



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:14 PM GMT

PDB ID : 2DU2
Title : Crystal Structure Analysis of the L-Lactate Oxidase
Authors : Morimoto, Y.
Deposited on : 2006-07-19
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

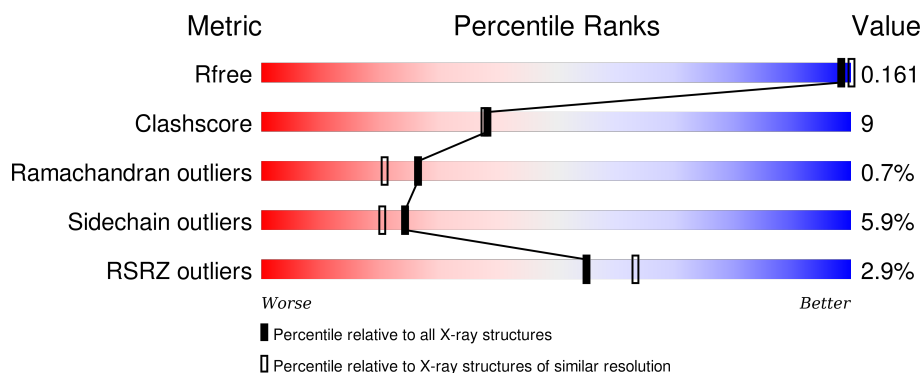
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	<div> <div>0%</div> <div>85% 12% ..</div> </div>
1	B	374	<div> <div>2%</div> <div>83% 13% ..</div> </div>
1	C	374	<div> <div>3%</div> <div>82% 13% 5% ..</div> </div>
1	D	374	<div> <div>5%</div> <div>81% 15% ..</div> </div>

2 Entry composition [i](#)

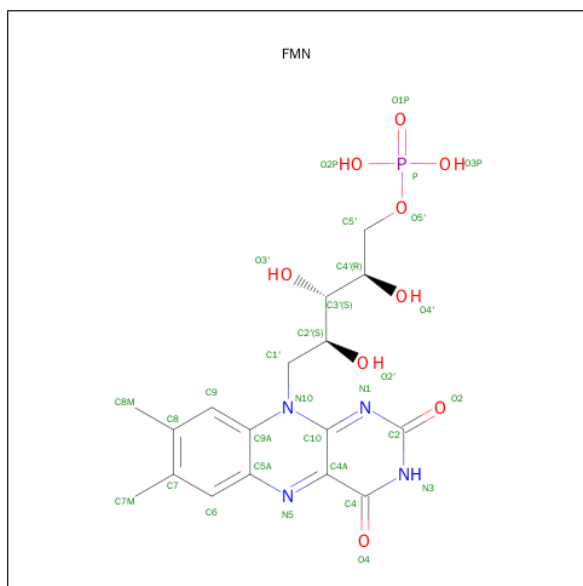
There are 3 unique types of molecules in this entry. The entry contains 12785 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			
1	B	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			
1	C	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			
1	D	374	Total	C	N	O	S	0	0	0
			2888	1821	503	556	8			

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



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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		

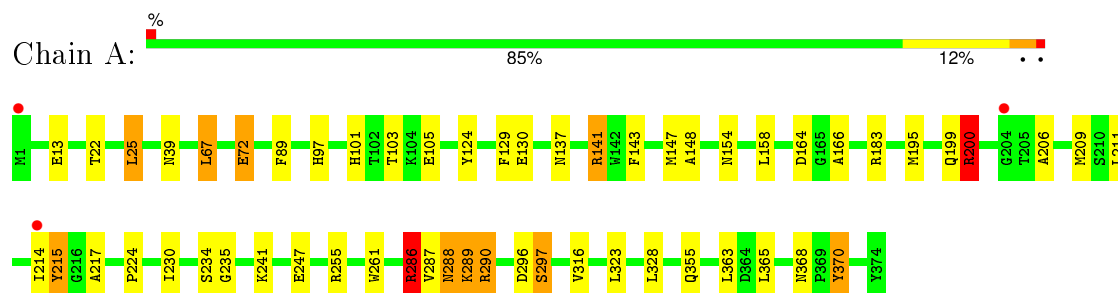
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	299	Total	O	0	0
			299	299		
3	B	266	Total	O	0	0
			266	266		
3	C	291	Total	O	0	0
			291	291		
3	D	253	Total	O	0	0
			253	253		

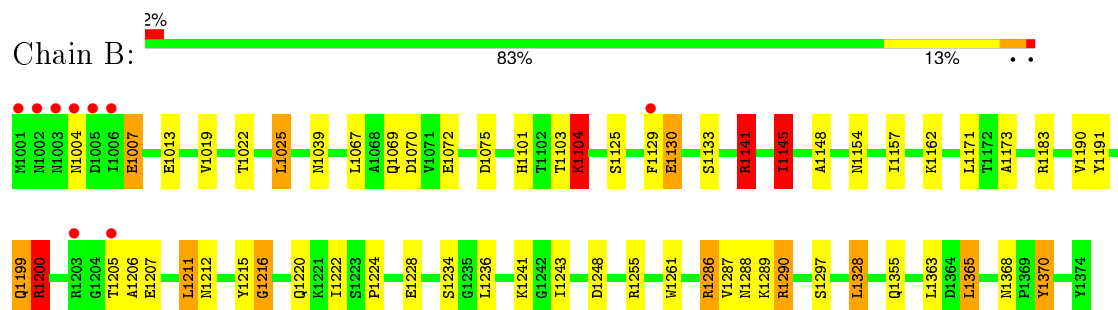
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

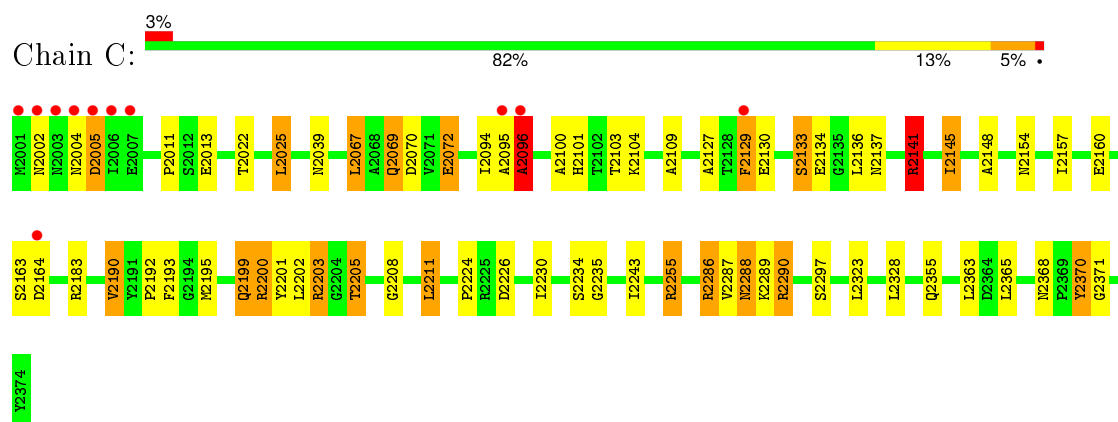
• Molecule 1: Lactate oxidase



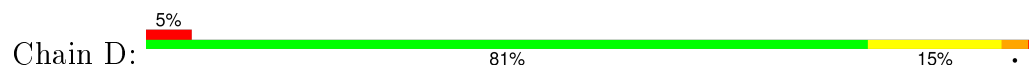
• Molecule 1: Lactate oxidase

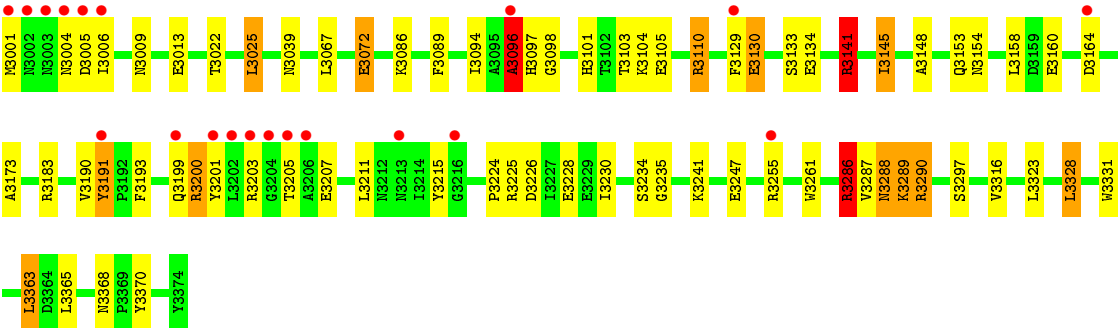


• Molecule 1: Lactate oxidase



• Molecule 1: Lactate oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	191.10Å 191.10Å 194.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 45.75 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.10) 100.0 (45.75-2.07)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.199 0.164 , 0.161	Depositor DCC
R_{free} test set	5219 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	EDS
Estimated twinning fraction	0.000 for -l,-k,-h 0.006 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 108566 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FMN

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	0.87	0/2952	0.94	8/4000 (0.2%)
1	B	0.88	1/2952 (0.0%)	0.99	20/4000 (0.5%)
1	C	0.87	2/2952 (0.1%)	0.96	16/4000 (0.4%)
1	D	0.90	1/2952 (0.0%)	0.93	12/4000 (0.3%)
All	All	0.88	4/11808 (0.0%)	0.96	56/16000 (0.3%)

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	C	0	2
1	D	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3096	ALA	CA-CB	7.14	1.67	1.52
1	C	2096	ALA	CA-CB	7.01	1.67	1.52
1	B	1104	LYS	CE-NZ	5.05	1.61	1.49
1	C	2070	ASP	N-CA	5.02	1.56	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH1	-16.29	112.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3290	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	A	290	ARG	NE-CZ-NH2	-15.05	112.77	120.30
1	C	2290	ARG	NE-CZ-NH2	-14.71	112.94	120.30
1	A	290	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	1286	ARG	NE-CZ-NH2	-11.87	114.36	120.30
1	D	3290	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	A	141	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	C	2290	ARG	NE-CZ-NH1	11.35	125.98	120.30
1	B	1290	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	D	3141	ARG	NE-CZ-NH1	-10.57	115.02	120.30
1	B	1290	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	370	TYR	C-N-CA	-10.24	100.80	122.30
1	B	1370	TYR	C-N-CA	-9.72	101.90	122.30
1	D	3286	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	C	2286	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	C	2370	TYR	C-N-CA	-9.04	103.32	122.30
1	C	2069	GLN	C-N-CA	-8.79	99.74	121.70
1	B	1200	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	1141	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	B	1069	GLN	C-N-CA	-8.44	100.60	121.70
1	B	1215	TYR	C-N-CA	-8.32	104.83	122.30
1	B	1200	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	B	1286	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	72	GLU	C-N-CA	-7.60	102.69	121.70
1	D	3145	ILE	CB-CA-C	-7.20	97.21	111.60
1	D	3141	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	C	2145	ILE	CB-CA-C	-6.90	97.81	111.60
1	B	1145	ILE	CB-CA-C	-6.89	97.81	111.60
1	D	3286	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	1104	LYS	CD-CE-NZ	6.71	127.13	111.70
1	D	3234	SER	C-N-CA	-6.68	108.28	122.30
1	A	286	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	1141	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	B	1286	ARG	CG-CD-NE	-6.31	98.56	111.80
1	D	3072	GLU	C-N-CA	-6.30	105.95	121.70
1	C	2286	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	2141	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	B	1070	ASP	CB-CA-C	5.90	122.20	110.40
1	C	2234	SER	C-N-CA	-5.83	110.05	122.30
1	A	234	SER	C-N-CA	-5.73	110.27	122.30
1	C	2200	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	2072	GLU	C-N-CA	-5.54	107.84	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3328	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	2070	ASP	CB-CA-C	5.44	121.29	110.40
1	C	2205	THR	CB-CA-C	-5.33	97.22	111.60
1	D	3215	TYR	C-N-CA	-5.30	111.17	122.30
1	D	3363	LEU	CB-CG-CD1	5.29	120.00	111.00
1	B	1075	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	2069	GLN	O-C-N	-5.28	114.26	122.70
1	B	1286	ARG	CD-NE-CZ	5.21	130.89	123.60
1	C	2211	LEU	CB-CG-CD2	5.18	119.81	111.00
1	C	2067	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	B	1365	LEU	CB-CG-CD1	5.06	119.60	111.00
1	B	1328	LEU	CA-CB-CG	5.02	126.85	115.30
1	B	1070	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	GLY	Peptide
1	B	1216	GLY	Peptide
1	C	2096	ALA	Peptide
1	C	2235	GLY	Peptide
1	D	3096	ALA	Peptide
1	D	3235	GLY	Peptide

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	2888	0	2815	52	0
1	B	2888	0	2812	48	0
1	C	2888	0	2812	57	0
1	D	2888	0	2812	57	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	299	0	0	4	1
3	B	266	0	0	10	0
3	C	291	0	0	6	0
3	D	253	0	0	0	0
All	All	12785	0	11327	210	1

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 (210) 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:D:3224:PRO:HB3	1:D:3255:ARG:HG3	1.33	1.11
1:D:3129:PHE:CD2	1:D:3164:ASP:HB3	1.83	1.11
1:C:2224:PRO:HB3	1:C:2255:ARG:HG3	1.34	1.07
1:A:199:GLN:O	1:A:200:ARG:HB3	1.26	1.03
1:A:148:ALA:H	1:A:154:ASN:HD21	1.08	0.99
1:D:3129:PHE:CE2	1:D:3164:ASP:HB3	1.98	0.98
1:B:1224:PRO:HB3	1:B:1255:ARG:HG3	1.45	0.98
1:A:224:PRO:HB3	1:A:255:ARG:HG3	1.47	0.96
1:D:3148:ALA:H	1:D:3154:ASN:HD21	1.02	0.96
1:B:1191:TYR:O	1:B:1207:GLU:O	1.84	0.96
1:C:2005:ASP:HA	1:C:2192:PRO:O	1.68	0.94
1:C:2095:ALA:C	3:C:5650:HOH:O	2.06	0.94
1:C:2129:PHE:CE2	1:C:2164:ASP:HB3	2.02	0.93
1:B:1216:GLY:HA2	1:B:1220:GLN:NE2	1.83	0.93
1:B:1148:ALA:H	1:B:1154:ASN:HD21	1.11	0.92
1:C:2129:PHE:CD2	1:C:2164:ASP:HB3	2.05	0.91
1:B:1234:SER:OG	1:B:1234:SER:O	1.67	0.91
1:B:1287:VAL:O	1:B:1290:ARG:HD3	1.68	0.91
1:A:199:GLN:O	1:A:200:ARG:CB	2.13	0.88
1:C:2255:ARG:HG2	3:C:5124:HOH:O	1.74	0.88
1:A:255:ARG:HG2	3:A:5122:HOH:O	1.75	0.86
1:C:2287:VAL:O	1:C:2290:ARG:HD3	1.77	0.84
1:D:3191:TYR:O	1:D:3207:GLU:O	1.96	0.84
1:D:3191:TYR:HE2	1:D:3193:PHE:CE1	1.96	0.82
1:B:1129:PHE:HB3	3:B:5321:HOH:O	1.78	0.81
1:D:3191:TYR:CE2	1:D:3193:PHE:CE1	2.68	0.81
1:C:2096:ALA:N	3:C:5650:HOH:O	2.13	0.79
1:C:2148:ALA:H	1:C:2154:ASN:HD21	1.29	0.78
1:D:3148:ALA:N	1:D:3154:ASN:HD21	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:HD22	1:A:183:ARG:HH11	1.28	0.77
1:D:3205:THR:HG22	1:D:3207:GLU:H	1.48	0.77
1:D:3287:VAL:O	1:D:3290:ARG:HD3	1.84	0.77
1:C:2287:VAL:O	1:C:2290:ARG:CD	2.33	0.76
1:A:287:VAL:O	1:A:290:ARG:HD3	1.86	0.75
1:B:1148:ALA:N	1:B:1154:ASN:HD21	1.83	0.74
1:A:287:VAL:O	1:A:290:ARG:CD	2.35	0.74
1:C:2226:ASP:O	1:C:2230:ILE:HG12	1.87	0.74
1:B:1039:ASN:HD22	1:B:1183:ARG:HH11	1.33	0.74
1:D:3153:GLN:HG2	1:D:3200:ARG:HG3	1.68	0.74
1:B:1216:GLY:HA2	1:B:1220:GLN:HE22	1.51	0.73
1:B:1224:PRO:CB	1:B:1255:ARG:HG3	2.18	0.72
1:C:2096:ALA:HB3	1:C:2323:LEU:HD21	1.72	0.72
1:D:3199:GLN:NE2	1:D:3205:THR:HA	2.05	0.71
1:B:1255:ARG:HG2	3:B:5289:HOH:O	1.90	0.71
1:D:3191:TYR:HE2	1:D:3193:PHE:HE1	1.36	0.71
1:D:3129:PHE:CE2	1:D:3133:SER:OG	2.42	0.71
1:A:101:HIS:HD2	1:A:103:THR:H	1.37	0.70
1:C:2004:ASN:HB3	1:C:2193:PHE:HA	1.74	0.69
1:B:1148:ALA:H	1:B:1154:ASN:ND2	1.89	0.69
1:D:3004:ASN:HB3	1:D:3193:PHE:CB	2.23	0.69
1:B:1287:VAL:O	1:B:1290:ARG:CD	2.39	0.68
1:D:3039:ASN:HD22	1:D:3183:ARG:HH11	1.41	0.67
1:D:3129:PHE:CD2	1:D:3164:ASP:CB	2.72	0.67
1:C:2072:GLU:H	1:C:2355:GLN:HE22	1.43	0.67
1:C:2039:ASN:HD22	1:C:2183:ARG:HH11	1.44	0.66
1:C:2129:PHE:CD2	1:C:2164:ASP:CB	2.79	0.65
1:B:1234:SER:HB2	3:B:5923:HOH:O	1.98	0.64
1:D:3148:ALA:H	1:D:3154:ASN:ND2	1.85	0.64
1:A:209:MET:CE	1:A:217:ALA:HB3	2.28	0.63
1:B:1133:SER:OG	1:B:1141:ARG:NH1	2.32	0.63
1:A:209:MET:HE3	1:A:217:ALA:HB1	1.81	0.62
1:C:2129:PHE:CE2	1:C:2133:SER:OG	2.50	0.62
1:C:2022:THR:HA	1:C:2025:LEU:HD22	1.81	0.62
1:A:209:MET:HE3	1:A:217:ALA:CB	2.30	0.61
1:B:1228:GLU:OE2	1:B:1255:ARG:HD3	2.00	0.61
1:B:1101:HIS:HD2	1:B:1103:THR:H	1.48	0.61
1:C:2157:ILE:HD11	1:C:2200:ARG:HD2	1.82	0.61
1:B:1234:SER:O	1:B:1236:LEU:N	2.27	0.61
1:C:2129:PHE:CE2	1:C:2164:ASP:CB	2.80	0.60
1:D:3287:VAL:O	1:D:3290:ARG:CD	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:GLY:CA	1:B:1220:GLN:HE22	2.15	0.60
1:D:3096:ALA:HA	1:D:3191:TYR:OH	2.03	0.59
1:A:209:MET:CE	1:A:217:ALA:CB	2.80	0.59
1:A:101:HIS:CD2	1:A:103:THR:H	2.20	0.58
1:C:2195:MET:H	1:C:2199:GLN:HE22	1.50	0.58
1:C:2133:SER:OG	1:C:2141:ARG:NH1	2.37	0.58
1:D:3199:GLN:HE22	1:D:3205:THR:HA	1.66	0.58
1:A:224:PRO:CB	1:A:255:ARG:HG3	2.30	0.57
1:B:1013:GLU:O	1:B:1101:HIS:HE1	1.86	0.57
1:B:1072:GLU:H	1:B:1355:GLN:HE22	1.51	0.57
1:A:147:MET:CE	1:A:147:MET:HA	2.35	0.57
1:A:22:THR:HA	1:A:25:LEU:HD22	1.85	0.57
1:A:209:MET:HE2	1:A:217:ALA:HB3	1.86	0.57
1:A:39:ASN:ND2	1:A:183:ARG:HH11	2.02	0.57
1:D:3228:GLU:OE2	1:D:3255:ARG:HD2	2.05	0.56
1:D:3368:ASN:HD21	1:D:3370:TYR:HB2	1.70	0.56
1:C:2190:VAL:HG13	1:C:2208:GLY:HA2	1.87	0.56
1:A:147:MET:HA	1:A:147:MET:HE2	1.88	0.56
1:B:1129:PHE:CG	1:B:1130:GLU:N	2.73	0.56
1:B:1072:GLU:O	3:B:5748:HOH:O	2.17	0.56
1:A:195:MET:CE	1:A:211:LEU:HD23	2.36	0.56
1:C:2095:ALA:CA	3:C:5650:HOH:O	2.50	0.55
1:B:1212:ASN:OD1	3:B:5956:HOH:O	2.17	0.55
1:C:2371:GLY:HA3	3:C:5759:HOH:O	2.08	0.55
1:D:3224:PRO:HB3	1:D:3255:ARG:CG	2.23	0.54
1:A:72:GLU:O	3:A:5618:HOH:O	2.18	0.54
1:D:3039:ASN:ND2	1:D:3183:ARG:HH11	2.06	0.54
1:B:1224:PRO:HB3	1:B:1255:ARG:CG	2.30	0.53
1:B:1368:ASN:HD21	1:B:1370:TYR:HB2	1.73	0.53
1:B:1039:ASN:ND2	1:B:1183:ARG:HH11	2.06	0.53
1:C:2002:ASN:HD21	1:C:2004:ASN:HD22	1.55	0.53
1:D:3096:ALA:HB3	1:D:3323:LEU:HD21	1.91	0.53
1:B:1200:ARG:HD2	3:B:5654:HOH:O	2.08	0.53
1:D:3013:GLU:O	1:D:3101:HIS:HE1	1.92	0.52
1:C:2134:GLU:HG3	3:C:5408:HOH:O	2.09	0.52
1:D:3001:MET:HG3	1:D:3005:ASP:HB2	1.90	0.52
1:A:287:VAL:O	1:A:290:ARG:HD2	2.10	0.52
1:B:1228:GLU:OE2	1:B:1255:ARG:CD	2.58	0.52
1:C:2101:HIS:HD2	1:C:2103:THR:H	1.58	0.52
1:D:3129:PHE:CE2	1:D:3164:ASP:CB	2.85	0.51
1:B:1101:HIS:CD2	1:B:1103:THR:H	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3129:PHE:HD1	1:D:3130:GLU:OE2	1.94	0.51
1:C:2002:ASN:ND2	1:C:2004:ASN:HD22	2.09	0.51
1:A:124:TYR:HB3	1:A:195:MET:HE2	1.93	0.50
1:B:1216:GLY:CA	1:B:1220:GLN:NE2	2.65	0.50
1:C:2160:GLU:O	1:C:2164:ASP:OD1	2.30	0.50
1:D:3160:GLU:O	1:D:3164:ASP:CG	2.50	0.50
1:A:130:GLU:H	1:A:130:GLU:CD	2.15	0.50
1:D:3158:LEU:HD11	1:D:3230:ILE:HD12	1.94	0.50
1:A:214:ILE:O	1:A:215:TYR:CD1	2.65	0.49
1:C:2129:PHE:CD2	1:C:2164:ASP:CG	2.85	0.49
1:C:2130:GLU:CD	1:C:2130:GLU:H	2.14	0.49
1:C:2022:THR:O	1:C:2025:LEU:HB2	2.12	0.49
1:B:1243:ILE:HD12	1:B:1248:ASP:HB3	1.95	0.49
1:A:206:ALA:HA	1:A:209:MET:HE3	1.94	0.49
1:B:1162:LYS:HB2	3:B:5923:HOH:O	2.11	0.49
1:A:72:GLU:H	1:A:355:GLN:HE22	1.59	0.49
1:A:195:MET:HE2	1:A:211:LEU:HD23	1.95	0.48
1:D:3224:PRO:CB	1:D:3255:ARG:HG3	2.23	0.48
1:D:3022:THR:HA	1:D:3025:LEU:HD22	1.94	0.48
1:B:1067:LEU:HD22	1:D:3173:ALA:HB3	1.95	0.48
1:C:2094:ILE:HG21	1:C:2323:LEU:HD22	1.95	0.48
1:B:1222:ILE:O	1:C:2069:GLN:O	2.32	0.48
1:C:2101:HIS:CD2	1:C:2103:THR:H	2.31	0.48
1:D:3130:GLU:H	1:D:3130:GLU:CD	2.17	0.47
1:B:1191:TYR:OH	1:B:1211:LEU:HG	2.14	0.47
1:C:2148:ALA:N	1:C:2154:ASN:HD21	2.05	0.47
1:A:158:LEU:HD11	1:A:230:ILE:HD12	1.96	0.47
1:A:97:HIS:CD2	1:A:105:GLU:HG3	2.49	0.47
1:C:2368:ASN:HD21	1:C:2370:TYR:HB2	1.79	0.47
1:C:2013:GLU:O	1:C:2101:HIS:HE1	1.97	0.47
1:C:2148:ALA:HB2	1:C:2201:TYR:CD2	2.49	0.47
1:D:3004:ASN:HB3	1:D:3193:PHE:HB3	1.95	0.47
1:B:1130:GLU:HG2	3:B:5414:HOH:O	2.13	0.47
1:B:1104:LYS:HE3	3:B:5435:HOH:O	2.15	0.47
1:D:3133:SER:OG	1:D:3141:ARG:NH1	2.48	0.47
1:A:241:LYS:HA	1:A:261:TRP:HB3	1.96	0.46
1:C:2101:HIS:CD2	1:C:2103:THR:OG1	2.69	0.46
1:C:2129:PHE:CG	1:C:2164:ASP:CG	2.89	0.46
1:B:1199:GLN:HG3	1:B:1205:THR:HG23	1.98	0.46
1:A:13:GLU:O	1:A:101:HIS:HE1	1.98	0.46
1:B:1022:THR:HA	1:B:1025:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASN:HD21	1:A:370:TYR:HB2	1.81	0.46
1:C:2101:HIS:HD2	1:C:2103:THR:OG1	1.98	0.46
1:A:214:ILE:O	1:A:215:TYR:CB	2.63	0.46
1:A:147:MET:CA	1:A:147:MET:HE2	2.46	0.46
1:A:67:LEU:HD11	1:C:2243:ILE:HG12	1.96	0.46
1:A:214:ILE:O	1:A:215:TYR:CG	2.69	0.45
1:D:3101:HIS:HD2	1:D:3103:THR:H	1.65	0.45
1:C:2104:LYS:HE3	1:C:2127:ALA:HB2	1.97	0.45
1:D:3004:ASN:HB3	1:D:3193:PHE:HB2	1.99	0.45
1:B:1173:ALA:HB3	1:C:2067:LEU:HD22	1.99	0.45
1:D:3226:ASP:O	1:D:3230:ILE:HG12	2.16	0.45
1:B:1241:LYS:HA	1:B:1261:TRP:HB3	1.98	0.45
1:A:143:PHE:CD2	1:A:166:ALA:HB2	2.51	0.45
1:A:206:ALA:O	1:A:209:MET:HB2	2.18	0.44
1:D:3153:GLN:NE2	1:D:3201:TYR:HB3	2.32	0.44
1:C:2288:ASN:ND2	1:C:2289:LYS:HE3	2.33	0.44
1:C:2255:ARG:HD3	1:C:2255:ARG:HA	1.84	0.44
1:C:2004:ASN:HB3	1:C:2193:PHE:CA	2.46	0.44
1:C:2011:PRO:HD2	1:C:2100:ALA:O	2.17	0.44
1:C:2190:VAL:CG1	1:C:2208:GLY:HA2	2.47	0.44
1:D:3129:PHE:CG	1:D:3164:ASP:CG	2.92	0.43
1:B:1145:ILE:HD12	1:B:1171:LEU:HA	2.00	0.43
1:C:2160:GLU:O	1:C:2164:ASP:CG	2.55	0.43
1:A:199:GLN:O	3:A:5718:HOH:O	2.21	0.43
1:A:247:GLU:OE2	1:A:286:ARG:NH2	2.51	0.43
1:B:1129:PHE:CD1	1:B:1130:GLU:N	2.87	0.43
1:D:3098:GLY:CA	1:D:3104:LYS:HG2	2.49	0.43
1:C:2109:ALA:HB1	1:C:2136:LEU:HG	1.99	0.43
1:C:2287:VAL:O	1:C:2290:ARG:HD2	2.16	0.43
1:A:296:ASP:O	1:A:297:SER:HB2	2.19	0.43
1:D:3255:ARG:HD3	1:D:3255:ARG:HA	1.85	0.42
1:D:3101:HIS:HD2	1:D:3103:THR:OG1	2.02	0.42
1:A:89:PHE:HA	1:A:316:VAL:O	2.19	0.42
1:D:3288:ASN:C	1:D:3289:LYS:HG3	2.39	0.42
1:D:3228:GLU:OE2	1:D:3255:ARG:CD	2.67	0.42
1:D:3094:ILE:HG21	1:D:3323:LEU:HD22	2.02	0.42
1:B:1129:PHE:CD1	1:B:1129:PHE:N	2.88	0.42
1:C:2202:LEU:O	1:C:2203:ARG:CB	2.68	0.42
1:A:147:MET:HE3	1:A:230:ILE:HG13	2.02	0.42
1:B:1129:PHE:HE1	3:B:5800:HOH:O	2.03	0.41
1:C:2129:PHE:HE2	1:C:2141:ARG:HH11	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2148:ALA:H	1:C:2154:ASN:ND2	2.07	0.41
1:D:3241:LYS:HA	1:D:3261:TRP:HB3	2.03	0.41
1:A:199:GLN:HG3	3:A:5723:HOH:O	2.21	0.41
1:D:3110:ARG:HG2	1:D:3331:TRP:CD2	2.56	0.41
1:A:143:PHE:HD2	1:A:166:ALA:HB2	1.85	0.41
1:D:3247:GLU:OE2	1:D:3286:ARG:NH2	2.51	0.41
1:A:288:ASN:C	1:A:289:LYS:HG3	2.41	0.41
1:A:129:PHE:CZ	1:A:164:ASP:HB3	2.55	0.41
1:A:209:MET:HE2	1:A:217:ALA:CB	2.46	0.41
1:A:255:ARG:HA	1:A:255:ARG:HD3	1.73	0.40
1:D:3101:HIS:CD2	1:D:3103:THR:H	2.38	0.40
1:D:3129:PHE:HE2	1:D:3141:ARG:HH11	1.68	0.40
1:D:3089:PHE:HA	1:D:3316:VAL:O	2.21	0.40
1:D:3148:ALA:HB2	1:D:3201:TYR:CD1	2.57	0.40
1:B:1157:ILE:HD11	1:B:1200:ARG:HD3	2.03	0.40
1:A:296:ASP:C	1:A:296:ASP:OD1	2.60	0.40
1:D:3097:HIS:CG	1:D:3105:GLU:HG3	2.56	0.40

All (1) 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)
3:A:5545:HOH:O	3:A:5873:HOH:O[16_444]	2.19	0.01

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	372/374 (100%)	361 (97%)	8 (2%)	3 (1%)	24	17
1	B	372/374 (100%)	355 (95%)	13 (4%)	4 (1%)	17	11
1	C	372/374 (100%)	358 (96%)	12 (3%)	2 (0%)	34	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	372/374 (100%)	358 (96%)	12 (3%)	2 (0%)	34	30
All	All	1488/1496 (100%)	1432 (96%)	45 (3%)	11 (1%)	26	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	TYR
1	A	297	SER
1	B	1206	ALA
1	B	1297	SER
1	C	2297	SER
1	D	3297	SER
1	A	200	ARG
1	B	1019	VAL
1	C	2005	ASP
1	B	1007	GLU
1	D	3006	ILE

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	298/298 (100%)	286 (96%)	12 (4%)	38	38
1	B	298/298 (100%)	280 (94%)	18 (6%)	24	20
1	C	298/298 (100%)	280 (94%)	18 (6%)	24	20
1	D	298/298 (100%)	276 (93%)	22 (7%)	17	13
All	All	1192/1192 (100%)	1122 (94%)	70 (6%)	24	20

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	67	LEU
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	141	ARG
1	A	200	ARG
1	A	286	ARG
1	A	288	ASN
1	A	289	LYS
1	A	323	LEU
1	A	328	LEU
1	A	363	LEU
1	A	365	LEU
1	B	1004	ASN
1	B	1007	GLU
1	B	1025	LEU
1	B	1104	LYS
1	B	1125	SER
1	B	1130	GLU
1	B	1141	ARG
1	B	1145	ILE
1	B	1190	VAL
1	B	1199	GLN
1	B	1200	ARG
1	B	1211	LEU
1	B	1286	ARG
1	B	1288	ASN
1	B	1289	LYS
1	B	1328	LEU
1	B	1363	LEU
1	B	1365	LEU
1	C	2025	LEU
1	C	2129	PHE
1	C	2133	SER
1	C	2137	ASN
1	C	2141	ARG
1	C	2145	ILE
1	C	2163	SER
1	C	2190	VAL
1	C	2199	GLN
1	C	2203	ARG
1	C	2205	THR
1	C	2211	LEU
1	C	2255	ARG
1	C	2286	ARG
1	C	2288	ASN

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Mol	Chain	Res	Type
1	C	2328	LEU
1	C	2363	LEU
1	C	2365	LEU
1	D	3009	ASN
1	D	3025	LEU
1	D	3067	LEU
1	D	3072	GLU
1	D	3086	LYS
1	D	3110	ARG
1	D	3130	GLU
1	D	3134	GLU
1	D	3141	ARG
1	D	3145	ILE
1	D	3190	VAL
1	D	3191	TYR
1	D	3200	ARG
1	D	3203	ARG
1	D	3211	LEU
1	D	3225	ARG
1	D	3286	ARG
1	D	3288	ASN
1	D	3289	LYS
1	D	3328	LEU
1	D	3363	LEU
1	D	3365	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	ASN
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
1	B	1039	ASN
1	B	1083	HIS
1	B	1101	HIS
1	B	1137	ASN

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Mol	Chain	Res	Type
1	B	1153	GLN
1	B	1154	ASN
1	B	1187	ASN
1	B	1199	GLN
1	B	1288	ASN
1	B	1355	GLN
1	B	1368	ASN
1	C	2002	ASN
1	C	2035	HIS
1	C	2039	ASN
1	C	2083	HIS
1	C	2101	HIS
1	C	2153	GLN
1	C	2154	ASN
1	C	2187	ASN
1	C	2199	GLN
1	C	2288	ASN
1	C	2355	GLN
1	C	2368	ASN
1	D	3004	ASN
1	D	3035	HIS
1	D	3039	ASN
1	D	3101	HIS
1	D	3137	ASN
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 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	A	512	-	32,33,33	1.27	2 (6%)	34,50,50	2.14	7 (20%)
2	FMN	B	1512	-	32,33,33	1.22	4 (12%)	34,50,50	2.09	6 (17%)
2	FMN	C	2512	-	32,33,33	1.06	3 (9%)	34,50,50	2.13	7 (20%)
2	FMN	D	3512	-	32,33,33	1.44	4 (12%)	34,50,50	2.32	7 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	512	-	-	0/18/18/18	0/3/3/3
2	FMN	B	1512	-	-	0/18/18/18	0/3/3/3
2	FMN	C	2512	-	-	0/18/18/18	0/3/3/3
2	FMN	D	3512	-	-	0/18/18/18	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2512	FMN	C1'-N10	2.01	1.50	1.48
2	D	3512	FMN	C10-N1	2.11	1.39	1.35
2	B	1512	FMN	C5A-N5	2.20	1.38	1.35
2	D	3512	FMN	C5A-N5	2.28	1.38	1.35
2	B	1512	FMN	C1'-N10	2.51	1.51	1.48
2	C	2512	FMN	C4A-N5	2.95	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2512	FMN	C4-N3	2.98	1.38	1.33
2	B	1512	FMN	C4-N3	3.13	1.38	1.33
2	A	512	FMN	C4-N3	3.37	1.39	1.33
2	B	1512	FMN	C4A-N5	3.62	1.38	1.33
2	A	512	FMN	C4A-N5	4.13	1.39	1.33
2	D	3512	FMN	C4A-N5	4.24	1.39	1.33
2	D	3512	FMN	C1'-N10	4.26	1.52	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2512	FMN	N3-C2-N1	-5.12	119.06	127.69
2	D	3512	FMN	N3-C2-N1	-4.82	119.58	127.69
2	B	1512	FMN	N3-C2-N1	-4.62	119.92	127.69
2	A	512	FMN	N3-C2-N1	-4.51	120.09	127.69
2	B	1512	FMN	C4A-C4-N3	-4.25	117.96	123.52
2	A	512	FMN	C4A-C4-N3	-4.14	118.11	123.52
2	C	2512	FMN	C4A-C4-N3	-3.98	118.33	123.52
2	D	3512	FMN	C4A-C4-N3	-3.70	118.69	123.52
2	A	512	FMN	C8M-C8-C9	-2.22	114.05	120.33
2	D	3512	FMN	C4-C4A-N5	2.02	121.15	118.70
2	C	2512	FMN	O3P-P-O5'	2.05	112.70	106.72
2	A	512	FMN	O3P-P-O2P	2.06	115.01	107.44
2	B	1512	FMN	C1'-N10-C9A	2.09	121.25	118.83
2	C	2512	FMN	C5A-C9A-N10	2.63	119.55	117.58
2	D	3512	FMN	C4A-N5-C5A	2.68	119.88	116.72
2	C	2512	FMN	C1'-N10-C9A	2.95	122.25	118.83
2	A	512	FMN	C1'-N10-C9A	3.37	122.74	118.83
2	C	2512	FMN	C4A-N5-C5A	3.47	120.81	116.72
2	B	1512	FMN	C4-C4A-N5	3.60	123.07	118.70
2	D	3512	FMN	C5A-C9A-N10	3.66	120.32	117.58
2	B	1512	FMN	C4A-N5-C5A	4.05	121.49	116.72
2	A	512	FMN	C5A-C9A-N10	4.23	120.75	117.58
2	D	3512	FMN	C1'-N10-C9A	4.57	124.13	118.83
2	C	2512	FMN	C4-N3-C2	7.42	121.35	115.16
2	B	1512	FMN	C4-N3-C2	7.75	121.63	115.16
2	A	512	FMN	C4-N3-C2	7.82	121.69	115.16
2	D	3512	FMN	C4-N3-C2	8.83	122.53	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/374 (100%)	-0.69	3 (0%) 87 90	8, 14, 31, 47	0
1	B	374/374 (100%)	-0.45	9 (2%) 62 68	9, 17, 31, 91	0
1	C	374/374 (100%)	-0.51	11 (2%) 55 63	9, 17, 30, 89	0
1	D	374/374 (100%)	-0.37	20 (5%) 30 39	9, 16, 41, 91	0
All	All	1496/1496 (100%)	-0.51	43 (2%) 55 63	8, 16, 33, 91	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2002	ASN	12.7
1	C	2005	ASP	12.2
1	B	1006	ILE	11.8
1	D	3001	MET	11.0
1	C	2001	MET	10.8
1	B	1001	MET	9.8
1	C	2003	ASN	9.4
1	D	3003	ASN	9.2
1	D	3005	ASP	8.9
1	D	3006	ILE	8.6
1	B	1003	ASN	7.5
1	B	1002	ASN	7.5
1	B	1005	ASP	7.4
1	D	3004	ASN	7.1
1	C	2004	ASN	6.1
1	C	2006	ILE	5.8
1	D	3203	ARG	5.7
1	B	1205	THR	5.0
1	D	3002	ASN	4.6
1	B	1129	PHE	4.3
1	D	3129	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	2129	PHE	3.9
1	D	3191	TYR	3.9
1	B	1203	ARG	3.6
1	C	2164	ASP	3.5
1	D	3255	ARG	3.2
1	D	3205	THR	3.2
1	D	3201	TYR	3.1
1	D	3204	GLY	3.0
1	C	2095	ALA	2.9
1	D	3096	ALA	2.7
1	D	3216	GLY	2.6
1	B	1004	ASN	2.6
1	C	2007	GLU	2.5
1	D	3202	LEU	2.4
1	C	2096	ALA	2.4
1	A	214	ILE	2.4
1	D	3164	ASP	2.3
1	D	3199	GLN	2.3
1	A	204	GLY	2.3
1	A	1	MET	2.2
1	D	3213	ASN	2.0
1	D	3206	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FMN	A	512	31/31	0.98	0.07	0.05	7,11,14,15	0
2	FMN	C	2512	31/31	0.98	0.09	-0.15	11,13,14,17	0
2	FMN	D	3512	31/31	0.98	0.08	-0.33	10,14,15,16	0
2	FMN	B	1512	31/31	0.98	0.07	-0.50	11,13,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.