



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:30 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

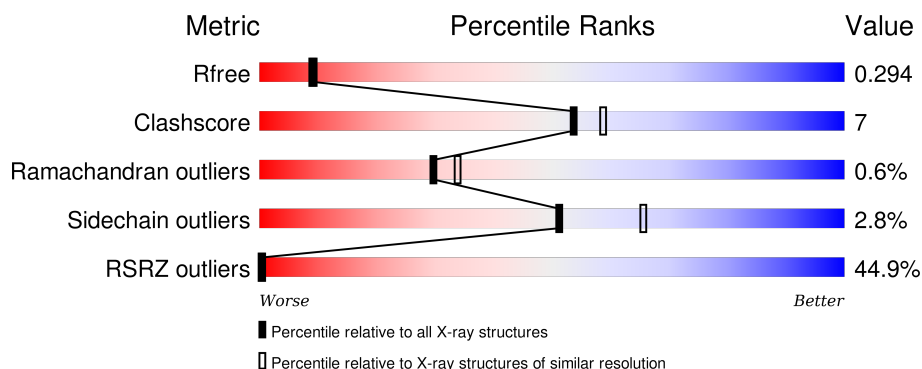
1 Overall quality at a glance

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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (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 ≥ 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>30%</div> <div>68% 10% • 21%</div> </div>
1	B	225	<div> <div>39%</div> <div>64% 14% • 21%</div> </div>
1	C	225	<div> <div>29%</div> <div>64% 14% • 20%</div> </div>
1	D	225	<div> <div>26%</div> <div>67% 12% • 20%</div> </div>
1	E	225	<div> <div>28%</div> <div>66% 12% 21%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	225	<div><div>44%</div><div><div></div><div></div><div></div><div></div></div><div>69%</div><div>9%</div><div>22%</div></div>
1	G	225	<div><div>44%</div><div><div></div><div></div><div></div><div></div></div><div>63%</div><div>14%</div><div>22%</div></div>
1	H	225	<div><div>42%</div><div><div></div><div></div><div></div><div></div></div><div>68%</div><div>10%</div><div>21%</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

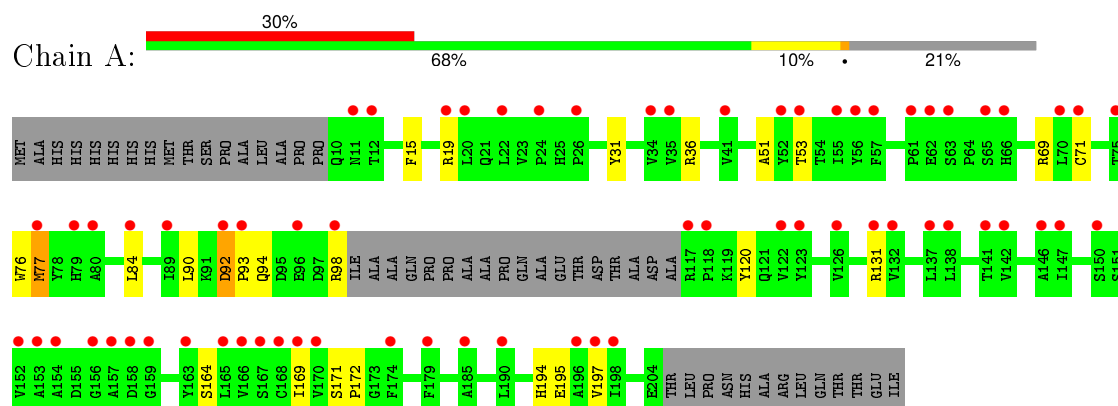
- Molecule 2 is water.

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

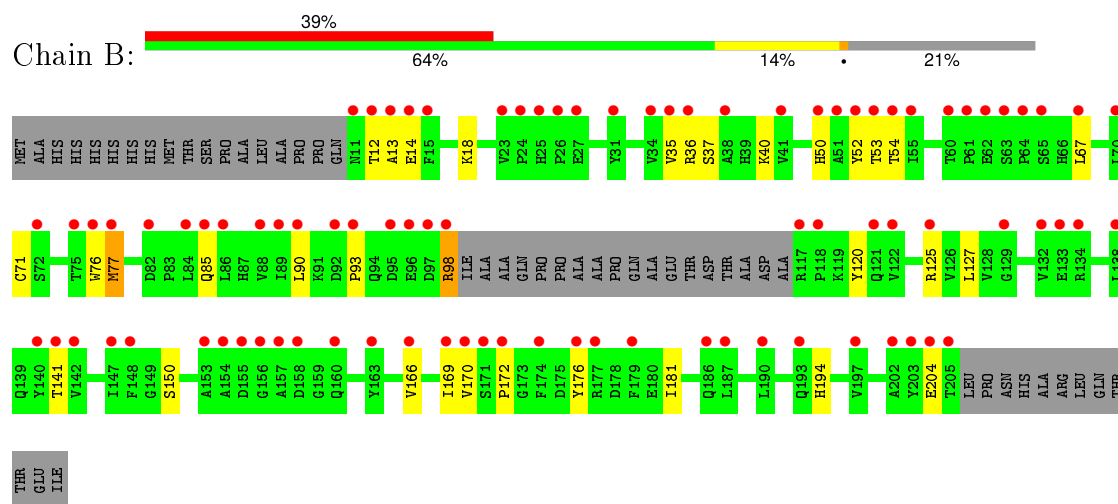
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

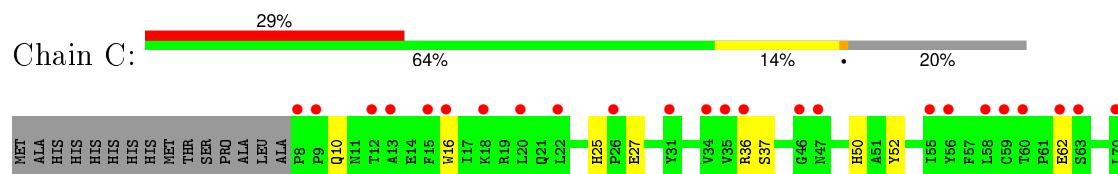
• Molecule 1: Putative uncharacterized protein



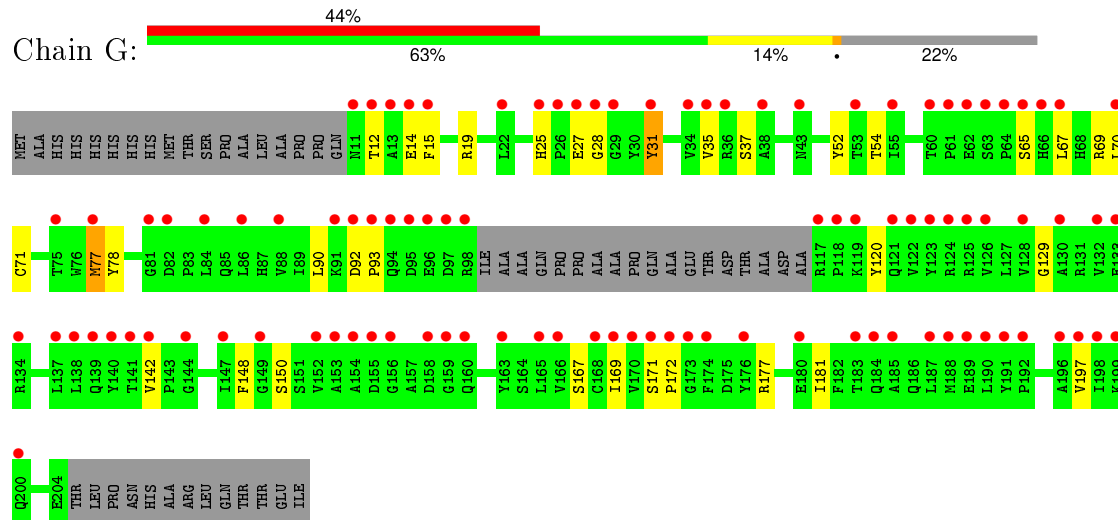
• Molecule 1: Putative uncharacterized protein



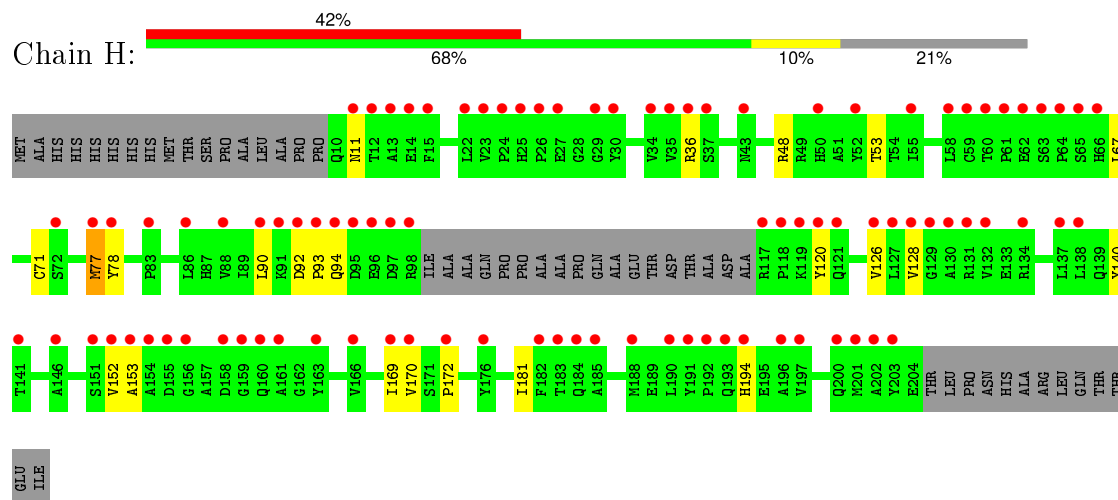
• Molecule 1: Putative uncharacterized protein



● 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, α , β , γ	52.98 Å 98.43 Å 100.76 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.5.0106	Depositor
R, R_{free}	0.239 , 0.290 0.249 , 0.294	Depositor DCC
R_{free} test set	3677 reflections (5.26%)	DCC
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 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 73637 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:H:92:ASP:O	1:H:94:GLN:N	2.36	0.59
1:B:169:ILE:HD12	1:E:169:ILE:HD12	1.84	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:77:MET:HE3	1:G:77:MET:HG2	1.86	0.57
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: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:95:ASP:O	1:D:98:ARG:HG3	2.08	0.53
1:D:10:GLN:HG2	1:D:15:PHE:CZ	2.43	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:E:134:ARG:HH12	1:E:157:ALA:HB1	1.81	0.45
1:C:193:GLN:HB3	1:E:133:GLU:HG3	1.98	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:B:12:THR:CG2	1:B:13:ALA:N	2.79	0.45
1:A:36:ARG:HG2	1:A:53:THR:HG22	1.98	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:H:11:ASN:HB2	2:H:225:HOH:O	2.16	0.45
1:F:37:SER:HB2	1:F:52:TYR:CD2	2.53	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: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: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:G:171:SER:HA	1:G:172:PRO:C	2.39	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: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:G:37:SER:HB2	1:G:52:TYR:CD2	2.54	0.42
1:D:34:VAL:HG12	1:D:35:VAL:HG12	2.00	0.42
1:B:76:TRP:CE3	1:B:166:VAL:HG21	2.54	0.42
1:G:12:THR:HG23	1:G:14:GLU:H	1.85	0.42
1:D:194:HIS:O	1:D:197:VAL:HG12	2.20	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:D:34:VAL:HG12	1:D:35:VAL:CG1	2.51	0.41
1:C:90:LEU:O	1:C:120:TYR:HA	2.20	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:G:142:VAL:HG11	1:G:148:PHE:CE1	2.54	0.41
1:B:77:MET:SD	1:E:77:MET:HE2	2.61	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:92:ASP:O	1:F:94:GLN:N	2.54	0.41
1:F:34:VAL:HG12	1:F:35:VAL:HG13	2.02	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:H:90:LEU:O	1:H:120:TYR:HA	2.21	0.40
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:92:ASP:HB2	1:H:94:GLN:HG3	2.03	0.40
1:D:194:HIS:HB3	1:D:197:VAL:HG12	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%)	30	34
1	B	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	30	34
1	C	176/225 (78%)	172 (98%)	3 (2%)	1 (1%)	30	34
1	D	175/225 (78%)	168 (96%)	6 (3%)	1 (1%)	30	34
1	E	174/225 (77%)	167 (96%)	6 (3%)	1 (1%)	30	34
1	F	173/225 (77%)	167 (96%)	5 (3%)	1 (1%)	30	34
1	G	173/225 (77%)	168 (97%)	4 (2%)	1 (1%)	30	34
1	H	174/225 (77%)	169 (97%)	4 (2%)	1 (1%)	30	34
All	All	1392/1800 (77%)	1347 (97%)	37 (3%)	8 (1%)	30	34

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%)	44	57
1	B	149/188 (79%)	144 (97%)	5 (3%)	44	57
1	C	149/188 (79%)	146 (98%)	3 (2%)	63	77
1	D	149/188 (79%)	145 (97%)	4 (3%)	52	67
1	E	146/188 (78%)	140 (96%)	6 (4%)	37	48
1	F	144/188 (77%)	142 (99%)	2 (1%)	74	86
1	G	145/188 (77%)	139 (96%)	6 (4%)	37	48
1	H	147/188 (78%)	145 (99%)	2 (1%)	74	86
All	All	1174/1504 (78%)	1141 (97%)	33 (3%)	51	65

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.96	67 (37%) 0 0	57, 69, 99, 135	0
1	B	177/225 (78%)	2.26	88 (49%) 0 0	61, 73, 101, 162	0
1	C	179/225 (79%)	1.77	65 (36%) 0 0	57, 65, 83, 101	0
1	D	179/225 (79%)	1.77	58 (32%) 1 0	57, 65, 84, 113	0
1	E	177/225 (78%)	1.86	64 (36%) 0 0	55, 66, 84, 124	0
1	F	176/225 (78%)	2.46	100 (56%) 0 0	59, 74, 113, 205	0
1	G	176/225 (78%)	2.53	100 (56%) 0 0	59, 77, 121, 180	0
1	H	177/225 (78%)	2.35	94 (53%) 0 0	59, 74, 107, 142	0
All	All	1418/1800 (78%)	2.12	636 (44%) 0 0	55, 70, 103, 205	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	117	ARG	16.6
1	F	118	PRO	10.9
1	H	118	PRO	8.9
1	G	117	ARG	8.3
1	H	117	ARG	7.7
1	E	117	ARG	7.7
1	B	156	GLY	7.0
1	G	98	ARG	6.9
1	G	188	MET	6.8
1	G	156	GLY	6.4
1	E	156	GLY	6.3
1	F	196	ALA	6.2
1	B	176[A]	TYR	6.1
1	A	168	CYS	6.1
1	A	117	ARG	5.9
1	F	188	MET	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	205	THR	5.8
1	A	156	GLY	5.7
1	B	154	ALA	5.7
1	G	176[A]	TYR	5.6
1	F	186	GLN	5.6
1	F	92	ASP	5.6
1	B	62	GLU	5.5
1	G	190	LEU	5.5
1	H	26	PRO	5.5
1	B	117	ARG	5.4
1	H	62	GLU	5.3
1	G	118	PRO	5.2
1	F	119	LYS	5.2
1	B	26	PRO	5.2
1	H	92	ASP	5.1
1	G	154	ALA	5.1
1	E	152	VAL	5.1
1	G	191	TYR	5.0
1	B	118	PRO	5.0
1	G	12	THR	5.0
1	B	12	THR	4.8
1	G	119	LYS	4.8
1	A	166	VAL	4.8
1	G	63	SER	4.7
1	H	35	VAL	4.7
1	H	154	ALA	4.7
1	F	98	ARG	4.7
1	F	185	ALA	4.7
1	F	121	GLN	4.7
1	G	95	ASP	4.7
1	B	98	ARG	4.7
1	E	12	THR	4.6
1	G	126	VAL	4.6
1	E	157	ALA	4.6
1	F	190	LEU	4.6
1	G	155	ASP	4.5
1	B	93	PRO	4.5
1	H	24	PRO	4.4
1	G	60	THR	4.4
1	H	12	THR	4.4
1	B	121	GLN	4.4
1	H	155	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	157	ALA	4.3
1	F	176[A]	TYR	4.3
1	H	190	LEU	4.3
1	G	92	ASP	4.3
1	G	124	ARG	4.3
1	B	63	SER	4.3
1	C	9	PRO	4.3
1	D	9	PRO	4.3
1	C	132	VAL	4.3
1	F	63	SER	4.3
1	H	156	GLY	4.3
1	H	188	MET	4.3
1	G	152	VAL	4.2
1	G	123	TYR	4.2
1	F	25	HIS	4.2
1	H	121	GLN	4.2
1	A	165	LEU	4.2
1	F	26	PRO	4.1
1	F	61	PRO	4.1
1	H	138	LEU	4.1
1	H	132	VAL	4.1
1	F	191	TYR	4.1
1	B	153	ALA	4.1
1	B	160	GLN	4.1
1	D	117	ARG	4.1
1	E	131	ARG	4.1
1	A	185	ALA	4.1
1	D	92	ASP	4.1
1	C	62	GLU	4.1
1	B	92	ASP	4.0
1	B	204	GLU	4.0
1	F	62	GLU	4.0
1	G	94	GLN	4.0
1	H	160	GLN	4.0
1	A	20	LEU	4.0
1	B	64	PRO	4.0
1	F	189	GLU	4.0
1	B	23	VAL	4.0
1	G	34	VAL	4.0
1	D	98	ARG	4.0
1	E	158	ASP	4.0
1	A	93	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	26	PRO	3.9
1	B	158	ASP	3.9
1	F	96	GLU	3.9
1	D	132	VAL	3.9
1	B	155	ASP	3.9
1	G	36	ARG	3.9
1	G	185	ALA	3.9
1	C	165	LEU	3.9
1	G	61	PRO	3.9
1	F	126	VAL	3.9
1	G	35	VAL	3.9
1	F	12	THR	3.9
1	F	60	THR	3.9
1	E	62	GLU	3.8
1	F	194	HIS	3.8
1	H	197	VAL	3.8
1	C	118	PRO	3.8
1	H	129	GLY	3.8
1	H	152	VAL	3.8
1	H	176	TYR	3.8
1	E	153	ALA	3.7
1	H	95	ASP	3.7
1	H	134	ARG	3.7
1	F	198	ILE	3.7
1	B	35	VAL	3.7
1	A	154	ALA	3.7
1	E	20	LEU	3.7
1	G	198	ILE	3.7
1	E	98	ARG	3.7
1	A	159	GLY	3.7
1	F	91	LYS	3.7
1	A	126	VAL	3.7
1	E	170	VAL	3.7
1	H	128	VAL	3.7
1	G	91	LYS	3.7
1	A	92	ASP	3.6
1	H	185	ALA	3.6
1	H	193	GLN	3.6
1	A	34	VAL	3.6
1	F	94	GLN	3.6
1	H	158	ASP	3.6
1	G	82	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	158	ASP	3.6
1	G	170	VAL	3.6
1	G	132	VAL	3.6
1	G	138	LEU	3.6
1	A	198	ILE	3.6
1	G	96	GLU	3.6
1	H	127	LEU	3.6
1	H	203	TYR	3.6
1	F	34	VAL	3.5
1	H	159	GLY	3.5
1	D	26	PRO	3.5
1	H	153	ALA	3.5
1	H	25	HIS	3.5
1	F	183	THR	3.5
1	G	183	THR	3.5
1	B	169	ILE	3.5
1	F	138	LEU	3.5
1	A	118	PRO	3.5
1	B	157	ALA	3.5
1	C	36	ARG	3.5
1	G	65	SER	3.5
1	C	26	PRO	3.5
1	D	10	GLN	3.5
1	B	163	TYR	3.5
1	C	35	VAL	3.4
1	G	197	VAL	3.4
1	A	196	ALA	3.4
1	A	98	ARG	3.4
1	H	65	SER	3.4
1	A	158	ASP	3.4
1	F	179	PHE	3.4
1	H	63	SER	3.4
1	B	166	VAL	3.4
1	D	35	VAL	3.4
1	F	155	ASP	3.4
1	H	163	TYR	3.4
1	B	141	THR	3.3
1	B	36	ARG	3.3
1	G	196	ALA	3.3
1	E	169	ILE	3.3
1	F	124	ARG	3.3
1	G	125	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	93	PRO	3.3
1	B	88	VAL	3.3
1	E	70	LEU	3.3
1	F	23	VAL	3.3
1	G	168	CYS	3.3
1	C	117	ARG	3.3
1	H	98	ARG	3.3
1	G	160	GLN	3.3
1	H	126	VAL	3.3
1	C	157	ALA	3.3
1	H	97	ASP	3.3
1	G	169	ILE	3.3
1	C	88	VAL	3.3
1	B	89	ILE	3.3
1	A	12	THR	3.3
1	A	123	TYR	3.3
1	A	167	SER	3.3
1	G	67	LEU	3.3
1	D	196	ALA	3.3
1	H	202	ALA	3.3
1	G	199	LYS	3.2
1	H	15	PHE	3.2
1	C	125	ARG	3.2
1	F	123	TYR	3.2
1	G	184	GLN	3.2
1	H	137	LEU	3.2
1	F	166	VAL	3.2
1	H	94	GLN	3.2
1	C	34	VAL	3.2
1	C	98	ARG	3.2
1	E	34	VAL	3.2
1	D	63	SER	3.2
1	A	141	THR	3.2
1	F	27	GLU	3.2
1	D	170	VAL	3.2
1	A	77	MET	3.2
1	H	36	ARG	3.2
1	D	157	ALA	3.2
1	G	62	GLU	3.2
1	A	96	GLU	3.1
1	E	93	PRO	3.1
1	F	156	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	196	ALA	3.1
1	H	120	TYR	3.1
1	B	170	VAL	3.1
1	B	75	THR	3.1
1	B	133	GLU	3.1
1	H	30	TYR	3.1
1	F	170	VAL	3.1
1	H	23	VAL	3.1
1	H	34	VAL	3.1
1	E	75	THR	3.1
1	D	55	ILE	3.1
1	F	192	PRO	3.1
1	H	59	CYS	3.1
1	C	92	ASP	3.1
1	E	123	TYR	3.1
1	F	65	SER	3.1
1	H	60	THR	3.1
1	F	146	ALA	3.1
1	A	22	LEU	3.1
1	B	142	VAL	3.1
1	E	82	ASP	3.1
1	G	77	MET	3.0
1	G	149	GLY	3.0
1	G	142	VAL	3.0
1	A	75	THR	3.0
1	C	128	VAL	3.0
1	B	52	TYR	3.0
1	B	86	LEU	3.0
1	E	23	VAL	3.0
1	E	159	GLY	3.0
1	F	36	ARG	3.0
1	F	125	ARG	3.0
1	B	129	GLY	3.0
1	E	160	GLN	3.0
1	F	22	LEU	3.0
1	G	84	LEU	3.0
1	A	62	GLU	3.0
1	B	197	VAL	3.0
1	C	166	VAL	3.0
1	F	128	VAL	3.0
1	F	199	LYS	3.0
1	H	93	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	2.9
1	F	38	ALA	2.9
1	A	174	PHE	2.9
1	F	66	HIS	2.9
1	G	86	LEU	2.9
1	F	35	VAL	2.9
1	H	37	SER	2.9
1	E	15	PHE	2.9
1	F	90	LEU	2.9
1	F	201	MET	2.9
1	A	132	VAL	2.9
1	D	126	VAL	2.9
1	D	166	VAL	2.9
1	F	165	LEU	2.9
1	D	36	ARG	2.9
1	A	131	ARG	2.9
1	B	134	ARG	2.9
1	D	15	PHE	2.9
1	F	72	SER	2.9
1	E	61	PRO	2.9
1	B	15	PHE	2.9
1	E	10	GLN	2.9
1	F	202	ALA	2.8
1	H	130	ALA	2.8
1	B	90	LEU	2.8
1	A	26	PRO	2.8
1	C	156	GLY	2.8
1	C	97	ASP	2.8
1	B	190	LEU	2.8
1	G	22	LEU	2.8
1	G	163	TYR	2.8
1	D	37	SER	2.8
1	G	121	GLN	2.8
1	D	161	ALA	2.8
1	F	184	GLN	2.8
1	G	38	ALA	2.8
1	B	97	ASP	2.8
1	G	64	PRO	2.8
1	F	29	GLY	2.8
1	H	11	ASN	2.8
1	B	61	PRO	2.8
1	C	71	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	197	VAL	2.8
1	B	85	GLN	2.8
1	G	165	LEU	2.8
1	C	80	ALA	2.8
1	G	13	ALA	2.8
1	C	59	CYS	2.8
1	E	36	ARG	2.7
1	G	97	ASP	2.7
1	D	52	TYR	2.7
1	G	171	SER	2.7
1	E	35	VAL	2.7
1	H	169	ILE	2.7
1	E	52	TYR	2.7
1	E	154	ALA	2.7
1	B	25	HIS	2.7
1	E	174	PHE	2.7
1	G	153	ALA	2.7
1	A	19	ARG	2.7
1	D	134	ARG	2.7
1	B	172	PRO	2.7
1	F	64	PRO	2.7
1	H	182	PHE	2.7
1	B	27	GLU	2.7
1	F	142	VAL	2.7
1	A	70	LEU	2.7
1	C	150	SER	2.7
1	B	54	THR	2.7
1	H	66	HIS	2.7
1	C	120	TYR	2.7
1	H	191	TYR	2.7
1	D	20	LEU	2.6
1	A	63	SER	2.6
1	B	55	ILE	2.6
1	G	174	PHE	2.6
1	H	131	ARG	2.6
1	H	96	GLU	2.6
1	D	93	PRO	2.6
1	F	152	VAL	2.6
1	B	77	MET	2.6
1	D	22	LEU	2.6
1	F	174	PHE	2.6
1	F	54	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	140	TYR	2.6
1	B	11	ASN	2.6
1	D	21	GLN	2.6
1	G	11	ASN	2.6
1	B	96	GLU	2.6
1	F	132	VAL	2.6
1	A	55	ILE	2.6
1	G	147	ILE	2.6
1	H	141	THR	2.6
1	G	128	VAL	2.6
1	G	166	VAL	2.6
1	H	170	VAL	2.6
1	B	60	THR	2.6
1	D	95	ASP	2.6
1	D	58	LEU	2.6
1	F	86	LEU	2.6
1	D	125	ARG	2.6
1	G	75	THR	2.6
1	C	76	TRP	2.6
1	G	93	PRO	2.6
1	G	172	PRO	2.6
1	E	92	ASP	2.6
1	F	162	GLY	2.6
1	H	27	GLU	2.6
1	B	31	TYR	2.6
1	C	31	TYR	2.6
1	C	163	TYR	2.6
1	F	13	ALA	2.6
1	A	138	LEU	2.6
1	F	84	LEU	2.6
1	D	97	ASP	2.5
1	F	28	GLY	2.5
1	G	28	GLY	2.5
1	G	134	ARG	2.5
1	F	163	TYR	2.5
1	B	202	ALA	2.5
1	B	147	ILE	2.5
1	E	168	CYS	2.5
1	E	179	PHE	2.5
1	D	19	ARG	2.5
1	F	137	LEU	2.5
1	H	183	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	166	VAL	2.5
1	D	96	GLU	2.5
1	G	27	GLU	2.5
1	H	146	ALA	2.5
1	H	161	ALA	2.5
1	A	190	LEU	2.5
1	B	67	LEU	2.5
1	B	125	ARG	2.5
1	C	60	THR	2.5
1	E	141	THR	2.5
1	A	79	HIS	2.5
1	G	25	HIS	2.5
1	H	61	PRO	2.5
1	E	134	ARG	2.5
1	E	96	GLU	2.5
1	D	90	LEU	2.5
1	A	152	VAL	2.5
1	C	142	VAL	2.5
1	D	8	PRO	2.5
1	G	122	VAL	2.5
1	H	194	HIS	2.5
1	H	119	LYS	2.5
1	C	15	PHE	2.5
1	B	82	ASP	2.5
1	C	22	LEU	2.5
1	C	190	LEU	2.5
1	H	90	LEU	2.5
1	D	88	VAL	2.5
1	B	193	GLN	2.5
1	D	121	GLN	2.5
1	H	184	GLN	2.5
1	G	29	GLY	2.4
1	H	196	ALA	2.4
1	B	171	SER	2.4
1	H	72	SER	2.4
1	C	95	ASP	2.4
1	F	78	TYR	2.4
1	A	122	VAL	2.4
1	D	151	SER	2.4
1	B	187	LEU	2.4
1	C	20	LEU	2.4
1	C	137	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	137	LEU	2.4
1	F	120	TYR	2.4
1	A	41	VAL	2.4
1	A	142	VAL	2.4
1	C	85[A]	GLN	2.4
1	E	171	SER	2.4
1	C	155	ASP	2.4
1	F	95	ASP	2.4
1	C	138	LEU	2.4
1	E	22	LEU	2.4
1	H	22	LEU	2.4
1	D	41	VAL	2.4
1	H	200	GLN	2.4
1	B	13	ALA	2.4
1	H	83	PRO	2.4
1	B	84	LEU	2.4
1	A	89	ILE	2.4
1	D	142	VAL	2.4
1	E	197	VAL	2.4
1	F	197	VAL	2.4
1	C	63	SER	2.4
1	B	177	ARG	2.4
1	F	129	GLY	2.4
1	G	31	TYR	2.4
1	D	169	ILE	2.4
1	E	55	ILE	2.4
1	E	122	VAL	2.4
1	F	204	GLU	2.4
1	G	66	HIS	2.4
1	B	76	TRP	2.4
1	C	8	PRO	2.4
1	C	196	ALA	2.4
1	D	168	CYS	2.4
1	B	186	GLN	2.4
1	C	58	LEU	2.3
1	E	190	LEU	2.3
1	G	173	GLY	2.3
1	H	58	LEU	2.3
1	B	132	VAL	2.3
1	E	166	VAL	2.3
1	G	88	VAL	2.3
1	A	80	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	51	ALA	2.3
1	C	16	TRP	2.3
1	H	29	GLY	2.3
1	D	165	LEU	2.3
1	E	84	LEU	2.3
1	F	20	LEU	2.3
1	D	34	VAL	2.3
1	A	61	PRO	2.3
1	B	148	PHE	2.3
1	B	179	PHE	2.3
1	G	189	GLU	2.3
1	A	52	TYR	2.3
1	E	89	ILE	2.3
1	C	141	THR	2.3
1	G	15	PHE	2.3
1	E	121	GLN	2.3
1	E	151	SER	2.3
1	F	127	LEU	2.3
1	A	35	VAL	2.3
1	A	53	THR	2.3
1	B	122	VAL	2.3
1	D	64	PRO	2.3
1	G	55	ILE	2.3
1	G	14	GLU	2.3
1	E	188	MET	2.3
1	F	71	CYS	2.3
1	E	193	GLN	2.3
1	B	203	TYR	2.3
1	E	163	TYR	2.3
1	H	52	TYR	2.3
1	F	32	SER	2.3
1	C	158	ASP	2.3
1	C	84	LEU	2.3
1	E	165	LEU	2.3
1	G	70	LEU	2.3
1	G	187	LEU	2.3
1	H	43	ASN	2.3
1	F	193	GLN	2.2
1	C	12	THR	2.2
1	D	12	THR	2.2
1	F	141	THR	2.2
1	G	53	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	71	CYS	2.2
1	C	56	TYR	2.2
1	C	78	TYR	2.2
1	G	140	TYR	2.2
1	A	179	PHE	2.2
1	G	139	GLN	2.2
1	H	86	LEU	2.2
1	B	24	PRO	2.2
1	D	158	ASP	2.2
1	F	180	GLU	2.2
1	H	88	VAL	2.2
1	F	203	TYR	2.2
1	C	18	LYS	2.2
1	A	137	LEU	2.2
1	H	77	MET	2.2
1	B	72	SER	2.2
1	F	169	ILE	2.2
1	F	181	ILE	2.2
1	G	200	GLN	2.2
1	A	24	PRO	2.2
1	H	64	PRO	2.2
1	B	50	HIS	2.2
1	C	13	ALA	2.2
1	C	185	ALA	2.2
1	D	146	ALA	2.2
1	E	51	ALA	2.2
1	C	181	ILE	2.2
1	A	57	PHE	2.2
1	D	156	GLY	2.2
1	E	71	CYS	2.2
1	E	118	PRO	2.2
1	E	90	LEU	2.2
1	C	121	GLN	2.2
1	D	94	GLN	2.2
1	F	18	LYS	2.2
1	A	146	ALA	2.2
1	H	13	ALA	2.2
1	A	169	ILE	2.2
1	D	122	VAL	2.2
1	B	95	ASP	2.2
1	H	91	LYS	2.2
1	D	24	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	2.2
1	B	65	SER	2.2
1	C	47	ASN	2.2
1	E	37	SER	2.2
1	B	53	THR	2.2
1	B	38	ALA	2.2
1	E	132	VAL	2.1
1	D	174	PHE	2.1
1	A	65	SER	2.1
1	C	70	LEU	2.1
1	H	50	HIS	2.1
1	A	71	CYS	2.1
1	G	159	GLY	2.1
1	D	118	PRO	2.1
1	F	67	LEU	2.1
1	F	158	ASP	2.1
1	D	153	ALA	2.1
1	E	189	GLU	2.1
1	F	14	GLU	2.1
1	F	154	ALA	2.1
1	H	14	GLU	2.1
1	C	126	VAL	2.1
1	F	172	PRO	2.1
1	C	174	PHE	2.1
1	A	56	TYR	2.1
1	A	84	LEU	2.1
1	F	58	LEU	2.1
1	F	77	MET	2.1
1	F	200	GLN	2.1
1	G	141	THR	2.1
1	B	14	GLU	2.1
1	E	19	ARG	2.1
1	F	195	GLU	2.1
1	H	192	PRO	2.1
1	H	151	SER	2.1
1	F	187	LEU	2.1
1	C	167	SER	2.1
1	B	41	VAL	2.1
1	C	46	GLY	2.1
1	A	11	ASN	2.1
1	A	163	TYR	2.1
1	E	30	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	180	GLU	2.1
1	G	130	ALA	2.1
1	D	76	TRP	2.1
1	H	55	ILE	2.1
1	E	41	VAL	2.1
1	G	133	GLU	2.0
1	G	144	GLY	2.0
1	B	174	PHE	2.0
1	B	138	LEU	2.0
1	D	70	LEU	2.0
1	C	55	ILE	2.0
1	C	134	ARG	2.0
1	B	34	VAL	2.0
1	F	122	VAL	2.0
1	D	60	THR	2.0
1	C	203	TYR	2.0
1	F	52	TYR	2.0
1	A	66	HIS	2.0
1	A	150	SER	2.0
1	E	65	SER	2.0
1	H	172	PRO	2.0
1	A	147	ILE	2.0
1	G	43	ASN	2.0
1	G	81	GLY	2.0
1	A	153	ALA	2.0
1	C	86	LEU	2.0
1	H	201	MET	2.0
1	E	150	SER	2.0
1	D	31	TYR	2.0
1	G	192	PRO	2.0
1	H	78	TYR	2.0
1	C	168	CYS	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.