



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:58 am GMT

PDB ID : 3M3I  
Title : Hypothetical protein from Leishmania major  
Authors : Merritt, E.A.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)  
Deposited on : 2010-03-09  
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/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:

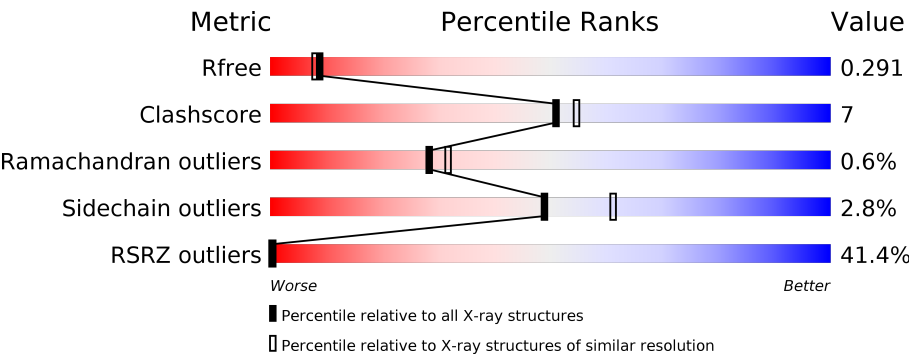
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 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 2.35 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))
$R_{free}$	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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. 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	225	<div><div>26%</div><div><div>68%</div><div>10%</div><div>•</div><div>21%</div></div></div>
1	B	225	<div><div>37%</div><div><div>64%</div><div>14%</div><div>•</div><div>21%</div></div></div>
1	C	225	<div><div>25%</div><div><div>64%</div><div>14%</div><div>•</div><div>20%</div></div></div>
1	D	225	<div><div>24%</div><div><div>67%</div><div>12%</div><div>•</div><div>20%</div></div></div>
1	E	225	<div><div>27%</div><div><div>66%</div><div>12%</div><div></div><div>21%</div></div></div>
1	F	225	<div><div>42%</div><div><div>69%</div><div>9%</div><div></div><div>22%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	225	<div><div><div>41%</div><div>63%</div><div>14%</div><div>22%</div></div></div>
1	H	225	<div><div><div>39%</div><div>68%</div><div>10%</div><div>21%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11442 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1404	893	245	260	6			
1	B	177	Total	C	N	O	S	0	1	0
			1424	904	245	269	6			
1	C	179	Total	C	N	O	S	0	1	0
			1431	909	250	266	6			
1	D	179	Total	C	N	O	S	0	0	0
			1425	906	248	265	6			
1	E	177	Total	C	N	O	S	0	1	0
			1413	898	247	262	6			
1	F	176	Total	C	N	O	S	0	1	0
			1401	893	241	261	6			
1	G	176	Total	C	N	O	S	0	1	0
			1407	896	244	261	6			
1	H	177	Total	C	N	O	S	0	1	0
			1416	898	247	265	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
A	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
A	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
A	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
A	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
A	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
A	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
A	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
B	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
B	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
B	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
B	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
B	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
B	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
B	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
C	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
C	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
C	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
C	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
C	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
C	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
C	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
C	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
D	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
D	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
D	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
D	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
D	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
D	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
D	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
D	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
E	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
E	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
E	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
E	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
E	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
E	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
E	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
E	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
F	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
F	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
F	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
F	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
F	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
F	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
F	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
F	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
G	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
G	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
G	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
G	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
G	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
G	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
G	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP Q4FX13
H	-7	MET	-	EXPRESSION TAG	UNP Q4FX13
H	-6	ALA	-	EXPRESSION TAG	UNP Q4FX13
H	-5	HIS	-	EXPRESSION TAG	UNP Q4FX13
H	-4	HIS	-	EXPRESSION TAG	UNP Q4FX13
H	-3	HIS	-	EXPRESSION TAG	UNP Q4FX13
H	-2	HIS	-	EXPRESSION TAG	UNP Q4FX13
H	-1	HIS	-	EXPRESSION TAG	UNP Q4FX13
H	0	HIS	-	EXPRESSION TAG	UNP Q4FX13

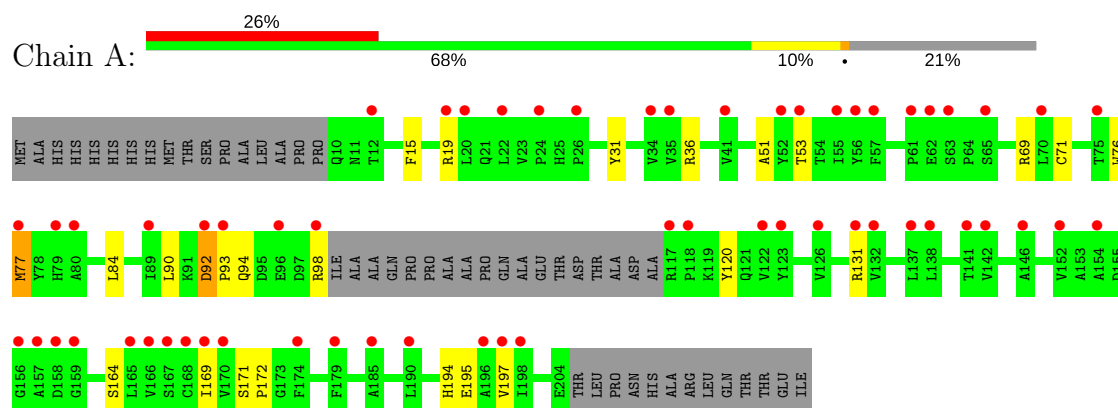
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	18	Total O 18 18	0	0
2	C	19	Total O 19 19	0	0
2	D	22	Total O 22 22	0	0
2	E	17	Total O 17 17	0	0
2	F	10	Total O 10 10	0	0
2	G	6	Total O 6 6	0	0
2	H	14	Total O 14 14	0	0

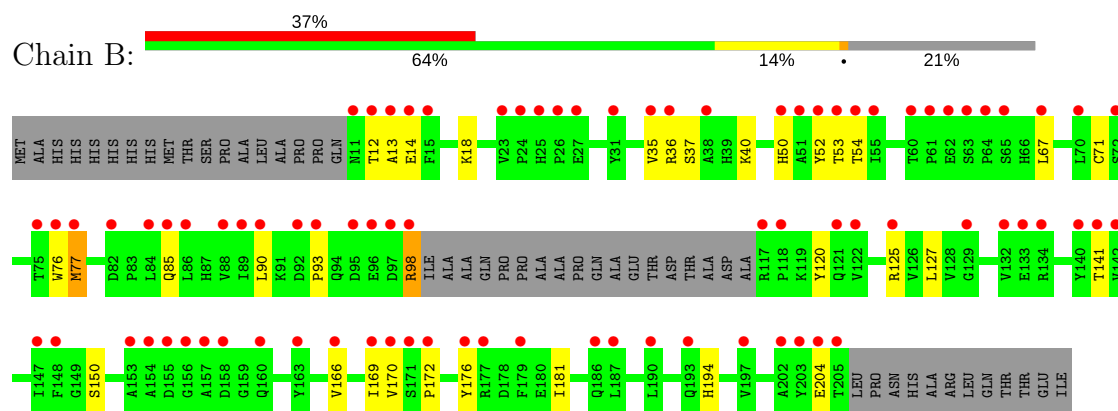
### 3 Residue-property plots [i](#)

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.

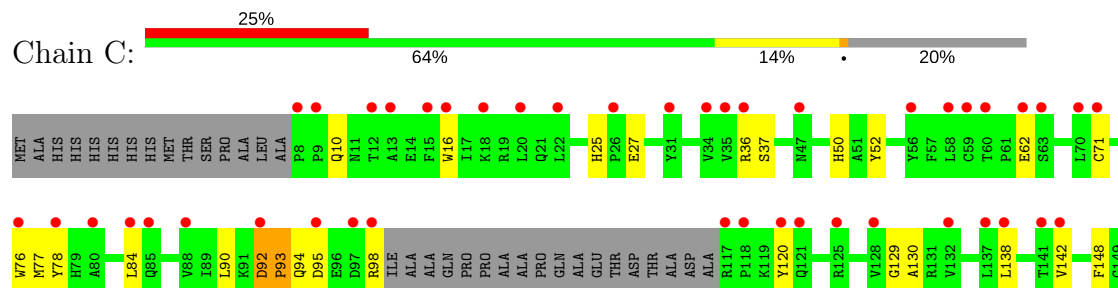
#### • Molecule 1: Putative uncharacterized protein

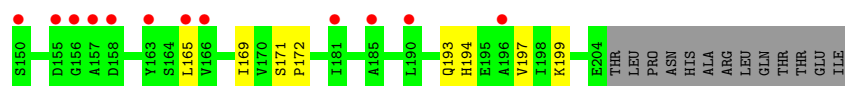


#### • Molecule 1: Putative uncharacterized protein

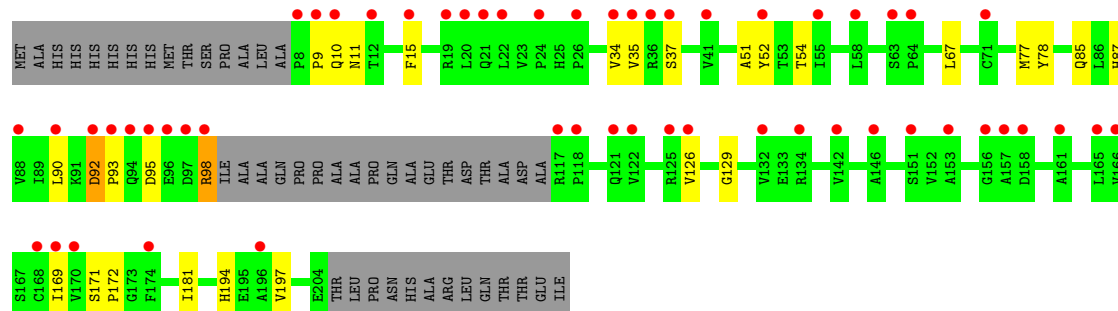


#### • Molecule 1: Putative uncharacterized protein

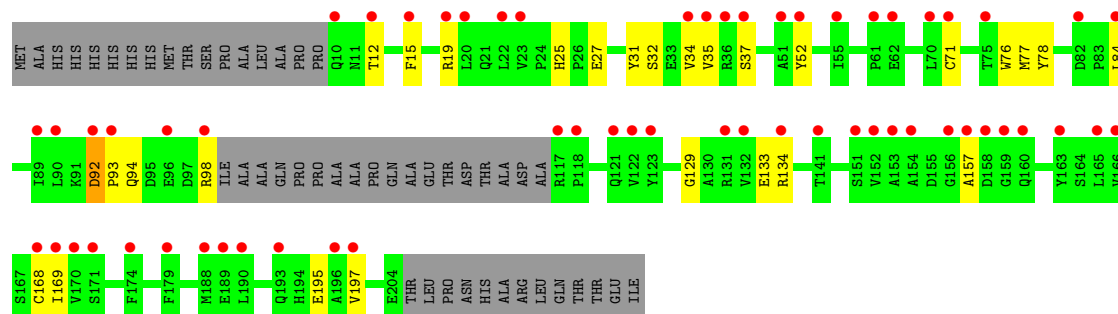




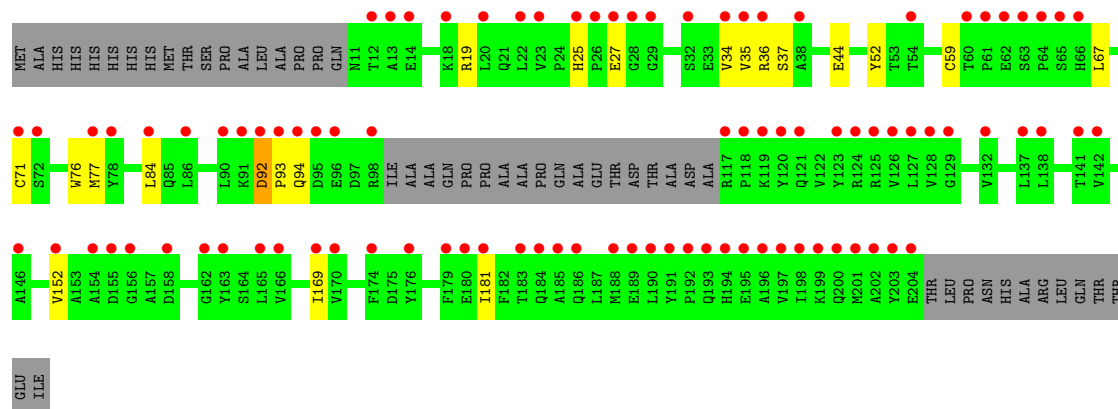
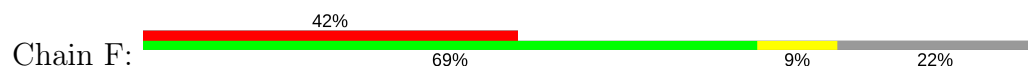
• Molecule 1: Putative uncharacterized protein



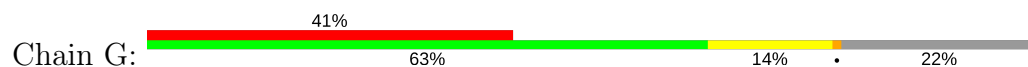
• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.98Å 98.43Å 100.76Å 71.87° 80.19° 89.57°	Depositor
Resolution (Å)	46.72 – 2.35 46.72 – 2.35	Depositor EDS
% Data completeness (in resolution range)	92.8 (46.72-2.35) 82.9 (46.72-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0106	Depositor
R, $R_{free}$	0.239 , 0.290 0.245 , 0.291	Depositor DCC
$R_{free}$ test set	3678 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.62% 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	0.51	0/1442	0.63	0/1959
1	B	0.48	0/1463	0.58	0/1989
1	C	0.53	0/1471	0.63	0/2000
1	D	0.53	0/1465	0.65	0/1991
1	E	0.53	1/1451 (0.1%)	0.64	0/1971
1	F	0.48	0/1440	0.59	0/1959
1	G	0.47	0/1446	0.58	0/1966
1	H	0.48	0/1454	0.60	0/1976
All	All	0.50	1/11632 (0.0%)	0.61	0/15811

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	168	CYS	CB-SG	-5.14	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1404	0	1328	18	0
1	B	1424	0	1338	23	0
1	C	1431	0	1351	26	0
1	D	1425	0	1351	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1413	0	1335	17	0
1	F	1401	0	1312	16	0
1	G	1407	0	1323	27	0
1	H	1416	0	1332	18	0
2	A	15	0	0	2	0
2	B	18	0	0	1	0
2	C	19	0	0	3	0
2	D	22	0	0	0	0
2	E	17	0	0	0	0
2	F	10	0	0	1	0
2	G	6	0	0	0	0
2	H	14	0	0	1	0
All	All	11442	0	10670	144	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 7.

All (144) 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:A:169:ILE:CD1	1:H:169:ILE:HD12	1.85	1.06
1:A:169:ILE:HD12	1:H:169:ILE:HD12	1.06	1.06
1:E:195:GLU:OE1	1:F:19:ARG:NH1	1.95	0.99
1:A:169:ILE:HD12	1:H:169:ILE:CD1	1.95	0.96
1:A:195:GLU:OE1	1:G:19:ARG:NH1	2.04	0.91
1:G:54:THR:HG22	1:G:169:ILE:HG12	1.56	0.88
1:F:77:MET:HE1	1:F:169:ILE:CD1	2.13	0.79
1:G:77:MET:HE1	1:G:169:ILE:HD12	1.67	0.77
1:C:92:ASP:O	1:C:94:GLN:N	2.20	0.75
1:F:77:MET:HE1	1:F:169:ILE:HD13	1.69	0.75
1:C:62:GLU:OE2	1:H:48:ARG:NE	2.22	0.72
1:C:62:GLU:OE2	1:H:48:ARG:CZ	2.38	0.71
1:D:54:THR:HG22	1:D:169:ILE:HG12	1.73	0.70
1:B:98:ARG:NH1	1:B:141:THR:O	2.26	0.68
1:E:34:VAL:HG12	1:E:35:VAL:HG13	1.75	0.67
1:H:36:ARG:HG2	1:H:53:THR:HG22	1.77	0.66
1:D:98:ARG:HD3	1:G:35:VAL:HG11	1.78	0.66
1:G:25:HIS:HD2	1:G:31:TYR:CG	2.14	0.66
1:B:12:THR:HG22	1:B:14:GLU:H	1.61	0.65
1:G:142:VAL:HG11	1:G:148:PHE:CD1	2.35	0.62
1:C:169:ILE:HD12	1:F:169:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HG22	1:B:14:GLU:N	2.15	0.60
1:B:169:ILE:HD12	1:E:169:ILE:HD12	1.84	0.59
1:H:92:ASP:O	1:H:94:GLN:N	2.36	0.59
1:A:131:ARG:NH1	2:A:225:HOH:O	2.36	0.58
1:C:25:HIS:ND1	1:C:27:GLU:HG2	2.18	0.58
1:D:54:THR:HG22	1:D:169:ILE:CG1	2.33	0.57
1:D:77:MET:HE3	1:G:77:MET:HG2	1.86	0.57
1:B:36:ARG:HG2	1:B:53:THR:HG22	1.85	0.57
1:A:92:ASP:O	1:A:94:GLN:N	2.37	0.57
1:E:92:ASP:OD2	1:E:94:GLN:NE2	2.38	0.57
1:C:199:LYS:O	2:C:233:HOH:O	2.17	0.56
1:B:77:MET:HG2	1:E:77:MET:HE2	1.88	0.56
1:B:120:TYR:O	1:B:194:HIS:NE2	2.29	0.55
1:F:59:CYS:SG	1:F:152:VAL:HG23	2.46	0.55
1:C:93:PRO:O	2:C:234:HOH:O	2.18	0.55
1:A:169:ILE:HD11	1:H:77:MET:HE1	1.87	0.55
1:D:77:MET:HE3	1:G:77:MET:SD	2.47	0.55
1:F:77:MET:CE	1:F:169:ILE:CD1	2.85	0.54
1:D:10:GLN:HG2	1:D:15:PHE:CZ	2.43	0.53
1:D:95:ASP:O	1:D:98:ARG:HG3	2.08	0.53
1:G:25:HIS:ND1	1:G:27:GLU:HG2	2.23	0.53
1:B:40:LYS:NZ	2:B:232:HOH:O	2.42	0.53
1:C:77:MET:HE3	1:C:169:ILE:HD12	1.89	0.52
1:C:95:ASP:OD1	1:C:98:ARG:NH2	2.42	0.52
1:D:67:LEU:O	1:D:181:ILE:HD12	2.08	0.52
1:C:62:GLU:OE2	1:H:48:ARG:NH2	2.42	0.52
1:A:84:LEU:HD12	1:A:164:SER:HB3	1.90	0.52
1:E:12:THR:HG21	1:G:177:ARG:HD2	1.92	0.51
1:B:40:LYS:NZ	1:B:50:HIS:CE1	2.79	0.51
1:F:36:ARG:NH2	2:F:227:HOH:O	2.29	0.50
1:D:98:ARG:HD2	1:G:35:VAL:HG12	1.94	0.50
1:B:54:THR:HG22	1:B:169:ILE:HG12	1.93	0.50
1:C:194:HIS:O	1:C:197:VAL:HG12	2.12	0.50
1:F:44:GLU:OE1	1:F:44:GLU:N	2.43	0.50
1:C:36:ARG:NH2	1:C:50:HIS:NE2	2.61	0.49
1:A:69:ARG:NH2	2:A:230:HOH:O	2.27	0.49
1:D:37:SER:HB2	1:D:52:TYR:CD2	2.48	0.49
1:A:15:PHE:CZ	1:A:19:ARG:HD2	2.48	0.49
1:F:67:LEU:O	1:F:181:ILE:HD12	2.12	0.49
1:A:194:HIS:HB3	1:A:197:VAL:CG1	2.43	0.48
1:C:130:ALA:HA	1:C:138:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:VAL:HG12	1:H:172:PRO:O	2.13	0.48
1:C:169:ILE:CD1	1:F:169:ILE:HD13	2.42	0.48
1:C:77:MET:HG2	1:F:77:MET:HE3	1.96	0.48
1:E:37:SER:HB2	1:E:52:TYR:CD2	2.49	0.48
1:B:176[B]:TYR:CD1	1:B:176[B]:TYR:C	2.87	0.48
1:C:171:SER:HA	1:C:172:PRO:C	2.34	0.47
1:G:12:THR:CG2	1:G:15:PHE:H	2.27	0.47
1:C:94:GLN:HA	2:C:234:HOH:O	2.13	0.47
1:A:77:MET:HE1	1:A:169:ILE:CD1	2.45	0.47
1:B:170:VAL:HG12	1:B:172:PRO:O	2.15	0.47
1:D:78:TYR:CD2	1:D:129:GLY:HA2	2.49	0.47
1:B:67:LEU:O	1:B:181:ILE:HD12	2.14	0.47
1:B:37:SER:HB2	1:B:52:TYR:CD2	2.50	0.47
1:A:51:ALA:O	1:A:172:PRO:HA	2.16	0.46
1:F:25:HIS:NE2	1:F:27:GLU:OE2	2.49	0.46
1:G:25:HIS:HB3	1:G:28:GLY:O	2.16	0.46
1:B:125:ARG:NH2	1:B:127:LEU:HD11	2.31	0.46
1:E:37:SER:HB2	1:E:52:TYR:CE2	2.50	0.46
1:D:77:MET:HE3	1:G:77:MET:CG	2.45	0.45
1:A:171:SER:HA	1:A:172:PRO:C	2.37	0.45
1:C:193:GLN:HB3	1:E:133:GLU:HG3	1.98	0.45
1:E:134:ARG:HH12	1:E:157:ALA:HB1	1.81	0.45
1:C:37:SER:HB2	1:C:52:TYR:CD2	2.51	0.45
1:B:90:LEU:O	1:B:120:TYR:HA	2.17	0.45
1:A:36:ARG:HG2	1:A:53:THR:HG22	1.98	0.45
1:B:12:THR:CG2	1:B:13:ALA:N	2.79	0.45
1:F:76:TRP:CZ3	1:F:84:LEU:HD21	2.51	0.45
1:G:67:LEU:O	1:G:181:ILE:HD12	2.16	0.45
1:B:37:SER:HB2	1:B:52:TYR:CE2	2.52	0.45
1:F:37:SER:HB2	1:F:52:TYR:CD2	2.53	0.45
1:H:11:ASN:HB2	2:H:225:HOH:O	2.16	0.45
1:D:54:THR:HG22	1:D:169:ILE:CD1	2.47	0.44
1:A:76:TRP:CZ3	1:A:84:LEU:HD21	2.52	0.44
1:C:78:TYR:CD2	1:C:129:GLY:HA2	2.52	0.44
1:G:12:THR:HG23	1:G:14:GLU:N	2.32	0.44
1:C:16:TRP:CD2	1:C:165:LEU:HD22	2.52	0.44
1:D:9:PRO:O	1:D:15:PHE:HB2	2.18	0.44
1:D:98:ARG:HD3	1:G:35:VAL:CG1	2.47	0.43
1:C:76:TRP:CZ3	1:C:84:LEU:HD21	2.54	0.43
1:H:152:VAL:HG12	1:H:153:ALA:O	2.18	0.43
1:G:90:LEU:O	1:G:120:TYR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:GLN:O	1:B:150:SER:HA	2.18	0.43
1:D:85:GLN:NE2	1:D:87:HIS:CE1	2.87	0.43
1:A:90:LEU:O	1:A:120:TYR:HA	2.19	0.43
1:D:90:LEU:HB3	1:D:92:ASP:O	2.18	0.43
1:E:92:ASP:O	1:E:94:GLN:N	2.51	0.43
1:H:120:TYR:O	1:H:194:HIS:NE2	2.47	0.43
1:E:76:TRP:CZ3	1:E:84:LEU:HD21	2.54	0.43
1:G:171:SER:HA	1:G:172:PRO:C	2.39	0.43
1:D:37:SER:OG	1:D:51:ALA:HB3	2.19	0.42
1:G:65:SER:HB3	1:G:150:SER:OG	2.19	0.42
1:H:67:LEU:O	1:H:181:ILE:HD12	2.20	0.42
1:D:77:MET:HE1	1:G:169:ILE:CD1	2.49	0.42
1:D:34:VAL:HG12	1:D:35:VAL:HG12	2.00	0.42
1:G:37:SER:HB2	1:G:52:TYR:CD2	2.54	0.42
1:B:76:TRP:CE3	1:B:166:VAL:HG21	2.54	0.42
1:D:194:HIS:O	1:D:197:VAL:HG12	2.20	0.42
1:G:12:THR:HG23	1:G:14:GLU:H	1.85	0.42
1:C:142:VAL:HG11	1:C:148:PHE:CG	2.55	0.41
1:E:25:HIS:ND1	1:E:27:GLU:HG2	2.34	0.41
1:C:90:LEU:O	1:C:120:TYR:HA	2.20	0.41
1:D:34:VAL:HG12	1:D:35:VAL:CG1	2.51	0.41
1:G:69:ARG:O	1:G:70:LEU:HD23	2.20	0.41
1:C:16:TRP:CG	1:C:165:LEU:HD22	2.55	0.41
1:D:98:ARG:CD	1:G:35:VAL:CG1	2.98	0.41
1:B:77:MET:SD	1:E:77:MET:HE2	2.61	0.41
1:G:142:VAL:HG11	1:G:148:PHE:CE1	2.54	0.41
1:B:40:LYS:HZ1	1:B:50:HIS:CE1	2.39	0.41
1:E:78:TYR:CD2	1:E:129:GLY:HA2	2.56	0.41
1:C:130:ALA:HA	1:C:138:LEU:CD2	2.51	0.41
1:F:34:VAL:HG12	1:F:35:VAL:HG13	2.02	0.41
1:F:92:ASP:O	1:F:94:GLN:N	2.54	0.41
1:A:92:ASP:OD2	1:A:94:GLN:NE2	2.54	0.41
1:H:78:TYR:HB2	1:H:128:VAL:HG12	2.02	0.41
1:E:12:THR:HG23	1:E:15:PHE:H	1.86	0.41
1:D:171:SER:HA	1:D:172:PRO:C	2.41	0.40
1:G:78:TYR:CD2	1:G:129:GLY:HA2	2.56	0.40
1:H:90:LEU:O	1:H:120:TYR:HA	2.21	0.40
1:D:194:HIS:HB3	1:D:197:VAL:HG12	2.03	0.40
1:H:92:ASP:HB2	1:H:94:GLN:HG3	2.03	0.40
1:H:126:VAL:HG21	1:H:140:TYR:CZ	2.56	0.40
1:B:35:VAL:HG11	1:E:98:ARG:HH11	1.87	0.40

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	173/225 (77%)	167 (96%)	5 (3%)	1 (1%)	28	32
1	B	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	28	32
1	C	176/225 (78%)	172 (98%)	3 (2%)	1 (1%)	28	32
1	D	175/225 (78%)	168 (96%)	6 (3%)	1 (1%)	28	32
1	E	174/225 (77%)	167 (96%)	6 (3%)	1 (1%)	28	32
1	F	173/225 (77%)	167 (96%)	5 (3%)	1 (1%)	28	32
1	G	173/225 (77%)	168 (97%)	4 (2%)	1 (1%)	28	32
1	H	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	28	32
All	All	1392/1800 (77%)	1347 (97%)	37 (3%)	8 (1%)	28	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	93	PRO
1	A	93	PRO
1	E	93	PRO
1	H	93	PRO
1	D	93	PRO
1	F	93	PRO
1	B	93	PRO
1	G	93	PRO

### 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	145/188 (77%)	140 (97%)	5 (3%)	42	53
1	B	149/188 (79%)	144 (97%)	5 (3%)	42	53
1	C	149/188 (79%)	146 (98%)	3 (2%)	60	73
1	D	149/188 (79%)	145 (97%)	4 (3%)	50	63
1	E	146/188 (78%)	140 (96%)	6 (4%)	35	44
1	F	144/188 (77%)	142 (99%)	2 (1%)	71	82
1	G	145/188 (77%)	139 (96%)	6 (4%)	35	44
1	H	147/188 (78%)	145 (99%)	2 (1%)	71	82
All	All	1174/1504 (78%)	1141 (97%)	33 (3%)	49	61

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	TYR
1	A	71	CYS
1	A	77	MET
1	A	92	ASP
1	A	98	ARG
1	B	18	LYS
1	B	71	CYS
1	B	77	MET
1	B	98	ARG
1	B	204	GLU
1	C	10	GLN
1	C	71	CYS
1	C	92	ASP
1	D	11	ASN
1	D	92	ASP
1	D	98	ARG
1	D	126	VAL
1	E	19	ARG
1	E	31	TYR
1	E	32	SER
1	E	71	CYS
1	E	92	ASP
1	E	197	VAL
1	F	71	CYS

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Mol	Chain	Res	Type
1	F	92	ASP
1	G	31	TYR
1	G	71	CYS
1	G	77	MET
1	G	92	ASP
1	G	167	SER
1	G	197	VAL
1	H	71	CYS
1	H	77	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	D	85	GLN
1	G	21	GLN
1	G	25	HIS
1	G	68	HIS
1	G	121	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 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](#)

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	177/225 (78%)	1.86	59 (33%) 0 0	57, 69, 99, 135	0
1	B	177/225 (78%)	2.15	84 (47%) 0 0	61, 73, 101, 162	0
1	C	179/225 (79%)	1.67	56 (31%) 0 0	57, 65, 83, 101	0
1	D	179/225 (79%)	1.67	54 (30%) 1 0	57, 65, 84, 113	0
1	E	177/225 (78%)	1.76	60 (33%) 0 0	55, 66, 84, 124	0
1	F	176/225 (78%)	2.35	94 (53%) 0 0	59, 74, 113, 205	0
1	G	176/225 (78%)	2.42	92 (52%) 0 0	59, 77, 121, 180	0
1	H	177/225 (78%)	2.24	88 (49%) 0 0	59, 74, 107, 142	0
All	All	1418/1800 (78%)	2.01	587 (41%) 0 0	55, 70, 103, 205	0

All (587) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	ARG	16.3
1	F	118	PRO	10.5
1	H	118	PRO	8.6
1	G	117	ARG	8.1
1	H	117	ARG	7.6
1	E	117	ARG	7.5
1	G	98	ARG	6.8
1	B	156	GLY	6.7
1	G	188	MET	6.6
1	G	156	GLY	6.2
1	E	156	GLY	6.1
1	F	196	ALA	6.0
1	B	176[A]	TYR	6.0
1	A	168	CYS	5.8
1	A	117	ARG	5.8
1	F	188	MET	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	205	THR	5.6
1	A	156	GLY	5.5
1	G	176[A]	TYR	5.5
1	B	154	ALA	5.5
1	F	186	GLN	5.5
1	F	92	ASP	5.4
1	B	62	GLU	5.4
1	G	190	LEU	5.3
1	H	26	PRO	5.3
1	B	117	ARG	5.3
1	H	62	GLU	5.2
1	F	119	LYS	5.1
1	G	118	PRO	5.0
1	B	26	PRO	5.0
1	H	92	ASP	4.9
1	G	154	ALA	4.9
1	G	191	TYR	4.9
1	E	152	VAL	4.9
1	B	118	PRO	4.8
1	G	12	THR	4.8
1	G	119	LYS	4.7
1	B	12	THR	4.6
1	F	98	ARG	4.6
1	G	63	SER	4.6
1	B	98	ARG	4.6
1	F	121	GLN	4.6
1	A	166	VAL	4.6
1	H	154	ALA	4.5
1	G	95	ASP	4.5
1	H	35	VAL	4.5
1	F	185	ALA	4.5
1	E	12	THR	4.4
1	E	157	ALA	4.4
1	F	190	LEU	4.4
1	G	126	VAL	4.4
1	G	155	ASP	4.3
1	B	93	PRO	4.3
1	B	121	GLN	4.2
1	H	24	PRO	4.2
1	F	176[A]	TYR	4.2
1	H	155	ASP	4.2
1	G	124	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	60	THR	4.2
1	H	12	THR	4.2
1	H	190	LEU	4.2
1	A	157	ALA	4.2
1	G	92	ASP	4.2
1	B	63	SER	4.1
1	F	63	SER	4.1
1	C	9	PRO	4.1
1	D	9	PRO	4.1
1	H	188	MET	4.1
1	H	156	GLY	4.1
1	C	132	VAL	4.1
1	G	123	TYR	4.1
1	H	121	GLN	4.1
1	F	25	HIS	4.1
1	G	152	VAL	4.0
1	A	165	LEU	4.0
1	B	160	GLN	4.0
1	D	117	ARG	4.0
1	E	131	ARG	4.0
1	F	191	TYR	4.0
1	H	138	LEU	4.0
1	F	26	PRO	4.0
1	F	61	PRO	4.0
1	C	62	GLU	4.0
1	B	153	ALA	3.9
1	H	132	VAL	3.9
1	D	92	ASP	3.9
1	B	204	GLU	3.9
1	F	62	GLU	3.9
1	A	185	ALA	3.9
1	G	94	GLN	3.9
1	H	160	GLN	3.9
1	F	189	GLU	3.9
1	B	92	ASP	3.9
1	D	98	ARG	3.9
1	A	20	LEU	3.9
1	B	64	PRO	3.8
1	E	158	ASP	3.8
1	F	96	GLU	3.8
1	B	23	VAL	3.8
1	G	34	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	36	ARG	3.8
1	A	93	PRO	3.8
1	B	158	ASP	3.8
1	G	26	PRO	3.8
1	B	155	ASP	3.8
1	G	185	ALA	3.7
1	D	132	VAL	3.7
1	C	165	LEU	3.7
1	G	61	PRO	3.7
1	F	12	THR	3.7
1	F	126	VAL	3.7
1	G	35	VAL	3.7
1	F	60	THR	3.7
1	E	62	GLU	3.7
1	H	176	TYR	3.6
1	H	134	ARG	3.6
1	F	194	HIS	3.6
1	C	118	PRO	3.6
1	H	129	GLY	3.6
1	E	98	ARG	3.6
1	H	197	VAL	3.6
1	E	153	ALA	3.6
1	H	95	ASP	3.6
1	F	91	LYS	3.6
1	G	91	LYS	3.6
1	F	198	ILE	3.6
1	E	20	LEU	3.6
1	H	152	VAL	3.6
1	A	154	ALA	3.5
1	A	159	GLY	3.5
1	G	198	ILE	3.5
1	B	35	VAL	3.5
1	F	94	GLN	3.5
1	H	193	GLN	3.5
1	A	92	ASP	3.5
1	A	126	VAL	3.5
1	E	170	VAL	3.5
1	H	128	VAL	3.5
1	H	158	ASP	3.5
1	H	185	ALA	3.5
1	G	82	ASP	3.5
1	G	158	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	96	GLU	3.5
1	A	34	VAL	3.4
1	H	203	TYR	3.4
1	G	138	LEU	3.4
1	G	170	VAL	3.4
1	A	198	ILE	3.4
1	H	127	LEU	3.4
1	H	159	GLY	3.4
1	G	132	VAL	3.4
1	H	25	HIS	3.4
1	F	183	THR	3.4
1	H	153	ALA	3.4
1	F	34	VAL	3.4
1	D	26	PRO	3.4
1	G	183	THR	3.4
1	C	36	ARG	3.4
1	A	98	ARG	3.3
1	B	163	TYR	3.3
1	D	10	GLN	3.3
1	F	138	LEU	3.3
1	B	169	ILE	3.3
1	A	118	PRO	3.3
1	G	65	SER	3.3
1	C	26	PRO	3.3
1	B	157	ALA	3.3
1	H	65	SER	3.3
1	A	158	ASP	3.3
1	A	196	ALA	3.3
1	C	35	VAL	3.3
1	G	197	VAL	3.3
1	H	63	SER	3.3
1	F	179	PHE	3.3
1	B	36	ARG	3.3
1	H	163	TYR	3.2
1	F	124	ARG	3.2
1	G	125	ARG	3.2
1	F	155	ASP	3.2
1	B	166	VAL	3.2
1	D	35	VAL	3.2
1	C	117	ARG	3.2
1	H	98	ARG	3.2
1	B	141	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	160	GLN	3.2
1	E	169	ILE	3.2
1	F	93	PRO	3.2
1	G	196	ALA	3.2
1	E	70	LEU	3.2
1	G	199	LYS	3.2
1	C	125	ARG	3.2
1	A	123	TYR	3.1
1	B	88	VAL	3.1
1	F	23	VAL	3.1
1	C	157	ALA	3.1
1	H	97	ASP	3.1
1	G	184	GLN	3.1
1	G	169	ILE	3.1
1	A	167	SER	3.1
1	C	98	ARG	3.1
1	H	126	VAL	3.1
1	D	196	ALA	3.1
1	H	94	GLN	3.1
1	G	168	CYS	3.1
1	A	12	THR	3.1
1	B	89	ILE	3.1
1	H	15	PHE	3.1
1	C	88	VAL	3.1
1	F	123	TYR	3.1
1	H	202	ALA	3.1
1	G	67	LEU	3.1
1	H	137	LEU	3.1
1	F	27	GLU	3.1
1	H	36	ARG	3.1
1	D	63	SER	3.1
1	F	166	VAL	3.1
1	A	77	MET	3.1
1	A	141	THR	3.1
1	G	62	GLU	3.1
1	C	34	VAL	3.0
1	E	34	VAL	3.0
1	A	96	GLU	3.0
1	D	170	VAL	3.0
1	B	133	GLU	3.0
1	H	120	TYR	3.0
1	D	157	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	30	TYR	3.0
1	F	156	GLY	3.0
1	E	93	PRO	3.0
1	E	196	ALA	3.0
1	B	75	THR	3.0
1	E	123	TYR	3.0
1	C	92	ASP	3.0
1	F	65	SER	3.0
1	D	55	ILE	3.0
1	B	170	VAL	3.0
1	F	170	VAL	3.0
1	F	192	PRO	3.0
1	H	34	VAL	3.0
1	E	75	THR	3.0
1	H	23	VAL	2.9
1	H	60	THR	2.9
1	A	22	LEU	2.9
1	G	77	MET	2.9
1	E	82	ASP	2.9
1	F	146	ALA	2.9
1	H	59	CYS	2.9
1	G	149	GLY	2.9
1	B	142	VAL	2.9
1	F	36	ARG	2.9
1	F	125	ARG	2.9
1	B	52	TYR	2.9
1	F	199	LYS	2.9
1	A	75	THR	2.9
1	G	142	VAL	2.9
1	B	86	LEU	2.9
1	E	160	GLN	2.9
1	A	62	GLU	2.9
1	C	128	VAL	2.9
1	E	159	GLY	2.9
1	B	129	GLY	2.8
1	E	23	VAL	2.8
1	F	22	LEU	2.8
1	G	84	LEU	2.8
1	F	38	ALA	2.8
1	H	93	PRO	2.8
1	D	36	ARG	2.8
1	A	174	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	197	VAL	2.8
1	C	166	VAL	2.8
1	F	128	VAL	2.8
1	F	66	HIS	2.8
1	F	201	MET	2.8
1	G	86	LEU	2.8
1	H	37	SER	2.8
1	A	131	ARG	2.8
1	B	134	ARG	2.8
1	E	15	PHE	2.8
1	A	170	VAL	2.8
1	F	35	VAL	2.8
1	F	90	LEU	2.8
1	F	165	LEU	2.8
1	E	10	GLN	2.8
1	A	132	VAL	2.7
1	D	15	PHE	2.7
1	D	126	VAL	2.7
1	D	166	VAL	2.7
1	F	72	SER	2.7
1	E	61	PRO	2.7
1	B	15	PHE	2.7
1	G	163	TYR	2.7
1	F	202	ALA	2.7
1	H	130	ALA	2.7
1	B	90	LEU	2.7
1	C	97	ASP	2.7
1	C	156	GLY	2.7
1	A	26	PRO	2.7
1	F	184	GLN	2.7
1	G	121	GLN	2.7
1	D	37	SER	2.7
1	B	190	LEU	2.7
1	B	97	ASP	2.7
1	G	22	LEU	2.7
1	B	85	GLN	2.7
1	E	36	ARG	2.7
1	G	64	PRO	2.7
1	D	161	ALA	2.7
1	G	38	ALA	2.7
1	H	11	ASN	2.7
1	B	61	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	52	TYR	2.6
1	F	29	GLY	2.6
1	G	165	LEU	2.6
1	G	97	ASP	2.6
1	C	80	ALA	2.6
1	G	13	ALA	2.6
1	A	197	VAL	2.6
1	E	52	TYR	2.6
1	G	171	SER	2.6
1	A	19	ARG	2.6
1	C	71	CYS	2.6
1	D	134	ARG	2.6
1	B	25	HIS	2.6
1	E	154	ALA	2.6
1	H	169	ILE	2.6
1	C	59	CYS	2.6
1	B	27	GLU	2.6
1	E	35	VAL	2.6
1	E	174	PHE	2.6
1	G	153	ALA	2.6
1	H	131	ARG	2.6
1	B	172	PRO	2.6
1	F	64	PRO	2.6
1	C	120	TYR	2.6
1	H	191	TYR	2.6
1	H	96	GLU	2.6
1	C	150	SER	2.5
1	A	70	LEU	2.5
1	H	182	PHE	2.5
1	D	21	GLN	2.5
1	H	66	HIS	2.5
1	A	63	SER	2.5
1	B	54	THR	2.5
1	B	96	GLU	2.5
1	D	20	LEU	2.5
1	B	77	MET	2.5
1	G	174	PHE	2.5
1	B	140	TYR	2.5
1	B	55	ILE	2.5
1	D	93	PRO	2.5
1	D	22	LEU	2.5
1	B	11	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	142	VAL	2.5
1	F	174	PHE	2.5
1	G	11	ASN	2.5
1	F	54	THR	2.5
1	D	125	ARG	2.5
1	F	152	VAL	2.5
1	H	141	THR	2.5
1	G	134	ARG	2.5
1	A	55	ILE	2.5
1	G	147	ILE	2.5
1	H	27	GLU	2.5
1	D	95	ASP	2.5
1	F	132	VAL	2.5
1	B	31	TYR	2.5
1	B	60	THR	2.5
1	C	163	TYR	2.5
1	G	75	THR	2.5
1	D	58	LEU	2.5
1	E	92	ASP	2.5
1	D	19	ARG	2.4
1	G	128	VAL	2.4
1	G	166	VAL	2.4
1	C	76	TRP	2.4
1	G	93	PRO	2.4
1	G	172	PRO	2.4
1	C	31	TYR	2.4
1	F	162	GLY	2.4
1	F	163	TYR	2.4
1	A	138	LEU	2.4
1	F	84	LEU	2.4
1	F	86	LEU	2.4
1	F	13	ALA	2.4
1	H	170	VAL	2.4
1	F	28	GLY	2.4
1	D	97	ASP	2.4
1	B	125	ARG	2.4
1	D	96	GLU	2.4
1	G	27	GLU	2.4
1	B	202	ALA	2.4
1	G	28	GLY	2.4
1	E	134	ARG	2.4
1	H	119	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	137	LEU	2.4
1	E	96	GLU	2.4
1	E	179	PHE	2.4
1	H	183	THR	2.4
1	B	147	ILE	2.4
1	H	184	GLN	2.4
1	A	190	LEU	2.4
1	B	67	LEU	2.4
1	A	79	HIS	2.4
1	G	25	HIS	2.4
1	H	61	PRO	2.4
1	H	146	ALA	2.4
1	H	161	ALA	2.4
1	C	60	THR	2.4
1	E	141	THR	2.4
1	E	168	CYS	2.4
1	H	166	VAL	2.4
1	B	193	GLN	2.4
1	D	121	GLN	2.4
1	B	82	ASP	2.4
1	D	90	LEU	2.4
1	D	8	PRO	2.4
1	C	15	PHE	2.4
1	F	78	TYR	2.3
1	H	194	HIS	2.3
1	C	22	LEU	2.3
1	C	190	LEU	2.3
1	H	90	LEU	2.3
1	A	152	VAL	2.3
1	C	142	VAL	2.3
1	G	122	VAL	2.3
1	H	72	SER	2.3
1	C	95	ASP	2.3
1	G	29	GLY	2.3
1	C	85[A]	GLN	2.3
1	F	120	TYR	2.3
1	B	171	SER	2.3
1	D	151	SER	2.3
1	D	88	VAL	2.3
1	H	200	GLN	2.3
1	C	20	LEU	2.3
1	C	137	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	137	LEU	2.3
1	H	196	ALA	2.3
1	E	171	SER	2.3
1	F	95	ASP	2.3
1	A	122	VAL	2.3
1	B	177	ARG	2.3
1	C	155	ASP	2.3
1	B	187	LEU	2.3
1	C	138	LEU	2.3
1	E	22	LEU	2.3
1	H	22	LEU	2.3
1	A	41	VAL	2.3
1	A	142	VAL	2.3
1	F	204	GLU	2.3
1	B	13	ALA	2.3
1	B	84	LEU	2.3
1	C	63	SER	2.3
1	B	186	GLN	2.3
1	G	31	TYR	2.3
1	D	41	VAL	2.3
1	H	83	PRO	2.3
1	A	89	ILE	2.3
1	F	129	GLY	2.2
1	G	66	HIS	2.2
1	D	142	VAL	2.2
1	E	197	VAL	2.2
1	F	197	VAL	2.2
1	B	76	TRP	2.2
1	C	8	PRO	2.2
1	C	196	ALA	2.2
1	D	169	ILE	2.2
1	E	55	ILE	2.2
1	C	58	LEU	2.2
1	E	190	LEU	2.2
1	G	173	GLY	2.2
1	H	58	LEU	2.2
1	E	122	VAL	2.2
1	C	16	TRP	2.2
1	A	80	ALA	2.2
1	B	51	ALA	2.2
1	H	29	GLY	2.2
1	E	84	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	20	LEU	2.2
1	E	121	GLN	2.2
1	A	52	TYR	2.2
1	G	189	GLU	2.2
1	A	61	PRO	2.2
1	B	132	VAL	2.2
1	B	148	PHE	2.2
1	B	179	PHE	2.2
1	D	168	CYS	2.2
1	E	166	VAL	2.2
1	G	14	GLU	2.2
1	D	165	LEU	2.2
1	E	151	SER	2.2
1	G	88	VAL	2.2
1	G	15	PHE	2.2
1	C	141	THR	2.2
1	E	193	GLN	2.2
1	E	89	ILE	2.2
1	F	127	LEU	2.2
1	E	188	MET	2.2
1	D	64	PRO	2.2
1	B	203	TYR	2.2
1	E	163	TYR	2.2
1	H	52	TYR	2.2
1	D	34	VAL	2.2
1	F	193	GLN	2.2
1	A	53	THR	2.2
1	G	55	ILE	2.2
1	C	158	ASP	2.2
1	C	18	LYS	2.1
1	G	139	GLN	2.2
1	H	43	ASN	2.1
1	C	56	TYR	2.1
1	C	78	TYR	2.1
1	G	140	TYR	2.1
1	A	35	VAL	2.1
1	B	122	VAL	2.1
1	D	12	THR	2.1
1	F	180	GLU	2.1
1	C	84	LEU	2.1
1	D	158	ASP	2.1
1	E	165	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	70	LEU	2.1
1	G	187	LEU	2.1
1	F	32	SER	2.1
1	F	203	TYR	2.1
1	A	179	PHE	2.1
1	C	12	THR	2.1
1	F	141	THR	2.1
1	G	53	THR	2.1
1	G	200	GLN	2.1
1	B	24	PRO	2.1
1	H	86	LEU	2.1
1	F	71	CYS	2.1
1	H	77	MET	2.1
1	F	18	LYS	2.1
1	B	72	SER	2.1
1	A	137	LEU	2.1
1	D	71	CYS	2.1
1	H	91	LYS	2.1
1	C	121	GLN	2.1
1	D	94	GLN	2.1
1	H	88	VAL	2.1
1	A	24	PRO	2.1
1	H	64	PRO	2.1
1	F	169	ILE	2.1
1	F	181	ILE	2.1
1	C	13	ALA	2.1
1	C	185	ALA	2.1
1	E	51	ALA	2.1
1	A	57	PHE	2.1
1	D	156	GLY	2.1
1	E	118	PRO	2.1
1	B	50	HIS	2.1
1	E	90	LEU	2.1
1	B	95	ASP	2.1
1	C	47	ASN	2.1
1	A	146	ALA	2.1
1	D	146	ALA	2.1
1	H	13	ALA	2.1
1	B	65	SER	2.1
1	E	37	SER	2.1
1	D	24	PRO	2.1
1	A	169	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	2.0
1	C	181	ILE	2.0
1	B	53	THR	2.0
1	B	38	ALA	2.0
1	A	65	SER	2.0
1	E	189	GLU	2.0
1	F	14	GLU	2.0
1	H	14	GLU	2.0
1	D	122	VAL	2.0
1	D	174	PHE	2.0
1	E	71	CYS	2.0
1	C	70	LEU	2.0
1	F	154	ALA	2.0
1	F	200	GLN	2.0
1	G	159	GLY	2.0
1	D	118	PRO	2.0
1	E	19	ARG	2.0
1	F	158	ASP	2.0
1	E	132	VAL	2.0
1	H	50	HIS	2.0
1	A	56	TYR	2.0
1	B	14	GLU	2.0
1	F	195	GLU	2.0
1	F	77	MET	2.0
1	D	153	ALA	2.0

## 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 [i](#)

There are no such residues in this entry.