



Full wwPDB X-ray Structure Validation Report

May 7, 2014 – 03:22 AM EDT

PDB ID : 4KB3
Title : Crystal structure of the mitochondrial peroxiredoxin from *Leishmania braziliensis* in the decameric form
Authors : Giuseppe, P.O.; Souza, T.A.C.B.; Morais, M.A.B.; Murakami, M.T.
Deposited on : 2013-04-23
Resolution : 2.93 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

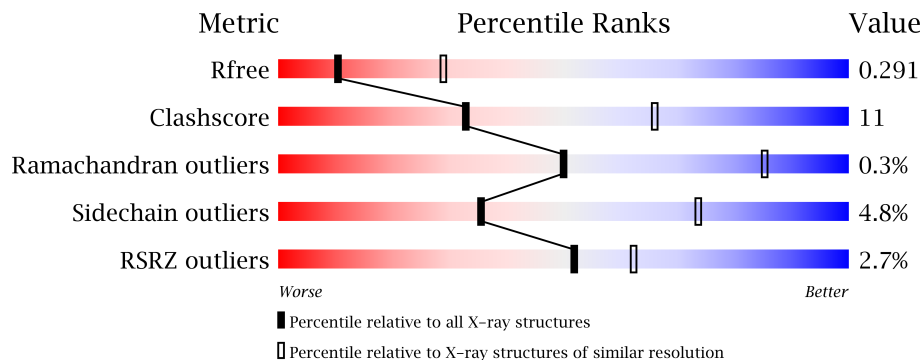
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	
1	C	192	
1	D	192	
1	E	192	
1	F	192	
1	G	192	
1	H	192	
1	I	192	
1	J	192	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12942 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peroxidoxin.

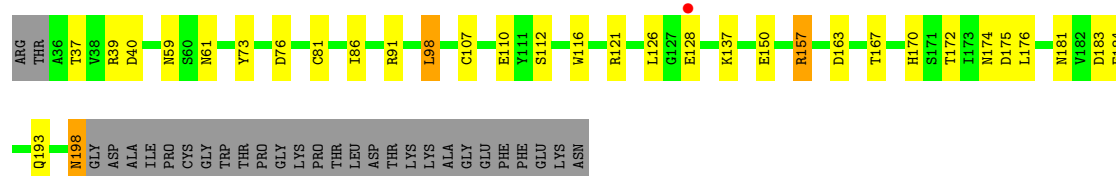
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	B	169	Total	C	N	O	S	0	0	0
			1321	846	219	250	6			
1	C	162	Total	C	N	O	S	0	0	0
			1275	819	211	240	5			
1	D	169	Total	C	N	O	S	0	0	0
			1321	846	219	250	6			
1	E	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	F	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	G	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	H	169	Total	C	N	O	S	0	0	0
			1327	853	220	248	6			
1	I	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			
1	J	163	Total	C	N	O	S	0	0	0
			1283	823	213	242	5			

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.

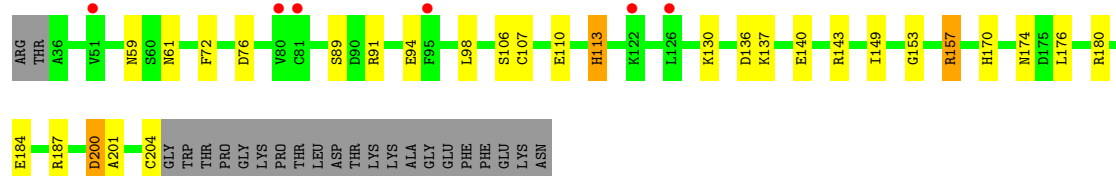
• Molecule 1: Peroxidoxin

Chain A: 



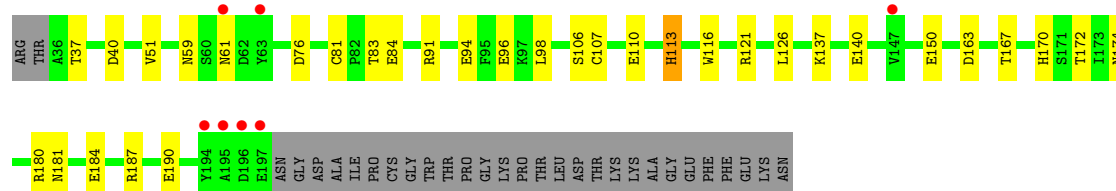
• Molecule 1: Peroxidoxin

Chain B: 



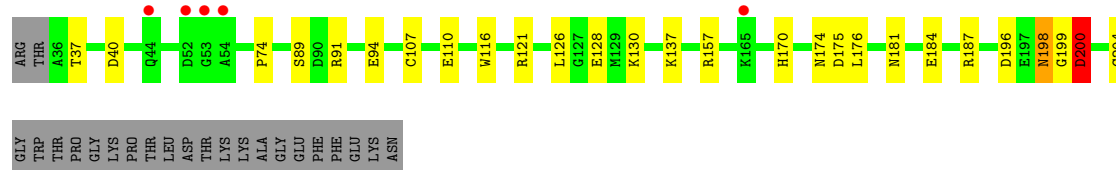
• Molecule 1: Peroxidoxin

Chain C: 



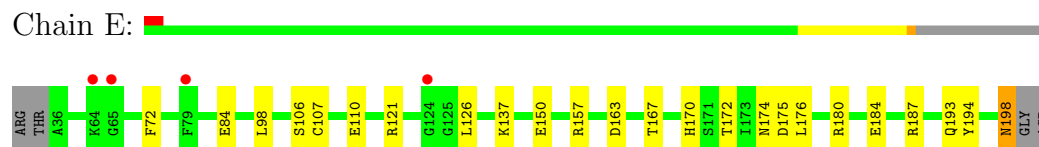
• Molecule 1: Peroxidoxin

Chain D: 



• Molecule 1: Peroxidoxin

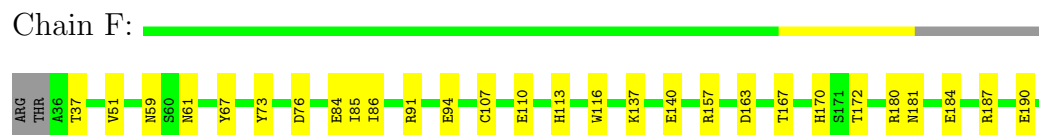
Chain E:



GLY
TRP
THR
PRO
GLY
LYS
PRO
THR
LEU
ASP
THR
LYS
ALA
GLY
PHE
PHE
GLY
LYS
ASN

- Molecule 1: Peroxidoxin

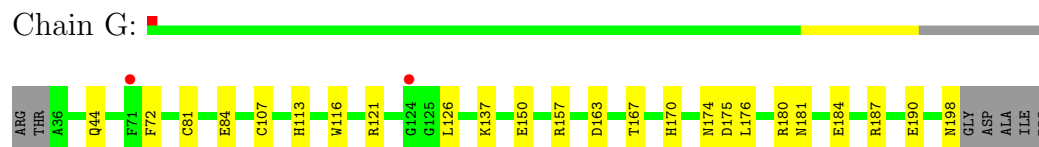
Chain F:



ASP
ALA
ILE
PRO
CYS
GLY
TRP
THR
PRO
GLY
LYS
THR
PRO
THR
LEU
ASP
THR
LYS
ALA
GLY
PHE
PHE
GLY
LYS
ASN

- Molecule 1: Peroxidoxin

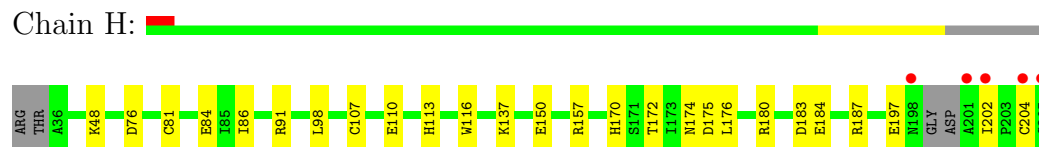
Chain G:



PRO
GLY
LYS
PRO
THR
LEU
ASP
THR
LYS
LYS
ALA
GLY
PHE
PHE
GLY
LYS
ASN

- Molecule 1: Peroxidoxin

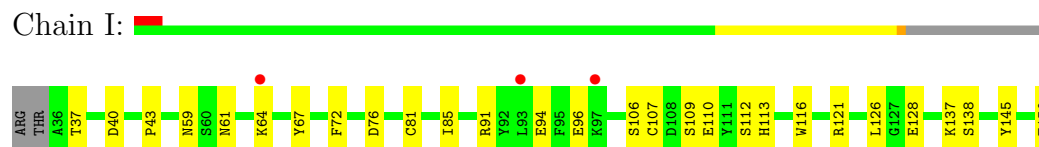
Chain H:



LYS
PRO
THR
LEU
ASP
THR
LYS
LYS
ALA
GLY
PHE
PHE
GLY
LYS
ASN

- Molecule 1: Peroxidoxin

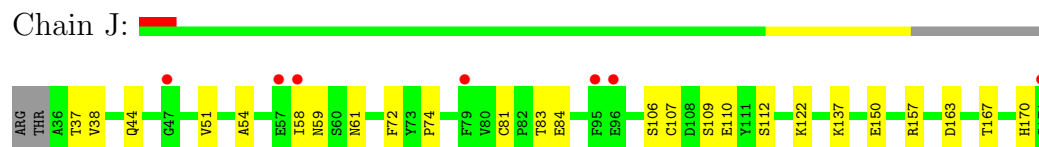
Chain I:



T167
S171
I173
N174
D175
R180
N181
V182
D183
E184
R187
D196
E197
E198
GLY
ASP
ALA
ILE
PRO
CYS
GLY
TRP
THR
PRO
GLY
LYS
PRO
THR
LEU
ASP
THR
LYS
LYS
ALA
GLY
PHE
PHE
GLY
LYS
ASN

- Molecule 1: Peroxidoxin

Chain J:



R180	N181	E184	N188	GLY	ASP	ALA	ILE	PRO	CYS	GLY	TRP	THR	PRO	GLY	LYS	PRO	THR	LEU	ASP	THR	LYS	LYS	ALA	GLY	GLU	PHE	PHE	GLU	LYS	ASN
------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.21Å 98.90Å 228.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.93 38.02 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.93) 99.4 (38.02-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.85Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8-1069)	Depositor
R, R_{free}	0.231 , 0.282 0.242 , 0.291	Depositor DCC
R_{free} test set	2433 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 47913 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12942	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.32	0/1309	0.55	0/1772
1	B	0.33	0/1348	0.55	0/1826
1	C	0.33	0/1301	0.58	0/1761
1	D	0.34	0/1348	0.56	0/1826
1	E	0.32	0/1309	0.54	0/1772
1	F	0.31	0/1309	0.54	0/1772
1	G	0.33	0/1309	0.56	0/1772
1	H	0.33	0/1355	0.56	0/1835
1	I	0.31	0/1309	0.56	0/1772
1	J	0.32	0/1309	0.59	0/1772
All	All	0.32	0/13206	0.56	0/17880

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1283	0	0	18	0
1	B	1321	0	0	17	0
1	C	1275	0	0	18	0
1	D	1321	0	0	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1283	0	0	15	0
1	F	1283	0	0	13	0
1	G	1283	0	0	14	0
1	H	1327	0	12	13	0
1	I	1283	0	0	23	0
1	J	1283	0	0	16	0
All	All	12942	0	12	145	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (145) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:137:LYS:NZ	1:I:107:CYS:O	2.18	0.77
1:G:174:ASN:OD1	1:H:170:HIS:ND1	2.20	0.75
1:B:137:LYS:NZ	1:C:107:CYS:O	2.22	0.73
1:J:37:THR:OG1	1:J:38:VAL:N	2.21	0.72
1:B:107:CYS:O	1:C:137:LYS:NZ	2.23	0.71
1:D:121:ARG:NH2	1:D:128:GLU:O	2.24	0.71
1:E:194:TYR:O	1:E:198:ASN:ND2	2.25	0.69
1:D:157:ARG:NH1	1:D:176:LEU:O	2.28	0.67
1:I:121:ARG:NH2	1:I:128:GLU:O	2.26	0.67
1:D:137:LYS:NZ	1:E:107:CYS:O	2.28	0.67
1:D:184:GLU:OE2	1:D:187:ARG:NE	2.28	0.66
1:A:170:HIS:ND1	1:B:174:ASN:OD1	2.28	0.66
1:D:107:CYS:O	1:E:137:LYS:NZ	2.29	0.65
1:B:157:ARG:NH1	1:B:176:LEU:O	2.29	0.65
1:F:107:CYS:O	1:G:137:LYS:NZ	2.29	0.65
1:H:107:CYS:O	1:I:137:LYS:NZ	2.30	0.65
1:A:137:LYS:NZ	1:J:107:CYS:O	2.30	0.65
1:G:170:HIS:ND1	1:H:174:ASN:OD1	2.29	0.64
1:E:174:ASN:OD1	1:F:170:HIS:ND1	2.33	0.62
1:E:157:ARG:NH1	1:E:176:LEU:O	2.33	0.62
1:F:181:ASN:OD1	1:F:184:GLU:N	2.33	0.61
1:C:84:GLU:OE1	1:C:180:ARG:N	2.34	0.61
1:D:121:ARG:NE	1:D:126:LEU:O	2.35	0.60
1:A:121:ARG:NH2	1:A:128:GLU:O	2.35	0.60
1:C:91:ARG:NE	1:C:94:GLU:OE2	2.34	0.59
1:F:184:GLU:OE2	1:F:187:ARG:NH2	2.35	0.59
1:C:76:ASP:OD1	1:C:113:HIS:ND1	2.36	0.59
1:H:157:ARG:NH1	1:H:176:LEU:O	2.36	0.58
1:I:76:ASP:OD1	1:I:113:HIS:ND1	2.35	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:184:GLU:OE2	1:C:187:ARG:NH2	2.36	0.58
1:E:72:PHE:O	1:E:180:ARG:NH2	2.36	0.58
1:I:157:ARG:NH1	1:I:176:LEU:O	2.36	0.58
1:J:84:GLU:OE2	1:J:180:ARG:NE	2.37	0.58
1:F:84:GLU:OE2	1:F:180:ARG:N	2.36	0.58
1:B:91:ARG:NE	1:B:94:GLU:OE1	2.37	0.58
1:A:121:ARG:NE	1:A:126:LEU:O	2.37	0.57
1:G:181:ASN:OD1	1:G:184:GLU:N	2.38	0.56
1:E:170:HIS:NE2	1:E:172:THR:OG1	2.39	0.56
1:C:163:ASP:OD2	1:C:167:THR:N	2.39	0.56
1:J:157:ARG:NH1	1:J:176:LEU:O	2.39	0.56
1:A:107:CYS:O	1:J:137:LYS:NZ	2.38	0.56
1:A:198:ASN:N	1:A:198:ASN:OD1	2.40	0.55
1:G:184:GLU:OE2	1:G:187:ARG:NH2	2.39	0.55
1:A:175:ASP:OD1	1:A:176:LEU:N	2.40	0.55
1:A:91:ARG:NH2	1:A:183:ASP:OD1	2.40	0.55
1:B:200:ASP:OD1	1:B:201:ALA:N	2.41	0.54
1:A:157:ARG:NH1	1:A:176:LEU:O	2.41	0.54
1:A:181:ASN:OD1	1:A:184:GLU:N	2.40	0.54
1:H:184:GLU:OE1	1:H:187:ARG:NH1	2.40	0.54
1:A:163:ASP:OD2	1:A:167:THR:N	2.41	0.54
1:D:200:ASP:OD2	1:D:200:ASP:N	2.40	0.54
1:I:67:TYR:OH	1:I:196:ASP:OD2	2.26	0.54
1:C:174:ASN:OD1	1:D:170:HIS:ND1	2.41	0.53
1:H:76:ASP:OD1	1:H:113:HIS:ND1	2.41	0.53
1:E:121:ARG:NE	1:E:126:LEU:O	2.42	0.53
1:J:170:HIS:NE2	1:J:172:THR:OG1	2.42	0.53
1:J:175:ASP:OD2	1:J:176:LEU:N	2.41	0.53
1:E:184:GLU:OE2	1:E:187:ARG:NH2	2.42	0.53
1:A:174:ASN:OD1	1:B:170:HIS:ND1	2.42	0.52
1:C:170:HIS:ND1	1:D:174:ASN:OD1	2.43	0.52
1:B:91:ARG:NH2	1:B:94:GLU:OE2	2.42	0.52
1:F:67:TYR:OH	1:F:196:ASP:OD2	2.27	0.52
1:I:121:ARG:NE	1:I:126:LEU:O	2.41	0.52
1:E:163:ASP:OD1	1:E:167:THR:N	2.43	0.52
1:I:163:ASP:OD2	1:I:167:THR:N	2.42	0.52
1:G:163:ASP:OD1	1:G:167:THR:N	2.43	0.52
1:J:72:PHE:O	1:J:180:ARG:NH2	2.42	0.52
1:B:184:GLU:OE1	1:B:187:ARG:NH2	2.44	0.51
1:I:43:PRO:O	1:I:145:TYR:OH	2.28	0.51
1:I:175:ASP:OD1	1:I:176:LEU:N	2.44	0.51
1:F:137:LYS:NZ	1:G:107:CYS:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:163:ASP:OD1	1:F:167:THR:N	2.45	0.50
1:E:110:GLU:N	1:E:110:GLU:OE1	2.44	0.50
1:E:84:GLU:OE2	1:E:180:ARG:N	2.45	0.50
1:I:110:GLU:N	1:I:110:GLU:OE1	2.44	0.50
1:D:198:ASN:N	1:D:198:ASN:OD1	2.43	0.49
1:H:110:GLU:N	1:H:110:GLU:OE1	2.45	0.49
1:I:37:THR:OG1	1:I:40:ASP:OD2	2.29	0.49
1:C:81:CYS:SG	1:D:204:CYS:N	2.82	0.49
1:J:59:ASN:OD1	1:J:61:ASN:ND2	2.46	0.48
1:D:110:GLU:OE1	1:D:110:GLU:N	2.47	0.48
1:F:110:GLU:N	1:F:110:GLU:OE1	2.47	0.48
1:C:91:ARG:NH2	1:C:94:GLU:OE1	2.46	0.48
1:I:91:ARG:NE	1:I:94:GLU:OE1	2.47	0.48
1:C:37:THR:OG1	1:C:40:ASP:OD1	2.31	0.48
1:C:59:ASN:OD1	1:C:61:ASN:N	2.47	0.48
1:I:72:PHE:O	1:I:180:ARG:NH2	2.47	0.48
1:E:175:ASP:OD1	1:E:176:LEU:N	2.47	0.48
1:B:76:ASP:OD1	1:B:113:HIS:ND1	2.47	0.47
1:I:163:ASP:OD1	1:I:167:THR:OG1	2.31	0.47
1:C:121:ARG:NE	1:C:126:LEU:O	2.48	0.47
1:C:170:HIS:NE2	1:C:172:THR:OG1	2.47	0.47
1:F:170:HIS:NE2	1:F:172:THR:OG1	2.48	0.47
1:G:72:PHE:O	1:G:180:ARG:NH1	2.48	0.47
1:H:91:ARG:NH2	1:H:183:ASP:OD1	2.47	0.47
1:J:110:GLU:N	1:J:110:GLU:OE1	2.48	0.47
1:G:175:ASP:OD1	1:G:176:LEU:N	2.48	0.47
1:D:175:ASP:OD2	1:D:176:LEU:N	2.48	0.46
1:I:181:ASN:OD1	1:I:184:GLU:N	2.48	0.46
1:H:175:ASP:OD1	1:H:176:LEU:N	2.48	0.46
1:J:51:VAL:N	1:J:54:ALA:O	2.47	0.46
1:C:110:GLU:N	1:C:110:GLU:OE1	2.49	0.46
1:I:59:ASN:OD1	1:I:61:ASN:N	2.48	0.46
1:D:181:ASN:OD1	1:D:184:GLU:N	2.49	0.45
1:J:181:ASN:OD1	1:J:184:GLU:N	2.49	0.45
1:A:37:THR:OG1	1:A:40:ASP:OD2	2.34	0.45
1:B:140:GLU:OE1	1:B:143:ARG:NH1	2.49	0.45
1:I:106:SER:OG	1:I:107:CYS:N	2.50	0.45
1:G:121:ARG:NE	1:G:126:LEU:O	2.50	0.44
1:B:110:GLU:N	1:B:110:GLU:OE1	2.51	0.44
1:A:98:LEU:O	1:A:193:GLN:NE2	2.50	0.44
1:D:89:SER:OG	1:D:130:LYS:N	2.51	0.44
1:H:84:GLU:OE2	1:H:180:ARG:NE	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:184:GLU:OE1	1:I:187:ARG:NH2	2.51	0.44
1:J:163:ASP:OD1	1:J:167:THR:N	2.51	0.44
1:A:110:GLU:OE1	1:A:110:GLU:N	2.51	0.43
1:A:170:HIS:NE2	1:A:172:THR:OG1	2.51	0.43
1:G:163:ASP:OD2	1:G:167:THR:OG1	2.37	0.43
1:G:84:GLU:OE2	1:G:180:ARG:N	2.52	0.43
1:B:72:PHE:O	1:B:180:ARG:NH2	2.51	0.43
1:B:106:SER:O	1:B:136:ASP:N	2.52	0.43
1:A:73:TYR:OH	1:A:76:ASP:OD1	2.36	0.43
1:B:149:ILE:O	1:B:153:GLY:N	2.53	0.42
1:H:84:GLU:OE2	1:H:180:ARG:N	2.53	0.42
1:C:106:SER:OG	1:C:107:CYS:N	2.53	0.42
1:D:37:THR:OG1	1:D:40:ASP:OD2	2.37	0.42
1:D:91:ARG:NE	1:D:94:GLU:OE1	2.52	0.42
1:G:157:ARG:NH1	1:G:176:LEU:O	2.52	0.42
1:I:174:ASN:OD1	1:J:170:HIS:ND1	2.53	0.42
1:I:109:SER:OG	1:I:112:SER:OG	2.37	0.41
1:I:91:ARG:NH1	1:I:183:ASP:OD1	2.53	0.41
1:B:89:SER:OG	1:B:130:LYS:N	2.54	0.41
1:B:59:ASN:OD1	1:B:61:ASN:N	2.54	0.41
1:A:59:ASN:OD1	1:A:61:ASN:ND2	2.53	0.41
1:C:181:ASN:OD1	1:C:184:GLU:N	2.53	0.41
1:F:59:ASN:OD1	1:F:61:ASN:N	2.54	0.41
1:F:73:TYR:OH	1:F:76:ASP:OD1	2.39	0.41
1:J:109:SER:OG	1:J:112:SER:OG	2.38	0.41
1:H:170:HIS:NE2	1:H:172:THR:OG1	2.54	0.41
1:I:157:ARG:O	1:I:174:ASN:N	2.54	0.41
1:F:91:ARG:NE	1:F:94:GLU:OE1	2.54	0.41
1:E:106:SER:OG	1:E:107:CYS:N	2.53	0.40
1:J:106:SER:OG	1:J:107:CYS:N	2.54	0.40
1:E:98:LEU:O	1:E:193:GLN:NE2	2.54	0.40
1:G:184:GLU:OE1	1:G:187:ARG:NE	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	B	167/192 (87%)	158 (95%)	8 (5%)	1 (1%)	33	75
1	C	160/192 (83%)	156 (98%)	4 (2%)	0	100	100
1	D	167/192 (87%)	159 (95%)	5 (3%)	3 (2%)	13	43
1	E	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	F	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	G	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	H	165/192 (86%)	161 (98%)	4 (2%)	0	100	100
1	I	161/192 (84%)	157 (98%)	4 (2%)	0	100	100
1	J	161/192 (84%)	155 (96%)	5 (3%)	1 (1%)	33	75
All	All	1625/1920 (85%)	1574 (97%)	46 (3%)	5 (0%)	50	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	ASP
1	D	199	GLY
1	B	200	ASP
1	J	74	PRO
1	D	74	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/162 (86%)	130 (94%)	9 (6%)	24	58
1	B	143/162 (88%)	139 (97%)	4 (3%)	56	89
1	C	138/162 (85%)	129 (94%)	9 (6%)	24	58
1	D	143/162 (88%)	139 (97%)	4 (3%)	56	89
1	E	139/162 (86%)	137 (99%)	2 (1%)	78	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	139/162 (86%)	130 (94%)	9 (6%)	24	58
1	G	139/162 (86%)	132 (95%)	7 (5%)	34	72
1	H	143/162 (88%)	134 (94%)	9 (6%)	25	60
1	I	139/162 (86%)	131 (94%)	8 (6%)	28	64
1	J	139/162 (86%)	133 (96%)	6 (4%)	40	77
All	All	1401/1620 (86%)	1334 (95%)	67 (5%)	35	73

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	81	CYS
1	A	86	ILE
1	A	98	LEU
1	A	112	SER
1	A	116	TRP
1	A	150	GLU
1	A	157	ARG
1	A	198	ASN
1	B	98	LEU
1	B	113	HIS
1	B	157	ARG
1	B	204	CYS
1	C	51	VAL
1	C	83	THR
1	C	96	GLU
1	C	98	LEU
1	C	113	HIS
1	C	116	TRP
1	C	140	GLU
1	C	150	GLU
1	C	190	GLU
1	D	116	TRP
1	D	196	ASP
1	D	198	ASN
1	D	200	ASP
1	E	150	GLU
1	E	198	ASN
1	F	37	THR
1	F	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	85	ILE
1	F	86	ILE
1	F	113	HIS
1	F	116	TRP
1	F	140	GLU
1	F	157	ARG
1	F	190	GLU
1	G	44	GLN
1	G	81	CYS
1	G	113	HIS
1	G	116	TRP
1	G	150	GLU
1	G	190	GLU
1	G	198	ASN
1	H	48	LYS
1	H	81	CYS
1	H	86	ILE
1	H	98	LEU
1	H	116	TRP
1	H	150	GLU
1	H	197	GLU
1	H	202	ILE
1	H	204	CYS
1	I	64	LYS
1	I	81	CYS
1	I	85	ILE
1	I	96	GLU
1	I	116	TRP
1	I	138	SER
1	I	150	GLU
1	I	157	ARG
1	J	44	GLN
1	J	58	ILE
1	J	81	CYS
1	J	83	THR
1	J	122	LYS
1	J	150	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	163/192 (84%)	-0.30	1 (0%) 86 92	54, 78, 107, 136	10 (6%)
1	B	169/192 (88%)	-0.07	6 (3%) 41 50	56, 82, 112, 176	18 (10%)
1	C	162/192 (84%)	-0.03	7 (4%) 34 42	58, 83, 114, 149	21 (12%)
1	D	169/192 (88%)	0.01	5 (2%) 48 58	60, 85, 115, 146	18 (10%)
1	E	163/192 (84%)	-0.07	4 (2%) 54 65	54, 79, 107, 122	11 (6%)
1	F	163/192 (84%)	-0.26	0 100 100	52, 78, 105, 122	14 (8%)
1	G	163/192 (84%)	-0.04	2 (1%) 75 84	53, 78, 104, 121	14 (8%)
1	H	169/192 (88%)	0.21	6 (3%) 41 50	50, 78, 107, 158	13 (7%)
1	I	163/192 (84%)	-0.08	5 (3%) 47 57	54, 81, 106, 134	24 (14%)
1	J	163/192 (84%)	0.03	8 (4%) 28 36	54, 81, 121, 157	21 (12%)
All	All	1647/1920 (85%)	-0.06	44 (2%) 52 62	50, 81, 111, 176	164 (9%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	204	CYS	4.7
1	H	205	GLY	4.5
1	E	79	PHE	4.3
1	H	206	TRP	3.8
1	J	172	THR	3.6
1	B	81	CYS	3.6
1	C	196	ASP	3.5
1	I	64	LYS	3.5
1	H	201	ALA	3.1
1	C	63	TYR	3.0
1	J	171	SER	3.0
1	C	195	ALA	2.9
1	C	61	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	64	LYS	2.8
1	J	58	ILE	2.8
1	D	52	ASP	2.6
1	B	80	VAL	2.6
1	D	54	ALA	2.6
1	G	124	GLY	2.6
1	J	57	GLU	2.5
1	H	202	ILE	2.5
1	C	194	TYR	2.5
1	E	65	GLY	2.5
1	I	172	THR	2.4
1	D	165	LYS	2.4
1	J	47	GLY	2.4
1	G	71	PHE	2.3
1	B	95	PHE	2.2
1	D	53	GLY	2.2
1	C	197	GLU	2.2
1	B	126	LEU	2.2
1	I	97	LYS	2.2
1	D	44	GLN	2.2
1	E	124	GLY	2.2
1	H	198	ASN	2.2
1	B	51	VAL	2.1
1	J	96	GLU	2.1
1	I	171	SER	2.1
1	B	122	LYS	2.1
1	C	147	VAL	2.1
1	A	128	GLU	2.1
1	J	79	PHE	2.0
1	I	93	LEU	2.0
1	J	95	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.