS
1	I	168	THR
1	I	172	ARG
1	J	17	PHE
1	J	19	ILE
1	J	31	LEU
1	J	39	MET
1	J	42	LEU
1	J	56	GLU
1	J	108	LYS
1	J	112	PHE
1	J	121	ILE
1	J	122	HIS
1	J	136	GLU
1	J	142	ILE
1	J	159	GLN

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Mol	Chain	Res	Type
1	J	162	GLU
1	J	172	ARG
1	J	184	LEU
1	K	17	PHE
1	K	111	ARG
1	K	113	CYS
1	K	115	PRO
1	K	122	HIS
1	K	123	GLN
1	K	136	GLU
1	K	155	LEU
1	K	163	GLN
1	K	180	VAL
1	K	181	GLU
1	L	17	PHE
1	L	31	LEU
1	L	56	GLU
1	L	91	CYS
1	L	108	LYS
1	L	122	HIS
1	L	155	LEU
1	L	174	LEU
1	M	17	PHE
1	M	19	ILE
1	M	22	ARG
1	M	31	LEU
1	M	34	GLN
1	M	56	GLU
1	M	113	CYS
1	M	122	HIS
1	M	124	PRO
1	M	161	LEU
1	M	172	ARG
1	M	190	THR
1	N	22	ARG
1	N	26	GLU
1	N	31	LEU
1	N	39	MET
1	N	104	THR
1	N	113	CYS
1	N	122	HIS
1	N	123	GLN

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Mol	Chain	Res	Type
1	N	172	ARG
1	O	17	PHE
1	O	19	ILE
1	O	31	LEU
1	O	79	THR
1	O	81	GLN
1	O	87	VAL
1	O	114	LEU
1	O	115	PRO
1	O	122	HIS
1	O	164	ILE
1	O	167	ASP
1	O	177	PRO
1	O	189	LEU
1	P	31	LEU
1	P	56	GLU
1	P	66	PRO
1	P	81	GLN
1	P	104	THR
1	P	112	PHE
1	P	122	HIS
1	P	166	ARG
1	P	178	GLU
1	P	185	VAL
1	Q	25	LYS
1	Q	31	LEU
1	Q	56	GLU
1	Q	114	LEU
1	Q	118	ARG
1	Q	122	HIS
1	Q	123	GLN
1	Q	155	LEU
1	Q	186	ASP
1	R	15	ARG
1	R	19	ILE
1	R	31	LEU
1	R	56	GLU
1	R	113	CYS
1	R	118	ARG
1	R	120	MET
1	R	122	HIS
1	R	136	GLU

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Mol	Chain	Res	Type
1	R	172	ARG
1	R	174	LEU
1	R	184	LEU
1	R	193	ASN
1	S	15	ARG
1	S	17	PHE
1	S	22	ARG
1	S	31	LEU
1	S	56	GLU
1	S	122	HIS
1	S	136	GLU
1	S	161	LEU
1	S	163	GLN
1	S	189	LEU
1	T	15	ARG
1	T	17	PHE
1	T	22	ARG
1	T	122	HIS
1	T	167	ASP
1	T	172	ARG
1	T	184	LEU
1	U	31	LEU
1	U	47	MET
1	U	81	GLN
1	U	91	CYS
1	U	108	LYS
1	U	122	HIS
1	U	162	GLU
1	V	17	PHE
1	V	19	ILE
1	V	81	GLN
1	V	118	ARG
1	V	122	HIS
1	V	142	ILE
1	V	155	LEU
1	V	184	LEU
1	W	31	LEU
1	W	36	GLU
1	W	66	PRO
1	W	121	ILE
1	W	122	HIS
1	W	170	ARG

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Mol	Chain	Res	Type
1	W	172	ARG
1	W	175	SER
1	W	184	LEU
1	W	192	ARG
1	X	15	ARG
1	X	17	PHE
1	X	31	LEU
1	X	71	THR
1	X	113	CYS
1	X	118	ARG
1	X	122	HIS
1	X	149	MET
1	X	165	GLU
1	X	166	ARG
1	X	167	ASP
1	X	190	THR
1	X	191	HIS
1	Y	31	LEU
1	Y	88	SER
1	Y	94	GLN
1	Y	104	THR
1	Y	118	ARG
1	Y	122	HIS
1	Y	155	LEU
1	Y	162	GLU
1	Y	184	LEU
1	Z	17	PHE
1	Z	19	ILE
1	Z	22	ARG
1	Z	31	LEU
1	Z	56	GLU
1	Z	81	GLN
1	Z	114	LEU
1	Z	116	ASN
1	Z	122	HIS
1	Z	123	GLN
1	Z	129	GLN
1	Z	136	GLU
1	Z	155	LEU
1	Z	160	SER
1	Z	172	ARG
1	Z	184	LEU

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Mol	Chain	Res	Type
1	Z	185	VAL
1	Z	192	ARG
1	a	15	ARG
1	a	19	ILE
1	a	22	ARG
1	a	31	LEU
1	a	56	GLU
1	a	65	SER
1	a	71	THR
1	a	122	HIS
1	a	184	LEU
1	b	17	PHE
1	b	19	ILE
1	b	31	LEU
1	b	34	GLN
1	b	36	GLU
1	b	91	CYS
1	b	122	HIS
1	b	136	GLU
1	b	148	ARG
1	b	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	116	ASN
1	A	123	GLN
1	A	156	HIS
1	B	41	ASN
1	B	123	GLN
1	B	156	HIS
1	C	41	ASN
1	C	116	ASN
1	C	123	GLN
1	C	129	GLN
1	C	156	HIS
1	D	34	GLN
1	D	41	ASN
1	D	116	ASN
1	D	123	GLN
1	D	156	HIS

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Mol	Chain	Res	Type
1	E	34	GLN
1	E	116	ASN
1	E	123	GLN
1	E	156	HIS
1	E	163	GLN
1	E	191	HIS
1	F	41	ASN
1	F	116	ASN
1	F	123	GLN
1	F	129	GLN
1	F	156	HIS
1	F	163	GLN
1	G	34	GLN
1	G	41	ASN
1	G	116	ASN
1	G	123	GLN
1	G	156	HIS
1	H	116	ASN
1	H	123	GLN
1	H	156	HIS
1	H	163	GLN
1	I	41	ASN
1	I	116	ASN
1	I	123	GLN
1	I	156	HIS
1	J	34	GLN
1	J	41	ASN
1	J	94	GLN
1	J	116	ASN
1	J	123	GLN
1	J	150	ASN
1	J	156	HIS
1	J	159	GLN
1	J	191	HIS
1	K	41	ASN
1	K	46	GLN
1	K	116	ASN
1	K	123	GLN
1	K	156	HIS
1	K	163	GLN
1	K	191	HIS
1	L	41	ASN

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Mol	Chain	Res	Type
1	L	46	GLN
1	L	123	GLN
1	L	156	HIS
1	L	193	ASN
1	M	34	GLN
1	M	41	ASN
1	M	116	ASN
1	M	123	GLN
1	M	156	HIS
1	M	163	GLN
1	N	34	GLN
1	N	123	GLN
1	N	129	GLN
1	N	156	HIS
1	O	34	GLN
1	O	41	ASN
1	O	122	HIS
1	O	123	GLN
1	O	129	GLN
1	O	156	HIS
1	O	159	GLN
1	O	163	GLN
1	O	191	HIS
1	O	193	ASN
1	P	41	ASN
1	P	94	GLN
1	P	116	ASN
1	P	123	GLN
1	P	156	HIS
1	Q	41	ASN
1	Q	116	ASN
1	Q	123	GLN
1	Q	129	GLN
1	Q	156	HIS
1	Q	163	GLN
1	R	41	ASN
1	R	46	GLN
1	R	116	ASN
1	R	123	GLN
1	R	156	HIS
1	R	193	ASN
1	S	34	GLN

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Mol	Chain	Res	Type
1	S	41	ASN
1	S	116	ASN
1	S	123	GLN
1	S	129	GLN
1	S	156	HIS
1	T	116	ASN
1	T	123	GLN
1	T	156	HIS
1	T	163	GLN
1	U	41	ASN
1	U	54	ASN
1	U	81	GLN
1	U	116	ASN
1	U	123	GLN
1	U	156	HIS
1	V	34	GLN
1	V	41	ASN
1	V	116	ASN
1	V	123	GLN
1	V	138	HIS
1	V	150	ASN
1	V	156	HIS
1	V	163	GLN
1	W	34	GLN
1	W	94	GLN
1	W	129	GLN
1	W	156	HIS
1	W	163	GLN
1	X	34	GLN
1	X	41	ASN
1	X	116	ASN
1	X	123	GLN
1	X	129	GLN
1	X	156	HIS
1	X	159	GLN
1	X	163	GLN
1	Y	41	ASN
1	Y	116	ASN
1	Y	123	GLN
1	Y	156	HIS
1	Z	41	ASN
1	Z	123	GLN

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Mol	Chain	Res	Type
1	Z	156	HIS
1	Z	163	GLN
1	a	41	ASN
1	a	116	ASN
1	a	122	HIS
1	a	123	GLN
1	a	156	HIS
1	a	163	GLN
1	b	34	GLN
1	b	41	ASN
1	b	116	ASN
1	b	123	GLN
1	b	150	ASN
1	b	156	HIS
1	b	163	GLN
1	b	191	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 [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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.