



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:25 am GMT

PDB ID : 3FY4  
Title : (6-4) Photolyase Crystal Structure  
Authors : Hitomi, K.; Arvai, A.S.; Tainer, J.A.; Getzoff, E.D.  
Deposited on : 2009-01-21  
Resolution : 2.70 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

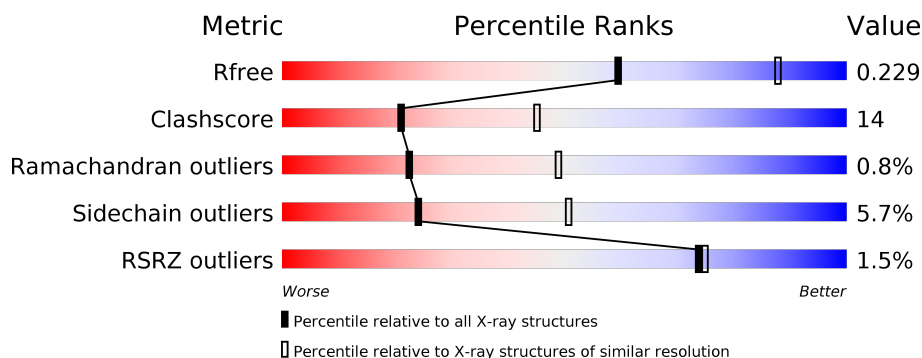
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	537	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>• •</div> </div> </div>
1	B	537	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	C	537	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</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
2	IMD	A	901	-	-	-	X
2	IMD	A	905	-	-	-	X
2	IMD	B	901	-	-	-	X
2	IMD	B	906	-	-	-	X
2	IMD	C	901	-	-	-	X
3	MES	A	920	-	-	-	X
3	MES	B	920	-	-	-	X
3	MES	C	920	-	-	-	X
4	PO4	A	930	-	-	-	X
4	PO4	B	930	-	-	-	X
4	PO4	C	930	-	-	-	X

## 2 Entry composition [i](#)

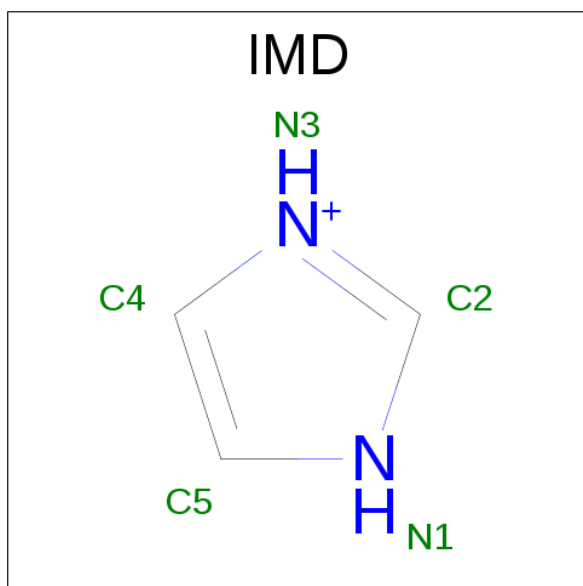
There are 6 unique types of molecules in this entry. The entry contains 13491 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-4 photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4194	2709	702	759	24			
1	B	521	Total	C	N	O	S	0	0	0
			4178	2697	699	758	24			
1	C	520	Total	C	N	O	S	0	0	0
			4181	2702	700	755	24			

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



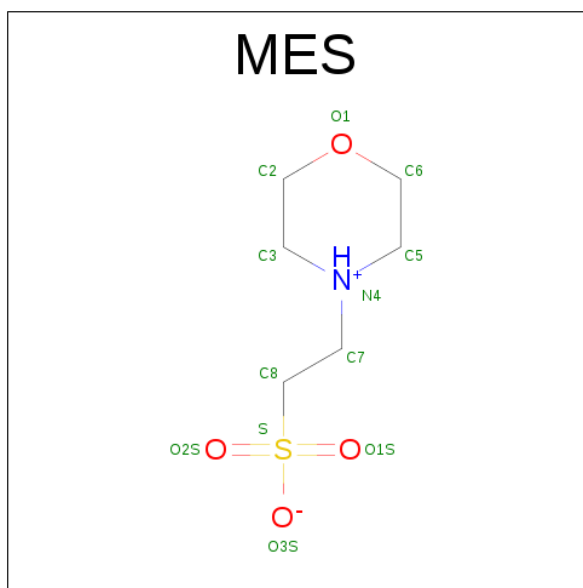
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	A	1	Total	C	N	0	0
			5	3	2		
2	A	1	Total	C	N	0	0
			5	3	2		

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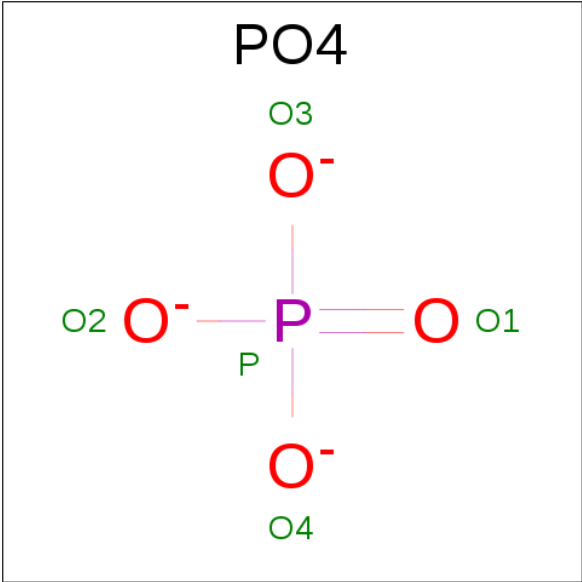
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



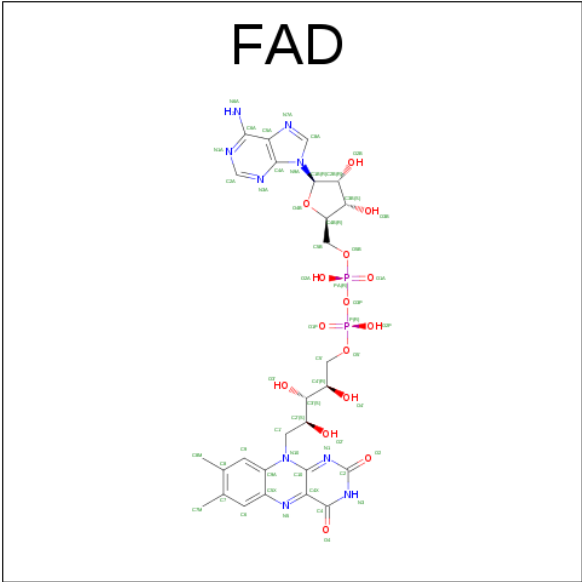
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



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

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

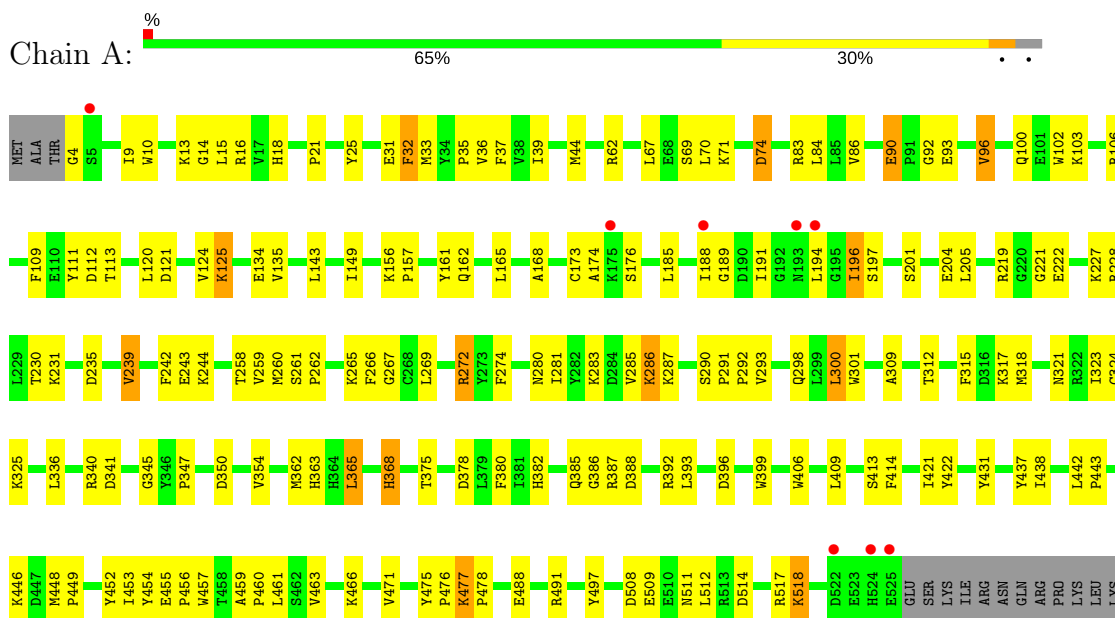
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	244	Total	O	0	0
			244	244		
6	C	247	Total	O	0	0
			247	247		
6	B	187	Total	O	0	0
			187	187		

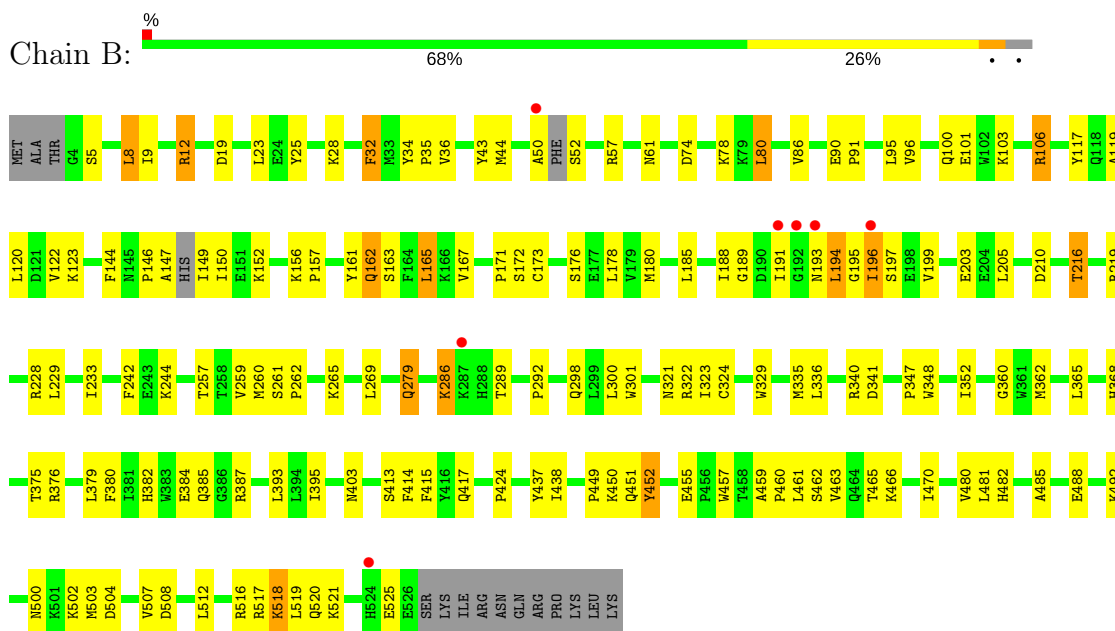
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 6-4 photolyase

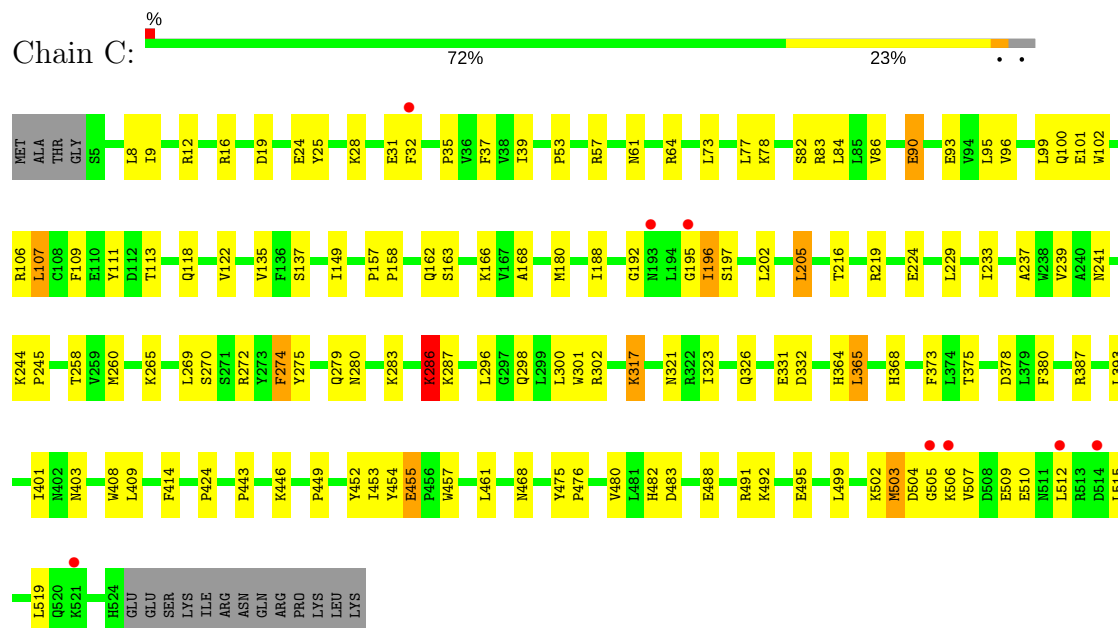


#### • Molecule 1: 6-4 photolyase





● Molecule 1: 6-4 photolyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.45Å 139.03Å 143.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.38 – 2.70 56.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (55.38-2.70) 95.7 (56.22-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.202 , 0.237 0.195 , 0.229	Depositor DCC
$R_{free}$ test set	3016 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13491	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 2.70% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, IMD, FAD, MES

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	0.38	0/4319	0.58	0/5846
1	B	0.37	0/4299	0.58	0/5816
1	C	0.38	0/4306	0.59	1/5829 (0.0%)
All	All	0.38	0/12924	0.58	1/17491 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	GLU	N-CA-C	-5.45	96.30	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	4194	0	4108	132	0
1	B	4178	0	4092	118	0
1	C	4181	0	4099	96	0
2	A	15	0	15	0	0
2	B	25	0	25	1	0
2	C	10	0	10	4	0
3	A	12	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	3	0
3	C	12	0	13	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	53	0	31	1	0
5	B	53	0	31	0	0
5	C	53	0	31	0	0
6	A	244	0	0	7	0
6	B	187	0	0	2	0
6	C	247	0	0	2	0
All	All	13491	0	12481	346	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.

All (346) 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:C:286:LYS:H	1:C:286:LYS:HD3	1.19	1.06
1:A:4:GLY:N	1:A:103:LYS:HZ3	1.64	0.94
1:A:285:VAL:HG23	1:A:286:LYS:H	1.29	0.93
1:C:387:ARG:HH11	1:C:403:ASN:HD21	1.18	0.86
1:A:508:ASP:HB3	1:A:511:ASN:HD22	1.43	0.83
1:A:165:LEU:HD21	1:A:300:LEU:HG	1.59	0.82
1:C:286:LYS:N	1:C:286:LYS:HD3	1.95	0.81
1:A:368:HIS:NE2	3:A:920:MES:H22	1.98	0.79
1:A:31:GLU:HG3	1:A:32:PHE:CD2	2.21	0.76
1:B:91:PRO:HB2	1:B:120:LEU:HD21	1.68	0.76
1:A:285:VAL:O	1:A:286:LYS:HB3	1.85	0.74
1:C:96:VAL:O	1:C:100:GLN:HG2	1.88	0.74
1:C:387:ARG:HH11	1:C:403:ASN:ND2	1.86	0.73
1:B:162:GLN:NE2	1:B:162:GLN:H	1.87	0.73
1:C:302:ARG:HG3	1:C:401:ILE:HD11	1.71	0.73
1:A:286:LYS:HG2	1:A:287:LYS:N	2.05	0.71
1:C:317:LYS:HB3	1:C:317:LYS:NZ	2.05	0.71
1:C:245:PRO:HG3	3:C:920:MES:O3S	1.91	0.71
1:C:387:ARG:NH1	1:C:403:ASN:HD21	1.88	0.71
1:A:196:ILE:HD12	1:A:196:ILE:H	1.56	0.70
1:C:286:LYS:HG2	1:C:287:LYS:H	1.54	0.70
1:C:408:TRP:HE1	2:C:901:IMD:H2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TRP:HB3	1:A:109:PHE:HB3	1.74	0.70
1:A:113:THR:OG1	6:A:3245:HOH:O	2.10	0.70
1:B:80:LEU:HD23	1:B:185:LEU:HD22	1.75	0.69
1:C:488:GLU:HG3	1:C:492:LYS:HE3	1.74	0.69
1:A:106:ARG:HD3	1:A:134:GLU:OE2	1.92	0.68
1:B:292:PRO:HB2	3:B:920:MES:O3S	1.91	0.68
1:C:443:PRO:O	1:C:446:LYS:HB2	1.93	0.68
1:B:74:ASP:OD2	1:B:78:LYS:HE2	1.94	0.68
1:A:508:ASP:HB3	1:A:511:ASN:ND2	2.08	0.68
1:B:86:VAL:O	1:B:197:SER:HB3	1.94	0.68
1:A:121:ASP:O	1:A:125:LYS:HB2	1.93	0.67
1:B:8:LEU:C	1:B:8:LEU:HD12	2.15	0.67
1:C:364:HIS:NE2	3:C:920:MES:H32	2.09	0.67
1:B:228:ARG:NH1	1:B:259:VAL:HB	2.09	0.67
1:B:340:ARG:HD2	1:B:341:ASP:OD1	1.95	0.67
1:B:28:LYS:NZ	1:B:28:LYS:HB2	2.10	0.67
1:B:455:GLU:HA	1:B:457:TRP:CZ3	2.29	0.67
1:A:286:LYS:HG2	1:A:287:LYS:H	1.59	0.67
1:C:286:LYS:H	1:C:286:LYS:CD	2.01	0.66
1:A:25:TYR:CE1	1:A:106:ARG:HD2	2.30	0.66
1:A:191:ILE:HG21	1:A:196:ILE:HG12	1.77	0.66
1:A:86:VAL:O	1:A:197:SER:HB3	1.96	0.66
1:A:188:ILE:HG23	1:A:189:GLY:H	1.59	0.66
1:C:24:GLU:HG2	1:C:28:LYS:HE2	1.78	0.65
1:B:382:HIS:CE1	1:B:384:GLU:HG3	2.32	0.65
1:A:285:VAL:HG23	1:A:286:LYS:N	2.08	0.65
1:A:9:ILE:HG23	1:A:35:PRO:HA	1.78	0.65
1:B:119:ALA:O	1:B:122:VAL:HG12	1.97	0.64
1:A:239:VAL:HG21	1:A:281:ILE:HD11	1.79	0.64
1:B:368:HIS:NE2	3:B:920:MES:H22	2.13	0.64
1:A:188:ILE:HG23	1:A:189:GLY:N	2.14	0.63
1:B:9:ILE:HG23	1:B:35:PRO:HA	1.81	0.63
1:B:335:MET:HE1	1:B:379:LEU:HD22	1.80	0.62
1:B:147:ALA:O	1:B:149:ILE:N	2.31	0.62
1:C:326:GLN:HB3	1:C:512:LEU:HD11	1.82	0.61
1:B:260:MET:HE2	1:B:269:LEU:HD22	1.82	0.61
1:B:61:ASN:ND2	1:B:216:THR:HG22	2.16	0.60
1:C:244:LYS:HG3	1:C:298:GLN:OE1	2.01	0.60
1:A:453:ILE:HG23	1:A:454:TYR:CD1	2.36	0.60
1:C:25:TYR:CE1	1:C:106:ARG:HD3	2.36	0.60
1:A:286:LYS:CG	1:A:287:LYS:N	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLY:HA3	1:A:31:GLU:OE2	2.01	0.60
1:A:201:SER:OG	1:A:204:GLU:HG3	2.02	0.59
1:A:228:ARG:NH1	1:A:259:VAL:HB	2.18	0.59
1:B:375:THR:O	1:B:380:PHE:HA	2.03	0.59
1:B:452:TYR:CD2	1:B:459:ALA:HA	2.38	0.59
1:B:516:ARG:O	1:B:520:GLN:CG	2.50	0.58
1:A:13:LYS:O	1:A:267:GLY:HA3	2.04	0.58
1:B:242:PHE:O	1:B:289:THR:HG21	2.03	0.58
1:B:286:LYS:HE2	1:B:286:LYS:H	1.69	0.58
1:B:260:MET:CE	1:B:269:LEU:HD22	2.33	0.57
1:A:165:LEU:CD2	1:A:300:LEU:HG	2.33	0.57
1:B:19:ASP:HB2	1:B:180:MET:HE1	1.86	0.57
1:B:8:LEU:HD13	1:B:36:VAL:HG13	1.87	0.57
1:A:460:PRO:HD2	1:A:463:VAL:HG21	1.87	0.57
1:A:514:ASP:O	1:A:517:ARG:CG	2.52	0.57
1:B:387:ARG:O	1:B:387:ARG:HD2	2.05	0.57
1:A:477:LYS:HB3	1:A:477:LYS:NZ	2.20	0.57
1:A:31:GLU:HG3	1:A:32:PHE:HD2	1.69	0.57
1:A:32:PHE:N	1:A:32:PHE:CD2	2.73	0.56
1:A:32:PHE:N	1:A:32:PHE:HD2	2.03	0.56
1:A:111:TYR:OH	1:A:113:THR:HG22	2.06	0.56
1:B:229:LEU:O	1:B:233:ILE:HG12	2.05	0.56
1:B:321:ASN:HB3	1:B:324:CYS:HB3	1.87	0.56
1:B:101:GLU:HG2	1:B:194:LEU:HD13	1.87	0.56
1:C:280:ASN:O	1:C:283:LYS:HG2	2.05	0.56
1:A:431:TYR:HE2	6:A:3312:HOH:O	1.88	0.56
1:A:74:ASP:HB2	1:A:84:LEU:HB3	1.88	0.56
1:B:188:ILE:HD12	1:B:188:ILE:N	2.21	0.56
1:A:460:PRO:HB2	1:A:463:VAL:HG23	1.87	0.56
1:C:86:VAL:O	1:C:197:SER:HB3	2.05	0.56
1:C:90:GLU:HG3	1:C:93:GLU:H	1.71	0.55
1:A:173:CYS:HA	1:A:176:SER:HB3	1.87	0.55
1:A:13:LYS:O	1:A:266:PHE:O	2.23	0.55
1:A:292:PRO:HB2	3:A:920:MES:O3S	2.06	0.55
1:B:336:LEU:HD22	1:B:385:GLN:HG2	1.89	0.55
1:B:25:TYR:CE1	1:B:106:ARG:HD2	2.42	0.55
1:C:317:LYS:HB3	1:C:317:LYS:HZ2	1.72	0.55
1:B:191:ILE:HG21	1:B:196:ILE:HB	1.89	0.55
1:A:448:MET:SD	1:A:449:PRO:HD2	2.47	0.54
1:A:111:TYR:CE1	1:A:113:THR:HG23	2.42	0.54
1:A:461:LEU:HD13	1:A:461:LEU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:MET:HB2	1:C:507:VAL:HG22	1.89	0.54
1:A:452:TYR:CD2	1:A:459:ALA:HA	2.42	0.54
1:B:80:LEU:HB3	1:B:185:LEU:HB2	1.89	0.54
1:A:340:ARG:HD2	1:A:341:ASP:OD1	2.08	0.54
1:B:360:GLY:HA3	1:B:395:ILE:HG23	1.90	0.54
1:B:450:LYS:H	1:B:450:LYS:CD	2.20	0.54
1:A:457:TRP:CE3	1:A:478:PRO:HG3	2.43	0.54
1:A:452:TYR:CE2	1:A:459:ALA:HA	2.43	0.54
1:A:96:VAL:O	1:A:100:GLN:HG2	2.08	0.53
1:A:244:LYS:HG3	1:A:298:GLN:OE1	2.08	0.53
1:A:317:LYS:O	1:A:321:ASN:HB2	2.09	0.53
1:C:279:GLN:OE1	1:C:279:GLN:HA	2.08	0.53
1:C:9:ILE:HG23	1:C:35:PRO:HA	1.90	0.53
1:A:67:LEU:O	1:A:71:LYS:HG3	2.08	0.53
1:B:5:SER:HB2	1:B:103:LYS:O	2.08	0.53
1:A:149:ILE:HD12	1:A:168:ALA:HA	1.90	0.53
1:A:39:ILE:HG23	1:A:44:MET:HG3	1.90	0.53
1:B:500:ASN:HA	1:B:507:VAL:CG2	2.39	0.53
1:B:450:LYS:HD2	1:B:450:LYS:H	1.73	0.53
1:A:125:LYS:HD2	1:A:135:VAL:HG11	1.91	0.52
1:B:460:PRO:HB2	1:B:463:VAL:HG23	1.91	0.52
1:B:517:ARG:O	1:B:520:GLN:HB2	2.09	0.52
1:C:495:GLU:OE1	1:C:519:LEU:HD21	2.10	0.52
1:B:28:LYS:HZ2	1:B:28:LYS:HB2	1.75	0.52
1:C:275:TYR:CE1	1:C:296:LEU:HD11	2.45	0.52
1:C:229:LEU:HD22	1:C:269:LEU:HD11	1.92	0.52
1:C:83:ARG:HB3	1:C:188:ILE:HD12	1.92	0.52
1:B:228:ARG:HG2	1:B:260:MET:SD	2.50	0.51
1:C:258:THR:HB	1:C:260:MET:HG2	1.92	0.51
1:B:244:LYS:HE3	1:B:257:THR:HG21	1.90	0.51
1:A:227:LYS:HE3	1:A:231:LYS:HZ1	1.75	0.51
1:B:50:ALA:O	1:B:52:SER:N	2.43	0.51
1:C:449:PRO:HG2	1:C:452:TYR:HD1	1.75	0.51
1:B:460:PRO:HD2	1:B:463:VAL:HG21	1.93	0.51
1:B:279:GLN:HA	1:B:279:GLN:OE1	2.11	0.51
1:B:462:SER:O	1:B:466:LYS:HB2	2.11	0.51
1:B:492:LYS:HG2	1:B:519:LEU:HD22	1.93	0.51
1:B:521:LYS:O	1:B:525:GLU:HG2	2.10	0.51
1:A:290:SER:HB3	1:A:291:PRO:HD2	1.92	0.50
1:A:321:ASN:OD1	1:A:323:ILE:HG12	2.11	0.50
1:B:28:LYS:O	1:B:106:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:CD1	1:B:36:VAL:HG13	2.40	0.50
1:C:244:LYS:HG3	1:C:298:GLN:CD	2.32	0.50
1:C:499:LEU:HD23	1:C:515:LEU:HD22	1.92	0.50
1:A:239:VAL:HG11	1:A:281:ILE:HD12	1.92	0.50
1:B:286:LYS:H	1:B:286:LYS:CE	2.24	0.50
1:C:368:HIS:CG	1:C:409:LEU:HD11	2.46	0.50
1:A:239:VAL:HG21	1:A:281:ILE:CD1	2.41	0.50
1:B:146:PRO:O	1:B:150:ILE:HG13	2.12	0.49
1:C:35:PRO:HD2	1:C:188:ILE:HD11	1.94	0.49
1:B:163:SER:O	1:B:167:VAL:HG23	2.12	0.49
1:B:352:ILE:HA	1:B:437:TYR:OH	2.13	0.49
1:A:102:TRP:CZ2	1:A:194:LEU:HD12	2.48	0.49
1:A:227:LYS:HE3	1:A:231:LYS:NZ	2.28	0.49
1:A:477:LYS:HB3	1:A:477:LYS:HZ2	1.77	0.49
1:A:382:HIS:HB3	1:A:385:GLN:HG2	1.94	0.49
1:A:157:PRO:HG2	6:A:3590:HOH:O	2.13	0.49
1:A:21:PRO:HD2	6:A:3157:HOH:O	2.12	0.49
1:C:57:ARG:HH11	1:C:57:ARG:HG3	1.78	0.49
1:B:508:ASP:C	1:B:508:ASP:OD2	2.51	0.49
1:C:492:LYS:NZ	2:C:902:IMD:HN1	2.10	0.49
1:A:259:VAL:O	1:A:259:VAL:HG12	2.12	0.49
1:B:91:PRO:CB	1:B:120:LEU:HD21	2.40	0.49
1:C:25:TYR:CD1	1:C:106:ARG:HD3	2.46	0.49
1:A:368:HIS:CG	1:A:409:LEU:HD11	2.47	0.49
1:A:517:ARG:CG	1:A:518:LYS:N	2.76	0.49
1:C:118:GLN:O	1:C:122:VAL:HG23	2.12	0.49
1:A:161:TYR:CE2	1:A:292:PRO:HB3	2.48	0.48
1:A:325:LYS:HD2	1:A:497:TYR:CE1	2.48	0.48
1:C:502:LYS:C	1:C:504:ASP:H	2.16	0.48
1:A:260:MET:CE	1:A:269:LEU:HD22	2.44	0.48
1:B:162:GLN:HG3	6:B:3474:HOH:O	2.13	0.48
1:C:16:ARG:NE	1:C:270:SER:HB2	2.28	0.48
1:B:156:LYS:NZ	1:B:322:ARG:HD3	2.28	0.48
1:A:121:ASP:O	1:A:125:LYS:HE3	2.13	0.48
1:A:438:ILE:HG23	1:A:442:LEU:HD12	1.95	0.48
1:A:69:SER:HA	1:A:221:GLY:HA2	1.96	0.48
1:B:502:LYS:C	1:B:504:ASP:H	2.17	0.48
1:C:149:ILE:CD1	1:C:168:ALA:HA	2.43	0.48
1:A:365:LEU:O	1:A:368:HIS:HB2	2.13	0.48
1:B:480:VAL:HG22	1:B:485:ALA:HB2	1.95	0.48
1:A:14:GLY:O	1:A:16:ARG:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:SER:O	1:B:414:PHE:HB2	2.13	0.48
1:C:8:LEU:HD23	1:C:8:LEU:C	2.34	0.48
1:B:321:ASN:OD1	1:B:323:ILE:HG12	2.14	0.48
1:A:437:TYR:HB3	6:A:3164:HOH:O	2.13	0.47
1:B:375:THR:OG1	1:B:376:ARG:N	2.45	0.47
1:C:499:LEU:O	1:C:499:LEU:HD12	2.15	0.47
1:C:503:MET:CB	1:C:507:VAL:HG22	2.43	0.47
1:C:77:LEU:HD12	1:C:84:LEU:HB2	1.96	0.47
1:B:348:TRP:O	1:B:352:ILE:HG13	2.15	0.47
1:A:449:PRO:HG2	1:A:452:TYR:HD1	1.79	0.47
1:C:163:SER:O	1:C:166:LYS:HB3	2.15	0.47
1:B:301:TRP:CZ2	3:B:920:MES:H71	2.50	0.47
1:B:387:ARG:C	1:B:387:ARG:HD2	2.34	0.47
1:C:19:ASP:N	1:C:180:MET:HE1	2.29	0.47
1:A:345:GLY:O	1:A:347:PRO:HD3	2.14	0.47
1:C:106:ARG:HG3	1:C:106:ARG:HH21	1.79	0.47
1:A:228:ARG:NH1	1:A:258:THR:O	2.48	0.46
1:A:318:MET:HE2	1:A:382:HIS:HE2	1.79	0.46
1:B:165:LEU:HD11	1:B:300:LEU:HG	1.96	0.46
1:C:25:TYR:CZ	1:C:106:ARG:NH2	2.83	0.46
1:A:149:ILE:CD1	1:A:168:ALA:HA	2.46	0.46
1:A:347:PRO:HG2	1:A:456:PRO:HD3	1.98	0.46
1:C:260:MET:HE2	1:C:269:LEU:HD22	1.97	0.46
1:C:31:GLU:HB3	1:C:32:PHE:CD1	2.51	0.46
1:B:12:ARG:HB3	1:B:117:TYR:CE2	2.50	0.46
1:B:156:LYS:HB3	1:B:157:PRO:HD2	1.98	0.46
1:B:244:LYS:HG3	1:B:298:GLN:OE1	2.15	0.46
1:C:453:ILE:HG23	1:C:454:TYR:CD1	2.51	0.46
1:A:243:GLU:HG2	1:A:293:VAL:HG21	1.97	0.46
1:B:244:LYS:HG3	1:B:298:GLN:CD	2.36	0.46
1:B:466:LYS:HD3	1:B:466:LYS:O	2.15	0.46
1:C:101:GLU:CG	1:C:192:GLY:HA3	2.45	0.46
1:A:156:LYS:HB3	1:A:157:PRO:HD2	1.97	0.46
1:A:312:THR:O	1:A:315:PHE:HB2	2.16	0.46
1:A:471:VAL:HA	1:A:475:TYR:O	2.15	0.45
1:B:101:GLU:OE1	1:B:193:ASN:HB3	2.16	0.45
1:C:102:TRP:HE1	1:C:192:GLY:H	1.64	0.45
1:B:449:PRO:O	1:B:450:LYS:C	2.55	0.45
1:C:301:TRP:CZ2	3:C:920:MES:H81	2.50	0.45
1:C:504:ASP:O	1:C:506:LYS:N	2.45	0.45
1:C:205:LEU:HA	1:C:205:LEU:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:TYR:CE2	1:B:460:PRO:HD3	2.51	0.45
1:A:318:MET:CE	1:A:382:HIS:HE2	2.30	0.45
1:B:43:TYR:CE1	1:B:57:ARG:HD3	2.52	0.45
1:C:53:PRO:HA	6:C:3655:HOH:O	2.16	0.45
1:A:258:THR:HB	1:A:260:MET:HG2	1.99	0.45
1:A:260:MET:HE2	1:A:269:LEU:HD22	1.98	0.45
1:A:309:ALA:HB1	1:A:399:TRP:CZ3	2.52	0.45
1:B:96:VAL:O	1:B:100:GLN:HG3	2.17	0.45
1:C:99:LEU:HA	1:C:99:LEU:HD12	1.85	0.45
1:B:415:PHE:CZ	1:B:417:GLN:HB2	2.53	0.45
1:A:235:ASP:O	1:A:239:VAL:HG12	2.17	0.44
1:B:165:LEU:HD11	1:B:300:LEU:CG	2.48	0.44
1:B:461:LEU:HD12	1:B:461:LEU:O	2.16	0.44
1:C:237:ALA:O	1:C:241:ASN:ND2	2.50	0.44
1:B:171:PRO:O	1:B:173:CYS:N	2.44	0.44
1:B:122:VAL:HG13	1:B:123:LYS:N	2.33	0.44
1:C:321:ASN:OD1	1:C:323:ILE:HG12	2.17	0.44
1:B:286:LYS:N	1:B:286:LYS:HD3	2.33	0.44
1:A:13:LYS:HB2	6:A:3247:HOH:O	2.16	0.44
1:A:508:ASP:OD1	1:A:509:GLU:N	2.50	0.44
1:B:195:GLY:O	1:B:196:ILE:C	2.55	0.44
1:B:518:LYS:C	1:B:518:LYS:HD3	2.38	0.44
1:C:286:LYS:HG2	1:C:287:LYS:N	2.29	0.44
1:C:449:PRO:HG2	1:C:452:TYR:CD1	2.52	0.44
1:C:455:GLU:HA	1:C:457:TRP:CZ3	2.53	0.44
1:A:508:ASP:CB	1:A:511:ASN:HD22	2.24	0.44
1:A:363:HIS:HE1	1:A:365:LEU:HD22	1.83	0.44
1:B:191:ILE:CD1	1:B:196:ILE:HD12	2.47	0.44
1:C:475:TYR:CD1	1:C:476:PRO:HD2	2.53	0.43
1:B:161:TYR:OH	1:B:300:LEU:HB2	2.18	0.43
1:C:229:LEU:O	1:C:233:ILE:HG12	2.19	0.43
1:A:33:MET:O	1:A:188:ILE:HA	2.18	0.43
1:B:152:LYS:HD2	1:B:167:VAL:O	2.18	0.43
1:B:466:LYS:NZ	6:B:3633:HOH:O	2.50	0.43
1:C:509:GLU:HG3	1:C:510:GLU:N	2.33	0.43
1:B:261:SER:OG	1:B:262:PRO:HD3	2.18	0.43
1:C:111:TYR:CE1	1:C:113:THR:HG23	2.54	0.43
1:C:408:TRP:NE1	2:C:901:IMD:H2	2.31	0.43
1:A:191:ILE:O	1:A:191:ILE:HG22	2.19	0.43
1:C:195:GLY:O	1:C:196:ILE:C	2.57	0.43
1:A:443:PRO:O	1:A:446:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ARG:HG3	1:B:516:ARG:HH11	1.83	0.43
1:C:78:LYS:HA	1:C:82:SER:O	2.18	0.43
1:A:191:ILE:HG21	1:A:196:ILE:CG1	2.47	0.43
1:A:386:GLY:HA3	1:A:406:TRP:CH2	2.54	0.43
1:B:347:PRO:HB2	1:B:438:ILE:HD13	2.00	0.43
1:B:452:TYR:CE2	1:B:459:ALA:HA	2.53	0.43
1:B:86:VAL:HG21	1:B:199:VAL:HG22	2.00	0.43
1:B:329:TRP:CG	1:B:382:HIS:HA	2.54	0.42
1:B:500:ASN:HA	1:B:507:VAL:HG23	2.01	0.42
1:C:57:ARG:HG3	1:C:57:ARG:NH1	2.34	0.42
1:C:25:TYR:OH	1:C:106:ARG:NH2	2.52	0.42
1:A:162:GLN:CD	1:A:162:GLN:H	2.21	0.42
1:B:178:LEU:HB2	1:B:180:MET:HE2	2.02	0.42
1:B:188:ILE:HG22	1:B:189:GLY:O	2.20	0.42
1:C:424:PRO:HD3	1:C:482:HIS:CE1	2.55	0.42
1:B:25:TYR:CZ	1:B:106:ARG:NH1	2.87	0.42
1:A:321:ASN:HB3	1:A:324:CYS:HB3	2.02	0.42
1:B:156:LYS:HZ3	1:B:322:ARG:HD3	1.85	0.42
1:C:224:GLU:HG2	6:C:3114:HOH:O	2.19	0.42
1:A:375:THR:O	1:A:380:PHE:HA	2.20	0.42
1:A:92:GLY:O	1:A:96:VAL:HG13	2.19	0.42
1:C:107:LEU:HB3	1:C:135:VAL:HG22	2.02	0.42
1:C:37:PHE:O	1:C:86:VAL:HA	2.19	0.42
1:A:120:LEU:O	1:A:124:VAL:HG23	2.20	0.42
1:C:157:PRO:HA	1:C:158:PRO:HD3	1.91	0.42
1:A:421:ILE:HG22	1:A:422:TYR:O	2.20	0.41
1:A:62:ARG:HH12	1:A:392:ARG:HA	1.84	0.41
1:A:301:TRP:CZ2	3:A:920:MES:H71	2.55	0.41
1:A:413:SER:O	1:A:414:PHE:HB2	2.20	0.41
1:A:90:GLU:HG3	1:A:93:GLU:H	1.84	0.41
1:B:233:ILE:HD11	2:B:906:IMD:N1	2.35	0.41
1:C:373:PHE:O	1:C:378:ASP:HB2	2.19	0.41
1:A:227:LYS:O	1:A:230:THR:HB	2.20	0.41
1:A:261:SER:HB3	1:A:262:PRO:CD	2.50	0.41
1:A:475:TYR:CD1	1:A:476:PRO:HD2	2.55	0.41
1:B:5:SER:HA	1:B:32:PHE:CZ	2.54	0.41
1:A:18:HIS:ND1	1:A:222:GLU:OE2	2.34	0.41
1:B:188:ILE:N	1:B:188:ILE:CD1	2.83	0.41
1:B:387:ARG:NH1	1:B:403:ASN:OD1	2.47	0.41
1:C:488:GLU:CD	1:C:491:ARG:HE	2.23	0.41
1:A:350:ASP:O	1:A:354:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PHE:O	1:B:146:PRO:HD3	2.20	0.41
1:C:162:GLN:N	1:C:162:GLN:OE1	2.43	0.41
1:C:274:PHE:HD2	1:C:274:PHE:O	2.04	0.41
1:C:64:ARG:HH11	1:C:64:ARG:HG3	1.86	0.41
1:C:502:LYS:C	1:C:504:ASP:N	2.73	0.41
1:A:336:LEU:HD13	1:A:385:GLN:HB3	2.03	0.41
1:C:260:MET:CE	1:C:269:LEU:HD22	2.50	0.41
1:C:375:THR:O	1:C:380:PHE:HA	2.21	0.41
1:C:95:LEU:O	1:C:99:LEU:HB2	2.20	0.41
1:C:93:GLU:O	1:C:96:VAL:HG22	2.19	0.41
1:A:111:TYR:CG	1:A:112:ASP:N	2.89	0.41
1:B:465:THR:OG1	1:B:470:ILE:HD11	2.21	0.41
1:B:8:LEU:HD13	1:B:36:VAL:CG1	2.49	0.41
1:A:242:PHE:HB3	6:A:3143:HOH:O	2.21	0.41
1:A:261:SER:HB3	1:A:262:PRO:HD3	2.03	0.41
1:A:387:ARG:NE	1:A:388:ASP:OD2	2.50	0.41
1:B:261:SER:N	1:B:262:PRO:HD2	2.36	0.41
1:C:408:TRP:CE3	1:C:414:PHE:HB3	2.55	0.41
1:B:424:PRO:HD3	1:B:482:HIS:CE1	2.56	0.41
1:C:37:PHE:HE2	1:C:39:ILE:HD13	1.86	0.41
1:A:196:ILE:CD1	1:A:196:ILE:H	2.18	0.40
1:A:36:VAL:HG12	1:A:37:PHE:N	2.36	0.40
1:A:453:ILE:HG23	1:A:454:TYR:HD1	1.82	0.40
1:A:261:SER:HB2	5:A:900:FAD:C5'	2.51	0.40
1:B:32:PHE:HD2	1:B:34:TYR:HE1	1.69	0.40
1:A:280:ASN:O	1:A:283:LYS:HG2	2.21	0.40
1:B:259:VAL:O	1:B:259:VAL:HG12	2.21	0.40
1:B:382:HIS:HE1	1:B:384:GLU:HG3	1.84	0.40
1:B:460:PRO:HD2	1:B:463:VAL:CG2	2.51	0.40
1:B:194:LEU:HD12	1:B:194:LEU:HA	1.91	0.40
1:C:492:LYS:HZ2	2:C:902:IMD:HN1	1.67	0.40
1:A:261:SER:HG	1:A:396:ASP:CG	2.25	0.40
1:A:488:GLU:OE2	1:A:491:ARG:NH1	2.54	0.40
1:C:109:PHE:O	1:C:137:SER:HA	2.20	0.40
1:C:365:LEU:HD12	1:C:365:LEU:HA	1.86	0.40
1:A:143:LEU:HD23	1:A:272:ARG:HG3	2.03	0.40
1:C:83:ARG:HG2	1:C:84:LEU:N	2.35	0.40

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	520/537 (97%)	471 (91%)	46 (9%)	3 (1%)	28	56
1	B	515/537 (96%)	471 (92%)	38 (7%)	6 (1%)	15	37
1	C	518/537 (96%)	486 (94%)	28 (5%)	4 (1%)	22	49
All	All	1553/1611 (96%)	1428 (92%)	112 (7%)	13 (1%)	22	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	LYS
1	B	172	SER
1	B	176	SER
1	B	286	LYS
1	B	451	GLN
1	A	15	LEU
1	B	503	MET
1	A	174	ALA
1	C	332	ASP
1	B	196	ILE
1	C	196	ILE
1	C	286	LYS
1	C	505	GLY

### 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	453/473 (96%)	427 (94%)	26 (6%)	24	51
1	B	451/473 (95%)	424 (94%)	27 (6%)	22	48
1	C	452/473 (96%)	428 (95%)	24 (5%)	26	54
All	All	1356/1419 (96%)	1279 (94%)	77 (6%)	24	51

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	70	LEU
1	A	74	ASP
1	A	83	ARG
1	A	90	GLU
1	A	96	VAL
1	A	125	LYS
1	A	185	LEU
1	A	196	ILE
1	A	205	LEU
1	A	219	ARG
1	A	239	VAL
1	A	265	LYS
1	A	272	ARG
1	A	274	PHE
1	A	300	LEU
1	A	362	MET
1	A	365	LEU
1	A	368	HIS
1	A	378	ASP
1	A	393	LEU
1	A	455	GLU
1	A	466	LYS
1	A	477	LYS
1	A	512	LEU
1	A	518	LYS
1	B	8	LEU
1	B	12	ARG
1	B	23	LEU
1	B	32	PHE
1	B	44	MET
1	B	80	LEU
1	B	90	GLU
1	B	95	LEU

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Mol	Chain	Res	Type
1	B	106	ARG
1	B	162	GLN
1	B	165	LEU
1	B	194	LEU
1	B	203	GLU
1	B	205	LEU
1	B	210	ASP
1	B	216	THR
1	B	219	ARG
1	B	265	LYS
1	B	279	GLN
1	B	362	MET
1	B	365	LEU
1	B	393	LEU
1	B	452	TYR
1	B	481	LEU
1	B	488	GLU
1	B	512	LEU
1	B	518	LYS
1	C	12	ARG
1	C	61	ASN
1	C	73	LEU
1	C	90	GLU
1	C	107	LEU
1	C	202	LEU
1	C	205	LEU
1	C	216	THR
1	C	219	ARG
1	C	239	VAL
1	C	265	LYS
1	C	272	ARG
1	C	274	PHE
1	C	286	LYS
1	C	300	LEU
1	C	317	LYS
1	C	365	LEU
1	C	393	LEU
1	C	455	GLU
1	C	461	LEU
1	C	468	ASN
1	C	480	VAL
1	C	483	ASP

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Mol	Chain	Res	Type
1	C	503	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	385	GLN
1	A	451	GLN
1	A	511	ASN
1	B	61	ASN
1	B	100	GLN
1	B	162	GLN
1	B	451	GLN
1	C	61	ASN
1	C	403	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](#)

19 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
5	FAD	A	900	-	51,58,58	2.07	10 (19%)	54,89,89	2.01	9 (16%)
2	IMD	A	901	-	3,5,5	0.61	0	4,5,5	0.51	0
2	IMD	A	902	-	3,5,5	0.66	0	4,5,5	0.45	0
2	IMD	A	905	-	3,5,5	0.61	0	4,5,5	0.45	0
3	MES	A	920	-	12,12,12	1.56	3 (25%)	14,16,16	0.84	1 (7%)
4	PO4	A	930	-	4,4,4	1.33	0	6,6,6	0.39	0
5	FAD	B	900	-	51,58,58	2.06	11 (21%)	54,89,89	2.03	9 (16%)
2	IMD	B	901	-	3,5,5	0.59	0	4,5,5	0.46	0
2	IMD	B	903	-	3,5,5	0.59	0	4,5,5	0.46	0
2	IMD	B	904	-	3,5,5	0.63	0	4,5,5	0.49	0
2	IMD	B	905	-	3,5,5	0.61	0	4,5,5	0.41	0
2	IMD	B	906	-	3,5,5	0.61	0	4,5,5	0.48	0
3	MES	B	920	-	12,12,12	1.63	4 (33%)	14,16,16	0.96	2 (14%)
4	PO4	B	930	-	4,4,4	1.33	0	6,6,6	0.40	0
5	FAD	C	900	-	51,58,58	2.00	10 (19%)	54,89,89	1.96	8 (14%)
2	IMD	C	901	-	3,5,5	0.63	0	4,5,5	0.53	0
2	IMD	C	902	-	3,5,5	0.65	0	4,5,5	0.42	0
3	MES	C	920	-	12,12,12	1.34	3 (25%)	14,16,16	0.93	1 (7%)
4	PO4	C	930	-	4,4,4	1.32	0	6,6,6	0.39	0

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
5	FAD	A	900	-	-	0/28/50/50	0/6/6/6
2	IMD	A	901	-	-	0/0/0/0	0/1/1/1
2	IMD	A	902	-	-	0/0/0/0	0/1/1/1
2	IMD	A	905	-	-	0/0/0/0	0/1/1/1
3	MES	A	920	-	-	0/6/14/14	0/1/1/1
4	PO4	A	930	-	-	0/0/0/0	0/0/0/0
5	FAD	B	900	-	-	0/28/50/50	0/6/6/6
2	IMD	B	901	-	-	0/0/0/0	0/1/1/1
2	IMD	B	903	-	-	0/0/0/0	0/1/1/1
2	IMD	B	904	-	-	0/0/0/0	0/1/1/1
2	IMD	B	905	-	-	0/0/0/0	0/1/1/1
2	IMD	B	906	-	-	0/0/0/0	0/1/1/1
3	MES	B	920	-	-	0/6/14/14	0/1/1/1
4	PO4	B	930	-	-	0/0/0/0	0/0/0/0
5	FAD	C	900	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	C	901	-	-	0/0/0/0	0/1/1/1
2	IMD	C	902	-	-	0/0/0/0	0/1/1/1
3	MES	C	920	-	-	0/6/14/14	0/1/1/1
4	PO4	C	930	-	-	0/0/0/0	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	FAD	C2B-C1B	-2.20	1.50	1.53
5	B	900	FAD	C9-C8	2.01	1.43	1.37
5	B	900	FAD	C2-N3	2.03	1.42	1.38
3	B	920	MES	C8-S	2.03	1.80	1.77
3	C	920	MES	C7-N4	2.07	1.52	1.47
5	C	900	FAD	C6-C7	2.09	1.43	1.37
5	B	900	FAD	C6-C7	2.16	1.43	1.37
5	A	900	FAD	C6-C7	2.24	1.43	1.37
3	C	920	MES	C3-N4	2.25	1.53	1.47
3	B	920	MES	C3-N4	2.32	1.53	1.47
3	A	920	MES	C3-N4	2.45	1.53	1.47
3	C	920	MES	C5-N4	2.47	1.53	1.47
5	C	900	FAD	C9-C8	2.52	1.44	1.37
5	B	900	FAD	C9A-N10	2.57	1.42	1.38
3	B	920	MES	C5-N4	2.75	1.54	1.47
3	A	920	MES	C5-N4	2.78	1.54	1.47
3	A	920	MES	C7-N4	2.97	1.54	1.47
3	B	920	MES	C7-N4	3.18	1.54	1.47
5	C	900	FAD	C9A-N10	3.34	1.43	1.38
5	C	900	FAD	C4-N3	3.41	1.39	1.33
5	B	900	FAD	C4-N3	3.44	1.39	1.33
5	A	900	FAD	C4-N3	3.47	1.39	1.33
5	A	900	FAD	C9A-N10	3.49	1.43	1.38
5	A	900	FAD	C2A-N1A	4.10	1.41	1.33
5	C	900	FAD	C5X-N5	4.15	1.41	1.35
5	A	900	FAD	C5X-N5	4.24	1.41	1.35
5	B	900	FAD	C2A-N1A	4.29	1.42	1.33
5	B	900	FAD	C5X-N5	4.31	1.41	1.35
5	C	900	FAD	C2A-N1A	4.45	1.42	1.33
5	C	900	FAD	C1'-N10	4.49	1.53	1.48
5	C	900	FAD	C4X-N5	4.57	1.39	1.33
5	B	900	FAD	C4X-N5	4.67	1.40	1.33
5	A	900	FAD	C2A-N3A	4.87	1.40	1.32
5	B	900	FAD	C2A-N3A	5.00	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	FAD	C1'-N10	5.27	1.53	1.48
5	A	900	FAD	C4X-N5	5.37	1.41	1.33
5	C	900	FAD	C2A-N3A	5.52	1.41	1.32
5	C	900	FAD	C10-N1	5.76	1.41	1.33
5	B	900	FAD	C1'-N10	5.78	1.54	1.48
5	A	900	FAD	C10-N1	5.85	1.41	1.33
5	B	900	FAD	C10-N1	6.02	1.41	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	900	FAD	N3A-C2A-N1A	-9.27	120.78	128.86
5	C	900	FAD	N3A-C2A-N1A	-9.07	120.96	128.86
5	A	900	FAD	N3A-C2A-N1A	-8.96	121.06	128.86
5	B	900	FAD	C4X-C4-N3	-3.36	118.70	123.48
5	A	900	FAD	C4X-C4-N3	-3.27	118.83	123.48
5	C	900	FAD	C4X-C4-N3	-3.02	119.18	123.48
5	B	900	FAD	C1B-N9A-C4A	-2.54	122.25	126.64
5	A	900	FAD	C4A-C5A-N7A	-2.37	107.12	109.41
5	C	900	FAD	C4A-C5A-N7A	-2.36	107.13	109.41
5	B	900	FAD	C4A-C5A-N7A	-2.18	107.30	109.41
3	A	920	MES	C2-C3-N4	-2.17	107.06	110.11
5	A	900	FAD	C1B-N9A-C4A	-2.17	122.89	126.64
3	B	920	MES	C2-C3-N4	-2.14	107.11	110.11
5	C	900	FAD	C1B-N9A-C4A	-2.13	122.96	126.64
3	B	920	MES	O1S-S-C8	2.01	108.52	106.79
3	C	920	MES	O1S-S-C8	2.07	108.57	106.79
5	C	900	FAD	C4-C4X-N5	2.13	121.02	118.68
5	B	900	FAD	C5X-C9A-N10	2.20	119.29	117.66
5	A	900	FAD	C5X-C9A-N10	2.42	119.45	117.66
5	A	900	FAD	C1'-N10-C9A	2.45	120.59	118.35
5	B	900	FAD	C4-C4X-N5	2.50	121.42	118.68
5	A	900	FAD	C4-C4X-N5	2.56	121.49	118.68
5	C	900	FAD	C1'-N10-C9A	2.80	120.91	118.35
5	B	900	FAD	C1'-N10-C9A	2.84	120.95	118.35
5	B	900	FAD	C4X-N5-C5X	4.24	121.23	116.76
5	A	900	FAD	C4X-N5-C5X	4.29	121.29	116.76
5	C	900	FAD	C4X-N5-C5X	4.32	121.32	116.76
5	C	900	FAD	C4-N3-C2	6.39	120.75	115.16
5	B	900	FAD	C4-N3-C2	6.82	121.13	115.16
5	A	900	FAD	C4-N3-C2	6.89	121.18	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	FAD	1	0
3	A	920	MES	3	0
2	B	906	IMD	1	0
3	B	920	MES	3	0
2	C	901	IMD	2	0
2	C	902	IMD	2	0
3	C	920	MES	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

### 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	522/537 (97%)	-0.14	8 (1%) 74 75	18, 36, 65, 100	0
1	B	521/537 (97%)	-0.13	7 (1%) 77 78	20, 39, 67, 100	0
1	C	520/537 (96%)	-0.24	8 (1%) 74 75	16, 36, 76, 101	0
All	All	1563/1611 (97%)	-0.17	23 (1%) 74 75	16, 37, 67, 101	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	ILE	3.6
1	B	193	ASN	3.4
1	A	193	ASN	3.2
1	A	188	ILE	3.1
1	C	195	GLY	3.1
1	C	32	PHE	3.1
1	B	191	ILE	3.0
1	A	524	HIS	3.0
1	C	193	ASN	2.8
1	B	524	HIS	2.7
1	C	512	LEU	2.6
1	A	5	SER	2.5
1	C	514	ASP	2.5
1	C	521	LYS	2.4
1	A	525	GLU	2.3
1	B	50	ALA	2.3
1	A	194	LEU	2.2
1	C	506	LYS	2.2
1	A	522	ASP	2.1
1	B	192	GLY	2.1
1	C	505	GLY	2.1
1	A	175	LYS	2.0
1	B	287	LYS	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, 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
3	MES	C	920	12/12	0.68	0.49	21.03	97,100,111,111	0
3	MES	B	920	12/12	0.58	0.50	18.41	85,90,101,102	0
3	MES	A	920	12/12	0.70	0.41	13.86	85,88,97,97	0
2	IMD	A	905	5/5	0.74	0.34	13.82	83,84,84,84	0
4	PO4	C	930	5/5	0.81	0.28	9.03	98,98,99,100	0
2	IMD	B	901	5/5	0.89	0.27	7.30	68,69,69,70	0
4	PO4	A	930	5/5	0.88	0.24	4.43	92,93,93,94	0
2	IMD	A	901	5/5	0.93	0.22	4.14	72,72,72,72	0
4	PO4	B	930	5/5	0.80	0.24	3.19	94,96,96,96	0
2	IMD	C	901	5/5	0.94	0.19	2.76	52,53,54,54	0
2	IMD	B	906	5/5	0.90	0.19	2.31	90,90,90,90	0
2	IMD	A	902	5/5	0.89	0.17	1.32	54,56,56,56	0
5	FAD	A	900	53/53	0.99	0.16	0.14	18,23,26,29	0
2	IMD	B	905	5/5	0.89	0.17	-0.00	65,66,66,67	0
2	IMD	C	902	5/5	0.91	0.15	-0.13	48,48,49,49	0
5	FAD	B	900	53/53	0.98	0.15	-0.38	20,25,31,32	0
5	FAD	C	900	53/53	0.98	0.14	-0.42	16,18,22,26	0
2	IMD	B	904	5/5	0.84	0.22	-	73,74,74,74	0
2	IMD	B	903	5/5	0.81	0.13	-	88,88,89,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.