



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 08:51 am GMT

PDB ID : 1KBI  
Title : Crystallographic Study of the Recombinant Flavin-binding Domain of Baker's Yeast Flavocytochrome b2: Comparison with the Intact Wild-type Enzyme  
Authors : Cunane, L.M.; Barton, J.D.; Chen, Z.-W.; Welsh, F.E.; Chapman, S.K.; Reid, G.A.; Mathews, F.S.  
Deposited on : 2001-11-06  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

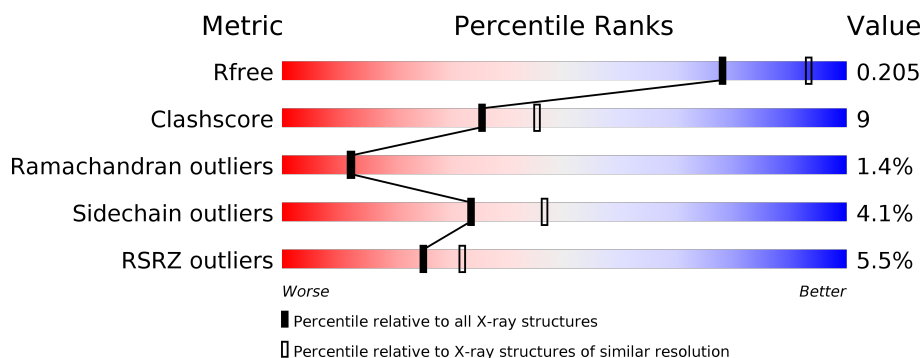
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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	511	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div> </div>
1	B	511	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>14%</div> <div>••</div> <div>21%</div> </div> </div>

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
5	PO4	B	900	-	-	X	-

## 2 Entry composition [i](#)

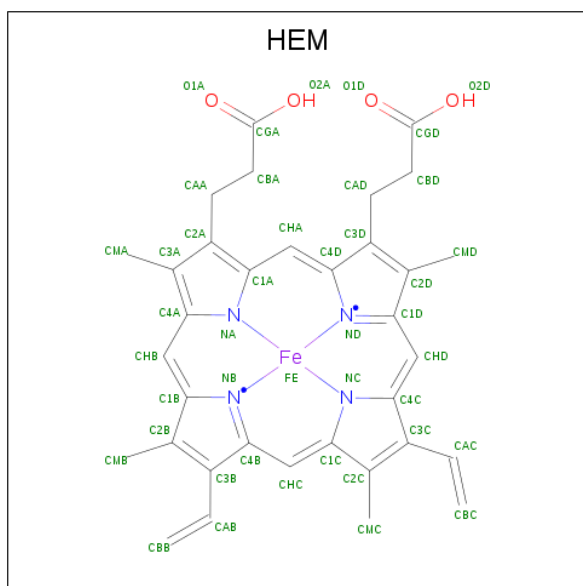
There are 7 unique types of molecules in this entry. The entry contains 7863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

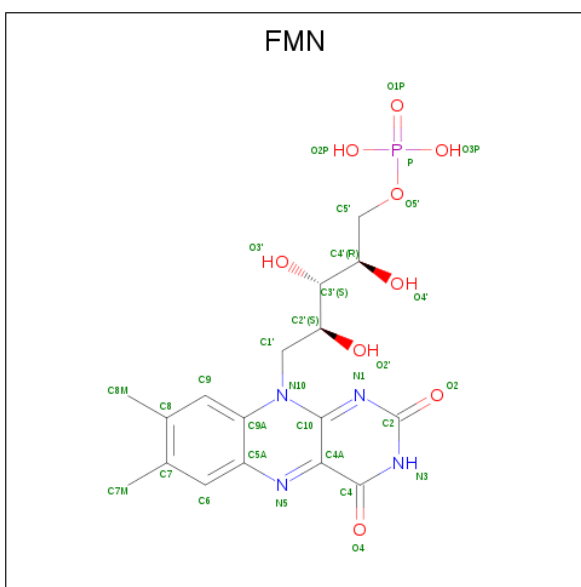
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	4	0
			3939	2498	668	758	15			
1	B	405	Total	C	N	O	S	0	0	0
			3152	1994	538	609	11			

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



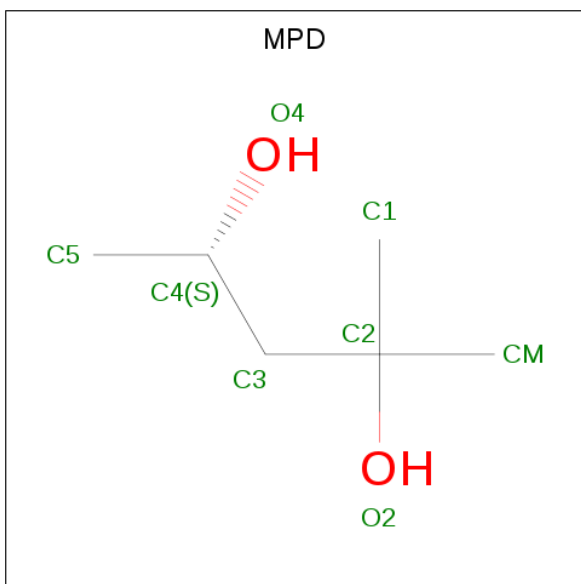
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



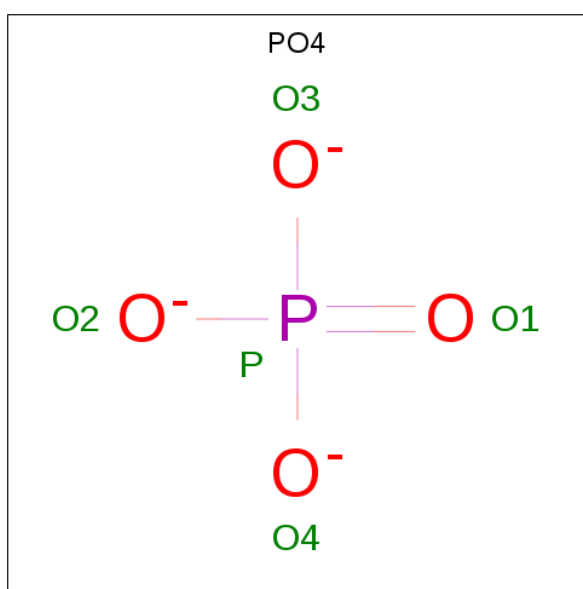
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

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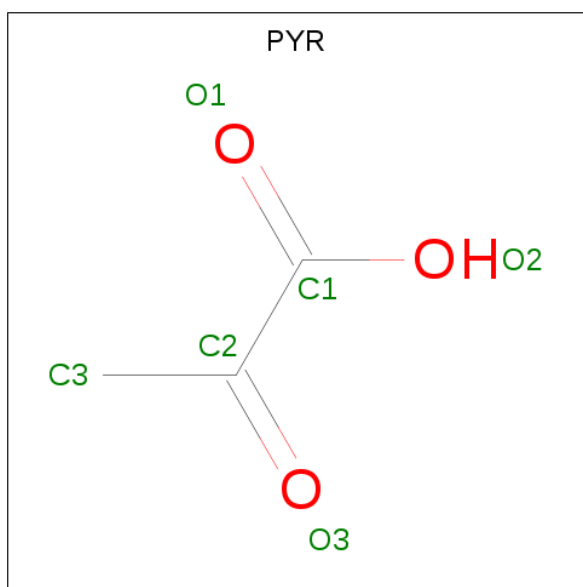
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			3	2	1		

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



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

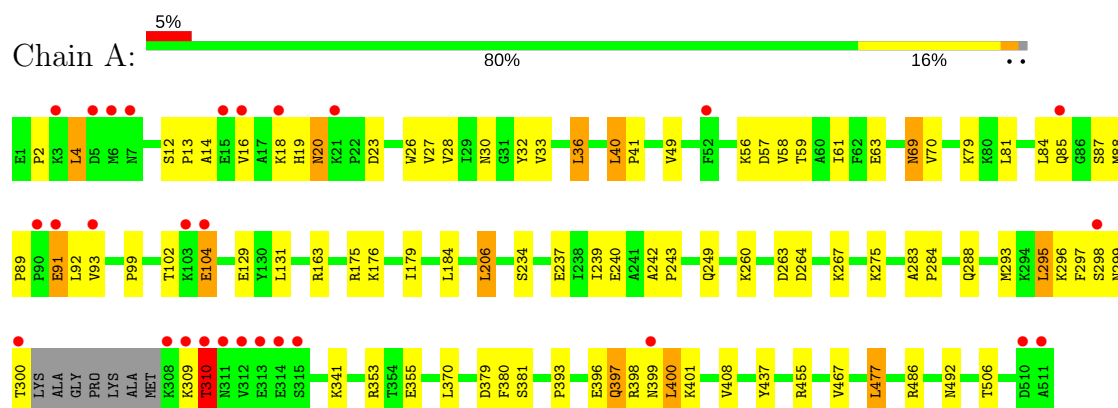
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	371	Total	O	0	0
			371	371		
7	B	247	Total	O	0	0
			247	247		

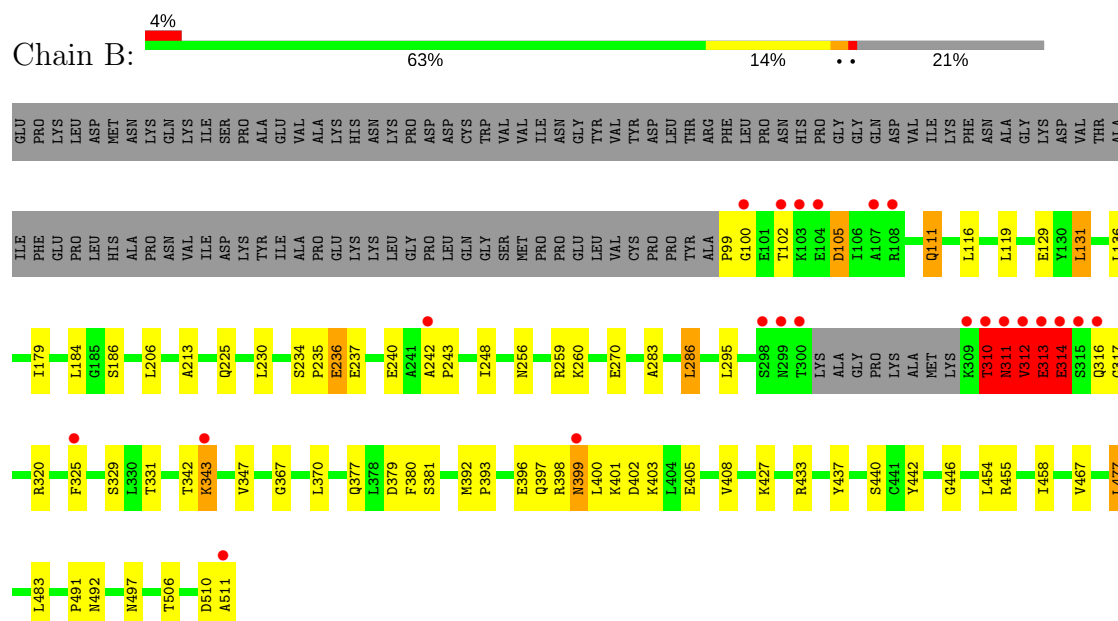
### 3 Residue-property plots [i](#)

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.16Å 164.16Å 111.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 28.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	80.5 (30.00-2.30) 80.6 (28.16-2.30)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.29 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.170 , 0.211 0.164 , 0.205	Depositor DCC
$R_{free}$ test set	6657 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.333 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, MPD, PYR, PO4

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	0.52	0/4014	0.89	5/5439 (0.1%)
1	B	0.60	3/3202 (0.1%)	0.93	10/4326 (0.2%)
All	All	0.56	3/7216 (0.0%)	0.91	15/9765 (0.2%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	GLU	C-N	5.57	1.46	1.34
1	B	314	GLU	N-CA	5.17	1.56	1.46
1	B	311	ASN	C-N	-5.05	1.22	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	GLU	O-C-N	-23.79	84.63	122.70
1	A	310	THR	CA-C-O	-22.65	72.54	120.10
1	A	310	THR	CA-C-N	20.68	162.70	117.20
1	A	310	THR	O-C-N	-16.77	95.87	122.70
1	B	313	GLU	CA-C-N	16.26	152.97	117.20
1	B	310	THR	O-C-N	-9.82	106.98	122.70
1	B	312	VAL	O-C-N	6.84	133.65	122.70
1	A	310	THR	N-CA-C	6.12	127.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	GLU	O-C-N	6.11	132.48	122.70
1	B	312	VAL	CA-C-N	-6.09	103.80	117.20
1	B	310	THR	CA-C-N	5.78	129.91	117.20
1	A	381	SER	N-CA-C	-5.32	96.64	111.00
1	B	311	ASN	O-C-N	-5.26	114.29	122.70
1	B	100	GLY	N-CA-C	-5.14	100.25	113.10
1	B	381	SER	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	THR	Mainchain

## 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	3939	0	3956	81	1
1	B	3152	0	3205	46	1
2	A	43	0	30	8	0
3	A	31	0	19	0	0
3	B	31	0	19	1	0
4	A	32	0	56	3	0
4	B	8	0	14	0	0
5	B	3	0	0	0	2
6	B	6	0	3	0	0
7	A	371	0	0	6	0
7	B	247	0	0	4	0
All	All	7863	0	7302	128	3

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 9.

All (128) 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:506:THR:HB	7:B:1098:HOH:O	1.75	0.85
1:B:270:GLU:OE2	1:B:343:LYS:HG2	1.76	0.84
1:B:317:GLY:O	1:B:320:ARG:HG2	1.82	0.80
1:A:20:ASN:H	1:A:20:ASN:HD22	1.29	0.78
1:B:186:SER:HB3	1:B:248:ILE:HD11	1.66	0.77
1:A:28:VAL:CG2	1:A:57:ASP:HA	2.16	0.76
1:B:313:GLU:O	1:B:314:GLU:CB	2.33	0.76
1:B:343:LYS:N	1:B:343:LYS:HD3	2.02	0.75
1:A:355:GLU:HG2	4:A:702:MPD:H51	1.69	0.73
1:A:58:VAL:HG21	2:A:760:HEM:HBC1	1.71	0.73
1:B:235:PRO:HG2	1:B:236:GLU:OE1	1.90	0.71
1:A:396:GLU:C	1:A:398:ARG:H	1.95	0.68
1:A:28:VAL:HG22	1:A:57:ASP:HA	1.75	0.68
1:B:399:ASN:C	1:B:401:LYS:H	1.92	0.67
1:A:49:VAL:HG21	2:A:760:HEM:HMD3	1.76	0.67
1:B:136:LEU:HD21	1:B:440:SER:HB3	1.75	0.66
1:A:399:ASN:O	1:A:401:LYS:N	2.29	0.65
1:A:19:HIS:HB2	1:A:26:TRP:HB2	1.77	0.65
1:A:58:VAL:CG2	1:A:61:ILE:HD12	2.29	0.62
1:A:263:ASP:OD1	4:A:701:MPD:H51	2.00	0.61
1:B:99:PRO:HA	7:B:1073:HOH:O	1.98	0.61
1:A:58:VAL:HG23	1:A:61:ILE:HD12	1.81	0.61
1:A:89:PRO:HB3	1:A:91:GLU:OE2	2.01	0.60
1:B:396:GLU:HG2	1:B:401:LYS:HG2	1.84	0.59
1:B:186:SER:CB	1:B:248:ILE:HD11	2.31	0.59
1:B:379:ASP:O	1:B:380:PHE:HB2	2.01	0.59
1:A:40:LEU:HG	1:A:41:PRO:HD3	1.84	0.58
1:B:399:ASN:C	1:B:401:LYS:N	2.55	0.58
1:A:56:LYS:HE3	7:A:1132:HOH:O	2.04	0.57
1:A:93:VAL:HG23	1:A:93:VAL:O	2.05	0.57
1:B:396:GLU:C	1:B:398:ARG:H	2.07	0.57
1:A:28:VAL:HG23	1:A:57:ASP:HA	1.87	0.57
1:B:343:LYS:CD	1:B:343:LYS:N	2.65	0.57
1:A:63:GLU:HG3	7:A:1086:HOH:O	2.03	0.56
1:A:36:LEU:O	1:A:40:LEU:HD23	2.05	0.56
1:A:16:VAL:HB	1:A:88:MET:HE1	1.88	0.56
1:A:102:THR:OG1	1:A:104[B]:GLU:HG2	2.05	0.56
1:B:230:LEU:HD21	1:B:325:PHE:CE2	2.41	0.55
1:B:129:GLU:HG3	1:B:437:TYR:CE2	2.41	0.55
1:A:2:PRO:HB2	1:A:4:LEU:CD2	2.37	0.55
1:A:26:TRP:CE2	1:A:81:LEU:HD11	2.42	0.54
1:A:396:GLU:C	1:A:398:ARG:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASN:N	1:A:20:ASN:HD22	1.96	0.53
1:B:405:GLU:HG2	1:B:427:LYS:HD3	1.90	0.53
1:A:129:GLU:HG3	1:A:437:TYR:CE2	2.44	0.53
1:B:370:LEU:HB2	1:B:408:VAL:HG12	1.90	0.53
1:A:89:PRO:HB2	1:A:92:LEU:HB2	1.91	0.52
1:B:400:LEU:HA	1:B:403:LYS:HG2	1.90	0.52
1:A:234:SER:OG	1:A:237:GLU:HG2	2.10	0.52
1:A:260:LYS:HE2	1:A:264:ASP:OD1	2.10	0.51
1:A:33:VAL:HG12	1:A:81:LEU:HD12	1.92	0.51
1:A:239:ILE:HA	1:A:249:GLN:HE22	1.76	0.51
1:B:310:THR:O	1:B:311:ASN:ND2	2.44	0.51
1:A:396:GLU:O	1:A:398:ARG:N	2.44	0.50
1:B:329:SER:O	1:B:331:THR:HG23	2.12	0.50
1:B:234:SER:OG	1:B:237:GLU:HG2	2.12	0.50
1:A:296:LYS:HE2	7:A:1081:HOH:O	2.12	0.49
1:A:370:LEU:HB2	1:A:408:VAL:HG12	1.92	0.49
1:A:275:LYS:NZ	7:A:1063:HOH:O	2.45	0.49
1:B:467:VAL:HG11	1:B:477:LEU:HD21	1.94	0.49
1:A:379:ASP:O	1:A:380:PHE:HB2	2.13	0.49
1:A:20:ASN:ND2	1:A:20:ASN:H	2.04	0.49
1:B:506:THR:CB	7:B:1098:HOH:O	2.46	0.49
1:A:49:VAL:HG21	2:A:760:HEM:CMD	2.42	0.49
1:A:58:VAL:HG21	2:A:760:HEM:CBC	2.42	0.49
1:A:206:LEU:HB2	7:A:1033:HOH:O	2.11	0.48
1:B:310:THR:O	1:B:311:ASN:CG	2.51	0.48
1:A:20:ASN:N	1:A:20:ASN:ND2	2.62	0.48
1:A:2:PRO:HB2	1:A:4:LEU:HD21	1.94	0.48
1:B:433:ARG:HG3	3:B:870:FMN:O1P	2.14	0.47
7:A:847:HOH:O	1:B:491:PRO:HD3	2.13	0.47
1:A:19:HIS:N	1:A:19:HIS:CD2	2.82	0.47
1:A:70:VAL:HB	2:A:760:HEM:HMB2	1.96	0.47
1:A:288[A]:GLN:HG3	1:A:293:MET:SD	2.55	0.47
1:A:33:VAL:CG1	1:A:81:LEU:HD12	2.43	0.47
1:A:263:ASP:OD2	1:A:267:LYS:HE2	2.14	0.47
1:A:30:ASN:ND2	1:A:59:THR:HG21	2.30	0.47
1:A:16:VAL:C	1:A:18:LYS:N	2.69	0.46
1:B:283:ALA:HA	1:B:377:GLN:NE2	2.30	0.46
1:B:179:ILE:HD11	1:B:455:ARG:HG3	1.98	0.46
1:B:454:LEU:O	1:B:458:ILE:HG13	2.16	0.46
1:A:70:VAL:HB	2:A:760:HEM:CMB	2.46	0.45
1:A:467:VAL:HG11	1:A:477:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASN:O	1:B:259:ARG:HD3	2.17	0.45
1:A:57:ASP:HB3	1:A:93:VAL:HG12	1.98	0.45
1:A:4:LEU:HB3	1:A:32:TYR:CZ	2.52	0.44
1:A:99:PRO:HB2	1:A:295:LEU:HD13	1.98	0.44
1:A:40:LEU:HG	1:A:41:PRO:CD	2.47	0.44
1:A:393:PRO:O	1:A:397:GLN:HG3	2.17	0.44
1:A:398:ARG:C	1:A:400:LEU:H	2.21	0.44
1:B:442:TYR:HB2	1:B:446:GLY:HA3	1.99	0.44
1:A:299:ASN:O	1:A:300:THR:C	2.56	0.44
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.81	0.43
1:A:16:VAL:O	1:A:18:LYS:N	2.51	0.43
1:A:399:ASN:C	1:A:401:LYS:N	2.71	0.43
1:A:23:ASP:OD1	1:A:23:ASP:N	2.51	0.43
1:B:116:LEU:CD2	1:B:131:LEU:HG	2.48	0.43
1:A:12:SER:C	1:A:14:ALA:H	2.22	0.43
1:A:27:VAL:CG1	1:A:36:LEU:HD22	2.48	0.43
1:A:353:ARG:HH22	4:A:702:MPD:HM1	1.84	0.43
1:B:242:ALA:HA	1:B:243:PRO:HD3	1.81	0.43
1:A:506:THR:HB	7:B:1099:HOH:O	2.19	0.42
1:B:102:THR:HG23	1:B:105:ASP:OD2	2.19	0.42
1:A:297:PHE:C	1:A:299:ASN:N	2.73	0.42
1:A:399:ASN:C	1:A:401:LYS:H	2.23	0.42
1:A:58:VAL:HG22	1:A:61:ILE:HB	2.02	0.42
1:A:179:ILE:HD11	1:A:455:ARG:HG3	2.01	0.42
1:A:93:VAL:CG2	1:A:93:VAL:O	2.68	0.42
1:B:111:GLN:HB3	1:B:111:GLN:HE21	1.56	0.42
1:B:510:ASP:O	1:B:511:ALA:OXT	2.37	0.42
1:A:163:ARG:NH2	1:A:486:ARG:HG3	2.35	0.41
1:B:347:VAL:HG13	1:B:367:GLY:C	2.41	0.41
1:A:283:ALA:N	1:A:284:PRO:CD	2.84	0.41
1:A:27:VAL:HG12	1:A:36:LEU:HD22	2.02	0.41
1:A:297:PHE:O	1:A:299:ASN:N	2.54	0.41
1:B:342:THR:C	1:B:343:LYS:HD3	2.41	0.41
1:A:16:VAL:C	1:A:18:LYS:H	2.24	0.41
1:A:242:ALA:HA	1:A:243:PRO:HD3	1.89	0.41
1:A:58:VAL:CG2	2:A:760:HEM:HBC1	2.47	0.41
1:B:286:LEU:HD22	1:B:286:LEU:HA	1.89	0.41
1:A:84:LEU:HG	1:A:85:GLN:N	2.35	0.41
1:A:87:SER:O	1:A:88:MET:HG2	2.19	0.41
1:B:492:ASN:OD1	1:B:497:ASN:ND2	2.54	0.41
1:B:392:MET:HB2	1:B:393:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:N	1:A:69:ASN:HD22	2.19	0.40
1:B:119:LEU:HD13	1:B:442:TYR:CG	2.57	0.40
2:A:760:HEM:HBC2	2:A:760:HEM:HHD	2.02	0.40
1:B:213:ALA:HB2	1:B:225:GLN:HE22	1.87	0.40

All (3) 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)
5:B:900:PO4:P	5:B:900:PO4:O1[4_555]	1.53	0.67
5:B:900:PO4:P	5:B:900:PO4:O2[4_555]	1.57	0.63
1:A:341:LYS:O	1:B:312:VAL:CG1[3_665]	1.92	0.28

## 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	504/511 (99%)	465 (92%)	33 (6%)	6 (1%)	14	15
1	B	401/511 (78%)	378 (94%)	16 (4%)	7 (2%)	10	9
All	All	905/1022 (89%)	843 (93%)	49 (5%)	13 (1%)	12	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	THR
1	A	400	LEU
1	B	312	VAL
1	B	313	GLU
1	B	314	GLU
1	A	397	GLN
1	B	310	THR

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Mol	Chain	Res	Type
1	B	311	ASN
1	A	309	LYS
1	B	397	GLN
1	B	399	ASN
1	A	298	SER
1	A	13	PRO

### 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	433/440 (98%)	415 (96%)	18 (4%)	32	45
1	B	348/440 (79%)	332 (95%)	16 (5%)	29	41
All	All	781/880 (89%)	747 (96%)	34 (4%)	33	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	20	ASN
1	A	36	LEU
1	A	40	LEU
1	A	69	ASN
1	A	79	LYS
1	A	91	GLU
1	A	104[A]	GLU
1	A	104[B]	GLU
1	A	131	LEU
1	A	175	ARG
1	A	184	LEU
1	A	206	LEU
1	A	240	GLU
1	A	295	LEU
1	A	477	LEU
1	A	492[A]	ASN

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Mol	Chain	Res	Type
1	A	492[B]	ASN
1	B	105	ASP
1	B	111	GLN
1	B	131	LEU
1	B	184	LEU
1	B	206	LEU
1	B	236	GLU
1	B	240	GLU
1	B	260	LYS
1	B	286	LEU
1	B	295	LEU
1	B	312	VAL
1	B	316	GLN
1	B	343	LYS
1	B	402	ASP
1	B	477	LEU
1	B	483	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	30	ASN
1	A	47	GLN
1	A	53	ASN
1	A	69	ASN
1	A	85	GLN
1	A	111	GLN
1	A	149	ASN
1	A	159	ASN
1	A	225	GLN
1	A	249	GLN
1	A	316	GLN
1	A	397	GLN
1	B	111	GLN
1	B	149	ASN
1	B	159	ASN
1	B	225	GLN
1	B	311	ASN
1	B	316	GLN
1	B	397	GLN

### 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 ⓘ

10 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	$\# Z  > 2$
4	MPD	A	701	-	7,7,7	0.51	0	9,10,10	0.60	0
4	MPD	A	702	-	7,7,7	0.47	0	9,10,10	0.55	0
4	MPD	A	703	-	7,7,7	0.51	0	9,10,10	0.60	0
4	MPD	A	704	-	7,7,7	0.59	0	9,10,10	0.59	0
2	HEM	A	760	1	27,50,50	1.83	9 (33%)	17,82,82	2.02	6 (35%)
3	FMN	A	770	-	31,33,33	2.05	9 (29%)	39,50,50	2.46	6 (15%)
6	PYR	B	800	-	2,5,5	0.73	0	2,6,6	0.23	0
4	MPD	B	801	-	7,7,7	0.61	0	9,10,10	0.42	0
3	FMN	B	870	-	31,33,33	1.95	9 (29%)	39,50,50	2.36	5 (12%)
5	PO4	B	900	-	0,2,4	0.00	-	0,1,6	0.00	-

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
4	MPD	A	701	-	-	0/5/5/5	0/0/0/0
4	MPD	A	702	-	-	0/5/5/5	0/0/0/0
4	MPD	A	703	-	-	0/5/5/5	0/0/0/0
4	MPD	A	704	-	-	0/5/5/5	0/0/0/0
2	HEM	A	760	1	-	0/6/54/54	0/0/8/8
3	FMN	A	770	-	-	0/16/18/18	0/3/3/3
6	PYR	B	800	-	-	0/0/4/4	0/0/0/0
4	MPD	B	801	-	-	0/5/5/5	0/0/0/0
3	FMN	B	870	-	-	0/16/18/18	0/3/3/3
5	PO4	B	900	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	870	FMN	C1'-N10	-3.42	1.44	1.48
2	A	760	HEM	C3C-C2C	-2.82	1.36	1.40
2	A	760	HEM	C3B-CAB	-2.75	1.42	1.47
2	A	760	HEM	C3C-CAC	-2.48	1.42	1.47
3	A	770	FMN	C1'-N10	-2.30	1.46	1.48
2	A	760	HEM	C4B-NB	2.02	1.40	1.36
3	A	770	FMN	C9A-C5A	2.11	1.46	1.42
3	A	770	FMN	C2-N3	2.13	1.42	1.38
2	A	760	HEM	C1B-C2B	2.33	1.48	1.42
3	B	870	FMN	C4A-N5	2.48	1.36	1.33
2	A	760	HEM	CBC-CAC	2.61	1.46	1.29
3	B	870	FMN	C2-N3	2.63	1.43	1.38
3	B	870	FMN	C4A-C10	2.68	1.45	1.41
3	B	870	FMN	C5A-N5	2.79	1.39	1.35
2	A	760	HEM	C1A-NA	2.84	1.42	1.36
3	B	870	FMN	C4-C4A	2.95	1.46	1.41
3	A	770	FMN	C4-C4A	3.13	1.46	1.41
2	A	760	HEM	C1D-ND	3.48	1.43	1.36
3	A	770	FMN	C4-N3	3.56	1.39	1.33
3	A	770	FMN	C5A-N5	3.60	1.40	1.35
3	B	870	FMN	C4-N3	3.80	1.39	1.33
3	A	770	FMN	C4A-N5	3.81	1.38	1.33
3	B	870	FMN	C10-N1	3.87	1.38	1.33
2	A	760	HEM	C4A-NA	3.88	1.44	1.36
3	A	770	FMN	C4A-C10	3.97	1.47	1.41
3	B	870	FMN	C9A-N10	4.67	1.44	1.38
3	A	770	FMN	C9A-N10	5.03	1.44	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	770	FMN	C4A-C4-N3	-5.50	115.65	123.47
3	B	870	FMN	C4A-C4-N3	-4.98	116.39	123.47
2	A	760	HEM	C4C-C3C-C2C	-3.88	104.19	106.90
3	B	870	FMN	C4A-C10-N10	-3.67	116.98	120.40
2	A	760	HEM	C1D-C2D-C3D	-3.67	104.45	107.00
2	A	760	HEM	C4A-C3A-C2A	-3.05	104.87	107.00
3	A	770	FMN	C4-C4A-C10	-2.89	117.80	119.95
3	A	770	FMN	C4A-C10-N10	-2.66	117.93	120.40
2	A	760	HEM	CBD-CAD-C3D	-2.58	107.54	112.47
2	A	760	HEM	CAD-C3D-C2D	-2.41	122.11	129.00
3	B	870	FMN	P-O5'-C5'	2.03	123.90	118.30
2	A	760	HEM	CMB-C2B-C3B	2.17	128.84	124.88
3	A	770	FMN	P-O5'-C5'	2.81	126.03	118.30
3	A	770	FMN	C4A-N5-C5A	3.47	120.40	116.76
3	B	870	FMN	C4A-N5-C5A	4.79	121.78	116.76
3	B	870	FMN	C4-N3-C2	11.36	124.81	115.14
3	A	770	FMN	C4-N3-C2	12.23	125.56	115.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	MPD	1	0
4	A	702	MPD	2	0
2	A	760	HEM	8	0
3	B	870	FMN	1	0
5	B	900	PO4	0	2

## 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, 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	504/511 (98%)	-0.22	28 (5%) 24 31	17, 29, 83, 99	0
1	B	405/511 (79%)	-0.22	22 (5%) 26 33	17, 29, 70, 99	0
All	All	909/1022 (88%)	-0.22	50 (5%) 25 32	17, 29, 80, 99	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	THR	10.7
1	B	311	ASN	9.2
1	A	311	ASN	8.7
1	B	312	VAL	8.1
1	A	314	GLU	8.0
1	A	310	THR	7.9
1	B	313	GLU	7.4
1	A	313	GLU	7.1
1	A	315	SER	6.7
1	B	300	THR	6.2
1	B	315	SER	6.2
1	B	299	ASN	6.1
1	B	511	ALA	6.0
1	B	309	LYS	6.0
1	A	511	ALA	5.1
1	A	312	VAL	4.8
1	A	309	LYS	4.7
1	A	7	ASN	4.5
1	B	298	SER	4.0
1	B	314	GLU	3.8
1	B	325	PHE	3.7
1	A	308	LYS	3.6
1	A	90	PRO	3.6
1	A	300	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	102	THR	3.4
1	B	399	ASN	3.2
1	A	6	MET	3.1
1	A	399	ASN	3.1
1	B	100	GLY	3.1
1	A	93	VAL	3.1
1	B	107	ALA	2.9
1	B	316	GLN	2.9
1	A	18	LYS	2.8
1	A	91	GLU	2.6
1	B	104	GLU	2.6
1	A	85	GLN	2.5
1	A	52	PHE	2.4
1	A	5	ASP	2.4
1	A	15	GLU	2.3
1	A	103	LYS	2.3
1	B	108	ARG	2.3
1	A	16	VAL	2.3
1	A	21	LYS	2.3
1	A	510	ASP	2.3
1	A	3	LYS	2.2
1	B	343	LYS	2.2
1	A	298	SER	2.2
1	B	242	ALA	2.2
1	B	103	LYS	2.1
1	A	104[A]	GLU	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MPD	A	704	8/8	0.80	0.31	96,96,99,99	0
4	MPD	A	702	8/8	0.81	0.27	80,82,84,84	0
4	MPD	A	703	8/8	0.86	0.36	91,91,92,92	0
4	MPD	B	801	8/8	0.90	0.21	70,72,72,73	0
4	MPD	A	701	8/8	0.95	0.13	39,43,52,54	0
5	PO4	B	900	3/5	0.96	0.21	65,65,68,72	1
6	PYR	B	800	6/6	0.96	0.13	41,45,51,52	0
2	HEM	A	760	43/43	0.98	0.09	21,28,34,39	0
3	FMN	B	870	31/31	0.98	0.14	18,23,27,29	0
3	FMN	A	770	31/31	0.99	0.11	15,19,24,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.