



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:11 pm GMT

PDB ID : 2GMH  
Title : Structure of Porcine Electron Transfer Flavoprotein-Ubiquinone Oxidoreductase in Complexed with Ubiquinone  
Authors : Zhang, J.; Frerman, F.E.; Kim, J.-J.P.  
Deposited on : 2006-04-06  
Resolution : 2.50 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](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

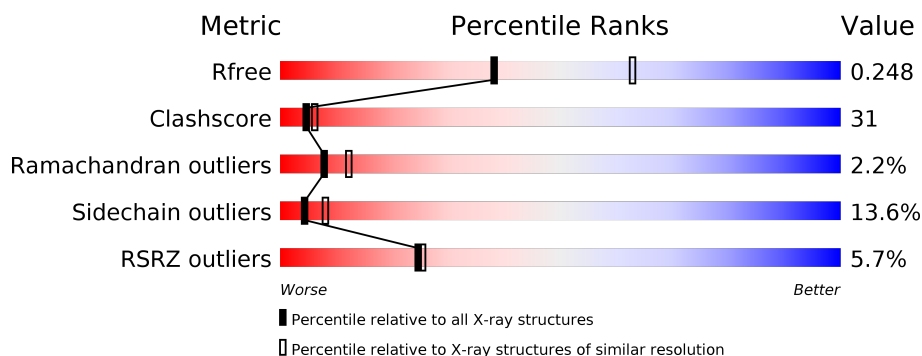
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	584	<div> <div>2%</div> <div>64%</div> <div>29%</div> <div>5% ..</div> </div>
1	B	584	<div> <div>10%</div> <div>41%</div> <div>47%</div> <div>11% ..</div> </div>

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	BHG	A	616	X	-	-	X
2	BHG	A	617	X	-	-	X
2	BHG	B	618	X	-	-	-
6	UQ5	A	612	-	-	-	X
6	UQ5	B	615	-	-	-	X
7	EDO	A	619	-	-	-	X
7	EDO	A	621	-	-	-	X
7	EDO	A	622	-	-	-	X
7	EDO	A	623	-	-	X	X
7	EDO	A	624	-	-	-	X

## 2 Entry composition [i](#)

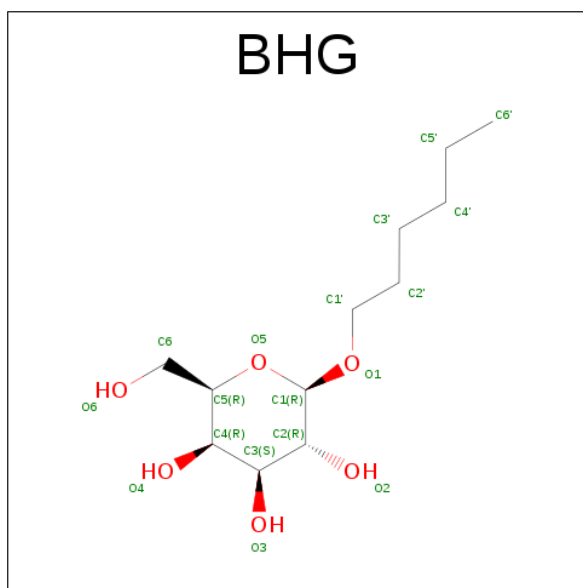
There are 8 unique types of molecules in this entry. The entry contains 9751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Electron transfer flavoprotein-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4558	2910	792	836	20			
1	B	578	Total	C	N	O	S	0	0	0
			4531	2893	787	832	19			

- Molecule 2 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: C<sub>12</sub>H<sub>24</sub>O<sub>6</sub>).

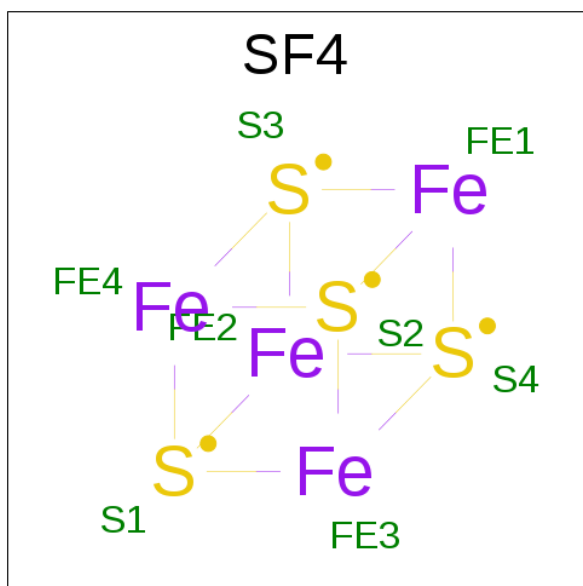


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	12	6		
2	A	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

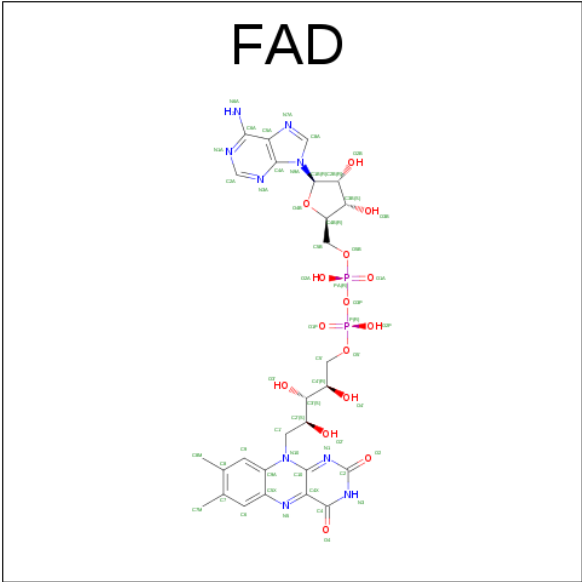
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



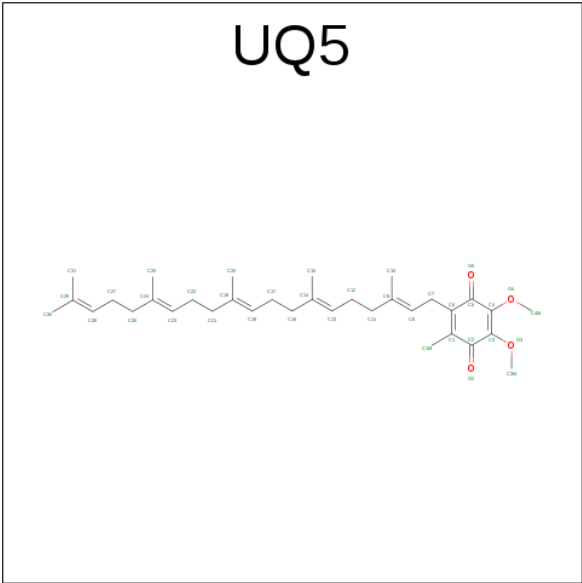
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



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

- Molecule 6 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>4</sub>).



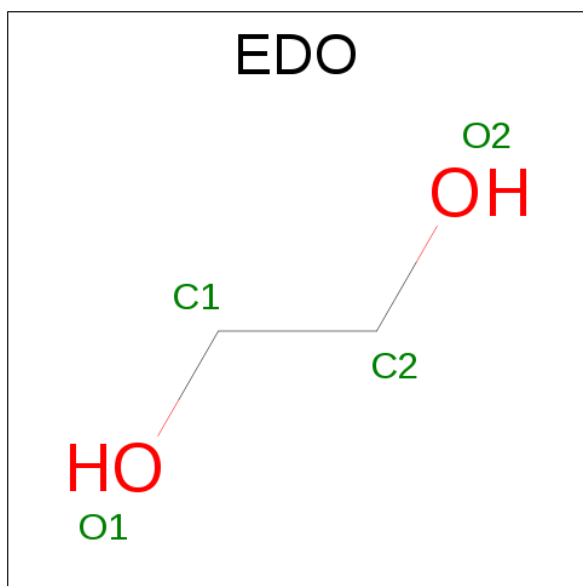
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			38	34	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			38	34	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	301	Total 301	O 301	0	0
8	B	68	Total 68	O 68	0	0





H278	V361	M448	P523
L279	P362	E449	E524
M280		P450	Q525
	K365	W451	R526
L286		T452	P527
A287	H368		V532
L288		K456	
G289	T375	G457	P535
		S458	V536
L294		D459	P537
	E379	S460	L538
P299	S380	D461	E539
Y300	I381	G462	Q540
L301	F382	L463	G541
S302	N383		D542
P303	Q384	K467	G543
F304	L385		P544
R305	T386	P471	R545
E306	S387		L546
F307	E388	Y474	Q547
	N389	P475	T548
	L390	K476	N549
W310	Q391		A550
	S392	T481	Q551
H313	K393	S482	N552
P314	T394	F483	
S315	T395	D484	H555
I316	G396	L485	C556
K317	L397	L486	K557
P318	H398	S487	
T319	V399	S488	T561
L320	T400	V489	K562
	E401		
R325	Y402	T494	S565
I326	E403	M495	Q566
A327		H496	
	K407	E497	N569
R331		H498	W570
A332	W410	D499	V571
L333		Q500	V572
N334	V418	P501	P573
E335	R419	A502	E574
G336	N420	H503	G575
	I421	L504	
S340	R422	T505	
I341	P423	L506	G578
	V431	K507	P579
L344	Y432	D508	
T345		D509	N584
F346	M435	S510	
P347		V511	
G348	T438	P512	
G349		V513	
L350		N514	
L351	F441	R515	
I352	Y442	N516	
G353		L517	
C354	F445		
S355	R446	D521	
P356	G447	G522	
G357			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.32Å 154.32Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.50 29.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.67-2.50) 98.8 (29.66-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.94 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.254 0.216 , 0.248	Depositor DCC
$R_{free}$ test set	4358 reflections (8.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</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: NA, SF4, EDO, BHG, UQ5, 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	0.59	0/4687	0.96	18/6363 (0.3%)
1	B	0.50	0/4660	0.88	10/6326 (0.2%)
All	All	0.55	0/9347	0.92	28/12689 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	VAL	C-N-CD	-15.72	86.01	120.60
1	A	542	ASP	N-CA-C	9.67	137.11	111.00
1	A	5	LYS	N-CA-C	8.39	133.65	111.00
1	A	6	VAL	C-N-CA	8.38	157.20	122.00
1	A	8	ARG	NE-CZ-NH1	-8.31	116.15	120.30

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	4558	0	4457	204	0
1	B	4531	0	4424	365	0
2	A	36	0	48	6	0
2	B	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	53	0	31	2	0
5	B	53	0	31	4	0
6	A	38	0	50	17	0
6	B	38	0	50	13	0
7	A	36	0	54	18	0
7	B	4	0	6	0	0
8	A	301	0	0	8	0
8	B	68	0	0	5	0
All	All	9751	0	9175	576	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 31.

The worst 5 of 576 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:38:VAL:HG12	1:B:67:VAL:HG12	1.26	1.13
1:B:55:LYS:HB2	1:B:157:LEU:HD12	1.30	1.08
1:B:351:LEU:HB3	1:B:356:PRO:HG3	1.43	1.00
1:B:510:SER:O	1:B:514:ASN:HB2	1.62	0.99
1:B:203:GLU:HG2	1:B:205:HIS:CE1	1.97	0.99

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	579/584 (99%)	544 (94%)	31 (5%)	4 (1%)	25 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	576/584 (99%)	493 (86%)	62 (11%)	21 (4%)	4	5
All	All	1155/1168 (99%)	1037 (90%)	93 (8%)	25 (2%)	8	12

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ARG
1	B	74	ALA
1	B	84	ALA
1	B	99	LYS
1	B	391	GLN

### 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	483/486 (99%)	428 (89%)	55 (11%)	7	12
1	B	479/486 (99%)	403 (84%)	76 (16%)	3	5
All	All	962/972 (99%)	831 (86%)	131 (14%)	4	8

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	VAL
1	B	112	ASP
1	B	500	GLN
1	B	31	ARG
1	B	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	551	GLN
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	498	HIS
1	A	525	GLN
1	B	516	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](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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	$\# Z  > 2$
4	SF4	A	610	1	0,12,12	0.00	-	0,24,24	0.00	-
5	FAD	A	611	-	51,58,58	2.72	19 (37%)	54,89,89	2.62	11 (20%)
6	UQ5	A	612	-	38,38,38	2.54	15 (39%)	46,49,49	2.33	14 (30%)
2	BHG	A	616	-	18,18,18	1.07	2 (11%)	23,23,23	3.54	4 (17%)
2	BHG	A	617	-	18,18,18	1.40	3 (16%)	23,23,23	2.35	6 (26%)
7	EDO	A	619	-	3,3,3	0.60	0	2,2,2	0.45	0
7	EDO	A	621	-	3,3,3	0.61	0	2,2,2	0.45	0
7	EDO	A	622	-	3,3,3	0.72	0	2,2,2	0.08	0
7	EDO	A	623	-	3,3,3	0.52	0	2,2,2	0.64	0
7	EDO	A	624	-	3,3,3	0.64	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	625	-	3,3,3	0.71	0	2,2,2	0.48	0
7	EDO	A	626	-	3,3,3	0.77	0	2,2,2	0.52	0
7	EDO	A	627	-	3,3,3	0.82	0	2,2,2	0.46	0
7	EDO	A	628	-	3,3,3	0.84	0	2,2,2	0.35	0
4	SF4	B	613	1	0,12,12	0.00	-	0,24,24	0.00	-
5	FAD	B	614	-	51,58,58	2.39	17 (33%)	54,89,89	2.94	15 (27%)
6	UQ5	B	615	-	38,38,38	2.57	17 (44%)	46,49,49	2.16	18 (39%)
2	BHG	B	618	-	18,18,18	1.04	1 (5%)	23,23,23	2.81	3 (13%)
7	EDO	B	620	-	3,3,3	0.63	0	2,2,2	0.59	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
4	SF4	A	610	1	-	0/0/48/48	0/6/5/5
5	FAD	A	611	-	-	0/28/50/50	0/6/6/6
6	UQ5	A	612	-	-	0/33/57/57	0/1/1/1
2	BHG	A	616	-	1/1/5/5	0/9/29/29	0/1/1/1
2	BHG	A	617	-	1/1/5/5	1/9/29/29	0/1/1/1
7	EDO	A	619	-	-	0/1/1/1	0/0/0/0
7	EDO	A	621	-	-	0/1/1/1	0/0/0/0
7	EDO	A	622	-	-	0/1/1/1	0/0/0/0
7	EDO	A	623	-	-	0/1/1/1	0/0/0/0
7	EDO	A	624	-	-	0/1/1/1	0/0/0/0
7	EDO	A	625	-	-	0/1/1/1	0/0/0/0
7	EDO	A	626	-	-	0/1/1/1	0/0/0/0
7	EDO	A	627	-	-	0/1/1/1	0/0/0/0
7	EDO	A	628	-	-	0/1/1/1	0/0/0/0
4	SF4	B	613	1	-	0/0/48/48	0/6/5/5
5	FAD	B	614	-	-	0/28/50/50	0/6/6/6
6	UQ5	B	615	-	-	0/33/57/57	0/1/1/1
2	BHG	B	618	-	1/1/5/5	0/9/29/29	0/1/1/1
7	EDO	B	620	-	-	0/1/1/1	0/0/0/0

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	611	FAD	C1'-N10	-10.01	1.38	1.48
5	B	614	FAD	C1'-N10	-6.45	1.41	1.48
6	B	615	UQ5	C7-C8	-4.84	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	612	UQ5	C7-C8	-3.61	1.45	1.50
5	B	614	FAD	C2-N1	-3.52	1.31	1.38

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	614	FAD	C4X-C4-N3	-7.50	112.80	123.48
5	A	611	FAD	C4X-C4-N3	-7.08	113.40	123.48
5	B	614	FAD	C4X-C10-N10	-6.87	115.75	120.52
5	A	611	FAD	C4X-C10-N10	-5.30	116.84	120.52
6	A	612	UQ5	C12-C11-C9	-5.09	95.72	112.93

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	618	BHG	C4
2	A	616	BHG	C4
2	A	617	BHG	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	617	BHG	C1-O1-C1'-C2'

There are no ring outliers.

11 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	FAD	2	0
6	A	612	UQ5	17	0
2	A	617	BHG	6	0
7	A	619	EDO	3	0
7	A	621	EDO	3	0
7	A	622	EDO	3	0
7	A	623	EDO	7	0
7	A	627	EDO	1	0
7	A	628	EDO	1	0
5	B	614	FAD	4	0
6	B	615	UQ5	13	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	581/584 (99%)	-0.25	10 (1%) 70 72	13, 30, 57, 84	0
1	B	578/584 (98%)	0.62	56 (9%) 8 8	38, 64, 79, 86	0
All	All	1159/1168 (99%)	0.19	66 (5%) 24 25	13, 49, 77, 86	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	CYS	7.8
1	B	176	GLY	5.4
1	B	540	GLN	5.4
1	B	390	LEU	5.2
1	A	540	GLN	5.0

### 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, 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	BHG	A	617	18/18	0.59	0.57	16.72	55,75,78,79	0
7	EDO	A	623	4/4	0.92	0.45	15.56	48,49,49,53	0
2	BHG	A	616	18/18	0.59	0.38	14.60	52,76,78,79	0
7	EDO	A	622	4/4	0.84	0.38	11.07	51,55,55,57	0
7	EDO	A	621	4/4	0.94	0.27	8.76	45,47,48,49	0
7	EDO	A	624	4/4	0.95	0.32	7.81	35,41,42,42	0
7	EDO	A	619	4/4	0.89	0.20	4.70	37,37,38,43	0
6	UQ5	A	612	38/38	0.88	0.26	3.08	39,48,62,63	0
6	UQ5	B	615	38/38	0.85	0.27	2.28	51,56,68,71	0
7	EDO	B	620	4/4	0.88	0.15	0.34	49,53,54,56	0
5	FAD	A	611	53/53	0.98	0.17	-0.02	16,20,24,26	0
5	FAD	B	614	53/53	0.92	0.19	-0.31	44,60,68,69	0
4	SF4	A	610	8/8	0.99	0.11	-0.35	16,19,22,22	0
4	SF4	B	613	8/8	0.98	0.09	-2.33	55,58,59,59	0
7	EDO	A	626	4/4	0.89	0.16	-	43,45,45,46	0
7	EDO	A	628	4/4	0.77	0.34	-	53,54,55,55	0
3	NA	A	1070	1/1	0.95	0.07	-	37,37,37,37	0
7	EDO	A	627	4/4	0.81	0.56	-	57,58,58,58	0
2	BHG	B	618	18/18	0.53	0.36	-	61,76,78,78	0
7	EDO	A	625	4/4	0.90	0.15	-	49,55,55,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.