wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:07 PM GMT

PDB ID	:	1FCB
Title	:	MOLECULAR STRUCTURE OF FLAVOCYTOCHROME B2 AT 2.4 ANGSTROMS RESOLUTION
Authors	:	Mathews, F.S.; Xia, Z.-X.
Deposited on	:	1990-01-16
Resolution	:	2.40 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 (i) symbol.

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

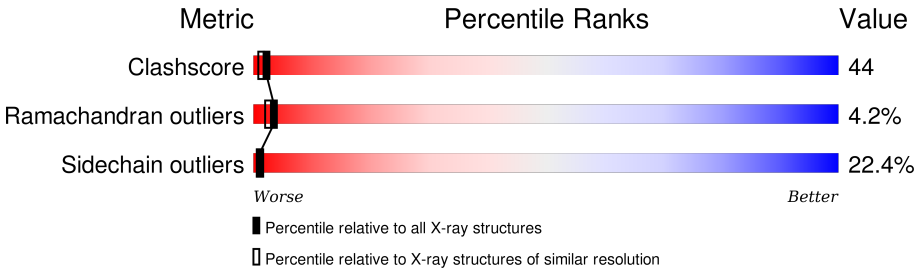
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	35% 33% 19% 10% •
1	B	511	26% 29% 17% 6% 22%

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	570	X	-	-	-

2 Entry composition

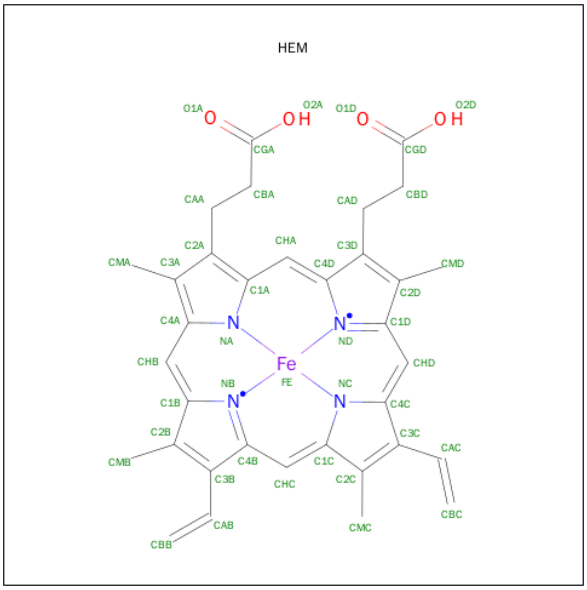
There are 5 unique types of molecules in this entry. The entry contains 7342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOCYTOCHROME B2.

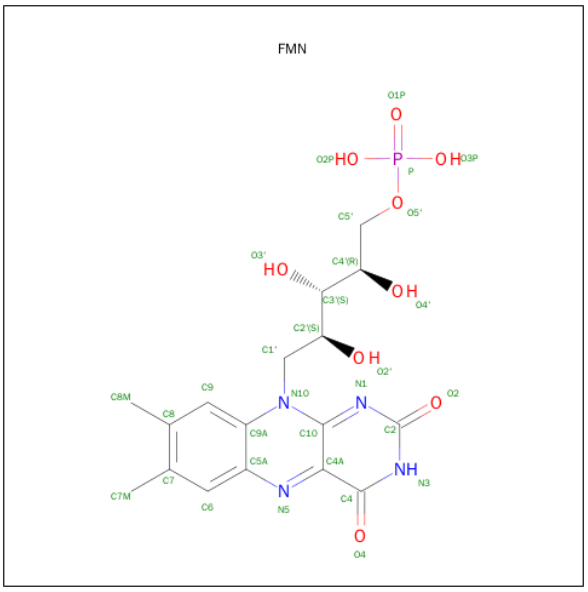
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3841	2446	652	728	15			
1	B	400	Total	C	N	O	S	0	0	0
			3107	1968	529	599	11			

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



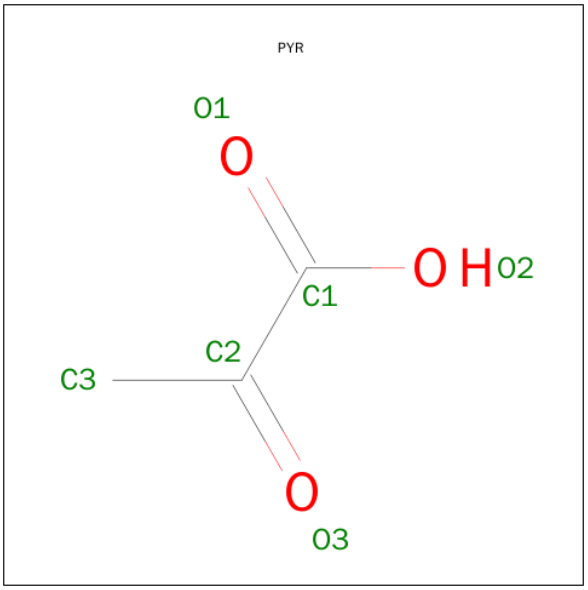
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	182	Total O 182 182	0	0
5	B	101	Total O 101 101	0	0

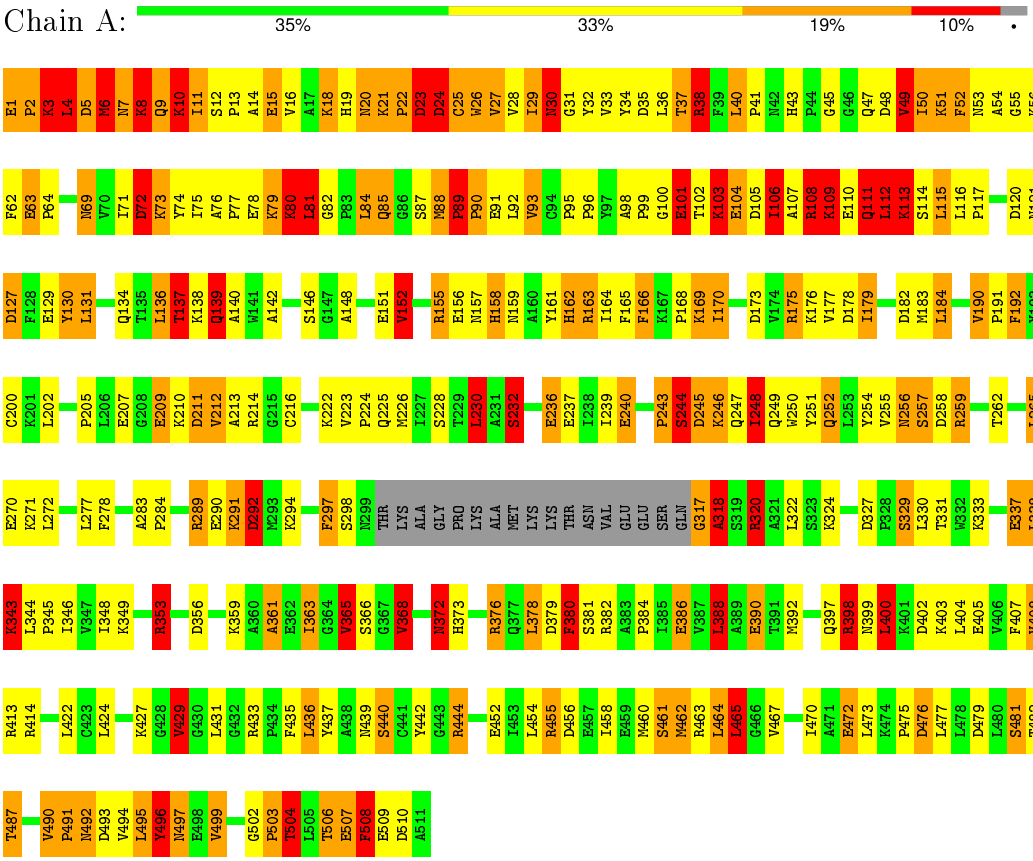
3 Residue-property plots (i)

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.

Note EDS was not executed.

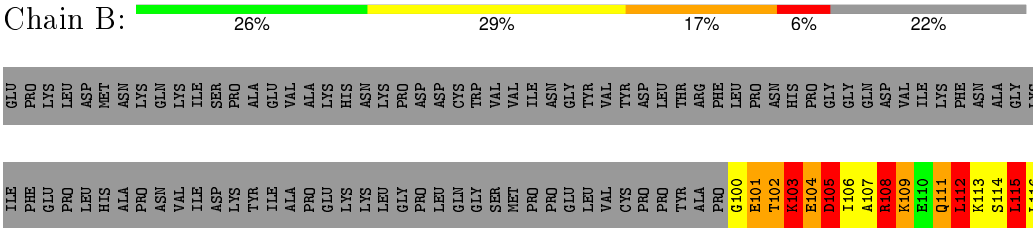
- Molecule 1: FLAVOCYTOCHROME B2

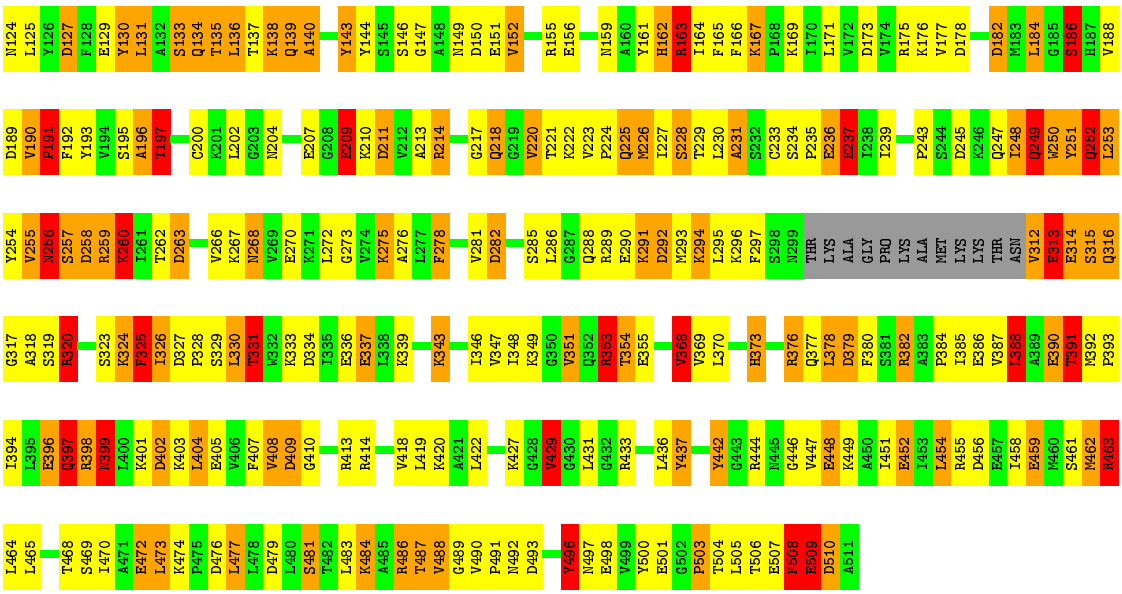
Chain A:



- Molecule 1: FLAVOCYTOCHROME B2

Chain B:




N124 L125 Y126 D127 F128 E129 Y130 L131 A132 S133 Q134 T135 L136 T137 K138 Q139 A140 Y143 Y144 S145 S146 G147 A148 N149 D150 E151 V152 R155 E156 N159 A160 Y161 H162 R163 I164 F165 F166 K167 P168 K169 I170 L171 V172 D173 Y174 R175 K176 V177 D178 D182 M183 L184 G185 S186 H187 V188
D189 V190 P191 F192 Y193 V194 S195 A196 T197 C200 K201 L202 G203 N204 E207 G208 E209 K210 D211 V212 A213 R214 G217 Q218 G219 V220 T221 K222 V223 P224 Q225 M226 I227 S228 T229 L230 A231 S232 C233 S234 P235 E236 E237 I238 I239 P243 S244 D245 K246 Q247 I248 Q249 W250 Y251 Q252 L253
Y254 V255 N256 S257 D258 R259 K260 I261 T262 D263 V266 K267 N268 V269 E270 K271 L272 G273 V274 K275 A276 L277 F278 V281 D282 S285 L286 G287 Q288 R289 E290 K291 D292 M293 K294 L295 K296 F297 S298 N299 THR LYS ALA GLY PRO LYS ALA MET LYS LYS THR ASN V312 E313 E314 S315 Q316
G317 A318 S319 R320 S323 M324 F325 I326 D327 P328 S329 L330 T331 M332 K333 D334 I335 E336 E337 I338 N339 K343 I346 V347 I348 K349 G350 V351 Q352 R353 T354 E355 V368 V369 L370 H373 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 R413 R414 V418 L419 K420 A421 L422 K427 G428 V429 G430 L431 G432 R433 L436 Y437 Y442 G443 R444 N445 G446 V447 E448 K449 A450 I451 E452 I453 L454 R455 D456 E457 I458 E459 M460 S461 M462 R463
L464 L465 T468 S469 I470 A471 E472 L473 K474 P475 D476 L477 L478 D479 L480 S481 T482 L483 K484 A485 R486 T487 V488 G489 V490 P491 N492 D493 Y496 N497 E498 V499 Y500 E501 G502 P503 T504 L505 T506 E507 F508 E509 D510 A511

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	165.51Å 165.51Å 113.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

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	1.00	2/3916 (0.1%)	2.80	286/5303 (5.4%)
1	B	0.97	0/3156	2.83	233/4263 (5.5%)
All	All	0.99	2/7072 (0.0%)	2.81	519/9566 (5.4%)

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	0	4
1	B	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CD-OE1	-5.64	1.19	1.25
1	A	232	SER	CB-OG	-5.27	1.35	1.42

The worst 5 of 519 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	353	ARG	NE-CZ-NH1	41.59	141.09	120.30
1	B	259	ARG	NE-CZ-NH2	32.94	136.77	120.30
1	A	155	ARG	NE-CZ-NH2	32.52	136.56	120.30
1	A	376	ARG	NE-CZ-NH1	30.93	135.76	120.30
1	A	353	ARG	NE-CZ-NH2	-26.04	107.28	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	A	353	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	38	ARG	Sidechain
1	B	163	ARG	Sidechain

5.2 Too-close contacts (i)

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	3841	0	3899	403	2
1	B	3107	0	3156	259	0
2	A	43	0	30	9	0
3	A	31	0	17	0	0
3	B	31	0	18	2	0
4	B	6	0	3	0	0
5	A	182	0	0	9	0
5	B	101	0	0	11	0
All	All	7342	0	7123	628	2

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 44.

The worst 5 of 628 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:10:LYS:O	1:A:10:LYS:HD3	1.18	1.33
1:A:24:ASP:HA	1:A:37:THR:CG2	1.60	1.27
1:A:1:GLU:N	1:A:71:ILE:HD12	1.49	1.27
1:A:1:GLU:H3	1:A:2:PRO:CD	1.50	1.25
1:A:24:ASP:CA	1:A:37:THR:HG21	1.66	1.25

All (2) 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:38:ARG:NH2	1:A:245:ASP:OD1[3_665]	2.09	0.11
1:A:38:ARG:CZ	1:A:245:ASP:OD1[3_665]	2.12	0.08

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	490/511 (96%)	438 (89%)	27 (6%)	25 (5%)	2 1
1	B	396/511 (78%)	353 (89%)	31 (8%)	12 (3%)	5 4
All	All	886/1022 (87%)	791 (89%)	58 (6%)	37 (4%)	3 2

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	ASP
1	A	7	ASN
1	A	10	LYS
1	A	22	PRO

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	423/440 (96%)	330 (78%)	93 (22%)	1 1
1	B	342/440 (78%)	264 (77%)	78 (23%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	765/880 (87%)	594 (78%)	171 (22%)	1 1

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	B	105	ASP
1	B	463	ARG
1	A	399	ASN
1	A	472	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	439	ASN
1	B	377	GLN
1	A	372	ASN
1	B	121	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	24,50,50	2.20	7 (29%)	16,82,82	3.20	7 (43%)
3	FMN	A	570	-	32,33,33	1.12	2 (6%)	34,50,50	4.23	15 (44%)
3	FMN	B	570	-	32,33,33	1.46	4 (12%)	34,50,50	3.85	19 (55%)
4	PYR	B	580	-	2,5,5	5.49	2 (100%)	2,6,6	5.77	2 (100%)

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	570	-	1/1/4/4	0/18/18/18	0/3/3/3
3	FMN	B	570	-	-	0/18/18/18	0/3/3/3
4	PYR	B	580	-	-	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	C3B-C2B	-5.72	1.33	1.40
2	A	560	HEM	C3C-C2C	-4.13	1.35	1.40
3	A	570	FMN	C10-N1	-2.96	1.30	1.35
3	B	570	FMN	C10-N1	-2.78	1.30	1.35
3	B	570	FMN	P-O5'	-2.22	1.53	1.59

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	570	FMN	C4A-C10-N10	-9.30	113.76	120.52
3	A	570	FMN	C4A-C10-N10	-7.85	114.81	120.52
3	A	570	FMN	C4-C4A-C10	-7.68	115.03	119.94
3	A	570	FMN	N3-C2-N1	-7.65	114.81	127.69
3	B	570	FMN	C4-C4A-C10	-7.57	115.10	119.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	570	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	560	HEM	9	0
3	B	570	FMN	2	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.