wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:47 PM GMT

PDB ID	:	1H6V
Title	:	MAMMALIAN THIOREDOXIN REDUCTASE
Authors	:	Sandalova, T.; Zhong, L.; Lindqvist, Y.; Holmgren, A.; Schneider, G.
Deposited on	:	2001-06-27
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

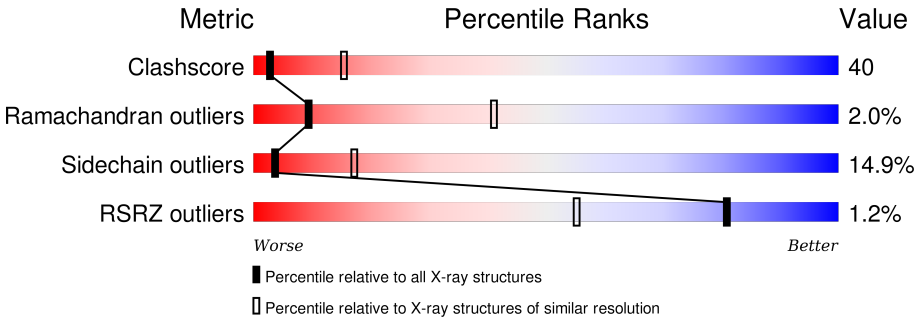
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	499	40% 49% 8%
1	B	499	44% 43% 10%
1	C	499	3% 28% 54% 14%
1	D	499	% 44% 40% 11%
1	E	499	% 47% 41% 9%
1	F	499	% 44% 43% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	D	600	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23075 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.

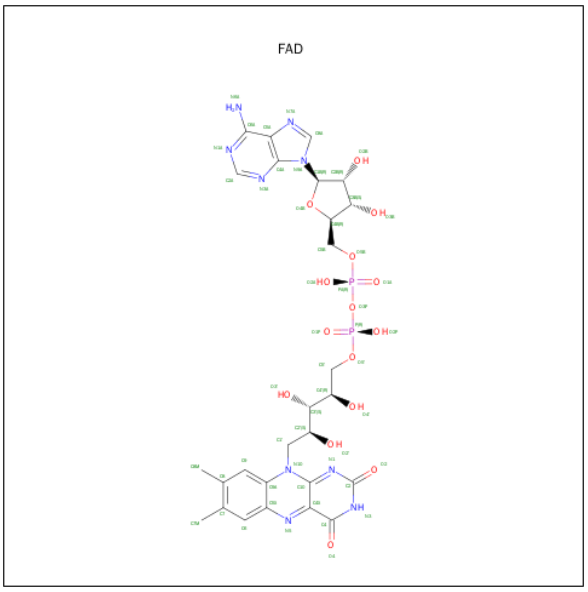
- Molecule 1 is a protein called THIOREDOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3764	2391	635	716	22			
1	B	487	Total	C	N	O	S	0	0	0
			3753	2387	633	713	20			
1	C	482	Total	C	N	O	S	0	0	0
			3707	2356	627	704	20			
1	D	487	Total	C	N	O	S	0	0	0
			3753	2387	633	713	20			
1	E	491	Total	C	N	O	S	0	0	0
			3773	2397	637	717	22			
1	F	490	Total	C	N	O	S	0	0	0
			3764	2391	635	716	22			

There are 11 discrepancies between the modelled and reference sequences:

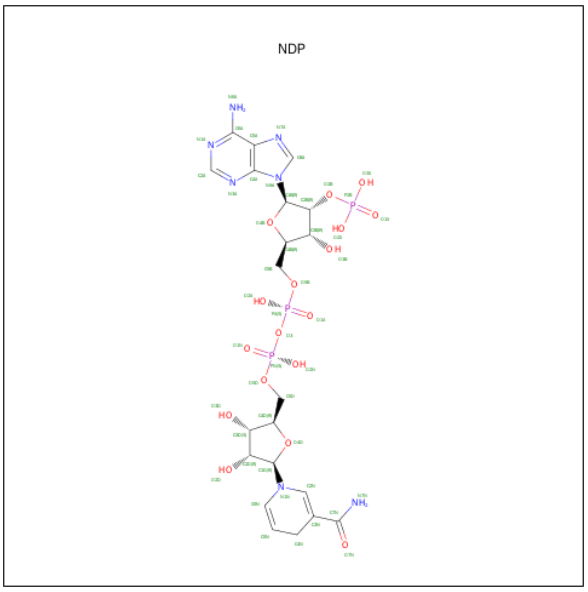
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ASN	ARG	CONFLICT	UNP O89049
B	52	ASN	ARG	CONFLICT	UNP O89049
C	52	ASN	ARG	CONFLICT	UNP O89049
D	52	ASN	ARG	CONFLICT	UNP O89049
E	52	ASN	ARG	CONFLICT	UNP O89049
F	52	ASN	ARG	CONFLICT	UNP O89049
A	497	CYS	SEL	ENGINEERED MUTATION	UNP O89049
B	497	CYS	SEL	ENGINEERED MUTATION	UNP O89049
C	497	CYS	SEL	ENGINEERED MUTATION	UNP O89049
D	497	CYS	SEL	ENGINEERED MUTATION	UNP O89049
E	497	CYS	SEL	ENGINEERED MUTATION	UNP O89049

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	B	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	C	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	D	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	E	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
3	F	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

- Molecule 4 is water.

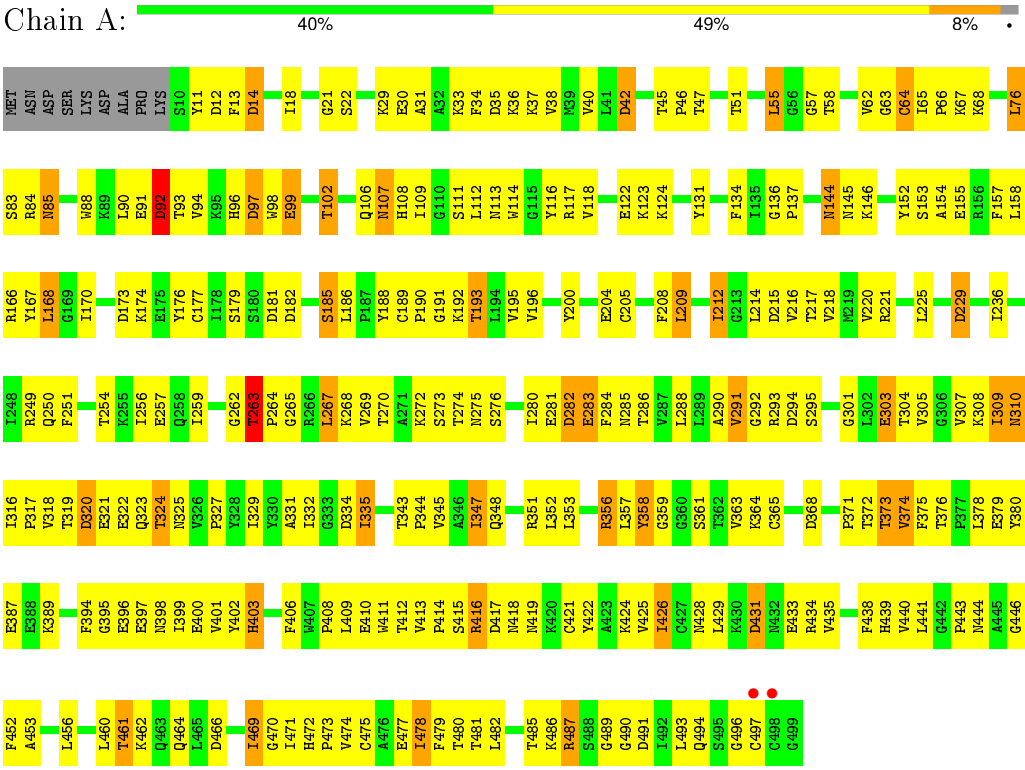
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	3	Total	O	0	0
			3	3		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		

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.

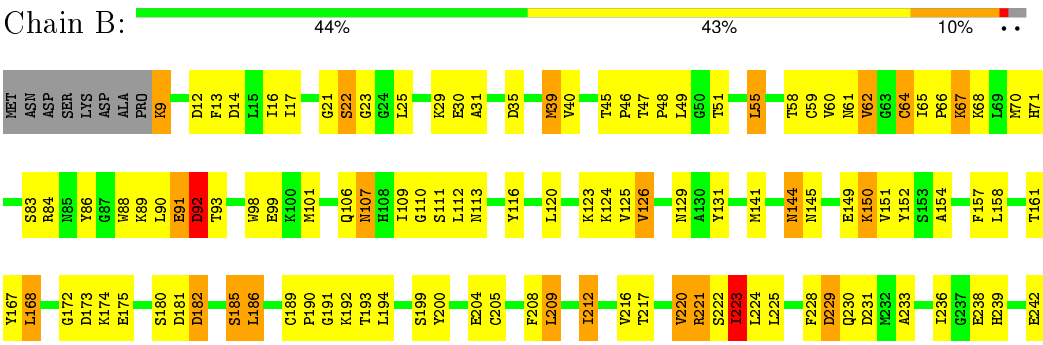
- Molecule 1: THIOREDOXIN REDUCTASE

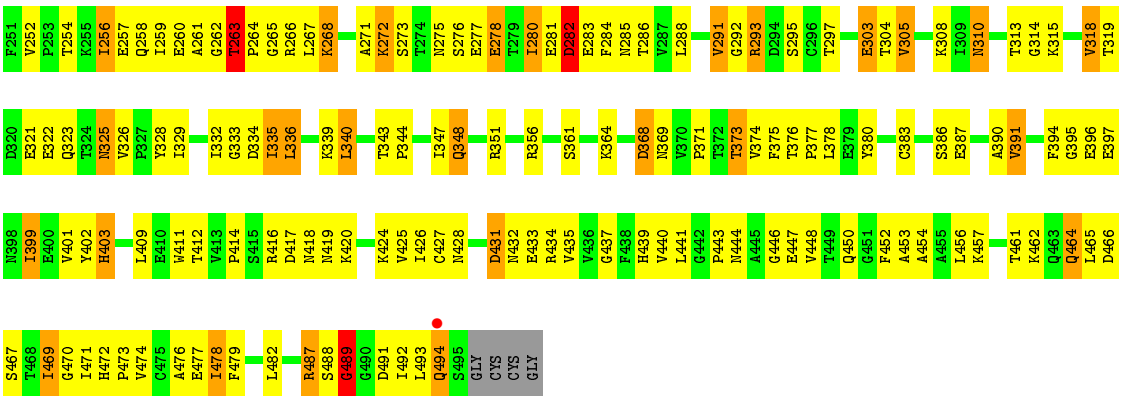
Chain A:



- Molecule 1: THIOREDOXIN REDUCTASE

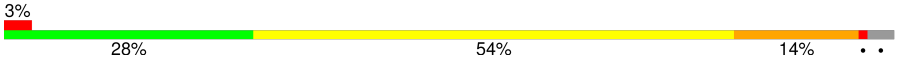
Chain B:

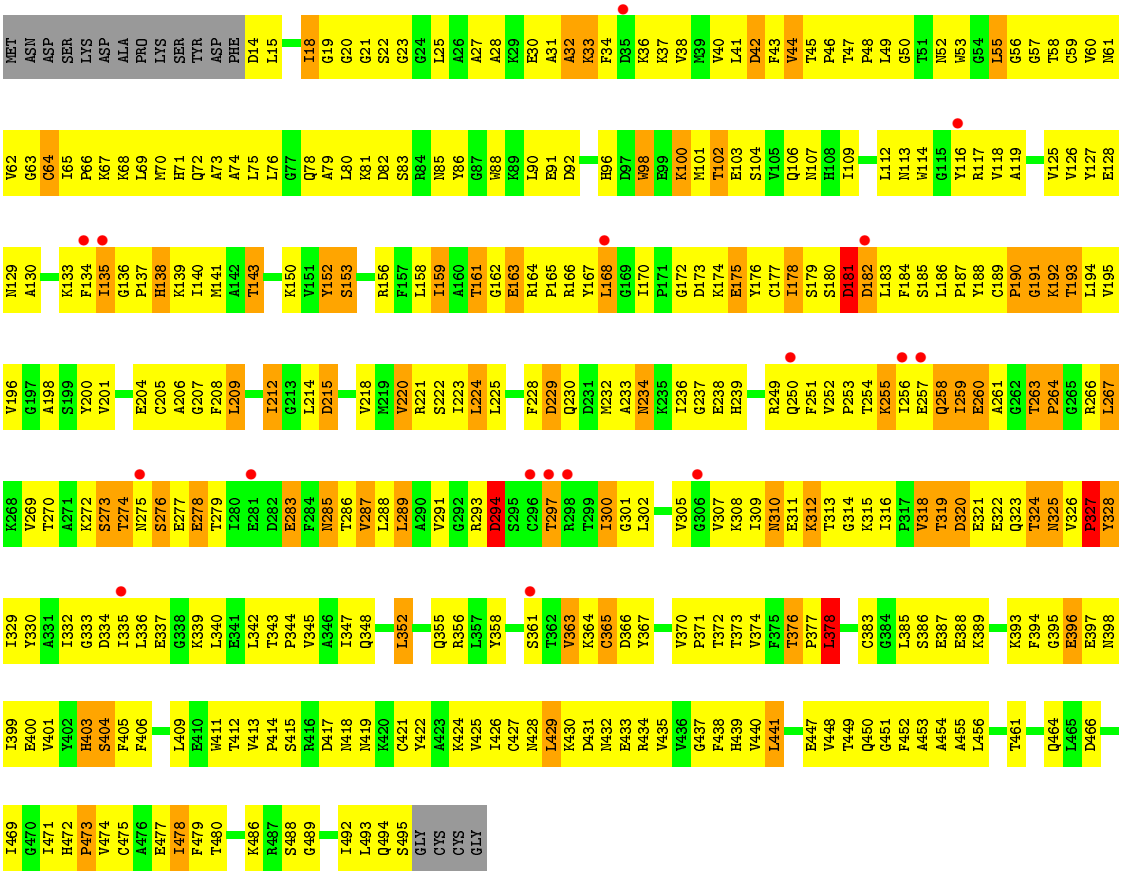




• Molecule 1: THIOREDOXIN REDUCTASE

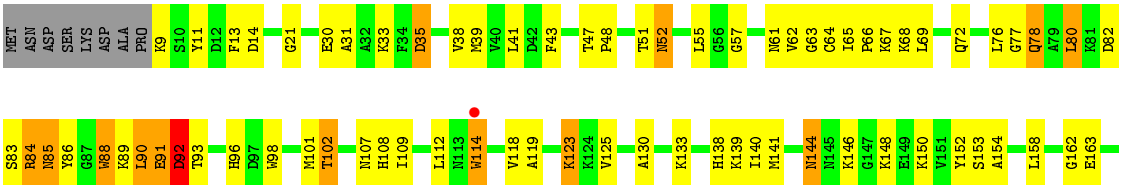
Chain C:

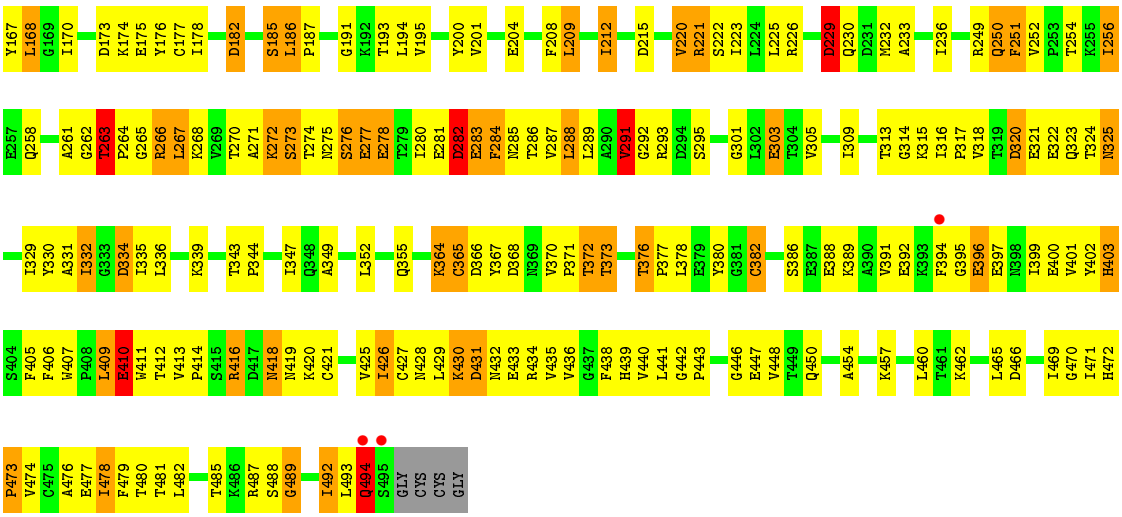




• Molecule 1: THIOREDOXIN REDUCTASE

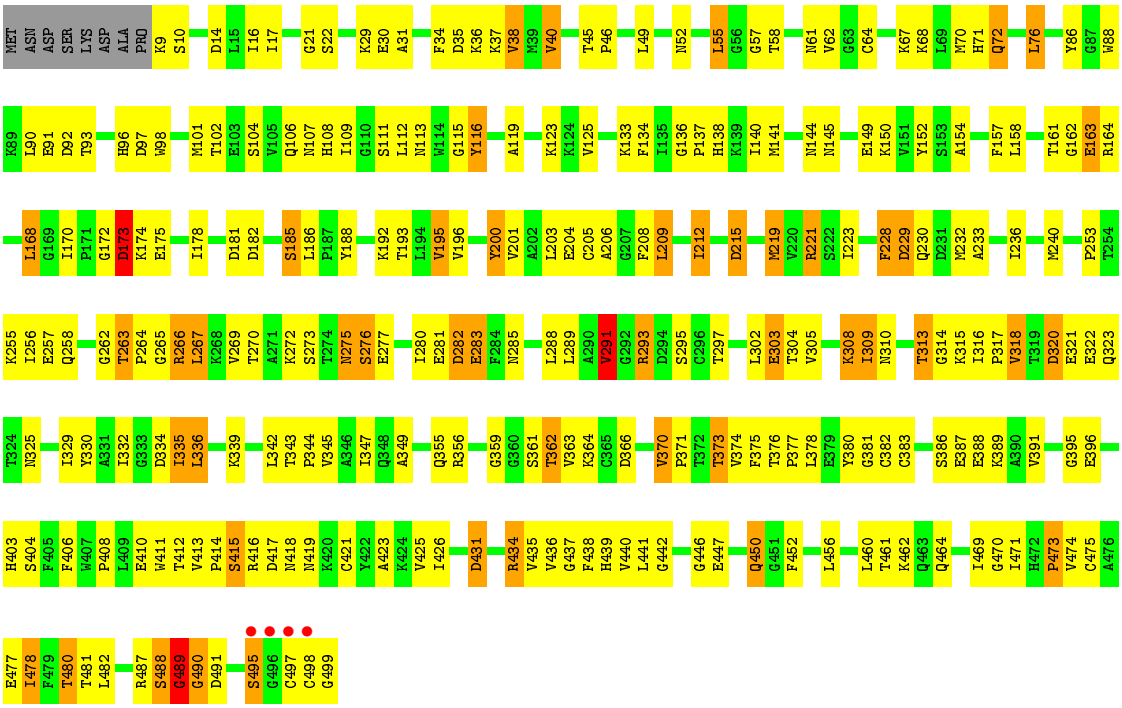
Chain D:





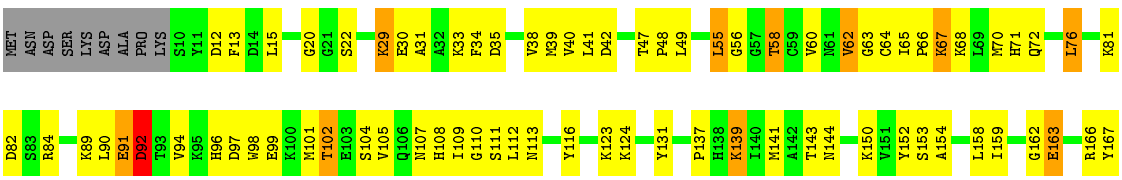
• Molecule 1: THIOREDOXIN REDUCTASE

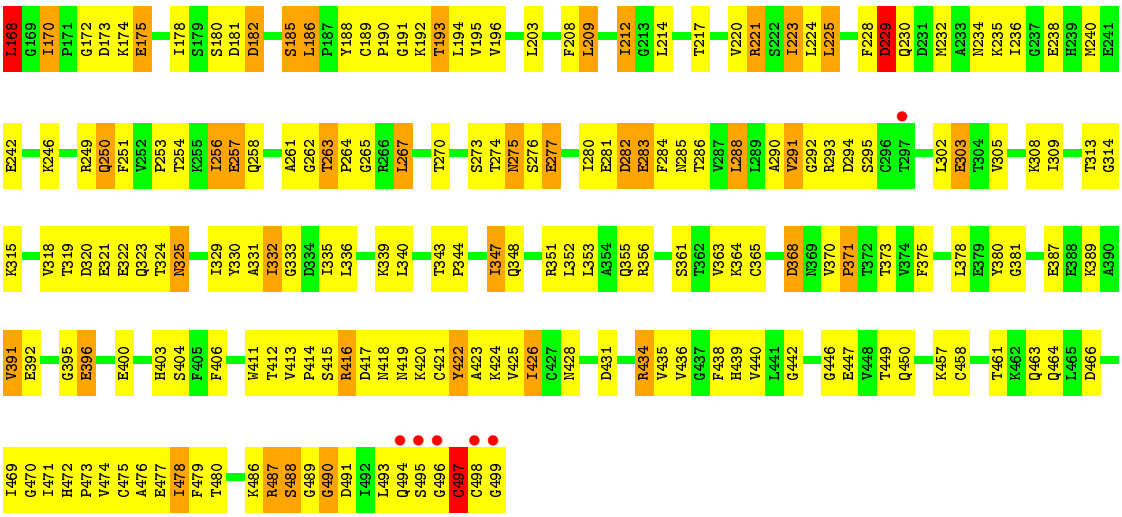
Chain E:



• Molecule 1: THIOREDOXIN REDUCTASE

Chain F:




L168 G169 I170 P171 G172 D173 K174 E175 I178 S179 S180 D181 D182 S185 L186 P187 Y188 C189 P190 G191 K192 T193 L194 Y195 V196 L203 F208 L209 I212 G213 L214 T217 V220 R221 S222 I223 L224 L225 F228 D229 Q230 D231 M232 A233 N234 K235 I236 G237 E238 H239 M240 E241
E242 K246 R249 Q250 F251 V252 P253 T254 K255 I256 E257 Q258 A261 G262 T263 P264 G265 R266 L267 T270 S273 T274 N275 S276 E277 I280 E281 D282 E283 F284 N285 T286 V287 L288 L289 A290 V291 G292 R293 D294 S295 C296 T297 L302 E303 T304 V305 K308 I309 T313 G314
K315 V318 T319 D320 E321 E322 Q323 T324 N325 I329 Y330 A331 I332 G333 D334 I335 L336 K339 L340 T343 P344 I347 Q348 R351 L352 L353 A354 Q355 R356 S361 T362 V363 K364 C365 D368 N369 V370 P371 T372 T373 V374 F375 L378 E379 Y380 G381 E387 E388 K389 A390
V391 E392 G395 E396 E400 H403 S404 F405 F406 W411 T412 V413 P414 S415 R416 D417 N418 N419 K420 C421 Y422 A423 K424 V425 I426 G427 N428 D431 R434 V435 V436 G437 F438 H439 V440 L441 G442 G446 E447 V448 T449 Q450 K457 C458 T461 K462 Q463 Q464 L465 D466
I469 G470 I471 H472 P473 V474 C475 A476 E477 I478 F479 T480 K486 R487 S488 G489 G490 D491 I492 L493 Q494 S495 G496 C497 C498 G499

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.92Å 140.46Å 170.83Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.00) 92.5 (29.86-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.263 0.263 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 4.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 69328 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23075	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FAD

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	0.92	0/3838	1.07	15/5193 (0.3%)
1	B	0.90	0/3827	1.04	14/5178 (0.3%)
1	C	0.82	1/3779 (0.0%)	1.03	15/5114 (0.3%)
1	D	0.97	3/3827 (0.1%)	1.08	16/5178 (0.3%)
1	E	0.99	2/3847 (0.1%)	1.11	16/5204 (0.3%)
1	F	0.80	0/3838	1.03	14/5193 (0.3%)
All	All	0.90	6/22956 (0.0%)	1.06	90/31060 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	489	GLY	C-O	-6.05	1.14	1.23
1	D	410	GLU	CD-OE1	5.80	1.32	1.25
1	D	114	TRP	CB-CG	-5.08	1.41	1.50
1	C	300	ILE	C-O	-5.07	1.13	1.23
1	D	88	TRP	CB-CG	-5.03	1.41	1.50

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	ASP	CB-CG-OD2	9.47	126.82	118.30
1	F	229	ASP	CB-CG-OD2	9.21	126.59	118.30
1	F	417	ASP	CB-CG-OD2	8.16	125.65	118.30
1	E	282	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	466	ASP	CB-CG-OD2	7.83	125.35	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3764	0	3764	309	0
1	B	3753	0	3763	287	0
1	C	3707	0	3721	463	0
1	D	3753	0	3761	294	0
1	E	3773	0	3777	257	0
1	F	3764	0	3764	300	0
2	A	53	0	31	5	0
2	B	53	0	31	10	0
2	C	53	0	31	17	0
2	D	53	0	31	4	0
2	E	53	0	31	3	0
2	F	53	0	31	5	0
3	A	39	0	18	2	0
3	B	39	0	18	8	0
3	C	39	0	18	6	0
3	D	39	0	18	6	0
3	E	39	0	18	1	0
3	F	39	0	18	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	2	0
4	D	1	0	0	0	0
4	E	2	0	0	1	0
4	F	1	0	0	0	0
All	All	23075	0	22844	1832	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 40.

The worst 5 of 1832 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:C:98:TRP:NE1	1:C:190:PRO:HD2	1.54	1.21
1:C:98:TRP:CD1	1:C:189:CYS:HA	1.76	1.20
1:D:477:GLU:O	1:D:480:THR:HG22	1.49	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:HD13	1:C:441:LEU:HD11	1.13	1.12
1:C:98:TRP:CZ3	1:C:102:THR:HG23	1.85	1.12

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	488/499 (98%)	445 (91%)	36 (7%)	7 (1%)	14 51
1	B	485/499 (97%)	436 (90%)	40 (8%)	9 (2%)	10 43
1	C	480/499 (96%)	395 (82%)	70 (15%)	15 (3%)	5 28
1	D	485/499 (97%)	439 (90%)	37 (8%)	9 (2%)	10 43
1	E	489/499 (98%)	441 (90%)	39 (8%)	9 (2%)	11 45
1	F	488/499 (98%)	438 (90%)	40 (8%)	10 (2%)	9 41
All	All	2915/2994 (97%)	2594 (89%)	262 (9%)	59 (2%)	9 41

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	THR
1	A	489	GLY
1	B	92	ASP
1	B	263	THR
1	B	314	GLY

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/414 (98%)	352 (87%)	54 (13%)	5	21
1	B	405/414 (98%)	344 (85%)	61 (15%)	3	17
1	C	400/414 (97%)	325 (81%)	75 (19%)	2	10
1	D	405/414 (98%)	342 (84%)	63 (16%)	3	16
1	E	407/414 (98%)	354 (87%)	53 (13%)	5	22
1	F	406/414 (98%)	349 (86%)	57 (14%)	4	19
All	All	2429/2484 (98%)	2066 (85%)	363 (15%)	4	17

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	310	ASN
1	D	168	LEU
1	F	250	GLN
1	C	325	ASN
1	C	404	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	418	ASN
1	D	108	HIS
1	F	250	GLN
1	C	444	ASN
1	D	61	ASN

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)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	600	-	48,58,58	1.38	6 (12%)	54,89,89	2.42	12 (22%)
3	NDP	A	601	-	35,42,52	1.62	5 (14%)	46,65,80	1.94	12 (26%)
2	FAD	B	600	-	48,58,58	1.37	7 (14%)	54,89,89	2.30	12 (22%)
3	NDP	B	601	-	35,42,52	1.84	8 (22%)	46,65,80	1.72	11 (23%)
2	FAD	C	600	-	48,58,58	1.34	7 (14%)	54,89,89	2.47	12 (22%)
3	NDP	C	601	-	35,42,52	1.65	7 (20%)	46,65,80	1.97	10 (21%)
2	FAD	D	600	-	48,58,58	1.54	8 (16%)	54,89,89	2.29	8 (14%)
3	NDP	D	601	-	35,42,52	1.58	5 (14%)	46,65,80	1.95	7 (15%)
2	FAD	E	600	-	48,58,58	1.42	5 (10%)	54,89,89	2.43	16 (29%)
3	NDP	E	601	-	35,42,52	1.60	5 (14%)	46,65,80	1.74	7 (15%)
2	FAD	F	600	-	48,58,58	1.16	4 (8%)	54,89,89	2.38	10 (18%)
3	NDP	F	601	-	35,42,52	1.64	6 (17%)	46,65,80	1.94	12 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	NDP	A	601	-	-	0/23/56/77	0/4/4/5
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	NDP	B	601	-	-	0/23/56/77	0/4/4/5
2	FAD	C	600	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	C	601	-	-	0/23/56/77	0/4/4/5
2	FAD	D	600	-	-	0/30/50/50	0/6/6/6
3	NDP	D	601	-	-	0/23/56/77	0/4/4/5
2	FAD	E	600	-	-	0/30/50/50	0/6/6/6
3	NDP	E	601	-	-	0/23/56/77	0/4/4/5
2	FAD	F	600	-	-	0/30/50/50	0/6/6/6
3	NDP	F	601	-	-	0/23/56/77	0/4/4/5

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C10-N10	-3.35	1.35	1.39
2	B	600	FAD	C4X-C10	-2.73	1.35	1.41
2	A	600	FAD	C9A-C5X	-2.45	1.37	1.42
2	A	600	FAD	C10-N10	-2.37	1.36	1.39
2	D	600	FAD	C9A-C5X	-2.17	1.38	1.42

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	FAD	N3A-C2A-N1A	-12.04	119.68	128.89
2	C	600	FAD	N3A-C2A-N1A	-11.79	119.87	128.89
2	F	600	FAD	N3A-C2A-N1A	-11.63	119.99	128.89
2	D	600	FAD	N3A-C2A-N1A	-11.20	120.32	128.89
2	A	600	FAD	N3A-C2A-N1A	-10.55	120.81	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	5	0
3	A	601	NDP	2	0
2	B	600	FAD	10	0
3	B	601	NDP	8	0
2	C	600	FAD	17	0
3	C	601	NDP	6	0
2	D	600	FAD	4	0
3	D	601	NDP	6	0
2	E	600	FAD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	NDP	1	0
2	F	600	FAD	5	0
3	F	601	NDP	4	0

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, 95^{th} 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	490/499 (98%)	-0.37	2 (0%) 93 80	7, 13, 20, 49	0
1	B	487/499 (97%)	-0.47	1 (0%) 95 87	6, 13, 20, 39	0
1	C	482/499 (96%)	0.14	17 (3%) 48 21	6, 13, 19, 44	0
1	D	487/499 (97%)	-0.31	4 (0%) 87 67	6, 12, 19, 38	0
1	E	491/499 (98%)	-0.37	4 (0%) 87 67	7, 13, 20, 48	0
1	F	490/499 (98%)	-0.22	6 (1%) 81 55	6, 13, 20, 48	0
All	All	2927/2994 (97%)	-0.27	34 (1%) 81 55	6, 13, 20, 49	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	497	CYS	7.1
1	E	495	SER	5.8
1	C	297	THR	5.3
1	F	495	SER	5.2
1	A	498	CYS	3.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FAD	D	600	53/53	0.95	0.29	2.70	20,29,40,47	0
2	FAD	E	600	53/53	0.94	0.28	1.61	10,17,54,56	0
3	NDP	F	601	39/48	0.78	0.29	1.50	72,95,112,112	0
2	FAD	B	600	53/53	0.95	0.25	1.45	18,26,42,46	0
2	FAD	F	600	53/53	0.92	0.26	1.40	27,33,53,55	0
2	FAD	A	600	53/53	0.94	0.22	0.91	14,24,36,36	0
3	NDP	B	601	39/48	0.89	0.21	0.73	31,50,69,71	0
2	FAD	C	600	53/53	0.86	0.28	0.37	34,45,49,51	0
3	NDP	D	601	39/48	0.85	0.20	0.05	44,55,77,77	0
3	NDP	E	601	39/48	0.91	0.21	-0.01	45,52,76,79	0
3	NDP	A	601	39/48	0.86	0.21	-0.08	41,49,78,78	0
3	NDP	C	601	39/48	0.77	0.26	-0.34	82,92,100,101	0

6.5 Other polymers

There are no such residues in this entry.