



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:15 PM BST

PDB ID : 6KMV
Title : caspase-11 C254A P22/P10 in complex with mouse GSDMD-C domain
Authors : Ding, J.; Sun, Q.
Deposited on : 2019-08-01
Resolution : 3.35 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) : 1.13
EDS : 2.13
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) : 2.13

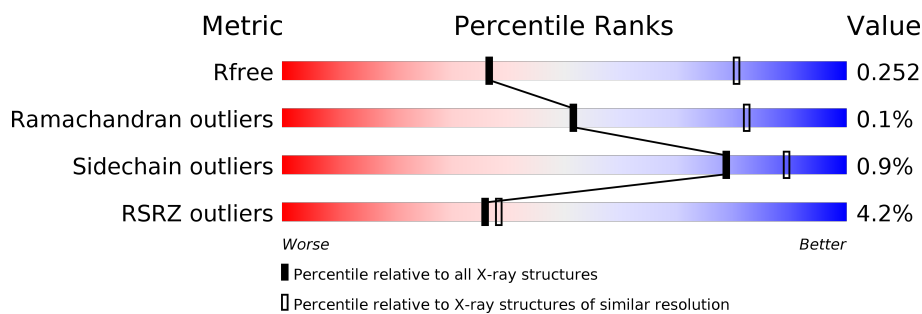
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. 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	161	99% .
2	B	167	99% .
2	V	167	10% 99% .
3	C	198	3% 100%
3	G	198	2% 100%
3	O	198	4% 97% .
4	D	197	5% 99% .

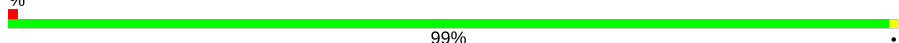





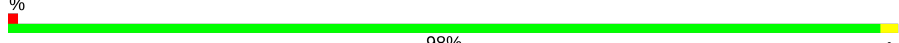




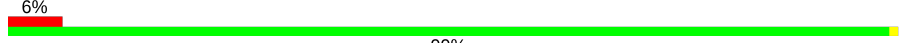




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Mol	Chain	Length	Quality of chain
4	K	197	
4	S	197	
4	T	197	
4	W	197	
4	b	197	
4	f	197	
5	E	166	
5	F	166	
5	Z	166	
5	d	166	
6	H	191	
7	I	165	
7	M	165	
7	N	165	
7	Q	165	
7	Y	165	
8	J	149	
9	L	214	
9	P	214	
9	e	214	
10	R	150	
10	c	150	
11	U	165	
12	X	199	
13	a	196	

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Mol	Chain	Length	Quality of chain
14	g	88	%  99% .
14	h	88	 98% .
14	i	88	 97% .
14	j	88	 99% .
14	k	88	 98% .
14	l	88	%  99% .
14	m	88	%  98% .
14	n	88	 99% .
14	o	88	 98% .
14	p	88	%  99% .
14	q	88	%  99% .
14	r	88	6%  99% .
14	t	88	7%  98% .
14	u	88	%  98% .
14	v	88	2%  99% .
15	s	87	%  99% .

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 56064 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 Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1258	788	217	242	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 2 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1316	825	226	253	12			
2	V	167	Total	C	N	O	S	0	0	0
			1316	825	226	253	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	254	ALA	CYS	engineered mutation	UNP P70343
V	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 3 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	198	Total	C	N	O	S	0	0	0
			1506	960	237	301	8			
3	G	198	Total	C	N	O	S	0	0	0
			1506	960	237	301	8			
3	O	198	Total	C	N	O	S	0	0	0
			1506	960	237	301	8			

- Molecule 4 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1501	957	236	300	8			
4	K	197	Total	C	N	O	S	0	0	0
			1501	957	236	300	8			
4	S	197	Total	C	N	O	S	0	0	0
			1501	957	236	300	8			
4	T	197	Total	C	N	O	S	0	0	0
			1501	957	236	300	8			
4	W	197	Total	C	N	O	S	0	0	0
			1501	957	236	300	8			
4	b	180	Total	C	N	O	S	0	0	0
			1363	870	211	275	7			
4	f	197	Total	C	N	O	S	0	0	0
			1501	957	236	300	8			

- Molecule 5 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	166	Total	C	N	O	S	0	0	0
			1310	822	225	251	12			
5	F	166	Total	C	N	O	S	0	0	0
			1310	822	225	251	12			
5	Z	166	Total	C	N	O	S	0	0	0
			1310	822	225	251	12			
5	d	166	Total	C	N	O	S	0	0	0
			1310	822	225	251	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	254	ALA	CYS	engineered mutation	UNP P70343
F	254	ALA	CYS	engineered mutation	UNP P70343
Z	254	ALA	CYS	engineered mutation	UNP P70343
d	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 6 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	171	Total	C	N	O	S	0	0	0
			1304	830	206	261	7			

- Molecule 7 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	165	Total	C	N	O	S	0	0	0
			1303	818	224	249	12			
7	M	165	Total	C	N	O	S	0	0	0
			1303	818	224	249	12			
7	N	165	Total	C	N	O	S	0	0	0
			1303	818	224	249	12			
7	Q	165	Total	C	N	O	S	0	0	0
			1303	818	224	249	12			
7	Y	165	Total	C	N	O	S	0	0	0
			1303	818	224	249	12			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	254	ALA	CYS	engineered mutation	UNP P70343
M	254	ALA	CYS	engineered mutation	UNP P70343
N	254	ALA	CYS	engineered mutation	UNP P70343
Q	254	ALA	CYS	engineered mutation	UNP P70343
Y	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 8 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	149	Total	C	N	O	S	0	0	0
			1169	734	200	225	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 9 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	214	Total	C	N	O	S	0	0	0
			1627	1035	253	331	8			
9	P	214	Total	C	N	O	S	0	0	0
			1627	1035	253	331	8			
9	e	214	Total	C	N	O	S	0	0	0
			1627	1035	253	331	8			

- Molecule 10 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	R	150	Total	C	N	O	S	0	0	0
			1175	737	201	227	10			
10	c	150	Total	C	N	O	S	0	0	0
			1175	737	201	227	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	254	ALA	CYS	engineered mutation	UNP P70343
c	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 11 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	U	165	Total	C	N	O	S	0	0	0
			1301	817	224	248	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 12 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	199	Total	C	N	O	S	0	0	0
			1511	963	238	302	8			

- Molecule 13 is a protein called Gasdermin-D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	a	183	Total	C	N	O	S	0	0	0
			1405	898	222	278	7			

- Molecule 14 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	g	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	h	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	i	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	j	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	k	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	l	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	m	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	n	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	o	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	p	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	q	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	r	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	t	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	u	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			
14	v	88	Total	C	N	O	S	0	0	0
			726	471	125	126	4			

- Molecule 15 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	s	87	Total	C	N	O	S	0	0	0
			721	468	124	125	4			

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: Caspase-4

Chain A:  99%



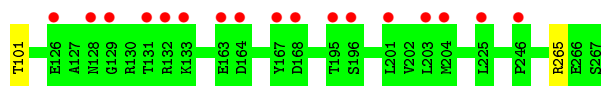
- Molecule 2: Caspase-4

Chain B:  99%



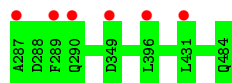
- Molecule 2: Caspase-4

Chain V:  10% 99%



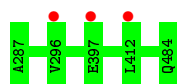
- Molecule 3: Gasdermin-D

Chain C:  3% 100%

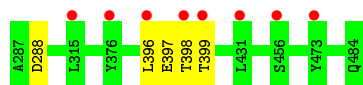


- Molecule 3: Gasdermin-D

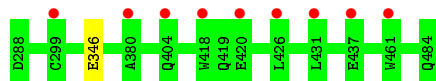
Chain G:  2% 100%



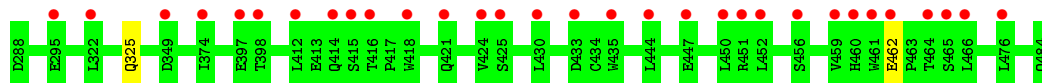
- Molecule 3: Gasdermin-D



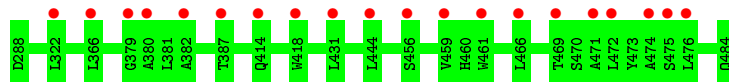
• Molecule 4: Gasdermin-D



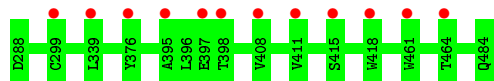
• Molecule 4: Gasdermin-D



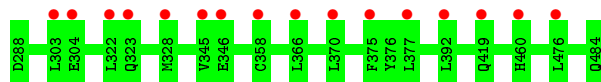
• Molecule 4: Gasdermin-D



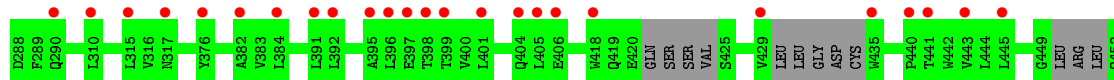
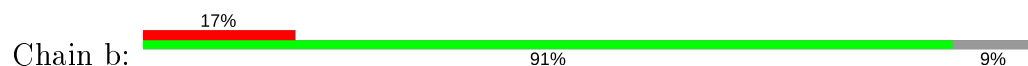
• Molecule 4: Gasdermin-D

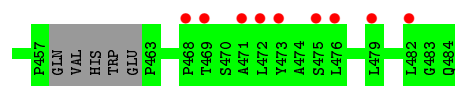


• Molecule 4: Gasdermin-D

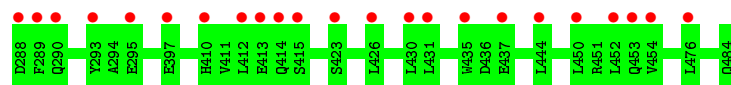


• Molecule 4: Gasdermin-D

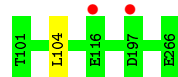




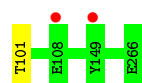
● Molecule 4: Gasdermin-D



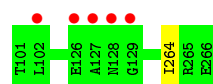
● Molecule 5: Caspase-4



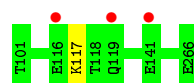
● Molecule 5: Caspase-4



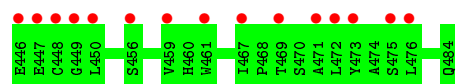
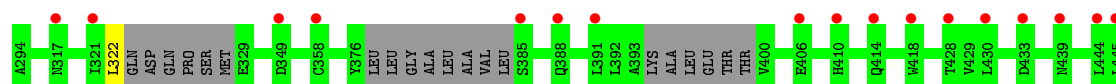
● Molecule 5: Caspase-4



● Molecule 5: Caspase-4



● Molecule 6: Gasdermin-D



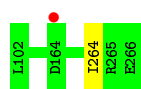
- Molecule 7: Caspase-4

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Caspase-4

Chain M:  99%



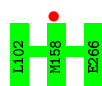
- Molecule 7: Caspase-4

Chain N:  99%



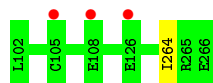
- Molecule 7: Caspase-4

Chain Q:  100%



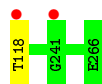
- Molecule 7: Caspase-4

Chain Y:  99%



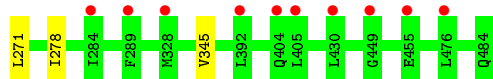
- Molecule 8: Caspase-4

Chain J:  99%



- Molecule 9: Gasdermin-D

Chain L:  99%



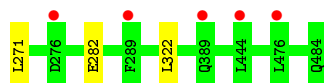
- Molecule 9: Gasdermin-D

Chain P:  99%



- Molecule 9: Gasdermin-D

Chain e:  99%



- Molecule 10: Caspase-4

Chain R:  100%

There are no outlier residues recorded for this chain.

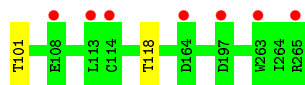
- Molecule 10: Caspase-4

Chain c:  100%



- Molecule 11: Caspase-4

Chain U:  99%

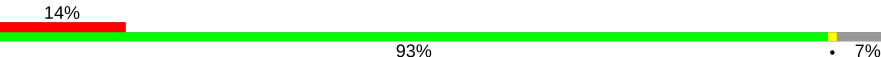


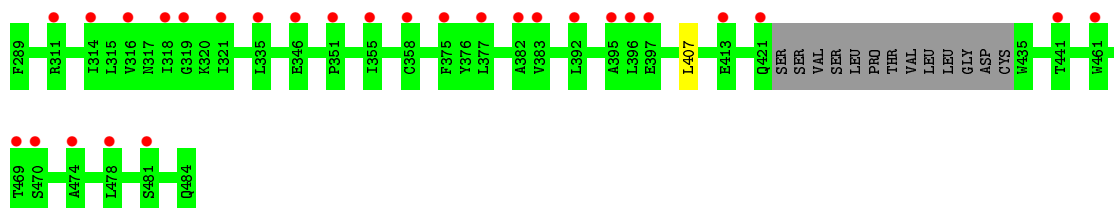
- Molecule 12: Gasdermin-D

Chain X:  100%

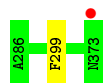
There are no outlier residues recorded for this chain.

- Molecule 13: Gasdermin-D

Chain a:  93% 7%



● Molecule 14: Caspase-4



● Molecule 14: Caspase-4



● Molecule 14: Caspase-4



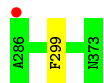
● Molecule 14: Caspase-4



● Molecule 14: Caspase-4



● Molecule 14: Caspase-4



● Molecule 14: Caspase-4



- Molecule 14: Caspase-4

Chain n:  99% .



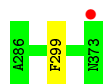
- Molecule 14: Caspase-4

Chain o:  98% .



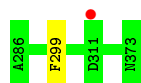
- Molecule 14: Caspase-4

Chain p:  99% .



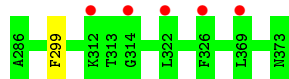
- Molecule 14: Caspase-4

Chain q:  99% .



- Molecule 14: Caspase-4

Chain r:  99% .



- Molecule 14: Caspase-4

Chain t:  98% .

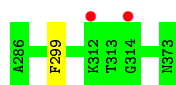


- Molecule 14: Caspase-4

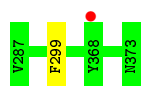
Chain u:  98% .



- Molecule 14: Caspase-4



- Molecule 15: Caspase-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.80Å 139.21Å 175.94Å 92.43° 99.06° 96.35°	Depositor
Resolution (Å)	37.44 – 3.35 45.07 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.44-3.35) 94.2 (45.07-3.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.252 0.220 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	81.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	56064	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.31	0/1280	0.50	0/1724
2	B	0.24	0/1339	0.43	0/1802
2	V	0.24	0/1339	0.43	0/1802
3	C	0.23	0/1532	0.40	0/2089
3	G	0.24	0/1532	0.39	0/2089
3	O	0.29	0/1532	0.46	0/2089
4	D	0.24	0/1527	0.39	0/2082
4	K	0.23	0/1527	0.39	0/2082
4	S	0.24	0/1527	0.39	0/2082
4	T	0.23	0/1527	0.39	0/2082
4	W	0.23	0/1527	0.39	0/2082
4	b	0.24	0/1382	0.39	0/1877
4	f	0.24	0/1527	0.39	0/2082
5	E	0.24	0/1333	0.43	0/1794
5	F	0.24	0/1333	0.43	0/1794
5	Z	0.24	0/1333	0.43	0/1794
5	d	0.24	0/1333	0.43	0/1794
6	H	0.23	0/1324	0.40	0/1801
7	I	0.24	0/1326	0.42	0/1784
7	M	0.24	0/1326	0.42	0/1784
7	N	0.24	0/1326	0.42	0/1784
7	Q	0.24	0/1326	0.42	0/1784
7	Y	0.24	0/1326	0.42	0/1784
8	J	0.24	0/1190	0.43	0/1603
9	L	0.24	0/1653	0.40	0/2253
9	P	0.31	0/1653	0.46	0/2253
9	e	0.24	0/1653	0.40	0/2253
10	R	0.24	0/1196	0.43	0/1611
10	c	0.24	0/1196	0.43	0/1611
11	U	0.24	0/1324	0.43	0/1782
12	X	0.25	0/1537	0.41	0/2096
13	a	0.24	0/1429	0.39	0/1945
14	g	0.24	0/748	0.44	0/1007
14	h	0.24	0/748	0.43	0/1007

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	i	0.24	0/748	0.44	0/1007
14	j	0.24	0/748	0.42	0/1007
14	k	0.24	0/748	0.44	0/1007
14	l	0.24	0/748	0.42	0/1007
14	m	0.24	0/748	0.43	0/1007
14	n	0.24	0/748	0.42	0/1007
14	o	0.24	0/748	0.44	0/1007
14	p	0.24	0/748	0.43	0/1007
14	q	0.24	0/748	0.44	0/1007
14	r	0.24	0/748	0.42	0/1007
14	t	0.24	0/748	0.42	0/1007
14	u	0.24	0/748	0.44	0/1007
14	v	0.25	0/748	0.42	0/1007
15	s	0.24	0/743	0.44	0/1000
All	All	0.24	0/57178	0.42	0/77373

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	B	165/167 (99%)	157 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	165/167 (99%)	156 (94%)	8 (5%)	1 (1%)	25	59
3	C	196/198 (99%)	195 (100%)	1 (0%)	0	100	100
3	G	196/198 (99%)	195 (100%)	1 (0%)	0	100	100
3	O	196/198 (99%)	193 (98%)	2 (1%)	1 (0%)	29	63
4	D	195/197 (99%)	193 (99%)	2 (1%)	0	100	100
4	K	195/197 (99%)	194 (100%)	1 (0%)	0	100	100
4	S	195/197 (99%)	194 (100%)	1 (0%)	0	100	100
4	T	195/197 (99%)	194 (100%)	1 (0%)	0	100	100
4	W	195/197 (99%)	194 (100%)	1 (0%)	0	100	100
4	b	170/197 (86%)	169 (99%)	1 (1%)	0	100	100
4	f	195/197 (99%)	194 (100%)	1 (0%)	0	100	100
5	E	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
5	F	164/166 (99%)	157 (96%)	7 (4%)	0	100	100
5	Z	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
5	d	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
6	H	163/191 (85%)	163 (100%)	0	0	100	100
7	I	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
7	M	163/165 (99%)	154 (94%)	9 (6%)	0	100	100
7	N	163/165 (99%)	155 (95%)	7 (4%)	1 (1%)	25	59
7	Q	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
7	Y	163/165 (99%)	154 (94%)	9 (6%)	0	100	100
8	J	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
9	L	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
9	P	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
9	e	212/214 (99%)	206 (97%)	5 (2%)	1 (0%)	29	63
10	R	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
10	c	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
11	U	163/165 (99%)	155 (95%)	8 (5%)	0	100	100
12	X	197/199 (99%)	196 (100%)	1 (0%)	0	100	100
13	a	179/196 (91%)	178 (99%)	1 (1%)	0	100	100
14	g	86/88 (98%)	83 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	h	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	i	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	j	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	k	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	l	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	m	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
14	n	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	o	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	p	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	q	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	r	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	t	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	u	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	v	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	s	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
All	All	7044/7206 (98%)	6838 (97%)	202 (3%)	4 (0%)	51	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	e	282	GLU
2	V	265	ARG
3	O	398	THR
7	N	128	ASN

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	139/139 (100%)	137 (99%)	2 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	146/146 (100%)	144 (99%)	2 (1%)	67	83
2	V	146/146 (100%)	145 (99%)	1 (1%)	84	92
3	C	171/171 (100%)	171 (100%)	0	100	100
3	G	171/171 (100%)	171 (100%)	0	100	100
3	O	171/171 (100%)	167 (98%)	4 (2%)	50	75
4	D	171/171 (100%)	170 (99%)	1 (1%)	86	93
4	K	171/171 (100%)	169 (99%)	2 (1%)	71	85
4	S	171/171 (100%)	171 (100%)	0	100	100
4	T	171/171 (100%)	171 (100%)	0	100	100
4	W	171/171 (100%)	171 (100%)	0	100	100
4	b	155/171 (91%)	155 (100%)	0	100	100
4	f	171/171 (100%)	171 (100%)	0	100	100
5	E	145/145 (100%)	144 (99%)	1 (1%)	84	92
5	F	145/145 (100%)	144 (99%)	1 (1%)	84	92
5	Z	145/145 (100%)	144 (99%)	1 (1%)	84	92
5	d	145/145 (100%)	144 (99%)	1 (1%)	84	92
6	H	150/166 (90%)	149 (99%)	1 (1%)	84	92
7	I	144/144 (100%)	144 (100%)	0	100	100
7	M	144/144 (100%)	143 (99%)	1 (1%)	84	92
7	N	144/144 (100%)	143 (99%)	1 (1%)	84	92
7	Q	144/144 (100%)	144 (100%)	0	100	100
7	Y	144/144 (100%)	143 (99%)	1 (1%)	84	92
8	J	128/128 (100%)	127 (99%)	1 (1%)	81	91
9	L	185/185 (100%)	182 (98%)	3 (2%)	62	81
9	P	185/185 (100%)	182 (98%)	3 (2%)	62	81
9	e	185/185 (100%)	183 (99%)	2 (1%)	73	86
10	R	129/129 (100%)	129 (100%)	0	100	100
10	c	129/129 (100%)	129 (100%)	0	100	100
11	U	144/144 (100%)	142 (99%)	2 (1%)	67	83
12	X	171/171 (100%)	171 (100%)	0	100	100
13	a	158/170 (93%)	157 (99%)	1 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	g	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	h	80/80 (100%)	78 (98%)	2 (2%)	47	73
14	i	80/80 (100%)	77 (96%)	3 (4%)	33	63
14	j	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	k	80/80 (100%)	78 (98%)	2 (2%)	47	73
14	l	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	m	80/80 (100%)	78 (98%)	2 (2%)	47	73
14	n	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	o	80/80 (100%)	78 (98%)	2 (2%)	47	73
14	p	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	q	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	r	80/80 (100%)	79 (99%)	1 (1%)	69	84
14	t	80/80 (100%)	78 (98%)	2 (2%)	47	73
14	u	80/80 (100%)	78 (98%)	2 (2%)	47	73
14	v	80/80 (100%)	79 (99%)	1 (1%)	69	84
15	s	80/80 (100%)	79 (99%)	1 (1%)	69	84
All	All	6269/6313 (99%)	6213 (99%)	56 (1%)	78	89

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	278	LEU
2	B	264	ILE
2	B	266	GLU
4	D	346	GLU
5	E	104	LEU
5	F	101	THR
6	H	322	LEU
8	J	118	THR
4	K	325	GLN
4	K	462	GLU
9	L	271	LEU
9	L	278	ILE
9	L	345	VAL
7	M	264	ILE

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Mol	Chain	Res	Type
7	N	108	GLU
3	O	288	ASP
3	O	396	LEU
3	O	397	GLU
3	O	399	THR
9	P	272	SER
9	P	276	ASP
9	P	346	GLU
11	U	101	THR
11	U	118	THR
2	V	101	THR
7	Y	264	ILE
5	Z	264	ILE
13	a	407	LEU
5	d	117	LYS
9	e	271	LEU
9	e	322	LEU
14	g	299	PHE
14	h	299	PHE
14	h	326	PHE
14	i	299	PHE
14	i	321	ARG
14	i	326	PHE
14	j	299	PHE
14	k	299	PHE
14	k	321	ARG
14	l	299	PHE
14	m	299	PHE
14	m	321	ARG
14	n	299	PHE
14	o	299	PHE
14	o	321	ARG
14	p	299	PHE
14	q	299	PHE
14	r	299	PHE
15	s	299	PHE
14	t	299	PHE
14	t	326	PHE
14	u	299	PHE
14	u	321	ARG
14	v	299	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
14	r	344	GLN

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	161/161 (100%)	-0.05	0	100	100	41, 65, 104, 154	0
2	B	167/167 (100%)	-0.01	0	100	100	41, 63, 95, 109	0
2	V	167/167 (100%)	0.48	17 (10%)	6	8	70, 116, 140, 159	0
3	C	198/198 (100%)	0.27	6 (3%)	50	53	60, 88, 125, 139	0
3	G	198/198 (100%)	0.29	3 (1%)	73	76	70, 97, 121, 137	0
3	O	198/198 (100%)	0.18	8 (4%)	38	40	30, 94, 119, 140	0
4	D	197/197 (100%)	0.30	9 (4%)	32	35	66, 98, 140, 149	0
4	K	197/197 (100%)	0.85	31 (15%)	2	2	77, 122, 147, 154	0
4	S	197/197 (100%)	0.57	20 (10%)	6	8	68, 107, 148, 162	0
4	T	197/197 (100%)	0.48	12 (6%)	21	23	81, 116, 150, 160	0
4	W	197/197 (100%)	0.64	16 (8%)	12	13	99, 126, 146, 153	0
4	b	180/197 (91%)	0.89	34 (18%)	1	1	96, 123, 145, 153	0
4	f	197/197 (100%)	0.69	23 (11%)	4	5	80, 111, 150, 163	0
5	E	166/166 (100%)	-0.03	2 (1%)	79	82	48, 75, 111, 129	0
5	F	166/166 (100%)	-0.07	2 (1%)	79	82	53, 77, 111, 120	0
5	Z	166/166 (100%)	0.17	5 (3%)	50	53	68, 93, 127, 147	0
5	d	166/166 (100%)	-0.08	3 (1%)	68	71	41, 64, 96, 123	0
6	H	171/191 (89%)	1.02	32 (18%)	1	1	86, 126, 156, 165	0
7	I	165/165 (100%)	-0.04	0	100	100	45, 66, 105, 120	0
7	M	165/165 (100%)	0.09	1 (0%)	89	92	61, 91, 117, 132	0
7	N	165/165 (100%)	0.09	3 (1%)	68	71	72, 101, 130, 138	0
7	Q	165/165 (100%)	0.09	1 (0%)	89	92	56, 82, 109, 123	0
7	Y	165/165 (100%)	0.09	3 (1%)	68	71	66, 94, 129, 144	0
8	J	149/149 (100%)	0.06	2 (1%)	77	80	44, 64, 88, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
9	L	214/214 (100%)	0.30	10 (4%) 31 34	64, 100, 128, 138	0
9	P	214/214 (100%)	0.11	0 100 100	30, 77, 97, 114	0
9	e	214/214 (100%)	0.19	5 (2%) 60 63	51, 84, 121, 138	0
10	R	150/150 (100%)	-0.12	0 100 100	45, 61, 100, 118	0
10	c	150/150 (100%)	-0.01	1 (0%) 87 91	45, 74, 95, 136	0
11	U	165/165 (100%)	0.19	7 (4%) 36 38	66, 87, 121, 130	0
12	X	199/199 (100%)	0.12	0 100 100	30, 73, 97, 109	0
13	a	183/196 (93%)	0.84	28 (15%) 2 2	86, 120, 142, 148	0
14	g	88/88 (100%)	0.08	1 (1%) 80 84	43, 59, 86, 104	0
14	h	88/88 (100%)	-0.01	0 100 100	41, 58, 95, 118	0
14	i	88/88 (100%)	-0.02	0 100 100	53, 69, 93, 104	0
14	j	88/88 (100%)	0.01	0 100 100	50, 72, 92, 102	0
14	k	88/88 (100%)	0.07	0 100 100	44, 66, 87, 94	0
14	l	88/88 (100%)	0.07	1 (1%) 80 84	43, 64, 94, 109	0
14	m	88/88 (100%)	0.11	1 (1%) 80 84	67, 87, 110, 119	0
14	n	88/88 (100%)	0.12	0 100 100	69, 90, 124, 130	0
14	o	88/88 (100%)	-0.02	0 100 100	42, 68, 96, 105	0
14	p	88/88 (100%)	-0.00	1 (1%) 80 84	44, 61, 82, 112	0
14	q	88/88 (100%)	0.26	1 (1%) 80 84	69, 95, 114, 128	0
14	r	88/88 (100%)	0.36	5 (5%) 23 26	78, 107, 136, 144	0
14	t	88/88 (100%)	0.40	6 (6%) 17 20	71, 93, 122, 132	0
14	u	88/88 (100%)	0.11	1 (1%) 80 84	43, 63, 100, 105	0
14	v	88/88 (100%)	0.14	2 (2%) 60 63	43, 64, 99, 130	0
15	s	87/87 (100%)	0.08	1 (1%) 80 84	67, 88, 112, 128	0
All	All	7156/7206 (99%)	0.25	304 (4%) 36 38	30, 89, 137, 165	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	a	396	LEU	6.7
4	f	431	LEU	6.2
13	a	441	THR	6.0
4	K	450	LEU	6.0
4	b	398	THR	5.5

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Mol	Chain	Res	Type	RSRZ
4	S	418	TRP	5.4
14	t	373	ASN	5.3
2	V	129	GLY	5.1
4	W	476	LEU	5.1
6	H	449	GLY	5.0
4	b	472	LEU	5.0
4	b	469	THR	4.9
6	H	476	LEU	4.9
4	f	289	PHE	4.8
13	a	382	ALA	4.8
6	H	444	LEU	4.8
4	b	406	GLU	4.7
4	f	435	TRP	4.7
4	b	471	ALA	4.7
13	a	474	ALA	4.6
6	H	448	CYS	4.6
13	a	397	GLU	4.5
13	a	319	GLY	4.5
6	H	473	TYR	4.4
6	H	414	GLN	4.4
4	f	452	LEU	4.3
6	H	461	TRP	4.3
6	H	450	LEU	4.1
6	H	391	LEU	4.1
4	K	466	LEU	4.1
4	T	418	TRP	4.1
4	b	384	LEU	4.0
4	S	472	LEU	4.0
4	S	474	ALA	4.0
4	f	450	LEU	4.0
4	K	418	TRP	4.0
4	b	441	THR	4.0
13	a	318	ILE	3.9
4	b	395	ALA	3.9
5	Z	129	GLY	3.8
6	H	447	GLU	3.8
4	W	358	CYS	3.8
4	W	345	VAL	3.7
14	g	373	ASN	3.7
5	Z	126	GLU	3.7
4	f	412	LEU	3.6
3	O	431	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
7	N	129	GLY	3.6
9	e	444	LEU	3.6
13	a	316	VAL	3.6
2	V	168	ASP	3.6
4	K	452	LEU	3.6
4	b	396	LEU	3.6
14	l	286	ALA	3.6
14	m	373	ASN	3.5
2	V	201	LEU	3.5
2	V	163	GLU	3.5
14	v	312	LYS	3.5
3	G	412	LEU	3.5
4	S	387	THR	3.5
4	b	392	LEU	3.5
13	a	395	ALA	3.4
6	H	472	LEU	3.4
2	V	203	LEU	3.4
6	H	456	SER	3.4
4	f	453	GLN	3.4
4	b	468	PRO	3.4
4	b	475	SER	3.4
2	V	131	THR	3.3
4	K	424	VAL	3.3
4	T	299	CYS	3.3
4	W	322	LEU	3.3
13	a	481	SER	3.3
4	S	471	ALA	3.2
4	b	404	GLN	3.2
6	H	358	CYS	3.2
6	H	388	GLN	3.2
6	H	410	HIS	3.2
5	Z	128	ASN	3.2
11	U	265	ARG	3.2
4	S	456	SER	3.2
4	W	377	LEU	3.2
6	H	321	ILE	3.2
4	S	382	ALA	3.1
3	C	431	LEU	3.1
4	D	431	LEU	3.1
9	L	476	LEU	3.1
4	S	469	THR	3.1
4	f	295	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	b	382	ALA	3.1
4	W	419	GLN	3.1
13	a	311	ARG	3.1
4	S	444	LEU	3.1
2	V	246	PRO	3.1
4	f	430	LEU	3.1
13	a	335	LEU	3.1
6	H	406	GLU	3.0
14	t	286	ALA	3.0
4	K	398	THR	3.0
4	D	437	GLU	3.0
4	b	310	LEU	3.0
11	U	263	TRP	3.0
6	H	439	ASN	3.0
6	H	475	SER	3.0
4	b	435	TRP	3.0
7	M	164	ASP	3.0
6	H	418	TRP	2.9
6	H	467	ILE	2.9
4	K	464	THR	2.9
13	a	314	ILE	2.9
14	p	373	ASN	2.9
6	H	469	THR	2.9
4	f	397	GLU	2.9
13	a	421	GLN	2.9
4	b	397	GLU	2.9
4	b	429	VAL	2.9
4	f	413	GLU	2.8
6	H	428	THR	2.8
2	V	133	LYS	2.8
4	f	288	ASP	2.8
2	V	195	THR	2.8
4	W	323	GLN	2.8
4	b	290	GLN	2.8
4	b	401	LEU	2.8
4	b	399	THR	2.8
8	J	118	THR	2.8
4	S	475	SER	2.8
4	K	451	ARG	2.7
4	b	418	TRP	2.7
4	K	456	SER	2.7
14	r	312	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
4	K	349	ASP	2.7
2	V	128	ASN	2.7
4	S	380	ALA	2.7
4	b	473	TYR	2.7
4	T	395	ALA	2.7
3	O	315	LEU	2.7
3	O	398	THR	2.7
4	f	414	GLN	2.7
11	U	108	GLU	2.7
4	K	461	TRP	2.7
14	r	369	LEU	2.7
14	t	372	GLY	2.6
9	L	284	ILE	2.6
9	e	276	ASP	2.6
4	W	346	GLU	2.6
4	K	459	VAL	2.6
14	r	314	GLY	2.6
4	D	461	TRP	2.6
13	a	355	ILE	2.6
6	H	385	SER	2.6
11	U	197	ASP	2.6
4	T	397	GLU	2.6
4	b	440	PRO	2.6
4	D	418	TRP	2.6
4	K	397	GLU	2.6
4	W	304	GLU	2.6
3	G	397	GLU	2.6
4	T	398	THR	2.6
2	V	126	GLU	2.5
3	C	396	LEU	2.5
4	K	412	LEU	2.5
4	S	476	LEU	2.5
13	a	377	LEU	2.5
3	O	399	THR	2.5
14	r	322	LEU	2.5
4	S	461	TRP	2.5
6	H	445	LEU	2.5
4	K	465	SER	2.5
11	U	113	LEU	2.5
9	L	430	LEU	2.5
3	O	456	SER	2.5
4	W	303	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
9	L	289	PHE	2.5
4	S	379	GLY	2.5
3	C	289	PHE	2.5
5	F	108	GLU	2.5
13	a	413	GLU	2.5
4	b	315	LEU	2.5
4	K	460	HIS	2.5
4	f	423	SER	2.5
3	G	296	VAL	2.4
4	T	408	VAL	2.4
14	u	312	LYS	2.4
4	W	375	PHE	2.4
4	K	433	ASP	2.4
4	b	445	LEU	2.4
14	t	326	PHE	2.4
4	K	447	GLU	2.4
4	W	328	MET	2.4
7	N	139	ASN	2.4
4	T	411	VAL	2.4
4	W	370	LEU	2.4
4	T	461	TRP	2.4
14	r	326	PHE	2.4
6	H	433	ASP	2.4
7	Y	126	GLU	2.4
13	a	351	PRO	2.4
6	H	446	GLU	2.4
5	Z	102	LEU	2.4
4	f	290	GLN	2.4
6	H	471	ALA	2.4
4	W	460	HIS	2.4
13	a	478	LEU	2.4
4	S	414	GLN	2.4
4	f	410	HIS	2.4
9	L	405	LEU	2.4
4	W	392	LEU	2.4
9	L	392	LEU	2.3
14	q	311	ASP	2.3
4	D	420	GLU	2.3
4	b	317	ASN	2.3
6	H	317	ASN	2.3
5	E	197	ASP	2.3
3	O	376	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
7	N	115	ARG	2.3
6	H	349	ASP	2.3
3	O	473	TYR	2.3
14	t	287	VAL	2.3
2	V	204	MET	2.3
4	D	299	CYS	2.3
4	K	444	LEU	2.3
4	b	391	LEU	2.3
4	K	430	LEU	2.3
4	T	339	LEU	2.3
13	a	392	LEU	2.3
4	K	421	GLN	2.3
3	C	349	ASP	2.3
2	V	225	LEU	2.3
4	S	366	LEU	2.3
2	V	196	SER	2.2
4	f	437	GLU	2.2
4	K	476	LEU	2.2
4	K	462	GLU	2.2
4	f	293	TYR	2.2
4	f	415	SER	2.2
7	Y	105	CYS	2.2
4	K	415	SER	2.2
13	a	469	THR	2.2
4	S	466	LEU	2.2
13	a	375	PHE	2.2
6	H	430	LEU	2.2
9	e	389	GLN	2.2
4	b	443	VAL	2.2
9	L	328	MET	2.2
13	a	383	VAL	2.2
3	C	287	ALA	2.2
2	V	132	ARG	2.2
4	b	476	LEU	2.2
2	V	164	ASP	2.2
4	K	416	THR	2.2
4	T	376	TYR	2.2
3	C	290	GLN	2.2
9	L	404	GLN	2.2
4	K	374	ILE	2.2
4	K	322	LEU	2.2
4	f	444	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
9	e	476	LEU	2.2
14	t	367	PHE	2.2
13	a	358	CYS	2.2
4	T	464	THR	2.2
4	S	431	LEU	2.1
4	f	476	LEU	2.1
4	f	454	VAL	2.1
4	T	415	SER	2.1
13	a	461	TRP	2.1
13	a	321	ILE	2.1
11	U	164	ASP	2.1
5	E	116	GLU	2.1
6	H	459	VAL	2.1
5	d	116	GLU	2.1
7	Y	108	GLU	2.1
4	D	426	LEU	2.1
7	Q	158	MET	2.1
13	a	470	SER	2.1
3	O	396	LEU	2.1
4	S	322	LEU	2.1
4	W	366	LEU	2.1
4	D	380	ALA	2.1
5	Z	127	ALA	2.1
4	S	459	VAL	2.1
14	v	314	GLY	2.1
2	V	167	TYR	2.1
4	b	479	LEU	2.1
4	b	482	LEU	2.1
4	K	414	GLN	2.1
4	b	376	TYR	2.1
4	K	425	SER	2.1
8	J	241	GLY	2.1
5	d	119	GLN	2.0
4	f	426	LEU	2.0
11	U	114	CYS	2.0
9	L	449	GLY	2.0
10	c	118	THR	2.0
4	D	404	GLN	2.0
4	K	435	TRP	2.0
9	L	455	GLU	2.0
15	s	368	TYR	2.0
9	e	289	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
5	d	141	GLU	2.0
4	b	405	LEU	2.0
5	F	149	TYR	2.0
4	K	295	GLU	2.0
13	a	346	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.