Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 10:00 AM EST

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*
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:

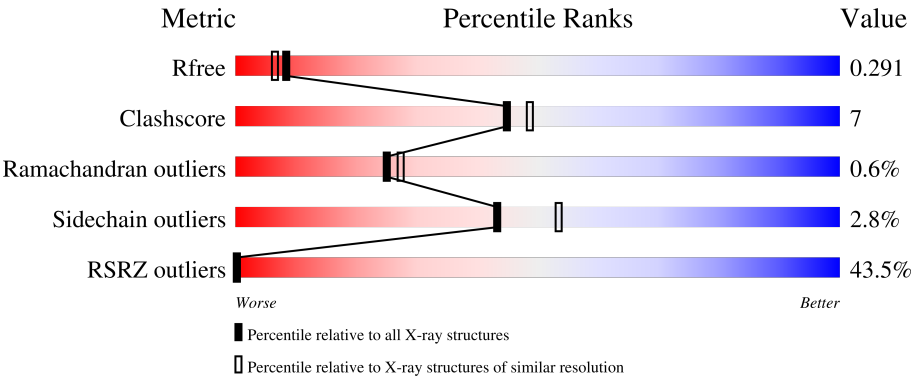
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	29% 68% 10% • 21%
1	B	225	38% 64% 14% • 21%
1	C	225	26% 64% 14% • 20%
1	D	225	25% 67% 12% • 20%
1	E	225	28% 66% 12% 21%

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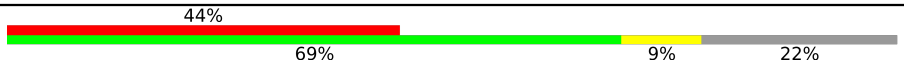
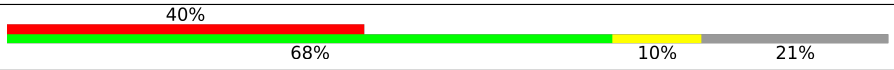
Mol	Chain	Length	Quality of chain
1	F	225	
1	G	225	
1	H	225	

2 Entry composition (i)

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.

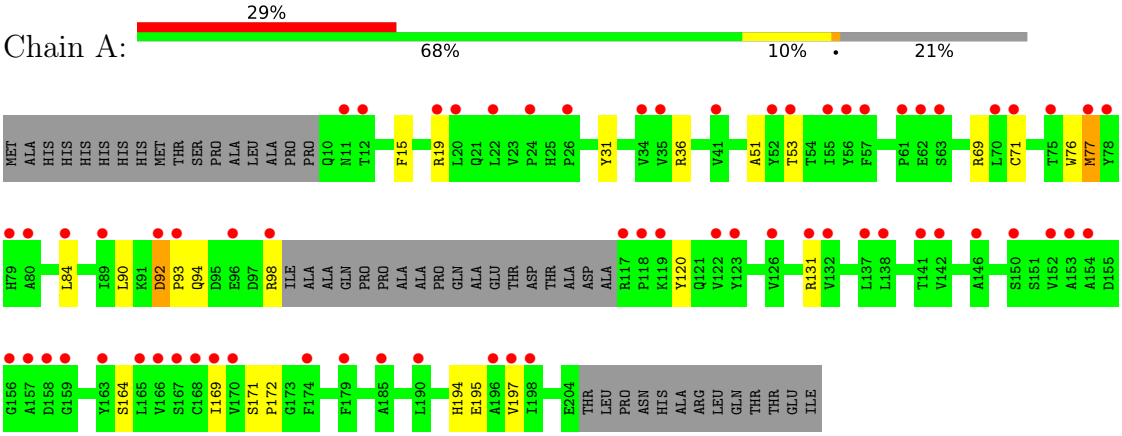
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	18	Total O 18 18	0	0
2	C	19	Total O 19 19	0	0
2	D	22	Total O 22 22	0	0
2	E	17	Total O 17 17	0	0
2	F	10	Total O 10 10	0	0
2	G	6	Total O 6 6	0	0
2	H	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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.

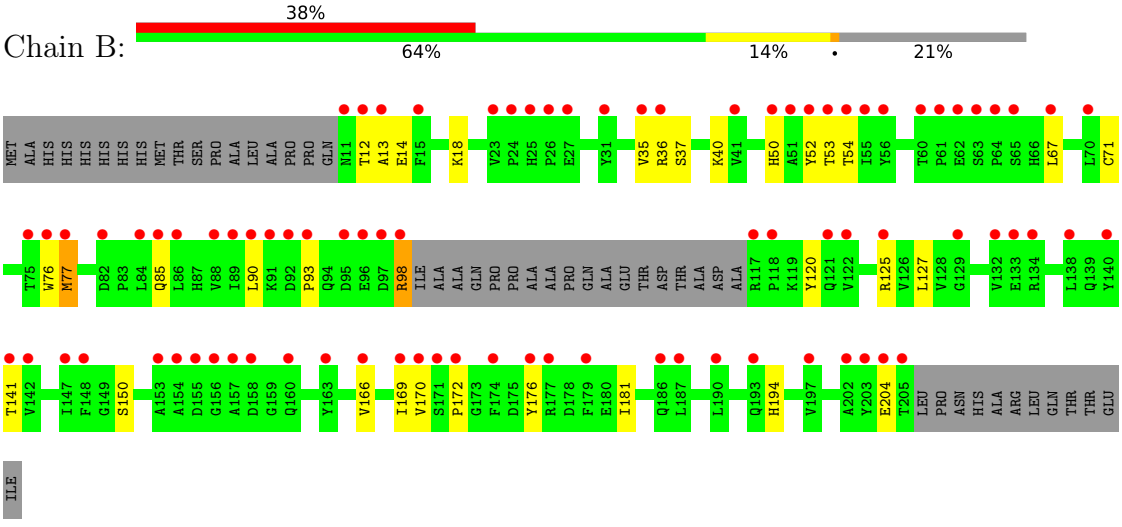
• Molecule 1: Putative uncharacterized protein

Chain A:



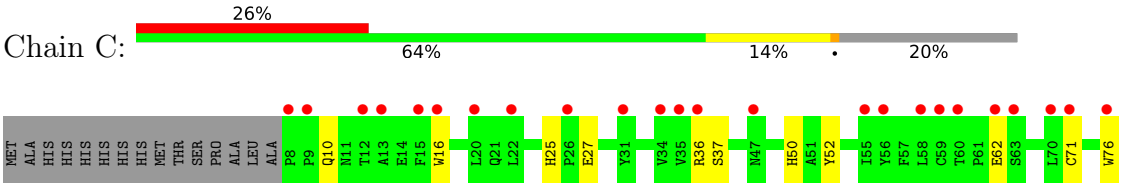
• Molecule 1: Putative uncharacterized protein

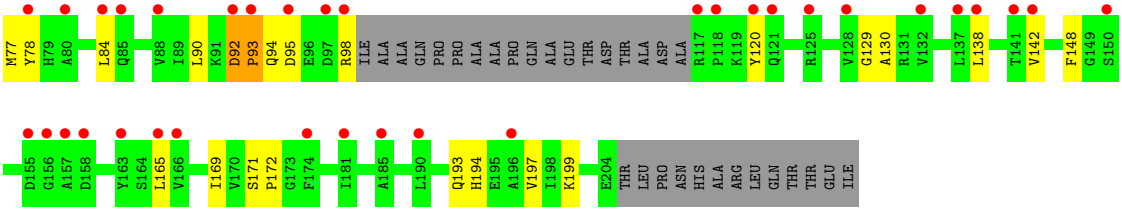
Chain B:



• Molecule 1: Putative uncharacterized protein

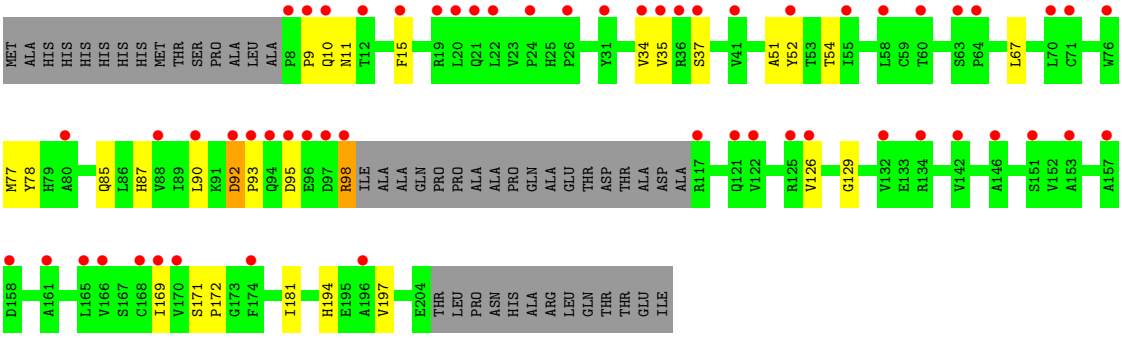
Chain C:





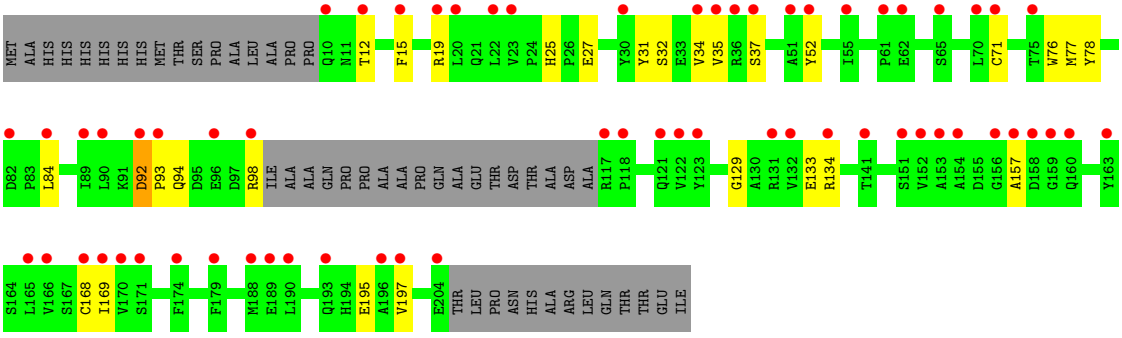
• Molecule 1: Putative uncharacterized protein

Chain D:



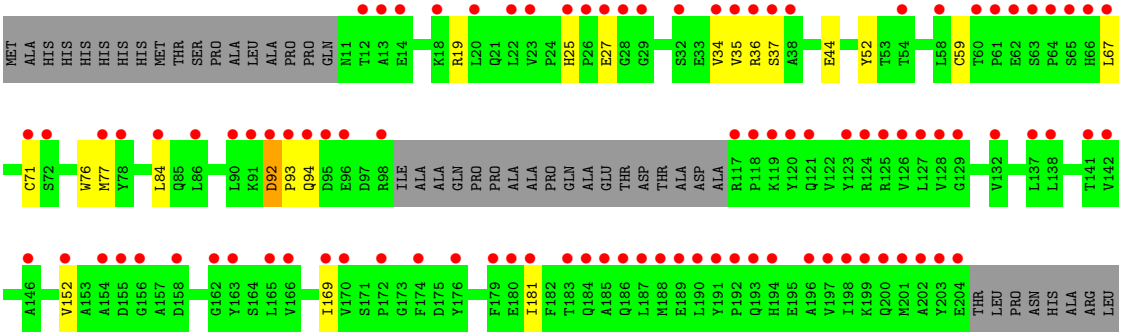
• Molecule 1: Putative uncharacterized protein

Chain E:



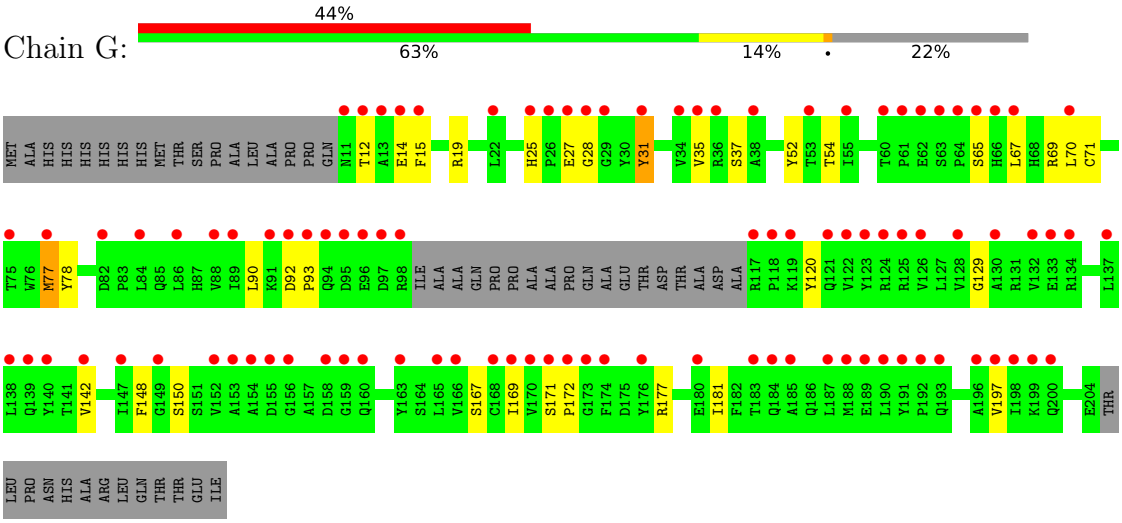
• Molecule 1: Putative uncharacterized protein

Chain F:



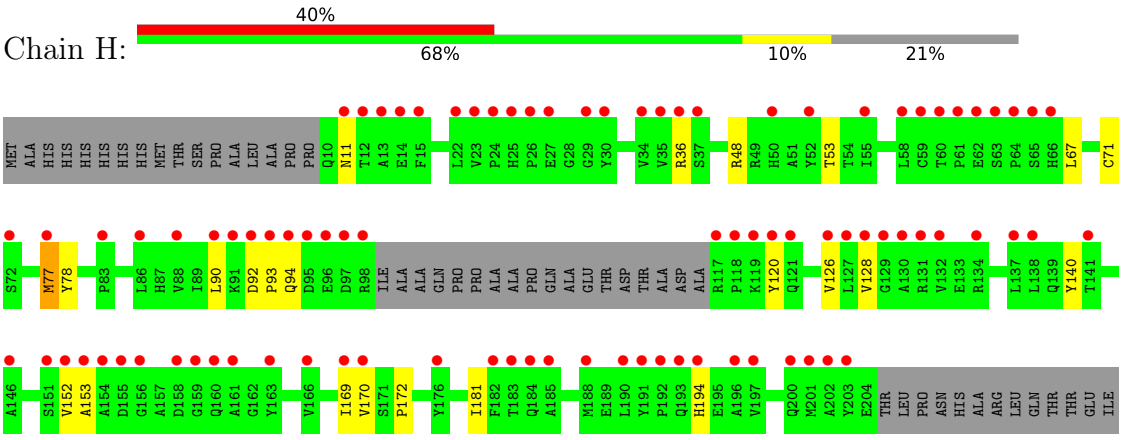
• Molecule 1: Putative uncharacterized protein

Chain G:



• Molecule 1: Putative uncharacterized protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 92.8 (46.72-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.290 0.245 , 0.291	Depositor DCC
R_{free} test set	3678 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

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:A:169:ILE:HD11	1:H:77:MET:HE1	1.87	0.55
1:C:93:PRO:O	2:C:234:HOH:O	2.18	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:N	1:F:44:GLU:OE1	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:37:SER:HB2	1:B:52:TYR:CD2	2.50	0.47
1:B:67:LEU:O	1:B:181:ILE:HD12	2.14	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:B:77:MET:SD	1:E:77:MET:HE2	2.61	0.41
1:D:98:ARG:CD	1:G:35:VAL:CG1	2.98	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:A:92:ASP:OD2	1:A:94:GLN:NE2	2.54	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: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%)	25	27
1	B	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	25	27
1	C	176/225 (78%)	172 (98%)	3 (2%)	1 (1%)	25	27
1	D	175/225 (78%)	168 (96%)	6 (3%)	1 (1%)	25	27
1	E	174/225 (77%)	167 (96%)	6 (3%)	1 (1%)	25	27
1	F	173/225 (77%)	167 (96%)	5 (3%)	1 (1%)	25	27
1	G	173/225 (77%)	168 (97%)	4 (2%)	1 (1%)	25	27
1	H	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	25	27
All	All	1392/1800 (77%)	1347 (97%)	37 (3%)	8 (1%)	25	27

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%)	37	46
1	B	149/188 (79%)	144 (97%)	5 (3%)	37	46
1	C	149/188 (79%)	146 (98%)	3 (2%)	55	66
1	D	149/188 (79%)	145 (97%)	4 (3%)	44	55
1	E	146/188 (78%)	140 (96%)	6 (4%)	30	37
1	F	144/188 (77%)	142 (99%)	2 (1%)	67	78
1	G	145/188 (77%)	139 (96%)	6 (4%)	30	37
1	H	147/188 (78%)	145 (99%)	2 (1%)	67	78
All	All	1174/1504 (78%)	1141 (97%)	33 (3%)	43	53

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

Sometimes 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 monosaccharides 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^{th} 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	177/225 (78%)	1.91	66 (37%)	0	0	57, 69, 99, 135	0
1	B	177/225 (78%)	2.21	86 (48%)	0	0	61, 73, 101, 162	0
1	C	179/225 (79%)	1.72	58 (32%)	0	0	57, 65, 83, 101	0
1	D	179/225 (79%)	1.73	57 (31%)	0	0	57, 65, 84, 113	0
1	E	177/225 (78%)	1.82	63 (35%)	0	0	55, 66, 84, 124	0
1	F	176/225 (78%)	2.41	98 (55%)	0	0	59, 74, 113, 205	0
1	G	176/225 (78%)	2.48	98 (55%)	0	0	59, 77, 121, 180	0
1	H	177/225 (78%)	2.28	91 (51%)	0	0	59, 74, 107, 142	0
All	All	1418/1800 (78%)	2.07	617 (43%)	0	0	55, 70, 103, 205	0

All (617) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	ARG	16.7
1	F	118	PRO	10.8
1	H	118	PRO	8.7
1	G	117	ARG	8.2
1	E	117	ARG	7.6
1	H	117	ARG	7.4
1	G	98	ARG	6.7
1	G	188	MET	6.6
1	B	156	GLY	6.6
1	G	156	GLY	6.2
1	B	176[A]	TYR	6.1
1	E	156	GLY	6.1
1	A	117	ARG	6.0
1	A	168	CYS	5.9
1	F	196	ALA	5.8
1	G	176[A]	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	205	THR	5.6
1	F	188	MET	5.6
1	F	92	ASP	5.6
1	F	186	GLN	5.5
1	G	190	LEU	5.5
1	B	154	ALA	5.4
1	A	156	GLY	5.4
1	B	117	ARG	5.4
1	B	62	GLU	5.4
1	H	26	PRO	5.3
1	H	62	GLU	5.3
1	F	119	LYS	5.1
1	H	92	ASP	5.1
1	G	118	PRO	5.1
1	B	26	PRO	5.0
1	B	93	PRO	5.0
1	G	154	ALA	4.9
1	E	152	VAL	4.9
1	G	191	TYR	4.8
1	B	98	ARG	4.7
1	G	119	LYS	4.7
1	H	154	ALA	4.7
1	F	121	GLN	4.7
1	B	12	THR	4.7
1	B	118	PRO	4.7
1	G	12	THR	4.6
1	F	98	ARG	4.6
1	G	95	ASP	4.6
1	G	63	SER	4.5
1	A	166	VAL	4.5
1	H	35	VAL	4.5
1	G	126	VAL	4.4
1	F	185	ALA	4.4
1	F	190	LEU	4.4
1	H	155	ASP	4.4
1	A	157	ALA	4.4
1	F	176[A]	TYR	4.4
1	G	155	ASP	4.3
1	E	12	THR	4.3
1	H	12	THR	4.3
1	G	92	ASP	4.3
1	B	121	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	157	ALA	4.2
1	H	156	GLY	4.2
1	H	121	GLN	4.2
1	C	9	PRO	4.2
1	G	124	ARG	4.2
1	B	92	ASP	4.2
1	H	24	PRO	4.2
1	F	63	SER	4.2
1	G	60	THR	4.2
1	A	20	LEU	4.2
1	D	9	PRO	4.2
1	F	61	PRO	4.2
1	H	190	LEU	4.2
1	D	117	ARG	4.2
1	A	165	LEU	4.1
1	C	132	VAL	4.1
1	G	152	VAL	4.1
1	H	188	MET	4.1
1	B	63	SER	4.1
1	D	92	ASP	4.1
1	A	185	ALA	4.0
1	G	123	TYR	4.0
1	B	204	GLU	4.0
1	B	64	PRO	4.0
1	F	62	GLU	4.0
1	B	160	GLN	4.0
1	E	158	ASP	4.0
1	G	61	PRO	4.0
1	E	131	ARG	4.0
1	F	25	HIS	4.0
1	B	153	ALA	4.0
1	C	62	GLU	4.0
1	F	96	GLU	4.0
1	G	94	GLN	3.9
1	H	160	GLN	3.9
1	H	138	LEU	3.9
1	F	26	PRO	3.9
1	A	93	PRO	3.9
1	G	185	ALA	3.9
1	D	98	ARG	3.9
1	F	189	GLU	3.9
1	D	132	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	158	ASP	3.9
1	H	132	VAL	3.8
1	B	155	ASP	3.8
1	G	82	ASP	3.8
1	G	26	PRO	3.8
1	G	34	VAL	3.8
1	F	12	THR	3.8
1	F	191	TYR	3.8
1	B	23	VAL	3.8
1	G	36	ARG	3.8
1	G	91	LYS	3.8
1	E	20	LEU	3.8
1	E	98	ARG	3.8
1	C	165	LEU	3.7
1	G	35	VAL	3.7
1	H	134	ARG	3.7
1	F	126	VAL	3.7
1	F	198	ILE	3.7
1	H	128	VAL	3.7
1	H	152	VAL	3.7
1	F	60	THR	3.7
1	F	91	LYS	3.7
1	A	159	GLY	3.7
1	C	118	PRO	3.7
1	G	198	ILE	3.7
1	E	62	GLU	3.6
1	H	158	ASP	3.6
1	B	163	TYR	3.6
1	H	197	VAL	3.6
1	G	96	GLU	3.6
1	F	194	HIS	3.6
1	A	154	ALA	3.6
1	H	95	ASP	3.6
1	E	153	ALA	3.6
1	E	170	VAL	3.6
1	H	203	TYR	3.6
1	H	193	GLN	3.6
1	B	35	VAL	3.5
1	C	117	ARG	3.5
1	H	129	GLY	3.5
1	H	176	TYR	3.5
1	F	94	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	34	VAL	3.5
1	A	92	ASP	3.5
1	C	26	PRO	3.5
1	D	26	PRO	3.5
1	G	138	LEU	3.5
1	A	126	VAL	3.5
1	G	132	VAL	3.5
1	H	185	ALA	3.5
1	H	159	GLY	3.5
1	A	34	VAL	3.4
1	G	199	LYS	3.4
1	G	65	SER	3.4
1	B	169	ILE	3.4
1	G	197	VAL	3.4
1	H	163	TYR	3.4
1	H	153	ALA	3.4
1	D	35	VAL	3.4
1	A	118	PRO	3.4
1	H	25	HIS	3.4
1	C	35	VAL	3.4
1	C	36	ARG	3.4
1	A	196	ALA	3.4
1	E	169	ILE	3.4
1	F	138	LEU	3.4
1	F	93	PRO	3.3
1	H	63	SER	3.3
1	A	12	THR	3.3
1	F	183	THR	3.3
1	D	10	GLN	3.3
1	H	127	LEU	3.3
1	A	198	ILE	3.3
1	G	158	ASP	3.3
1	G	125	ARG	3.3
1	E	70	LEU	3.3
1	A	123	TYR	3.3
1	A	158	ASP	3.3
1	F	155	ASP	3.3
1	G	170	VAL	3.3
1	G	160	GLN	3.3
1	G	183	THR	3.3
1	A	98	ARG	3.3
1	B	166	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	3.3
1	B	36	ARG	3.3
1	H	65	SER	3.3
1	F	23	VAL	3.3
1	C	98	ARG	3.3
1	F	179	PHE	3.2
1	C	157	ALA	3.2
1	H	97	ASP	3.2
1	D	55	ILE	3.2
1	B	141	THR	3.2
1	G	62	GLU	3.2
1	B	157	ALA	3.2
1	A	96	GLU	3.2
1	F	27	GLU	3.2
1	E	75	THR	3.2
1	F	124	ARG	3.2
1	H	98	ARG	3.2
1	H	93	PRO	3.2
1	F	123	TYR	3.2
1	B	88	VAL	3.2
1	A	167	SER	3.2
1	G	196	ALA	3.2
1	H	94	GLN	3.2
1	G	184	GLN	3.2
1	B	133	GLU	3.2
1	A	141	THR	3.1
1	F	166	VAL	3.1
1	D	196	ALA	3.1
1	G	67	LEU	3.1
1	B	89	ILE	3.1
1	D	63	SER	3.1
1	D	170	VAL	3.1
1	E	34	VAL	3.1
1	H	126	VAL	3.1
1	A	75	THR	3.1
1	C	125	ARG	3.1
1	H	15	PHE	3.1
1	H	34	VAL	3.1
1	A	131	ARG	3.1
1	E	196	ALA	3.1
1	B	52	TYR	3.1
1	F	36	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	169	ILE	3.1
1	H	23	VAL	3.1
1	H	30	TYR	3.0
1	A	77	MET	3.0
1	B	75	THR	3.0
1	F	156	GLY	3.0
1	G	168	CYS	3.0
1	C	166	VAL	3.0
1	E	123	TYR	3.0
1	F	192	PRO	3.0
1	G	149	GLY	3.0
1	H	36	ARG	3.0
1	E	160	GLN	3.0
1	E	159	GLY	3.0
1	E	93	PRO	3.0
1	C	92	ASP	3.0
1	H	137	LEU	3.0
1	F	146	ALA	3.0
1	H	202	ALA	3.0
1	C	34	VAL	3.0
1	C	128	VAL	3.0
1	G	142	VAL	3.0
1	G	121	GLN	3.0
1	B	86	LEU	3.0
1	A	197	VAL	3.0
1	F	125	ARG	3.0
1	B	197	VAL	2.9
1	F	66	HIS	2.9
1	B	170	VAL	2.9
1	G	84	LEU	2.9
1	H	60	THR	2.9
1	E	82	ASP	2.9
1	F	65	SER	2.9
1	B	190	LEU	2.9
1	G	165	LEU	2.9
1	E	15	PHE	2.9
1	E	23	VAL	2.9
1	D	157	ALA	2.9
1	F	199	LYS	2.9
1	G	97	ASP	2.9
1	B	134	ARG	2.9
1	D	36	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	142	VAL	2.9
1	F	201	MET	2.9
1	G	163	TYR	2.9
1	A	62	GLU	2.8
1	F	170	VAL	2.8
1	C	71	CYS	2.8
1	H	59	CYS	2.8
1	A	22	LEU	2.8
1	F	22	LEU	2.8
1	F	165	LEU	2.8
1	G	77	MET	2.8
1	B	129	GLY	2.8
1	B	97	ASP	2.8
1	D	166	VAL	2.8
1	A	26	PRO	2.8
1	H	120	TYR	2.8
1	F	142	VAL	2.8
1	F	38	ALA	2.8
1	D	20	LEU	2.8
1	C	97	ASP	2.8
1	A	174	PHE	2.8
1	B	15	PHE	2.8
1	E	61	PRO	2.8
1	G	64	PRO	2.8
1	B	61	PRO	2.8
1	H	130	ALA	2.8
1	F	72	SER	2.8
1	G	22	LEU	2.8
1	B	25	HIS	2.8
1	A	170	VAL	2.7
1	D	15	PHE	2.7
1	F	128	VAL	2.7
1	G	86	LEU	2.7
1	F	202	ALA	2.7
1	H	37	SER	2.7
1	C	120	TYR	2.7
1	D	52	TYR	2.7
1	B	90	LEU	2.7
1	H	11	ASN	2.7
1	B	55	ILE	2.7
1	E	10	GLN	2.7
1	G	171	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	VAL	2.7
1	D	125	ARG	2.7
1	F	90	LEU	2.7
1	H	169	ILE	2.7
1	A	19	ARG	2.7
1	E	36	ARG	2.7
1	E	52	TYR	2.7
1	B	85	GLN	2.7
1	G	27	GLU	2.7
1	C	80	ALA	2.7
1	B	27	GLU	2.7
1	H	66	HIS	2.7
1	E	35	VAL	2.7
1	F	35	VAL	2.7
1	G	75	THR	2.7
1	C	59	CYS	2.6
1	H	131	ARG	2.6
1	F	184	GLN	2.6
1	G	38	ALA	2.6
1	D	126	VAL	2.6
1	G	174	PHE	2.6
1	D	21	GLN	2.6
1	E	154	ALA	2.6
1	C	156	GLY	2.6
1	F	29	GLY	2.6
1	F	64	PRO	2.6
1	D	134	ARG	2.6
1	G	153	ALA	2.6
1	C	163	TYR	2.6
1	E	174	PHE	2.6
1	F	174	PHE	2.6
1	D	37	SER	2.6
1	D	93	PRO	2.6
1	H	61	PRO	2.6
1	H	191	TYR	2.6
1	B	82	ASP	2.6
1	G	147	ILE	2.6
1	B	11	ASN	2.6
1	A	63	SER	2.6
1	B	96	GLU	2.6
1	H	170	VAL	2.6
1	E	92	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	202	ALA	2.6
1	B	60	THR	2.5
1	C	150	SER	2.5
1	A	70	LEU	2.5
1	B	77	MET	2.5
1	F	71	CYS	2.5
1	B	172	PRO	2.5
1	B	193	GLN	2.5
1	F	86	LEU	2.5
1	E	179	PHE	2.5
1	G	13	ALA	2.5
1	B	54	THR	2.5
1	G	93	PRO	2.5
1	H	96	GLU	2.5
1	G	25	HIS	2.5
1	G	28	GLY	2.5
1	F	152	VAL	2.5
1	G	128	VAL	2.5
1	B	140	TYR	2.5
1	H	27	GLU	2.5
1	B	177	ARG	2.5
1	G	134	ARG	2.5
1	F	162	GLY	2.5
1	H	166	VAL	2.5
1	D	161	ALA	2.5
1	H	200	GLN	2.5
1	B	125	ARG	2.5
1	E	134	ARG	2.5
1	B	147	ILE	2.5
1	A	138	LEU	2.5
1	B	67	LEU	2.5
1	C	138	LEU	2.5
1	D	22	LEU	2.5
1	D	58	LEU	2.5
1	D	90	LEU	2.5
1	D	88	VAL	2.5
1	H	161	ALA	2.5
1	C	31	TYR	2.5
1	E	141	THR	2.5
1	C	20	LEU	2.5
1	C	15	PHE	2.4
1	G	166	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	182	PHE	2.4
1	F	54	THR	2.4
1	B	31	TYR	2.4
1	F	163	TYR	2.4
1	D	95	ASP	2.4
1	B	171	SER	2.4
1	D	19	ARG	2.4
1	G	137	LEU	2.4
1	B	51	ALA	2.4
1	A	79	HIS	2.4
1	G	172	PRO	2.4
1	F	28	GLY	2.4
1	D	151	SER	2.4
1	H	72	SER	2.4
1	C	142	VAL	2.4
1	D	8	PRO	2.4
1	F	132	VAL	2.4
1	F	197	VAL	2.4
1	C	60	THR	2.4
1	F	84	LEU	2.4
1	F	137	LEU	2.4
1	G	11	ASN	2.4
1	E	168	CYS	2.4
1	H	183	THR	2.4
1	H	151	SER	2.4
1	A	55	ILE	2.4
1	B	186	GLN	2.4
1	C	76	TRP	2.4
1	B	187	LEU	2.4
1	C	190	LEU	2.4
1	H	22	LEU	2.4
1	H	194	HIS	2.4
1	G	88	VAL	2.4
1	C	63	SER	2.4
1	E	171	SER	2.4
1	A	89	ILE	2.4
1	D	169	ILE	2.4
1	F	95	ASP	2.4
1	G	173	GLY	2.4
1	A	190	LEU	2.4
1	D	165	LEU	2.4
1	G	187	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	90	LEU	2.4
1	H	141	THR	2.4
1	A	35	VAL	2.4
1	B	132	VAL	2.4
1	E	96	GLU	2.4
1	E	197	VAL	2.4
1	E	151	SER	2.4
1	D	97	ASP	2.3
1	G	29	GLY	2.3
1	C	16	TRP	2.3
1	E	190	LEU	2.3
1	H	58	LEU	2.3
1	E	71	CYS	2.3
1	D	96	GLU	2.3
1	G	66	HIS	2.3
1	C	85[A]	GLN	2.3
1	D	121	GLN	2.3
1	F	172	PRO	2.3
1	H	83	PRO	2.3
1	C	58	LEU	2.3
1	C	84	LEU	2.3
1	F	127	LEU	2.3
1	B	76	TRP	2.3
1	H	119	LYS	2.3
1	F	169	ILE	2.3
1	C	22	LEU	2.3
1	C	137	LEU	2.3
1	D	146	ALA	2.3
1	F	78	TYR	2.3
1	G	70	LEU	2.3
1	H	146	ALA	2.3
1	C	95	ASP	2.3
1	F	180	GLU	2.3
1	F	204	GLU	2.3
1	G	189	GLU	2.3
1	A	122	VAL	2.3
1	A	152	VAL	2.3
1	A	179	PHE	2.3
1	H	184	GLN	2.3
1	E	55	ILE	2.3
1	B	95	ASP	2.3
1	D	71	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	52	TYR	2.3
1	B	84	LEU	2.3
1	B	203	TYR	2.3
1	D	12	THR	2.3
1	G	31	TYR	2.3
1	G	140	TYR	2.3
1	F	200	GLN	2.3
1	F	120	TYR	2.3
1	H	29	GLY	2.3
1	B	148	PHE	2.3
1	D	34	VAL	2.3
1	D	142	VAL	2.3
1	H	88	VAL	2.3
1	F	181	ILE	2.3
1	E	84	LEU	2.2
1	F	20	LEU	2.2
1	F	141	THR	2.2
1	A	41	VAL	2.2
1	D	41	VAL	2.2
1	A	61	PRO	2.2
1	F	13	ALA	2.2
1	G	55	ILE	2.2
1	H	196	ALA	2.2
1	C	141	THR	2.2
1	G	53	THR	2.2
1	H	86	LEU	2.2
1	C	155	ASP	2.2
1	C	158	ASP	2.2
1	E	122	VAL	2.2
1	G	14	GLU	2.2
1	H	64	PRO	2.2
1	C	12	THR	2.2
1	E	51	ALA	2.2
1	H	50	HIS	2.2
1	E	121	GLN	2.2
1	D	64	PRO	2.2
1	B	179	PHE	2.2
1	D	168	CYS	2.2
1	G	122	VAL	2.2
1	F	129	GLY	2.2
1	D	76	TRP	2.2
1	E	89	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	84	LEU	2.2
1	E	22	LEU	2.2
1	E	188	MET	2.2
1	C	56	TYR	2.2
1	C	78	TYR	2.2
1	F	203	TYR	2.2
1	H	52	TYR	2.2
1	A	142	VAL	2.2
1	F	32	SER	2.2
1	A	146	ALA	2.2
1	E	132	VAL	2.2
1	B	174	PHE	2.2
1	D	174	PHE	2.2
1	E	193	GLN	2.2
1	G	139	GLN	2.2
1	G	193	GLN	2.2
1	B	13	ALA	2.2
1	B	70	LEU	2.2
1	E	204	GLU	2.2
1	C	8	PRO	2.2
1	A	80	ALA	2.1
1	C	196	ALA	2.1
1	F	154	ALA	2.1
1	H	55	ILE	2.1
1	A	137	LEU	2.1
1	B	24	PRO	2.1
1	B	65	SER	2.1
1	E	118	PRO	2.1
1	B	41	VAL	2.1
1	A	57	PHE	2.1
1	D	158	ASP	2.1
1	A	169	ILE	2.1
1	E	37	SER	2.1
1	E	65	SER	2.1
1	A	71	CYS	2.1
1	B	50	HIS	2.1
1	A	53	THR	2.1
1	B	53	THR	2.1
1	E	163	TYR	2.1
1	E	166	VAL	2.1
1	A	24	PRO	2.1
1	D	24	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	189	GLU	2.1
1	F	14	GLU	2.1
1	F	67	LEU	2.1
1	G	159	GLY	2.1
1	C	121	GLN	2.1
1	F	158	ASP	2.1
1	F	193	GLN	2.1
1	A	153	ALA	2.1
1	A	163	TYR	2.1
1	C	13	ALA	2.1
1	D	122	VAL	2.1
1	E	30	TYR	2.1
1	G	15	PHE	2.1
1	G	133	GLU	2.1
1	G	192	PRO	2.1
1	E	165	LEU	2.1
1	F	18	LYS	2.1
1	H	13	ALA	2.1
1	A	56	TYR	2.1
1	B	56	TYR	2.1
1	C	174	PHE	2.1
1	F	37	SER	2.1
1	H	91	LYS	2.1
1	H	192	PRO	2.1
1	A	119	LYS	2.1
1	C	185	ALA	2.1
1	G	130	ALA	2.1
1	B	138	LEU	2.0
1	C	70	LEU	2.0
1	C	47	ASN	2.0
1	B	122	VAL	2.0
1	D	94	GLN	2.0
1	A	78	TYR	2.0
1	D	31	TYR	2.0
1	C	181	ILE	2.0
1	D	70	LEU	2.0
1	A	11	ASN	2.0
1	H	14	GLU	2.0
1	A	150	SER	2.0
1	G	200	GLN	2.0
1	C	93	PRO	2.0
1	E	19	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	91	LYS	2.0
1	C	55	ILE	2.0
1	E	90	LEU	2.0
1	F	58	LEU	2.0
1	F	187	LEU	2.0
1	G	89	ILE	2.0
1	G	180	GLU	2.0
1	F	77	MET	2.0
1	H	77	MET	2.0
1	H	201	MET	2.0
1	D	60	THR	2.0
1	D	80	ALA	2.0
1	D	153	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.