



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:27 PM GMT

PDB ID : 4LLR
Title : Tryparedoxin peroxidase (TXNPX) from trypanosoma cruzi in the reduced state
Authors : Pineyro, M.D.; Pizarro, J.C.; Lema, F.; Pritsch, O.; Cayota, A.; Bentley, G.A.; Robello, C.
Deposited on : 2013-07-09
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

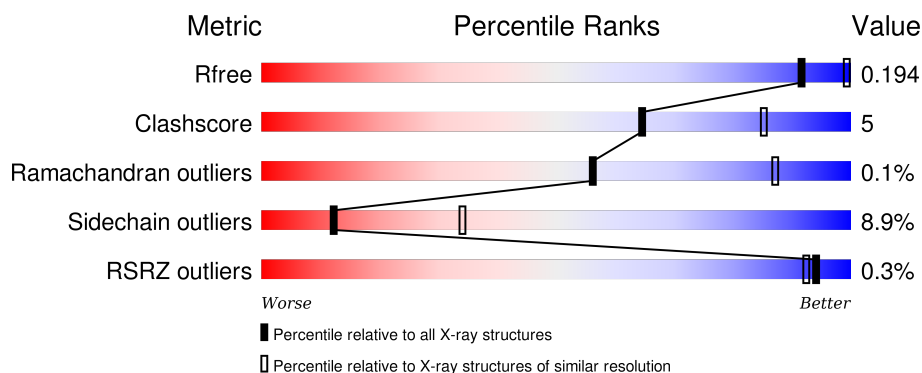
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	197	<div> <div>83%</div> <div>12%</div> <div>...</div> </div>
1	B	197	<div> <div>85%</div> <div>12%</div> <div>...</div> </div>
1	C	197	<div> <div>83%</div> <div>12%</div> <div>...</div> </div>
1	D	197	<div> <div>82%</div> <div>14%</div> <div>...</div> </div>
1	E	197	<div> <div>82%</div> <div>15%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	197	<div><div></div><div>82%</div><div>12%</div><div></div><div></div></div>
1	G	197	<div>%<div><div></div><div>85%</div><div>11%</div><div></div><div></div></div></div>
1	H	197	<div><div></div><div>83%</div><div>13%</div><div></div><div></div></div>
1	I	197	<div><div></div><div>83%</div><div>12%</div><div></div><div></div></div>
1	J	197	<div>%<div><div></div><div>83%</div><div>11%</div><div></div><div></div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15833 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 Tryparedoxin peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	B	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	C	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	D	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	E	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	F	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	G	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	H	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	I	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			
1	J	194	Total	C	N	O	S	0	0	0
			1538	987	255	284	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	49	Total	O	0	0
			49	49		
2	B	43	Total	O	0	0
			43	43		
2	C	48	Total	O	0	0
			48	48		
2	D	50	Total	O	0	0
			50	50		

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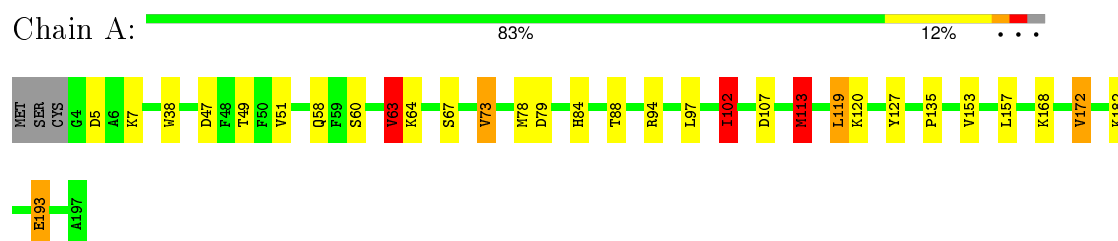
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	50	Total 50	O 50	0	0
2	F	50	Total 50	O 50	0	0
2	G	48	Total 48	O 48	0	0
2	H	37	Total 37	O 37	0	0
2	I	38	Total 38	O 38	0	0
2	J	40	Total 40	O 40	0	0

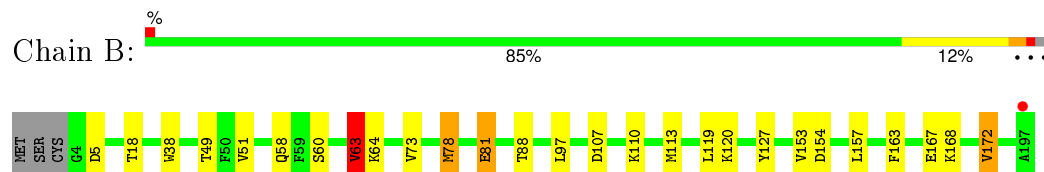
3 Residue-property plots [i](#)

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.

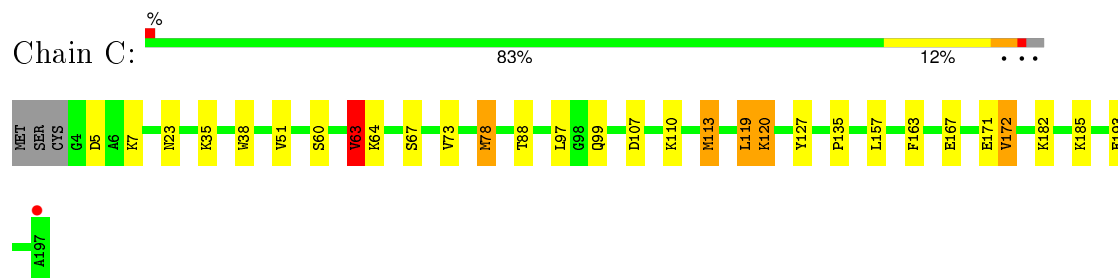
- Molecule 1: Tryparedoxin peroxidase



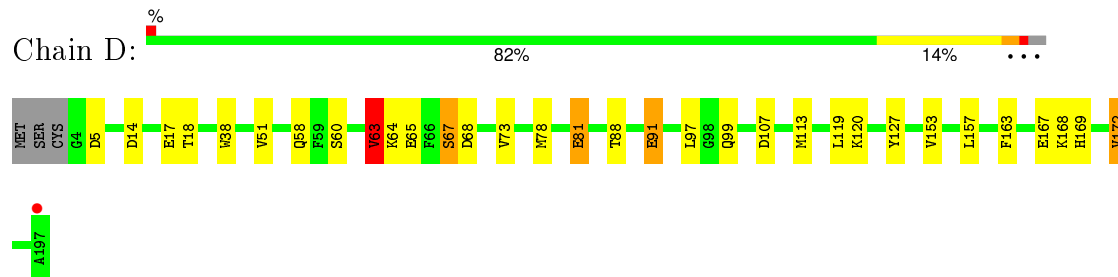
- Molecule 1: Tryparedoxin peroxidase



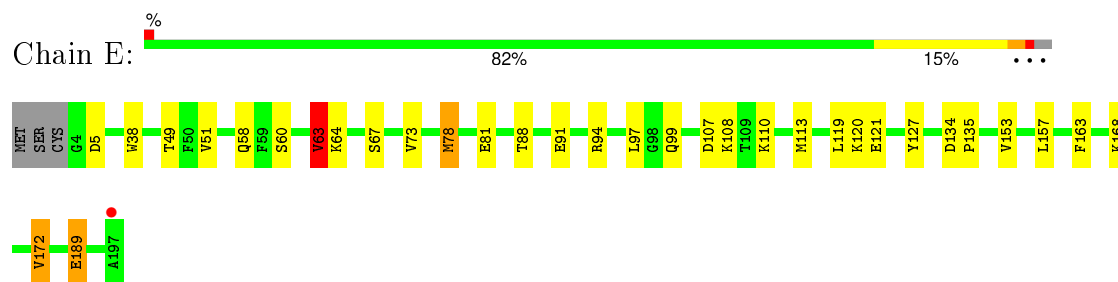
- Molecule 1: Tryparedoxin peroxidase



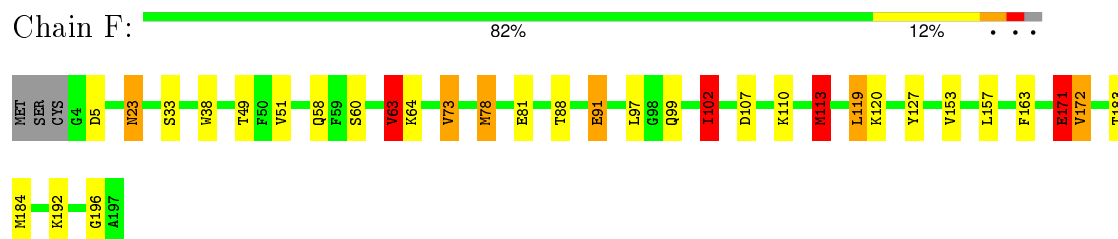
- Molecule 1: Tryparedoxin peroxidase



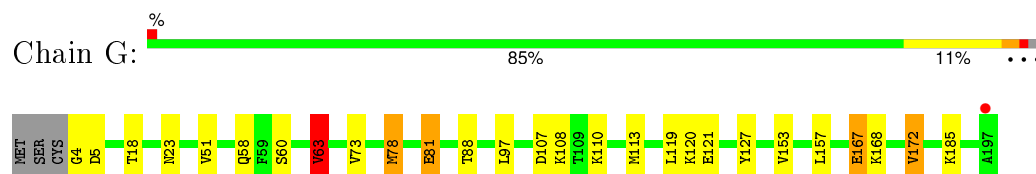
- Molecule 1: Tryparedoxin peroxidase



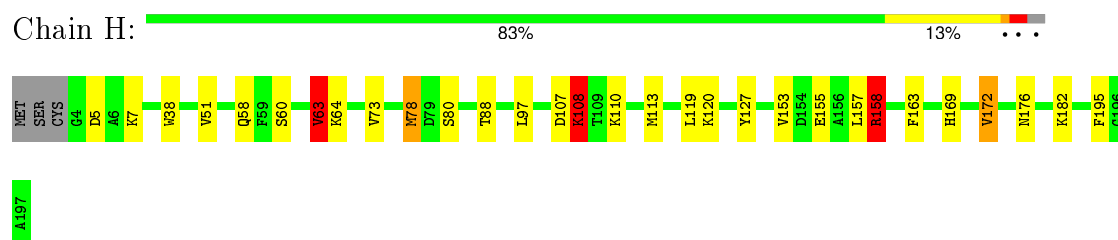
- Molecule 1: Tryparedoxin peroxidase



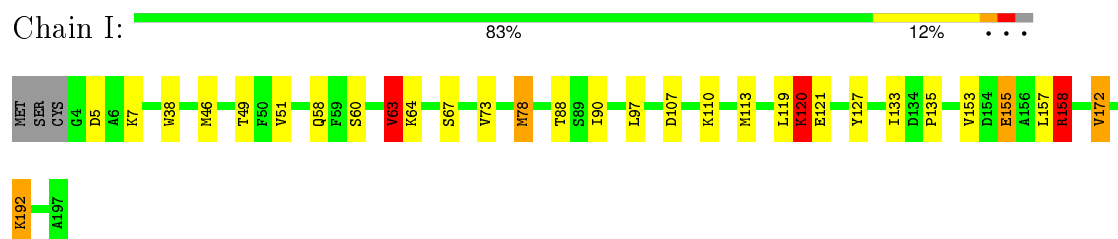
- Molecule 1: Tryparedoxin peroxidase



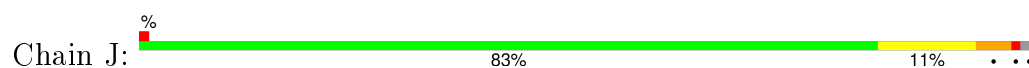
- Molecule 1: Tryparedoxin peroxidase

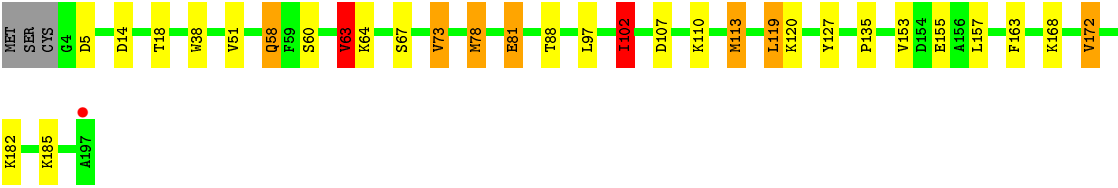


- Molecule 1: Tryparedoxin peroxidase



- Molecule 1: Tryparedoxin peroxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.56 Å 87.02 Å 127.14 Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	29.97 – 2.80 29.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.97-2.80) 99.9 (29.97-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.162 , 0.195 0.167 , 0.194	Depositor DCC
R_{free} test set	3354 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.7	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66035 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15833	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

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	0.76	1/1576 (0.1%)	0.94	8/2127 (0.4%)
1	B	0.74	0/1576	0.88	3/2127 (0.1%)
1	C	0.77	0/1576	0.92	3/2127 (0.1%)
1	D	0.76	1/1576 (0.1%)	0.87	5/2127 (0.2%)
1	E	0.73	0/1576	0.88	4/2127 (0.2%)
1	F	0.81	1/1576 (0.1%)	0.93	5/2127 (0.2%)
1	G	0.80	2/1576 (0.1%)	0.90	3/2127 (0.1%)
1	H	0.74	0/1576	0.91	5/2127 (0.2%)
1	I	0.77	1/1576 (0.1%)	0.95	9/2127 (0.4%)
1	J	0.74	0/1576	0.92	7/2127 (0.3%)
All	All	0.76	6/15760 (0.0%)	0.91	52/21270 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	7

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	171	GLU	CB-CG	6.47	1.64	1.52
1	D	65	GLU	CD-OE2	5.82	1.32	1.25
1	A	193	GLU	CD-OE1	-5.73	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	167	GLU	CG-CD	5.09	1.59	1.51
1	I	192	LYS	CD-CE	5.04	1.63	1.51

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	MET	CG-SD-CE	-11.11	82.42	100.20
1	J	113	MET	CG-SD-CE	-10.26	83.79	100.20
1	I	133	ILE	CA-CB-CG1	8.65	127.43	111.00
1	I	90	ILE	CG1-CB-CG2	-8.21	93.34	111.40
1	F	113	MET	CA-CB-CG	7.77	126.50	113.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	THR	Peptide
1	B	49	THR	Peptide
1	E	49	THR	Peptide
1	F	49	THR	Peptide
1	G	4	GLY	Peptide

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	1538	0	1525	22	0
1	B	1538	0	1525	12	0
1	C	1538	0	1525	15	0
1	D	1538	0	1525	14	0
1	E	1538	0	1525	17	0
1	F	1538	0	1525	29	0
1	G	1538	0	1525	12	0
1	H	1538	0	1525	16	0
1	I	1538	0	1525	13	0
1	J	1538	0	1525	23	0
2	A	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	0	1	0
2	C	48	0	0	0	0
2	D	50	0	0	4	0
2	E	50	0	0	3	0
2	F	50	0	0	1	0
2	G	48	0	0	2	0
2	H	37	0	0	3	0
2	I	38	0	0	0	0
2	J	40	0	0	0	0
All	All	15833	0	15250	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 5.

The worst 5 of 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:J:63:VAL:HG13	1:J:102:ILE:HD12	1.57	0.87
1:F:63:VAL:HG13	1:F:102:ILE:HD12	1.55	0.87
1:F:63:VAL:HG13	1:F:102:ILE:CD1	2.05	0.86
1:J:63:VAL:HG13	1:J:102:ILE:CD1	2.07	0.84
1:D:68:ASP:OD2	2:D:232:HOH:O	1.99	0.80

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	192/197 (98%)	185 (96%)	7 (4%)	0	100	100
1	B	192/197 (98%)	187 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	192/197 (98%)	187 (97%)	5 (3%)	0	100	100
1	D	192/197 (98%)	186 (97%)	6 (3%)	0	100	100
1	E	192/197 (98%)	188 (98%)	4 (2%)	0	100	100
1	F	192/197 (98%)	187 (97%)	4 (2%)	1 (0%)	34	69
1	G	192/197 (98%)	186 (97%)	6 (3%)	0	100	100
1	H	192/197 (98%)	188 (98%)	4 (2%)	0	100	100
1	I	192/197 (98%)	186 (97%)	6 (3%)	0	100	100
1	J	192/197 (98%)	188 (98%)	4 (2%)	0	100	100
All	All	1920/1970 (98%)	1868 (97%)	51 (3%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	196	GLY

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	168/171 (98%)	151 (90%)	17 (10%)	9	27
1	B	168/171 (98%)	157 (94%)	11 (6%)	21	52
1	C	168/171 (98%)	150 (89%)	18 (11%)	8	24
1	D	168/171 (98%)	154 (92%)	14 (8%)	14	38
1	E	168/171 (98%)	154 (92%)	14 (8%)	14	38
1	F	168/171 (98%)	150 (89%)	18 (11%)	8	24
1	G	168/171 (98%)	156 (93%)	12 (7%)	18	46
1	H	168/171 (98%)	154 (92%)	14 (8%)	14	38
1	I	168/171 (98%)	152 (90%)	16 (10%)	11	30
1	J	168/171 (98%)	153 (91%)	15 (9%)	12	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1680/1710 (98%)	1531 (91%)	149 (9%)	12	34

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	97	LEU
1	F	91	GLU
1	J	73	VAL
1	E	119	LEU
1	F	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	169	HIS
1	J	99	GLN
1	G	23	ASN
1	C	23	ASN
1	F	23	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	194/197 (98%)	-0.55	0 100 100	16, 27, 55, 63	0
1	B	194/197 (98%)	-0.55	1 (0%) 91 88	17, 25, 55, 83	0
1	C	194/197 (98%)	-0.53	1 (0%) 91 88	19, 29, 57, 73	0
1	D	194/197 (98%)	-0.56	1 (0%) 91 88	18, 27, 56, 70	0
1	E	194/197 (98%)	-0.67	1 (0%) 91 88	14, 23, 51, 72	0
1	F	194/197 (98%)	-0.67	0 100 100	14, 22, 49, 60	0
1	G	194/197 (98%)	-0.61	1 (0%) 91 88	15, 25, 56, 89	0
1	H	194/197 (98%)	-0.51	0 100 100	19, 31, 56, 75	0
1	I	194/197 (98%)	-0.41	0 100 100	20, 32, 61, 69	0
1	J	194/197 (98%)	-0.52	1 (0%) 91 88	18, 28, 62, 82	0
All	All	1940/1970 (98%)	-0.56	6 (0%) 94 92	14, 27, 57, 89	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	197	ALA	3.9
1	C	197	ALA	3.6
1	B	197	ALA	3.6
1	E	197	ALA	2.7
1	G	197	ALA	2.6

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.