



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:27 AM GMT

PDB ID : 2E77  
Title : Crystal structure of L-lactate oxidase with pyruvate complex  
Authors : Morimoto, Y.  
Deposited on : 2007-01-06  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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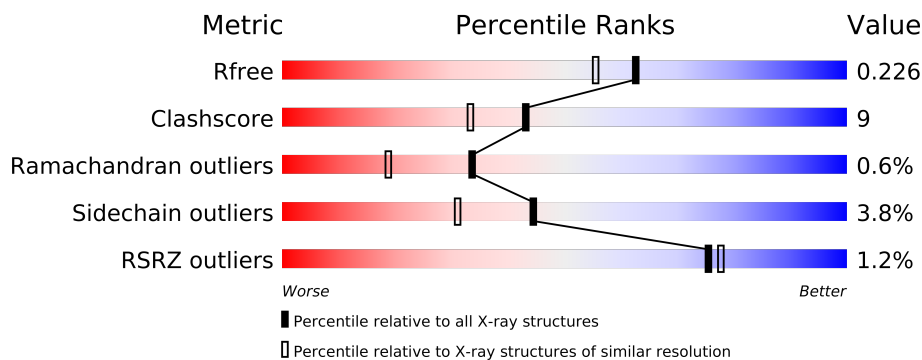
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	
1	C	374	
1	D	374	

## 2 Entry composition i

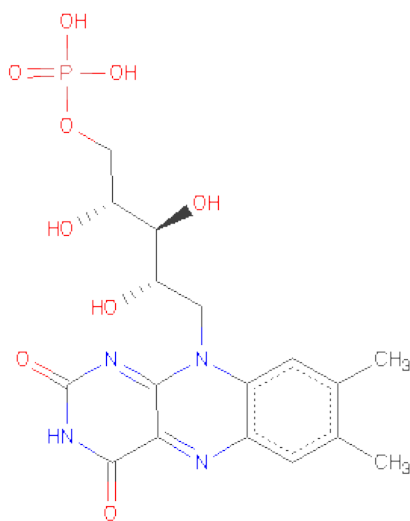
There are 4 unique types of molecules in this entry. The entry contains 12571 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2738	1732	475	525	6			
1	B	368	Total	C	N	O	S	0	0	0
			2840	1794	494	545	7			
1	C	350	Total	C	N	O	S	0	0	0
			2700	1708	467	519	6			
1	D	368	Total	C	N	O	S	0	0	0
			2840	1794	494	545	7			

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



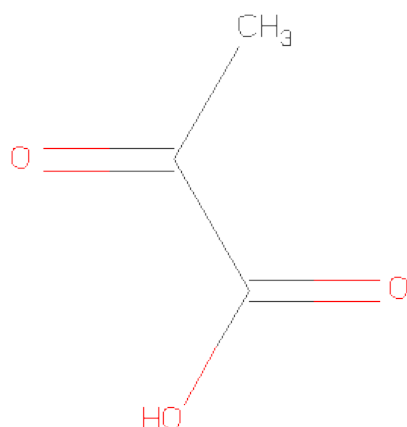
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



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

- Molecule 4 is water.

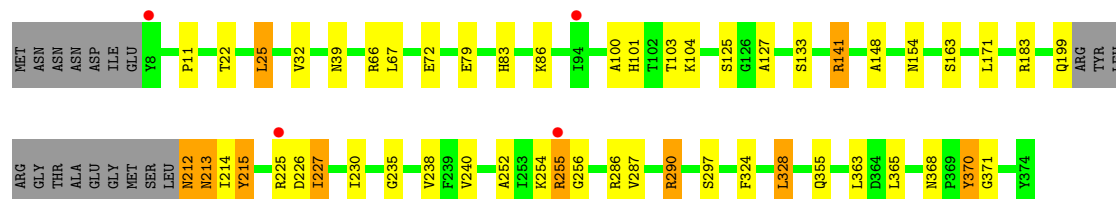
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	292	Total	O	0	0
			292	292		
4	B	370	Total	O	0	0
			370	370		
4	C	289	Total	O	0	0
			289	289		
4	D	360	Total	O	0	0
			360	360		

### 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.

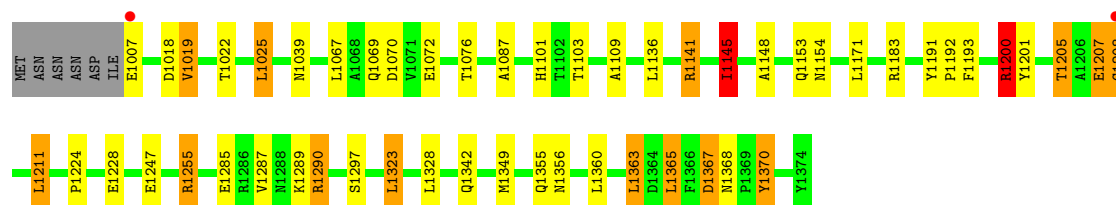
#### • Molecule 1: Lactate oxidase

Chain A: 



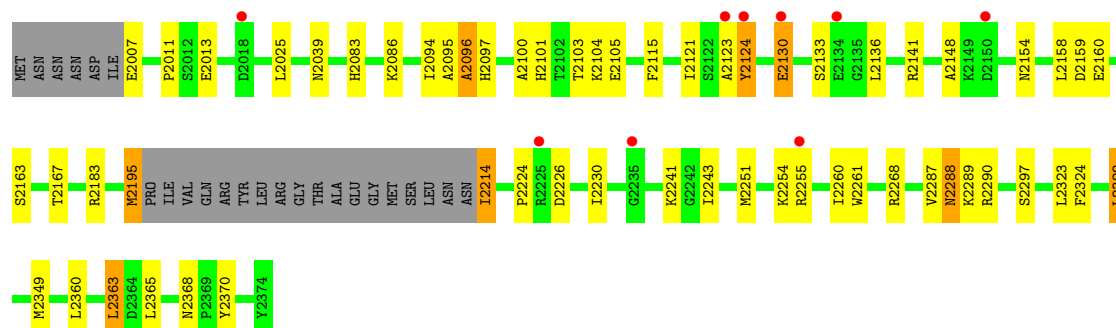
#### • Molecule 1: Lactate oxidase

Chain B: 



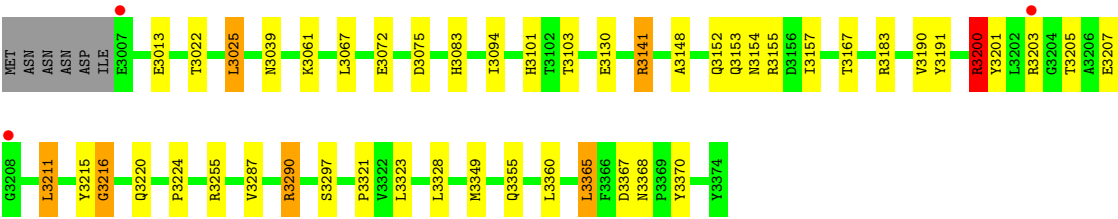
#### • Molecule 1: Lactate oxidase

Chain C: 



#### • Molecule 1: Lactate oxidase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.84Å 118.57Å 107.24Å 90.00° 121.07° 90.00°	Depositor
Resolution (Å)	37.40 – 1.90 37.39 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.40-1.90) 99.2 (37.39-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.227 0.176 , 0.226	Depositor DCC
$R_{free}$ test set	5676 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 113365 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12571	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.73	0/2800	0.78	3/3795 (0.1%)
1	B	0.93	4/2904 (0.1%)	0.98	17/3935 (0.4%)
1	C	0.77	0/2761	0.75	1/3740 (0.0%)
1	D	0.87	0/2904	0.95	10/3935 (0.3%)
All	All	0.83	4/11369 (0.0%)	0.87	31/15405 (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
1	B	0	1
1	D	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1285	GLU	CG-CD	7.33	1.62	1.51
1	B	1070	ASP	N-CA	5.66	1.57	1.46
1	B	1285	GLU	CB-CG	5.32	1.62	1.52
1	B	1255	ARG	CG-CD	5.06	1.64	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3290	ARG	NE-CZ-NH2	-18.76	110.92	120.30
1	D	3290	ARG	NE-CZ-NH1	14.97	127.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1290	ARG	NE-CZ-NH1	13.33	126.96	120.30
1	B	1290	ARG	NE-CZ-NH2	-12.51	114.04	120.30
1	B	1069	GLN	C-N-CA	-10.63	95.11	121.70
1	B	1141	ARG	NE-CZ-NH1	-9.93	115.33	120.30
1	D	3141	ARG	NE-CZ-NH1	-9.47	115.57	120.30
1	B	1370	TYR	C-N-CA	-9.08	103.23	122.30
1	B	1323	LEU	CA-CB-CG	-8.86	94.93	115.30
1	D	3200	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	D	3215	TYR	C-N-CA	-8.33	104.81	122.30
1	B	1070	ASP	CB-CG-OD2	7.95	125.45	118.30
1	D	3200	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	1141	ARG	NE-CZ-NH2	7.55	124.07	120.30
1	B	1069	GLN	O-C-N	-7.20	111.17	122.70
1	D	3141	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	B	1145	ILE	CB-CA-C	-7.05	97.49	111.60
1	A	290	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	B	1363	LEU	CB-CG-CD1	5.69	120.68	111.00
1	B	1207	GLU	C-N-CA	-5.65	110.44	122.30
1	B	1367	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	328	LEU	CA-CB-CG	5.42	127.76	115.30
1	D	3075	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	1070	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	C	2363	LEU	CB-CG-CD1	5.29	119.99	111.00
1	B	1200	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	370	TYR	C-N-CA	-5.27	111.24	122.30
1	B	1365	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	1070	ASP	CB-CA-C	5.15	120.70	110.40
1	D	3290	ARG	CD-NE-CZ	5.12	130.78	123.60
1	D	3365	LEU	CB-CG-CD1	5.05	119.58	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	GLY	Peptide
1	B	1208	GLY	Peptide
1	D	3216	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2738	0	2668	51	0
1	B	2840	0	2770	46	0
1	C	2700	0	2627	55	0
1	D	2840	0	2770	43	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
3	A	6	0	3	0	0
3	B	6	0	3	0	0
3	D	6	0	3	0	0
4	A	292	0	0	10	0
4	B	370	0	0	13	0
4	C	289	0	0	23	0
4	D	360	0	0	11	0
All	All	12571	0	10920	195	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (195) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2123:ALA:HB2	4:C:2716:HOH:O	1.31	1.25
1:B:1356:ASN:HB3	4:B:1826:HOH:O	1.35	1.20
1:A:227:ILE:HB	1:A:255:ARG:NE	1.62	1.14
1:B:1228:GLU:OE2	1:B:1255:ARG:HD2	1.52	1.06
1:D:3287:VAL:O	1:D:3290:ARG:HD3	1.52	1.06
1:D:3216:GLY:HA2	1:D:3220:GLN:NE2	1.74	1.03
1:B:1367:ASP:HB2	4:B:1830:HOH:O	1.59	1.00
1:B:1289:LYS:HD3	4:B:1876:HOH:O	1.60	0.99
1:D:3130:GLU:HG3	4:D:3712:HOH:O	1.63	0.98
1:B:1287:VAL:O	1:B:1290:ARG:HD3	1.63	0.97
1:C:2195:MET:C	4:C:2744:HOH:O	2.02	0.97
1:A:286:ARG:HD2	4:A:4731:HOH:O	1.66	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2007:GLU:N	4:C:2797:HOH:O	2.00	0.95
1:A:148:ALA:H	1:A:154:ASN:HD21	0.96	0.95
1:C:2083:HIS:HE1	4:C:2775:HOH:O	1.49	0.94
1:D:3224:PRO:HB3	1:D:3255:ARG:HG3	1.52	0.91
1:C:2123:ALA:O	1:C:2124:TYR:HD1	1.53	0.91
1:C:2214:ILE:HG12	4:C:2769:HOH:O	1.68	0.91
1:B:1148:ALA:H	1:B:1154:ASN:HD21	1.17	0.91
1:D:3287:VAL:O	1:D:3290:ARG:CD	2.19	0.90
1:D:3205:THR:HG22	1:D:3207:GLU:H	1.35	0.90
1:C:2083:HIS:CE1	4:C:2775:HOH:O	2.21	0.88
1:D:3216:GLY:HA2	1:D:3220:GLN:HE22	1.39	0.86
1:A:225:ARG:HD2	4:A:4752:HOH:O	1.75	0.86
1:C:2148:ALA:H	1:C:2154:ASN:HD21	1.23	0.84
1:C:2039:ASN:HD22	1:C:2183:ARG:HH11	1.22	0.83
1:C:2095:ALA:O	1:C:2096:ALA:CB	2.26	0.83
1:B:1255:ARG:HG2	4:B:1542:HOH:O	1.77	0.83
1:D:3148:ALA:H	1:D:3154:ASN:HD21	1.27	0.82
1:C:2254:LYS:HD2	4:C:2736:HOH:O	1.79	0.82
1:B:1007:GLU:HA	4:B:1739:HOH:O	1.78	0.81
1:C:2104:LYS:HD3	4:C:2752:HOH:O	1.80	0.80
1:A:212:ASN:ND2	4:A:4803:HOH:O	2.13	0.80
1:B:1205:THR:HG22	1:B:1207:GLU:H	1.45	0.79
1:A:227:ILE:CB	1:A:255:ARG:NE	2.46	0.79
1:D:3255:ARG:HG2	4:D:3559:HOH:O	1.82	0.78
1:C:2123:ALA:O	1:C:2124:TYR:CD1	2.36	0.78
1:D:3039:ASN:HD22	1:D:3183:ARG:HH11	1.29	0.78
1:C:2243:ILE:HD12	1:C:2260:ILE:HG23	1.66	0.76
1:C:2159:ASP:HB3	4:C:2767:HOH:O	1.84	0.76
1:C:2214:ILE:CD1	4:C:2793:HOH:O	2.33	0.75
1:B:1039:ASN:HD22	1:B:1183:ARG:HH11	1.34	0.75
1:C:2254:LYS:CD	4:C:2736:HOH:O	2.32	0.75
1:C:2287:VAL:O	1:C:2290:ARG:HD3	1.87	0.74
1:D:3061:LYS:HE2	4:D:3805:HOH:O	1.87	0.73
1:A:287:VAL:O	1:A:290:ARG:HD3	1.89	0.73
1:A:148:ALA:N	1:A:154:ASN:HD21	1.79	0.72
1:B:1205:THR:CG2	1:B:1207:GLU:H	2.02	0.71
1:D:3323:LEU:HB2	4:D:3804:HOH:O	1.91	0.70
1:C:2214:ILE:HD11	4:C:2793:HOH:O	1.91	0.70
1:A:39:ASN:HD22	1:A:183:ARG:HH11	1.38	0.69
1:D:3224:PRO:CB	1:D:3255:ARG:HG3	2.21	0.69
1:B:1191:TYR:OH	1:B:1211:LEU:HG	1.93	0.69
1:A:226:ASP:O	1:A:230:ILE:HG12	1.93	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:ALA:H	1:A:154:ASN:ND2	1.81	0.68
1:B:1148:ALA:N	1:B:1154:ASN:HD21	1.89	0.68
1:B:1200:ARG:HD2	4:B:1598:HOH:O	1.93	0.68
1:D:3323:LEU:HD13	4:D:3804:HOH:O	1.94	0.68
1:D:3224:PRO:HB3	1:D:3255:ARG:CG	2.24	0.68
1:A:227:ILE:HG22	1:A:255:ARG:HH11	1.61	0.66
1:D:3148:ALA:N	1:D:3154:ASN:HD21	1.94	0.66
1:B:1228:GLU:OE2	1:B:1255:ARG:CD	2.39	0.65
1:C:2158:LEU:HD11	1:C:2230:ILE:HD12	1.78	0.65
1:C:2039:ASN:ND2	1:C:2183:ARG:HH11	1.95	0.65
1:A:227:ILE:HB	1:A:255:ARG:CD	2.25	0.65
1:D:3216:GLY:CA	1:D:3220:GLN:HE22	2.10	0.64
1:D:3205:THR:HG21	4:D:3627:HOH:O	1.96	0.64
1:C:2254:LYS:HG2	4:C:2649:HOH:O	1.97	0.64
1:A:227:ILE:HB	1:A:255:ARG:HE	1.57	0.64
1:C:2095:ALA:O	1:C:2096:ALA:HB3	1.97	0.63
1:B:1287:VAL:O	1:B:1290:ARG:CD	2.42	0.63
1:D:3072:GLU:H	1:D:3355:GLN:HE22	1.44	0.62
1:A:324:PHE:O	1:A:328:LEU:HD22	2.01	0.61
1:C:2104:LYS:CD	4:C:2752:HOH:O	2.42	0.61
1:A:227:ILE:HG21	1:A:240:VAL:HG22	1.82	0.61
1:B:1247:GLU:HB2	4:B:1879:HOH:O	2.00	0.61
1:C:2324:PHE:O	1:C:2328:LEU:HD22	2.02	0.60
1:A:171:LEU:CD2	1:A:227:ILE:HG23	2.31	0.60
1:C:2368:ASN:HD21	1:C:2370:TYR:HB2	1.67	0.59
1:A:104:LYS:HD2	1:A:127:ALA:HB2	1.82	0.59
1:A:171:LEU:HD23	1:A:227:ILE:HG23	1.84	0.59
1:A:199:GLN:HA	4:A:4801:HOH:O	2.01	0.59
1:C:2289:LYS:HD2	4:C:2683:HOH:O	2.03	0.59
1:B:1019:VAL:N	4:B:1878:HOH:O	1.72	0.58
1:B:1205:THR:HG22	1:B:1207:GLU:N	2.15	0.58
1:A:213:ASN:HA	4:A:4725:HOH:O	2.03	0.58
1:D:3191:TYR:O	1:D:3207:GLU:O	2.21	0.58
1:D:3022:THR:HA	1:D:3025:LEU:HD22	1.84	0.58
1:D:3083:HIS:HD2	4:D:3664:HOH:O	1.86	0.56
1:D:3039:ASN:ND2	1:D:3183:ARG:HH11	2.02	0.56
1:C:2095:ALA:O	1:C:2096:ALA:HB2	2.03	0.56
1:C:2214:ILE:HD12	4:C:2799:HOH:O	2.06	0.56
1:B:1148:ALA:H	1:B:1154:ASN:ND2	1.97	0.56
1:A:227:ILE:HB	1:A:255:ARG:CZ	2.33	0.56
1:D:3216:GLY:CA	1:D:3220:GLN:NE2	2.61	0.56
1:A:227:ILE:CB	1:A:255:ARG:HE	2.14	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1072:GLU:H	1:B:1355:GLN:HE22	1.53	0.55
1:A:227:ILE:CG2	1:A:255:ARG:HE	2.20	0.55
1:B:1153:GLN:HE22	1:B:1201:TYR:HB3	1.71	0.55
1:B:1101:HIS:CD2	1:B:1103:THR:H	2.25	0.54
1:B:1224:PRO:HB3	1:B:1255:ARG:HG3	1.89	0.54
1:D:3094:ILE:HG21	1:D:3323:LEU:HD22	1.90	0.54
1:D:3157:ILE:HD11	1:D:3200:ARG:HD3	1.90	0.54
1:A:214:ILE:O	1:A:215:TYR:HB2	2.08	0.54
1:A:11:PRO:HG3	1:A:32:VAL:O	2.07	0.53
1:B:1101:HIS:HD2	1:B:1103:THR:H	1.56	0.53
1:C:2094:ILE:O	1:C:2097:HIS:CD2	2.61	0.53
1:D:3153:GLN:HE22	1:D:3201:TYR:HB3	1.74	0.53
1:A:368:ASN:HD21	1:A:370:TYR:HB2	1.74	0.53
1:B:1228:GLU:OE2	1:B:1255:ARG:NH2	2.28	0.53
1:C:2086:LYS:HD3	1:C:2115:PHE:O	2.09	0.53
1:D:3152:GLN:NE2	1:D:3155:ARG:HH11	2.06	0.52
1:C:2101:HIS:HD2	1:C:2103:THR:H	1.58	0.52
1:A:252:ALA:O	1:A:255:ARG:HD3	2.09	0.52
1:C:2097:HIS:CD2	1:C:2105:GLU:HG3	2.44	0.52
1:B:1145:ILE:HD12	1:B:1171:LEU:HA	1.92	0.51
1:A:101:HIS:HD2	1:A:103:THR:H	1.59	0.51
1:C:2104:LYS:CE	4:C:2752:HOH:O	2.58	0.51
1:A:199:GLN:HB2	4:A:4624:HOH:O	2.11	0.51
1:B:1247:GLU:OE2	4:B:1879:HOH:O	2.19	0.50
1:C:2241:LYS:HA	1:C:2261:TRP:HB3	1.94	0.50
1:C:2121:ILE:HD11	1:C:2136:LEU:HD11	1.93	0.50
1:D:3013:GLU:O	1:D:3101:HIS:HE1	1.94	0.49
1:B:1109:ALA:HB1	1:B:1136:LEU:HG	1.93	0.49
1:B:1224:PRO:CB	1:B:1255:ARG:HG3	2.43	0.49
1:A:227:ILE:HD12	1:A:255:ARG:HD2	1.95	0.49
1:B:1368:ASN:HD21	1:B:1370:TYR:HB2	1.78	0.48
1:D:3224:PRO:HB2	1:D:3255:ARG:NH2	2.28	0.48
1:B:1039:ASN:ND2	1:B:1183:ARG:HH11	2.08	0.48
1:D:3368:ASN:HD21	1:D:3370:TYR:HB2	1.79	0.47
1:A:101:HIS:CD2	1:A:103:THR:H	2.32	0.47
1:B:1067:LEU:HD23	4:D:3609:HOH:O	2.14	0.47
1:D:3349:MET:HG2	1:D:3360:LEU:HD21	1.96	0.47
1:C:2268:ARG:NH2	4:C:2637:HOH:O	2.47	0.47
1:D:3148:ALA:H	1:D:3154:ASN:ND2	2.03	0.47
1:B:1076:THR:O	1:B:1087:ALA:HA	2.15	0.47
1:B:1224:PRO:HB3	1:B:1255:ARG:CG	2.45	0.47
1:A:227:ILE:HG21	1:A:240:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2086:LYS:CG	4:C:2684:HOH:O	2.61	0.46
1:D:3153:GLN:NE2	1:D:3201:TYR:HB3	2.31	0.46
1:A:255:ARG:HH21	1:A:255:ARG:C	2.20	0.46
1:A:227:ILE:HB	1:A:255:ARG:CG	2.45	0.45
1:A:39:ASN:ND2	1:A:183:ARG:HH11	2.09	0.45
1:B:1022:THR:HA	1:B:1025:LEU:HD22	1.98	0.45
1:C:2130:GLU:CD	1:C:2130:GLU:H	2.18	0.45
1:D:3101:HIS:HD2	1:D:3103:THR:H	1.65	0.45
1:B:1208:GLY:HA3	4:B:1785:HOH:O	2.17	0.45
1:C:2224:PRO:CB	1:C:2255:ARG:HD2	2.46	0.44
1:A:371:GLY:HA3	4:A:4587:HOH:O	2.15	0.44
1:A:227:ILE:HG22	1:A:255:ARG:NH1	2.29	0.44
1:C:2254:LYS:HD3	4:C:2736:HOH:O	2.07	0.44
1:C:2013:GLU:O	1:C:2101:HIS:HE1	2.01	0.44
1:A:225:ARG:HG3	4:A:4787:HOH:O	2.18	0.44
1:B:1191:TYR:O	1:B:1207:GLU:O	2.35	0.44
1:B:1367:ASP:CB	4:B:1830:HOH:O	2.38	0.44
1:A:255:ARG:NH2	1:A:256:GLY:C	2.71	0.44
1:A:290:ARG:NH2	4:A:4784:HOH:O	2.50	0.44
1:C:2226:ASP:O	1:C:2230:ILE:HG12	2.18	0.44
1:A:11:PRO:HD2	1:A:100:ALA:O	2.18	0.44
1:C:2101:HIS:CD2	1:C:2103:THR:H	2.34	0.44
1:D:3101:HIS:CD2	1:D:3103:THR:H	2.36	0.44
1:A:79:GLU:HA	1:A:83:HIS:O	2.17	0.44
1:B:1153:GLN:NE2	1:B:1201:TYR:HB3	2.32	0.43
1:C:2251:MET:O	1:C:2255:ARG:HG2	2.17	0.43
1:C:2094:ILE:O	1:C:2097:HIS:NE2	2.51	0.43
1:D:3130:GLU:CG	4:D:3712:HOH:O	2.40	0.43
1:B:1018:ASP:CA	4:B:1878:HOH:O	2.65	0.43
1:C:2224:PRO:HB3	1:C:2255:ARG:HG3	2.00	0.43
1:A:238:VAL:HG11	1:A:255:ARG:HH11	1.83	0.43
1:C:2011:PRO:HD2	1:C:2100:ALA:O	2.18	0.43
1:A:199:GLN:CB	4:A:4624:HOH:O	2.66	0.42
1:D:3022:THR:HB	1:D:3321:PRO:HB3	2.01	0.42
1:C:2160:GLU:HG3	4:C:2734:HOH:O	2.20	0.42
1:A:66:ARG:C	1:A:67:LEU:HD23	2.40	0.42
1:B:1022:THR:O	1:B:1025:LEU:HB2	2.20	0.42
1:A:133:SER:OG	1:A:141:ARG:NH1	2.53	0.42
1:C:2349:MET:HG2	1:C:2360:LEU:HD21	2.01	0.42
1:D:3148:ALA:HB2	1:D:3201:TYR:CD1	2.54	0.42
1:D:3083:HIS:CE1	1:D:3167:THR:OG1	2.73	0.42
1:C:2101:HIS:HD2	1:C:2103:THR:OG1	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1192:PRO:HG2	1:B:1193:PHE:CD2	2.55	0.41
1:C:2214:ILE:HD12	4:C:2793:HOH:O	2.07	0.41
1:A:22:THR:HA	1:A:25:LEU:HD22	2.01	0.41
1:A:171:LEU:HD22	1:A:227:ILE:HG23	2.01	0.41
1:B:1205:THR:CG2	1:B:1207:GLU:HB3	2.50	0.41
1:B:1349:MET:HG2	1:B:1360:LEU:HD21	2.03	0.41
1:A:72:GLU:H	1:A:355:GLN:HE22	1.68	0.41
1:C:2288:ASN:HD22	1:C:2288:ASN:HA	1.55	0.41
1:D:3191:TYR:OH	1:D:3211:LEU:HG	2.21	0.40
1:C:2101:HIS:CD2	1:C:2103:THR:OG1	2.75	0.40
1:D:3323:LEU:CB	4:D:3804:HOH:O	2.56	0.40
1:A:101:HIS:HD2	1:A:103:THR:OG1	2.04	0.40
1:C:2104:LYS:HE2	4:C:2752:HOH:O	2.19	0.40
1:D:3367:ASP:OD1	4:D:3849:HOH:O	2.22	0.40
1:B:1153:GLN:NE2	4:B:1659:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 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	351/374 (94%)	339 (97%)	9 (3%)	3 (1%)	25	10
1	B	366/374 (98%)	355 (97%)	9 (2%)	2 (0%)	38	23
1	C	346/374 (92%)	333 (96%)	10 (3%)	3 (1%)	25	10
1	D	366/374 (98%)	355 (97%)	10 (3%)	1 (0%)	50	37
All	All	1429/1496 (96%)	1382 (97%)	38 (3%)	9 (1%)	33	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	215	TYR
1	A	297	SER

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Mol	Chain	Res	Type
1	B	1297	SER
1	C	2096	ALA
1	C	2124	TYR
1	D	3297	SER
1	C	2297	SER
1	B	1019	VAL

### 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	282/298 (95%)	271 (96%)	11 (4%)	43	30
1	B	292/298 (98%)	281 (96%)	11 (4%)	44	31
1	C	277/298 (93%)	264 (95%)	13 (5%)	36	22
1	D	292/298 (98%)	283 (97%)	9 (3%)	52	41
All	All	1143/1192 (96%)	1099 (96%)	44 (4%)	44	31

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	86	LYS
1	A	125	SER
1	A	141	ARG
1	A	163	SER
1	A	212	ASN
1	A	227	ILE
1	A	254	LYS
1	A	255	ARG
1	A	363	LEU
1	A	365	LEU
1	B	1025	LEU
1	B	1141	ARG
1	B	1145	ILE
1	B	1200	ARG
1	B	1205	THR

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Mol	Chain	Res	Type
1	B	1211	LEU
1	B	1323	LEU
1	B	1328	LEU
1	B	1342	GLN
1	B	1363	LEU
1	B	1365	LEU
1	C	2025	LEU
1	C	2130	GLU
1	C	2133	SER
1	C	2141	ARG
1	C	2163	SER
1	C	2167	THR
1	C	2195	MET
1	C	2214	ILE
1	C	2288	ASN
1	C	2323	LEU
1	C	2328	LEU
1	C	2363	LEU
1	C	2365	LEU
1	D	3025	LEU
1	D	3067	LEU
1	D	3141	ARG
1	D	3190	VAL
1	D	3200	ARG
1	D	3203	ARG
1	D	3211	LEU
1	D	3328	LEU
1	D	3365	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	ASN
1	A	83	HIS
1	A	101	HIS
1	A	137	ASN
1	A	154	ASN
1	A	187	ASN
1	A	288	ASN
1	A	355	GLN
1	A	368	ASN

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Mol	Chain	Res	Type
1	B	1039	ASN
1	B	1083	HIS
1	B	1101	HIS
1	B	1153	GLN
1	B	1154	ASN
1	B	1187	ASN
1	B	1288	ASN
1	B	1342	GLN
1	B	1355	GLN
1	B	1368	ASN
1	C	2039	ASN
1	C	2083	HIS
1	C	2101	HIS
1	C	2137	ASN
1	C	2154	ASN
1	C	2187	ASN
1	C	2288	ASN
1	C	2355	GLN
1	C	2368	ASN
1	D	3009	ASN
1	D	3035	HIS
1	D	3039	ASN
1	D	3083	HIS
1	D	3101	HIS
1	D	3152	GLN
1	D	3153	GLN
1	D	3154	ASN
1	D	3187	ASN
1	D	3288	ASN
1	D	3355	GLN
1	D	3368	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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

7 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$
3	PYR	A	4442	-	5,5,5	3.38	3 (60%)	6,6,6	1.47	1 (16%)
2	FMN	A	4512	-	33,33,33	0.92	2 (6%)	46,50,50	1.51	7 (15%)
3	PYR	B	1442	-	5,5,5	3.26	3 (60%)	6,6,6	1.80	3 (50%)
2	FMN	B	1512	-	33,33,33	1.36	3 (9%)	46,50,50	1.55	10 (21%)
2	FMN	C	2512	-	33,33,33	0.99	2 (6%)	46,50,50	1.59	8 (17%)
3	PYR	D	3442	-	5,5,5	3.22	3 (60%)	6,6,6	1.54	2 (33%)
2	FMN	D	3512	-	33,33,33	1.18	4 (12%)	46,50,50	1.67	5 (10%)

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
3	PYR	A	4442	-	-	0/4/4/4	0/0/0/0
2	FMN	A	4512	-	-	0/18/18/18	0/0/3/3
3	PYR	B	1442	-	-	0/4/4/4	0/0/0/0
2	FMN	B	1512	-	-	0/18/18/18	0/0/3/3
2	FMN	C	2512	-	-	0/18/18/18	0/0/3/3
3	PYR	D	3442	-	-	0/4/4/4	0/0/0/0
2	FMN	D	3512	-	-	0/18/18/18	0/0/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4442	PYR	C2-C1	-5.83	1.39	1.53
3	B	1442	PYR	C2-C1	-5.81	1.39	1.53
3	D	3442	PYR	C2-C1	-5.71	1.40	1.53
2	B	1512	FMN	C1'-N10	3.84	1.52	1.48
3	A	4442	PYR	O3-C2	3.70	1.31	1.23
3	B	1442	PYR	O3-C2	3.55	1.31	1.23
3	D	3442	PYR	O3-C2	3.52	1.31	1.23
3	A	4442	PYR	O1-C1	2.97	1.31	1.22
3	B	1442	PYR	O1-C1	2.53	1.30	1.22
3	D	3442	PYR	O1-C1	2.51	1.30	1.22
2	C	2512	FMN	C10-N1	2.42	1.40	1.35
2	C	2512	FMN	C5A-N5	2.41	1.39	1.35
2	D	3512	FMN	C1'-N10	2.31	1.50	1.48
2	B	1512	FMN	C5'-C4'	2.28	1.55	1.51
2	A	4512	FMN	C1'-N10	2.26	1.50	1.48
2	A	4512	FMN	C6-C5A	-2.21	1.39	1.41
2	D	3512	FMN	C1'-C2'	2.20	1.53	1.51
2	B	1512	FMN	C9A-N10	2.14	1.42	1.38
2	D	3512	FMN	C5'-C4'	2.09	1.55	1.51
2	D	3512	FMN	C5A-N5	2.06	1.38	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3512	FMN	C2-N1-C10	6.22	121.25	114.98
2	B	1512	FMN	C2-N1-C10	4.72	119.74	114.98
2	A	4512	FMN	C2-N1-C10	4.51	119.53	114.98
2	C	2512	FMN	C2-N1-C10	4.30	119.31	114.98
2	D	3512	FMN	C2'-C1'-N10	-4.21	106.86	112.45
2	C	2512	FMN	C2'-C1'-N10	-3.59	107.69	112.45
2	A	4512	FMN	C4A-N5-C5A	3.56	120.69	116.69
2	C	2512	FMN	C1'-N10-C9A	3.39	122.17	118.87
2	D	3512	FMN	C4A-N5-C5A	3.34	120.44	116.69
2	C	2512	FMN	C4A-N5-C5A	3.27	120.36	116.69
2	B	1512	FMN	C1'-N10-C9A	3.19	121.98	118.87
3	B	1442	PYR	O2-C1-C2	3.16	121.33	114.37
2	C	2512	FMN	C4A-C10-N1	-3.10	119.63	122.73
2	A	4512	FMN	O4'-C4'-C5'	-2.98	104.01	110.12
2	B	1512	FMN	C5A-C9A-N10	2.96	119.72	116.80
2	C	2512	FMN	C5A-C9A-N10	2.95	119.71	116.80
2	B	1512	FMN	C4A-N5-C5A	2.92	119.97	116.69
2	B	1512	FMN	C4A-C10-N1	-2.92	119.82	122.73
2	A	4512	FMN	C1'-N10-C9A	2.87	121.66	118.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1512	FMN	C2'-C1'-N10	-2.86	108.65	112.45
2	A	4512	FMN	C4A-C10-N1	-2.77	119.96	122.73
3	A	4442	PYR	O2-C1-C2	2.73	120.39	114.37
2	D	3512	FMN	C5A-C9A-N10	2.66	119.42	116.80
2	A	4512	FMN	C5A-C9A-N10	2.45	119.21	116.80
2	B	1512	FMN	O2P-P-O1P	2.41	118.33	110.44
2	D	3512	FMN	C4A-C10-N1	-2.35	120.38	122.73
3	D	3442	PYR	O2-C1-C2	2.29	119.42	114.37
2	C	2512	FMN	C4-C4A-C10	2.26	120.60	116.95
2	B	1512	FMN	C8M-C8-C9	-2.21	115.04	120.38
2	B	1512	FMN	C9A-N10-C10	-2.21	119.60	121.77
3	B	1442	PYR	O2-C1-O1	-2.20	118.41	123.62
3	D	3442	PYR	O2-C1-O1	-2.12	118.61	123.62
2	C	2512	FMN	O3P-P-O5'	2.11	112.47	106.65
2	B	1512	FMN	O4'-C4'-C5'	-2.09	105.82	110.12
3	B	1442	PYR	C3-C2-C1	2.08	122.31	117.47
2	A	4512	FMN	C4-N3-C2	-2.03	121.23	125.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	355/374 (94%)	-0.00	4 (1%) 77 79	16, 29, 43, 51	0
1	B	368/374 (98%)	-0.23	2 (0%) 88 90	11, 19, 30, 46	0
1	C	350/374 (93%)	0.09	9 (2%) 53 55	14, 27, 43, 49	0
1	D	368/374 (98%)	-0.24	3 (0%) 83 85	11, 19, 30, 46	0
All	All	1441/1496 (96%)	-0.10	18 (1%) 75 78	11, 23, 40, 51	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	4.5
1	D	3203	ARG	4.2
1	D	3208	GLY	3.8
1	C	2124	TYR	3.6
1	D	3007	GLU	3.4
1	C	2130	GLU	3.2
1	B	1007	GLU	3.1
1	C	2123	ALA	2.9
1	A	225	ARG	2.9
1	C	2235	GLY	2.7
1	C	2134	GLU	2.6
1	C	2255	ARG	2.3
1	A	8	TYR	2.3
1	C	2018	ASP	2.2
1	C	2225	ARG	2.1
1	A	94	ILE	2.0
1	B	1208	GLY	2.0
1	C	2150	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMN	B	1512	31/31	0.17	1.52	9,16,19,19	0
3	PYR	D	3442	6/6	0.14	1.34	19,23,26,27	0
3	PYR	B	1442	6/6	0.14	0.64	25,29,33,33	0
2	FMN	D	3512	31/31	0.15	0.51	9,14,16,16	0
2	FMN	A	4512	31/31	0.14	0.44	17,23,25,27	0
2	FMN	C	2512	31/31	0.16	0.40	19,25,28,28	0
3	PYR	A	4442	6/6	0.13	0.03	34,35,36,37	0

## 6.5 Other polymers

There are no such residues in this entry.