



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 06:45 PM GMT

PDB ID : 3GH8  
Title : Crystal structure of Mus musculus iodotyrosine deiodinase (IYD) bound to FMN and di-iodotyrosine (DIT)  
Authors : Thomas, S.R.; McTamney, P.M.; Adler, J.M.; LaRonde-LeBlanc, N.; Rokita, S.E.  
Deposited on : 2009-03-03  
Resolution : 2.61 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



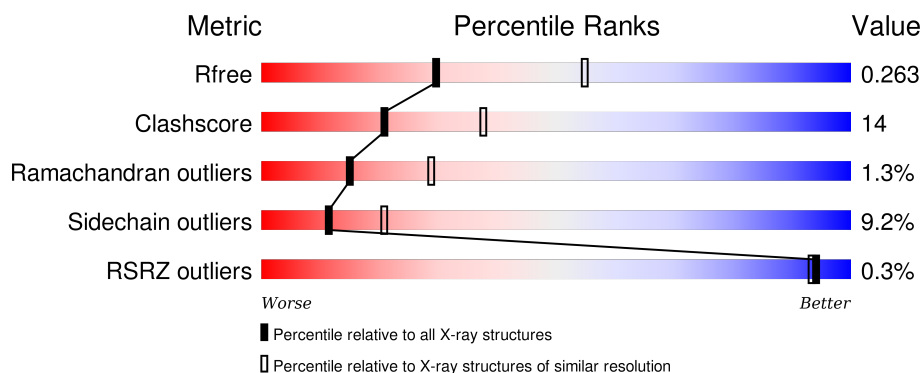
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	259	<div> <div>61%</div> <div>22%</div> <div>•</div> <div>15%</div> </div>
1	B	259	<div> <div>56%</div> <div>27%</div> <div>•</div> <div>15%</div> </div>
1	C	259	<div> <div>58%</div> <div>24%</div> <div>•</div> <div>15%</div> </div>
1	D	259	<div> <div>56%</div> <div>24%</div> <div>• •</div> <div>15%</div> </div>
1	E	259	<div> <div>60%</div> <div>23%</div> <div>•</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	259	<div><div></div><div>58%22%15%</div></div>
1	G	259	<div>%<div><div></div><div>58%23%15%</div></div></div>
1	H	259	<div><div></div><div>57%25%15%</div></div>



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14910 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 Iodotyrosine dehalogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1783	1142	317	315	9			
1	B	220	Total	C	N	O	S	0	0	0
			1773	1136	314	314	9			
1	C	221	Total	C	N	O	S	0	0	0
			1783	1142	317	315	9			
1	D	220	Total	C	N	O	S	0	0	0
			1777	1139	316	313	9			
1	E	221	Total	C	N	O	S	0	0	0
			1783	1142	317	315	9			
1	F	220	Total	C	N	O	S	0	0	0
			1773	1136	314	314	9			
1	G	221	Total	C	N	O	S	0	0	0
			1783	1142	317	315	9			
1	H	220	Total	C	N	O	S	0	0	0
			1777	1139	316	313	9			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
A	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
A	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
A	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
A	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
A	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8
A	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
B	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
B	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
B	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
B	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
B	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
B	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
C	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
C	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
C	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
C	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
C	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
C	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8
C	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
D	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
D	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
D	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
D	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
D	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
D	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8
D	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
E	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
E	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
E	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
E	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
E	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
E	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8
E	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
F	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
F	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
F	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
F	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
F	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
F	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8
F	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
G	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
G	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
G	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
G	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
G	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
G	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8
G	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8
H	33	MET	-	EXPRESSION TAG	UNP Q9DCX8
H	286	HIS	-	EXPRESSION TAG	UNP Q9DCX8
H	287	HIS	-	EXPRESSION TAG	UNP Q9DCX8
H	288	HIS	-	EXPRESSION TAG	UNP Q9DCX8
H	289	HIS	-	EXPRESSION TAG	UNP Q9DCX8
H	290	HIS	-	EXPRESSION TAG	UNP Q9DCX8

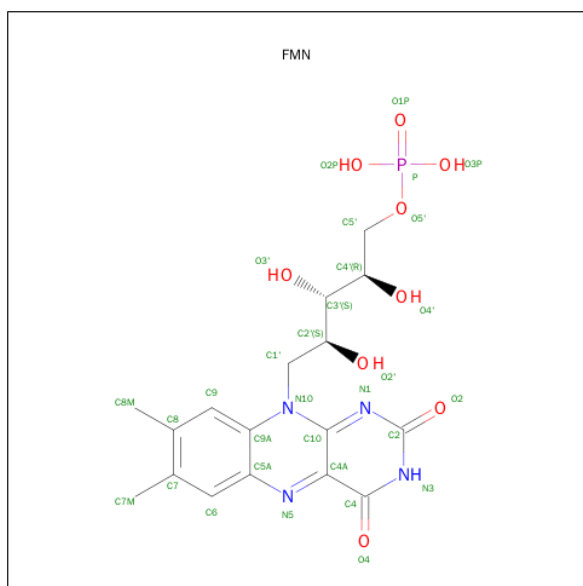
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Chain	Residue	Modelled	Actual	Comment	Reference
H	291	HIS	-	EXPRESSION TAG	UNP Q9DCX8

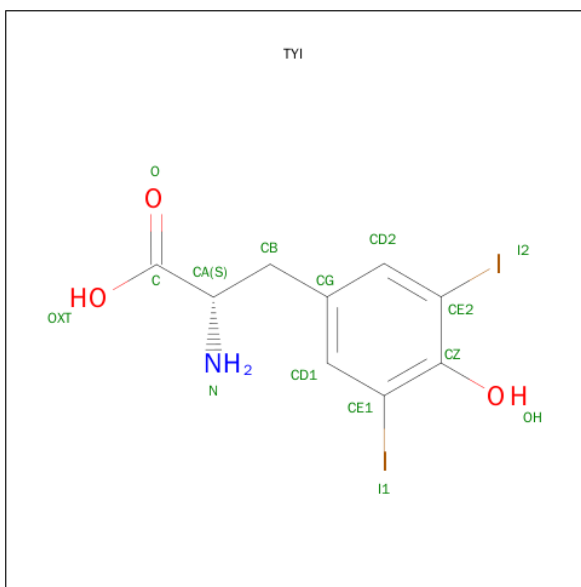
- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
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		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 3,5-DIODOTYROSINE (three-letter code: TYI) (formula:  $C_9H_9I_2NO_3$ ).

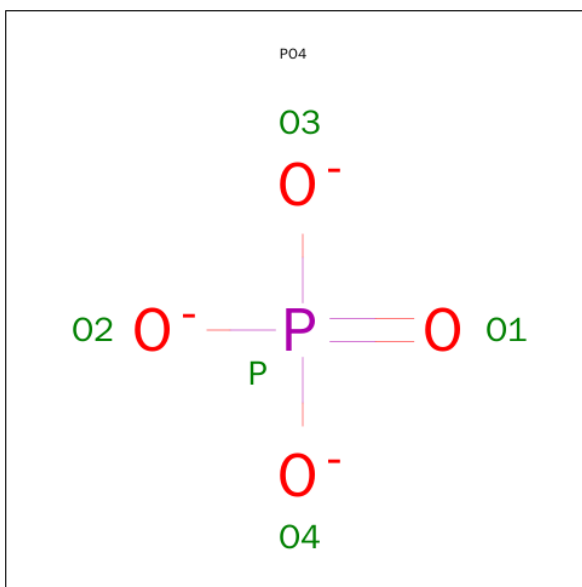




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	B	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	C	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	D	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	E	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	F	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	G	1	Total	C	I	N	O	0	0
			15	9	2	1	3		
3	H	1	Total	C	I	N	O	0	0
			15	9	2	1	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

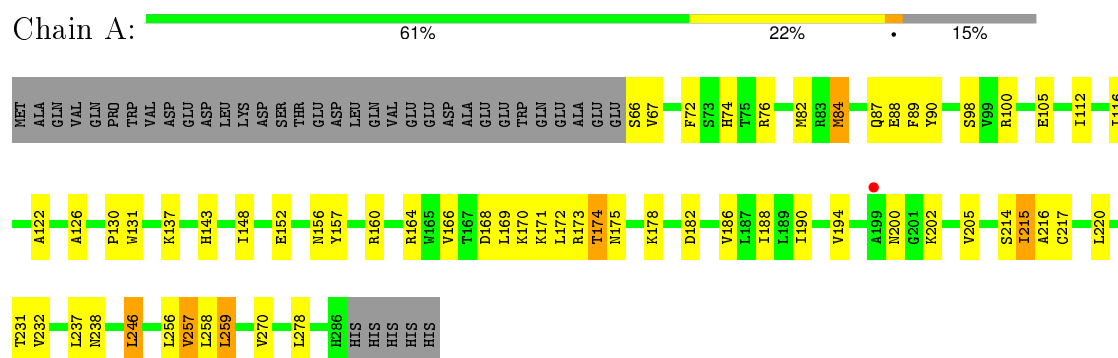
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	38	Total	O	0	0
			38	38		
5	C	39	Total	O	0	0
			39	39		
5	D	23	Total	O	0	0
			23	23		
5	E	48	Total	O	0	0
			48	48		
5	F	40	Total	O	0	0
			40	40		
5	G	38	Total	O	0	0
			38	38		
5	H	38	Total	O	0	0
			38	38		



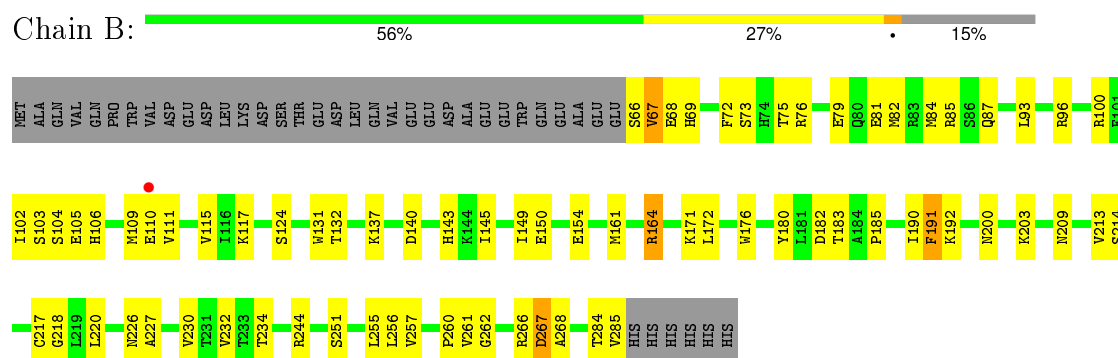
### 3 Residue-property plots

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.

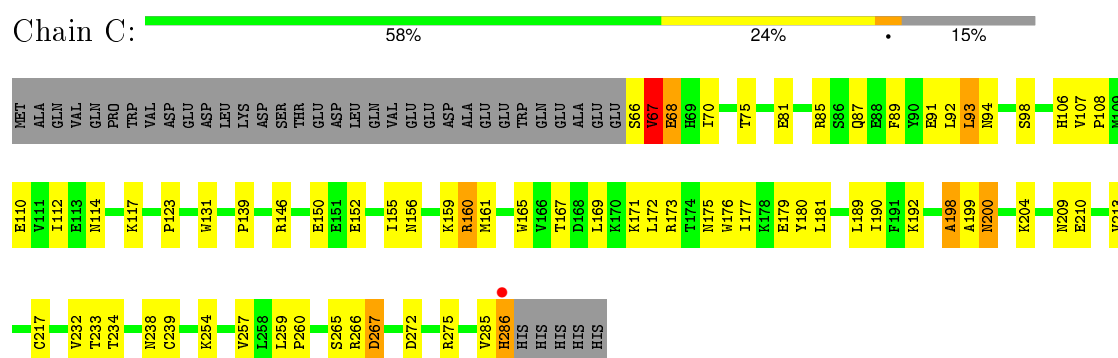
#### • Molecule 1: Iodotyrosine dehalogenase 1



#### • Molecule 1: Iodotyrosine dehalogenase 1

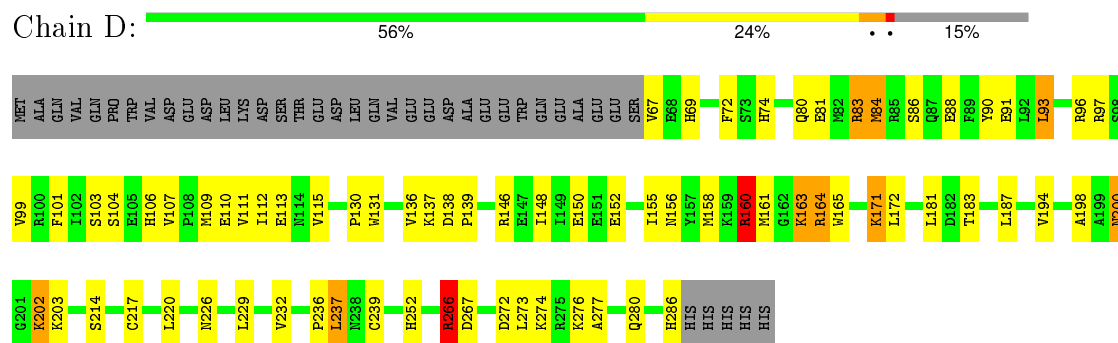


#### • Molecule 1: Iodotyrosine dehalogenase 1

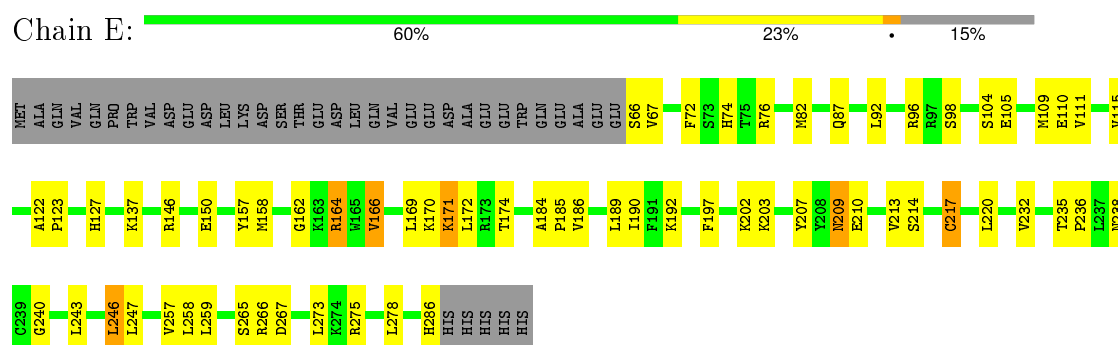




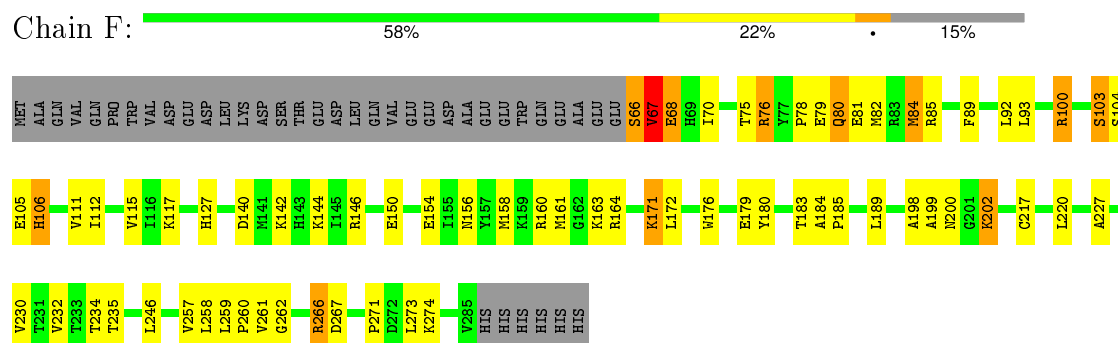
- Molecule 1: Iodotyrosine dehalogenase 1



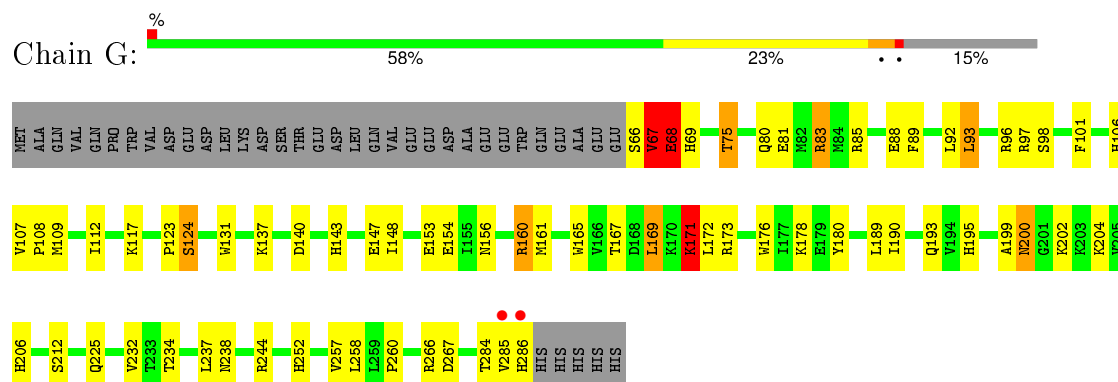
- Molecule 1: Iodotyrosine dehalogenase 1



- Molecule 1: Iodotyrosine dehalogenase 1

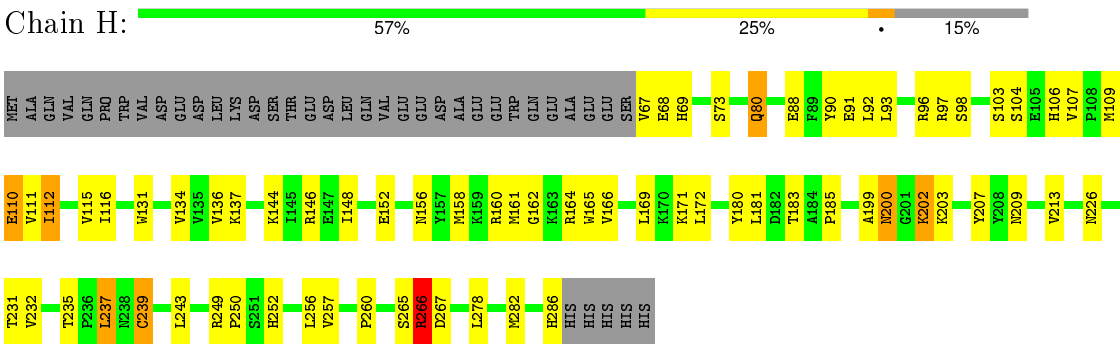


- Molecule 1: Iodotyrosine dehalogenase 1





● Molecule 1: Iodotyrosine dehalogenase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.61Å 112.57Å 189.25Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	30.00 – 2.61 48.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.61) 96.7 (48.37-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.181 , 0.264 0.182 , 0.263	Depositor DCC
$R_{free}$ test set	3195 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.986	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 14.6	EDS
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 62910 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PO4, TYI

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	0.92	0/1823	0.92	2/2468 (0.1%)
1	B	0.89	1/1812 (0.1%)	0.93	1/2453 (0.0%)
1	C	0.86	0/1823	0.91	1/2468 (0.0%)
1	D	0.88	0/1817	0.90	4/2460 (0.2%)
1	E	0.93	2/1823 (0.1%)	0.90	1/2468 (0.0%)
1	F	0.91	1/1812 (0.1%)	0.96	4/2453 (0.2%)
1	G	0.88	0/1823	0.92	0/2468
1	H	0.92	1/1817 (0.1%)	0.90	2/2460 (0.1%)
All	All	0.90	5/14550 (0.0%)	0.92	15/19698 (0.1%)

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	C	0	1
1	F	1	1
1	G	0	1
All	All	1	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	PHE	CE2-CZ	6.18	1.49	1.37
1	E	207	TYR	CE2-CZ	5.95	1.46	1.38
1	E	217	CYS	CB-SG	-5.74	1.72	1.81
1	H	239	CYS	CB-SG	-5.20	1.73	1.81
1	F	217	CYS	CB-SG	-5.05	1.73	1.81

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



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	100	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	F	100	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	246	LEU	CA-CB-CG	6.47	130.18	115.30
1	E	246	LEU	CA-CB-CG	6.33	129.85	115.30
1	H	237	LEU	CA-CB-CG	5.95	128.98	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	67	VAL	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	285	VAL	Peptide
1	F	66	SER	Peptide
1	G	285	VAL	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	1783	0	1839	42	0
1	B	1773	0	1832	58	0
1	C	1783	0	1839	69	0
1	D	1777	0	1834	70	0
1	E	1783	0	1839	34	0
1	F	1773	0	1832	58	0
1	G	1783	0	1839	55	0
1	H	1777	0	1834	68	0
2	A	31	0	19	3	0
2	B	31	0	19	4	0
2	C	31	0	19	2	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
2	F	31	0	19	1	0
2	G	31	0	19	1	0
2	H	31	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	8	3	0
3	B	15	0	8	4	0
3	C	15	0	8	2	0
3	D	15	0	7	2	0
3	E	15	0	8	0	0
3	F	15	0	8	3	0
3	G	15	0	8	1	0
3	H	15	0	7	3	0
4	C	5	0	0	0	0
4	G	5	0	0	0	0
5	A	36	0	0	8	0
5	B	38	0	0	12	0
5	C	39	0	0	10	0
5	D	23	0	0	7	0
5	E	48	0	0	8	0
5	F	40	0	0	13	0
5	G	38	0	0	12	0
5	H	38	0	0	19	0
All	All	14910	0	14902	424	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 14.

The worst 5 of 424 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:E:164:ARG:HD3	5:E:305:HOH:O	1.38	1.21
1:B:191:PHE:HB2	5:B:294:HOH:O	1.43	1.14
1:D:266:ARG:HH11	1:D:266:ARG:CB	1.61	1.13
1:B:132:THR:HB	5:B:294:HOH:O	1.51	1.08
1:E:110:GLU:HA	5:E:403:HOH:O	1.53	1.07

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	219/259 (85%)	201 (92%)	16 (7%)	2 (1%)	21	41
1	B	218/259 (84%)	199 (91%)	16 (7%)	3 (1%)	14	26
1	C	219/259 (85%)	202 (92%)	13 (6%)	4 (2%)	11	20
1	D	218/259 (84%)	204 (94%)	13 (6%)	1 (0%)	34	58
1	E	219/259 (85%)	206 (94%)	10 (5%)	3 (1%)	14	26
1	F	218/259 (84%)	201 (92%)	13 (6%)	4 (2%)	11	20
1	G	219/259 (85%)	200 (91%)	14 (6%)	5 (2%)	8	13
1	H	218/259 (84%)	203 (93%)	14 (6%)	1 (0%)	34	58
All	All	1748/2072 (84%)	1616 (92%)	109 (6%)	23 (1%)	15	29

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	126	ALA
1	B	67	VAL
1	B	79	GLU
1	C	68	GLU

### 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	198/233 (85%)	180 (91%)	18 (9%)	12	22
1	B	197/233 (84%)	178 (90%)	19 (10%)	10	19
1	C	198/233 (85%)	183 (92%)	15 (8%)	16	31
1	D	197/233 (84%)	178 (90%)	19 (10%)	10	19
1	E	198/233 (85%)	176 (89%)	22 (11%)	8	13
1	F	197/233 (84%)	178 (90%)	19 (10%)	10	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	198/233 (85%)	180 (91%)	18 (9%)	12	22
1	H	197/233 (84%)	181 (92%)	16 (8%)	15	27
All	All	1580/1864 (85%)	1434 (91%)	146 (9%)	11	21

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	220	LEU
1	E	170	LYS
1	H	92	LEU
1	D	232	VAL
1	E	105	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	HIS
1	E	74	HIS
1	H	156	ASN
1	D	156	ASN
1	D	200	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](#)

18 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	-	32,33,33	1.45	3 (9%)	34,50,50	2.35	8 (23%)
3	TYI	A	302	-	12,15,15	1.25	1 (8%)	15,21,21	1.77	3 (20%)
2	FMN	B	301	-	32,33,33	1.48	6 (18%)	34,50,50	2.40	9 (26%)
3	TYI	B	302	-	12,15,15	1.79	3 (25%)	15,21,21	1.88	4 (26%)
4	PO4	C	1	-	4,4,4	0.47	0	6,6,6	0.25	0
2	FMN	C	301	-	32,33,33	1.23	4 (12%)	34,50,50	1.85	7 (20%)
3	TYI	C	302	-	12,15,15	1.52	2 (16%)	15,21,21	1.99	5 (33%)
2	FMN	D	301	-	32,33,33	1.44	4 (12%)	34,50,50	2.39	10 (29%)
3	TYI	D	302	-	12,15,15	1.15	2 (16%)	15,21,21	2.23	6 (40%)
2	FMN	E	301	-	32,33,33	1.31	2 (6%)	34,50,50	2.26	9 (26%)
3	TYI	E	302	-	12,15,15	1.40	2 (16%)	15,21,21	1.57	5 (33%)
2	FMN	F	301	-	32,33,33	1.31	4 (12%)	34,50,50	1.96	6 (17%)
3	TYI	F	302	-	12,15,15	1.61	2 (16%)	15,21,21	1.68	4 (26%)
4	PO4	G	2	-	4,4,4	0.52	0	6,6,6	0.24	0
2	FMN	G	301	-	32,33,33	1.51	5 (15%)	34,50,50	2.01	11 (32%)
3	TYI	G	302	-	12,15,15	1.37	2 (16%)	15,21,21	2.01	3 (20%)
2	FMN	H	301	-	32,33,33	1.33	4 (12%)	34,50,50	2.08	7 (20%)
3	TYI	H	302	-	12,15,15	0.90	0	15,21,21	1.53	4 (26%)

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	TYI	A	302	-	-	0/4/8/8	0/1/1/1
2	FMN	B	301	-	-	0/18/18/18	0/3/3/3
3	TYI	B	302	-	-	0/4/8/8	0/1/1/1
4	PO4	C	1	-	-	0/0/0/0	0/0/0/0
2	FMN	C	301	-	-	0/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYI	C	302	-	-	0/4/8/8	0/1/1/1
2	FMN	D	301	-	-	0/18/18/18	0/3/3/3
3	TYI	D	302	-	-	0/4/8/8	0/1/1/1
2	FMN	E	301	-	-	0/18/18/18	0/3/3/3
3	TYI	E	302	-	-	0/4/8/8	0/1/1/1
2	FMN	F	301	-	-	0/18/18/18	0/3/3/3
3	TYI	F	302	-	-	0/4/8/8	0/1/1/1
4	PO4	G	2	-	-	0/0/0/0	0/0/0/0
2	FMN	G	301	-	-	0/18/18/18	0/3/3/3
3	TYI	G	302	-	-	0/4/8/8	0/1/1/1
2	FMN	H	301	-	-	0/18/18/18	0/3/3/3
3	TYI	H	302	-	-	0/4/8/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	FMN	C4'-C3'	-2.60	1.48	1.53
2	B	301	FMN	C10-N10	-2.31	1.36	1.39
2	G	301	FMN	C2'-C3'	-2.26	1.49	1.53
2	F	301	FMN	O3'-C3'	-2.20	1.37	1.43
2	F	301	FMN	C6-C5A	-2.14	1.38	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FMN	N3-C2-N1	-5.87	117.81	127.69
2	D	301	FMN	C4A-C4-N3	-5.05	116.92	123.52
2	F	301	FMN	N3-C2-N1	-5.01	119.25	127.69
2	B	301	FMN	N3-C2-N1	-4.88	119.47	127.69
2	E	301	FMN	C4A-C4-N3	-4.67	117.42	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FMN	3	0
3	A	302	TYI	3	0
2	B	301	FMN	4	0
3	B	302	TYI	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	FMN	2	0
3	C	302	TYI	2	0
3	D	302	TYI	2	0
2	E	301	FMN	1	0
2	F	301	FMN	1	0
3	F	302	TYI	3	0
2	G	301	FMN	1	0
3	G	302	TYI	1	0
2	H	301	FMN	1	0
3	H	302	TYI	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	221/259 (85%)	-0.41	1 (0%) 91 90	24, 33, 45, 56	2 (0%)
1	B	220/259 (84%)	-0.46	1 (0%) 91 90	22, 31, 47, 55	1 (0%)
1	C	221/259 (85%)	-0.38	1 (0%) 91 90	24, 35, 46, 68	0
1	D	220/259 (84%)	-0.46	0 100 100	25, 35, 45, 59	0
1	E	221/259 (85%)	-0.61	0 100 100	18, 35, 51, 63	2 (0%)
1	F	220/259 (84%)	-0.64	0 100 100	18, 33, 52, 61	1 (0%)
1	G	221/259 (85%)	-0.54	2 (0%) 85 83	20, 37, 53, 67	0
1	H	220/259 (84%)	-0.63	0 100 100	22, 36, 51, 56	0
All	All	1764/2072 (85%)	-0.51	5 (0%) 94 93	18, 34, 50, 68	6 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	286	HIS	3.8
1	A	199	ALA	2.8
1	C	286	HIS	2.4
1	B	110	GLU	2.3
1	G	285	VAL	2.2

### 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(Å <sup>2</sup> )	Q<0.9
2	FMN	E	301	31/31	0.97	0.14	0.51	18,25,28,29	0
3	TYI	G	302	15/15	0.99	0.14	0.22	42,44,48,49	1
3	TYI	F	302	15/15	0.99	0.13	0.00	38,42,43,50	1
3	TYI	A	302	15/15	0.98	0.14	-0.24	37,39,41,42	2
3	TYI	D	302	15/15	0.98	0.14	-0.30	39,41,44,50	1
2	FMN	A	301	31/31	0.97	0.13	-0.33	16,27,29,30	0
3	TYI	E	302	15/15	0.99	0.12	-0.39	35,38,41,43	2
2	FMN	G	301	31/31	0.98	0.12	-0.43	14,24,27,27	0
2	FMN	H	301	31/31	0.97	0.12	-0.50	23,27,30,32	0
3	TYI	H	302	15/15	0.98	0.11	-0.75	33,35,40,47	1
2	FMN	B	301	31/31	0.98	0.12	-0.97	15,24,26,30	0
2	FMN	C	301	31/31	0.98	0.11	-0.99	17,24,26,26	0
2	FMN	D	301	31/31	0.97	0.12	-1.00	24,28,29,31	0
2	FMN	F	301	31/31	0.99	0.10	-1.05	11,21,23,26	0
3	TYI	C	302	15/15	0.98	0.10	-1.59	39,40,45,49	1
3	TYI	B	302	15/15	0.99	0.10	-1.71	35,38,40,46	1
4	PO4	G	2	5/5	0.92	0.14	-	78,80,82,82	0
4	PO4	C	1	5/5	0.87	0.20	-	76,79,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.