



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 11:47 PM GMT

PDB ID : 2ZZC
Title : Crystal structure of NADP(H):human thioredoxin reductase I
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2009-02-09
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

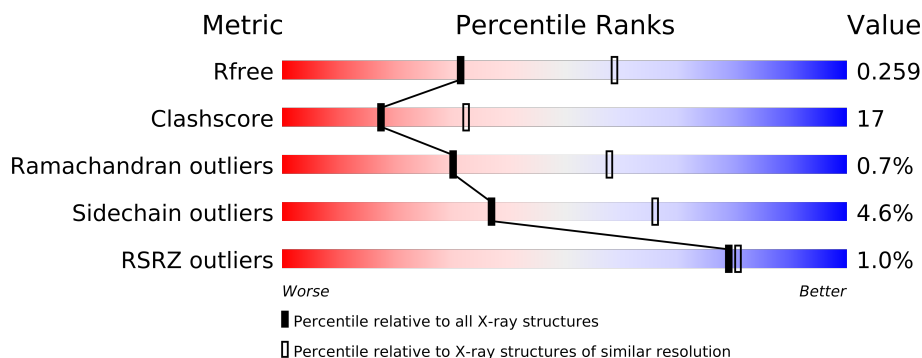
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. 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 4 unique types of molecules in this entry. The entry contains 16283 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	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	B	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			
1	C	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	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:

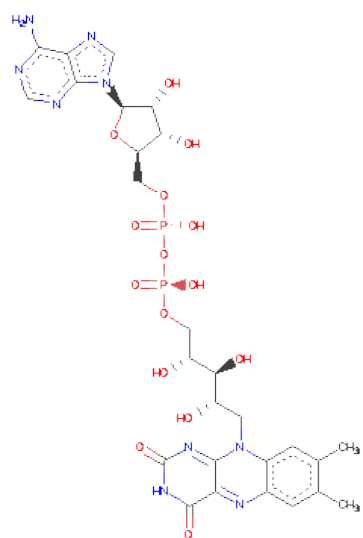
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q16881
A	-12	ALA	-	EXPRESSION TAG	UNP Q16881
A	-11	HIS	-	EXPRESSION TAG	UNP Q16881
A	-10	HIS	-	EXPRESSION TAG	UNP Q16881
A	-9	HIS	-	EXPRESSION TAG	UNP Q16881
A	-8	HIS	-	EXPRESSION TAG	UNP Q16881
A	-7	HIS	-	EXPRESSION TAG	UNP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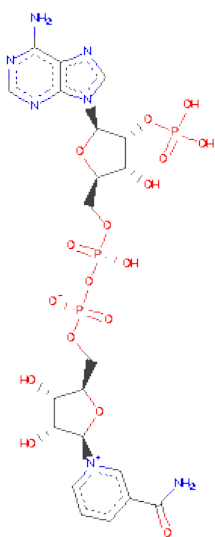
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	ASP	-	EXPRESSION TAG	UNP Q16881
B	-3	ASP	-	EXPRESSION TAG	UNP Q16881
B	-2	ASP	-	EXPRESSION TAG	UNP Q16881
B	-1	ASP	-	EXPRESSION TAG	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP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

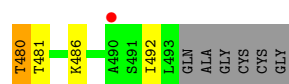
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

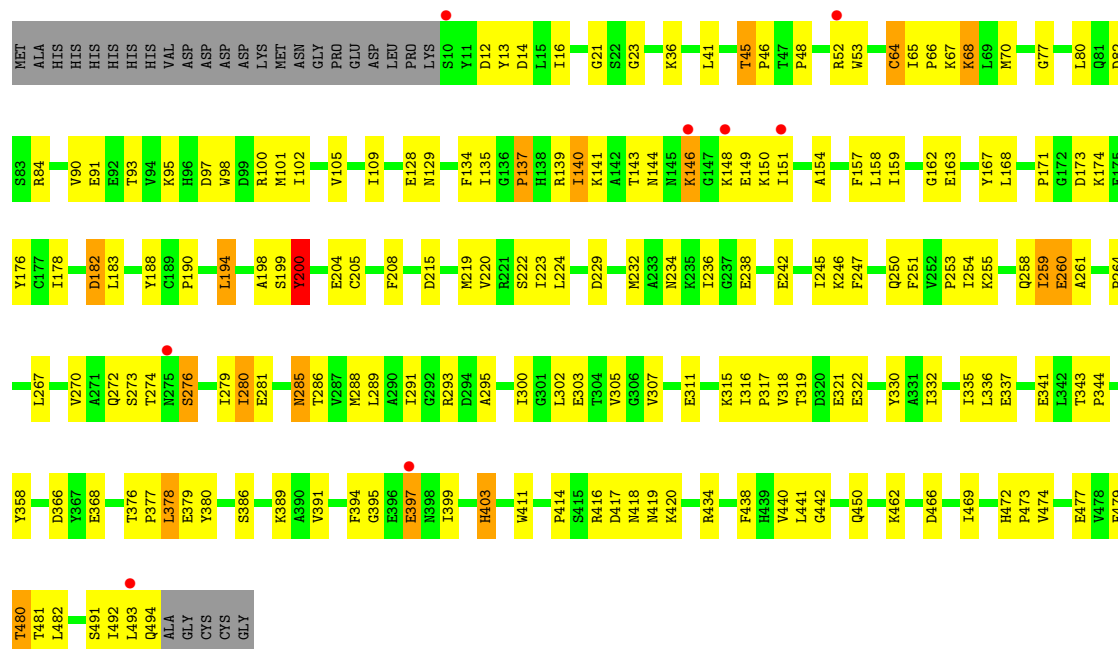
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total 246	O 246	0	0
4	B	260	Total 260	O 260	0	0
4	C	184	Total 184	O 184	0	0
4	D	207	Total 207	O 207	0	0



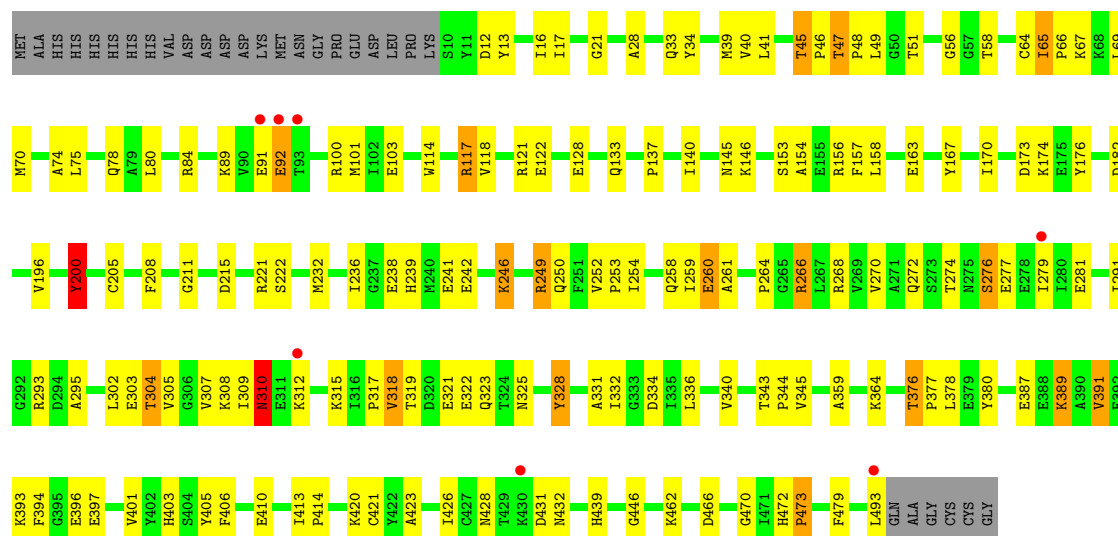
- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain C:



- Molecule 1: Thioredoxin reductase 1, cytoplasmic

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.86Å 135.17Å 346.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.60) 94.4 (29.92-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.260 0.210 , 0.259	Depositor DCC
R_{free} test set	4147 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 82282 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: NAP, 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	2/3824 (0.1%)	0.96	4/5178 (0.1%)
1	B	0.97	2/3815 (0.1%)	0.95	2/5166 (0.0%)
1	C	0.89	1/3824 (0.0%)	0.91	4/5178 (0.1%)
1	D	0.93	2/3815 (0.1%)	0.94	2/5166 (0.0%)
All	All	0.93	7/15278 (0.0%)	0.94	12/20688 (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	B	0	1
1	C	0	1
1	D	0	3
All	All	0	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	GLU	CG-CD	6.97	1.62	1.51
1	D	103	GLU	CG-CD	6.89	1.62	1.51
1	B	114	TRP	CB-CG	-6.17	1.39	1.50
1	D	397	GLU	CG-CD	5.87	1.60	1.51
1	C	53	TRP	CB-CG	-5.44	1.40	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	LEU	CA-CB-CG	-5.94	101.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	293	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	82	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	310	ASN	N-CA-C	-5.61	95.84	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	TYR	Sidechain
1	C	200	TYR	Sidechain
1	D	200	TYR	Sidechain
1	D	328	TYR	Sidechain
1	D	405	TYR	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	3750	0	3759	151	0
1	B	3741	0	3751	110	0
1	C	3750	0	3759	167	0
1	D	3741	0	3751	134	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
3	C	48	0	25	3	0
3	D	48	0	25	3	0
4	A	246	0	0	5	0
4	B	260	0	0	7	0
4	C	184	0	0	5	0
4	D	207	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16283	0	15244	534	0

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 17.

The worst 5 of 534 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:308:LYS:N	1:B:325:ASN:HD21	1.43	1.17
1:C:419:ASN:ND2	1:C:494:GLN:HB2	1.62	1.13
1:D:302:LEU:HD22	1:D:307:VAL:HG21	1.27	1.12
1:B:308:LYS:H	1:B:325:ASN:ND2	1.48	1.09
1:C:183:LEU:HD22	1:C:288:MET:HE1	1.37	1.06

There are no symmetry-related clashes.

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	483/513 (94%)	446 (92%)	33 (7%)	4 (1%)	27	53
1	B	482/513 (94%)	455 (94%)	26 (5%)	1 (0%)	56	82
1	C	483/513 (94%)	443 (92%)	34 (7%)	6 (1%)	19	39
1	D	482/513 (94%)	443 (92%)	36 (8%)	3 (1%)	33	63
All	All	1930/2052 (94%)	1787 (93%)	129 (7%)	14 (1%)	30	58

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	260	GLU
1	A	200	TYR
1	C	200	TYR
1	D	260	GLU
1	A	260	GLU

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	399/422 (94%)	383 (96%)	16 (4%)	42	73
1	B	398/422 (94%)	386 (97%)	12 (3%)	53	82
1	C	399/422 (94%)	378 (95%)	21 (5%)	32	58
1	D	398/422 (94%)	373 (94%)	25 (6%)	25	49
All	All	1594/1688 (94%)	1520 (95%)	74 (5%)	37	66

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	68	LYS
1	C	285	ASN
1	D	376	THR
1	C	129	ASN
1	C	146	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	432	ASN
1	C	129	ASN
1	D	355	GLN
1	C	113	ASN
1	C	145	ASN

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

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	-	58,58,58	1.60	6 (10%)	85,89,89	2.13	18 (21%)
3	NAP	A	901	-	52,52,52	1.47	6 (11%)	80,80,80	1.16	5 (6%)
2	FAD	B	900	-	58,58,58	1.63	10 (17%)	85,89,89	2.16	16 (18%)
3	NAP	B	901	-	52,52,52	1.49	8 (15%)	80,80,80	1.29	7 (8%)
2	FAD	C	900	-	58,58,58	1.79	9 (15%)	85,89,89	2.17	18 (21%)
3	NAP	C	901	-	52,52,52	1.52	9 (17%)	80,80,80	1.21	6 (7%)
2	FAD	D	900	-	58,58,58	1.74	7 (12%)	85,89,89	1.98	18 (21%)
3	NAP	D	901	-	52,52,52	1.35	7 (13%)	80,80,80	1.20	4 (5%)

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	-	-	0/34/50/50	0/1/6/6
3	NAP	A	901	-	-	0/35/67/67	0/3/5/5
2	FAD	B	900	-	-	0/34/50/50	0/1/6/6
3	NAP	B	901	-	-	0/35/67/67	0/3/5/5
2	FAD	C	900	-	-	0/34/50/50	0/1/6/6
3	NAP	C	901	-	-	0/35/67/67	0/3/5/5
2	FAD	D	900	-	-	0/34/50/50	0/1/6/6
3	NAP	D	901	-	-	0/35/67/67	0/3/5/5

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	FAD	C4X-C10	6.18	1.51	1.40
2	B	900	FAD	C4-C4X	5.65	1.50	1.41
2	D	900	FAD	C4-C4X	5.30	1.49	1.41
2	C	900	FAD	C4-C4X	5.24	1.49	1.41
3	B	901	NAP	C2N-N1N	5.20	1.42	1.35

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	N3A-C2A-N1A	-8.93	121.25	128.71
2	A	900	FAD	N3A-C2A-N1A	-8.90	121.27	128.71
2	B	900	FAD	N3A-C2A-N1A	-8.45	121.65	128.71
2	B	900	FAD	C2-N1-C10	7.21	122.25	114.98
2	A	900	FAD	P-O3P-PA	-6.94	111.34	131.68

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, 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	485/513 (94%)	-0.28	3 (0%) 86 89	26, 50, 70, 84	0
1	B	484/513 (94%)	-0.47	2 (0%) 90 91	28, 44, 63, 87	0
1	C	485/513 (94%)	-0.24	8 (1%) 68 69	34, 53, 74, 94	0
1	D	484/513 (94%)	-0.34	7 (1%) 72 72	28, 49, 70, 89	0
All	All	1938/2052 (94%)	-0.33	20 (1%) 79 81	26, 49, 71, 94	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	493	LEU	5.3
1	D	92	GLU	3.7
1	C	275	ASN	2.9
1	D	93	THR	2.8
1	C	493	LEU	2.7

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	A	900	53/53	0.17	0.30	42,50,68,68	0
2	FAD	C	900	53/53	0.16	0.27	38,48,65,66	0
2	FAD	B	900	53/53	0.13	0.11	30,37,43,43	0
2	FAD	D	900	53/53	0.13	-0.25	30,42,49,51	0
3	NAP	D	901	48/48	0.13	-0.35	51,60,83,85	0
3	NAP	B	901	48/48	0.12	-0.45	45,53,63,64	0
3	NAP	C	901	48/48	0.14	-0.64	61,72,86,87	0
3	NAP	A	901	48/48	0.14	-0.67	49,64,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.