



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:12 AM GMT

PDB ID : 2ZZ0
Title : Crystal structure of human thioredoxin reductase I (SeCys 498 Cys)
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2009-02-02
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

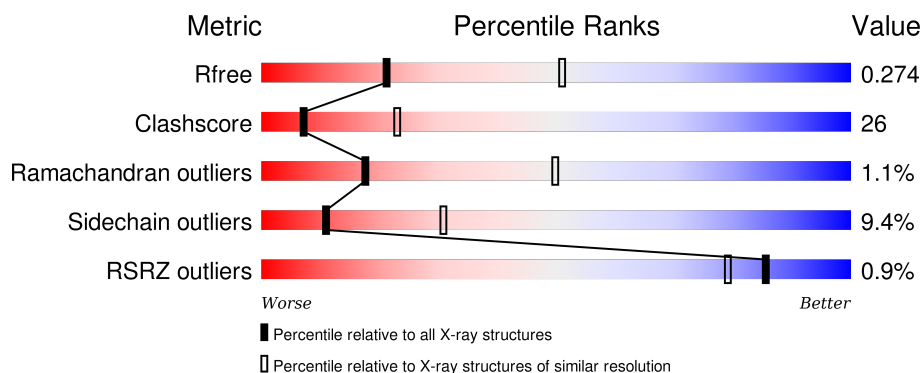
1 Overall quality at a glance ⓘ

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	513	<div> <div>51%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>
1	B	513	<div> <div>54%</div> <div>36%</div> <div>5%</div> <div>5%</div> </div>
1	C	513	<div> <div>51%</div> <div>39%</div> <div>5%</div> <div>5%</div> </div>
1	D	513	<div> <div>52%</div> <div>37%</div> <div>5%</div> <div>6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15818 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 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3785	2403	647	714	21			
1	B	487	Total	C	N	O	S	0	0	0
			3765	2396	642	708	19			
1	C	487	Total	C	N	O	S	0	0	0
			3765	2396	642	708	19			
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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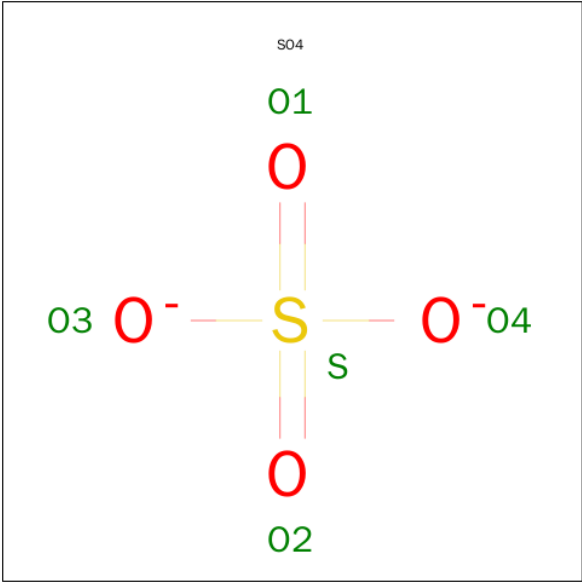
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	ASP	-	EXPRESSION TAG	UNP Q16881
B	-3	ASP	-	EXPRESSION TAG	UNP Q16881
B	-2	ASP	-	EXPRESSION TAG	UNP Q16881
B	-1	ASP	-	EXPRESSION TAG	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP 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: C₂₇H₃₃N₉O₁₅P₂).



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: O₄S).



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

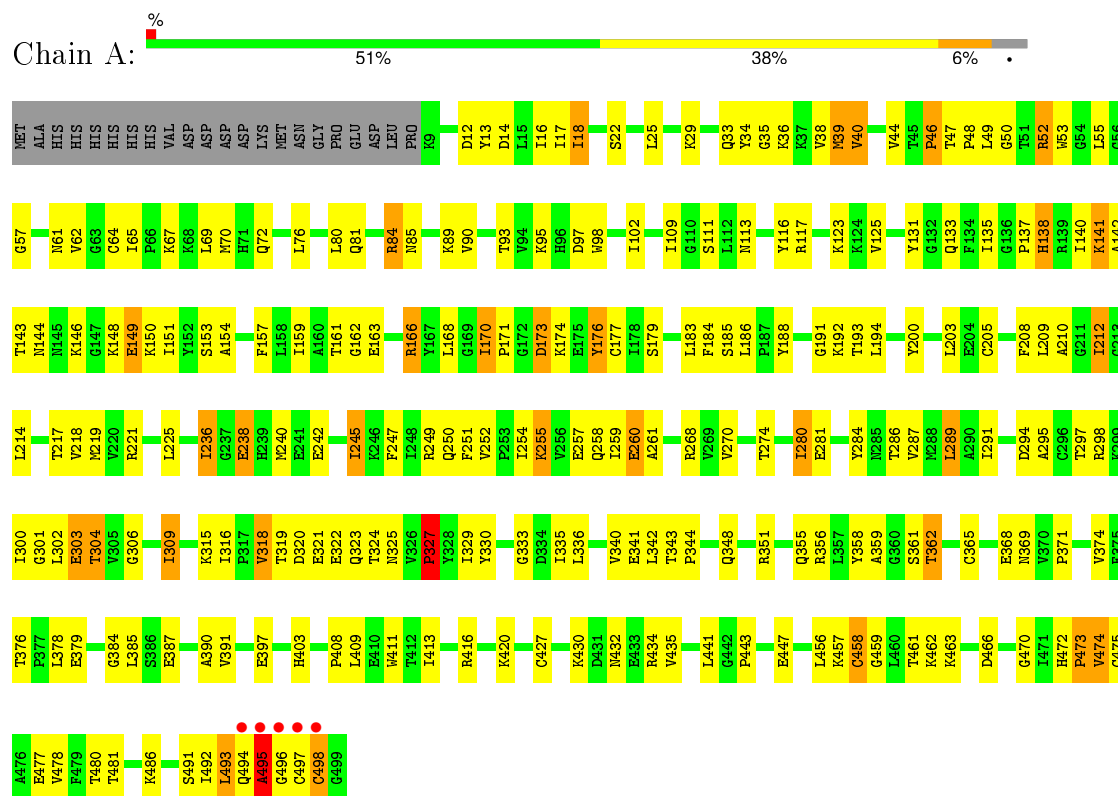
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	162	Total O 162 162	0	0
4	B	137	Total O 137 137	0	0
4	C	123	Total O 123 123	0	0
4	D	108	Total O 108 108	0	0

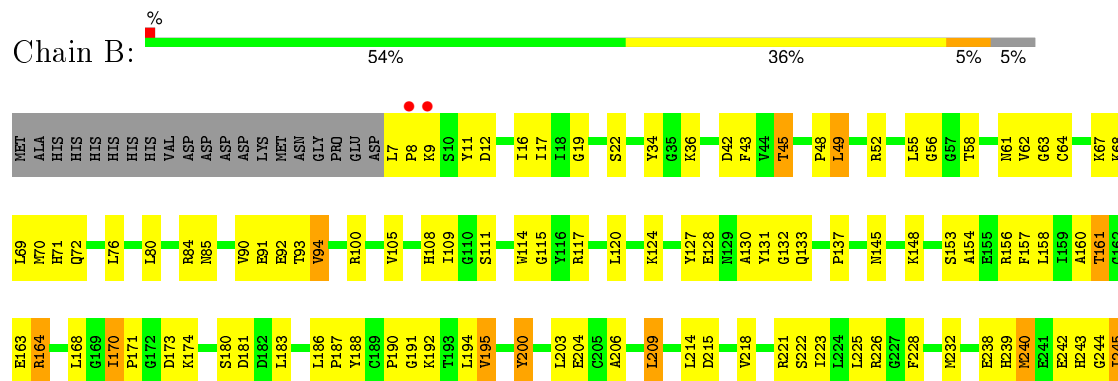
3 Residue-property plots

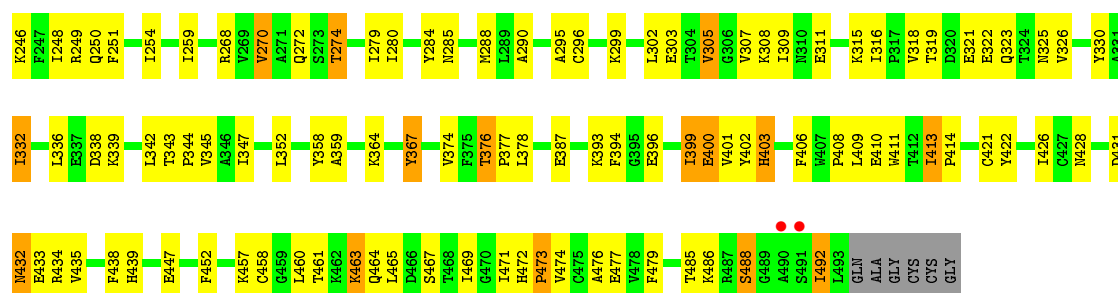
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

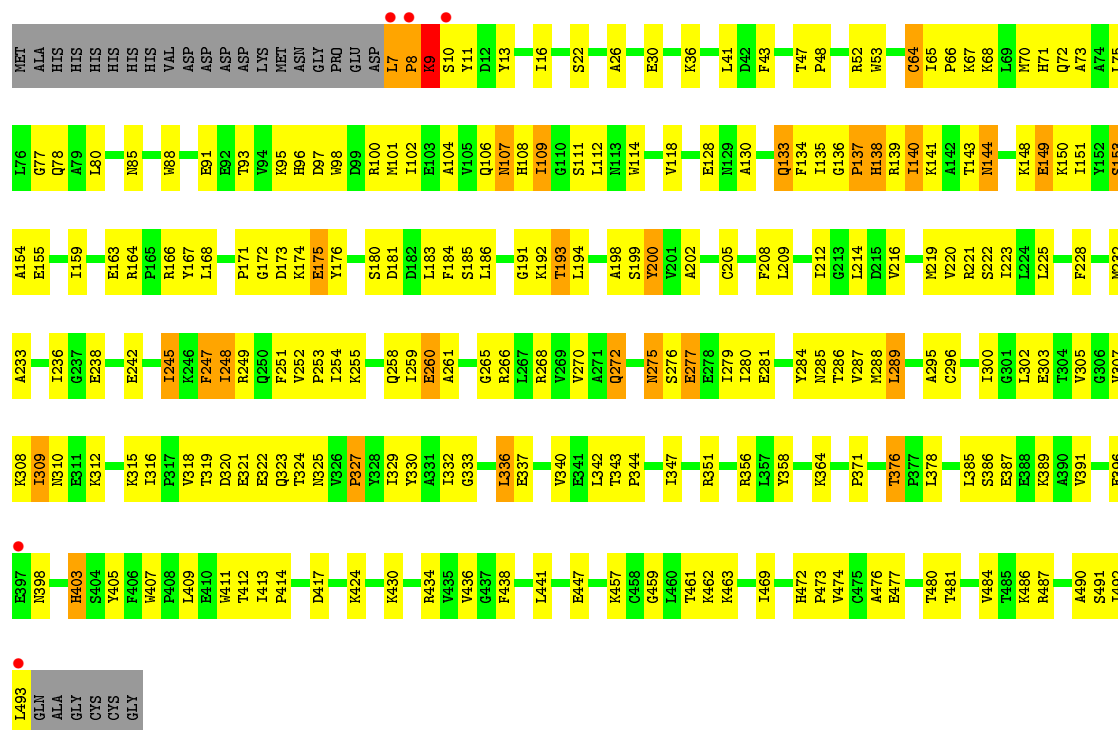


- Molecule 1: Thioredoxin reductase 1, cytoplasmic

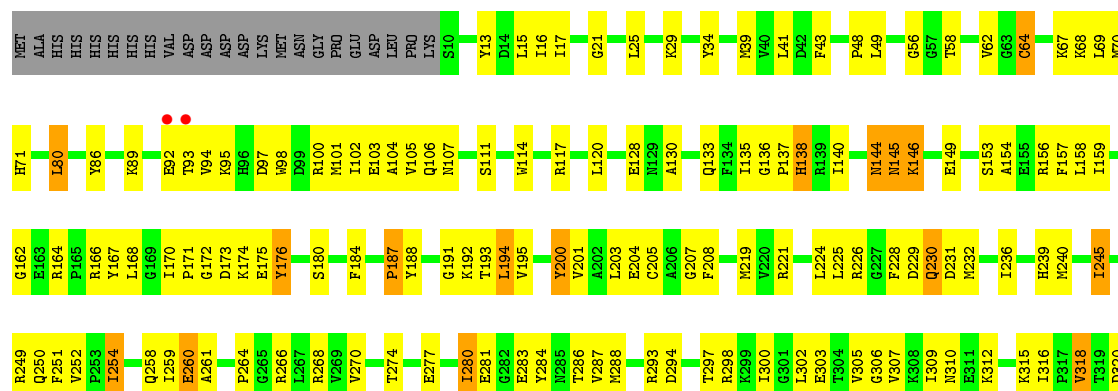




• Molecule 1: Thioredoxin reductase 1, cytoplasmic



• Molecule 1: Thioredoxin reductase 1, cytoplasmic



E321	E322	Q323	T324	N325	V326	E327	Y328	A331	I332	I335	L336	D338	K339	V340	T343	P344	V345	A359	E360	S361	D366	Y367	E368	T376	P377	L378	E379	Y380	C383	S386	E387	E388	E396	E397	N398	I399	E400	V401	Y402	H403	W407	P408	L409	E410	W411	T412	I413	P414
Y422	A423	K424	I425	I426	C427	M428	E433	R434	G446	E447	L456	K457	T461	K462	K463	Q464	L465	I471	E472	P473	V474	C475	A476	E477	W478	P479	T480	T481	L482	K486	R487	S488	G489	A490	S491	I492	L493	GLN	ALA	GLY	CYS	CYS	GLY					

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	121.09Å 135.41Å 345.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 90.9 (29.55-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.277 0.217 , 0.274	Depositor DCC
R_{free} test set	3229 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 64014 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15818	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.94	3/3859 (0.1%)	0.99	10/5222 (0.2%)
1	B	0.98	2/3840 (0.1%)	1.01	9/5200 (0.2%)
1	C	0.94	3/3840 (0.1%)	0.98	1/5200 (0.0%)
1	D	0.92	3/3815 (0.1%)	0.94	1/5166 (0.0%)
All	All	0.95	11/15354 (0.1%)	0.98	21/20788 (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	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	TRP	CB-CG	-7.36	1.36	1.50
1	B	200	TYR	CE2-CZ	6.48	1.47	1.38
1	C	296	CYS	CB-SG	-6.26	1.71	1.82
1	C	175	GLU	CG-CD	6.07	1.61	1.51
1	D	383	CYS	CB-SG	-5.82	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	TYR	CA-CB-CG	7.71	128.04	113.40
1	B	164	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	D	164	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	A	289	LEU	CA-CB-CG	7.21	131.88	115.30
1	A	495	ALA	C-N-CA	-6.93	107.74	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Sidechain
1	B	188	TYR	Sidechain
1	B	402	TYR	Sidechain
1	C	200	TYR	Sidechain
1	D	176	TYR	Sidechain

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	3785	0	3793	197	0
1	B	3765	0	3782	196	0
1	C	3765	0	3782	232	0
1	D	3741	0	3751	208	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	162	0	0	6	0
4	B	137	0	0	2	0
4	C	123	0	0	2	0
4	D	108	0	0	4	0
All	All	15818	0	15232	799	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 26.

The worst 5 of 799 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:B:308:LYS:N	1:B:325:ASN:HD21	1.40	1.18
1:B:308:LYS:H	1:B:325:ASN:ND2	1.45	1.15
1:D:270:VAL:HG22	1:D:281:GLU:HG2	1.31	1.13
1:D:461:THR:HG22	1:D:464:GLN:H	1.07	1.13
1:B:308:LYS:HB2	1:B:325:ASN:HD22	1.07	1.07

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	489/513 (95%)	442 (90%)	40 (8%)	7 (1%)	14	42
1	B	485/513 (94%)	441 (91%)	40 (8%)	4 (1%)	24	58
1	C	485/513 (94%)	435 (90%)	43 (9%)	7 (1%)	14	42
1	D	482/513 (94%)	437 (91%)	41 (8%)	4 (1%)	24	58
All	All	1941/2052 (95%)	1755 (90%)	164 (8%)	22 (1%)	17	50

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	ALA
1	C	9	LYS
1	C	138	HIS
1	A	138	HIS
1	B	476	ALA

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	402/422 (95%)	359 (89%)	43 (11%)	8	24
1	B	401/422 (95%)	361 (90%)	40 (10%)	9	27
1	C	401/422 (95%)	366 (91%)	35 (9%)	13	35
1	D	398/422 (94%)	365 (92%)	33 (8%)	14	38
All	All	1602/1688 (95%)	1451 (91%)	151 (9%)	11	31

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	305	VAL
1	C	9	LYS
1	D	368	GLU
1	B	347	ILE
1	B	403	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	133	GLN
1	C	258	GLN
1	D	258	GLN
1	C	144	ASN
1	C	272	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	900	-	48,58,58	1.71	9 (18%)	54,89,89	2.59	13 (24%)
3	SO4	A	901	-	4,4,4	0.52	0	6,6,6	0.64	0
2	FAD	B	900	-	48,58,58	1.76	7 (14%)	54,89,89	2.45	13 (24%)
3	SO4	B	901	-	4,4,4	0.44	0	6,6,6	0.50	0
2	FAD	C	900	-	48,58,58	1.70	8 (16%)	54,89,89	2.65	14 (25%)
3	SO4	C	901	-	4,4,4	0.58	0	6,6,6	0.44	0
2	FAD	D	900	-	48,58,58	1.56	6 (12%)	54,89,89	2.46	13 (24%)
3	SO4	D	901	-	4,4,4	0.35	0	6,6,6	0.41	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	900	-	-	0/30/50/50	0/6/6/6
3	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	FAD	B	900	-	-	0/30/50/50	0/6/6/6
3	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	FAD	C	900	-	-	0/30/50/50	0/6/6/6
3	SO4	C	901	-	-	0/0/0/0	0/0/0/0
2	FAD	D	900	-	-	0/30/50/50	0/6/6/6
3	SO4	D	901	-	-	0/0/0/0	0/0/0/0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	FAD	C8A-N7A	-3.15	1.28	1.34
2	C	900	FAD	C8A-N7A	-2.71	1.29	1.34
2	D	900	FAD	C10-N10	-2.26	1.36	1.39
2	C	900	FAD	O4B-C4B	-2.21	1.39	1.45
2	D	900	FAD	C5A-C4A	2.02	1.45	1.40

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	N3A-C2A-N1A	-9.63	121.52	128.89
2	A	900	FAD	N3A-C2A-N1A	-9.45	121.66	128.89
2	D	900	FAD	N3A-C2A-N1A	-8.86	122.11	128.89
2	B	900	FAD	N3A-C2A-N1A	-8.32	122.53	128.89
2	B	900	FAD	P-O3P-PA	-7.57	111.48	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	FAD	1	0
3	B	901	SO4	1	0
2	C	900	FAD	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	491/513 (95%)	-0.46	5 (1%) 84 77	21, 45, 65, 112	0
1	B	487/513 (94%)	-0.57	4 (0%) 87 81	21, 41, 65, 95	0
1	C	487/513 (94%)	-0.40	5 (1%) 84 77	27, 49, 69, 104	0
1	D	484/513 (94%)	-0.44	3 (0%) 90 86	25, 48, 73, 96	0
All	All	1949/2052 (94%)	-0.47	17 (0%) 85 79	21, 46, 69, 112	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	CYS	6.7
1	A	495	ALA	5.2
1	B	8	PRO	5.0
1	C	7	LEU	4.2
1	A	498	CYS	4.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th 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(\AA^2)	Q<0.9
2	FAD	A	900	53/53	0.97	0.18	0.54	37,49,55,56	0
2	FAD	C	900	53/53	0.96	0.16	0.09	39,45,53,53	0
2	FAD	B	900	53/53	0.98	0.13	-0.39	23,28,39,40	0
2	FAD	D	900	53/53	0.97	0.14	-0.39	27,33,48,49	0
3	SO4	A	901	5/5	0.95	0.12	-	68,69,71,71	0
3	SO4	C	901	5/5	0.96	0.10	-	67,67,68,68	0
3	SO4	B	901	5/5	0.95	0.10	-	63,65,66,66	0
3	SO4	D	901	5/5	0.93	0.15	-	71,73,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.