



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:10 AM GMT

PDB ID : 2BS3  
Title : GLU C180 -> GLN VARIANT QUINOL:FUMARATE REDUCTASE FROM  
WOLINELLA SUCCINOGENES  
Authors : Lancaster, C.R.D.  
Deposited on : 2005-05-14  
Resolution : 2.19 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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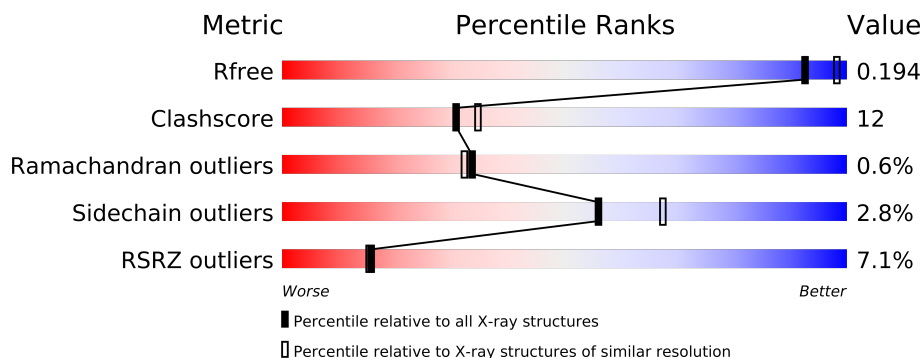
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.19 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	656	
1	D	656	
2	B	239	
2	E	239	
3	C	256	
3	F	256	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	LMT	C	1257	-	X
11	LMT	F	1257	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	CIT	A	1657[A]	-	X
5	CIT	A	1657[B]	-	X
5	CIT	D	1657[A]	-	X
5	CIT	D	1657[B]	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19737 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 QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	27	5	1
			5145	3219	927	967	32			
1	D	656	Total	C	N	O	S	38	3	1
			5125	3207	921	965	32			

- Molecule 2 is a protein called QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	6	2	0
			1908	1202	324	358	24			
2	E	239	Total	C	N	O	S	6	2	0
			1908	1202	324	358	24			

- Molecule 3 is a protein called QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	255	Total	C	N	O	S	16	3	1
			2110	1407	339	350	14			
3	F	255	Total	C	N	O	S	6	3	1
			2110	1407	339	350	14			

There are 2 discrepancies between the modelled and reference sequences:

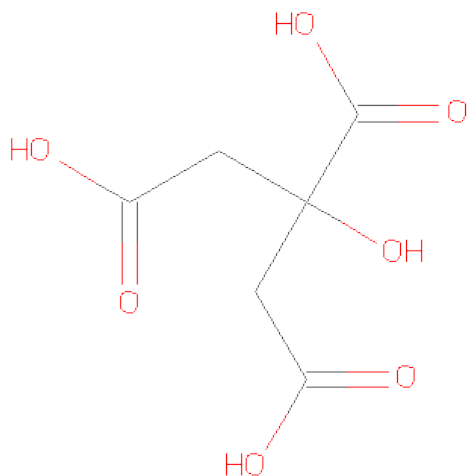
Chain	Residue	Modelled	Actual	Comment	Reference
C	180	GLN	GLU	CONFLICT SEE REMARK 9	UNP P17413
F	180	GLN	GLU	CONFLICT SEE REMARK 9	UNP P17413

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).

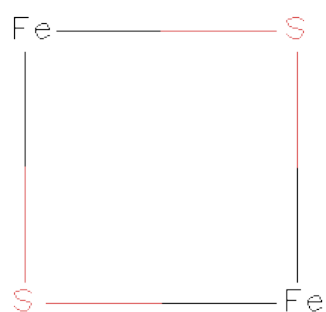


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			26	12	14		
5	D	1	Total	C	O	0	1
			26	12	14		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

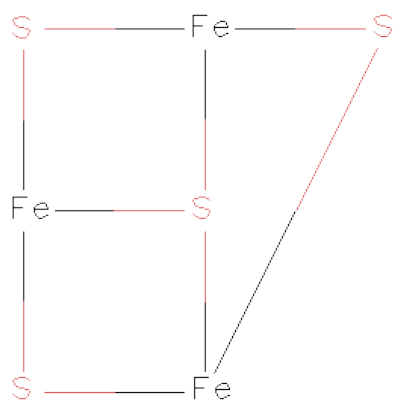
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



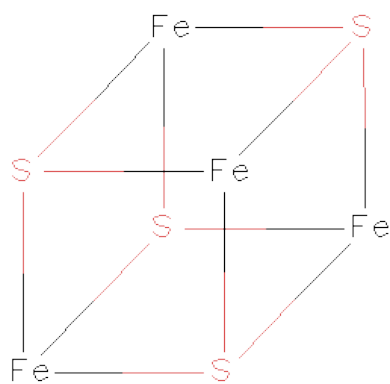
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



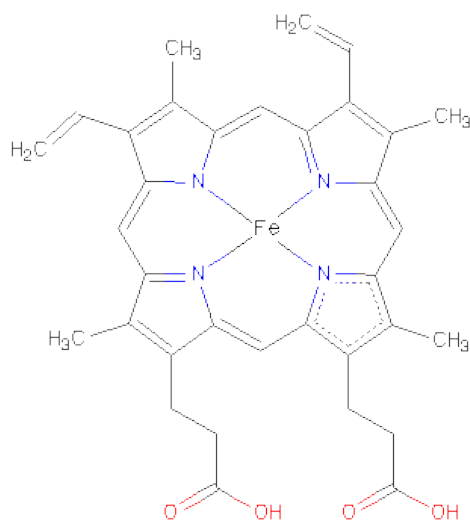
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

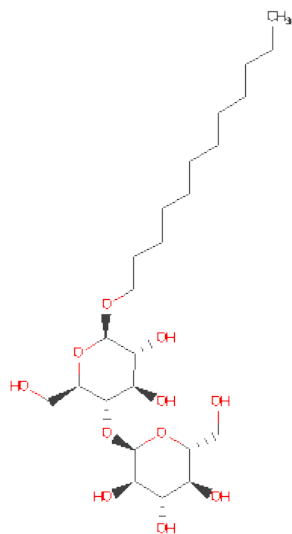
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	16	0
			35	24	11		
11	F	1	Total	C	O	16	0
			35	24	11		

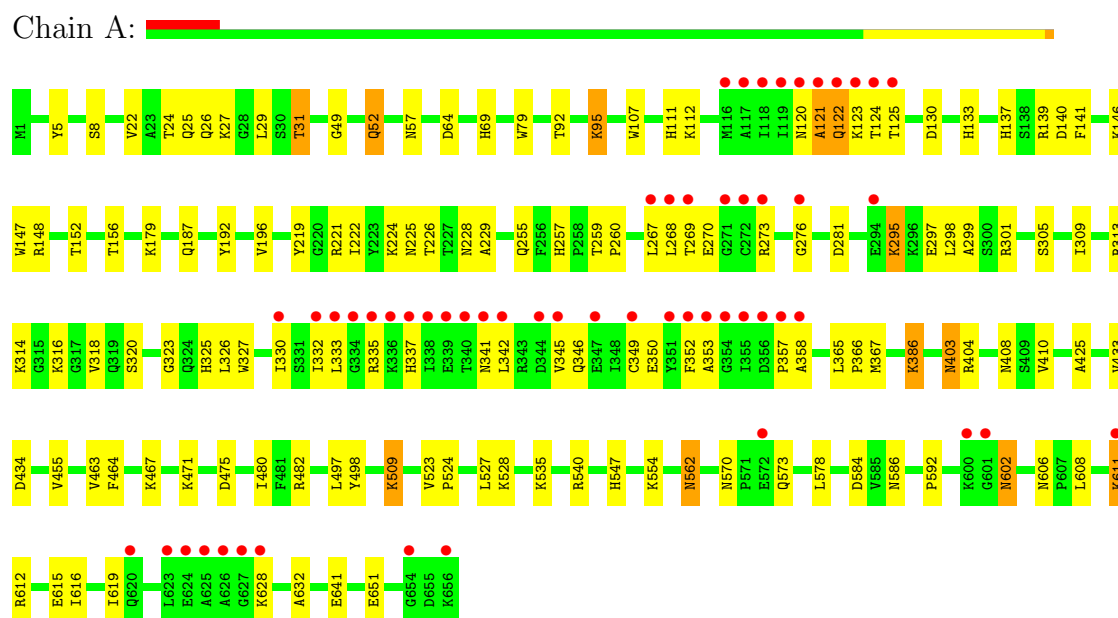
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	274	Total	O	0	0
			274	274		
12	B	156	Total	O	1	0
			156	156		
12	C	47	Total	O	0	0
			47	47		
12	D	291	Total	O	3	0
			291	291		
12	E	164	Total	O	1	0
			164	164		
12	F	59	Total	O	0	0
			59	59		

### 3 Residue-property plots

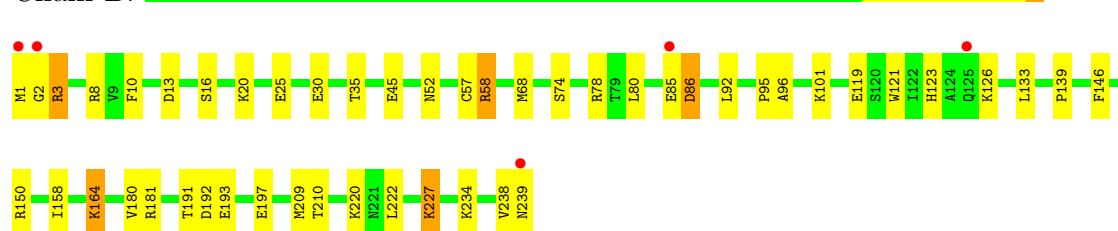
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



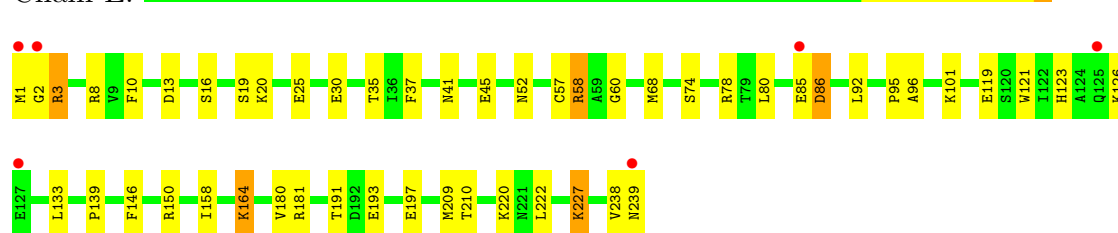
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

Chain B:



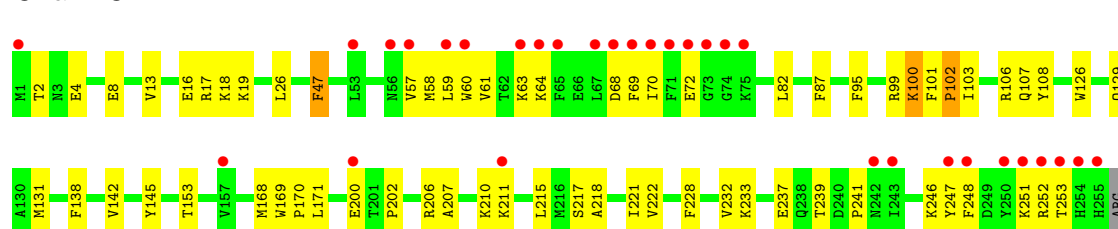
• Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

Chain E:



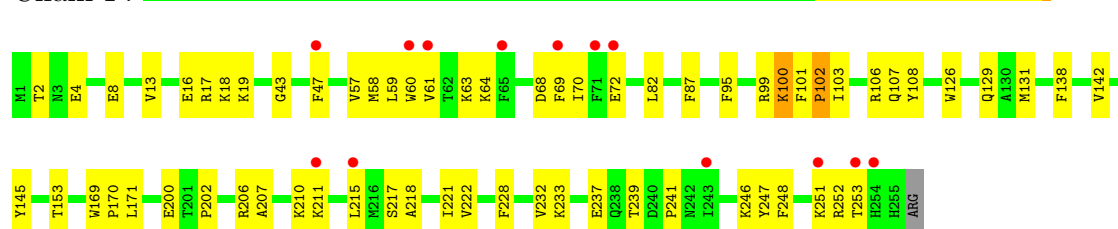
• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C

Chain C:



• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.10Å 188.77Å 117.82Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	38.58 – 2.19 48.59 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.58-2.19) 99.1 (48.59-2.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.89 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.183 , 0.198 0.180 , 0.194	Depositor DCC
$R_{free}$ test set	1000 reflections (0.55%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 182199 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: NA, SF4, LMT, F3S, FES, CIT, HEM, 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	0.30	0/5241	0.59	0/7063
1	D	0.30	0/5221	0.59	0/7038
2	B	0.32	0/1945	0.57	0/2622
2	E	0.32	0/1945	0.57	0/2622
3	C	0.33	0/2177	0.62	5/2946 (0.2%)
3	F	0.32	0/2177	0.49	1/2946 (0.0%)
All	All	0.31	0/18706	0.58	6/25237 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	47[A]	PHE	CB-CG-CD2	-10.33	113.57	120.80
3	C	47[B]	PHE	CB-CG-CD2	-10.33	113.57	120.80
3	C	47[A]	PHE	CB-CG-CD1	9.85	127.70	120.80
3	C	47[B]	PHE	CB-CG-CD1	9.85	127.70	120.80
3	C	102	PRO	N-CA-C	-5.87	96.84	112.10

There are no chirality outliers.

There are no planarity outliers.

### 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	5145	0	5124	139	0
1	D	5125	0	5100	132	0
2	B	1908	0	1873	40	0
2	E	1908	0	1873	44	0
3	C	2110	0	2123	52	0
3	F	2110	0	2123	49	0
4	A	53	0	29	3	0
4	D	53	0	29	4	0
5	A	26	0	10	11	0
5	D	26	0	10	11	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	1	0
8	B	7	0	0	0	0
8	E	7	0	0	0	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
10	C	86	0	60	0	0
10	F	86	0	60	0	0
11	C	35	0	46	7	0
11	F	35	0	46	9	0
12	A	274	0	0	2	0
12	B	156	0	0	1	0
12	C	47	0	0	1	0
12	D	291	0	0	4	0
12	E	164	0	0	1	0
12	F	59	0	0	0	0
All	All	19737	0	18506	434	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 12.

The worst 5 of 434 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273[B]:ARG:HE	1:A:301:ARG:HH21	1.07	0.91
3:F:131:MET:HG2	11:F:1257:LMT:H123	1.53	0.90
3:C:131:MET:HG2	11:C:1257:LMT:H123	1.52	0.89
1:D:120:ASN:HB3	1:D:298:LEU:HD13	1.58	0.86
1:A:120:ASN:HB3	1:A:298:LEU:HD13	1.57	0.86

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	659/656 (100%)	633 (96%)	22 (3%)	4 (1%)	33	32
1	D	657/656 (100%)	629 (96%)	24 (4%)	4 (1%)	33	32
2	B	239/239 (100%)	230 (96%)	7 (3%)	2 (1%)	27	24
2	E	239/239 (100%)	230 (96%)	7 (3%)	2 (1%)	27	24
3	C	256/256 (100%)	249 (97%)	6 (2%)	1 (0%)	43	45
3	F	256/256 (100%)	249 (97%)	6 (2%)	1 (0%)	43	45
All	All	2306/2302 (100%)	2220 (96%)	72 (3%)	14 (1%)	33	32

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
2	B	3	ARG
2	B	86	ASP
3	C	72	GLU
1	D	122	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	537/533 (101%)	522 (97%)	15 (3%)	56	67
1	D	535/533 (100%)	518 (97%)	17 (3%)	51	62
2	B	213/211 (101%)	208 (98%)	5 (2%)	63	74
2	E	213/211 (101%)	208 (98%)	5 (2%)	63	74
3	C	224/223 (100%)	216 (96%)	8 (4%)	47	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	224/223 (100%)	218 (97%)	6 (3%)	57	68
All	All	1946/1934 (101%)	1890 (97%)	56 (3%)	56	66

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	87	PHE
1	D	137	HIS
3	F	58	MET
3	C	100	LYS
1	D	31	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	123	HIS
1	D	57	ASN
2	E	116	GLN
1	D	26	GLN
1	D	111	HIS

### 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 ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	FAD	A	1656	1	58,58,58	2.13	13 (22%)	85,89,89	2.01	14 (16%)
5	CIT	A	1657[A]	-	12,12,12	1.21	2 (16%)	17,17,17	1.63	1 (5%)
5	CIT	A	1657[B]	-	12,12,12	1.04	1 (8%)	17,17,17	1.74	1 (5%)
7	FES	B	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	B	1241	2	3,9,9	9.87	1 (33%)	0,15,15	0.00	-
9	SF4	B	1242	2	12,12,12	9.65	10 (83%)	0,24,24	0.00	-
10	HEM	C	1255	3	49,50,50	1.79	13 (26%)	46,82,82	1.32	4 (8%)
10	HEM	C	1256	3	49,50,50	1.82	11 (22%)	46,82,82	1.37	4 (8%)
11	LMT	C	1257	-	36,36,36	1.08	2 (5%)	47,47,47	1.27	4 (8%)
4	FAD	D	1656	1	58,58,58	2.11	12 (20%)	85,89,89	2.04	14 (16%)
5	CIT	D	1657[A]	-	12,12,12	1.24	1 (8%)	17,17,17	1.60	1 (5%)
5	CIT	D	1657[B]	-	12,12,12	1.05	1 (8%)	17,17,17	1.68	1 (5%)
7	FES	E	1240	2	0,4,4	0.00	-	0,4,4	0.00	-
8	F3S	E	1241	2	3,9,9	8.76	2 (66%)	0,15,15	0.00	-
9	SF4	E	1242	2	12,12,12	9.68	9 (75%)	0,24,24	0.00	-
10	HEM	F	1255	3	49,50,50	1.80	12 (24%)	46,82,82	1.33	4 (8%)
10	HEM	F	1256	3	49,50,50	1.77	9 (18%)	46,82,82	1.38	5 (10%)
11	LMT	F	1257	-	36,36,36	1.07	2 (5%)	47,47,47	1.27	4 (8%)

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	FAD	A	1656	1	-	0/34/50/50	0/1/6/6
5	CIT	A	1657[A]	-	-	0/16/16/16	0/0/0/0
5	CIT	A	1657[B]	-	-	0/16/16/16	0/0/0/0
7	FES	B	1240	2	-	0/0/4/4	0/0/1/1
8	F3S	B	1241	2	-	0/0/24/24	0/0/3/3
9	SF4	B	1242	2	-	0/0/48/48	0/0/5/5
10	HEM	C	1255	3	-	0/14/114/114	0/0/8/8
10	HEM	C	1256	3	-	0/14/114/114	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMT	C	1257	-	-	0/21/61/61	0/2/2/2
4	FAD	D	1656	1	-	0/34/50/50	0/1/6/6
5	CIT	D	1657[A]	-	-	0/16/16/16	0/0/0/0
5	CIT	D	1657[B]	-	-	0/16/16/16	0/0/0/0
7	FES	E	1240	2	-	0/0/4/4	0/0/1/1
8	F3S	E	1241	2	-	0/0/24/24	0/0/3/3
9	SF4	E	1242	2	-	0/0/48/48	0/0/5/5
10	HEM	F	1255	3	-	0/14/114/114	0/0/8/8
10	HEM	F	1256	3	-	0/14/114/114	0/0/8/8
11	LMT	F	1257	-	-	0/21/61/61	0/2/2/2

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1242	SF4	S4-FE3	-18.90	2.20	2.33
9	B	1242	SF4	S1-FE3	-18.52	2.20	2.33
9	B	1242	SF4	S4-FE3	-18.38	2.20	2.33
9	E	1242	SF4	S1-FE3	-18.25	2.21	2.33
8	B	1241	F3S	S3-FE4	-17.04	2.21	2.33

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1656	FAD	C2'-C1'-N10	-7.79	102.11	112.45
4	A	1656	FAD	C2'-C1'-N10	-7.64	102.32	112.45
4	D	1656	FAD	C1'-N10-C9A	-7.02	112.04	118.87
4	D	1656	FAD	O4B-C1B-N9A	-6.99	101.94	108.44
4	A	1656	FAD	C1'-N10-C9A	-6.85	112.21	118.87

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	656/656 (100%)	0.31	55 (8%) 11 10	15, 29, 66, 78	13 (1%)
1	D	656/656 (100%)	0.35	52 (7%) 13 12	13, 28, 65, 78	16 (2%)
2	B	239/239 (100%)	-0.13	5 (2%) 60 61	16, 24, 46, 73	2 (0%)
2	E	239/239 (100%)	-0.15	6 (2%) 54 55	15, 23, 46, 72	2 (0%)
3	C	255/256 (99%)	0.65	31 (12%) 5 4	21, 37, 71, 93	11 (4%)
3	F	255/256 (99%)	0.34	13 (5%) 27 27	19, 37, 71, 92	9 (3%)
All	All	2300/2302 (99%)	0.27	162 (7%) 16 16	13, 29, 66, 93	53 (2%)

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	255	HIS	11.3
2	B	1	MET	9.6
3	C	254	HIS	8.9
3	C	72	GLU	7.2
3	C	253	THR	7.2

### 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(Å <sup>2</sup> )	Q<0.9
11	LMT	C	1257	35/35	0.43	12.88	55,59,65,66	16
11	LMT	F	1257	35/35	0.35	7.82	55,58,65,66	16
5	CIT	D	1657[B]	13/13	0.55	5.50	29,32,35,36	13
5	CIT	A	1657[A]	13/13	0.50	5.42	31,35,39,41	13
5	CIT	D	1657[A]	13/13	0.55	5.11	26,34,41,42	13
5	CIT	A	1657[B]	13/13	0.50	5.03	25,30,32,35	13
6	NA	A	1658	1/1	0.19	0.70	19,19,19,19	0
8	F3S	E	1241	7/7	0.11	0.60	19,19,20,20	0
4	FAD	A	1656	53/53	0.18	0.35	13,17,21,22	0
4	FAD	D	1656	53/53	0.19	0.34	11,16,21,23	0
6	NA	D	1658	1/1	0.20	0.26	16,16,16,16	0
8	F3S	B	1241	7/7	0.09	-0.09	20,20,21,21	0
10	HEM	F	1256	43/43	0.12	-0.20	31,33,37,40	0
9	SF4	E	1242	8/8	0.11	-0.21	17,18,18,20	0
10	HEM	C	1255	43/43	0.11	-0.24	22,27,29,34	0
10	HEM	F	1255	43/43	0.11	-0.43	21,26,29,33	0
10	HEM	C	1256	43/43	0.12	-0.43	32,34,39,42	0
9	SF4	B	1242	8/8	0.10	-1.12	18,19,19,19	0
7	FES	B	1240	4/4	0.11	-1.57	17,18,18,18	0
7	FES	E	1240	4/4	0.12	-1.72	16,17,17,18	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.