



# wwPDB X-ray Structure Validation Summary Report

May 17, 2020 – 12:40 am BST

PDB ID : 1F9E  
Title : CASPASE-8 SPECIFICITY PROBED AT SUBSITE S4: CRYSTAL STRUCTURE OF THE CASPASE-8-Z-DEVD-CHO  
Authors : Blanchard, H.; Donepudi, M.; Tschopp, M.; Kodandapani, L.; Wu, J.C.; Grutter, M.G.  
Deposited on : 2000-07-10  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

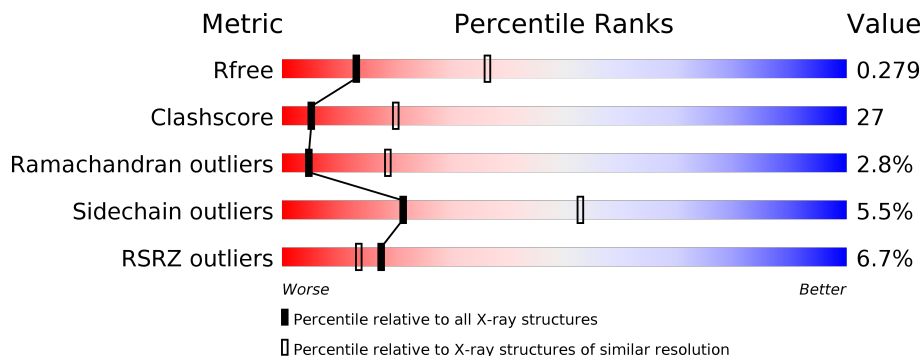
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	153	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 59% 38% .</p>
1	C	153	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 54% 40% 6%</p>
1	E	153	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 54% 41% 5% .</p>
1	G	153	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 63% 35% .</p>
1	I	153	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">9% 57% 37% 6%</p>
1	K	153	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 42%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">14% 56% 40% .</p>

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Mol	Chain	Length	Quality of chain
2	B	89	<p>%</p> <p>57% 36% 7%</p>
2	D	89	<p>6%</p> <p>52% 43% 6%</p>
2	F	89	<p>9%</p> <p>54% 38% 8%</p>
2	H	89	<p>2%</p> <p>63% 34%</p>
2	J	89	<p>7%</p> <p>56% 38%</p>
2	L	89	<p>20%</p> <p>57% 37%</p>
3	Q	5	<p>40% 60%</p>
3	R	5	<p>40% 60%</p>
3	S	5	<p>20%</p> <p>40% 40% 20%</p>
3	T	5	<p>100%</p>
3	U	5	<p>40% 40% 20%</p>
3	V	5	<p>20%</p> <p>40% 60%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ASA	V	4604	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11926 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-8 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1220	774	208	228	10	0	0	0
1	C	153	1220	774	208	228	10	0	0	0
1	E	153	1220	774	208	228	10	0	0	0
1	G	153	1220	774	208	228	10	0	0	0
1	I	153	1220	774	208	228	10	0	0	0
1	K	153	1220	774	208	228	10	0	0	0

- Molecule 2 is a protein called CASPASE-8 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	89	718	450	124	138	6	0	0	0
2	D	89	718	450	124	138	6	0	0	0
2	F	89	717	450	124	137	6	0	0	0
2	H	89	718	450	124	138	6	0	0	0
2	J	89	718	450	124	138	6	0	0	0
2	L	89	718	450	124	138	6	0	0	0

- Molecule 3 is a protein called (PHQ)DEVD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	R	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	S	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	T	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	U	5	Total	C	N	O	0	0	0
			42	26	4	12			
3	V	5	Total	C	N	O	0	0	0
			42	26	4	12			

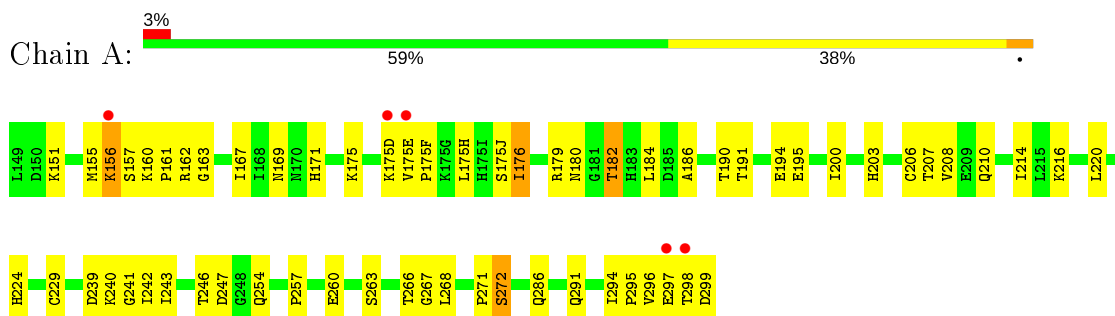
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	7	Total	O	0	0
			7	7		
4	Q	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	D	4	Total	O	0	0
			4	4		
4	E	4	Total	O	0	0
			4	4		
4	F	3	Total	O	0	0
			3	3		
4	G	11	Total	O	0	0
			11	11		
4	H	1	Total	O	0	0
			1	1		
4	I	5	Total	O	0	0
			5	5		
4	K	2	Total	O	0	0
			2	2		
4	L	1	Total	O	0	0
			1	1		

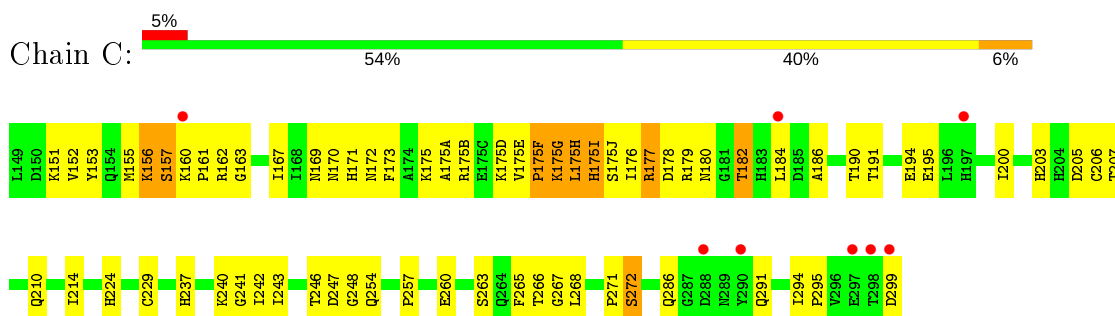
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

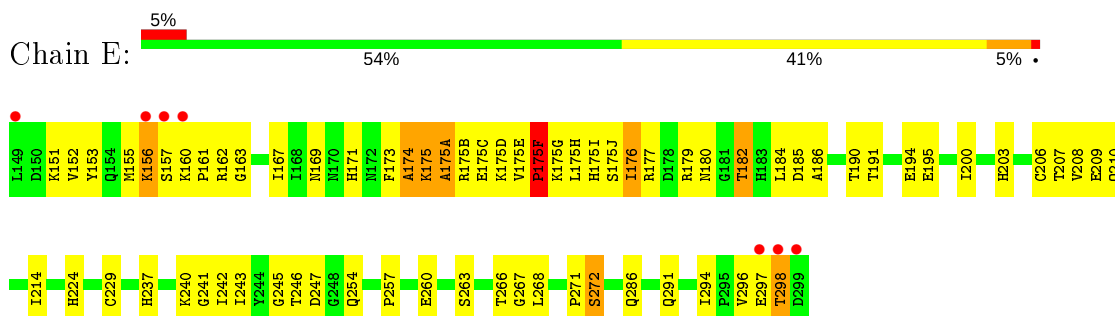
- Molecule 1: CASPASE-8 ALPHA CHAIN



- Molecule 1: CASPASE-8 ALPHA CHAIN

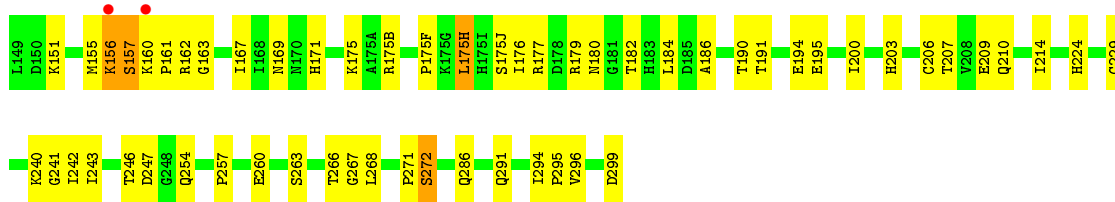


- Molecule 1: CASPASE-8 ALPHA CHAIN

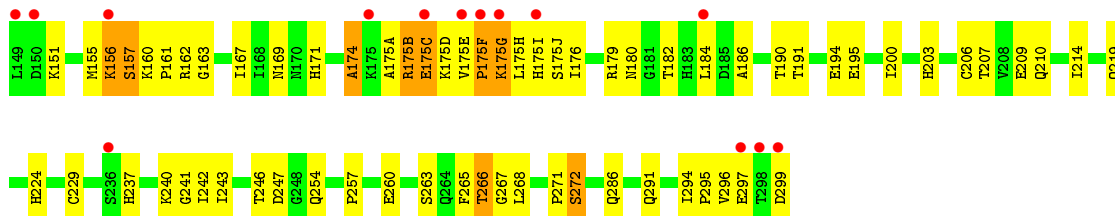


- Molecule 1: CASPASE-8 ALPHA CHAIN

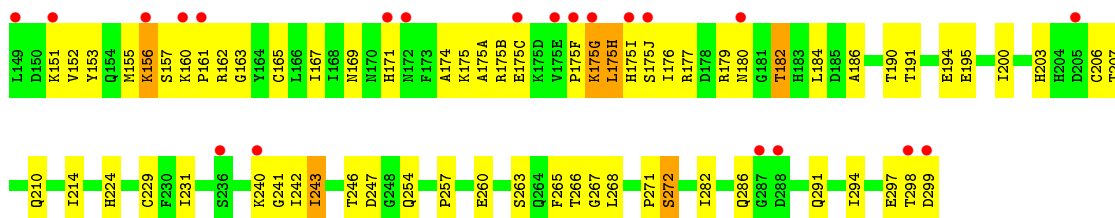




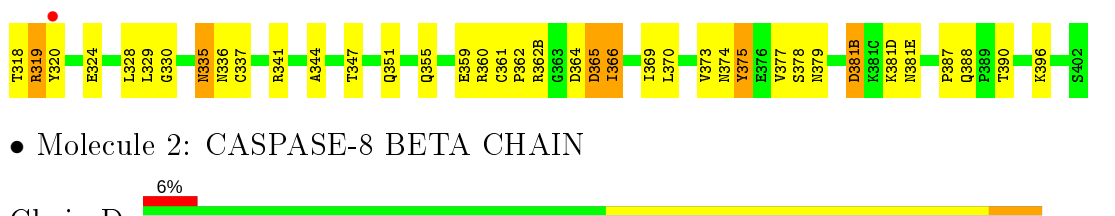
• Molecule 1: CASPASE-8 ALPHA CHAIN



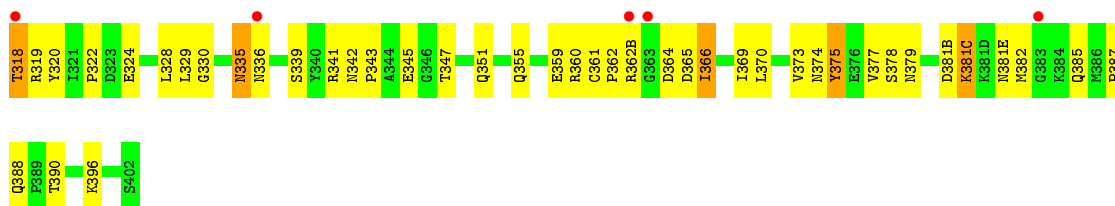
• Molecule 1: CASPASE-8 ALPHA CHAIN



• Molecule 2: CASPASE-8 BETA CHAIN

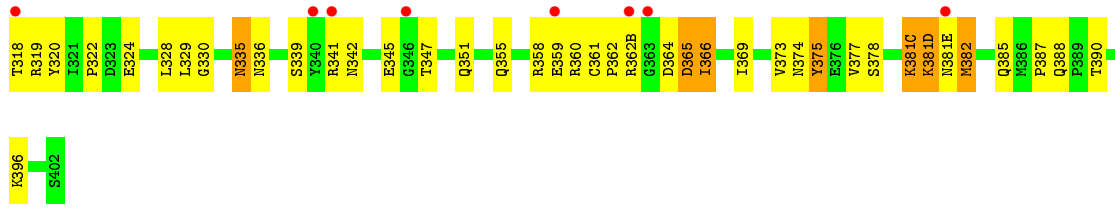


• Molecule 2: CASPASE-8 BETA CHAIN

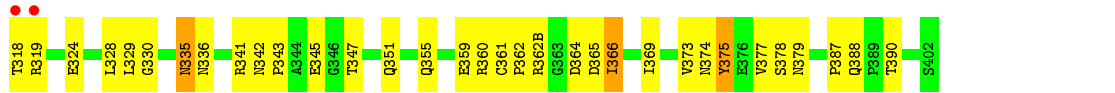


• Molecule 2: CASPASE-8 BETA CHAIN

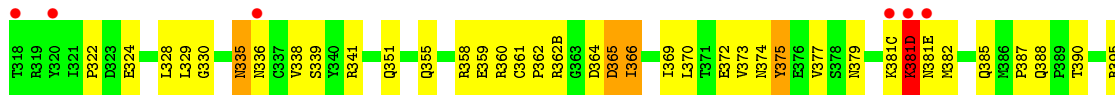




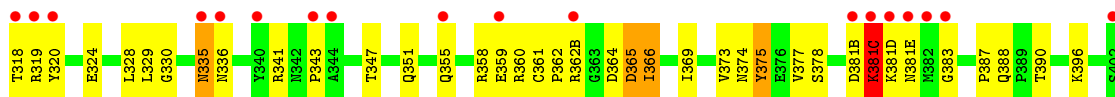
● Molecule 2: CASPASE-8 BETA CHAIN



● Molecule 2: CASPASE-8 BETA CHAIN



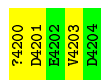
● Molecule 2: CASPASE-8 BETA CHAIN



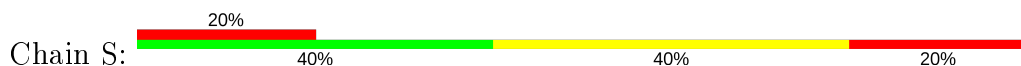
● Molecule 3: (PHQ)DEVD



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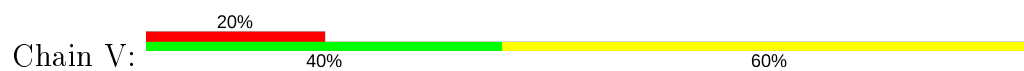
- Molecule 3: (PHQ)DEVD



- Molecule 3: (PHQ)DEVD



- Molecule 3: (PHQ)DEVD



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.03Å 188.75Å 209.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.93 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 99.5 (19.93-2.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.93Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.289 0.233 , 0.279	Depositor DCC
$R_{free}$ test set	4318 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtrriage
Anisotropy	0.078	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 72.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ASA, PHQ

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	0.54	0/1248	0.69	0/1682
1	C	0.52	0/1248	0.71	0/1682
1	E	0.50	0/1248	0.72	0/1682
1	G	0.55	0/1248	0.71	0/1682
1	I	0.49	0/1248	0.71	0/1682
1	K	0.48	0/1248	0.70	0/1682
2	B	0.51	0/732	0.74	0/989
2	D	0.48	0/732	0.71	0/989
2	F	0.54	0/731	0.74	0/989
2	H	0.53	0/732	0.71	0/989
2	J	0.46	0/732	0.69	0/989
2	L	0.49	0/732	0.71	0/989
3	Q	2.09	1/23 (4.3%)	1.84	0/30
3	R	2.35	0/23	1.96	0/30
3	S	2.16	1/23 (4.3%)	1.71	0/30
3	T	2.21	1/23 (4.3%)	2.06	1/30 (3.3%)
3	U	2.18	1/23 (4.3%)	1.68	0/30
3	V	2.16	0/23	1.89	0/30
All	All	0.56	4/12017 (0.0%)	0.73	1/16206 (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
3	Q	1	0
3	R	1	1
3	S	1	1
3	T	1	1
3	U	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	V	0	1
All	All	5	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	4102	GLU	CD-OE2	5.31	1.31	1.25
3	U	4502	GLU	CD-OE1	5.24	1.31	1.25
3	S	4302	GLU	CD-OE2	5.21	1.31	1.25
3	T	4402	GLU	CD-OE1	5.13	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	4401	ASP	N-CA-C	-5.57	95.95	111.00

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	Q	4101	ASP	CA
3	R	4201	ASP	CA
3	S	4301	ASP	CA
3	T	4401	ASP	CA
3	U	4501	ASP	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	R	4203	VAL	Mainchain
3	S	4303	VAL	Mainchain
3	T	4403	VAL	Mainchain
3	U	4503	VAL	Mainchain
3	V	4603	VAL	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1220	0	1198	72	0
1	C	1220	0	1198	84	0
1	E	1220	0	1198	87	0
1	G	1220	0	1198	60	0
1	I	1220	0	1198	80	0
1	K	1220	0	1198	85	0
2	B	718	0	712	53	0
2	D	718	0	712	53	0
2	F	717	0	712	49	0
2	H	718	0	712	39	0
2	J	718	0	712	47	0
2	L	718	0	712	54	0
3	Q	42	0	28	2	0
3	R	42	0	28	2	0
3	S	42	0	28	3	0
3	T	42	0	28	2	0
3	U	42	0	28	2	0
3	V	42	0	28	3	0
4	A	6	0	0	2	0
4	B	7	0	0	2	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	3	0	0	0	0
4	G	11	0	0	4	0
4	H	1	0	0	0	0
4	I	5	0	0	1	0
4	K	2	0	0	0	0
4	L	1	0	0	0	0
4	Q	1	0	0	0	0
All	All	11926	0	11628	630	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 630 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:THR:HG23	2:H:319:ARG:HH21	1.15	1.10
2:B:319:ARG:HH22	1:C:299:ASP:HB2	1.13	1.09
1:A:160:LYS:HB2	1:A:161:PRO:HD3	1.35	1.08
1:K:160:LYS:HB2	1:K:161:PRO:HD3	1.38	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HB2	1:C:161:PRO:HD3	1.38	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/153 (99%)	134 (89%)	15 (10%)	2 (1%)	12	37
1	C	151/153 (99%)	125 (83%)	19 (13%)	7 (5%)	2	9
1	E	151/153 (99%)	128 (85%)	13 (9%)	10 (7%)	1	3
1	G	151/153 (99%)	132 (87%)	17 (11%)	2 (1%)	12	37
1	I	151/153 (99%)	126 (83%)	16 (11%)	9 (6%)	1	4
1	K	151/153 (99%)	131 (87%)	15 (10%)	5 (3%)	4	15
2	B	87/89 (98%)	78 (90%)	7 (8%)	2 (2%)	6	23
2	D	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
2	F	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	14	42
2	H	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
2	J	87/89 (98%)	80 (92%)	5 (6%)	2 (2%)	6	23
2	L	87/89 (98%)	79 (91%)	7 (8%)	1 (1%)	14	42
3	Q	2/5 (40%)	2 (100%)	0	0	100	100
3	R	2/5 (40%)	2 (100%)	0	0	100	100
3	S	2/5 (40%)	2 (100%)	0	0	100	100
3	T	2/5 (40%)	2 (100%)	0	0	100	100
3	U	2/5 (40%)	2 (100%)	0	0	100	100
3	V	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1440/1482 (97%)	1264 (88%)	135 (9%)	41 (3%)	5	19

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	319	ARG
1	C	175(F)	PRO
1	C	175(G)	LYS
1	C	175(H)	LEU
1	C	175(J)	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/135 (100%)	129 (96%)	6 (4%)	28	61
1	C	135/135 (100%)	129 (96%)	6 (4%)	28	61
1	E	135/135 (100%)	128 (95%)	7 (5%)	23	55
1	G	135/135 (100%)	127 (94%)	8 (6%)	19	49
1	I	135/135 (100%)	131 (97%)	4 (3%)	41	75
1	K	135/135 (100%)	129 (96%)	6 (4%)	28	61
2	B	82/82 (100%)	77 (94%)	5 (6%)	18	48
2	D	82/82 (100%)	76 (93%)	6 (7%)	14	38
2	F	82/82 (100%)	75 (92%)	7 (8%)	10	31
2	H	82/82 (100%)	77 (94%)	5 (6%)	18	48
2	J	82/82 (100%)	77 (94%)	5 (6%)	18	48
2	L	82/82 (100%)	76 (93%)	6 (7%)	14	38
3	Q	3/3 (100%)	3 (100%)	0	100	100
3	R	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	S	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	T	3/3 (100%)	3 (100%)	0	100	100
3	U	3/3 (100%)	3 (100%)	0	100	100
3	V	3/3 (100%)	3 (100%)	0	100	100
All	All	1320/1320 (100%)	1247 (94%)	73 (6%)	21	53

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	365	ASP
1	G	175	LYS
2	L	335	ASN
2	F	382	MET
1	G	175(J)	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	286	GLN
1	G	210	GLN
1	K	286	GLN
1	E	291	GLN
2	F	336	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ASA	U	4504	1,3	3,7,7	1.77	1 (33%)	1,8,8	0.91	0
3	ASA	S	4304	1,3	3,7,7	1.96	1 (33%)	1,8,8	1.50	0
3	ASA	Q	4104	1,3	3,7,7	2.10	2 (66%)	1,8,8	0.84	0
3	ASA	V	4604	1	3,7,7	1.80	1 (33%)	1,8,8	0.80	0
3	ASA	R	4204	1,3	3,7,7	1.59	1 (33%)	1,8,8	0.95	0
3	ASA	T	4404	1,3	3,7,7	1.69	1 (33%)	1,8,8	0.63	0



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASA	U	4504	1,3	-	2/3/6/6	-
3	ASA	S	4304	1,3	-	0/3/6/6	-
3	ASA	Q	4104	1,3	-	2/3/6/6	-
3	ASA	V	4604	1	-	0/3/6/6	-
3	ASA	R	4204	1,3	-	2/3/6/6	-
3	ASA	T	4404	1,3	-	3/3/6/6	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	4304	ASA	O-C	3.30	1.33	1.19
3	U	4504	ASA	O-C	3.03	1.32	1.19
3	V	4604	ASA	O-C	3.02	1.32	1.19
3	T	4404	ASA	O-C	2.77	1.31	1.19
3	R	4204	ASA	O-C	2.70	1.30	1.19

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	4504	ASA	C-CA-CB-CG
3	Q	4104	ASA	C-CA-CB-CG
3	R	4204	ASA	C-CA-CB-CG
3	T	4404	ASA	O-C-CA-CB
3	T	4404	ASA	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	4504	ASA	1	0
3	Q	4104	ASA	1	0
3	T	4404	ASA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	4603:VAL	C	4604:ASA	N	1.20

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	153/153 (100%)	-0.01	5 (3%) 46 41	26, 51, 79, 97	0
1	C	153/153 (100%)	0.14	8 (5%) 27 23	30, 60, 85, 100	0
1	E	153/153 (100%)	0.33	7 (4%) 32 29	34, 65, 94, 99	0
1	G	153/153 (100%)	-0.06	2 (1%) 77 77	23, 49, 81, 96	0
1	I	153/153 (100%)	0.34	14 (9%) 9 6	42, 64, 96, 100	0
1	K	153/153 (100%)	0.66	21 (13%) 3 2	45, 72, 99, 100	0
2	B	89/89 (100%)	-0.10	1 (1%) 80 80	26, 48, 84, 95	0
2	D	89/89 (100%)	0.15	5 (5%) 24 20	27, 57, 91, 98	0
2	F	89/89 (100%)	0.54	8 (8%) 9 7	28, 66, 97, 99	0
2	H	89/89 (100%)	-0.16	2 (2%) 62 59	31, 49, 85, 96	0
2	J	89/89 (100%)	0.34	6 (6%) 17 13	37, 66, 97, 100	0
2	L	89/89 (100%)	0.81	18 (20%) 1 0	39, 70, 97, 100	0
3	Q	3/5 (60%)	-0.62	0 100 100	30, 30, 39, 42	0
3	R	3/5 (60%)	0.14	0 100 100	70, 70, 76, 87	0
3	S	3/5 (60%)	1.35	1 (33%) 0 0	72, 72, 86, 93	0
3	T	3/5 (60%)	-0.72	0 100 100	33, 33, 35, 48	0
3	U	3/5 (60%)	1.00	0 100 100	92, 92, 97, 99	0
3	V	3/5 (60%)	1.23	1 (33%) 0 0	100, 100, 100, 100	0
All	All	1470/1482 (99%)	0.25	99 (6%) 17 13	23, 60, 95, 100	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	402	SER	5.3
2	J	320	TYR	4.6
1	E	298	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	F	359	GLU	4.2
1	K	288	ASP	4.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ASA	V	4604	8/8	0.76	0.47	89,99,100,100	0
3	ASA	S	4304	8/8	0.77	0.33	68,89,96,100	0
3	ASA	U	4504	8/8	0.88	0.28	65,76,82,89	0
3	ASA	R	4204	8/8	0.94	0.17	60,65,72,80	0
3	ASA	T	4404	8/8	0.96	0.18	19,30,35,35	0
3	ASA	Q	4104	8/8	0.97	0.19	41,42,45,48	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.