



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:21 AM UTC

PDB ID : 3M3I / pdb_00003m3i
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

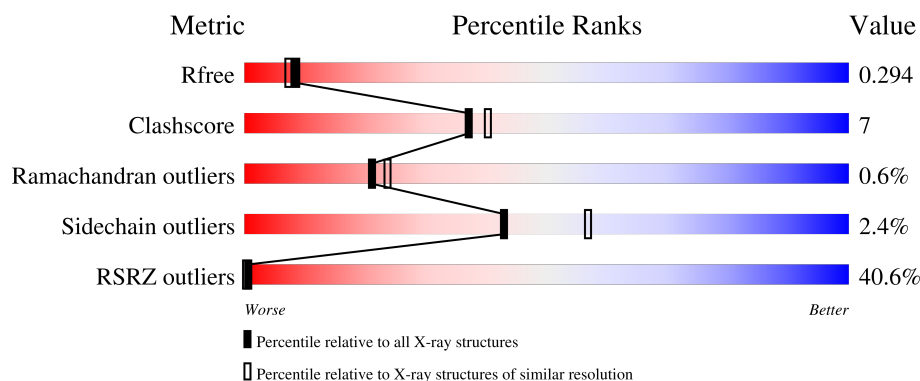
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



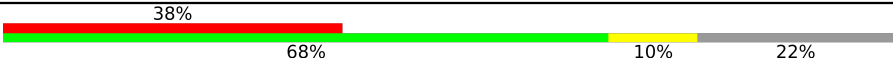
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	32% 67% 11% 21%
1	B	225	35% 64% 14% 21%
1	C	225	22% 64% 14% 20%
1	D	225	20% 65% 13% 20%
1	E	225	24% 67% 12% 21%

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

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

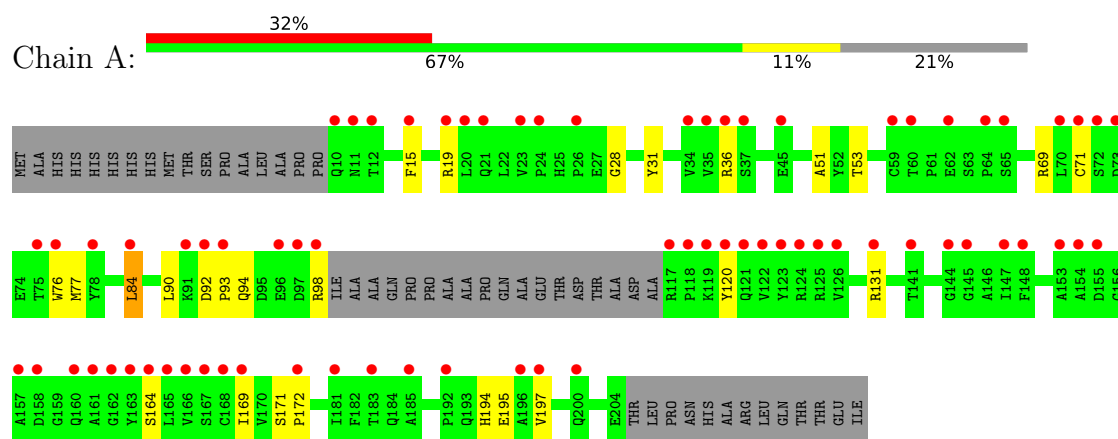
- Molecule 2 is water.

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

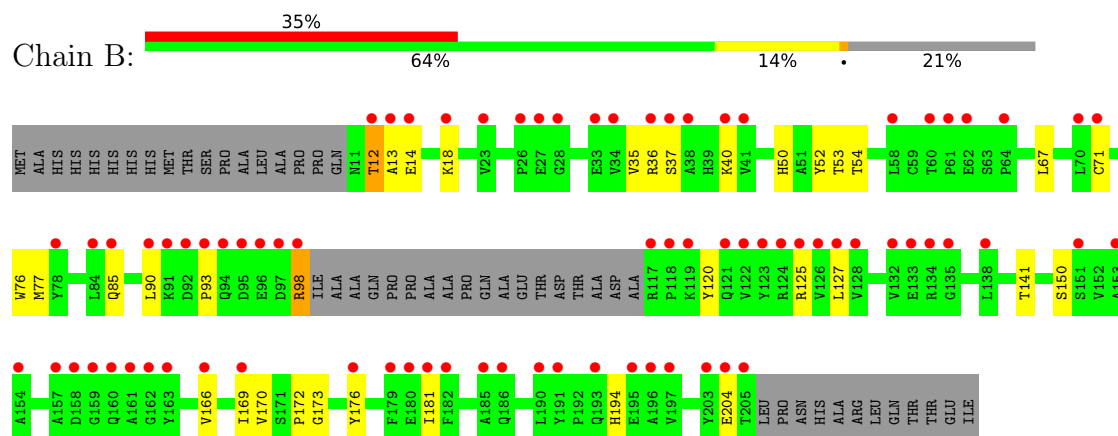
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

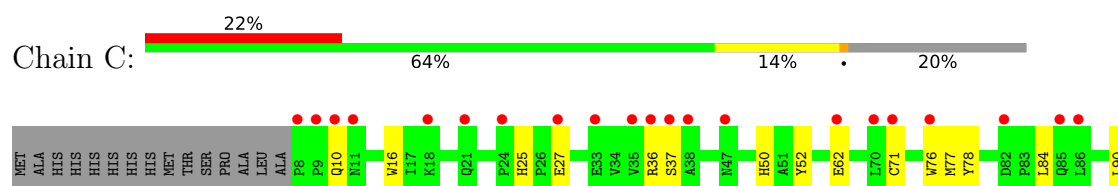
• Molecule 1: Putative uncharacterized protein

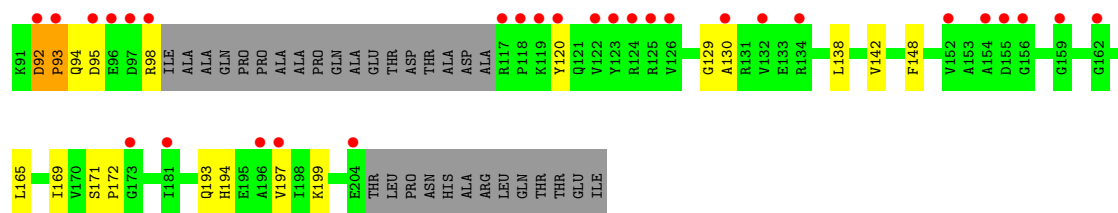


• Molecule 1: Putative uncharacterized protein

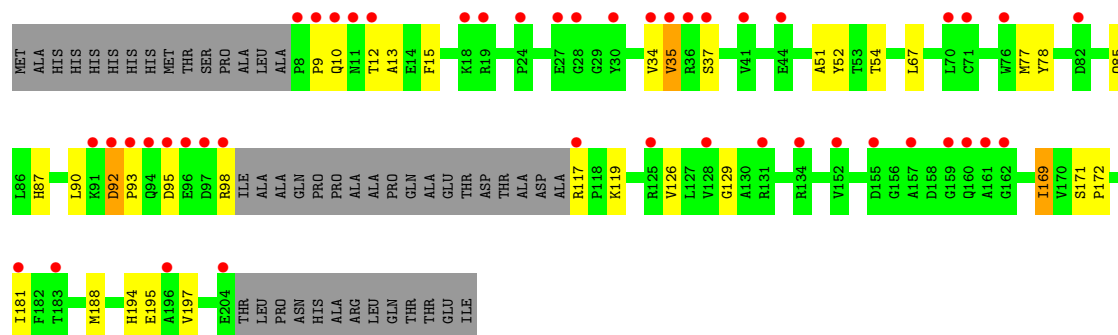


• Molecule 1: Putative uncharacterized protein

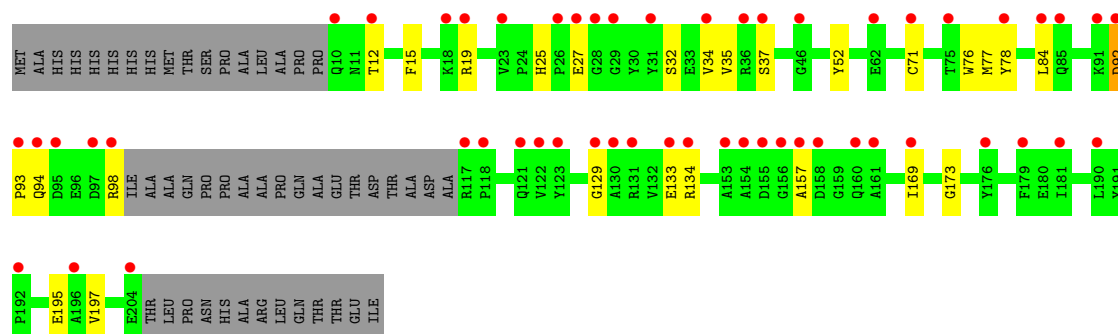




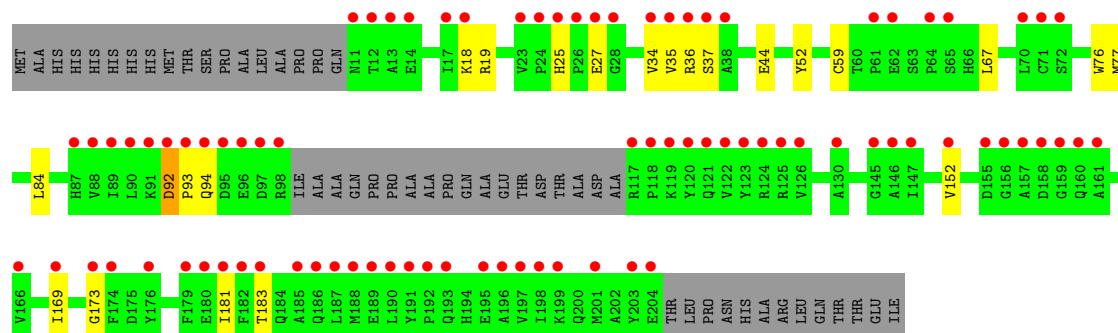
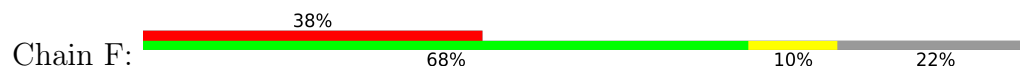
● Molecule 1: Putative uncharacterized protein



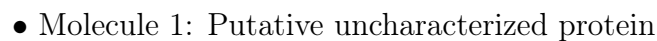
● Molecule 1: Putative uncharacterized protein



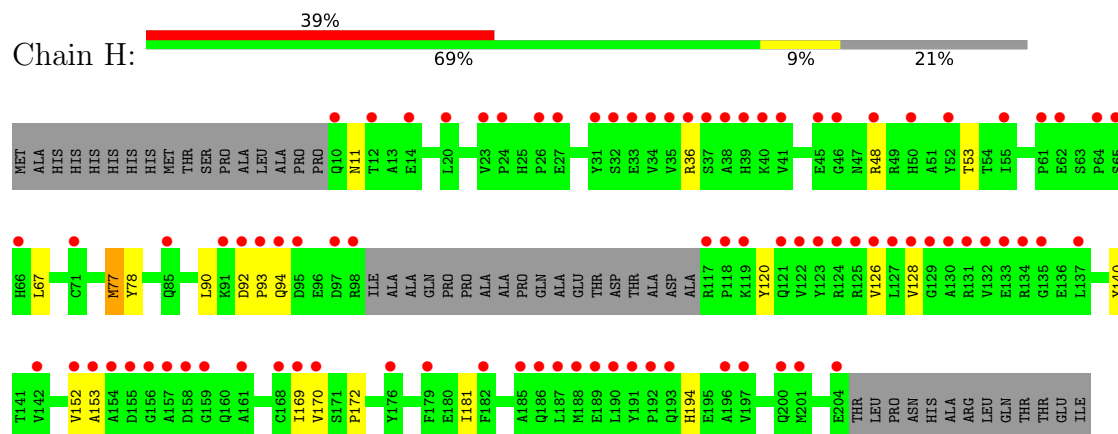
● Molecule 1: Putative uncharacterized protein



Chain G:



Chain H:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.290 0.249 , 0.294	Depositor DCC
R_{free} test set	3684 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)	0.38 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.66	0/1442	0.81	2/1959 (0.1%)
1	B	0.61	0/1463	0.77	1/1989 (0.1%)
1	C	0.70	0/1471	0.81	0/2000
1	D	0.68	0/1465	0.82	0/1991
1	E	0.67	0/1451	0.80	1/1971 (0.1%)
1	F	0.63	0/1440	0.81	1/1959 (0.1%)
1	G	0.61	0/1446	0.78	0/1966
1	H	0.61	0/1454	0.77	0/1976
All	All	0.65	0/11632	0.80	5/15811 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	173	GLY	N-CA-C	7.73	120.82	111.93
1	B	173	GLY	N-CA-C	6.29	119.25	112.33
1	A	31	TYR	N-CA-C	5.57	116.73	108.60
1	E	173	GLY	N-CA-C	5.16	118.01	112.33
1	A	28	GLY	N-CA-C	-5.15	105.71	111.63

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	19	0
1	B	1424	0	1338	25	0
1	C	1431	0	1351	27	0
1	D	1425	0	1351	29	0
1	E	1413	0	1335	20	0
1	F	1401	0	1312	20	0
1	G	1407	0	1323	28	0
1	H	1416	0	1332	20	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	156	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 (156) 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:D:77:MET:HE3	1:G:77:MET:HE3	1.48	0.93
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:C:77:MET:HE3	1:F:77:MET:HE3	1.55	0.86
1:B:77:MET:HE3	1:E:77:MET:HE3	1.63	0.80
1:D:77:MET:HE3	1:G:77:MET:CE	2.12	0.79
1:F:77:MET:HE1	1:F:169:ILE:CD1	2.12	0.79
1:C:92:ASP:O	1:C:94:GLN:N	2.20	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:C:77:MET:HE3	1:F:77:MET:CE	2.24	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:MET:HE3	1:G:77:MET:SD	2.34	0.66
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:F:77:MET:HE1	1:F:169:ILE:HD13	1.77	0.66
1:B:77:MET:CE	1:E:77:MET:HE3	2.25	0.66
1:B:12:THR:HG22	1:B:14:GLU:H	1.61	0.65
1:B:77:MET:SD	1:E:77:MET:HE3	2.40	0.62
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
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: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:F:77:MET:HE1	1:F:169:ILE:HD12	1.85	0.57
1:C:77:MET:CE	1:F:77:MET:HE3	2.30	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:A:77:MET:HE3	1:H:77:MET:SD	2.45	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: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:B:176[B]:TYR:CD1	1:B:176[B]:TYR:C	2.87	0.52
1:C:95:ASP:OD1	1:C:98:ARG:NH2	2.42	0.52
1:C:171:SER:HA	1:C:172:PRO:C	2.34	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:A:77:MET:HE3	1:H:77:MET:HE3	1.90	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:171:SER:HA	1:A:172:PRO:C	2.37	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
1:H:170:VAL:HG12	1:H:172:PRO:O	2.13	0.48
1:D:77:MET:CE	1:G:77:MET:HE3	2.33	0.48
1:C:169:ILE:CD1	1:F:169:ILE:HD13	2.42	0.48
1:E:37:SER:HB2	1:E:52:TYR:CD2	2.49	0.48
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: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:F:77:MET:HB2	1:F:77:MET:HE2	1.82	0.47
1:B:77:MET:HE3	1:E:77:MET:CE	2.42	0.46
1:A:51:ALA:O	1:A:172:PRO:HA	2.16	0.46
1:G:171:SER:HA	1:G:172:PRO:C	2.39	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:A:77:MET:HE3	1:H:77:MET:CE	2.46	0.46
1:E:37:SER:HB2	1:E:52:TYR:CE2	2.50	0.46
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:G:77:MET:HE1	1:G:169:ILE:HD12	1.99	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:D:171:SER:HA	1:D:172:PRO:C	2.41	0.45
1:G:67:LEU:O	1:G:181:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:188:MET:HE1	1:D:195:GLU:HB2	2.00	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:G:77:MET:CE	1:G:169:ILE:HD12	2.48	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:D:77:MET:HE2	1:D:77:MET:HB2	1.90	0.43
1:G:90:LEU:O	1:G:120:TYR:HA	2.19	0.43
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: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:D:12:THR:O	1:D:13:ALA:C	2.62	0.42
1:B:40:LYS:HZ1	1:B:50:HIS:CE1	2.38	0.42
1:D:117:ARG:O	1:D:119:LYS:NZ	2.47	0.42
1:H:67:LEU:O	1:H:181:ILE:HD12	2.20	0.42
1:D:34:VAL:HG12	1:D:35:VAL:HG12	2.00	0.42
1:E:77:MET:HE2	1:E:77:MET:HB2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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%)	21	24
1	B	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	21	24
1	C	176/225 (78%)	172 (98%)	3 (2%)	1 (1%)	21	24
1	D	175/225 (78%)	168 (96%)	6 (3%)	1 (1%)	21	24
1	E	174/225 (77%)	167 (96%)	6 (3%)	1 (1%)	21	24
1	F	173/225 (77%)	167 (96%)	5 (3%)	1 (1%)	21	24
1	G	173/225 (77%)	168 (97%)	4 (2%)	1 (1%)	21	24
1	H	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	21	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1392/1800 (77%)	1347 (97%)	37 (3%)	8 (1%)	21 24

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%)	142 (98%)	3 (2%)	47 61
1	B	149/188 (79%)	144 (97%)	5 (3%)	32 43
1	C	149/188 (79%)	146 (98%)	3 (2%)	48 63
1	D	149/188 (79%)	145 (97%)	4 (3%)	39 52
1	E	146/188 (78%)	141 (97%)	5 (3%)	32 43
1	F	144/188 (77%)	141 (98%)	3 (2%)	47 61
1	G	145/188 (77%)	141 (97%)	4 (3%)	38 51
1	H	147/188 (78%)	146 (99%)	1 (1%)	76 86
All	All	1174/1504 (78%)	1146 (98%)	28 (2%)	43 57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	CYS
1	A	84	LEU

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Mol	Chain	Res	Type
1	A	98	ARG
1	B	12	THR
1	B	18	LYS
1	B	71	CYS
1	B	98	ARG
1	B	204	GLU
1	C	10	GLN
1	C	71	CYS
1	C	92	ASP
1	D	35	VAL
1	D	92	ASP
1	D	126	VAL
1	D	169	ILE
1	E	19	ARG
1	E	32	SER
1	E	71	CYS
1	E	92	ASP
1	E	197	VAL
1	F	18	LYS
1	F	92	ASP
1	F	183	THR
1	G	18	LYS
1	G	71	CYS
1	G	167	SER
1	G	197	VAL
1	H	77	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	200	GLN
1	B	139	GLN
1	C	10	GLN
1	C	139	GLN
1	D	85	GLN
1	G	21	GLN
1	G	25	HIS
1	G	43	ASN
1	G	68	HIS
1	G	121	GLN
1	H	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	177/225 (78%)	2.04	73 (41%) 0 0	57, 69, 99, 135	0
1	B	177/225 (78%)	2.09	78 (44%) 0 0	37, 73, 101, 162	1 (0%)
1	C	179/225 (79%)	1.65	50 (27%) 1 1	32, 65, 83, 101	1 (0%)
1	D	179/225 (79%)	1.59	45 (25%) 1 1	57, 65, 84, 113	0
1	E	177/225 (78%)	1.70	53 (29%) 1 1	32, 66, 84, 124	1 (0%)
1	F	176/225 (78%)	2.23	85 (48%) 0 0	37, 74, 113, 205	1 (0%)
1	G	176/225 (78%)	2.44	103 (58%) 0 0	38, 77, 121, 180	1 (0%)
1	H	177/225 (78%)	2.16	88 (49%) 0 0	35, 74, 107, 142	1 (0%)
All	All	1418/1800 (78%)	1.99	575 (40%) 0 0	32, 70, 103, 205	6 (0%)

All (575) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	ARG	9.1
1	G	98	ARG	7.8
1	B	176[A]	TYR	7.8
1	G	176[A]	TYR	6.9
1	G	97	ASP	6.8
1	F	97	ASP	6.7
1	A	93	PRO	6.6
1	E	93	PRO	6.6
1	F	117	ARG	6.4
1	F	176[A]	TYR	6.3
1	G	125	ARG	6.2
1	B	93	PRO	6.2
1	H	93	PRO	6.2
1	B	118	PRO	6.2
1	F	93	PRO	6.1
1	B	98	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	H	36	ARG	5.8
1	A	118	PRO	5.8
1	E	117	ARG	5.6
1	D	93	PRO	5.6
1	G	93	PRO	5.5
1	F	118	PRO	5.4
1	H	35	VAL	5.3
1	E	97	ASP	5.3
1	G	204	GLU	5.3
1	D	98	ARG	5.3
1	G	190	LEU	5.3
1	G	117	ARG	5.2
1	A	10	GLN	5.1
1	F	95	ASP	5.0
1	B	36	ARG	5.0
1	H	129	GLY	4.9
1	G	38	ALA	4.9
1	A	154	ALA	4.8
1	G	91	LYS	4.8
1	A	98	ARG	4.8
1	A	168	CYS	4.7
1	C	93	PRO	4.7
1	A	121	GLN	4.7
1	C	117	ARG	4.7
1	B	121	GLN	4.6
1	H	98	ARG	4.6
1	H	117	ARG	4.6
1	F	155	ASP	4.6
1	H	130	ALA	4.6
1	E	98	ARG	4.6
1	E	36	ARG	4.5
1	F	124	ARG	4.5
1	B	117	ARG	4.4
1	G	191	TYR	4.4
1	C	125	ARG	4.4
1	D	97	ASP	4.4
1	G	124	ARG	4.4
1	F	94	GLN	4.4
1	F	204	GLU	4.4
1	H	92	ASP	4.4
1	A	125	ARG	4.3
1	G	126	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	131	ARG	4.3
1	H	132	VAL	4.3
1	A	119	LYS	4.3
1	B	97	ASP	4.3
1	H	155	ASP	4.3
1	F	190	LEU	4.3
1	H	134	ARG	4.2
1	F	12	THR	4.2
1	B	92	ASP	4.2
1	A	157	ALA	4.2
1	F	96	GLU	4.2
1	G	92	ASP	4.1
1	G	95	ASP	4.1
1	D	92	ASP	4.1
1	G	12	THR	4.1
1	H	185	ALA	4.1
1	C	98	ARG	4.1
1	H	118	PRO	4.1
1	B	91	LYS	4.0
1	F	36	ARG	4.0
1	A	62	GLU	4.0
1	E	62	GLU	4.0
1	H	176	TYR	4.0
1	G	185	ALA	3.9
1	C	36	ARG	3.9
1	G	122	VAL	3.9
1	B	193	GLN	3.9
1	B	28	GLY	3.9
1	E	118	PRO	3.9
1	A	122	VAL	3.9
1	A	117	ARG	3.9
1	G	121	GLN	3.8
1	H	190	LEU	3.8
1	G	130	ALA	3.8
1	H	12	THR	3.8
1	H	38	ALA	3.8
1	B	125	ARG	3.8
1	D	117	ARG	3.8
1	G	13	ALA	3.8
1	C	204	GLU	3.8
1	D	204	GLU	3.8
1	G	26	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	65	SER	3.8
1	B	205	THR	3.8
1	A	120	TYR	3.7
1	A	123	TYR	3.7
1	C	35	VAL	3.8
1	F	189	GLU	3.7
1	G	27	GLU	3.7
1	F	26	PRO	3.7
1	F	65	SER	3.7
1	B	196	ALA	3.7
1	G	36	ARG	3.7
1	G	203	TYR	3.7
1	F	122	VAL	3.7
1	H	135	GLY	3.6
1	A	153	ALA	3.6
1	G	183	THR	3.6
1	A	167	SER	3.6
1	G	188	MET	3.6
1	B	12	THR	3.6
1	F	126	VAL	3.6
1	A	161	ALA	3.6
1	H	27	GLU	3.6
1	E	131	ARG	3.6
1	G	179	PHE	3.6
1	G	71	CYS	3.6
1	B	166	VAL	3.5
1	G	34	VAL	3.5
1	G	96	GLU	3.5
1	F	125	ARG	3.5
1	H	124	ARG	3.5
1	A	163	TYR	3.5
1	G	35	VAL	3.5
1	F	181	ILE	3.5
1	H	33	GLU	3.5
1	F	179	PHE	3.5
1	D	94	GLN	3.5
1	C	97	ASP	3.4
1	F	186	GLN	3.4
1	C	196	ALA	3.4
1	G	137	LEU	3.4
1	C	85[A]	GLN	3.4
1	D	10	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	95	ASP	3.4
1	A	166	VAL	3.4
1	C	38	ALA	3.4
1	G	134	ARG	3.4
1	H	133	GLU	3.4
1	H	85[A]	GLN	3.4
1	G	181	ILE	3.3
1	C	76	TRP	3.3
1	G	62	GLU	3.3
1	A	126	VAL	3.3
1	F	185	ALA	3.3
1	B	94	GLN	3.3
1	B	13	ALA	3.3
1	F	196	ALA	3.3
1	A	64	PRO	3.3
1	A	12	THR	3.3
1	B	123	TYR	3.3
1	H	191	TYR	3.3
1	E	158	ASP	3.3
1	C	118	PRO	3.3
1	F	203	TYR	3.3
1	B	26	PRO	3.2
1	H	94	GLN	3.2
1	G	182	PHE	3.2
1	F	38	ALA	3.2
1	H	34	VAL	3.2
1	A	162	GLY	3.2
1	E	92	ASP	3.2
1	F	158	ASP	3.2
1	H	204	GLU	3.2
1	G	94	GLN	3.2
1	D	155	ASP	3.2
1	H	95	ASP	3.2
1	F	37	SER	3.2
1	H	119	LYS	3.2
1	E	12	THR	3.2
1	F	182	PHE	3.1
1	A	70	LEU	3.1
1	H	121	GLN	3.1
1	A	158	ASP	3.1
1	B	135	GLY	3.1
1	E	121	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	160	GLN	3.1
1	A	24	PRO	3.1
1	F	123	TYR	3.1
1	G	118	PRO	3.1
1	G	192	PRO	3.1
1	E	181	ILE	3.1
1	H	37	SER	3.1
1	A	97	ASP	3.1
1	F	159	GLY	3.1
1	G	144	GLY	3.1
1	B	122	VAL	3.1
1	E	26	PRO	3.1
1	B	133	GLU	3.1
1	C	162	GLY	3.1
1	G	196	ALA	3.1
1	B	64	PRO	3.1
1	G	197	VAL	3.1
1	G	127	LEU	3.1
1	H	14	GLU	3.0
1	A	160	GLN	3.0
1	D	91	LYS	3.0
1	B	157	ALA	3.0
1	E	157	ALA	3.0
1	B	197	VAL	3.0
1	G	170	VAL	3.0
1	H	122	VAL	3.0
1	D	181	ILE	3.0
1	A	131	ARG	3.0
1	D	19	ARG	3.0
1	B	154	ALA	3.0
1	G	33	GLU	3.0
1	B	186	GLN	3.0
1	F	18	LYS	3.0
1	H	40	LYS	3.0
1	G	63	SER	3.0
1	C	92	ASP	3.0
1	C	62	GLU	3.0
1	F	157	ALA	3.0
1	C	181	ILE	3.0
1	G	123	TYR	3.0
1	A	155	ASP	3.0
1	H	26	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	190	LEU	2.9
1	C	132	VAL	2.9
1	H	128	VAL	2.9
1	C	155	ASP	2.9
1	E	153	ALA	2.9
1	G	154	ALA	2.9
1	D	128	VAL	2.9
1	G	152	VAL	2.9
1	F	89	ILE	2.9
1	B	33	GLU	2.9
1	F	180	GLU	2.9
1	E	192	PRO	2.9
1	A	196	ALA	2.9
1	C	10	GLN	2.9
1	A	181	ILE	2.9
1	F	183	THR	2.9
1	F	188	MET	2.9
1	G	189	GLU	2.9
1	E	95	ASP	2.9
1	G	187	LEU	2.9
1	D	96	GLU	2.9
1	G	65	SER	2.8
1	B	38	ALA	2.8
1	C	126	VAL	2.8
1	B	14	GLU	2.8
1	F	14	GLU	2.8
1	F	27	GLU	2.8
1	C	18	LYS	2.8
1	G	162	GLY	2.8
1	B	61	PRO	2.8
1	G	64	PRO	2.8
1	G	120	TYR	2.8
1	F	62	GLU	2.8
1	C	71	CYS	2.8
1	F	71	CYS	2.8
1	G	131	ARG	2.8
1	E	37	SER	2.8
1	G	72	SER	2.8
1	G	151	SER	2.8
1	D	9	PRO	2.8
1	F	191	TYR	2.8
1	B	127	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	70	LEU	2.8
1	E	34	VAL	2.8
1	E	122	VAL	2.8
1	B	95	ASP	2.8
1	D	76	TRP	2.8
1	C	159	GLY	2.8
1	B	27	GLU	2.8
1	G	133	GLU	2.8
1	B	203	TYR	2.8
1	D	134	ARG	2.8
1	A	11	ASN	2.7
1	B	85	GLN	2.7
1	C	95	ASP	2.7
1	E	10	GLN	2.7
1	E	156	GLY	2.7
1	C	24	PRO	2.7
1	F	61	PRO	2.7
1	H	157	ALA	2.7
1	F	25	HIS	2.7
1	C	156	GLY	2.7
1	D	162	GLY	2.7
1	F	28	GLY	2.7
1	D	8	PRO	2.7
1	A	71	CYS	2.7
1	G	180	GLU	2.7
1	B	128	VAL	2.7
1	D	35	VAL	2.7
1	F	160	GLN	2.7
1	G	155	ASP	2.7
1	G	17	ILE	2.7
1	A	37	SER	2.7
1	G	61	PRO	2.7
1	B	58	LEU	2.7
1	E	154	ALA	2.7
1	E	196	ALA	2.7
1	F	146	ALA	2.7
1	F	120	TYR	2.7
1	B	181	ILE	2.7
1	A	19	ARG	2.7
1	A	76	TRP	2.7
1	G	186	GLN	2.6
1	G	202	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	161	ALA	2.6
1	E	176	TYR	2.6
1	G	18	LYS	2.6
1	H	152	VAL	2.6
1	A	192	PRO	2.6
1	B	134	ARG	2.6
1	F	147	ILE	2.6
1	F	192	PRO	2.6
1	G	24	PRO	2.6
1	H	169	ILE	2.6
1	F	119	LYS	2.6
1	G	156	GLY	2.6
1	H	188	MET	2.6
1	H	10	GLN	2.6
1	B	161	ALA	2.6
1	H	158	ASP	2.6
1	F	64	PRO	2.6
1	F	72	SER	2.6
1	B	160	GLN	2.6
1	H	193	GLN	2.6
1	B	204	GLU	2.6
1	B	185	ALA	2.6
1	H	154	ALA	2.6
1	F	92	ASP	2.6
1	F	145	GLY	2.6
1	G	30	TYR	2.6
1	A	124	ARG	2.5
1	G	157	ALA	2.5
1	A	73	ASP	2.5
1	E	155	ASP	2.5
1	G	145	GLY	2.5
1	B	37	SER	2.5
1	D	18	LYS	2.5
1	G	199	LYS	2.5
1	H	197	VAL	2.5
1	A	183	THR	2.5
1	G	139	GLN	2.5
1	A	169	ILE	2.5
1	B	169	ILE	2.5
1	A	36	ARG	2.5
1	A	185	ALA	2.5
1	B	40	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	11	ASN	2.5
1	G	40	LYS	2.5
1	G	158	ASP	2.5
1	H	196	ALA	2.5
1	E	28	GLY	2.5
1	G	28	GLY	2.5
1	A	60	THR	2.5
1	E	94	GLN	2.5
1	F	121	GLN	2.5
1	A	23	VAL	2.5
1	C	152	VAL	2.5
1	D	36	ARG	2.5
1	H	41	VAL	2.5
1	H	62	GLU	2.5
1	C	120	TYR	2.5
1	H	127	LEU	2.5
1	A	21	GLN	2.5
1	F	156	GLY	2.5
1	F	173	GLY	2.5
1	G	135	GLY	2.5
1	H	159	GLY	2.5
1	B	96	GLU	2.4
1	E	133	GLU	2.4
1	F	23	VAL	2.4
1	G	147	ILE	2.4
1	A	165	LEU	2.4
1	H	39	HIS	2.4
1	F	193	GLN	2.4
1	D	28	GLY	2.4
1	D	125	ARG	2.4
1	E	27	GLU	2.4
1	E	204	GLU	2.4
1	G	173	GLY	2.4
1	A	147	ILE	2.4
1	B	179	PHE	2.4
1	F	35	VAL	2.4
1	E	123	TYR	2.4
1	H	31	TYR	2.4
1	C	124	ARG	2.4
1	H	97	ASP	2.4
1	H	125	ARG	2.4
1	C	130	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	71	CYS	2.4
1	E	18	LYS	2.4
1	E	91	LYS	2.4
1	G	148	PHE	2.4
1	H	142	VAL	2.4
1	C	134	ARG	2.4
1	H	200	GLN	2.4
1	B	62	GLU	2.4
1	C	82	ASP	2.4
1	A	26	PRO	2.4
1	F	130	ALA	2.4
1	A	75	THR	2.4
1	A	35	VAL	2.4
1	B	23	VAL	2.4
1	B	132	VAL	2.4
1	D	71	CYS	2.4
1	E	169	ILE	2.4
1	F	169	ILE	2.4
1	H	48	ARG	2.4
1	A	200	GLN	2.4
1	G	184	GLN	2.4
1	B	180	GLU	2.4
1	B	195	GLU	2.4
1	C	27	GLU	2.4
1	H	189	GLU	2.4
1	B	191	TYR	2.3
1	C	123	TYR	2.3
1	H	192	PRO	2.3
1	C	119	LYS	2.3
1	G	129	GLY	2.3
1	D	161	ALA	2.3
1	D	12	THR	2.3
1	G	201	MET	2.3
1	A	59	CYS	2.3
1	G	128	VAL	2.3
1	H	168	CYS	2.3
1	D	27	GLU	2.3
1	H	186	GLN	2.3
1	G	82	ASP	2.3
1	B	119	LYS	2.3
1	E	31	TYR	2.3
1	H	61	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	157	ALA	2.3
1	F	13	ALA	2.3
1	H	153	ALA	2.3
1	D	183	THR	2.3
1	F	201	MET	2.3
1	F	87	HIS	2.3
1	F	197	VAL	2.3
1	G	14	GLU	2.3
1	H	170	VAL	2.3
1	B	153	ALA	2.3
1	D	196	ALA	2.3
1	A	164	SER	2.3
1	H	66	HIS	2.3
1	C	96	GLU	2.3
1	A	15	PHE	2.3
1	B	41	VAL	2.3
1	G	88	VAL	2.3
1	H	126	VAL	2.3
1	F	199	LYS	2.3
1	E	71	CYS	2.3
1	D	30	TYR	2.3
1	G	163	TYR	2.3
1	G	66	HIS	2.3
1	H	91	LYS	2.3
1	A	84	LEU	2.2
1	C	70	LEU	2.2
1	F	174	PHE	2.2
1	H	187	LEU	2.2
1	C	47	ASN	2.2
1	D	82	ASP	2.2
1	A	144	GLY	2.2
1	E	29	GLY	2.2
1	C	154	ALA	2.2
1	E	75	THR	2.2
1	G	31	TYR	2.2
1	H	50	HIS	2.2
1	A	65	SER	2.2
1	E	85[A]	GLN	2.2
1	A	34	VAL	2.2
1	A	197	VAL	2.2
1	B	90	LEU	2.2
1	C	122	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	88	VAL	2.2
1	B	162	GLY	2.2
1	G	195	GLU	2.2
1	B	18	LYS	2.2
1	F	91	LYS	2.2
1	F	161	ALA	2.2
1	H	52	TYR	2.2
1	E	84	LEU	2.2
1	H	20	LEU	2.2
1	F	34	VAL	2.2
1	F	152	VAL	2.2
1	D	11	ASN	2.2
1	E	19	ARG	2.2
1	C	8	PRO	2.2
1	H	64	PRO	2.2
1	E	129	GLY	2.2
1	C	21	GLN	2.2
1	D	160	GLN	2.2
1	E	78	TYR	2.2
1	C	86	LEU	2.2
1	D	41	VAL	2.2
1	H	182	PHE	2.2
1	H	46	GLY	2.2
1	H	156	GLY	2.2
1	B	151	SER	2.2
1	D	37	SER	2.2
1	B	124	ARG	2.1
1	B	163	TYR	2.1
1	E	134	ARG	2.1
1	A	20	LEU	2.1
1	B	138	LEU	2.1
1	F	90	LEU	2.1
1	C	197	VAL	2.1
1	F	166	VAL	2.1
1	A	96	GLU	2.1
1	E	179	PHE	2.1
1	F	195	GLU	2.1
1	G	21	GLN	2.1
1	H	71	CYS	2.1
1	D	131	ARG	2.1
1	A	78	TYR	2.1
1	H	123	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	2.1
1	B	84	LEU	2.1
1	F	187	LEU	2.1
1	F	198	ILE	2.1
1	G	70	LEU	2.1
1	D	44	GLU	2.1
1	E	23	VAL	2.1
1	A	145	GLY	2.1
1	D	159	GLY	2.1
1	A	72	SER	2.1
1	A	45	GLU	2.1
1	H	45	GLU	2.1
1	B	34	VAL	2.1
1	B	126	VAL	2.1
1	D	24	PRO	2.1
1	A	148	PHE	2.1
1	B	159	GLY	2.1
1	E	46	GLY	2.1
1	G	159	GLY	2.1
1	B	60	THR	2.1
1	G	119	LYS	2.1
1	G	161	ALA	2.1
1	H	201	MET	2.1
1	H	55	ILE	2.1
1	F	24	PRO	2.1
1	D	34	VAL	2.1
1	G	23	VAL	2.1
1	H	23	VAL	2.1
1	B	182	PHE	2.1
1	C	173	GLY	2.1
1	A	141	THR	2.0
1	C	37	SER	2.0
1	G	37	SER	2.0
1	G	153	ALA	2.0
1	B	158	ASP	2.0
1	D	70	LEU	2.0
1	E	190	LEU	2.0
1	F	11	ASN	2.0
1	H	137	LEU	2.0
1	F	17	ILE	2.0
1	G	169	ILE	2.0
1	A	172	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	9	PRO	2.0
1	B	78	TYR	2.0
1	D	152	VAL	2.0
1	G	81	GLY	2.0
1	H	179	PHE	2.0
1	A	91	LYS	2.0
1	C	33	GLU	2.0
1	H	32	SER	2.0
1	E	130	ALA	2.0
1	E	161	ALA	2.0
1	A	92	ASP	2.0
1	G	42	ASP	2.0
1	H	24	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.