



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:49 PM GMT

PDB ID : 2ZZB  
Title : Crystal structure of human thioredoxin reductase I and terpyridine platinum(II)  
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.  
Deposited on : 2009-02-09  
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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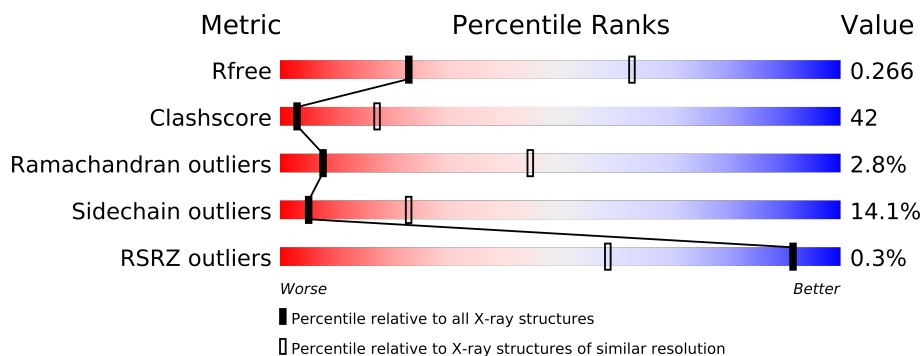
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	
1	D	513	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15394 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Thioredoxin reductase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	B	485	Total	C	N	O	S	0	0	0
			3750	2385	640	706	19			
1	C	493	Total	C	N	O	S	0	0	0
			3800	2414	649	716	21			
1	D	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q16881
A	-12	ALA	-	EXPRESSION TAG	UNP Q16881
A	-11	HIS	-	EXPRESSION TAG	UNP Q16881
A	-10	HIS	-	EXPRESSION TAG	UNP Q16881
A	-9	HIS	-	EXPRESSION TAG	UNP Q16881
A	-8	HIS	-	EXPRESSION TAG	UNP Q16881
A	-7	HIS	-	EXPRESSION TAG	UNP Q16881
A	-6	HIS	-	EXPRESSION TAG	UNP Q16881
A	-5	VAL	-	EXPRESSION TAG	UNP Q16881
A	-4	ASP	-	EXPRESSION TAG	UNP Q16881
A	-3	ASP	-	EXPRESSION TAG	UNP Q16881
A	-2	ASP	-	EXPRESSION TAG	UNP Q16881
A	-1	ASP	-	EXPRESSION TAG	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-13	MET	-	EXPRESSION TAG	UNP Q16881
B	-12	ALA	-	EXPRESSION TAG	UNP Q16881
B	-11	HIS	-	EXPRESSION TAG	UNP Q16881
B	-10	HIS	-	EXPRESSION TAG	UNP Q16881
B	-9	HIS	-	EXPRESSION TAG	UNP Q16881
B	-8	HIS	-	EXPRESSION TAG	UNP Q16881
B	-7	HIS	-	EXPRESSION TAG	UNP Q16881

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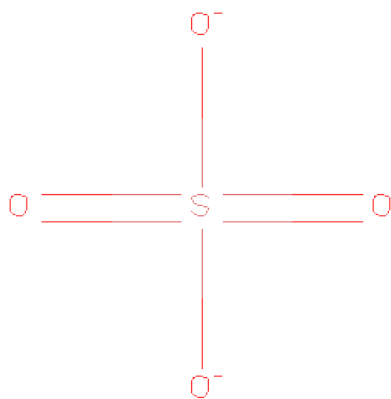
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	ASP	-	EXPRESSION TAG	UNP Q16881
B	-3	ASP	-	EXPRESSION TAG	UNP Q16881
B	-2	ASP	-	EXPRESSION TAG	UNP Q16881
B	-1	ASP	-	EXPRESSION TAG	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881
C	-13	MET	-	EXPRESSION TAG	UNP Q16881
C	-12	ALA	-	EXPRESSION TAG	UNP Q16881
C	-11	HIS	-	EXPRESSION TAG	UNP Q16881
C	-10	HIS	-	EXPRESSION TAG	UNP Q16881
C	-9	HIS	-	EXPRESSION TAG	UNP Q16881
C	-8	HIS	-	EXPRESSION TAG	UNP Q16881
C	-7	HIS	-	EXPRESSION TAG	UNP Q16881
C	-6	HIS	-	EXPRESSION TAG	UNP Q16881
C	-5	VAL	-	EXPRESSION TAG	UNP Q16881
C	-4	ASP	-	EXPRESSION TAG	UNP Q16881
C	-3	ASP	-	EXPRESSION TAG	UNP Q16881
C	-2	ASP	-	EXPRESSION TAG	UNP Q16881
C	-1	ASP	-	EXPRESSION TAG	UNP Q16881
C	498	CYS	U	SEE REMARK 999	UNP Q16881
D	-13	MET	-	EXPRESSION TAG	UNP Q16881
D	-12	ALA	-	EXPRESSION TAG	UNP Q16881
D	-11	HIS	-	EXPRESSION TAG	UNP Q16881
D	-10	HIS	-	EXPRESSION TAG	UNP Q16881
D	-9	HIS	-	EXPRESSION TAG	UNP Q16881
D	-8	HIS	-	EXPRESSION TAG	UNP Q16881
D	-7	HIS	-	EXPRESSION TAG	UNP Q16881
D	-6	HIS	-	EXPRESSION TAG	UNP Q16881
D	-5	VAL	-	EXPRESSION TAG	UNP Q16881
D	-4	ASP	-	EXPRESSION TAG	UNP Q16881
D	-3	ASP	-	EXPRESSION TAG	UNP Q16881
D	-2	ASP	-	EXPRESSION TAG	UNP Q16881
D	-1	ASP	-	EXPRESSION TAG	UNP Q16881
D	498	CYS	U	SEE REMARK 999	UNP Q16881

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



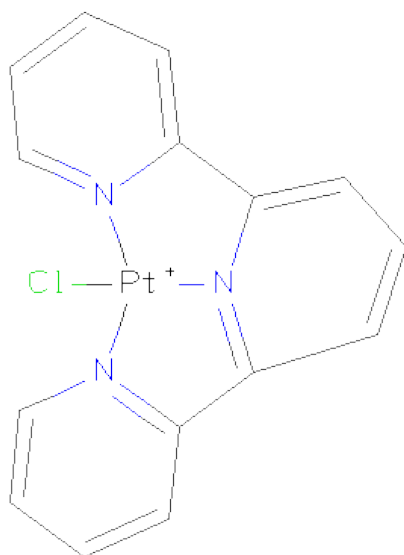
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is 2,2':6',2''-TERPYRIDINEPLATINUM(II) (three-letter code: TPT) (formula:  $C_{15}H_{11}ClN_3Pt$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N Pt 19 15 3 1	0	0
4	D	1	Total C N Pt 19 15 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0
5	B	17	Total O 17 17	0	0
5	C	13	Total O 13 13	0	0

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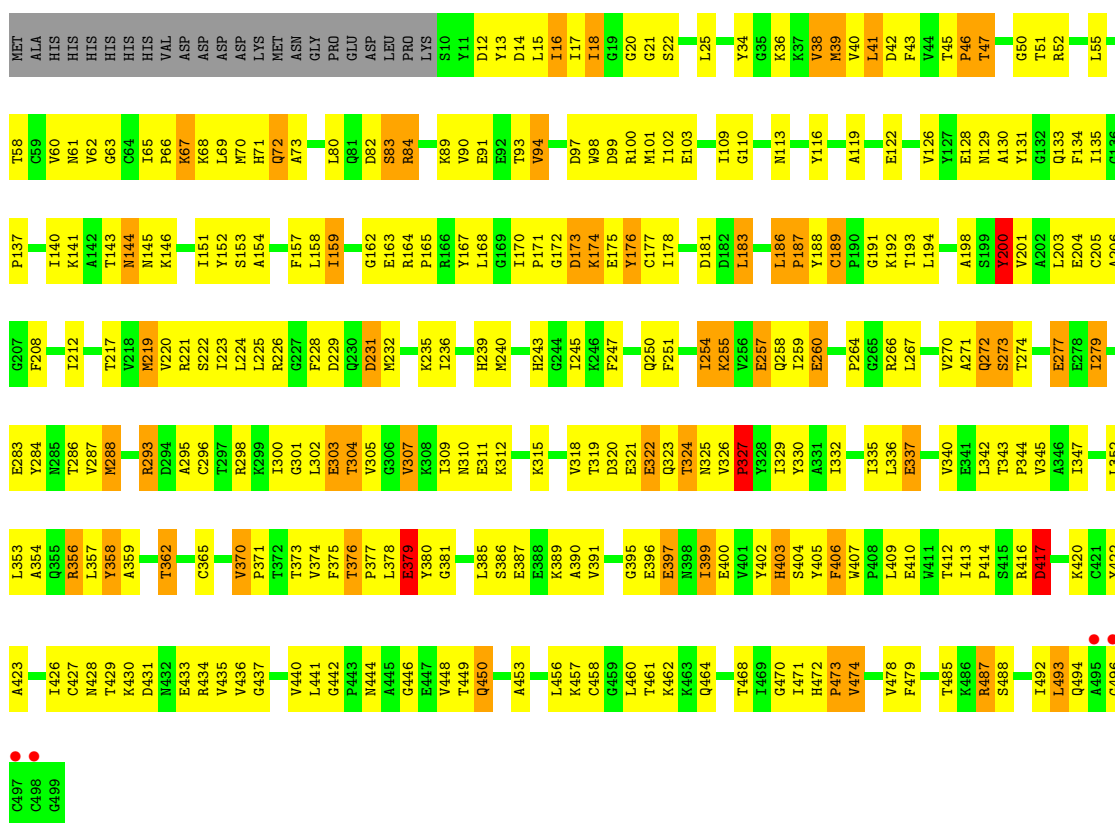
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

### 3 Residue-property plots

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

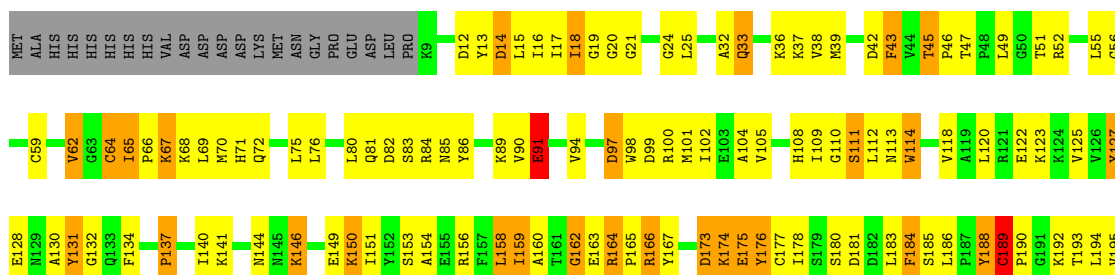
- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain A: 

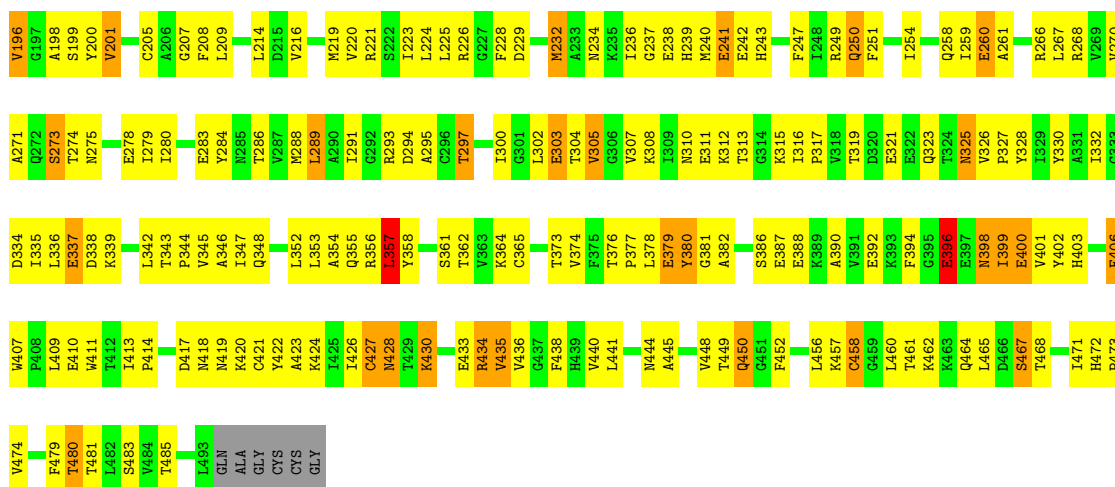


- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain B: 

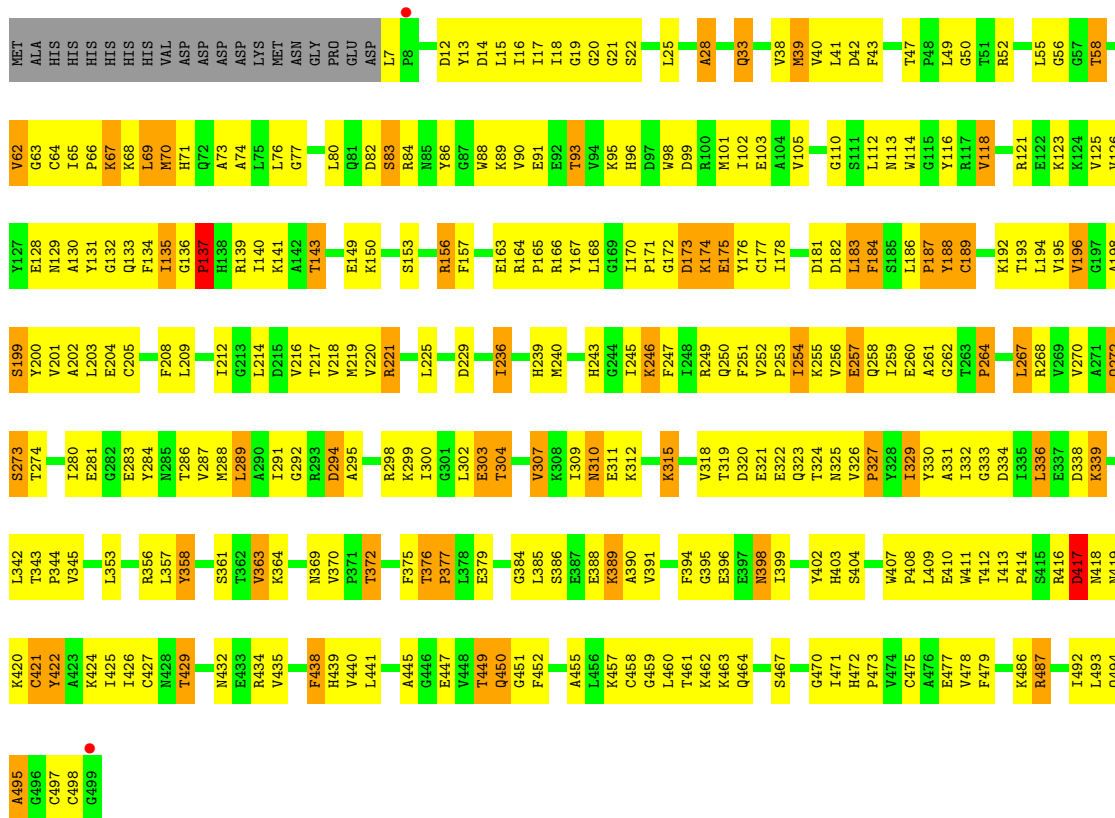






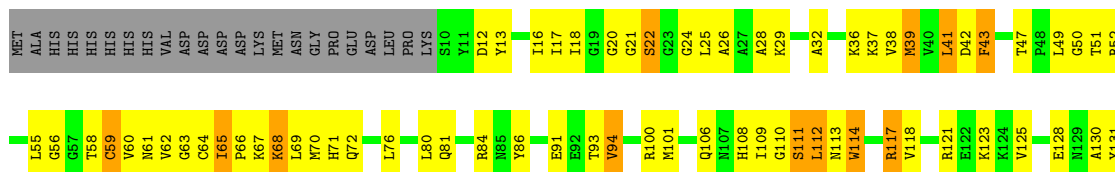
• Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain C:



• Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain D:



I492	A423	P344	R268	V195	G132
L493	K424	I347	V269		Q133
GLN		Q348	V270	A198	F134
ALA	C427		A271	S199	I135
GLY	N428	R351	Q272	Y200	G136
CYS	T429	L352	S273	V201	P137
CYS	K430	L353	T274	A202	H138
GLY		L354		L203	R139
	R434	A354	E277	E204	I140
		Q355	E278	C205	K141
F438		R356	I279	A206	A142
H439	F438	L357	I280	G207	T143
V440	H439	Y358		F208	N144
L441	L441		E283	L209	N145
G442	G442	K364	Y284		K146
N444	N444	C365	N285	I212	G147
		D366	T286	G213	K148
		Y367	V287	L214	E149
E447	E447	F368		D215	K150
V448	V448	N369	D294	V216	I151
T449	T449	V374	A295	T217	Y152
Q450	Q450	F375	C296	M218	S153
G451	G451	T376	T297	M219	A154
F452	F452	P377	R298	V220	E155
A453	A453	L378		R221	R156
A454	A454		E303		F157
A455	A455	G384	T304	L224	
L456	L456	L385	V305	L225	T161
K457	K457	S386	G306	F228	G162
C458	C458	E387	V307	D229	E163
G459	G459	A390	K308	Q230	R164
L460	L460		T309	D231	P165
T461	T461	F394	N310	M232	R166
K462	K462	G395	I316	A233	Y167
K463	K463	E396	P317	N234	G169
Q464	Q464	E397	V318	K235	I170
L465	L465	N398	T319		P171
D466	D466		D320	E238	G172
		V401	E321	H239	D173
I469	I469	H403	E322	M240	K174
G470	G470	S404	T324	I245	E175
H472	H472	Y405	N325		Y176
P473	P473	P406	V326	Q250	G177
V474	V474	W407	P327	P251	I178
C475	C475	P408	Y328	V252	
A476	A476	L409	I329	P253	D181
E477	E477	E410	Y330	I254	D182
V478	V478	W411	A331	K255	L183
F479	F479	W412	I332		F184
T480	T480	I413	G333	Q258	S185
L482	L482	D417	D334	I259	L186
S483	S483	N418	I335	E260	P187
		N419	L336	A261	Y188
K486	K486	K420			C189
R487	R487	C421	V340	P264	P190
S488	S488	Y422	E341	G265	G191
G489	G489		L342	R266	K192
			T343	L267	T193
					L194

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.95Å 135.16Å 346.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.93 – 3.21	Depositor EDS
% Data completeness (in resolution range)	95.3 (30.00-3.20) 95.5 (29.93-3.21)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.242 , 0.305 0.219 , 0.266	Depositor DCC
$R_{free}$ test set	2246 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 13.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 44790 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPT, SO4, 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	0.96	7/3850 (0.2%)	0.99	5/5211 (0.1%)
1	B	0.98	7/3824 (0.2%)	0.99	7/5177 (0.1%)
1	C	0.87	3/3875 (0.1%)	0.97	4/5245 (0.1%)
1	D	0.91	4/3815 (0.1%)	0.96	3/5166 (0.1%)
All	All	0.93	21/15364 (0.1%)	0.98	19/20799 (0.1%)

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	4
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	10

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	CYS	CB-SG	13.15	2.04	1.82
1	C	189	CYS	CB-SG	10.57	2.00	1.82
1	C	421	CYS	CB-SG	-7.38	1.69	1.82
1	A	277	GLU	CG-CD	7.03	1.62	1.51
1	A	277	GLU	CB-CG	6.12	1.63	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	458	CYS	CA-CB-SG	10.36	132.66	114.00
1	A	189	CYS	CA-CB-SG	9.46	131.03	114.00
1	A	458	CYS	CA-CB-SG	8.79	129.82	114.00
1	C	189	CYS	CA-CB-SG	8.15	128.67	114.00
1	B	458	CYS	CA-CB-SG	8.00	128.41	114.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	176	TYR	Sidechain
1	A	200	TYR	Sidechain
1	A	406	PHE	Sidechain
1	B	43	PHE	Sidechain

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3776	0	3779	326	0
1	B	3750	0	3763	324	0
1	C	3800	0	3809	361	2
1	D	3741	0	3750	338	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
2	C	53	0	31	4	0
2	D	53	0	31	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	B	19	0	11	0	0
4	D	19	0	11	3	0
5	A	19	0	0	0	0
5	B	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	13	0	0	1	0
5	D	8	0	0	0	0
All	All	15394	0	15247	1282	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 42.

The worst 5 of 1282 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:CYS:CB	1:A:189:CYS:SG	2.04	1.42
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.11	1.16
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.29	1.14
1:C:498:CYS:HB3	4:D:501:TPT:H15	1.27	1.12
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.33	1.11

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	Distance(Å)	Clash(Å)
1:C:497:CYS:O	1:C:497:CYS:O[3_554]	1.59	0.61
1:C:498:CYS:SG	1:C:498:CYS:SG[3_554]	1.70	0.50

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/513 (95%)	418 (86%)	57 (12%)	13 (3%)	8	46
1	B	483/513 (94%)	409 (85%)	64 (13%)	10 (2%)	11	55
1	C	491/513 (96%)	404 (82%)	67 (14%)	20 (4%)	4	32
1	D	482/513 (94%)	407 (84%)	63 (13%)	12 (2%)	9	49
All	All	1944/2052 (95%)	1638 (84%)	251 (13%)	55 (3%)	8	44

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	A	174	LYS
1	A	379	GLU
1	B	184	PHE
1	C	173	ASP

### 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	401/422 (95%)	341 (85%)	60 (15%)	4	19
1	B	399/422 (94%)	343 (86%)	56 (14%)	5	23
1	C	404/422 (96%)	343 (85%)	61 (15%)	4	19
1	D	398/422 (94%)	349 (88%)	49 (12%)	7	31
All	All	1602/1688 (95%)	1376 (86%)	226 (14%)	5	23

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	365	CYS
1	C	69	LEU
1	D	310	ASN
1	B	398	ASN
1	B	480	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	428	ASN
1	C	33	GLN
1	D	133	GLN
1	B	432	ASN
1	B	464	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	500	-	58,58,58	1.45	9 (15%)	85,89,89	2.12	14 (16%)
3	SO4	A	502	-	4,4,4	0.38	0	6,6,6	0.32	0
2	FAD	B	500	-	58,58,58	1.54	8 (13%)	85,89,89	2.15	15 (17%)
4	TPT	B	501	-	20,23,24	0.72	0	26,35,38	1.30	4 (15%)
3	SO4	B	502	-	4,4,4	0.34	0	6,6,6	0.17	0
2	FAD	C	500	-	58,58,58	1.67	8 (13%)	85,89,89	2.17	16 (18%)
3	SO4	C	502	-	4,4,4	0.30	0	6,6,6	0.23	0
2	FAD	D	500	-	58,58,58	1.65	9 (15%)	85,89,89	2.04	15 (17%)
4	TPT	D	501	-	20,23,24	0.71	0	26,35,38	1.27	4 (15%)
3	SO4	D	502	-	4,4,4	0.21	0	6,6,6	0.25	0

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	500	-	-	0/34/50/50	0/1/6/6
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	FAD	B	500	-	-	0/34/50/50	0/1/6/6
4	TPT	B	501	-	-	0/0/20/26	0/0/5/5
3	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	FAD	C	500	-	-	0/34/50/50	0/1/6/6
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	FAD	D	500	-	-	0/34/50/50	0/1/6/6
4	TPT	D	501	-	-	0/0/20/26	0/0/5/5
3	SO4	D	502	-	-	0/0/0/0	0/0/0/0

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	FAD	C4X-C10	5.82	1.51	1.40
2	B	500	FAD	C4-C4X	5.54	1.50	1.41
2	A	500	FAD	C4X-C10	5.03	1.49	1.40
2	D	500	FAD	C4X-C10	5.00	1.49	1.40
2	D	500	FAD	C9A-N10	4.70	1.45	1.38

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	FAD	N3A-C2A-N1A	-9.77	120.54	128.71
2	A	500	FAD	N3A-C2A-N1A	-9.62	120.67	128.71
2	B	500	FAD	N3A-C2A-N1A	-9.22	121.00	128.71
2	D	500	FAD	N3A-C2A-N1A	-8.87	121.29	128.71
2	B	500	FAD	C2-N1-C10	7.09	122.12	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	490/513 (95%)	-0.28	4 (0%) 83 35	15, 50, 81, 128	0
1	B	485/513 (94%)	-0.32	0 100 100	18, 45, 76, 107	0
1	C	493/513 (96%)	-0.25	2 (0%) 90 51	21, 58, 85, 137	0
1	D	484/513 (94%)	-0.28	0 100 100	23, 53, 83, 104	0
All	All	1952/2052 (95%)	-0.28	6 (0%) 91 58	15, 51, 83, 137	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	CYS	4.2
1	C	499	GLY	3.1
1	A	496	GLY	3.1
1	A	498	CYS	2.8
1	C	8	PRO	2.3

### 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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TPT	B	501	19/20	0.26	1.95	29,36,38,39	19
2	FAD	A	500	53/53	0.21	0.91	42,56,69,70	0
2	FAD	C	500	53/53	0.20	0.52	43,58,61,62	0
2	FAD	D	500	53/53	0.18	0.35	33,41,57,58	0
2	FAD	B	500	53/53	0.17	0.29	24,32,44,45	0
4	TPT	D	501	19/20	0.23	-0.26	42,46,48,48	19
3	SO4	D	502	5/5	0.13	-1.18	71,73,74,75	0
3	SO4	C	502	5/5	0.10	-1.37	83,83,83,83	0
3	SO4	B	502	5/5	0.11	-1.54	81,81,82,82	0
3	SO4	A	502	5/5	0.15	-1.73	72,73,75,75	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.