



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:37 am GMT

PDB ID : 1NPX  
Title : STRUCTURE OF NADH PEROXIDASE FROM STREPTOCOCCUS FAECALIS 10C1 REFINED AT 2.16 ANGSTROMS RESOLUTION  
Authors : Stehle, T.; Ahmed, S.A.; Claiborne, A.; Schulz, G.E.  
Deposited on : 1991-08-02  
Resolution : 2.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

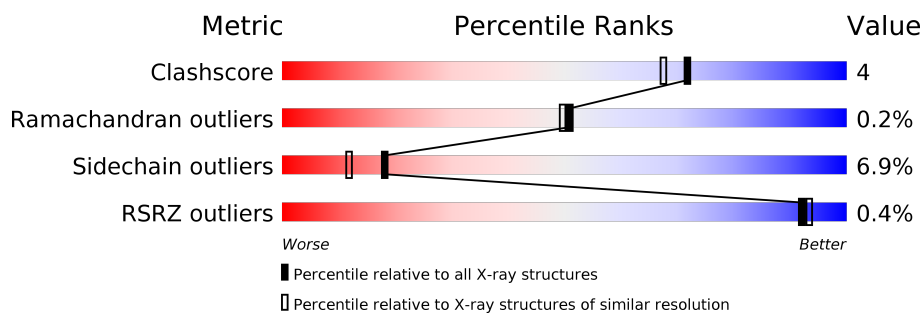
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.16 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	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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. 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	447	 82% <span style="float: right;">13% . .</span>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3915 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 NADH PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3493	2225	573	683	12	0	0	0

- 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
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

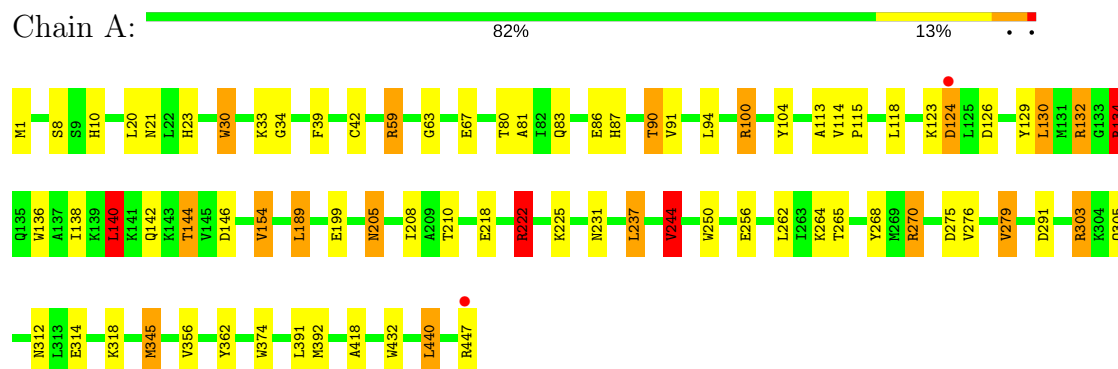
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	369	Total	O	0	0
			369	369		

### 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 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: NADH PEROXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.20Å 134.50Å 145.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.16 98.89 – 2.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.16) 92.0 (98.89-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.177 , (Not available) 0.171 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.4	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3915	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, 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	0.83	1/3547 (0.0%)	1.61	51/4807 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	VAL	CA-CB	5.99	1.67	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	-26.45	107.08	120.30
1	A	132	ARG	NE-CZ-NH1	25.58	133.09	120.30
1	A	303	ARG	NE-CZ-NH1	17.72	129.16	120.30
1	A	59	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	A	134	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	A	59	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	A	134	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	A	303	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	270	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	374	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	A	30	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A	432	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	A	270	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	374	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	124	ASP	CA-C-N	-7.24	101.28	117.20
1	A	136	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	30	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A	374	TRP	CB-CG-CD1	-6.96	117.95	127.00
1	A	432	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	136	TRP	CD1-CG-CD2	6.91	111.83	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	THR	N-CA-CB	-6.63	97.70	110.30
1	A	362	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	A	100	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	279	VAL	N-CA-CB	-6.43	97.35	111.50
1	A	345	MET	CG-SD-CE	-6.43	89.91	100.20
1	A	146	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	104	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	189	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	237	LEU	CA-CB-CG	6.22	129.61	115.30
1	A	250	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	A	250	TRP	CE2-CD2-CG	-6.04	102.47	107.30
1	A	100	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	140	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	144	THR	N-CA-CB	-5.80	99.27	110.30
1	A	432	TRP	CB-CG-CD1	-5.78	119.48	127.00
1	A	222	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	432	TRP	CG-CD2-CE3	5.73	139.06	133.90
1	A	114	VAL	N-CA-CB	-5.64	99.09	111.50
1	A	33	LYS	CB-CG-CD	-5.59	97.07	111.60
1	A	374	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	A	244	VAL	N-CA-CB	-5.55	99.29	111.50
1	A	34	GLY	CA-C-N	-5.50	105.11	117.20
1	A	374	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	A	222	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	391	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	432	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	A	205	ASN	N-CA-C	5.31	125.33	111.00
1	A	30	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	A	199	GLU	CA-CB-CG	5.18	124.80	113.40
1	A	356	VAL	CG1-CB-CG2	-5.03	102.86	110.90
1	A	392	MET	CG-SD-CE	5.01	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

## 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	3493	0	3489	28	0
2	A	53	0	31	1	0
3	A	369	0	0	3	0
All	All	3915	0	3520	28	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 4.

All (28) 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:A:268:TYR:HB2	1:A:270:ARG:HD2	1.74	0.68
1:A:418:ALA:HB1	1:A:440:LEU:HD13	1.77	0.67
1:A:23:HIS:HE1	3:A:573:HOH:O	1.82	0.61
1:A:312:ASN:HD21	1:A:318:LYS:H	1.51	0.58
1:A:83:GLN:HE22	1:A:90:THR:HG22	1.67	0.58
1:A:87:HIS:HE1	1:A:275:ASP:OD2	1.89	0.56
1:A:91:VAL:HG22	1:A:100:ARG:HG2	1.86	0.56
1:A:279:VAL:HG22	1:A:305:GLN:HB3	1.88	0.56
1:A:81:ALA:HB3	1:A:90:THR:HG23	1.87	0.55
1:A:115:PRO:HB2	1:A:130:LEU:HG	1.89	0.54
1:A:345:MET:HG2	3:A:758:HOH:O	2.08	0.52
1:A:132:ARG:NH2	1:A:244:VAL:HG21	2.26	0.50
1:A:39:PHE:CD1	1:A:134:ARG:HG2	2.48	0.48
1:A:218:GLU:HB2	1:A:225:LYS:HB2	1.96	0.47
1:A:208:ILE:HG22	1:A:210:THR:HG23	1.95	0.47
1:A:8:SER:HA	1:A:30:TRP:CZ2	2.50	0.46
1:A:126:ASP:HB2	1:A:222:ARG:HB3	1.98	0.46
1:A:129:TYR:HD2	1:A:140:LEU:HD13	1.81	0.45
1:A:10:HIS:ND1	1:A:303:ARG:HD2	2.32	0.45
1:A:63:GLY:O	1:A:67:GLU:HG3	2.17	0.45
1:A:312:ASN:HD21	1:A:318:LYS:N	2.13	0.44
1:A:91:VAL:CG2	1:A:100:ARG:HG2	2.49	0.43
1:A:42:OCS:OD2	2:A:449:FAD:C10	2.67	0.43
1:A:113:ALA:HB1	1:A:244:VAL:HG13	2.02	0.42
1:A:256:GLU:HB3	1:A:264:LYS:HE2	2.02	0.42
1:A:138:ILE:O	1:A:142:GLN:HG2	2.21	0.40
1:A:265:THR:HA	1:A:270:ARG:O	2.21	0.40
1:A:210:THR:HG22	3:A:812:HOH:O	2.20	0.40

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	444/447 (99%)	433 (98%)	10 (2%)	1 (0%)	51	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LYS

### 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	375/375 (100%)	349 (93%)	26 (7%)	18	12

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	20	LEU
1	A	21	ASN
1	A	59	ARG
1	A	86	GLU
1	A	90	THR
1	A	94	LEU
1	A	118	LEU
1	A	124	ASP
1	A	130	LEU

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Mol	Chain	Res	Type
1	A	134	ARG
1	A	140	LEU
1	A	144	THR
1	A	154	VAL
1	A	189	LEU
1	A	205	ASN
1	A	222	ARG
1	A	231	ASN
1	A	237	LEU
1	A	244	VAL
1	A	262	LEU
1	A	276	VAL
1	A	291	ASP
1	A	314	GLU
1	A	440	LEU
1	A	447	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	87	HIS
1	A	204	ASN
1	A	288	ASN
1	A	295	ASN
1	A	312	ASN
1	A	385	GLN
1	A	402	ASN
1	A	445	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	OCS	A	42	1	8,8,9	1.56	1 (12%)	7,11,13	6.70	6 (85%)

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
1	OCS	A	42	1	-	0/4/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	OCS	OD2-SG	-3.16	1.36	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	OCS	OD2-SG-OD1	-4.08	102.02	111.37
1	A	42	OCS	OD2-SG-OD3	-3.72	102.84	111.37
1	A	42	OCS	O-C-CA	-2.60	117.84	125.02
1	A	42	OCS	OD2-SG-CB	2.95	109.61	106.01
1	A	42	OCS	OD1-SG-CB	9.75	115.16	106.83
1	A	42	OCS	OD3-SG-CB	13.05	117.98	106.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	42	OCS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	449	-	51,58,58	1.19	3 (5%)	54,89,89	1.65	7 (12%)

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	449	-	-	0/28/50/50	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	449	FAD	C2-N1	-2.80	1.32	1.38
2	A	449	FAD	PA-O5B	-2.29	1.49	1.59
2	A	449	FAD	C4-N3	4.13	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	449	FAD	C4X-C4-N3	-5.61	115.49	123.48
2	A	449	FAD	C4X-C10-N10	-2.63	118.69	120.52
2	A	449	FAD	C6-C5X-N5	-2.04	116.57	118.97
2	A	449	FAD	N3A-C2A-N1A	2.02	130.62	128.86
2	A	449	FAD	C10-C4X-N5	2.68	123.68	120.59
2	A	449	FAD	C1'-N10-C9A	3.31	121.38	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	449	FAD	C4-N3-C2	6.89	121.18	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	449	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, 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	446/447 (99%)	-0.48	2 (0%) 92 93	6, 16, 35, 57	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ARG	3.7
1	A	124	ASP	2.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	OCS	A	42	9/10	0.98	0.11	-	10,11,13,15	0

### 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	449	53/53	0.99	0.08	-0.71	3,6,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.