



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2025 – 02:33 PM JST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

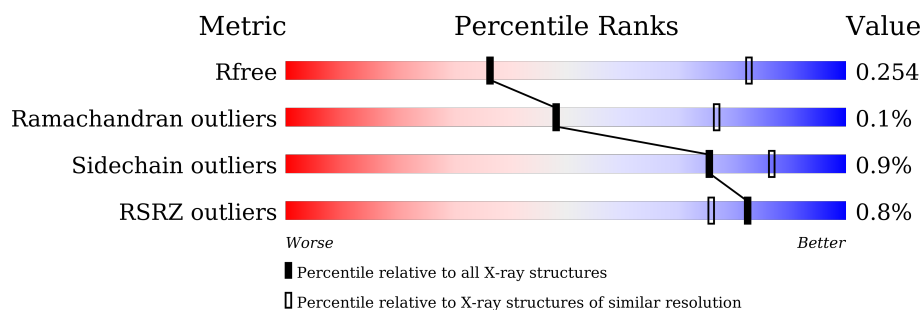
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



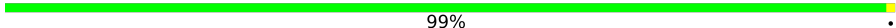
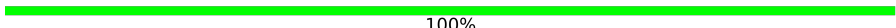

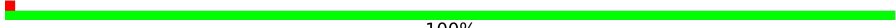









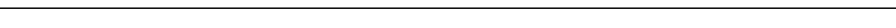

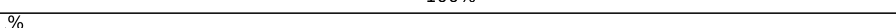
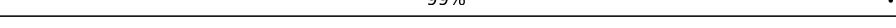
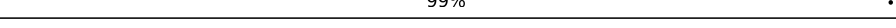
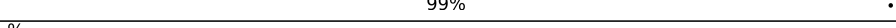
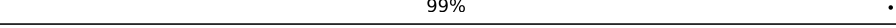
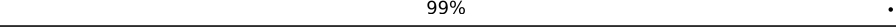
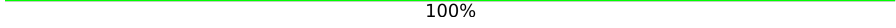
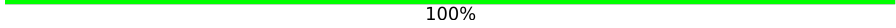
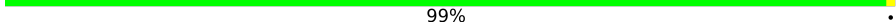

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1012 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)

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  $\geq 3$ , 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	<div> <div></div> <div>99%</div> <div>.</div> </div>
2	B	167	<div> <div></div> <div>99%</div> <div>.</div> </div>
2	V	167	<div> <div></div> <div>99%</div> <div>.</div> </div>
3	C	198	<div> <div></div> <div>100%</div> <div></div> </div>
3	G	198	<div> <div></div> <div>100%</div> <div></div> </div>
3	O	198	<div> <div>2%</div> <div>97%</div> <div>.</div> </div>
4	D	197	<div> <div></div> <div>99%</div> <div>.</div> </div>















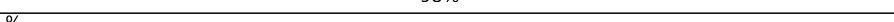
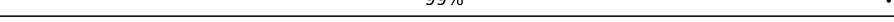
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Mol	Chain	Length	Quality of chain
4	K	197	 99% .
4	S	197	 100%
4	T	197	 2% 100%
4	W	197	 % 100%
4	b	197	 2% 91% 9%
4	f	197	 % 100%
5	E	166	 % 99% .
5	F	166	 99% .
5	Z	166	 99% .
5	d	166	 99% .
6	H	191	 6% 89% . 10%
7	I	165	 100%
7	M	165	 99% .
7	N	165	 99% .
7	Q	165	 % 100%
7	Y	165	 % 99% .
8	J	149	 99% .
9	L	214	 99% .
9	P	214	 % 99% .
9	e	214	 99% .
10	R	150	 100%
10	c	150	 100%
11	U	165	 % 99% .
12	X	199	 % 100%
13	a	196	 9% 93% . 7%

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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	 99% .
14	t	88	 98% .
14	u	88	 98% .
14	v	88	 99% .
15	s	87	 99% .

## 2 Entry composition

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			

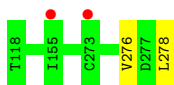
- Molecule 15 is a protein called Caspase-4.

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

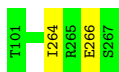
### 3 Residue-property plots

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



- Molecule 2: Caspase-4



- Molecule 2: Caspase-4



- Molecule 3: Gasdermin-D



There are no outlier residues recorded for this chain.

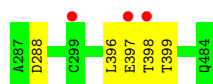
- Molecule 3: Gasdermin-D



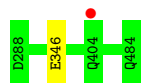
There are no outlier residues recorded for this chain.

- Molecule 3: Gasdermin-D





- Molecule 4: Gasdermin-D



- Molecule 4: Gasdermin-D

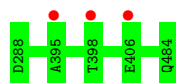


- Molecule 4: Gasdermin-D



There are no outlier residues recorded for this chain.

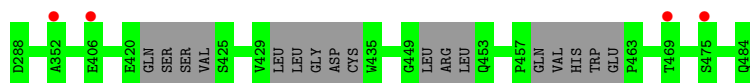
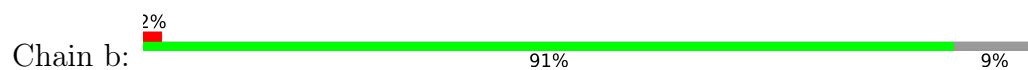
- Molecule 4: Gasdermin-D



- Molecule 4: Gasdermin-D

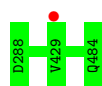


- Molecule 4: Gasdermin-D

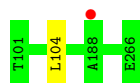


- Molecule 4: Gasdermin-D





- Molecule 5: Caspase-4



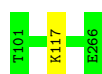
- Molecule 5: Caspase-4



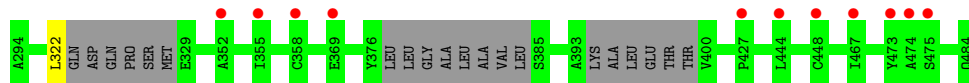
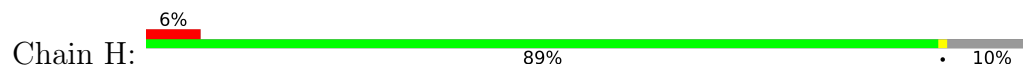
- Molecule 5: Caspase-4



- Molecule 5: Caspase-4



- Molecule 6: Gasdermin-D



- Molecule 7: Caspase-4



There are no outlier residues recorded for this chain.

- Molecule 7: Caspase-4





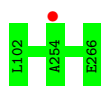
- Molecule 7: Caspase-4

Chain N: 99%



- Molecule 7: Caspase-4

Chain Q: 100%



- Molecule 7: Caspase-4

Chain Y: 99%



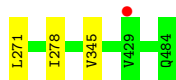
- Molecule 8: Caspase-4

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%

There are no outlier residues recorded for this chain.

- Molecule 11: Caspase-4

Chain U:  % 99%



- Molecule 12: Gasdermin-D

Chain X:  % 100%



- Molecule 13: Gasdermin-D

Chain a:  9% 93% 7%



- Molecule 14: Caspase-4

Chain g:  99%



- Molecule 14: Caspase-4

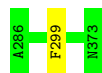
Chain h:  98%



## ● Molecule 14: Caspase-4

Chain i:  97% .

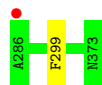
## ● Molecule 14: Caspase-4

Chain j:  99% .

## ● Molecule 14: Caspase-4

Chain k:  98% .

## ● Molecule 14: Caspase-4

Chain l:  99% .

## ● Molecule 14: Caspase-4

Chain m:  98% .

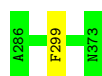
## ● Molecule 14: Caspase-4

Chain n:  99% .

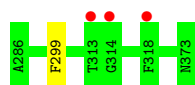
## ● Molecule 14: Caspase-4

Chain o:  98% .

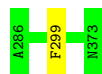
## ● Molecule 14: Caspase-4

Chain p:  99% .

## ● Molecule 14: Caspase-4

Chain q:  3% 99% .

## ● Molecule 14: Caspase-4

Chain r:  99% .

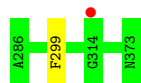
## ● Molecule 14: Caspase-4

Chain t:  98% .

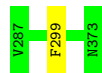
## ● Molecule 14: Caspase-4

Chain u:  98% .

## ● Molecule 14: Caspase-4

Chain v:  % 99% .

## ● Molecule 15: Caspase-4

Chain s:  99% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.80Å 139.21Å 175.94Å 92.43° 99.06° 96.35°	Depositor
Resolution (Å)	37.44 – 3.35 37.44 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.44-3.35) 94.3 (37.44-3.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.219 , 0.252 0.222 , 0.254	Depositor DCC
$R_{free}$ test set	116258 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

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

## 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	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%)	22	50
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%)	25	53
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%)	22	50
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%)	25	53
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%)	48	77

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%)	62	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	146/146 (100%)	144 (99%)	2 (1%)	62	78
2	V	146/146 (100%)	145 (99%)	1 (1%)	81	89
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%)	45	68
4	D	171/171 (100%)	170 (99%)	1 (1%)	84	91
4	K	171/171 (100%)	169 (99%)	2 (1%)	67	80
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%)	81	89
5	F	145/145 (100%)	144 (99%)	1 (1%)	81	89
5	Z	145/145 (100%)	144 (99%)	1 (1%)	81	89
5	d	145/145 (100%)	144 (99%)	1 (1%)	81	89
6	H	150/166 (90%)	149 (99%)	1 (1%)	81	89
7	I	144/144 (100%)	144 (100%)	0	100	100
7	M	144/144 (100%)	143 (99%)	1 (1%)	81	89
7	N	144/144 (100%)	143 (99%)	1 (1%)	81	89
7	Q	144/144 (100%)	144 (100%)	0	100	100
7	Y	144/144 (100%)	143 (99%)	1 (1%)	81	89
8	J	128/128 (100%)	127 (99%)	1 (1%)	79	88
9	L	185/185 (100%)	182 (98%)	3 (2%)	58	75
9	P	185/185 (100%)	182 (98%)	3 (2%)	58	75
9	e	185/185 (100%)	183 (99%)	2 (1%)	70	82
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%)	62	78
12	X	171/171 (100%)	171 (100%)	0	100	100
13	a	158/170 (93%)	157 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	g	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	h	80/80 (100%)	78 (98%)	2 (2%)	42	66
14	i	80/80 (100%)	77 (96%)	3 (4%)	28	54
14	j	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	k	80/80 (100%)	78 (98%)	2 (2%)	42	66
14	l	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	m	80/80 (100%)	78 (98%)	2 (2%)	42	66
14	n	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	o	80/80 (100%)	78 (98%)	2 (2%)	42	66
14	p	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	q	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	r	80/80 (100%)	79 (99%)	1 (1%)	65	79
14	t	80/80 (100%)	78 (98%)	2 (2%)	42	66
14	u	80/80 (100%)	78 (98%)	2 (2%)	42	66
14	v	80/80 (100%)	79 (99%)	1 (1%)	65	79
15	s	80/80 (100%)	79 (99%)	1 (1%)	65	79
All	All	6269/6313 (99%)	6213 (99%)	56 (1%)	75	87

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

Sometimes 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 oligosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	161/161 (100%)	-0.24	2 (1%) 76 69	41, 65, 104, 154	0
2	B	167/167 (100%)	-0.32	0 100 100	41, 63, 95, 109	0
2	V	167/167 (100%)	0.09	1 (0%) 85 81	70, 116, 140, 159	0
3	C	198/198 (100%)	-0.07	0 100 100	60, 88, 125, 139	0
3	G	198/198 (100%)	-0.12	0 100 100	70, 97, 121, 137	0
3	O	198/198 (100%)	0.03	3 (1%) 71 64	30, 94, 119, 140	0
4	D	197/197 (100%)	-0.14	1 (0%) 87 83	66, 98, 140, 149	0
4	K	197/197 (100%)	-0.01	0 100 100	77, 122, 147, 154	0
4	S	197/197 (100%)	0.10	0 100 100	68, 107, 148, 162	0
4	T	197/197 (100%)	0.11	3 (1%) 71 64	81, 116, 150, 160	0
4	W	197/197 (100%)	0.05	2 (1%) 79 72	99, 126, 146, 153	0
4	b	180/197 (91%)	0.30	4 (2%) 62 53	96, 123, 145, 153	0
4	f	197/197 (100%)	0.10	1 (0%) 87 83	80, 111, 150, 163	0
5	E	166/166 (100%)	-0.34	1 (0%) 85 81	48, 75, 111, 129	0
5	F	166/166 (100%)	-0.26	0 100 100	53, 77, 111, 120	0
5	Z	166/166 (100%)	-0.07	0 100 100	68, 93, 127, 147	0
5	d	166/166 (100%)	-0.40	0 100 100	41, 64, 96, 123	0
6	H	171/191 (89%)	0.54	11 (6%) 27 25	86, 126, 156, 165	0
7	I	165/165 (100%)	-0.34	0 100 100	45, 66, 105, 120	0
7	M	165/165 (100%)	-0.26	0 100 100	61, 91, 117, 132	0
7	N	165/165 (100%)	-0.14	0 100 100	72, 100, 130, 138	0
7	Q	165/165 (100%)	-0.17	1 (0%) 85 81	56, 82, 109, 123	0
7	Y	165/165 (100%)	-0.14	1 (0%) 85 81	66, 94, 129, 144	0
8	J	149/149 (100%)	-0.36	0 100 100	44, 64, 88, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
9	L	214/214 (100%)	0.01	1 (0%) 87 83	64, 100, 128, 138	0
9	P	214/214 (100%)	-0.21	3 (1%) 73 66	30, 77, 97, 114	0
9	e	214/214 (100%)	-0.12	0 100 100	51, 84, 121, 138	0
10	R	150/150 (100%)	-0.36	0 100 100	45, 61, 100, 118	0
10	c	150/150 (100%)	-0.27	0 100 100	45, 74, 95, 136	0
11	U	165/165 (100%)	-0.01	1 (0%) 85 81	66, 87, 121, 130	0
12	X	199/199 (100%)	-0.23	1 (0%) 87 83	30, 73, 97, 109	0
13	a	183/196 (93%)	0.53	17 (9%) 16 17	86, 120, 142, 148	0
14	g	88/88 (100%)	-0.18	0 100 100	43, 59, 86, 104	0
14	h	88/88 (100%)	-0.26	0 100 100	41, 58, 95, 118	0
14	i	88/88 (100%)	-0.25	0 100 100	52, 69, 93, 104	0
14	j	88/88 (100%)	-0.17	0 100 100	50, 72, 92, 102	0
14	k	88/88 (100%)	-0.16	0 100 100	44, 66, 87, 94	0
14	l	88/88 (100%)	-0.29	1 (1%) 77 70	43, 64, 94, 109	0
14	m	88/88 (100%)	-0.04	0 100 100	67, 87, 110, 119	0
14	n	88/88 (100%)	-0.14	0 100 100	69, 90, 124, 130	0
14	o	88/88 (100%)	-0.26	0 100 100	42, 68, 96, 105	0
14	p	88/88 (100%)	-0.19	0 100 100	44, 61, 82, 112	0
14	q	88/88 (100%)	0.29	3 (3%) 48 41	69, 95, 114, 128	0
14	r	88/88 (100%)	0.22	0 100 100	78, 107, 136, 144	0
14	t	88/88 (100%)	0.11	0 100 100	71, 93, 122, 132	0
14	u	88/88 (100%)	-0.25	0 100 100	43, 63, 100, 105	0
14	v	88/88 (100%)	-0.06	1 (1%) 77 70	43, 64, 99, 130	0
15	s	87/87 (100%)	-0.18	0 100 100	67, 88, 112, 128	0
All	All	7156/7206 (99%)	-0.08	59 (0%) 82 76	30, 89, 137, 165	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	475	SER	4.8
13	a	474	ALA	4.7
13	a	441	THR	4.7
13	a	396	LEU	3.8
4	W	377	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
6	H	358	CYS	3.3
14	q	314	GLY	3.3
3	O	398	THR	3.2
4	b	406	GLU	3.1
14	v	314	GLY	3.0
4	T	395	ALA	2.9
4	D	404	GLN	2.9
4	W	476	LEU	2.8
13	a	319	GLY	2.8
6	H	369	GLU	2.8
1	A	273	CYS	2.7
9	P	398	THR	2.7
4	b	469	THR	2.6
13	a	352	ALA	2.6
13	a	318	ILE	2.6
13	a	481	SER	2.5
6	H	352	ALA	2.4
14	q	313	THR	2.4
5	E	188	ALA	2.4
6	H	355	ILE	2.3
6	H	427	PRO	2.3
9	P	271	LEU	2.3
4	T	398	THR	2.3
12	X	287	ALA	2.3
9	P	397	GLU	2.3
13	a	315	LEU	2.3
11	U	164	ASP	2.2
3	O	299	CYS	2.2
6	H	448	CYS	2.2
6	H	473	TYR	2.2
6	H	467	ILE	2.2
14	l	286	ALA	2.2
4	T	406	GLU	2.2
4	b	352	ALA	2.1
7	Y	248	VAL	2.1
13	a	478	LEU	2.1
6	H	474	ALA	2.1
7	Q	254	ALA	2.1
13	a	393	ALA	2.1
13	a	358	CYS	2.1
1	A	155	ILE	2.1
4	b	475	SER	2.1

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Mol	Chain	Res	Type	RSRZ
6	H	444	LEU	2.1
13	a	391	LEU	2.1
9	L	429	VAL	2.1
13	a	311	ARG	2.1
13	a	355	ILE	2.1
14	q	318	PHE	2.1
4	f	429	VAL	2.1
2	V	213	CYS	2.1
3	O	397	GLU	2.1
13	a	377	LEU	2.0
13	a	392	LEU	2.0
13	a	382	ALA	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.