



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:42 pm BST

PDB ID : 4FH8
Title : Crystal Structure of Peroxiredoxin-1 from the human hookworm *Ancylostoma ceylanicum*
Authors : Nguyen, J.B.; Modis, Y.
Deposited on : 2012-06-05
Resolution : 2.11 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

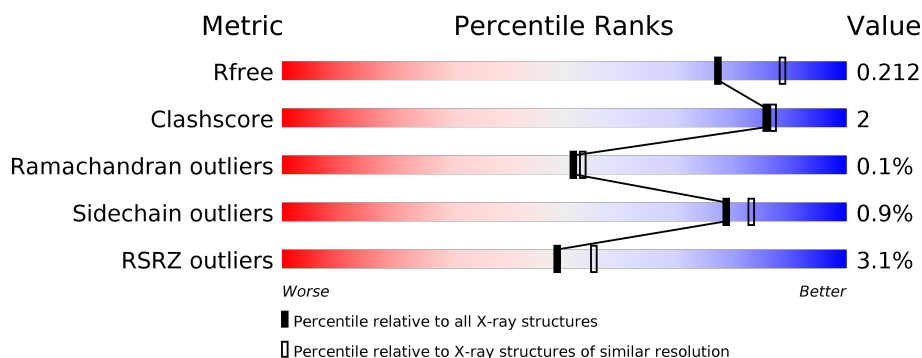
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 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	204	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	204	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>5%</div> <div>16%</div> </div> </div>
1	C	204	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	204	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	204	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>5%</div> <div>•</div> <div>18%</div> </div> </div>
1	F	204	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>•</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	204	<div><div>%</div><div><div></div><div>76%</div><div>6%</div><div>18%</div></div></div>
1	H	204	<div><div>2%</div><div><div></div><div>78%</div><div>5%</div><div>17%</div></div></div>
1	I	204	<div><div>3%</div><div><div></div><div>77%</div><div>6%</div><div>17%</div></div></div>
1	J	204	<div><div>4%</div><div><div></div><div>80%</div><div>•</div><div>17%</div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14009 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 AcePrx-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1348	877	220	246	5			
1	B	171	Total	C	N	O	S	0	0	0
			1353	880	222	246	5			
1	C	168	Total	C	N	O	S	0	0	0
			1330	866	217	243	4			
1	D	171	Total	C	N	O	S	0	0	0
			1353	880	222	246	5			
1	E	167	Total	C	N	O	S	0	0	0
			1321	861	216	240	4			
1	F	170	Total	C	N	O	S	0	0	0
			1347	877	221	245	4			
1	G	167	Total	C	N	O	S	0	0	0
			1321	861	216	240	4			
1	H	170	Total	C	N	O	S	0	0	0
			1347	877	221	245	4			
1	I	169	Total	C	N	O	S	0	0	0
			1337	871	218	244	4			
1	J	170	Total	C	N	O	S	0	0	0
			1347	877	221	245	4			

- Molecule 2 is water.

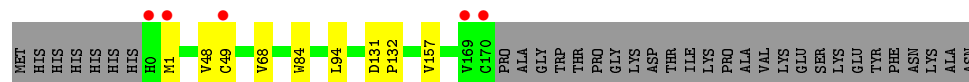
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	67	Total	O	0	0
			67	67		
2	C	47	Total	O	0	0
			47	47		
2	D	46	Total	O	0	0
			46	46		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	45	Total 45	O 45	0	0
2	F	51	Total 51	O 51	0	0
2	G	50	Total 50	O 50	0	0
2	H	69	Total 69	O 69	0	0
2	I	69	Total 69	O 69	0	0
2	J	70	Total 70	O 70	0	0

- Molecule 1: AcePrx-1



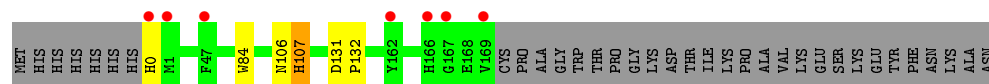
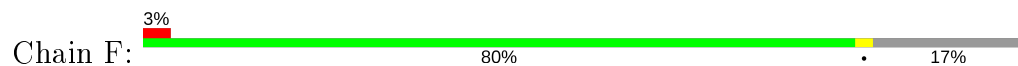
MET	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HO	M1	K90	M106	K107	K108	R125	D131	P132	M142	L154	Q158	E168	V169	C170	PRO	ALA	GLY	TRP	THR	PRO	GLY	LYS	ASP	THR	ILE	LYS	PRO	VAL	ALA	LYS	GLU	SER	LYS	GLU	TYR	PHE	ASN	LYS	ALA	ASN
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Residue	Score	Color
MET	0.00	Grey
HIS	0.00	Grey
HIS	0.00	Grey
HIS	0.00	Grey
HIS	0.00	Grey
HIS	0.00	Grey
HIS	0.00	Grey
HIS	0.00	Grey
M1	0.05	Red
Y35	0.05	Yellow
V68	0.05	Yellow
K90	0.05	Red
H91	0.05	Red
D131	0.05	Yellow
P132	0.05	Yellow
V157	0.05	Yellow
E168	0.05	Green
VAL	0.00	Grey
CYS	0.00	Grey
PRO	0.00	Grey
ALA	0.00	Grey
GLY	0.00	Grey
TRP	0.00	Grey
THR	0.00	Grey
PRO	0.00	Grey
GLY	0.00	Grey
LYS	0.00	Grey
ASP	0.00	Grey
THR	0.00	Grey
ILE	0.00	Grey
LYE	0.00	Grey
PRO	0.00	Grey
ALA	0.00	Grey
VAL	0.00	Grey
LYS	0.00	Grey
GLU	0.00	Grey
SER	0.00	Grey
LYS	0.00	Grey
GLU	0.00	Grey
TYR	0.00	Grey
PHE	0.00	Grey
ASN	0.00	Grey
LYS	0.00	Grey
ALA	0.00	Grey
ASN	0.00	Grey

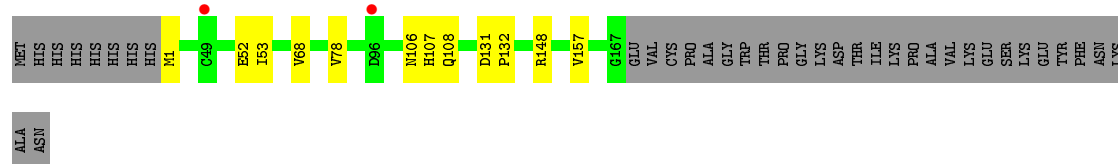
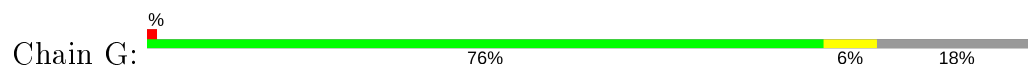
MET	HIS	HIS	HIS	HIS	HIS	HIS	HO	M1	F47	C49	K90	D96	M106	H107	D131	P132	K165	H166	V169	C170	PRO	ALA	GLY	TRP	THR	PRO	GLY	LYS	ASP	THR	THR	ILE	LYS	PRO	ALA	ALA	VAL	LYS	GLU	LYS	LYS	GLU	TYR	PHE	ASN	LYS	ALA	ALA
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Residue	Position	Score	Color	Label
GLU	1	0.00	Grey	MET
SER	2	0.00	Grey	HIS
LYS	3	0.00	Grey	HIS
GLU	4	0.00	Grey	HIS
THR	5	0.00	Grey	HIS
PRO	6	0.00	Grey	HIS
ASP	7	0.00	Grey	HIS
GLY	8	0.00	Grey	HIS
VAL	9	0.00	Grey	HIS
ASN	10	0.00	Grey	HIS
ALA	11	0.00	Grey	M1
ASN	12	0.00	Grey	V18
	13	0.00	Grey	P42
	14	0.00	Grey	F47
	15	0.00	Green	V49
	16	0.00	Green	C49
	17	0.00	Grey	E52
	18	0.00	Yellow	I53
	19	0.00	Yellow	V68
	20	0.00	Grey	V78
	21	0.00	Orange	W84
	22	0.00	Grey	H91
	23	0.00	Green	D96
	24	0.00	Grey	N106
	25	0.00	Yellow	H107
	26	0.00	Yellow	Q108
	27	0.00	Grey	D131
	28	0.00	Grey	P132
	29	0.00	Grey	V157
	30	0.00	Green	G167
	31	0.00	Grey	GLU
	32	0.00	Grey	VAL
	33	0.00	Grey	CYS
	34	0.00	Grey	PRO
	35	0.00	Grey	ALA
	36	0.00	Grey	GLY
	37	0.00	Grey	TRP
	38	0.00	Grey	THR
	39	0.00	Grey	PRO
	40	0.00	Grey	GLY
	41	0.00	Grey	LYS
	42	0.00	Grey	ASP
	43	0.00	Grey	THR
	44	0.00	Grey	ILE
	45	0.00	Grey	LYS
	46	0.00	Grey	PRO
	47	0.00	Grey	ALA
	48	0.00	Grey	VAL
	49	0.00	Grey	THR

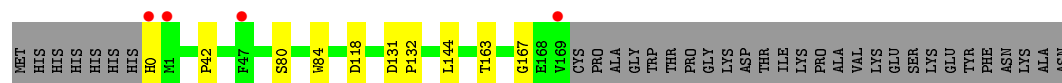
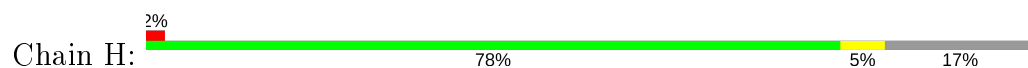
- Molecule 1: AcePrx-1



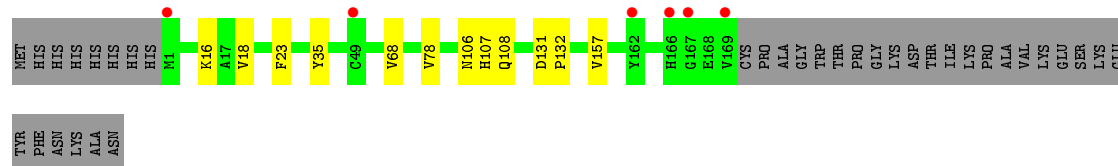
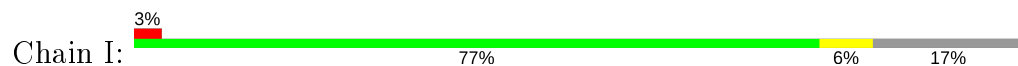
- Molecule 1: AcePrx-1



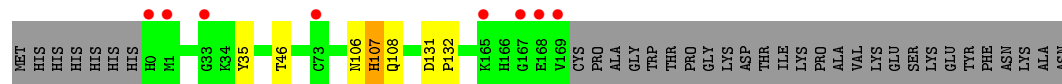
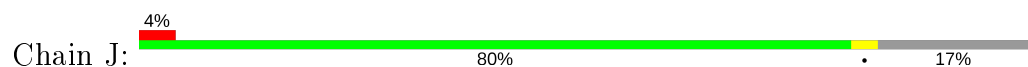
- Molecule 1: AcePrx-1



- Molecule 1: AcePrx-1



- Molecule 1: AcePrx-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.69Å 146.28Å 136.03Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	46.55 – 2.11 46.55 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.55-2.11) 99.8 (46.55-2.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.214 0.193 , 0.212	Depositor DCC
R_{free} test set	7231 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14009	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.27% 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

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	0.41	0/1382	0.52	0/1874
1	B	0.41	0/1388	0.50	0/1882
1	C	0.39	0/1364	0.48	0/1849
1	D	0.40	0/1388	0.49	0/1882
1	E	0.39	1/1355 (0.1%)	0.48	0/1837
1	F	0.40	1/1382 (0.1%)	0.48	0/1874
1	G	0.40	0/1355	0.49	0/1837
1	H	0.41	1/1382 (0.1%)	0.49	0/1874
1	I	0.40	0/1371	0.52	0/1859
1	J	0.41	0/1382	0.50	0/1874
All	All	0.40	3/13749 (0.0%)	0.50	0/18642

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	84	TRP	CD2-CE2	5.11	1.47	1.41
1	F	84	TRP	CD2-CE2	5.03	1.47	1.41
1	H	84	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1348	0	1339	5	0
1	B	1353	0	1344	8	0
1	C	1330	0	1323	4	0
1	D	1353	0	1344	5	0
1	E	1321	0	1318	6	0
1	F	1347	0	1340	4	0
1	G	1321	0	1318	6	0
1	H	1347	0	1340	4	0
1	I	1337	0	1333	13	0
1	J	1347	0	1340	7	0
2	A	91	0	0	0	0
2	B	67	0	0	0	0
2	C	47	0	0	0	0
2	D	46	0	0	1	0
2	E	45	0	0	0	0
2	F	51	0	0	1	0
2	G	50	0	0	0	0
2	H	69	0	0	0	0
2	I	69	0	0	0	0
2	J	70	0	0	2	0
All	All	14009	0	13339	60	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 2.

All (60) 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:I:23:PHE:CE1	1:I:78:VAL:HG12	2.33	0.64
1:A:68:VAL:HG21	1:A:157:VAL:HG11	1.82	0.59
1:B:106:ASN:HB3	1:B:108:GLN:H	1.68	0.58
1:A:49:CYS:HB2	1:B:170:CYS:SG	2.43	0.58
1:I:23:PHE:CD1	1:I:78:VAL:HG12	2.41	0.55
1:E:68:VAL:HG21	1:E:157:VAL:HG11	1.89	0.55
1:I:23:PHE:CD1	1:I:78:VAL:CG1	2.90	0.54
1:I:68:VAL:HG21	1:I:157:VAL:HG11	1.88	0.54
1:G:68:VAL:HG21	1:G:157:VAL:HG11	1.91	0.53
1:J:106:ASN:HB2	2:J:209:HOH:O	2.09	0.52
1:H:131:ASP:HB2	1:H:132:PRO:HD2	1.93	0.50
1:F:131:ASP:HB2	1:F:132:PRO:CD	2.42	0.50
1:I:16:LYS:HB3	1:I:78:VAL:HG21	1.95	0.49
1:B:125:ARG:HB2	1:B:142:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:ASP:HB2	1:J:132:PRO:CD	2.43	0.49
1:E:131:ASP:HB2	1:E:132:PRO:CD	2.44	0.48
1:G:106:ASN:HB3	1:G:108:GLN:H	1.78	0.48
1:F:131:ASP:HB2	1:F:132:PRO:HD2	1.94	0.48
1:G:131:ASP:HB2	1:G:132:PRO:CD	2.44	0.48
1:C:68:VAL:HG21	1:C:157:VAL:HG11	1.96	0.48
1:F:106:ASN:HB2	2:F:208:HOH:O	2.12	0.48
1:H:131:ASP:HB2	1:H:132:PRO:CD	2.44	0.47
1:H:42:PRO:HG3	1:H:144:LEU:HD22	1.95	0.47
1:D:131:ASP:HB2	1:D:132:PRO:CD	2.44	0.47
1:C:131:ASP:HB2	1:C:132:PRO:CD	2.45	0.46
1:E:106:ASN:O	1:E:107:HIS:HB2	2.14	0.46
1:J:106:ASN:O	1:J:107:HIS:HB2	2.16	0.46
1:D:165:LYS:HB2	1:D:166:HIS:CD2	2.51	0.46
1:J:46:THR:HG21	2:J:243:HOH:O	2.14	0.46
1:I:18:VAL:HG23	1:I:78:VAL:HG13	1.98	0.45
1:F:106:ASN:O	1:F:107:HIS:HB2	2.16	0.45
1:I:18:VAL:CG2	1:I:78:VAL:HG13	2.47	0.45
1:B:154:LEU:O	1:B:158:GLN:HG2	2.16	0.45
1:H:163:THR:HG22	1:H:167:GLY:O	2.17	0.45
1:G:131:ASP:HB2	1:G:132:PRO:HD2	1.98	0.45
1:J:131:ASP:HB2	1:J:132:PRO:HD2	1.99	0.45
1:B:106:ASN:O	1:B:107:HIS:HB2	2.17	0.44
1:B:131:ASP:HB2	1:B:132:PRO:HD2	2.00	0.44
1:G:106:ASN:O	1:G:107:HIS:HB2	2.18	0.44
1:J:106:ASN:HB3	1:J:108:GLN:H	1.82	0.44
1:D:131:ASP:HB2	1:D:132:PRO:HD2	2.00	0.43
1:A:131:ASP:HB2	1:A:132:PRO:CD	2.48	0.43
1:E:18:VAL:CG2	1:E:78:VAL:HG12	2.48	0.43
1:E:106:ASN:HB3	1:E:108:GLN:H	1.81	0.43
1:E:52:GLU:HG3	1:E:53:ILE:N	2.32	0.43
1:I:131:ASP:HB2	1:I:132:PRO:CD	2.49	0.42
1:B:131:ASP:HB2	1:B:132:PRO:CD	2.50	0.42
1:I:23:PHE:CD1	1:I:78:VAL:HG11	2.54	0.42
1:D:106:ASN:HB2	2:D:221:HOH:O	2.19	0.42
1:A:84:TRP:CE3	1:A:94:LEU:HG	2.55	0.41
1:I:106:ASN:O	1:I:107:HIS:HB2	2.20	0.41
1:C:35:TYR:CE2	1:C:132:PRO:HD3	2.55	0.41
1:I:106:ASN:HB3	1:I:108:GLN:H	1.84	0.41
1:I:35:TYR:CE1	1:I:132:PRO:HD3	2.56	0.41
1:D:106:ASN:O	1:D:107:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:GLU:HG3	1:G:53:ILE:N	2.35	0.41
1:I:131:ASP:HB2	1:I:132:PRO:HD2	2.03	0.41
1:A:48:VAL:HG21	1:B:168:GLU:OE1	2.20	0.40
1:C:131:ASP:HB2	1:C:132:PRO:HD2	2.04	0.40
1:J:35:TYR:CE1	1:J:132:PRO:HD3	2.56	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	169/204 (83%)	166 (98%)	3 (2%)	0	100	100
1	B	169/204 (83%)	166 (98%)	3 (2%)	0	100	100
1	C	166/204 (81%)	163 (98%)	3 (2%)	0	100	100
1	D	169/204 (83%)	167 (99%)	2 (1%)	0	100	100
1	E	165/204 (81%)	163 (99%)	1 (1%)	1 (1%)	25	20
1	F	168/204 (82%)	165 (98%)	3 (2%)	0	100	100
1	G	165/204 (81%)	163 (99%)	2 (1%)	0	100	100
1	H	168/204 (82%)	165 (98%)	3 (2%)	0	100	100
1	I	167/204 (82%)	163 (98%)	4 (2%)	0	100	100
1	J	168/204 (82%)	166 (99%)	2 (1%)	0	100	100
All	All	1674/2040 (82%)	1647 (98%)	26 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	42	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	146/175 (83%)	145 (99%)	1 (1%)	84	88
1	B	147/175 (84%)	147 (100%)	0	100	100
1	C	144/175 (82%)	144 (100%)	0	100	100
1	D	147/175 (84%)	146 (99%)	1 (1%)	84	88
1	E	143/175 (82%)	141 (99%)	2 (1%)	67	72
1	F	146/175 (83%)	144 (99%)	2 (1%)	67	72
1	G	143/175 (82%)	140 (98%)	3 (2%)	53	57
1	H	146/175 (83%)	143 (98%)	3 (2%)	53	57
1	I	145/175 (83%)	145 (100%)	0	100	100
1	J	146/175 (83%)	145 (99%)	1 (1%)	84	88
All	All	1453/1750 (83%)	1440 (99%)	13 (1%)	78	83

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	D	0	HIS
1	E	52	GLU
1	E	78	VAL
1	F	0	HIS
1	F	107	HIS
1	G	1	MET
1	G	78	VAL
1	G	148	ARG
1	H	0	HIS
1	H	80	SER
1	H	118	ASP
1	J	107	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS
1	B	166	HIS
1	D	166	HIS
1	F	91	HIS
1	H	158	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	171/204 (83%)	-0.18	5 (2%)	51	57	28, 37, 59, 90	0
1	B	171/204 (83%)	0.10	5 (2%)	51	57	33, 45, 71, 107	0
1	C	168/204 (82%)	-0.02	3 (1%)	68	72	35, 50, 70, 89	0
1	D	171/204 (83%)	0.07	8 (4%)	31	36	36, 51, 87, 115	0
1	E	167/204 (81%)	0.14	4 (2%)	59	64	37, 51, 72, 84	0
1	F	170/204 (83%)	-0.02	7 (4%)	37	43	35, 47, 76, 99	0
1	G	167/204 (81%)	-0.08	2 (1%)	79	82	34, 48, 68, 82	0
1	H	170/204 (83%)	-0.03	4 (2%)	59	64	33, 44, 64, 98	0
1	I	169/204 (82%)	0.03	6 (3%)	42	49	29, 42, 67, 101	0
1	J	170/204 (83%)	0.29	8 (4%)	31	36	32, 46, 68, 109	0
All	All	1694/2040 (83%)	0.03	52 (3%)	49	55	28, 46, 71, 115	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	169	VAL	9.3
1	J	169	VAL	9.0
1	D	169	VAL	6.6
1	D	170	CYS	5.9
1	F	169	VAL	5.6
1	A	49	CYS	5.2
1	H	0	HIS	5.1
1	A	170	CYS	5.0
1	H	169	VAL	5.0
1	J	168	GLU	4.5
1	B	169	VAL	4.1
1	D	49	CYS	3.7
1	H	1	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	0	HIS	3.6
1	F	0	HIS	3.5
1	I	162	TYR	3.5
1	A	1	MET	3.4
1	F	1	MET	3.4
1	B	0	HIS	3.4
1	A	169	VAL	3.3
1	D	0	HIS	3.1
1	D	96	ASP	3.1
1	J	167	GLY	3.1
1	I	49	CYS	3.1
1	A	0	HIS	3.1
1	D	47	PHE	3.0
1	B	90	LYS	2.9
1	G	96	ASP	2.9
1	C	90	LYS	2.8
1	E	49	CYS	2.6
1	F	47	PHE	2.6
1	B	170	CYS	2.6
1	D	90	LYS	2.5
1	I	1	MET	2.4
1	C	91	HIS	2.4
1	E	47	PHE	2.4
1	G	49	CYS	2.4
1	J	165	LYS	2.4
1	J	33	GLY	2.3
1	H	47	PHE	2.3
1	F	167	GLY	2.3
1	J	1	MET	2.3
1	B	1	MET	2.2
1	I	166	HIS	2.2
1	C	1	MET	2.2
1	E	96	ASP	2.1
1	F	166	HIS	2.1
1	I	167	GLY	2.1
1	J	73	CYS	2.1
1	D	1	MET	2.0
1	E	91	HIS	2.0
1	F	162	TYR	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 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.