



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:45 PM GMT

PDB ID : 2P2C  
Title : Inhibition of caspase-2 by a designed ankyrin repeat protein (DARPin)  
Authors : Roschitzki Voser, H; Briand, C.; Capitani, G.; Gruetter, M.G.  
Deposited on : 2007-03-07  
Resolution : 3.24 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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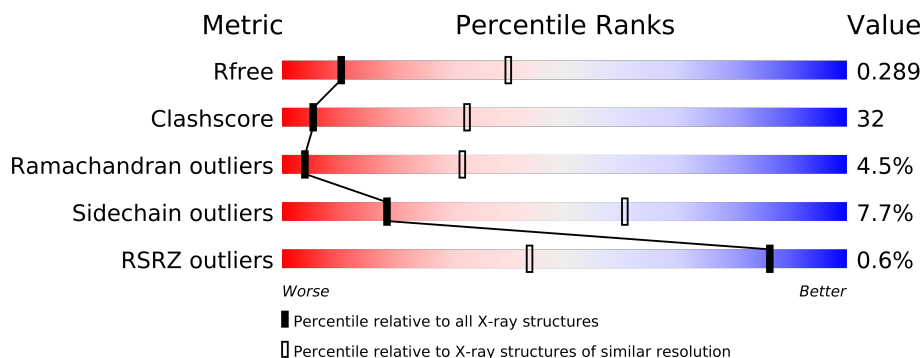
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.24 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.



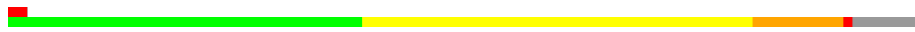
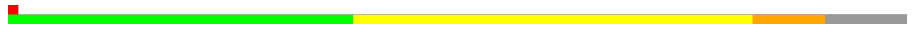


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1080 (3.30-3.18)
Clashscore	79885	1369 (3.30-3.18)
Ramachandran outliers	78287	1342 (3.30-3.18)
Sidechain outliers	78261	1340 (3.30-3.18)
RSRZ outliers	66119	1081 (3.30-3.18)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	169	
1	C	169	
1	E	169	
1	G	169	
1	I	169	
1	K	169	
2	B	106	
2	D	106	
2	F	106	
2	H	106	
2	J	106	
2	L	106	
3	P	169	
3	Q	169	

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Mol	Chain	Length	Quality of chain
3	R	169	
3	S	169	
3	T	169	
3	U	169	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19285 atoms, of which 0 are hydrogen and 0 are deuterium.

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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1284	810	223	243	8			
1	C	161	Total	C	N	O	S	0	0	0
			1276	804	222	242	8			
1	E	160	Total	C	N	O	S	0	0	0
			1267	800	221	238	8			
1	G	160	Total	C	N	O	S	0	0	0
			1267	800	221	238	8			
1	I	157	Total	C	N	O	S	0	0	0
			1244	786	217	234	7			
1	K	158	Total	C	N	O	S	0	0	0
			1252	792	218	235	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	CLONING ARTIFACT	UNP P42575
A	1	ALA	-	CLONING ARTIFACT	UNP P42575
A	7	LEU	VAL	VARIANT	UNP P42575
C	0	MET	-	CLONING ARTIFACT	UNP P42575
C	1	ALA	-	CLONING ARTIFACT	UNP P42575
C	7	LEU	VAL	VARIANT	UNP P42575
E	0	MET	-	CLONING ARTIFACT	UNP P42575
E	1	ALA	-	CLONING ARTIFACT	UNP P42575
E	7	LEU	VAL	VARIANT	UNP P42575
G	0	MET	-	CLONING ARTIFACT	UNP P42575
G	1	ALA	-	CLONING ARTIFACT	UNP P42575
G	7	LEU	VAL	VARIANT	UNP P42575
I	0	MET	-	CLONING ARTIFACT	UNP P42575
I	1	ALA	-	CLONING ARTIFACT	UNP P42575
I	7	LEU	VAL	VARIANT	UNP P42575
K	0	MET	-	CLONING ARTIFACT	UNP P42575
K	1	ALA	-	CLONING ARTIFACT	UNP P42575

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Chain	Residue	Modelled	Actual	Comment	Reference
K	7	LEU	VAL	VARIANT	UNP P42575

- Molecule 2 is a protein called Caspase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			760	477	137	134	12			
2	D	98	Total	C	N	O	S	0	0	0
			777	487	140	138	12			
2	F	96	Total	C	N	O	S	0	0	0
			760	477	137	134	12			
2	H	98	Total	C	N	O	S	0	0	0
			776	488	140	136	12			
2	J	94	Total	C	N	O	S	0	0	0
			746	467	135	132	12			
2	L	92	Total	C	N	O	S	0	0	0
			727	456	130	130	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	MET	-	CLONING ARTIFACT	UNP P42575
D	200	MET	-	CLONING ARTIFACT	UNP P42575
F	200	MET	-	CLONING ARTIFACT	UNP P42575
H	200	MET	-	CLONING ARTIFACT	UNP P42575
J	200	MET	-	CLONING ARTIFACT	UNP P42575
L	200	MET	-	CLONING ARTIFACT	UNP P42575

- Molecule 3 is a protein called Caspase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	158	Total	C	N	O	S	0	0	0
			1207	762	207	237	1			
3	Q	158	Total	C	N	O	S	0	0	0
			1209	764	205	239	1			
3	R	157	Total	C	N	O	S	0	0	0
			1198	757	205	235	1			
3	S	153	Total	C	N	O	S	0	0	0
			1168	740	197	230	1			
3	T	152	Total	C	N	O	S	0	0	0
			1161	735	197	228	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	154	Total	C	N	O	S	0	0	0
			1177	745	199	232	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	O	0	0
			4	4		
4	C	5	Total	O	0	0
			5	5		
4	D	5	Total	O	0	0
			5	5		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	G	2	Total	O	0	0
			2	2		
4	H	4	Total	O	0	0
			4	4		
4	I	1	Total	O	0	0
			1	1		
4	L	1	Total	O	0	0
			1	1		
4	P	1	Total	O	0	0
			1	1		
4	Q	2	Total	O	0	0
			2	2		
4	R	1	Total	O	0	0
			1	1		
4	S	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

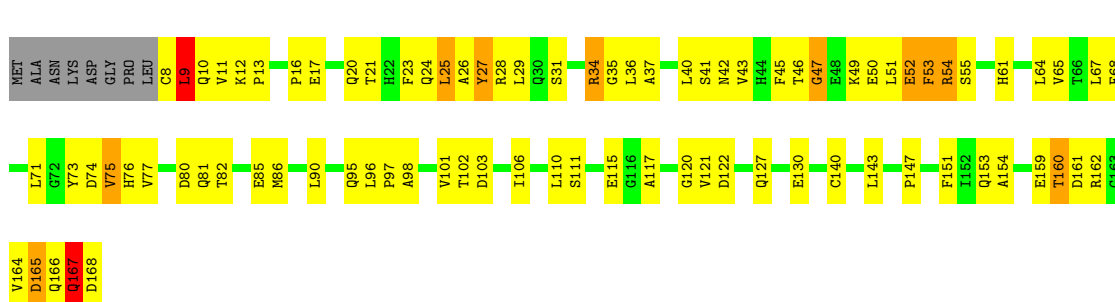
#### • Molecule 1: Caspase-2

Chain A:



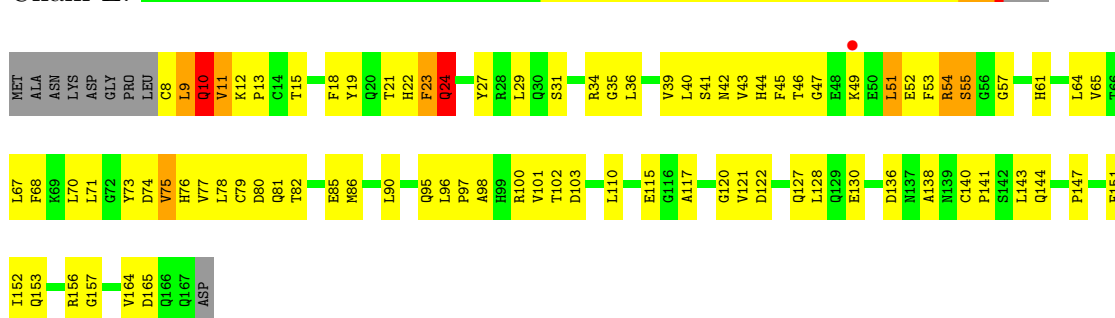
#### • Molecule 1: Caspase-2

Chain C:



#### • Molecule 1: Caspase-2

Chain E:



#### • Molecule 1: Caspase-2

Chain G:

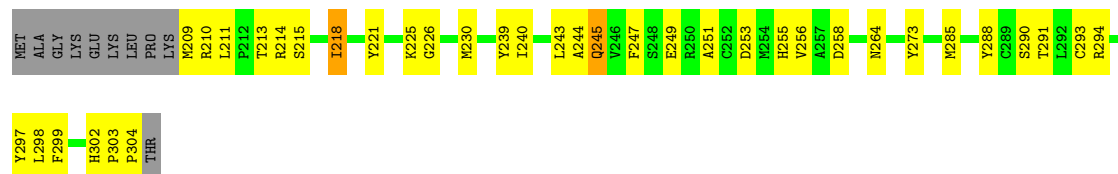






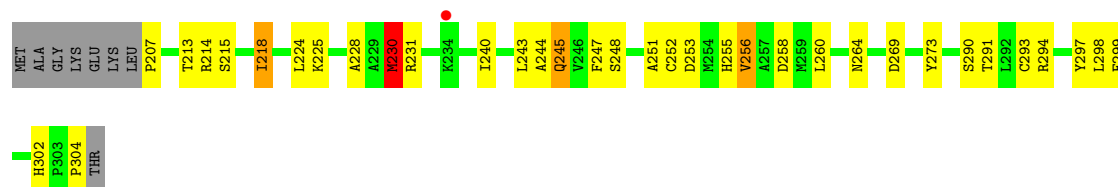
- Molecule 2: Caspase-2

Chain F:



- Molecule 2: Caspase-2

Chain H:



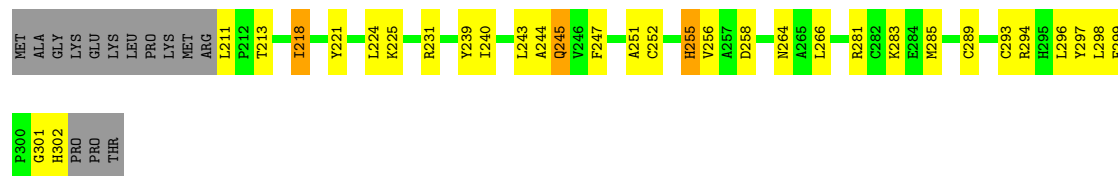
- Molecule 2: Caspase-2

Chain J:



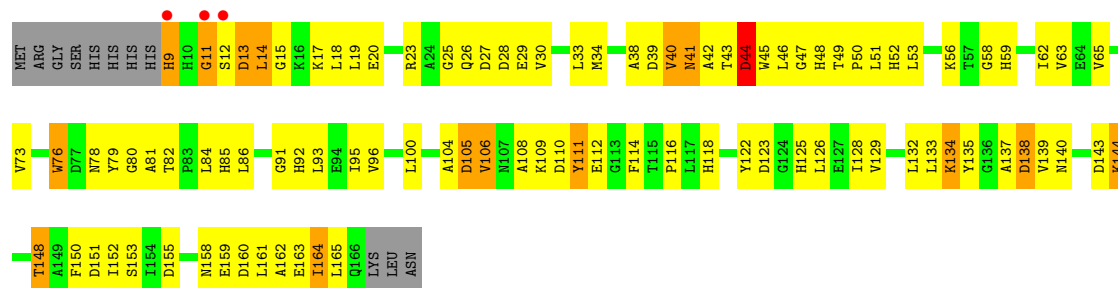
- Molecule 2: Caspase-2

Chain L:



- Molecule 3: Caspase-2

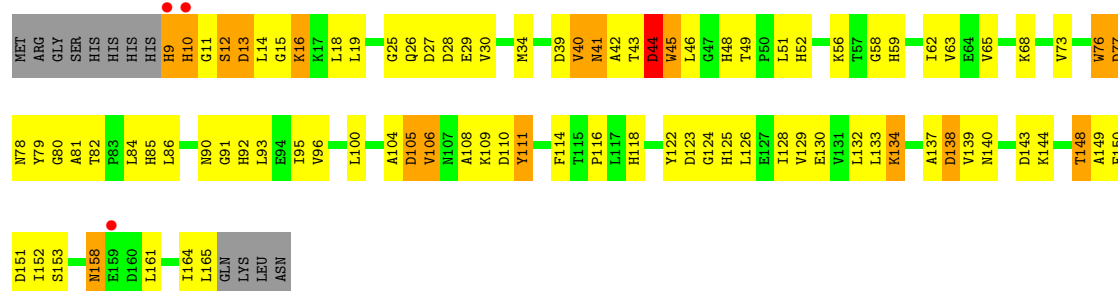
Chain P:



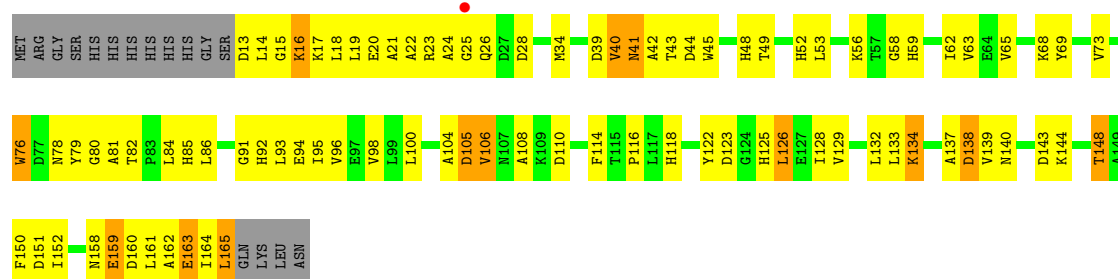
- Molecule 3: Caspase-2

F150	D77	ME1
D151	M78	ARG
I152	Y79	GLY
S153	G80	SER
	A81	HIS
M158	T82	HIS
E159	P83	HIS
D160	L84	HIS
L161	H85	HIS
A162	R86	HIS
E163		GLY
I164	G91	S12
L165	H92	D13
Q166	L93	L14
K167	E94	
L168	V95	L18
M169	Y96	
	E97	A21
	V98	A22
	L99	R23
	L100	A24
		G25
		Q26
	D105	
	M106	E29
	M107	V30
	A108	
	K109	L33
	D110	M34
	Y111	
	E112	D39
	G113	V40
	F114	M41
	T115	A42
	P116	M44
	L117	T43
	H118	D44
		W45
	Y122	L46
	D123	G47
	G124	H48
	H125	T49
	L126	P50
	E127	L51
	I128	H52
	V129	L53
	L132	K56
	L133	T57
	K134	G58
		H59
	A137	L60
	D138	E61
	V139	I62
	M140	V63
		E64
	D143	V65
	K144	
		V73
	T148	M76
	A149	

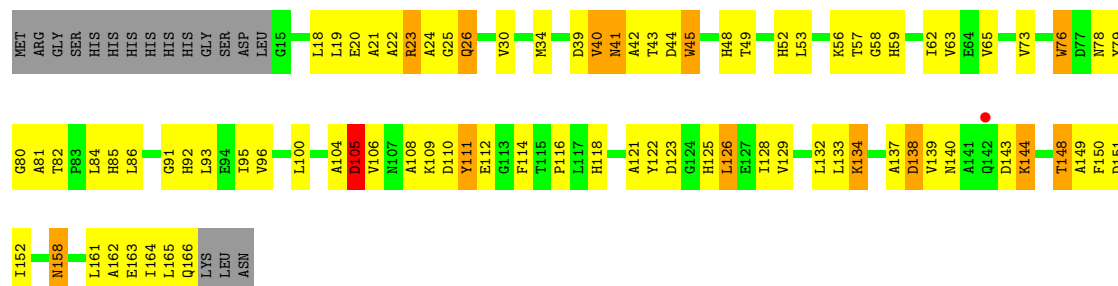
Chain R: 



Chain S:

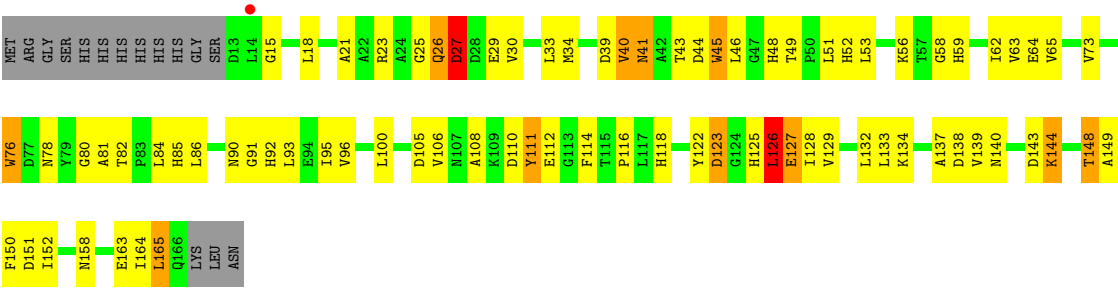


Chain T: 



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

Chain U:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.02Å 229.21Å 114.93Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.00 – 3.24 29.51 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.24) 97.6 (29.51-3.24)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	5.90	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.262 , 0.305 0.256 , 0.289	Depositor DCC
$R_{free}$ test set	1023 reflections (2.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 21.3	EDS
Estimated twinning fraction	0.235 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 46594 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.44	1/1309 (0.1%)	0.64	0/1769
1	C	0.38	0/1301	0.63	1/1758 (0.1%)
1	E	0.48	0/1292	0.68	2/1747 (0.1%)
1	G	0.42	0/1292	0.63	0/1747
1	I	0.38	0/1269	0.62	0/1716
1	K	0.39	0/1277	0.62	0/1727
2	B	0.41	0/778	0.63	0/1047
2	D	0.38	0/795	0.63	0/1068
2	F	0.39	0/778	0.65	0/1047
2	H	0.40	0/795	0.66	0/1069
2	J	0.38	0/762	0.64	0/1023
2	L	0.37	0/743	0.59	0/999
3	P	0.54	1/1231 (0.1%)	0.76	2/1674 (0.1%)
3	Q	0.50	0/1231	0.70	1/1672 (0.1%)
3	R	0.51	0/1222	0.73	2/1662 (0.1%)
3	S	0.61	3/1190 (0.3%)	0.78	3/1619 (0.2%)
3	T	0.51	0/1183	0.78	4/1609 (0.2%)
3	U	0.52	2/1199 (0.2%)	0.73	3/1631 (0.2%)
All	All	0.46	7/19647 (0.0%)	0.68	18/26584 (0.1%)

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
2	F	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	106	VAL	CB-CG1	-8.08	1.35	1.52
3	P	12	SER	CB-OG	7.92	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	127	GLU	CD-OE1	-7.16	1.17	1.25
1	A	69	LYS	CE-NZ	-7.09	1.31	1.49
3	S	106	VAL	CB-CG2	-6.92	1.38	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	126	LEU	CA-CB-CG	9.13	136.29	115.30
3	S	106	VAL	CG1-CB-CG2	-7.89	98.27	110.90
3	T	105	ASP	CB-CG-OD1	7.72	125.25	118.30
3	S	126	LEU	CB-CG-CD1	6.77	122.50	111.00
3	T	105	ASP	OD1-CG-OD2	-6.44	111.06	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	288	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1284	0	1256	95	0
1	C	1276	0	1245	89	0
1	E	1267	0	1241	104	0
1	G	1267	0	1241	93	0
1	I	1244	0	1217	99	0
1	K	1252	0	1228	99	0
2	B	760	0	748	46	0
2	D	777	0	768	48	0
2	F	760	0	748	35	0
2	H	776	0	769	39	0
2	J	746	0	734	47	0
2	L	727	0	712	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1207	0	1162	95	0
3	Q	1209	0	1175	81	0
3	R	1198	0	1154	89	0
3	S	1168	0	1132	88	0
3	T	1161	0	1125	99	0
3	U	1177	0	1140	86	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	4	0	0	1	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
All	All	19285	0	18795	1225	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 1225 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:T:25:GLY:HA2	3:T:59:HIS:CD2	1.74	1.21
2:J:255:HIS:HE1	2:J:258:ASP:OD2	1.24	1.17
2:L:255:HIS:HE1	2:L:258:ASP:OD2	1.27	1.16
2:D:255:HIS:HE1	2:D:258:ASP:OD2	1.33	1.12
2:H:255:HIS:HE1	2:H:258:ASP:OD2	1.35	1.10

There are no symmetry-related clashes.

## 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	160/169 (95%)	135 (84%)	21 (13%)	4 (2%)	9	52
1	C	159/169 (94%)	128 (80%)	26 (16%)	5 (3%)	7	45
1	E	158/169 (94%)	127 (80%)	26 (16%)	5 (3%)	6	43
1	G	158/169 (94%)	128 (81%)	24 (15%)	6 (4%)	5	37
1	I	155/169 (92%)	120 (77%)	28 (18%)	7 (4%)	4	32
1	K	156/169 (92%)	125 (80%)	21 (14%)	10 (6%)	2	20
2	B	94/106 (89%)	83 (88%)	7 (7%)	4 (4%)	4	34
2	D	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	11	58
2	F	94/106 (89%)	88 (94%)	4 (4%)	2 (2%)	11	58
2	H	96/106 (91%)	85 (88%)	8 (8%)	3 (3%)	7	45
2	J	92/106 (87%)	83 (90%)	5 (5%)	4 (4%)	4	34
2	L	90/106 (85%)	80 (89%)	7 (8%)	3 (3%)	6	43
3	P	156/169 (92%)	117 (75%)	26 (17%)	13 (8%)	1	12
3	Q	156/169 (92%)	121 (78%)	26 (17%)	9 (6%)	3	24
3	R	155/169 (92%)	124 (80%)	21 (14%)	10 (6%)	2	19
3	S	151/169 (89%)	117 (78%)	27 (18%)	7 (5%)	4	31
3	T	150/169 (89%)	113 (75%)	28 (19%)	9 (6%)	2	22
3	U	152/169 (90%)	119 (78%)	27 (18%)	6 (4%)	5	37
All	All	2428/2664 (91%)	1982 (82%)	337 (14%)	109 (4%)	4	32

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	52	GLU
3	P	27	ASP
3	P	126	LEU
3	P	162	ALA

### 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	142/147 (97%)	132 (93%)	10 (7%)	21	66
1	C	141/147 (96%)	130 (92%)	11 (8%)	18	60
1	E	140/147 (95%)	131 (94%)	9 (6%)	25	70
1	G	140/147 (95%)	133 (95%)	7 (5%)	34	78
1	I	137/147 (93%)	126 (92%)	11 (8%)	17	59
1	K	138/147 (94%)	131 (95%)	7 (5%)	33	77
2	B	81/89 (91%)	79 (98%)	2 (2%)	60	91
2	D	83/89 (93%)	80 (96%)	3 (4%)	47	86
2	F	81/89 (91%)	76 (94%)	5 (6%)	26	71
2	H	83/89 (93%)	78 (94%)	5 (6%)	27	73
2	J	79/89 (89%)	77 (98%)	2 (2%)	60	91
2	L	77/89 (86%)	75 (97%)	2 (3%)	59	90
3	P	122/132 (92%)	107 (88%)	15 (12%)	7	33
3	Q	123/132 (93%)	112 (91%)	11 (9%)	14	51
3	R	121/132 (92%)	103 (85%)	18 (15%)	4	22
3	S	118/132 (89%)	103 (87%)	15 (13%)	6	31
3	T	117/132 (89%)	105 (90%)	12 (10%)	10	42
3	U	119/132 (90%)	106 (89%)	13 (11%)	9	39
All	All	2042/2208 (92%)	1884 (92%)	158 (8%)	18	61

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	44	ASP
1	G	52	GLU
3	U	27	ASP
3	R	68	LYS
3	R	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	90	ASN
2	H	245	GLN
2	L	302	HIS
3	R	118	HIS

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Mol	Chain	Res	Type
1	G	76	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	162/169 (95%)	-0.11	0 100 100	41, 83, 113, 125	0
1	C	161/169 (95%)	-0.10	0 100 100	37, 81, 105, 121	0
1	E	160/169 (94%)	-0.09	1 (0%) 86 44	49, 88, 122, 142	0
1	G	160/169 (94%)	-0.09	0 100 100	36, 78, 105, 121	0
1	I	157/169 (92%)	-0.08	0 100 100	52, 91, 142, 160	0
1	K	158/169 (93%)	0.02	3 (1%) 64 19	55, 92, 156, 176	0
2	B	96/106 (90%)	-0.07	0 100 100	31, 72, 128, 136	0
2	D	98/106 (92%)	-0.08	0 100 100	35, 71, 125, 135	0
2	F	96/106 (90%)	-0.14	0 100 100	29, 73, 127, 136	0
2	H	98/106 (92%)	-0.05	1 (1%) 79 32	33, 71, 126, 136	0
2	J	94/106 (88%)	-0.06	1 (1%) 77 30	50, 75, 129, 136	0
2	L	92/106 (86%)	-0.12	0 100 100	49, 74, 122, 137	0
3	P	158/169 (93%)	0.10	3 (1%) 64 19	57, 106, 181, 191	0
3	Q	158/169 (93%)	-0.03	1 (0%) 86 44	64, 106, 177, 186	0
3	R	157/169 (92%)	0.03	3 (1%) 64 19	63, 107, 178, 186	0
3	S	153/169 (90%)	0.04	1 (0%) 84 40	67, 110, 177, 186	0
3	T	152/169 (89%)	0.21	1 (0%) 84 40	70, 112, 183, 191	0
3	U	154/169 (91%)	0.04	1 (0%) 86 44	66, 110, 182, 196	0
All	All	2464/2664 (92%)	-0.02	16 (0%) 86 44	29, 91, 168, 196	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	10	HIS	3.7
3	P	12	SER	3.1
3	Q	169	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
3	R	9	HIS	2.7
3	R	159	GLU	2.6

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.