



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:37 PM GMT

PDB ID : 4TMC  
Title : CRYSTAL STRUCTURE of OLD YELLOW ENZYME from CANDIDA MACEDONIENSIS AKU4588 COMPLEXED with P-HYDROXYBENZALDEHYDE  
Authors : Horita, S.; Kataoka, M.; Kitamura, N.; Nakagawa, T.; Miyakawa, T.; Ohtsuka, J.; Nagata, K.; Shimizu, S.; Tanokura, M.  
Deposited on : 2014-05-31  
Resolution : 1.80 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

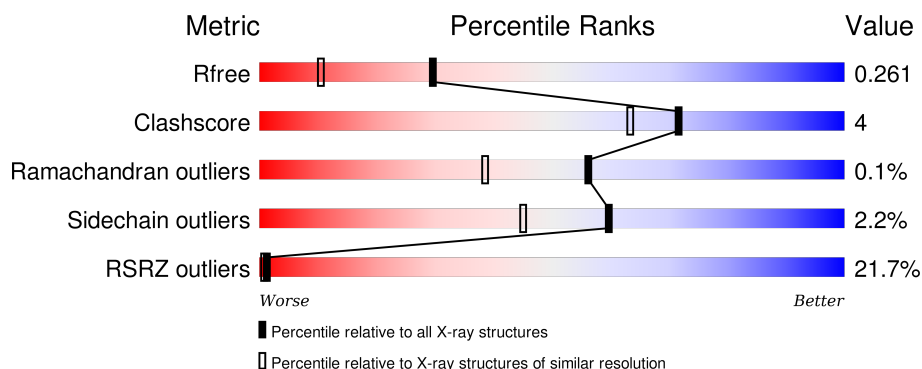
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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  $\geq 3$ , 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	403	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	B	403	<div> <div>5%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	C	403	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	D	403	<div> <div>76%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

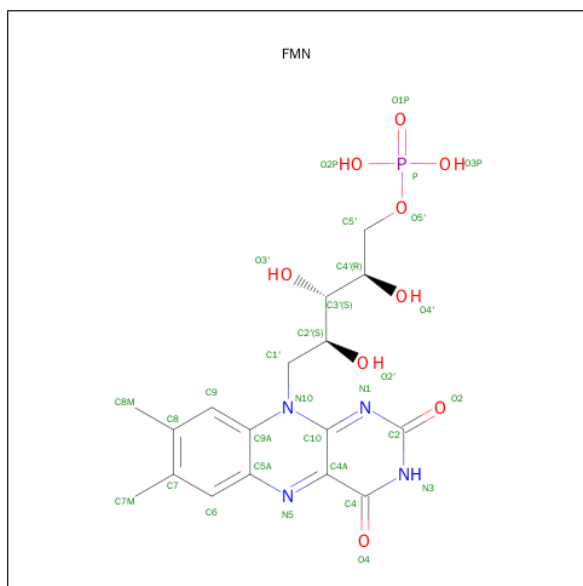
There are 4 unique types of molecules in this entry. The entry contains 14010 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Old yellow enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3209	2055	543	605	6			
1	B	398	Total	C	N	O	S	0	0	0
			3200	2050	542	602	6			
1	C	399	Total	C	N	O	S	0	0	0
			3209	2055	543	605	6			
1	D	396	Total	C	N	O	S	0	0	0
			3182	2038	538	600	6			

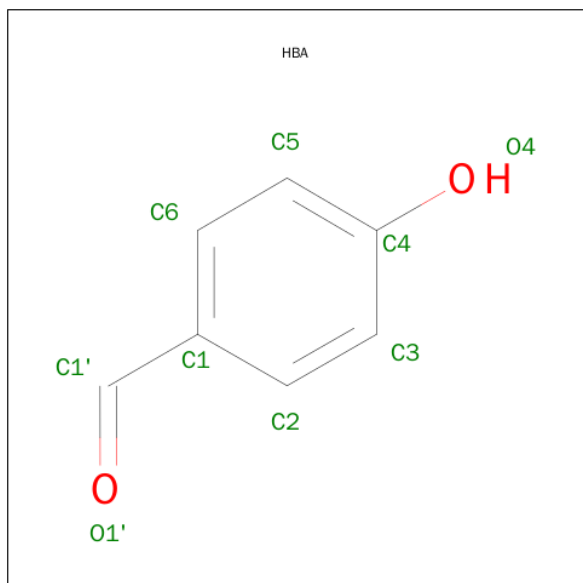
- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is P-HYDROXYBENZALDEHYDE (three-letter code: HBA) (formula:  $C_7H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		
3	B	1	Total	C	O	0	0
			9	7	2		
3	C	1	Total	C	O	0	0
			9	7	2		
3	D	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	254	Total	O	0	0
			254	254		
4	C	280	Total	O	0	0
			280	280		

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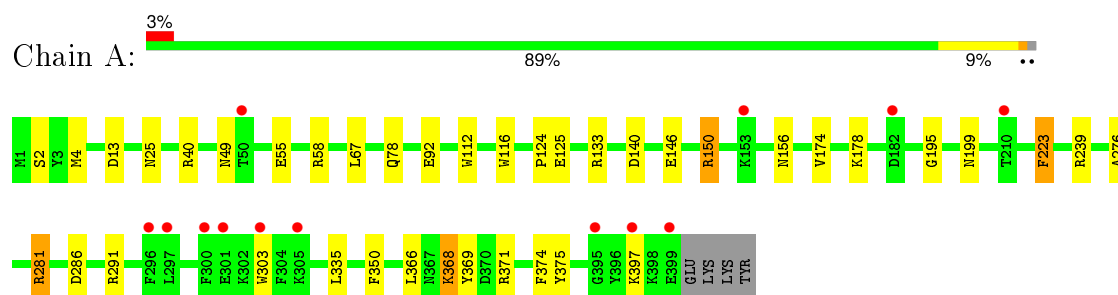
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	206	Total 206	O 206	0	0

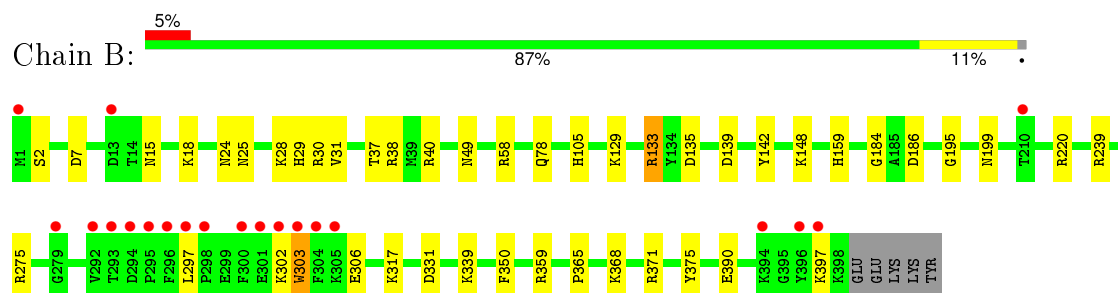
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

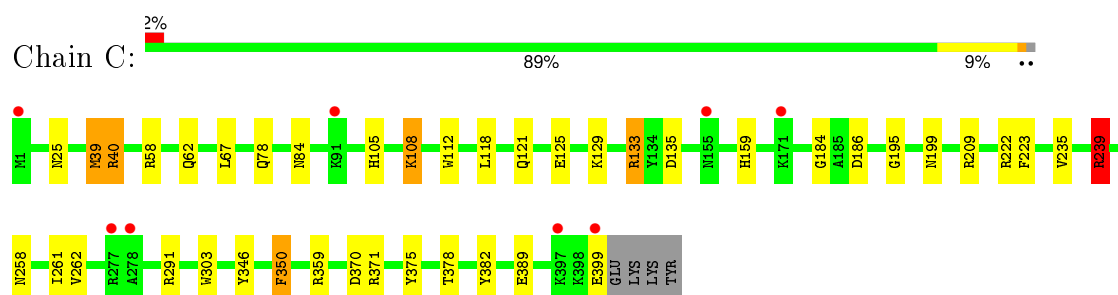
- Molecule 1: Old yellow enzyme



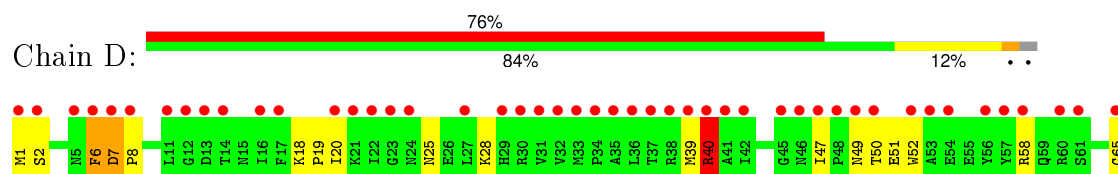
- Molecule 1: Old yellow enzyme



- Molecule 1: Old yellow enzyme



- Molecule 1: Old yellow enzyme



E390	K317	F250	I190	V126	T86
S391	G318	G251	H191	L127	L67
V392	P319	T252	S192	K128	I68
A393	V320	M253	A193	K129	I69
K394	L321	S254	M194	E130	T70
G395	R322	G255	G195	G131	E71
Y396	V323		Y196	L132	G72
LYS	G324	G260	L197	R133	T73
LYS	N325	I261	L198	L134	F74
GLU	V326	V262	M199	D135	P75
GLU	A327	A263	Q200	S136	S76
LYS	A333	Q264	F201	A137	A77
LYS	T334	T265	L202	T138	Q78
TYR	L335	A266	D203	D139	S79
		V267	P204	D140	G80
		V268	I205	L141	G81
		I269	S206	Y142	Y82
		G270	N207	M143	P83
		E271	N208		N84
		L272	R209	E146	V85
		E273	T210	E147	P86
		K274	D211	K148	G87
		R275	E212	E149	I88
		A276	Y213	A150	H89
			G214	A151	S90
			T215	L152	K91
			S216	K153	E92
			I217	A154	Q93
			E218	N155	L94
			N219	N156	A95
			R220	P157	E96
			A221	Q158	W87
			R222	H159	K98
			F223	G160	K99
			T224	I161	I100
			L225	T162	F101
			E226		N102
			V227	I166	A103
			V228		I104
			D229	Y169	H105
			A230	A170	E106
			V231	K171	N107
			D232	E172	K108
			D233	Y173	S109
			A234	V174	F110
			V235	D175	V111
			G236	A176	W112
			A237	A177	V113
			E238	K178	Q114
			R239	K179	L115
			T240	A180	W116
			S241	I181	V117
			I242	D182	G118
			R243	A183	G119
			F244	G184	R120
			S245	A185	Q121
			P246	D186	A122
			Y247	G187	W123
			I315	I315	P124
			H316	H316	E125

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.39Å 151.03Å 199.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 1.80 19.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.95-1.80) 99.8 (19.95-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.167 , 0.205 0.240 , 0.261	Depositor DCC
$R_{free}$ test set	7395 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 147412 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, HBA

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	0.97	2/3293 (0.1%)	1.03	9/4463 (0.2%)
1	B	0.97	2/3284 (0.1%)	1.06	19/4451 (0.4%)
1	C	0.95	2/3293 (0.1%)	1.18	21/4463 (0.5%)
1	D	0.89	3/3266 (0.1%)	1.05	13/4429 (0.3%)
All	All	0.94	9/13136 (0.1%)	1.08	62/17806 (0.3%)

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	D	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	GLU	CD-OE1	9.07	1.35	1.25
1	D	218	GLU	CD-OE1	7.03	1.33	1.25
1	D	218	GLU	CD-OE2	6.57	1.32	1.25
1	B	133	ARG	CD-NE	-6.40	1.35	1.46
1	B	239	ARG	CD-NE	-6.33	1.35	1.46

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	ARG	NE-CZ-NH1	24.27	132.43	120.30
1	C	40	ARG	NE-CZ-NH2	-22.28	109.16	120.30
1	B	133	ARG	NE-CZ-NH2	-20.77	109.91	120.30
1	D	40	ARG	NE-CZ-NH2	-18.41	111.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	40	ARG	NE-CZ-NH1	17.81	129.21	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1	MET	Peptide

## 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	3209	0	3138	27	0
1	B	3200	0	3132	26	0
1	C	3209	0	3138	24	0
1	D	3182	0	3106	35	0
2	A	31	0	19	2	0
2	B	31	0	19	2	0
2	C	31	0	19	0	0
2	D	31	0	19	3	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
4	A	310	0	0	1	0
4	B	254	0	0	3	0
4	C	280	0	0	1	0
4	D	206	0	0	5	0
All	All	14010	0	12610	111	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.

The worst 5 of 111 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:4:MET:HE3	1:A:366:LEU:HB2	1.37	1.07
1:B:368:LYS:HG3	4:B:823:HOH:O	1.52	1.07
1:D:371:ARG:NH2	4:D:641:HOH:O	2.01	0.93
1:A:55:GLU:HG2	4:A:673:HOH:O	1.75	0.87
1:A:4:MET:CE	1:A:366:LEU:HB2	2.06	0.85

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	397/403 (98%)	386 (97%)	11 (3%)	0	100	100
1	B	396/403 (98%)	382 (96%)	14 (4%)	0	100	100
1	C	397/403 (98%)	385 (97%)	12 (3%)	0	100	100
1	D	394/403 (98%)	379 (96%)	14 (4%)	1 (0%)	46	29
All	All	1584/1612 (98%)	1532 (97%)	51 (3%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	PHE

### 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	336/340 (99%)	330 (98%)	6 (2%)	66	54
1	B	335/340 (98%)	328 (98%)	7 (2%)	61	47
1	C	336/340 (99%)	332 (99%)	4 (1%)	78	71
1	D	333/340 (98%)	320 (96%)	13 (4%)	39	21
All	All	1340/1360 (98%)	1310 (98%)	30 (2%)	60	45

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	118	LEU
1	C	350	PHE
1	D	350	PHE
1	C	239	ARG
1	D	2	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	C	25	ASN
1	D	332	GLN
1	B	78	GLN
1	B	199	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

8 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	FMN	A	501	-	32,33,33	2.02	9 (28%)	34,50,50	2.74	14 (41%)
3	HBA	A	502	-	9,9,9	0.68	0	11,11,11	1.43	2 (18%)
2	FMN	B	501	-	32,33,33	1.79	7 (21%)	34,50,50	2.23	7 (20%)
3	HBA	B	502	-	9,9,9	0.95	0	11,11,11	1.07	0
2	FMN	C	501	-	32,33,33	1.49	4 (12%)	34,50,50	2.71	12 (35%)
3	HBA	C	502	-	9,9,9	0.92	0	11,11,11	1.04	0
2	FMN	D	501	-	32,33,33	1.67	9 (28%)	34,50,50	2.69	10 (29%)
3	HBA	D	502	-	9,9,9	0.84	0	11,11,11	1.12	1 (9%)

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	FMN	A	501	-	-	0/18/18/18	0/3/3/3
3	HBA	A	502	-	-	0/2/2/2	0/1/1/1
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
3	HBA	B	502	-	-	0/2/2/2	0/1/1/1
2	FMN	C	501	-	-	0/18/18/18	0/3/3/3
3	HBA	C	502	-	-	0/2/2/2	0/1/1/1
2	FMN	D	501	-	-	0/18/18/18	0/3/3/3
3	HBA	D	502	-	-	0/2/2/2	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FMN	C10-N1	-2.70	1.31	1.35
2	A	501	FMN	C6-C5A	-2.60	1.37	1.41
2	B	501	FMN	C6-C5A	-2.19	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FMN	C9A-N10	2.00	1.41	1.38
2	C	501	FMN	C4-N3	2.03	1.36	1.33

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FMN	C4-C4A-C10	-5.74	116.27	119.94
2	C	501	FMN	C4A-C4-N3	-5.58	116.23	123.52
2	A	501	FMN	C4-C4A-C10	-5.30	116.55	119.94
2	B	501	FMN	C4A-C4-N3	-5.22	116.70	123.52
2	D	501	FMN	C4A-C4-N3	-4.89	117.13	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FMN	2	0
2	B	501	FMN	2	0
2	D	501	FMN	3	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	399/403 (99%)	-0.13	13 (3%) 50 44	14, 21, 35, 49	0
1	B	398/403 (98%)	0.11	20 (5%) 32 27	15, 24, 45, 63	0
1	C	399/403 (99%)	0.05	8 (2%) 68 64	16, 24, 39, 50	0
1	D	396/403 (98%)	3.98	305 (77%) 0 0	49, 83, 121, 145	0
All	All	1592/1612 (98%)	1.00	346 (21%) 1 1	14, 26, 104, 145	0

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	TRP	13.7
1	D	134	TYR	12.5
1	D	197	LEU	12.1
1	D	201	PHE	11.5
1	D	136	SER	11.2

### 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
3	HBA	A	502	9/9	0.89	0.16	1.43	21,23,26,35	0
2	FMN	B	501	31/31	0.90	0.16	0.99	22,25,29,30	0
3	HBA	B	502	9/9	0.84	0.18	0.81	22,31,38,48	0
3	HBA	C	502	9/9	0.91	0.11	0.47	19,21,27,32	0
2	FMN	A	501	31/31	0.94	0.10	0.42	17,20,22,22	0
2	FMN	C	501	31/31	0.96	0.08	-0.45	17,19,21,22	0
3	HBA	D	502	9/9	0.92	0.14	-2.02	21,22,28,33	0
2	FMN	D	501	31/31	0.93	0.10	-3.73	19,22,28,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.