



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2017 – 02:34 PM EST

PDB ID : 5KO8
Title : Crystal structure of haliscomenobacter hydrossis iodotyrosine deiodinase (IYD) bound to FMN and mono-iodotyrosine (I-Tyr)
Authors : Ingavat, N.; Kavran, J.M.; Sun, Z.; Rokita, S.E.
Deposited on : 2016-06-29
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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-20028442

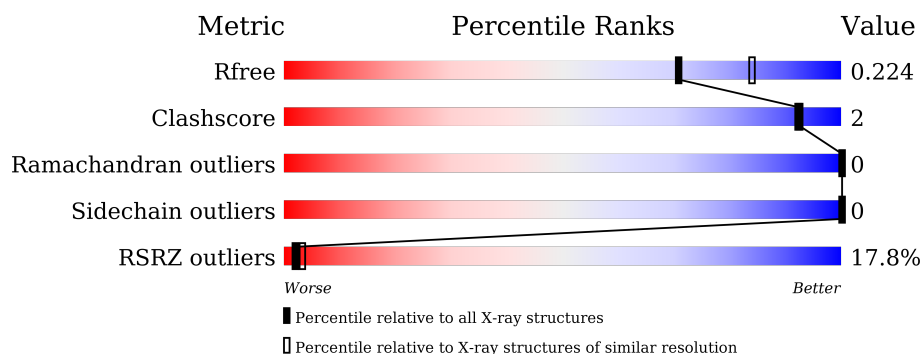
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	228	<div> <div>14%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	228	<div> <div>20%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7227 atoms, of which 3504 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.

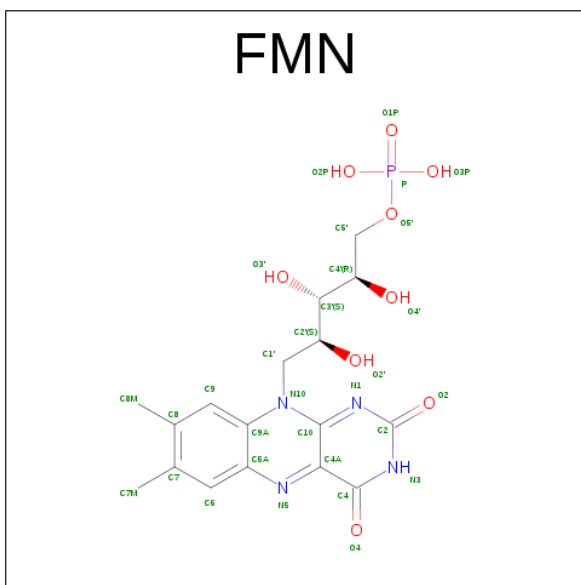
- Molecule 1 is a protein called Nitroreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	1	0
			3436	1121	1704	290	314	7			
1	B	218	Total	C	H	N	O	S	0	1	0
			3489	1135	1732	296	318	8			

There are 12 discrepancies between the modelled and reference sequences:

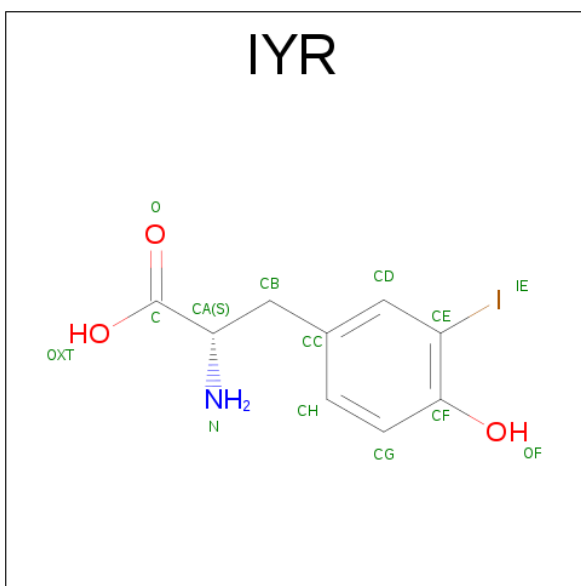
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	HIS	-	expression tag	UNP F4KU78
A	224	HIS	-	expression tag	UNP F4KU78
A	225	HIS	-	expression tag	UNP F4KU78
A	226	HIS	-	expression tag	UNP F4KU78
A	227	HIS	-	expression tag	UNP F4KU78
A	228	HIS	-	expression tag	UNP F4KU78
B	223	HIS	-	expression tag	UNP F4KU78
B	224	HIS	-	expression tag	UNP F4KU78
B	225	HIS	-	expression tag	UNP F4KU78
B	226	HIS	-	expression tag	UNP F4KU78
B	227	HIS	-	expression tag	UNP F4KU78
B	228	HIS	-	expression tag	UNP F4KU78

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

- Molecule 3 is 3-IODO-TYROSINE (three-letter code: IYR) (formula: $C_9H_{10}INO_3$).



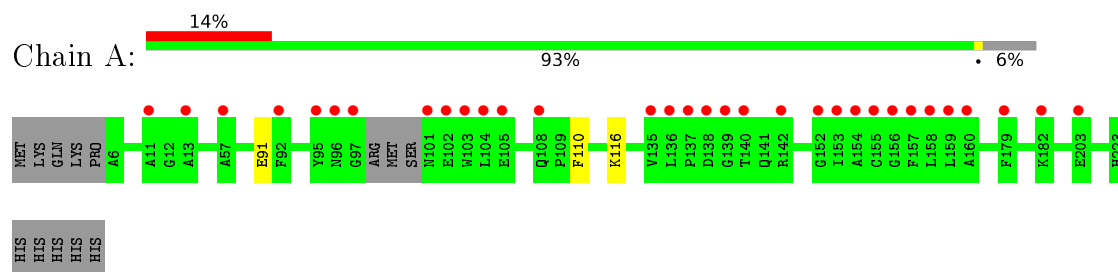
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total 84	O 84	0	0
4	B	44	Total 44	O 44	0	0

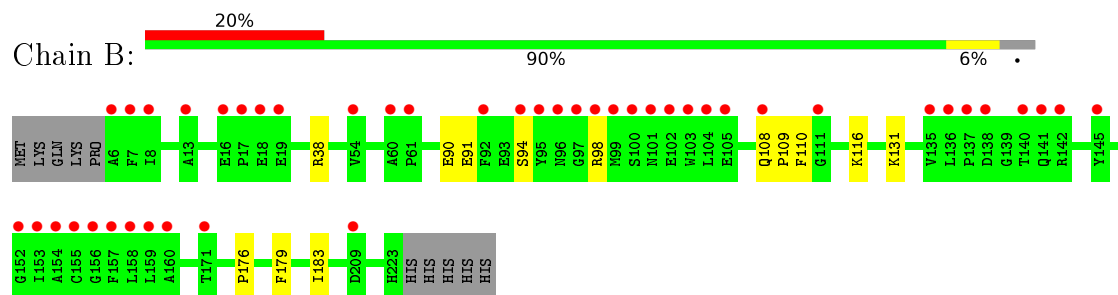
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Nitroreductase



• Molecule 1: Nitroreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.72Å 152.72Å 87.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.18 – 2.15 38.18 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.18-2.15) 89.2 (38.18-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.16Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.232 0.187 , 0.224	Depositor DCC
R_{free} test set	1454 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	40.4	Xtrriage
Anisotropy	0.116	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7227	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, IYR

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	0.29	0/1784	0.43	0/2427
1	B	0.27	0/1810	0.42	0/2462
All	All	0.28	0/3594	0.43	0/4889

There are no bond length outliers.

There are no bond angle outliers.

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	1732	1704	1704	5	0
1	B	1757	1732	1732	9	0
2	A	31	19	19	0	0
2	B	31	19	19	1	0
3	A	22	15	12	2	0
3	B	22	15	12	2	0
4	A	84	0	0	1	0
4	B	44	0	0	1	0
All	All	3723	3504	3498	14	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 2.

All (14) 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:ARG:NH1	2:B:301:FMN:O2	2.24	0.66
1:A:116:LYS:NZ	4:A:401:HOH:O	2.32	0.62
1:A:91:GLU:HG3	1:A:116:LYS:HE2	1.86	0.58
1:B:110:PHE:CD2	3:B:302[B]:IYR:IE	3.29	0.56
1:B:131:LYS:NZ	4:B:403:HOH:O	2.40	0.55
1:A:110:PHE:CD2	3:A:302[B]:IYR:IE	3.32	0.52
1:A:91:GLU:HG3	1:A:116:LYS:CE	2.43	0.48
1:B:90:GLU:HG3	1:B:176:PRO:HB3	1.97	0.47
1:B:108:GLN:N	1:B:109:PRO:CD	2.78	0.47
1:B:179:PHE:CE2	1:B:183:ILE:HG13	2.53	0.43
1:A:110:PHE:CG	3:A:302[B]:IYR:IE	3.42	0.42
1:B:94:SER:HA	1:B:98:ARG:HB2	2.01	0.42
1:B:91:GLU:HG3	1:B:116:LYS:CE	2.51	0.41
1:B:110:PHE:CG	3:B:302[B]:IYR:IE	3.43	0.41

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	212/228 (93%)	209 (99%)	3 (1%)	0	100	100
1	B	217/228 (95%)	214 (99%)	3 (1%)	0	100	100
All	All	429/456 (94%)	423 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	184/196 (94%)	184 (100%)	0	100	100
1	B	187/196 (95%)	187 (100%)	0	100	100
All	All	371/392 (95%)	371 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

6 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	301	-	31,33,33	1.16	2 (6%)	32,50,50	1.86	3 (9%)
3	IYR	A	302[A]	-	11,14,14	1.06	1 (9%)	14,19,19	1.56	2 (14%)
3	IYR	A	302[B]	-	11,14,14	1.14	1 (9%)	14,19,19	1.49	2 (14%)
2	FMN	B	301	-	31,33,33	1.14	2 (6%)	32,50,50	1.71	4 (12%)
3	IYR	B	302[A]	-	11,14,14	1.00	1 (9%)	14,19,19	1.71	2 (14%)
3	IYR	B	302[B]	-	11,14,14	1.10	1 (9%)	14,19,19	1.48	2 (14%)

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	301	-	-	0/18/18/18	0/3/3/3
3	IYR	A	302[A]	-	-	0/4/8/8	0/1/1/1
3	IYR	A	302[B]	-	-	0/4/8/8	0/1/1/1
2	FMN	B	301	-	-	0/18/18/18	0/3/3/3
3	IYR	B	302[A]	-	-	0/4/8/8	0/1/1/1
3	IYR	B	302[B]	-	-	0/4/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[B]	IYR	CE-IE	-3.14	2.02	2.10
3	B	302[B]	IYR	CE-IE	-3.01	2.02	2.10
3	A	302[A]	IYR	CE-IE	-2.75	2.02	2.10
3	B	302[A]	IYR	CE-IE	-2.60	2.03	2.10
2	A	301	FMN	C1'-N10	2.79	1.51	1.48
2	B	301	FMN	C4A-N5	3.14	1.38	1.33
2	B	301	FMN	C1'-N10	3.35	1.52	1.48
2	A	301	FMN	C4A-N5	3.61	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FMN	C1'-N10-C9A	2.02	121.17	118.83
3	B	302[B]	IYR	CF-CE-IE	2.66	122.91	119.77
2	B	301	FMN	C4A-N5-C5A	2.81	120.04	116.72
3	A	302[A]	IYR	CF-CE-IE	2.88	123.17	119.77
3	A	302[B]	IYR	CF-CE-IE	2.91	123.21	119.77
2	A	301	FMN	C4A-N5-C5A	3.03	120.30	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	IYR	CF-CE-IE	3.15	123.48	119.77
2	B	301	FMN	C5A-C9A-N10	3.27	120.03	117.58
2	A	301	FMN	C5A-C9A-N10	3.60	120.28	117.58
3	B	302[B]	IYR	OF-CF-CE	3.92	124.48	119.08
3	A	302[B]	IYR	OF-CF-CE	3.95	124.53	119.08
3	A	302[A]	IYR	OF-CF-CE	4.43	125.19	119.08
3	B	302[A]	IYR	OF-CF-CE	4.75	125.62	119.08
2	B	301	FMN	C2-N1-C10	7.62	119.89	113.39
2	A	301	FMN	C2-N1-C10	8.52	120.66	113.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302[B]	IYR	2	0
2	B	301	FMN	1	0
3	B	302[B]	IYR	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 ⓘ

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	215/228 (94%)	0.77	32 (14%) 3 5	29, 47, 90, 109	0
1	B	218/228 (95%)	1.10	45 (20%) 1 2	31, 56, 101, 126	0
All	All	433/456 (94%)	0.93	77 (17%) 2 3	29, 52, 98, 126	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	10.6
1	B	98	ARG	8.0
1	B	137	PRO	7.1
1	B	104	LEU	7.1
1	B	97	GLY	6.5
1	B	103	TRP	6.4
1	A	137	PRO	6.1
1	B	135	VAL	5.8
1	B	102	GLU	5.7
1	B	100	SER	5.6
1	A	140	THR	5.4
1	A	104	LEU	5.0
1	A	136	LEU	5.0
1	A	139	GLY	5.0
1	B	138	ASP	4.7
1	B	101	ASN	4.3
1	A	155	CYS	4.0
1	A	179	PHE	3.9
1	A	101	ASN	3.9
1	B	99	MET	3.8
1	B	153	ILE	3.7
1	B	140	THR	3.6
1	A	152	GLY	3.5
1	B	105	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	135	VAL	3.3
1	A	108	GLN	3.3
1	B	155	CYS	3.3
1	A	142	ARG	3.3
1	A	97	GLY	3.2
1	A	103	TRP	3.2
1	A	156	GLY	3.2
1	B	108	GLN	3.1
1	B	152	GLY	3.0
1	B	95	TYR	3.0
1	B	145	TYR	3.0
1	B	158	LEU	2.9
1	A	102	GLU	2.9
1	B	7	PHE	2.9
1	B	94	SER	2.9
1	A	95	TYR	2.9
1	A	13	ALA	2.9
1	A	157	PHE	2.8
1	A	154	ALA	2.8
1	A	153	ILE	2.8
1	B	142	ARG	2.8
1	B	18	GLU	2.8
1	B	159	LEU	2.6
1	B	96	ASN	2.6
1	A	138	ASP	2.6
1	A	160	ALA	2.6
1	B	8	ILE	2.5
1	B	92	PHE	2.5
1	B	154	ALA	2.5
1	B	19	GLU	2.5
1	A	92	PHE	2.5
1	B	6	ALA	2.5
1	A	11	ALA	2.4
1	B	60	ALA	2.4
1	A	105	GLU	2.4
1	A	182	LYS	2.4
1	B	16	GLU	2.4
1	B	156	GLY	2.4
1	B	13	ALA	2.3
1	B	171	THR	2.3
1	B	157	PHE	2.3
1	B	17	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	158	LEU	2.2
1	A	57	ALA	2.2
1	A	96	ASN	2.2
1	B	54	VAL	2.1
1	B	61	PRO	2.1
1	B	209	ASP	2.1
1	B	111	GLY	2.1
1	A	203	GLU	2.1
1	A	159	LEU	2.1
1	B	141	GLN	2.0
1	B	160	ALA	2.0

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, 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(Å ²)	Q<0.9
2	FMN	A	301	31/31	0.98	0.15	-0.24	31,42,51,58	0
2	FMN	B	301	31/31	0.96	0.16	-0.30	35,44,52,58	0
3	IYR	A	302[B]	14/14	0.97	0.14	-0.32	46,60,74,80	14
3	IYR	A	302[A]	14/14	0.97	0.14	-0.60	42,59,71,75	14
3	IYR	B	302[A]	14/14	0.97	0.12	-0.97	46,60,72,73	14
3	IYR	B	302[B]	14/14	0.97	0.12	-1.13	49,59,73,90	14

6.5 Other polymers [i](#)

There are no such residues in this entry.