



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:20 PM UTC

PDB ID : 3ZLP / pdb_00003zlp
Title : Crystal structure of Schistosoma mansoni Peroxiredoxin 1 C48P mutant form with four decamers in the asymmetric unit
Authors : Saccoccia, F.; Angelucci, F.; Ardini, M.; Boumis, G.; Brunori, M.; DiLeandro, L.; Ippoliti, R.; Miele, A.E.; Natoli, G.; Scotti, S.; Bellelli, A.
Deposited on : 2013-02-04
Resolution : 3.52 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

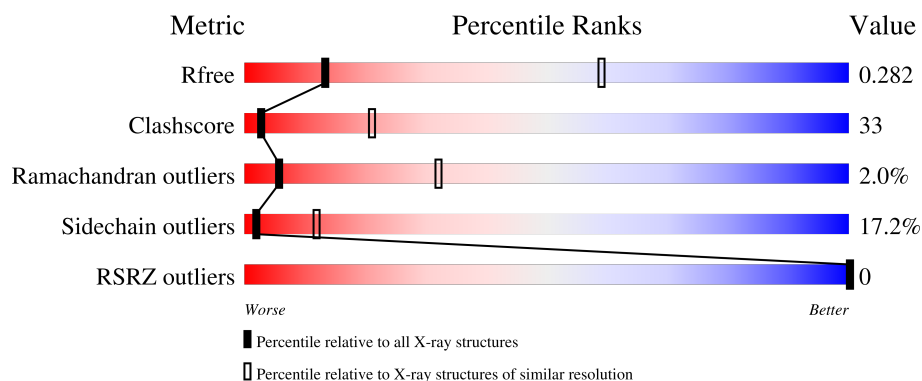
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 Å.

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



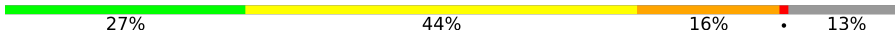
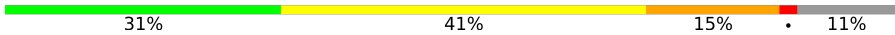
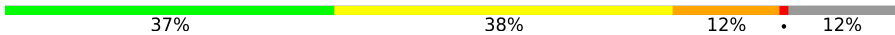
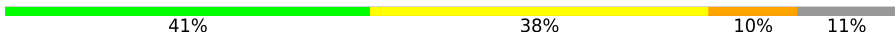
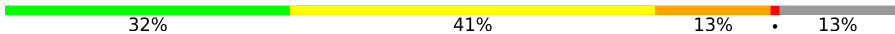
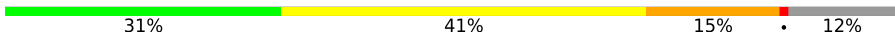
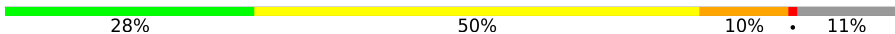
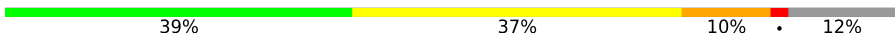
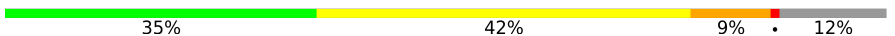
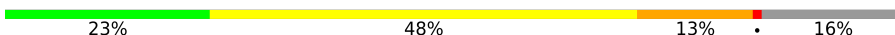
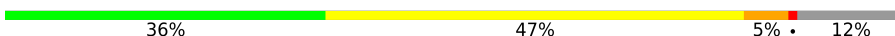
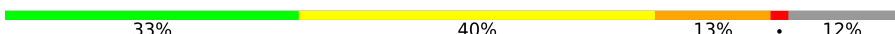
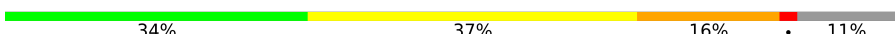
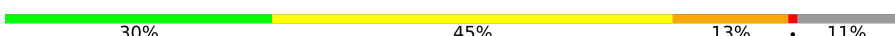
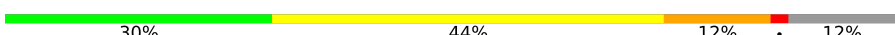
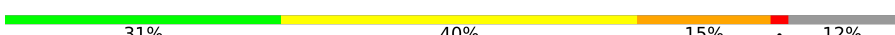
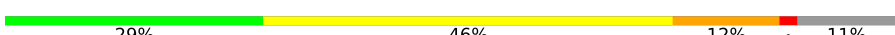
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	186	
1	B	186	
1	C	186	
1	D	186	
1	E	186	

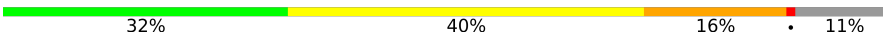
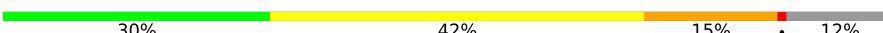
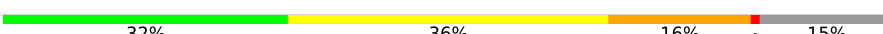
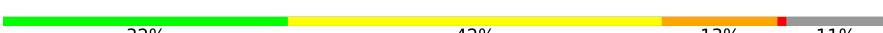
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Mol	Chain	Length	Quality of chain
1	F	186	
1	G	186	
1	H	186	
1	I	186	
1	J	186	
1	K	186	
1	L	186	
1	M	186	
1	N	186	
1	O	186	
1	P	186	
1	Q	186	
1	R	186	
1	S	186	
1	T	186	
1	U	186	
1	V	186	
1	W	186	
1	X	186	
1	Y	186	
1	Z	186	
1	a	186	
1	b	186	
1	c	186	
1	d	186	

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Mol	Chain	Length	Quality of chain
1	e	186	
1	f	186	
1	g	186	
1	h	186	
1	i	186	
1	j	186	
1	k	186	
1	l	186	
1	m	186	
1	n	186	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 52692 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 THIOREDOXIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	B	165	Total	C	N	O	S	0	2	0
			1337	860	226	246	5			
1	C	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	D	164	Total	C	N	O	S	0	2	0
			1331	854	227	246	4			
1	E	162	Total	C	N	O	S	0	0	0
			1300	834	219	243	4			
1	F	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	G	162	Total	C	N	O	S	0	1	0
			1306	838	219	245	4			
1	H	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	I	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	J	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			
1	K	161	Total	C	N	O	S	0	0	0
			1291	828	217	242	4			
1	L	164	Total	C	N	O	S	0	2	0
			1327	854	223	245	5			
1	M	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	N	164	Total	C	N	O	S	0	2	0
			1331	854	227	246	4			
1	O	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	P	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	157	Total	C	N	O	S	0	1	0
			1267	810	214	239	4			
1	R	164	Total	C	N	O	S	0	0	0
			1315	844	221	245	5			
1	S	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	T	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			
1	U	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	V	165	Total	C	N	O	S	0	2	0
			1337	860	226	246	5			
1	W	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	X	164	Total	C	N	O	S	0	2	0
			1331	854	227	246	4			
1	Y	163	Total	C	N	O	S	0	0	0
			1310	840	222	244	4			
1	Z	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	a	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	b	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	c	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			
1	d	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			
1	e	162	Total	C	N	O	S	0	0	0
			1300	834	219	243	4			
1	f	165	Total	C	N	O	S	0	2	0
			1337	860	226	246	5			
1	g	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	h	163	Total	C	N	O	S	0	2	0
			1321	848	224	245	4			
1	i	158	Total	C	N	O	S	0	0	0
			1271	812	217	238	4			
1	j	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	k	163	Total	C	N	O	S	0	1	0
			1316	844	222	246	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	165	Total	C	N	O	S	0	0	0
			1325	850	224	246	5			
1	m	157	Total	C	N	O	S	0	1	0
			1267	810	214	239	4			
1	n	166	Total	C	N	O	S	0	0	0
			1332	854	225	248	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	THR	-	expression tag	UNP O97161
A	48	PRO	CYS	engineered mutation	UNP O97161
B	0	THR	-	expression tag	UNP O97161
B	48	PRO	CYS	engineered mutation	UNP O97161
C	0	THR	-	expression tag	UNP O97161
C	48	PRO	CYS	engineered mutation	UNP O97161
D	0	THR	-	expression tag	UNP O97161
D	48	PRO	CYS	engineered mutation	UNP O97161
E	0	THR	-	expression tag	UNP O97161
E	48	PRO	CYS	engineered mutation	UNP O97161
F	0	THR	-	expression tag	UNP O97161
F	48	PRO	CYS	engineered mutation	UNP O97161
G	0	THR	-	expression tag	UNP O97161
G	48	PRO	CYS	engineered mutation	UNP O97161
H	0	THR	-	expression tag	UNP O97161
H	48	PRO	CYS	engineered mutation	UNP O97161
I	0	THR	-	expression tag	UNP O97161
I	48	PRO	CYS	engineered mutation	UNP O97161
J	0	THR	-	expression tag	UNP O97161
J	48	PRO	CYS	engineered mutation	UNP O97161
K	0	THR	-	expression tag	UNP O97161
K	48	PRO	CYS	engineered mutation	UNP O97161
L	0	THR	-	expression tag	UNP O97161
L	48	PRO	CYS	engineered mutation	UNP O97161
M	0	THR	-	expression tag	UNP O97161
M	48	PRO	CYS	engineered mutation	UNP O97161
N	0	THR	-	expression tag	UNP O97161
N	48	PRO	CYS	engineered mutation	UNP O97161
O	0	THR	-	expression tag	UNP O97161
O	48	PRO	CYS	engineered mutation	UNP O97161
P	0	THR	-	expression tag	UNP O97161
P	48	PRO	CYS	engineered mutation	UNP O97161

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	THR	-	expression tag	UNP O97161
Q	48	PRO	CYS	engineered mutation	UNP O97161
R	0	THR	-	expression tag	UNP O97161
R	48	PRO	CYS	engineered mutation	UNP O97161
S	0	THR	-	expression tag	UNP O97161
S	48	PRO	CYS	engineered mutation	UNP O97161
T	0	THR	-	expression tag	UNP O97161
T	48	PRO	CYS	engineered mutation	UNP O97161
U	0	THR	-	expression tag	UNP O97161
U	48	PRO	CYS	engineered mutation	UNP O97161
V	0	THR	-	expression tag	UNP O97161
V	48	PRO	CYS	engineered mutation	UNP O97161
W	0	THR	-	expression tag	UNP O97161
W	48	PRO	CYS	engineered mutation	UNP O97161
X	0	THR	-	expression tag	UNP O97161
X	48	PRO	CYS	engineered mutation	UNP O97161
Y	0	THR	-	expression tag	UNP O97161
Y	48	PRO	CYS	engineered mutation	UNP O97161
Z	0	THR	-	expression tag	UNP O97161
Z	48	PRO	CYS	engineered mutation	UNP O97161
a	0	THR	-	expression tag	UNP O97161
a	48	PRO	CYS	engineered mutation	UNP O97161
b	0	THR	-	expression tag	UNP O97161
b	48	PRO	CYS	engineered mutation	UNP O97161
c	0	THR	-	expression tag	UNP O97161
c	48	PRO	CYS	engineered mutation	UNP O97161
d	0	THR	-	expression tag	UNP O97161
d	48	PRO	CYS	engineered mutation	UNP O97161
e	0	THR	-	expression tag	UNP O97161
e	48	PRO	CYS	engineered mutation	UNP O97161
f	0	THR	-	expression tag	UNP O97161
f	48	PRO	CYS	engineered mutation	UNP O97161
g	0	THR	-	expression tag	UNP O97161
g	48	PRO	CYS	engineered mutation	UNP O97161
h	0	THR	-	expression tag	UNP O97161
h	48	PRO	CYS	engineered mutation	UNP O97161
i	0	THR	-	expression tag	UNP O97161
i	48	PRO	CYS	engineered mutation	UNP O97161
j	0	THR	-	expression tag	UNP O97161
j	48	PRO	CYS	engineered mutation	UNP O97161
k	0	THR	-	expression tag	UNP O97161
k	48	PRO	CYS	engineered mutation	UNP O97161

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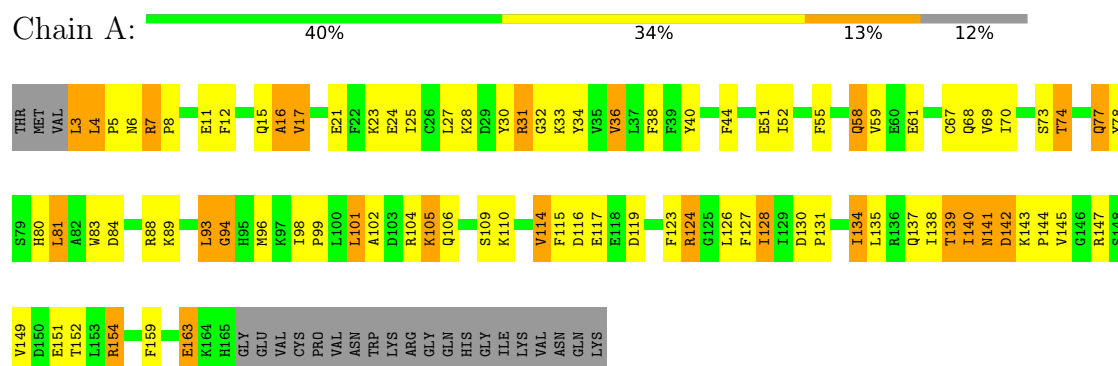
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Chain	Residue	Modelled	Actual	Comment	Reference
l	0	THR	-	expression tag	UNP O97161
l	48	PRO	CYS	engineered mutation	UNP O97161
m	0	THR	-	expression tag	UNP O97161
m	48	PRO	CYS	engineered mutation	UNP O97161
n	0	THR	-	expression tag	UNP O97161
n	48	PRO	CYS	engineered mutation	UNP O97161

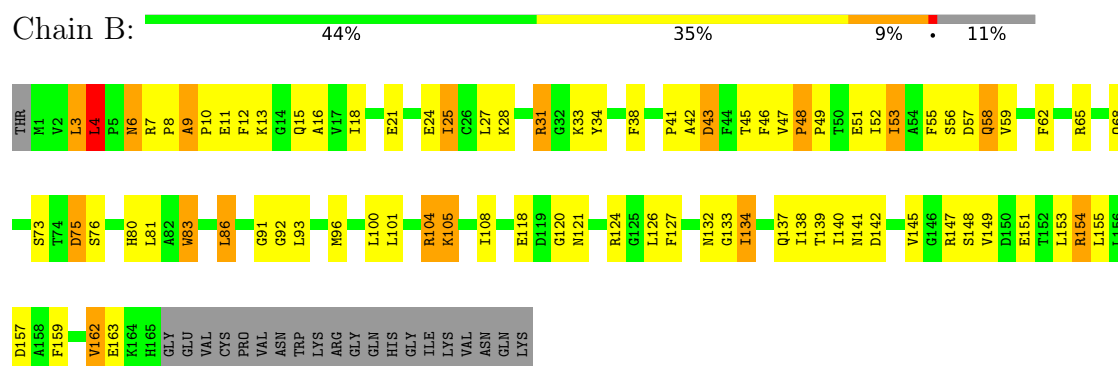
3 Residue-property plots [i](#)

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

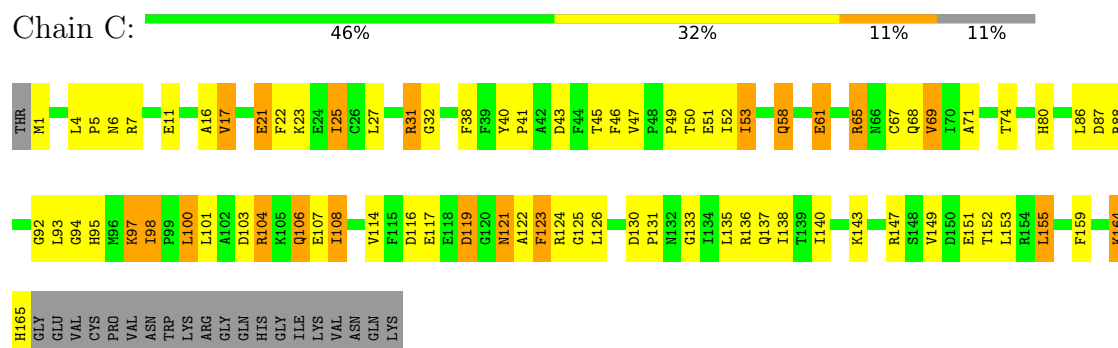
• Molecule 1: THIOREDOXIN PEROXIDASE



• Molecule 1: THIOREDOXIN PEROXIDASE

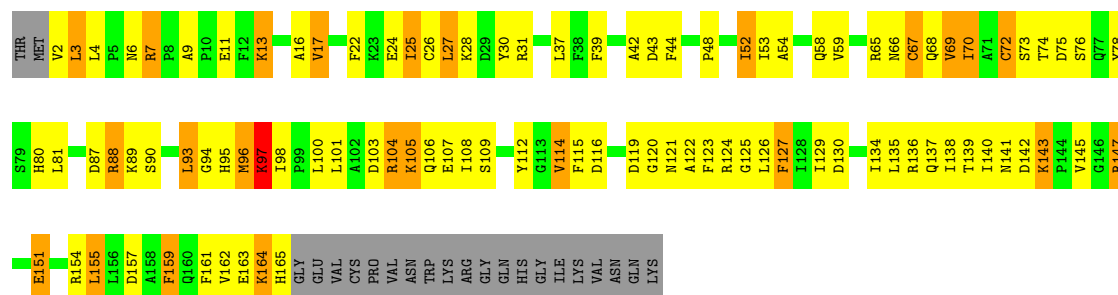


• Molecule 1: THIOREDOXIN PEROXIDASE



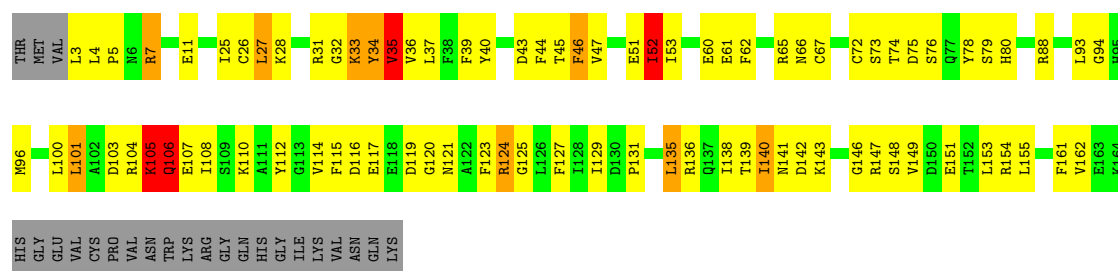
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain D: 35% 40% 13% • 12%



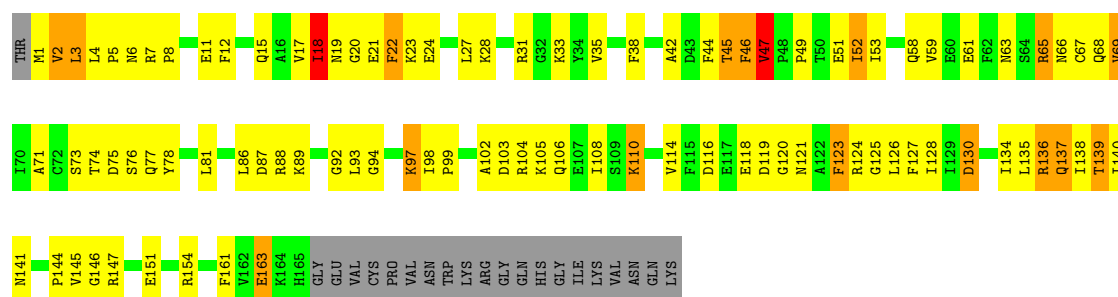
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain E: 41% 39% 5% • 13%



• Molecule 1: THIOREDOXIN PEROXIDASE

Chain F: 37% 42% 9% • 11%

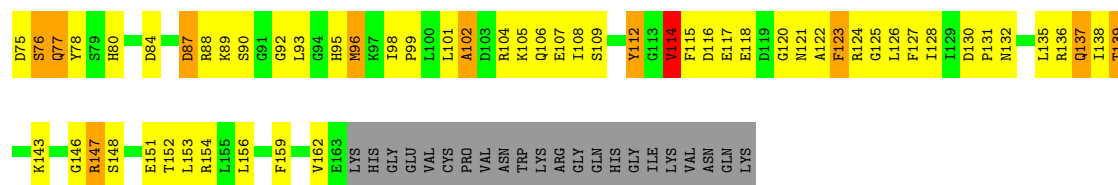


• Molecule 1: THIOREDOXIN PEROXIDASE

Chain G: 27% 44% 16% • 13%

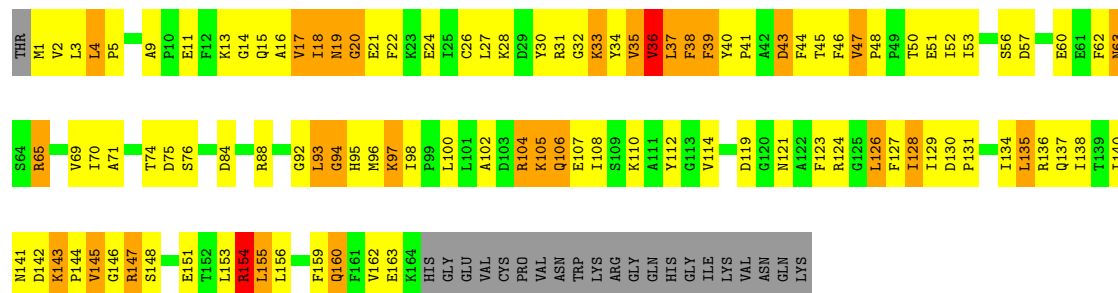






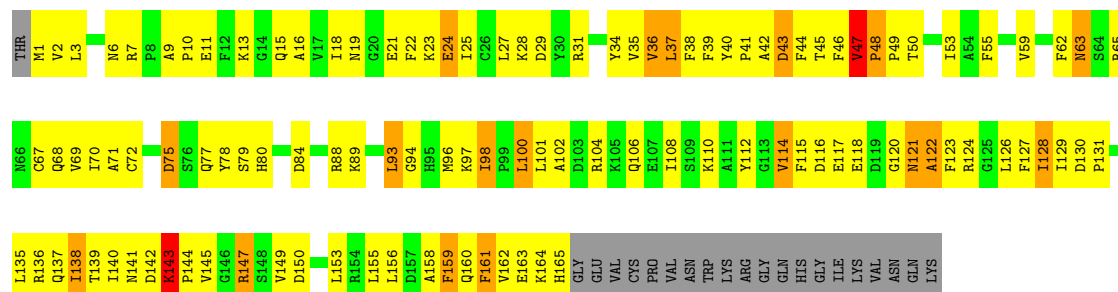
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain L: 31% 41% 15% 12%



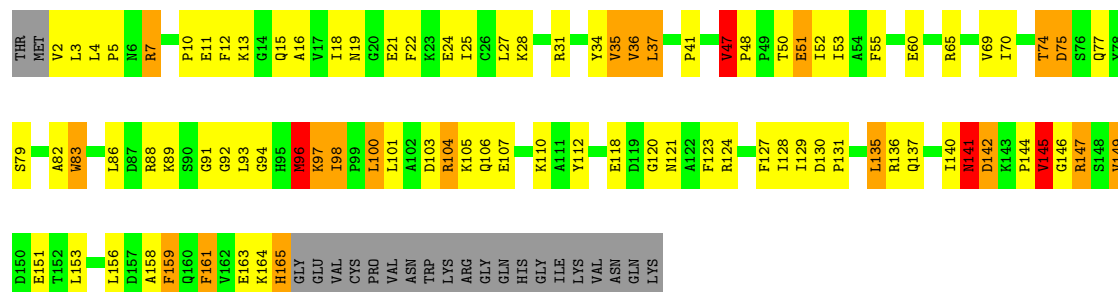
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain M: 28% 50% 10% 11%



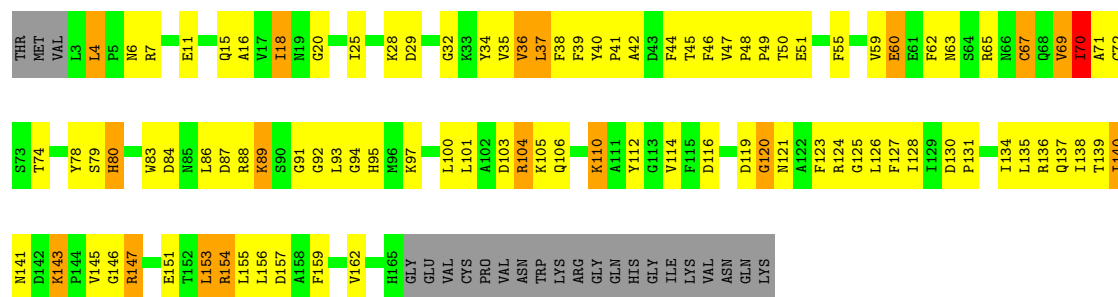
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain N: 39% 37% 10% 12%

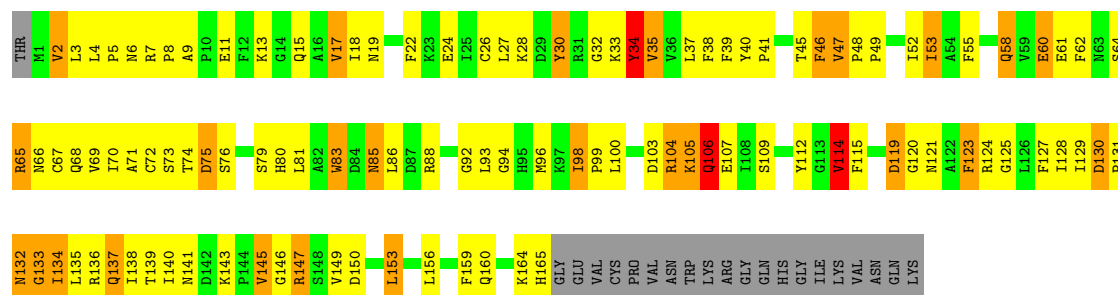


• Molecule 1: THIOREDOXIN PEROXIDASE

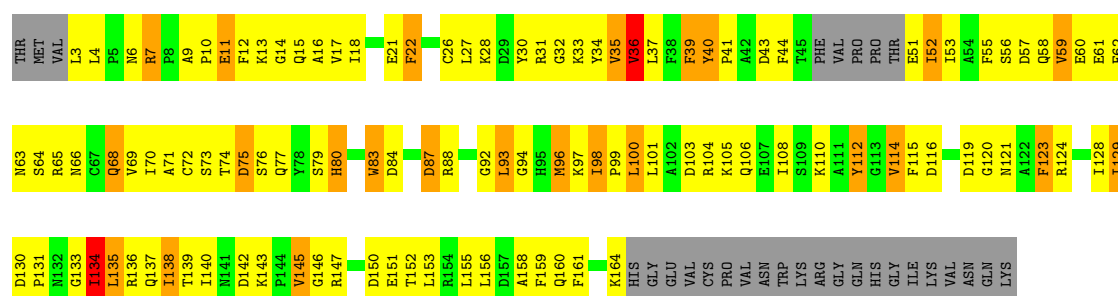
Chain O: 35% 42% 9% 12%



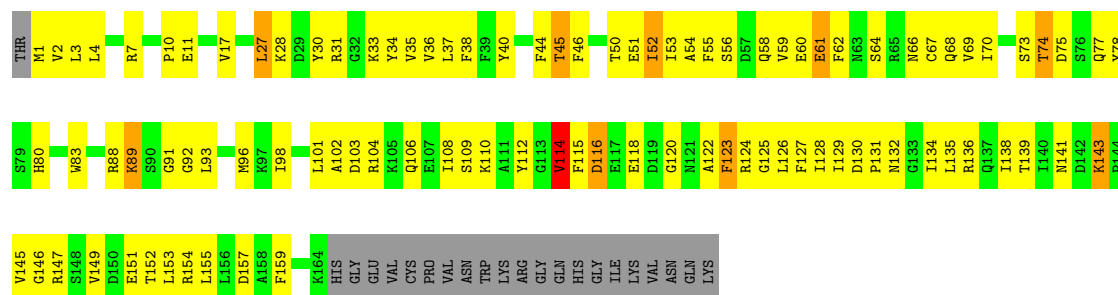
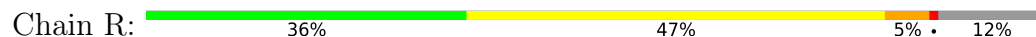
• Molecule 1: THIOREDOXIN PEROXIDASE



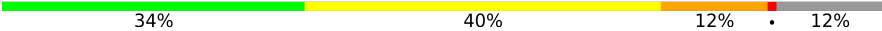
• Molecule 1: THIOREDOXIN PEROXIDASE

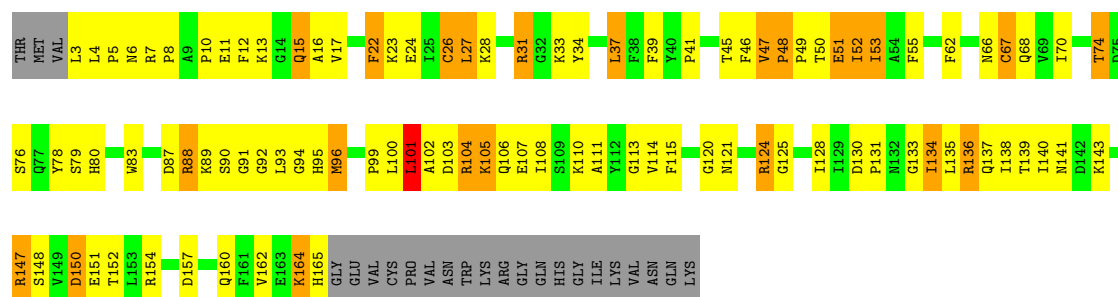


• Molecule 1: THIOREDOXIN PEROXIDASE



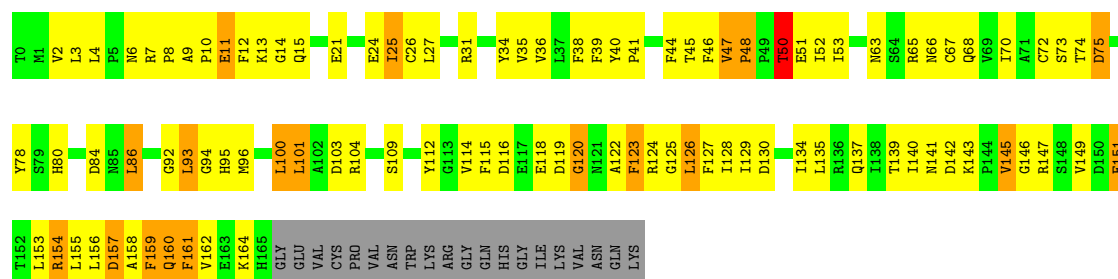
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain S: 



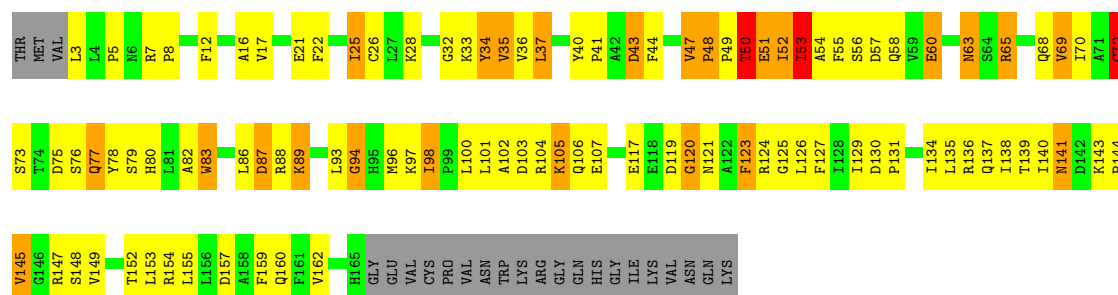
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain T: 

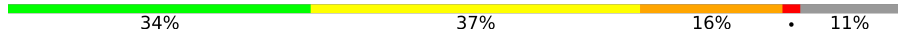


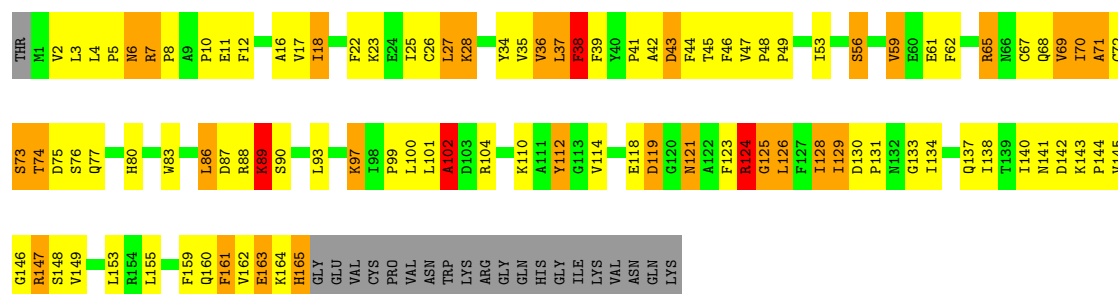
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain U: 

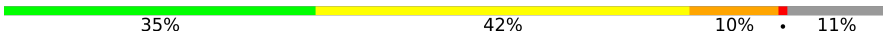


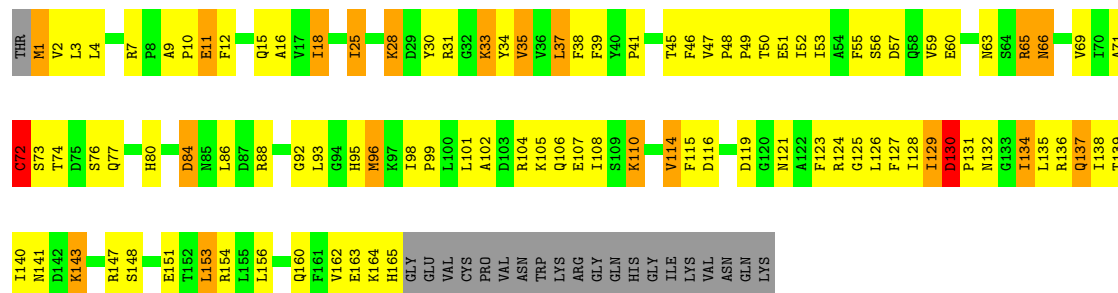
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain V: 



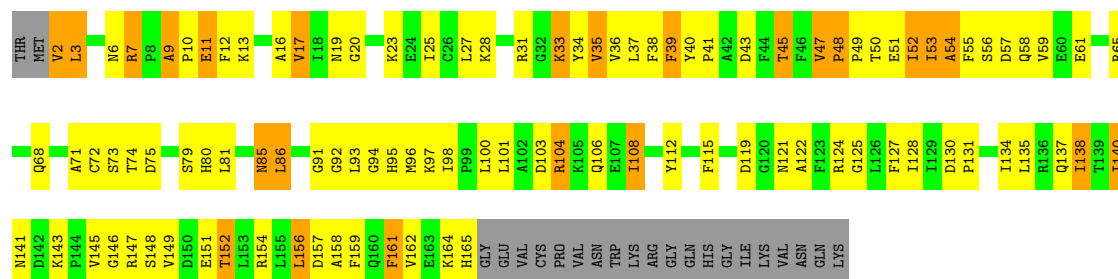
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain W: 

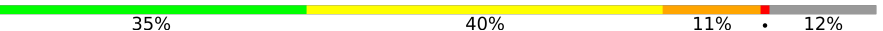


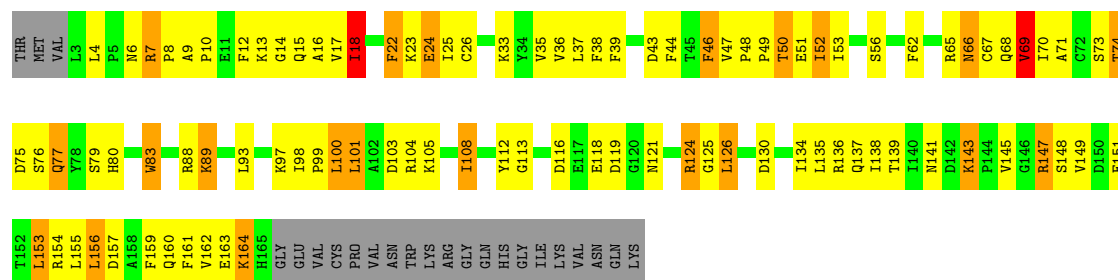
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain X: 

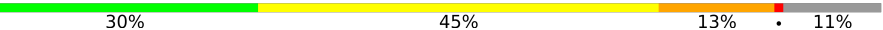


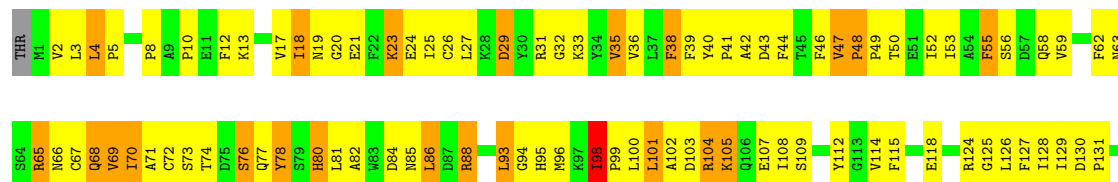
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain Y: 



• Molecule 1: THIOREDOXIN PEROXIDASE

Chain Z: 





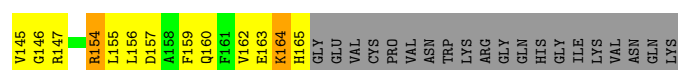
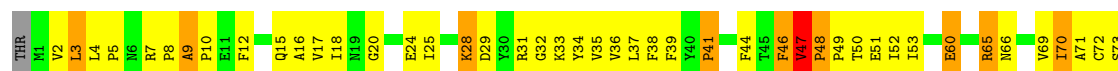
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain a: 30% 44% 12% 12%



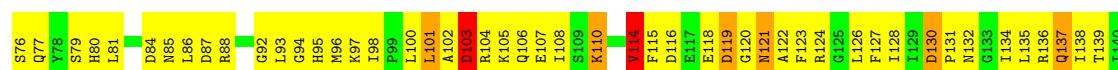
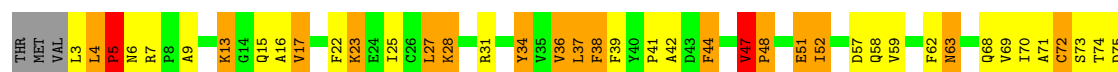
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain b: 32% 45% 10% 11%



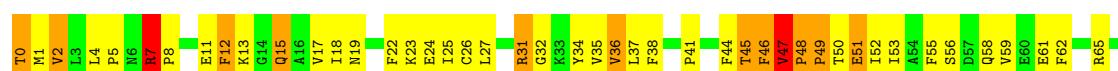
• Molecule 1: THIOREDOXIN PEROXIDASE

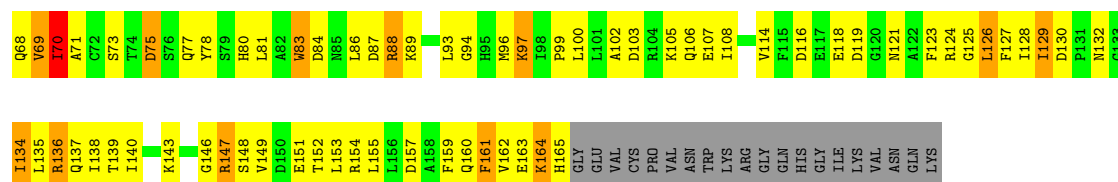
Chain c: 31% 40% 15% 12%



• Molecule 1: THIOREDOXIN PEROXIDASE

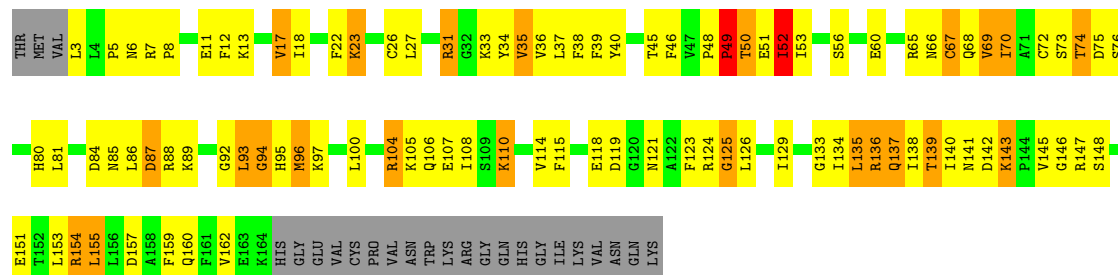
Chain d: 29% 46% 12% 11%





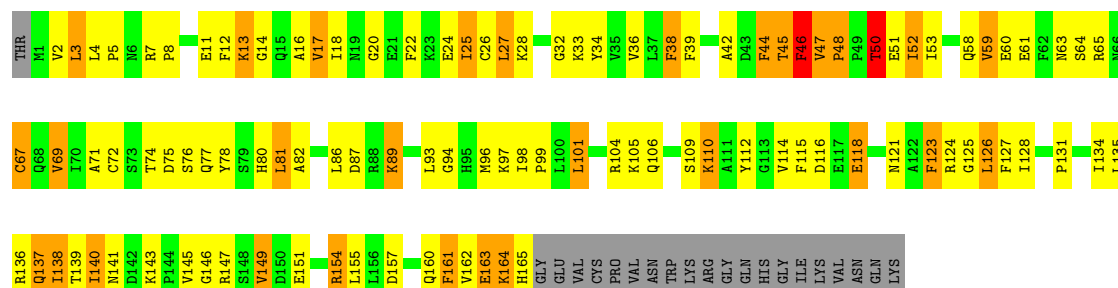
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain e: 34% 39% 12% 13%



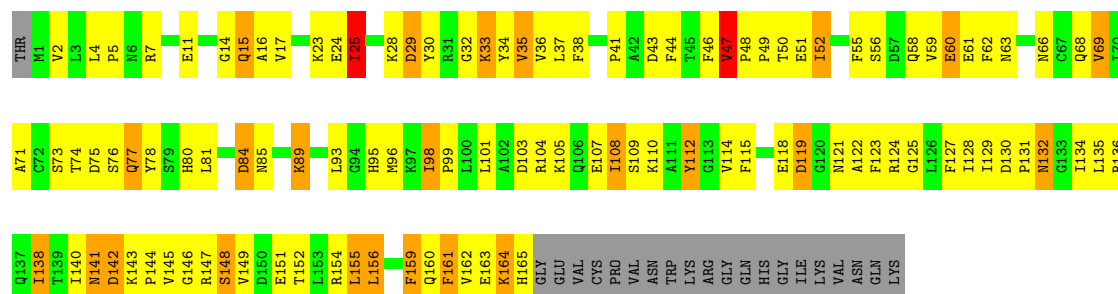
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain f: 32% 40% 16% 11%



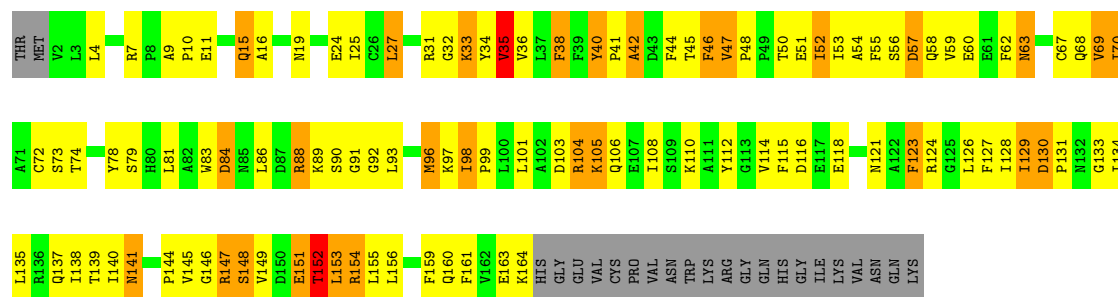
• Molecule 1: THIOREDOXIN PEROXIDASE

Chain g: 30% 45% 13% 11%

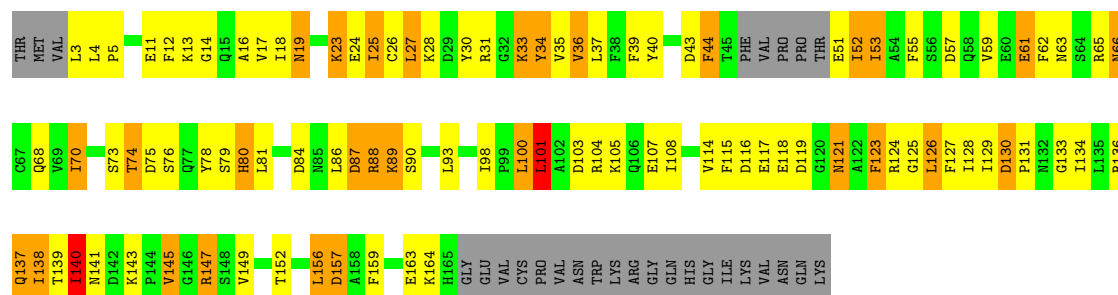


• Molecule 1: THIOREDOXIN PEROXIDASE

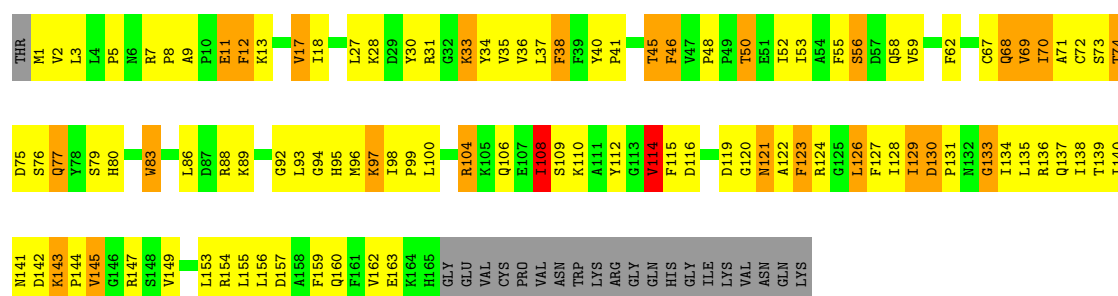
Chain h: 30% 42% 15% 12%



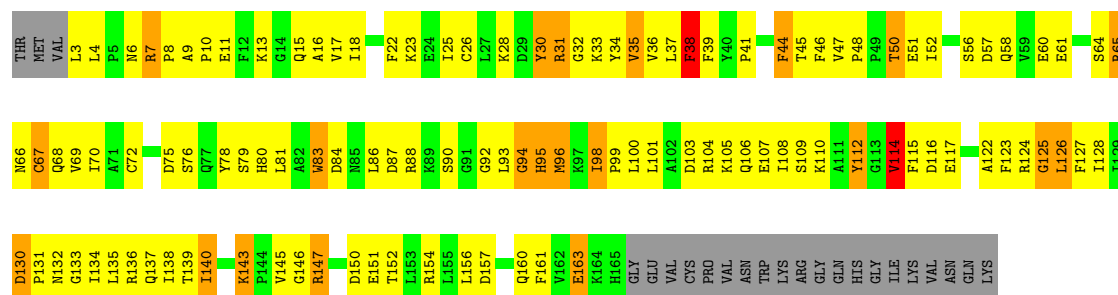
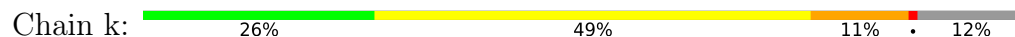
• Molecule 1: THIOREDOXIN PEROXIDASE



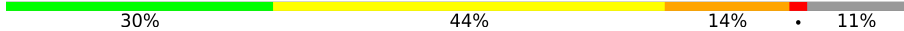
• Molecule 1: THIOREDOXIN PEROXIDASE

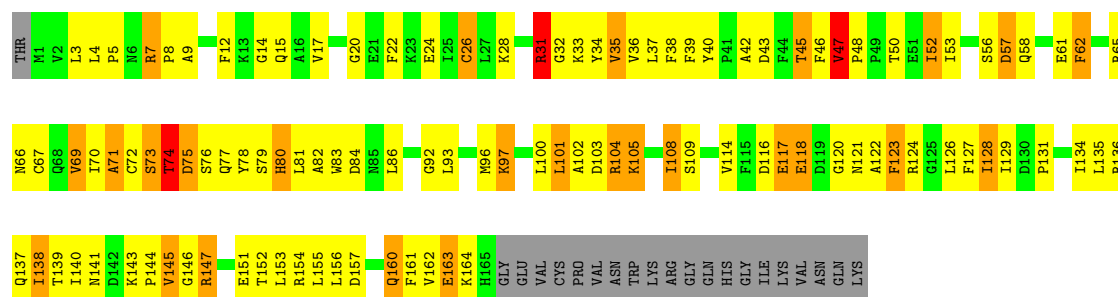


• Molecule 1: THIOREDOXIN PEROXIDASE



• Molecule 1: THIOREDOXIN PEROXIDASE

Chain l: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.18Å 190.30Å 212.00Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	48.76 – 3.52 48.76 – 3.52	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.76-3.52) 97.7 (48.76-3.52)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.277 , 0.289 0.274 , 0.282	Depositor DCC
R_{free} test set	4589 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.327 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	2 of 91789 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52692	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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	0.43	1/1341 (0.1%)	1.10	7/1813 (0.4%)
1	B	0.41	0/1374	1.05	7/1855 (0.4%)
1	C	0.39	0/1356	0.94	3/1833 (0.2%)
1	D	0.42	0/1368	1.15	14/1849 (0.8%)
1	E	0.40	0/1330	1.06	5/1798 (0.3%)
1	F	0.38	0/1356	0.95	2/1833 (0.1%)
1	G	0.40	0/1339	1.21	17/1810 (0.9%)
1	H	0.47	0/1356	1.20	13/1833 (0.7%)
1	I	0.45	0/1350	1.15	9/1825 (0.5%)
1	J	0.43	0/1363	1.04	6/1843 (0.3%)
1	K	0.42	0/1321	1.13	15/1787 (0.8%)
1	L	0.43	0/1363	1.13	7/1840 (0.4%)
1	M	0.45	0/1356	1.15	11/1833 (0.6%)
1	N	0.42	0/1368	1.21	15/1849 (0.8%)
1	O	0.41	0/1341	1.07	9/1813 (0.5%)
1	P	0.40	0/1356	1.12	9/1833 (0.5%)
1	Q	0.43	0/1296	1.00	4/1747 (0.2%)
1	R	0.42	0/1345	1.04	7/1818 (0.4%)
1	S	0.43	0/1350	1.20	7/1825 (0.4%)
1	T	0.39	0/1363	1.09	9/1843 (0.5%)
1	U	0.45	0/1341	1.13	11/1813 (0.6%)
1	V	0.44	0/1374	1.13	8/1855 (0.4%)
1	W	0.39	0/1356	1.04	3/1833 (0.2%)
1	X	0.43	0/1368	1.17	12/1849 (0.6%)
1	Y	0.46	1/1341 (0.1%)	1.04	4/1813 (0.2%)
1	Z	0.43	0/1356	1.16	16/1833 (0.9%)
1	a	0.48	0/1350	1.22	14/1825 (0.8%)
1	b	0.47	0/1356	1.21	13/1833 (0.7%)
1	c	0.43	0/1350	1.27	15/1825 (0.8%)
1	d	0.41	0/1363	1.15	14/1843 (0.8%)
1	e	0.41	0/1330	1.05	8/1798 (0.4%)
1	f	0.44	0/1374	1.15	10/1855 (0.5%)
1	g	0.42	0/1356	1.11	10/1833 (0.5%)
1	h	0.44	0/1357	1.27	19/1834 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.38	0/1298	0.86	2/1750 (0.1%)
1	j	0.43	0/1356	1.14	15/1833 (0.8%)
1	k	0.43	0/1350	1.21	8/1825 (0.4%)
1	l	0.43	0/1356	1.12	11/1833 (0.6%)
1	m	0.36	0/1296	0.92	6/1747 (0.3%)
1	n	0.44	0/1363	1.03	8/1843 (0.4%)
All	All	0.42	2/53983 (0.0%)	1.11	383/72953 (0.5%)

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	2
1	B	0	3
1	E	0	1
1	G	0	2
1	H	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	2
1	P	0	1
1	Q	0	2
1	R	0	1
1	S	0	2
1	T	0	1
1	U	0	1
1	V	0	4
1	W	0	1
1	X	0	1
1	Y	0	2
1	a	0	3
1	b	0	2
1	c	0	3
1	d	0	3
1	e	0	2
1	f	0	4
1	h	0	4
1	j	0	1
1	k	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	l	0	2
1	m	0	1
1	n	0	1
All	All	0	59

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	69	VAL	CA-CB	5.26	1.61	1.54
1	A	142	ASP	CA-C	5.17	1.55	1.52

The worst 5 of 383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	4	LEU	CA-C-N	13.26	136.41	119.84
1	c	4	LEU	C-N-CA	13.26	136.41	119.84
1	N	48	PRO	CA-C-N	-13.06	103.52	119.84
1	N	48	PRO	C-N-CA	-13.06	103.52	119.84
1	e	45	THR	N-CA-C	-12.45	97.45	112.89

There are no chirality outliers.

5 of 59 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	GLU	Peptide
1	A	94	GLY	Peptide
1	B	105	LYS	Peptide
1	B	31	ARG	Peptide
1	B	43	ASP	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	1310	0	1282	94	0
1	B	1337	0	1329	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1325	0	1303	85	0
1	D	1331	0	1312	106	0
1	E	1300	0	1275	78	0
1	F	1325	0	1303	92	0
1	G	1306	0	1281	114	0
1	H	1325	0	1303	101	0
1	I	1316	0	1288	86	0
1	J	1332	0	1310	85	0
1	K	1291	0	1262	78	0
1	L	1327	0	1322	105	0
1	M	1325	0	1303	103	0
1	N	1331	0	1312	80	1
1	O	1310	0	1282	88	0
1	P	1325	0	1303	108	0
1	Q	1267	0	1241	102	0
1	R	1315	0	1296	86	1
1	S	1316	0	1288	108	0
1	T	1332	0	1310	89	0
1	U	1310	0	1282	114	0
1	V	1337	0	1329	113	0
1	W	1325	0	1303	91	0
1	X	1331	0	1312	102	0
1	Y	1310	0	1282	89	1
1	Z	1325	0	1303	110	0
1	a	1316	0	1288	113	0
1	b	1325	0	1303	109	1
1	c	1316	0	1288	90	0
1	d	1332	0	1310	113	0
1	e	1300	0	1275	82	0
1	f	1337	0	1329	87	0
1	g	1325	0	1303	97	0
1	h	1321	0	1305	103	0
1	i	1271	0	1242	89	0
1	j	1325	0	1303	99	0
1	k	1316	0	1288	102	0
1	l	1325	0	1303	94	0
1	m	1267	0	1241	83	0
1	n	1332	0	1310	107	0
All	All	52692	0	51804	3465	2

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 33.

The worst 5 of 3465 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:65:ARG:NH1	1:i:157:ASP:OD2	1.84	1.09
1:H:76:SER:HB2	1:H:104:ARG:HH11	1.17	1.06
1:U:33:LYS:HZ3	1:U:68:GLN:HG3	1.15	1.06
1:D:119:ASP:OD2	1:D:143:LYS:NZ	1.89	1.06
1:g:11:GLU:OE1	1:g:28:LYS:NZ	1.89	1.04

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:ASN:ND2	1:b:60:GLU:OE2[2_655]	2.06	0.14
1:R:33:LYS:NZ	1:Y:66:ASN:OD1[1_565]	2.13	0.07

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	161/186 (87%)	132 (82%)	27 (17%)	2 (1%)	10	42
1	B	165/186 (89%)	145 (88%)	18 (11%)	2 (1%)	10	42
1	C	163/186 (88%)	141 (86%)	18 (11%)	4 (2%)	4	28
1	D	164/186 (88%)	148 (90%)	13 (8%)	3 (2%)	6	34
1	E	160/186 (86%)	134 (84%)	20 (12%)	6 (4%)	2	20
1	F	163/186 (88%)	140 (86%)	17 (10%)	6 (4%)	2	21
1	G	161/186 (87%)	135 (84%)	25 (16%)	1 (1%)	21	55
1	H	163/186 (88%)	131 (80%)	25 (15%)	7 (4%)	2	18
1	I	162/186 (87%)	131 (81%)	28 (17%)	3 (2%)	6	33
1	J	164/186 (88%)	144 (88%)	19 (12%)	1 (1%)	21	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	159/186 (86%)	133 (84%)	23 (14%)	3 (2%)	6	33
1	L	164/186 (88%)	140 (85%)	22 (13%)	2 (1%)	10	42
1	M	163/186 (88%)	137 (84%)	24 (15%)	2 (1%)	10	42
1	N	164/186 (88%)	143 (87%)	20 (12%)	1 (1%)	21	55
1	O	161/186 (87%)	139 (86%)	19 (12%)	3 (2%)	6	33
1	P	163/186 (88%)	134 (82%)	23 (14%)	6 (4%)	2	21
1	Q	154/186 (83%)	118 (77%)	29 (19%)	7 (4%)	2	17
1	R	162/186 (87%)	136 (84%)	25 (15%)	1 (1%)	21	55
1	S	162/186 (87%)	136 (84%)	23 (14%)	3 (2%)	6	33
1	T	164/186 (88%)	141 (86%)	20 (12%)	3 (2%)	6	34
1	U	161/186 (87%)	135 (84%)	21 (13%)	5 (3%)	3	24
1	V	165/186 (89%)	141 (86%)	21 (13%)	3 (2%)	6	34
1	W	163/186 (88%)	132 (81%)	28 (17%)	3 (2%)	6	34
1	X	164/186 (88%)	137 (84%)	23 (14%)	4 (2%)	4	29
1	Y	161/186 (87%)	133 (83%)	26 (16%)	2 (1%)	10	42
1	Z	163/186 (88%)	136 (83%)	25 (15%)	2 (1%)	10	42
1	a	162/186 (87%)	135 (83%)	24 (15%)	3 (2%)	6	33
1	b	163/186 (88%)	133 (82%)	28 (17%)	2 (1%)	10	42
1	c	162/186 (87%)	136 (84%)	23 (14%)	3 (2%)	6	33
1	d	164/186 (88%)	146 (89%)	17 (10%)	1 (1%)	21	55
1	e	160/186 (86%)	134 (84%)	21 (13%)	5 (3%)	3	24
1	f	165/186 (89%)	149 (90%)	14 (8%)	2 (1%)	10	42
1	g	163/186 (88%)	134 (82%)	25 (15%)	4 (2%)	4	28
1	h	163/186 (88%)	136 (83%)	25 (15%)	2 (1%)	10	42
1	i	154/186 (83%)	121 (79%)	31 (20%)	2 (1%)	9	40
1	j	163/186 (88%)	136 (83%)	24 (15%)	3 (2%)	6	34
1	k	162/186 (87%)	136 (84%)	23 (14%)	3 (2%)	6	33
1	l	163/186 (88%)	135 (83%)	23 (14%)	5 (3%)	3	24
1	m	154/186 (83%)	129 (84%)	24 (16%)	1 (1%)	21	55
1	n	164/186 (88%)	125 (76%)	32 (20%)	7 (4%)	2	18
All	All	6481/7440 (87%)	5437 (84%)	916 (14%)	128 (2%)	6	32

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	E	34	TYR
1	E	106	GLN
1	F	19	ASN
1	H	69	VAL

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	142/162 (88%)	121 (85%)	21 (15%)	3	17
1	B	146/162 (90%)	130 (89%)	16 (11%)	6	27
1	C	144/162 (89%)	125 (87%)	19 (13%)	4	21
1	D	145/162 (90%)	126 (87%)	19 (13%)	4	21
1	E	141/162 (87%)	126 (89%)	15 (11%)	6	28
1	F	144/162 (89%)	124 (86%)	20 (14%)	3	20
1	G	142/162 (88%)	114 (80%)	28 (20%)	1	8
1	H	144/162 (89%)	114 (79%)	30 (21%)	1	6
1	I	143/162 (88%)	123 (86%)	20 (14%)	3	19
1	J	145/162 (90%)	123 (85%)	22 (15%)	3	17
1	K	140/162 (86%)	112 (80%)	28 (20%)	1	7
1	L	145/162 (90%)	112 (77%)	33 (23%)	1	5
1	M	144/162 (89%)	125 (87%)	19 (13%)	4	21
1	N	145/162 (90%)	117 (81%)	28 (19%)	1	8
1	O	142/162 (88%)	120 (84%)	22 (16%)	2	16
1	P	144/162 (89%)	118 (82%)	26 (18%)	2	10
1	Q	137/162 (85%)	107 (78%)	30 (22%)	1	6
1	R	143/162 (88%)	126 (88%)	17 (12%)	5	24
1	S	143/162 (88%)	121 (85%)	22 (15%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	145/162 (90%)	123 (85%)	22 (15%)	3	17
1	U	142/162 (88%)	118 (83%)	24 (17%)	2	13
1	V	146/162 (90%)	119 (82%)	27 (18%)	1	9
1	W	144/162 (89%)	116 (81%)	28 (19%)	1	8
1	X	145/162 (90%)	123 (85%)	22 (15%)	3	17
1	Y	142/162 (88%)	117 (82%)	25 (18%)	2	11
1	Z	144/162 (89%)	118 (82%)	26 (18%)	2	10
1	a	143/162 (88%)	117 (82%)	26 (18%)	2	10
1	b	144/162 (89%)	124 (86%)	20 (14%)	3	20
1	c	143/162 (88%)	112 (78%)	31 (22%)	1	6
1	d	145/162 (90%)	121 (83%)	24 (17%)	2	13
1	e	141/162 (87%)	114 (81%)	27 (19%)	1	8
1	f	146/162 (90%)	114 (78%)	32 (22%)	1	6
1	g	144/162 (89%)	117 (81%)	27 (19%)	1	9
1	h	144/162 (89%)	119 (83%)	25 (17%)	2	11
1	i	137/162 (85%)	99 (72%)	38 (28%)	0	3
1	j	144/162 (89%)	119 (83%)	25 (17%)	2	11
1	k	143/162 (88%)	116 (81%)	27 (19%)	1	9
1	l	144/162 (89%)	113 (78%)	31 (22%)	1	6
1	m	137/162 (85%)	115 (84%)	22 (16%)	2	14
1	n	145/162 (90%)	126 (87%)	19 (13%)	4	21
All	All	5727/6480 (88%)	4744 (83%)	983 (17%)	2	12

5 of 983 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	50	THR
1	k	17	VAL
1	Y	108	ILE
1	j	124	ARG
1	m	25	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	63	ASN
1	f	58	GLN
1	b	58	GLN
1	d	77	GLN
1	g	77	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	163/186 (87%)	-1.46	0 100 100	110, 111, 112, 112	0
1	B	165/186 (88%)	-1.42	0 100 100	67, 111, 112, 112	2 (1%)
1	C	165/186 (88%)	-1.49	0 100 100	110, 111, 111, 112	0
1	D	164/186 (88%)	-1.49	0 100 100	64, 111, 111, 112	2 (1%)
1	E	162/186 (87%)	-1.43	0 100 100	110, 111, 111, 112	0
1	F	165/186 (88%)	-1.46	0 100 100	110, 111, 112, 112	0
1	G	162/186 (87%)	-1.45	0 100 100	67, 111, 112, 112	1 (0%)
1	H	165/186 (88%)	-1.43	0 100 100	110, 111, 112, 112	0
1	I	163/186 (87%)	-1.43	0 100 100	66, 111, 112, 112	1 (0%)
1	J	166/186 (89%)	-1.44	0 100 100	110, 111, 112, 112	0
1	K	161/186 (86%)	-1.44	0 100 100	110, 111, 112, 112	0
1	L	164/186 (88%)	-1.40	0 100 100	67, 111, 112, 112	2 (1%)
1	M	165/186 (88%)	-1.43	0 100 100	110, 111, 112, 112	0
1	N	164/186 (88%)	-1.39	0 100 100	64, 111, 112, 112	2 (1%)
1	O	163/186 (87%)	-1.38	0 100 100	110, 111, 112, 112	0
1	P	165/186 (88%)	-1.42	0 100 100	110, 111, 112, 112	0
1	Q	157/186 (84%)	-1.39	0 100 100	67, 111, 112, 112	1 (0%)
1	R	164/186 (88%)	-1.46	0 100 100	110, 111, 112, 112	0
1	S	163/186 (87%)	-1.50	0 100 100	67, 111, 111, 112	1 (0%)
1	T	166/186 (89%)	-1.48	0 100 100	109, 111, 111, 112	0
1	U	163/186 (87%)	-1.48	0 100 100	110, 111, 112, 112	0
1	V	165/186 (88%)	-1.43	0 100 100	67, 111, 112, 112	2 (1%)
1	W	165/186 (88%)	-1.48	0 100 100	109, 111, 111, 112	0
1	X	164/186 (88%)	-1.45	0 100 100	64, 111, 111, 112	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9		
1	Y	163/186 (87%)	-1.40	0	100	100	110, 111, 112, 112	0
1	Z	165/186 (88%)	-1.43	0	100	100	103, 111, 112, 112	0
1	a	163/186 (87%)	-1.44	0	100	100	66, 111, 112, 112	1 (0%)
1	b	165/186 (88%)	-1.44	0	100	100	110, 111, 112, 112	0
1	c	163/186 (87%)	-1.38	0	100	100	67, 111, 112, 113	1 (0%)
1	d	166/186 (89%)	-1.42	0	100	100	110, 111, 112, 112	0
1	e	162/186 (87%)	-1.46	0	100	100	110, 111, 111, 112	0
1	f	165/186 (88%)	-1.46	0	100	100	67, 111, 111, 112	2 (1%)
1	g	165/186 (88%)	-1.46	0	100	100	110, 111, 112, 112	0
1	h	163/186 (87%)	-1.41	0	100	100	64, 111, 112, 113	2 (1%)
1	i	158/186 (84%)	-1.44	0	100	100	110, 111, 112, 112	0
1	j	165/186 (88%)	-1.41	0	100	100	109, 111, 112, 112	0
1	k	163/186 (87%)	-1.39	0	100	100	67, 111, 112, 112	1 (0%)
1	l	165/186 (88%)	-1.43	0	100	100	110, 111, 112, 112	0
1	m	157/186 (84%)	-1.33	0	100	100	67, 111, 112, 112	1 (0%)
1	n	166/186 (89%)	-1.45	0	100	100	110, 111, 112, 112	0
All	All	6543/7440 (87%)	-1.43	0	100	100	64, 111, 112, 113	24 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.