



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 1F9E / pdb_00001f9e
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

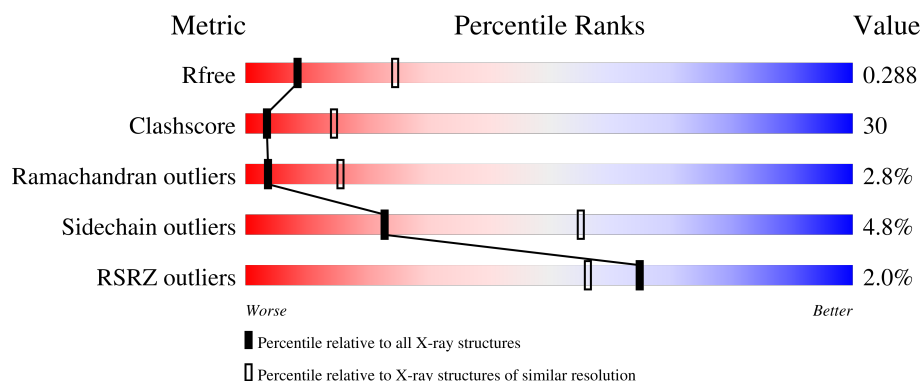
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	% 58% 38% 5%
1	C	153	% 52% 41% 7%
1	E	153	% 51% 39% 9%
1	G	153	% 57% 35% 7%
1	I	153	54% 39% 8%

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Mol	Chain	Length	Quality of chain
1	K	153	
2	B	89	
2	D	89	
2	F	89	
2	H	89	
2	J	89	
2	L	89	
3	Q	5	
3	R	5	
3	S	5	
3	T	5	
3	U	5	
3	V	5	

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 subunit p18.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	HIS	ASP	variant	UNP Q14790
C	204	HIS	ASP	variant	UNP Q14790
E	204	HIS	ASP	variant	UNP Q14790
G	204	HIS	ASP	variant	UNP Q14790
I	204	HIS	ASP	variant	UNP Q14790
K	204	HIS	ASP	variant	UNP Q14790

- Molecule 2 is a protein called Caspase-8 subunit p10.

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

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

- 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		

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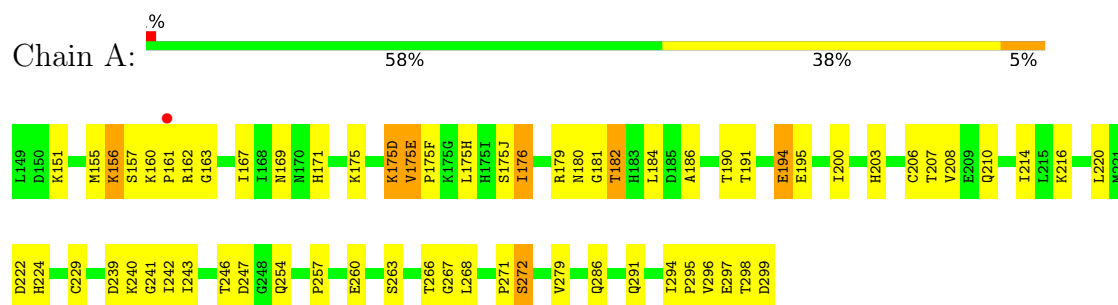
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	O 1	0	0
4	I	5	Total 5	O 5	0	0
4	K	2	Total 2	O 2	0	0
4	L	1	Total 1	O 1	0	0

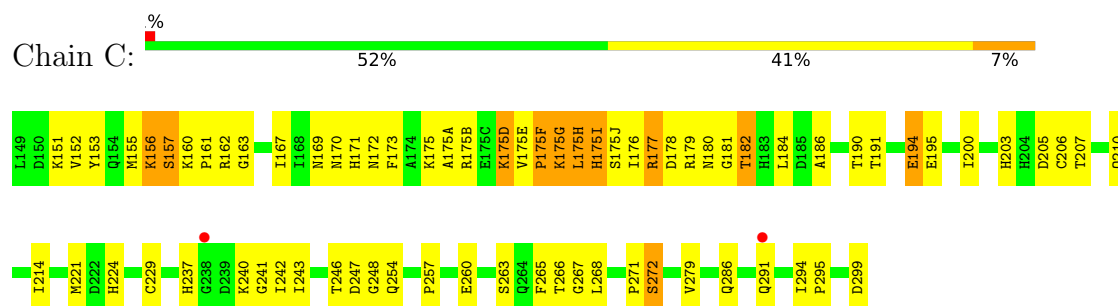
3 Residue-property plots

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.

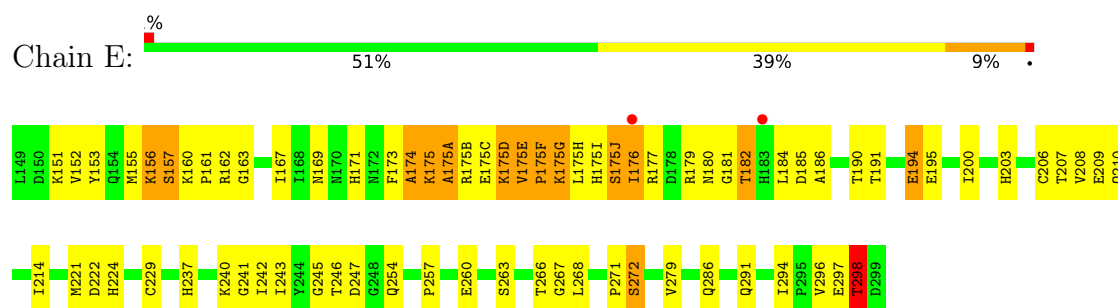
• Molecule 1: Caspase-8 subunit p18



• Molecule 1: Caspase-8 subunit p18

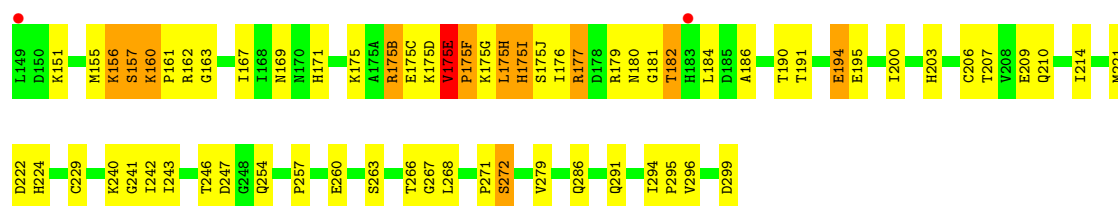


• Molecule 1: Caspase-8 subunit p18



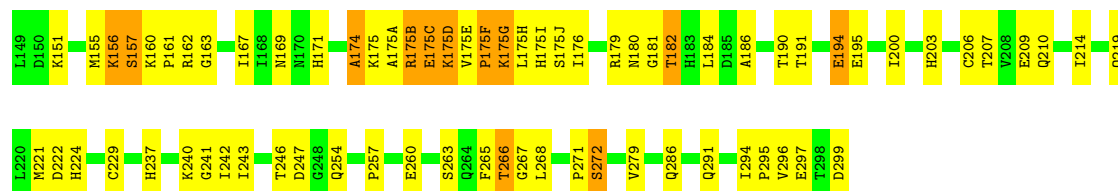
• Molecule 1: Caspase-8 subunit p18





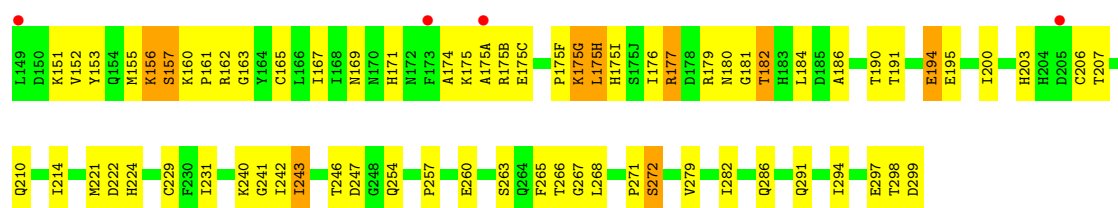
• Molecule 1: Caspase-8 subunit p18

Chain I: 54% 39% 8%



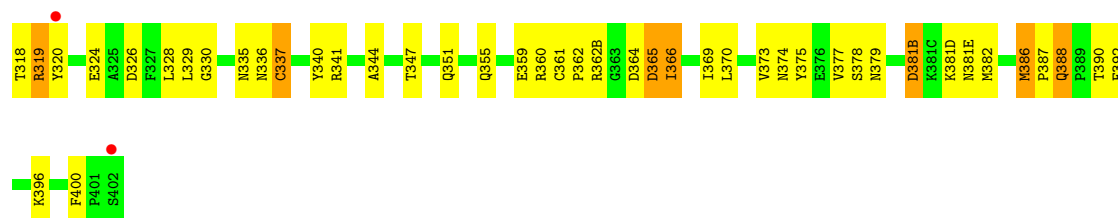
• Molecule 1: Caspase-8 subunit p18

Chain K: 54% 40% 6%



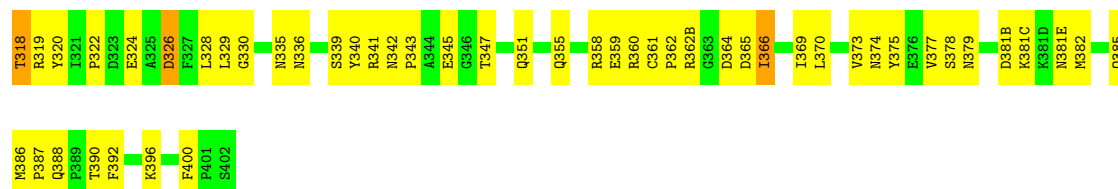
• Molecule 2: Caspase-8 subunit p10

Chain B: 51% 42% 8%

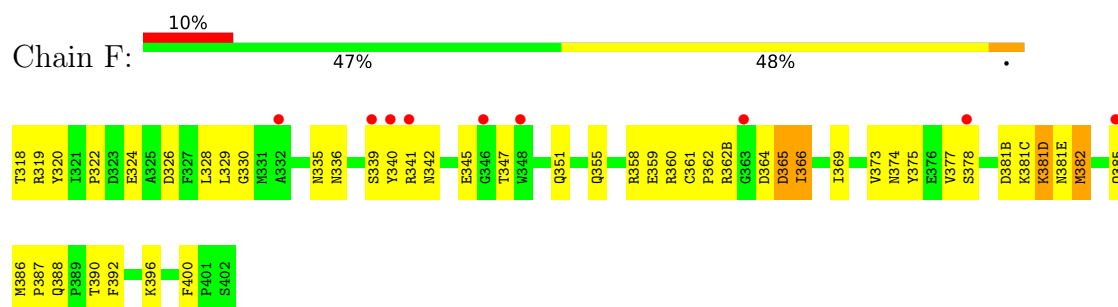


• Molecule 2: Caspase-8 subunit p10

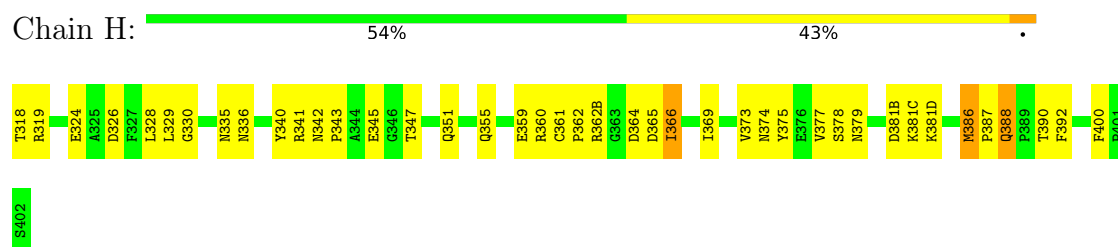
Chain D: 45% 52% 3%



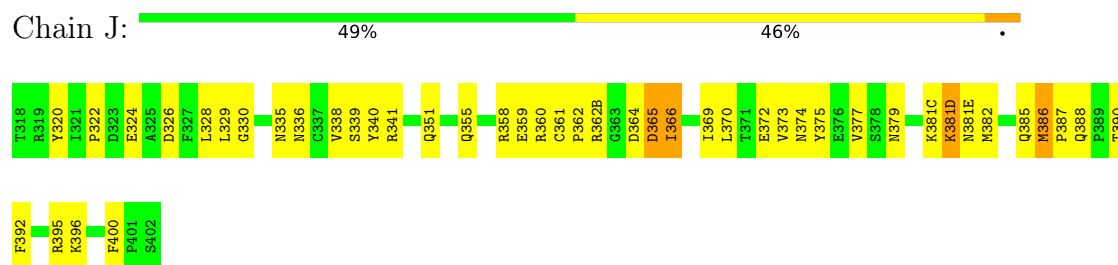
- Molecule 2: Caspase-8 subunit p10



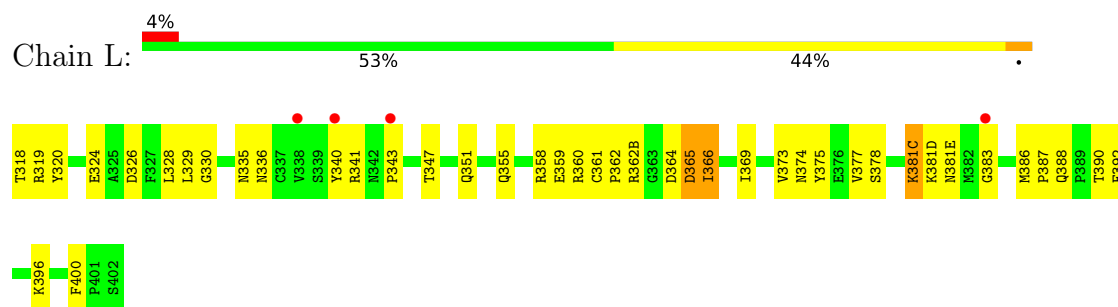
- Molecule 2: Caspase-8 subunit p10



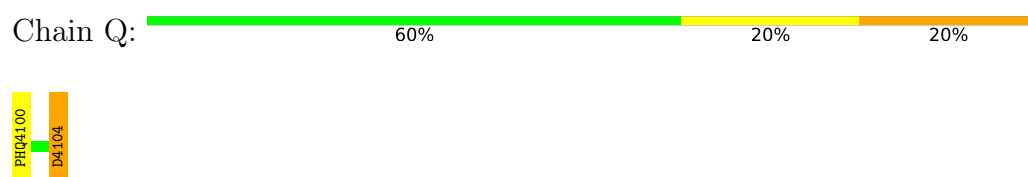
- Molecule 2: Caspase-8 subunit p10



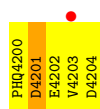
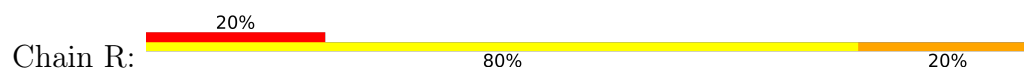
- Molecule 2: Caspase-8 subunit p10



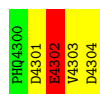
- Molecule 3: (PHQ)DEVD



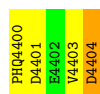
● Molecule 3: (PHQ)DEVD



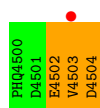
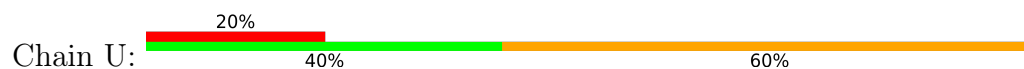
● Molecule 3: (PHQ)DEVD



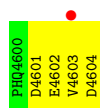
● Molecule 3: (PHQ)DEVD



● 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, α , β , γ	98.03Å 188.75Å 209.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 99.1 (19.94-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.93Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.289 0.240 , 0.288	Depositor DCC
R_{free} test set	4318 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11926	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.70	0/1248	1.02	4/1682 (0.2%)
1	C	0.64	0/1248	1.01	3/1682 (0.2%)
1	E	0.61	0/1248	1.05	6/1682 (0.4%)
1	G	0.71	0/1248	1.07	7/1682 (0.4%)
1	I	0.60	0/1248	1.02	3/1682 (0.2%)
1	K	0.57	0/1248	1.03	3/1682 (0.2%)
2	B	0.66	0/732	1.07	8/989 (0.8%)
2	D	0.59	0/732	1.04	4/989 (0.4%)
2	F	0.62	0/731	1.07	4/989 (0.4%)
2	H	0.65	0/732	1.07	6/989 (0.6%)
2	J	0.58	0/732	1.07	6/989 (0.6%)
2	L	0.57	0/732	1.04	3/989 (0.3%)
3	Q	1.93	0/23	1.81	0/30
3	R	2.74	2/23 (8.7%)	2.13	2/30 (6.7%)
3	S	2.28	1/23 (4.3%)	1.51	0/30
3	T	2.08	0/23	1.84	1/30 (3.3%)
3	U	2.21	1/23 (4.3%)	1.66	0/30
3	V	2.34	0/23	1.92	0/30
All	All	0.67	4/12017 (0.0%)	1.05	60/16206 (0.4%)

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	S	4302	GLU	N-CA	6.13	1.53	1.45
3	R	4202	GLU	N-CA	5.59	1.53	1.46
3	U	4502	GLU	N-CA	5.58	1.52	1.46
3	R	4201	ASP	CA-C	5.53	1.64	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	175(I)	HIS	N-CA-C	-10.15	97.92	110.41
1	E	175(E)	VAL	N-CA-C	9.40	118.14	107.89
1	G	175(E)	VAL	N-CA-C	8.78	116.99	107.60
1	A	175(D)	LYS	N-CA-C	7.76	119.82	111.36
1	C	175(D)	LYS	N-CA-C	7.67	120.72	111.82

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	79	0
1	C	1220	0	1198	90	0
1	E	1220	0	1198	97	0
1	G	1220	0	1198	68	0
1	I	1220	0	1198	89	0
1	K	1220	0	1198	91	0
2	B	718	0	712	59	0
2	D	718	0	712	58	0
2	F	717	0	712	54	0
2	H	718	0	712	46	0
2	J	718	0	712	52	0
2	L	718	0	712	58	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	697	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 30.

The worst 5 of 697 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
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%)	9	32
1	C	151/153 (99%)	125 (83%)	19 (13%)	7 (5%)	2	7
1	E	151/153 (99%)	128 (85%)	13 (9%)	10 (7%)	1	3
1	G	151/153 (99%)	132 (87%)	17 (11%)	2 (1%)	9	32
1	I	151/153 (99%)	126 (83%)	16 (11%)	9 (6%)	1	4
1	K	151/153 (99%)	131 (87%)	15 (10%)	5 (3%)	3	13
2	B	87/89 (98%)	78 (90%)	7 (8%)	2 (2%)	5	19
2	D	87/89 (98%)	81 (93%)	6 (7%)	0	100	100
2	F	87/89 (98%)	78 (90%)	8 (9%)	1 (1%)	11	36
2	H	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
2	J	87/89 (98%)	80 (92%)	5 (6%)	2 (2%)	5	19
2	L	87/89 (98%)	79 (91%)	7 (8%)	1 (1%)	11	36
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	4	15

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 ⓘ

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%)	25	59
1	C	135/135 (100%)	129 (96%)	6 (4%)	25	59
1	E	135/135 (100%)	129 (96%)	6 (4%)	25	59
1	G	135/135 (100%)	119 (88%)	16 (12%)	5	16
1	I	135/135 (100%)	130 (96%)	5 (4%)	30	64
1	K	135/135 (100%)	130 (96%)	5 (4%)	30	64
2	B	82/82 (100%)	80 (98%)	2 (2%)	43	75
2	D	82/82 (100%)	78 (95%)	4 (5%)	22	54
2	F	82/82 (100%)	78 (95%)	4 (5%)	22	54
2	H	82/82 (100%)	79 (96%)	3 (4%)	30	64
2	J	82/82 (100%)	80 (98%)	2 (2%)	43	75
2	L	82/82 (100%)	80 (98%)	2 (2%)	43	75
3	Q	3/3 (100%)	3 (100%)	0	100	100
3	R	3/3 (100%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	2 (67%)	1 (33%)	0	0
3	V	3/3 (100%)	3 (100%)	0	100	100
All	All	1320/1320 (100%)	1256 (95%)	64 (5%)	23	55

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	156	LYS
1	K	184	LEU
1	E	272	SER
1	E	243	ILE
1	K	243	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	171	HIS
1	K	204	HIS
2	L	336	ASN
1	E	169	ASN
2	D	379	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	T	4404	3,1	6,7,7	1.44	1 (16%)	4,8,8	1.06	0
3	ASA	V	4604	1	6,7,7	1.57	1 (16%)	4,8,8	1.16	0
3	ASA	Q	4104	3,1	6,7,7	1.87	3 (50%)	4,8,8	1.26	0
3	ASA	U	4504	3,1	6,7,7	1.51	1 (16%)	4,8,8	1.14	0
3	ASA	S	4304	3,1	6,7,7	1.63	1 (16%)	4,8,8	1.06	0
3	ASA	R	4204	3,1	6,7,7	1.39	1 (16%)	4,8,8	1.04	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	T	4404	3,1	-	3/5/6/6	-
3	ASA	V	4604	1	-	2/5/6/6	-
3	ASA	Q	4104	3,1	-	2/5/6/6	-
3	ASA	U	4504	3,1	-	2/5/6/6	-
3	ASA	S	4304	3,1	-	0/5/6/6	-
3	ASA	R	4204	3,1	-	2/5/6/6	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	4304	ASA	O-C	3.45	1.33	1.20
3	U	4504	ASA	O-C	3.16	1.32	1.20
3	V	4604	ASA	O-C	3.16	1.32	1.20
3	T	4404	ASA	O-C	2.90	1.31	1.20
3	R	4204	ASA	O-C	2.82	1.30	1.20

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
3	U	4504	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	T	4404	ASA	1	0
3	Q	4104	ASA	1	0
3	U	4504	ASA	1	0

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](#)

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

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	153/153 (100%)	-0.14	1 (0%) 84 79	26, 51, 78, 97	0
1	C	153/153 (100%)	0.11	2 (1%) 75 67	30, 60, 85, 100	0
1	E	153/153 (100%)	0.35	2 (1%) 75 67	34, 65, 94, 99	0
1	G	153/153 (100%)	-0.03	2 (1%) 75 67	23, 49, 81, 96	0
1	I	153/153 (100%)	0.17	0 100 100	42, 64, 96, 100	0
1	K	153/153 (100%)	0.41	4 (2%) 57 48	45, 72, 99, 100	0
2	B	89/89 (100%)	-0.05	2 (2%) 62 53	26, 48, 84, 95	0
2	D	89/89 (100%)	0.19	0 100 100	27, 57, 91, 98	0
2	F	89/89 (100%)	0.69	9 (10%) 12 10	28, 66, 97, 99	0
2	H	89/89 (100%)	-0.10	0 100 100	31, 49, 85, 96	0
2	J	89/89 (100%)	0.35	0 100 100	37, 66, 97, 100	0
2	L	89/89 (100%)	0.61	4 (4%) 38 30	39, 70, 97, 100	0
3	Q	3/5 (60%)	-0.52	0 100 100	30, 30, 39, 42	0
3	R	3/5 (60%)	1.27	1 (33%) 1 1	70, 70, 76, 87	0
3	S	3/5 (60%)	1.59	0 100 100	72, 72, 86, 93	0
3	T	3/5 (60%)	-0.73	0 100 100	33, 33, 35, 48	0
3	U	3/5 (60%)	1.25	1 (33%) 1 1	92, 92, 97, 99	0
3	V	3/5 (60%)	1.42	1 (33%) 1 1	100, 100, 100, 100	0
All	All	1470/1482 (99%)	0.20	29 (1%) 65 56	23, 60, 95, 100	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	175(A)	ALA	3.3
2	L	338	VAL	2.9
2	F	341	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	340	TYR	2.6
1	E	183	HIS	2.6

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, 95th 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 ²)	Q<0.9
3	ASA	V	4604	8/8	0.55	0.18	89,99,100,100	0
3	ASA	S	4304	8/8	0.79	0.15	68,89,96,100	0
3	ASA	U	4504	8/8	0.90	0.11	65,76,82,89	0
3	ASA	R	4204	8/8	0.90	0.10	60,65,72,80	0
3	ASA	T	4404	8/8	0.94	0.06	19,30,35,35	0
3	ASA	Q	4104	8/8	0.98	0.05	41,42,45,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.