



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:58 pm GMT

PDB ID : 2OZ0
Title : Mechanistic and Structural Studies of H373Q Flavocytochrome b2: Effects of Mutating the Active Site Base
Authors : Tsai, C.-L.; Gokulan, K.; Sobrado, P.; Sacchettini, J.C.; Fitzpatrick, P.F.
Deposited on : 2007-02-23
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 : 1.7.2 (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

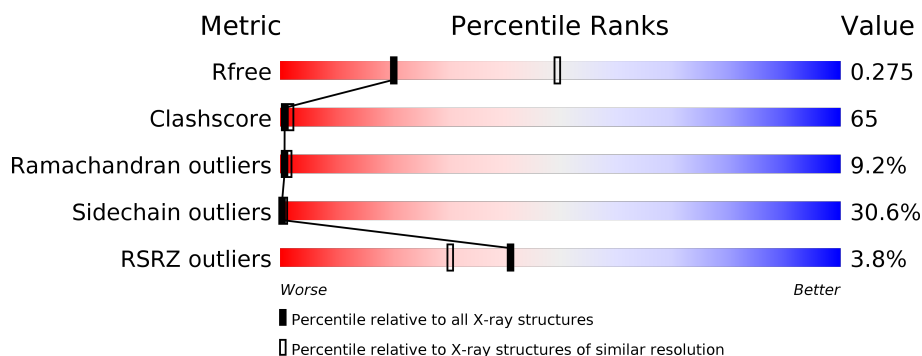
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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	511	
1	B	511	

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
3	FMN	A	569	X	-	X	-
3	FMN	B	570	-	-	X	-
4	PYR	B	571	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7042 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.

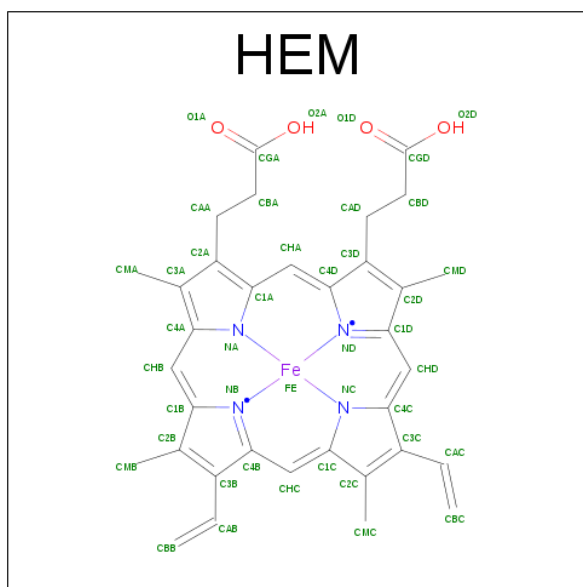
- Molecule 1 is a protein called Cytochrome b2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3833	2441	649	728	15			
1	B	396	Total	C	N	O	S	0	0	0
			3081	1953	524	593	11			

There are 2 discrepancies between the modelled and reference sequences:

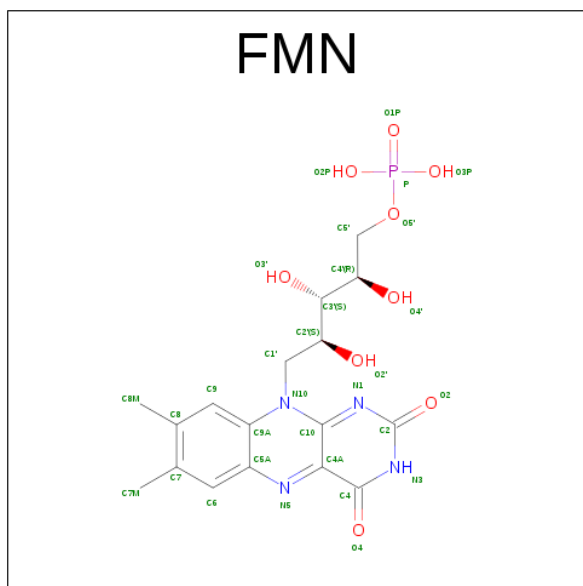
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLN	HIS	ENGINEERED	UNP P00175
B	373	GLN	HIS	ENGINEERED	UNP P00175

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



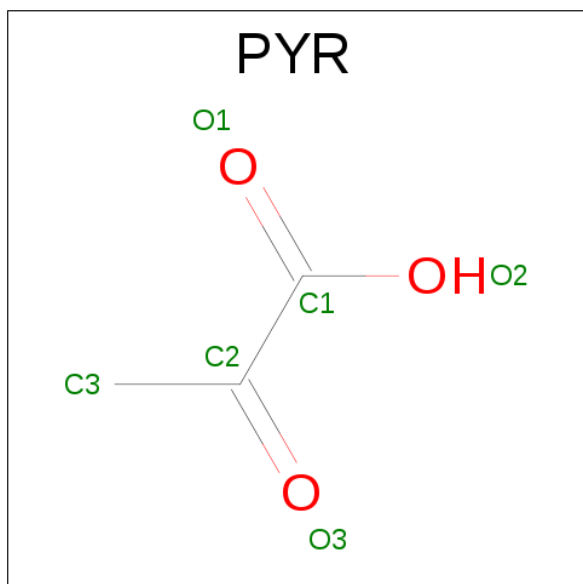
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

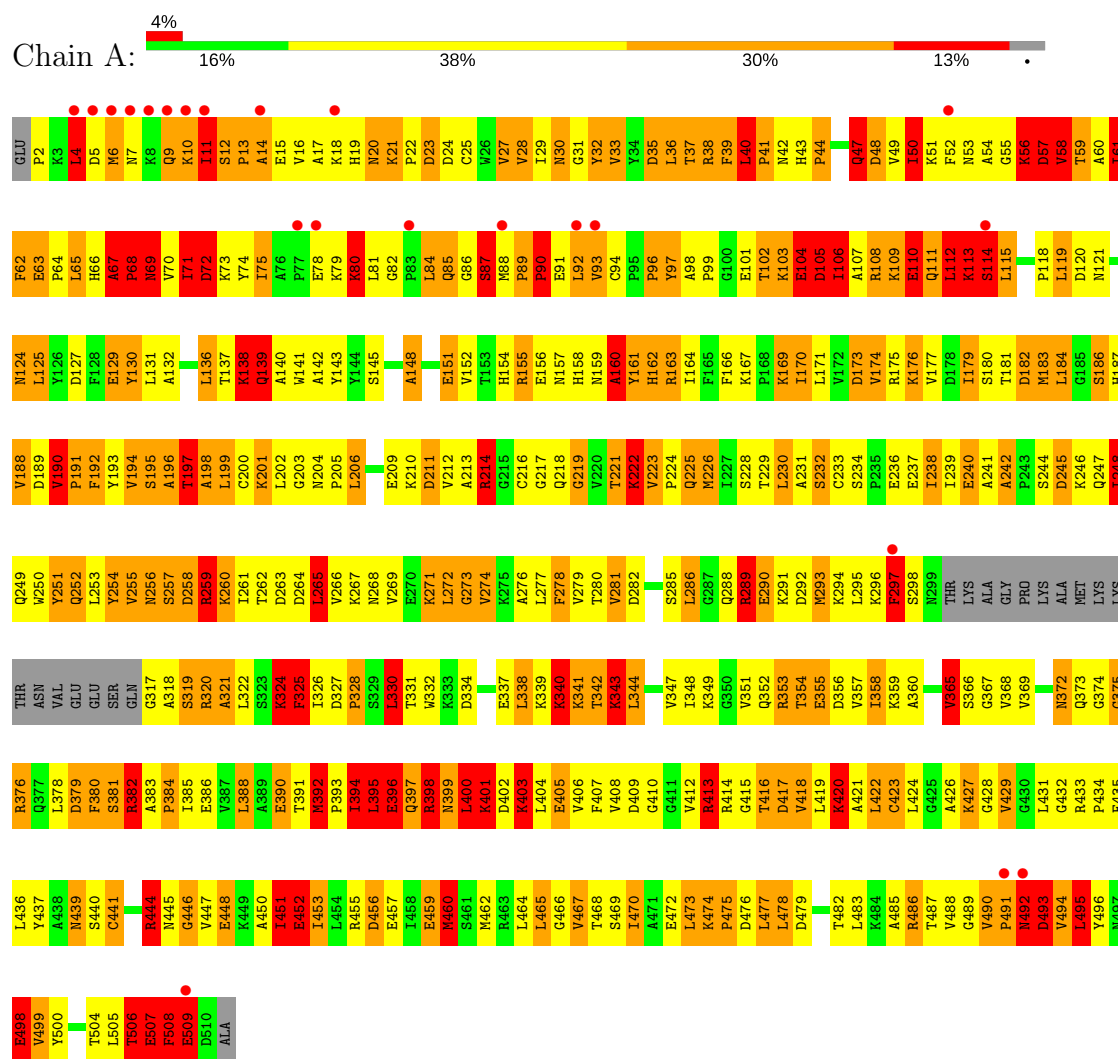
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	10	Total 10	O 10	0	0

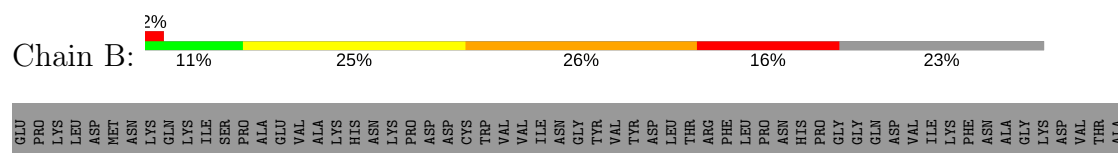
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Cytochrome b2



• Molecule 1: Cytochrome b2



G489	V490	P491	R492	D493	V494	L495	G496	R497	E498	V499	Y500	E501	T504	L505	T506	E507	F508	E509	D510	ALA																																								
K427	G428	V429	G430	L431	G432	R433	L436	Y437	A438	R439	S440	C441	Y442	C443	R444	N445	G446	V447	K449	A450	I451	E452	I453	L454	R455	D456	E457	I458	P459	M460	S461	M462	R463	L464	L465	G466	V467	T468	S469	I470	L473	K474	P475	D476	L477	L478	D479	L480	S481	T482	L483	R486	T487	V488						
V365	S366	G367	V368	V369	L370	S371	N372	Q373	G374	G375	R376	Q377	L378	D379	F380	S381	R382	A383	P384	I385	E386	V387	L388	A389	E390	T391	M392	P393	I394	L395	E396	Q397	R398	N399	L400	K401	D402	K403	L404	E405	V406	F407	V408	D409	G410	G411	V412	R413	R414	L415	G416	D417	V418	L419	K420	A421	L422	C423	L424	
LYS	ALA	MET	LYS	LYS	THR	ASN	VAL	GLU	GLU	SER	GLN	G317	A318	S319	R320	A321	L322	S323	K324	F325	I326	D327	P328	S329	L330	T331	W332	K333	D334	I335	E336	E337	L338	K339	K340	K341	T342	K343	L344	P345	I346	V347	I348	K349	G350	V351	Q352	R353	T354	E355	D356	V357	I358	V359	A360	A361	E362	T363	G364	
P243	S244	D245	K246	Q247	I248	Q249	W250	Y251	Q252	L253	Y254	V255	N256	S257	D258	R259	K260	T261	T262	D263	D264	L265	V266	K267	N268	V269	E270	K271	L272	G273	V274	K275	A276	L277	F278	V279	T280	V281	D282	A283	P284	S285	L286	R289	E290	K291	D292	L293	K296	F297	S298	N299	THR	LYS	ALA	GLY	PRO			
M183	L184	G185	S186	H187	V188	D189	V190	F191	Y192	Y193	A194	S195	A196	T197	L198	R199	C200	K201	L202	G203	N204	P205	L206	E207	G208	E209	K210	A211	D212	V213	V214	K215	G216	C217	Q218	G219	V220	T221	K222	V223	P224	Q225	M226	I227	S228	T229	L230	R231	A231	S232	C233	S234	P235	E236	K237	I238	I239	E240	A241	D242
ILE	PHE	GLU	PRO	LEU	HIS	ALA	PRO	ASN	VAL	ILE	ASP	LYS	LYS	TYR	ALA	PRO	GLU	LYS	LYS	LEU	GLY	PRO	LEU	GLN	GLY	SER	MET	PRO	PRO	GLU	LEU	VAL	CYS	PRO	PRO	TYR	A98	P99	G100	E101	T102	K103	E104	D105	I106	A107	R108	K109	E110	Q111	L112	K113	S114	L115	D116	P117	P118	L119	D120	
H121	I122	I123	M124	L125	Y126	D127	F128	E129	Y130	L131	A132	S133	Q134	T135	L136	K137	C200	K138	Q139	A140	W141	A142	Y143	Y144	S145	S146	G147	A148	N149	D150	F151	V152	T153	H154	R155	N159	A160	Y161	H162	R163	I164	F165	F166	K167	P168	K169	I170	L171	V172	D173	V174	R175	K176	V177	D178	I179	S180	T181	D182	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.69Å 163.69Å 112.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.34 – 2.45	Depositor EDS
% Data completeness (in resolution range)	87.6 (50.00-2.80) 64.2 (48.34-2.45)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.278 0.222 , 0.275	Depositor DCC
R_{free} test set	1937 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7042	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, 0.333 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: FMN, HEM, PYR

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	1.94	115/3907 (2.9%)	2.38	216/5291 (4.1%)
1	B	1.85	71/3130 (2.3%)	2.45	202/4230 (4.8%)
All	All	1.90	186/7037 (2.6%)	2.41	418/9521 (4.4%)

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	2	57
1	B	4	64
All	All	6	121

The worst 5 of 186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	CG-CD	12.01	1.81	1.51
1	B	441	CYS	CB-SG	11.82	2.02	1.82
1	A	413	ARG	CG-CD	10.79	1.78	1.51
1	A	266	VAL	CB-CG2	-10.57	1.30	1.52
1	A	421	ALA	CA-CB	-10.42	1.30	1.52

The worst 5 of 418 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	O-C-N	-25.98	81.14	122.70
1	A	395	LEU	O-C-N	-19.10	92.14	122.70
1	B	317	GLY	C-N-CA	18.27	167.38	121.70
1	A	245	ASP	CB-CG-OD1	-16.45	103.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLU	O-C-N	-16.19	96.79	122.70

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	11	ILE	CA
1	A	298	SER	CA
1	B	102	THR	CB
1	B	149	ASN	CA
1	B	272	LEU	CA

5 of 121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Mainchain
1	A	11	ILE	Peptide
1	A	31	GLY	Peptide
1	A	47	GLN	Peptide
1	A	50	ILE	Peptide

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	3833	0	3888	416	1
1	B	3081	0	3136	511	1
2	A	43	0	30	15	0
3	A	31	0	17	13	0
3	B	31	0	18	15	0
4	B	6	0	3	1	0
5	A	7	0	0	0	0
5	B	10	0	0	1	0
All	All	7042	0	7092	914	1

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 65.

The worst 5 of 914 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:175:ARG:CG	1:B:175:ARG:CD	1.77	1.63
1:A:413:ARG:CG	1:A:413:ARG:CD	1.78	1.61
1:A:343:LYS:CG	1:A:343:LYS:CB	1.79	1.60
1:A:286:LEU:CD1	1:A:286:LEU:CG	1.78	1.59
1:B:106:ILE:CD1	1:B:106:ILE:CG1	1.75	1.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:NH2	1:B:169:LYS:CG[6_555]	2.19	0.01

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	488/511 (96%)	381 (78%)	67 (14%)	40 (8%)	1	2
1	B	392/511 (77%)	273 (70%)	78 (20%)	41 (10%)	0	1
All	All	880/1022 (86%)	654 (74%)	145 (16%)	81 (9%)	1	1

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	11	ILE
1	A	20	ASN
1	A	37	THR
1	A	48	ASP

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	424/440 (96%)	298 (70%)	126 (30%)	0	1
1	B	340/440 (77%)	232 (68%)	108 (32%)	0	1
All	All	764/880 (87%)	530 (69%)	234 (31%)	0	1

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	VAL
1	B	104	GLU
1	B	420	LYS
1	A	448	GLU
1	A	483	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	B	124	ASN
1	B	439	ASN
1	A	439	ASN
1	A	497	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](#)

4 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	HEM	A	560	1	28,50,50	2.55	11 (39%)	17,82,82	3.64	6 (35%)
3	FMN	A	569	-	31,33,33	1.07	1 (3%)	38,50,50	3.99	18 (47%)
3	FMN	B	570	-	31,33,33	1.46	3 (9%)	38,50,50	3.83	21 (55%)
4	PYR	B	571	-	2,5,5	1.35	0	2,6,6	1.17	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	HEM	A	560	1	-	0/6/54/54	0/0/8/8
3	FMN	A	569	-	1/1/4/4	0/16/18/18	0/3/3/3
3	FMN	B	570	-	-	0/16/18/18	0/3/3/3
4	PYR	B	571	-	-	0/0/4/4	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	C3C-C2C	-6.21	1.32	1.40
2	A	560	HEM	C3B-C2B	-4.36	1.34	1.40
2	A	560	HEM	C4B-CHC	-2.09	1.34	1.40
3	B	570	FMN	P-O5'	-2.02	1.53	1.60
2	A	560	HEM	C1B-NB	2.02	1.39	1.36

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C4A-C10-N10	-9.75	113.75	120.52
3	A	569	FMN	C4A-C10-N10	-8.20	114.83	120.52
3	A	569	FMN	C4A-C4-N3	-6.31	114.50	123.48
3	A	569	FMN	C4-C4A-C10	-6.08	115.04	119.96
3	B	570	FMN	C4-C4A-C10	-6.03	115.09	119.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	569	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	560	HEM	15	0
3	A	569	FMN	13	0
3	B	570	FMN	15	0
4	B	571	PYR	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	492/511 (96%)	-0.22	22 (4%) 34 24	19, 52, 147, 183	0
1	B	396/511 (77%)	-0.28	12 (3%) 51 39	18, 65, 107, 171	0
All	All	888/1022 (86%)	-0.24	34 (3%) 41 30	18, 58, 138, 183	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASN	8.5
1	A	9	GLN	8.3
1	A	6	MET	6.7
1	B	99	PRO	6.4
1	A	5	ASP	5.9

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
4	PYR	B	571	6/6	0.80	0.43	8.43	120,125,128,133	0
3	FMN	A	569	31/31	0.88	0.17	0.80	10,14,17,18	0
2	HEM	A	560	43/43	0.97	0.21	0.57	90,98,116,122	0
3	FMN	B	570	31/31	0.87	0.18	0.49	16,21,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.