Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:09 PM GMT

PDB ID	:	1ICU
Title	:	THE STRUCTURE OF ESCHERICHIA COLI NITROREDUCTASE COMPLEXED WITH NICOTINIC ACID
Authors	:	Lovering, A.L.; Hyde, E.I.; Searle, P.F.; White, S.A.
Deposited on	:	2001-04-02
Resolution	:	1.80 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 (i) symbol.

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

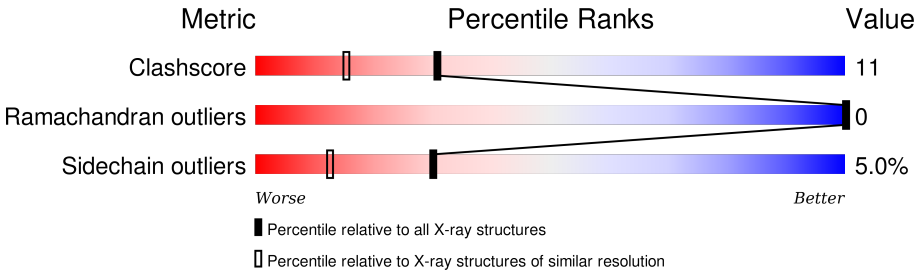
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	80% 17% •
1	B	217	81% 18% •
1	C	217	81% 16% •
1	D	217	75% 22% •

2 Entry composition

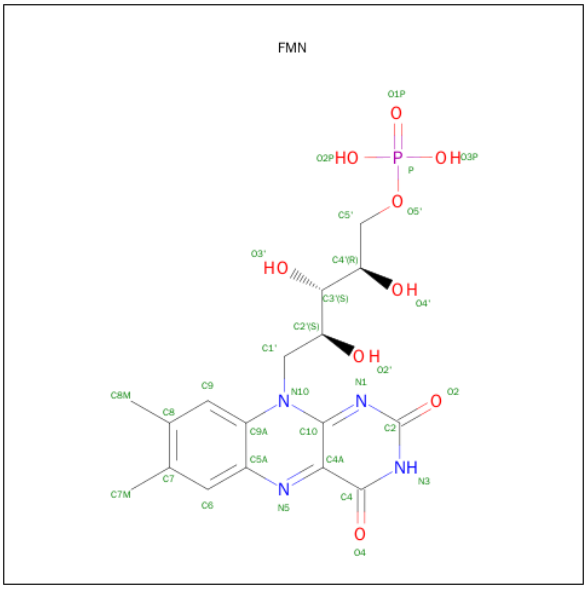
There are 4 unique types of molecules in this entry. The entry contains 7023 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OXYGEN-INSENSITIVE NAD(P)H NITROREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			
1	B	217	Total	C	N	O	S	0	0	0
			1685	1070	288	321	6			
1	C	216	Total	C	N	O	S	0	0	0
			1677	1065	287	320	5			
1	D	217	Total	C	N	O	S	0	0	0
			1685	1070	288	321	6			

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



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

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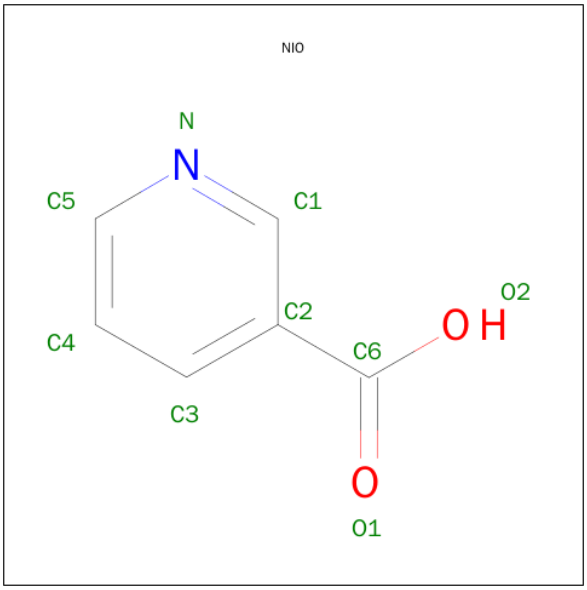
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 31 17 4 9 1	0	0
2	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 3 is NICOTINIC ACID (three-letter code: NIO) (formula: $C_6H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 9 6 1 2	0	0
3	A	1	Total C N O 9 6 1 2	0	0
3	D	1	Total C N O 9 6 1 2	0	0
3	C	1	Total C N O 9 6 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	42	Total O 42 42	0	0
4	C	32	Total O 32 32	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	30	Total O 30 30	0	0

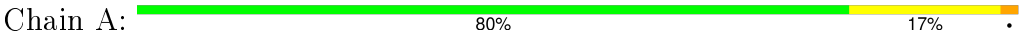
3 Residue-property plots (i)

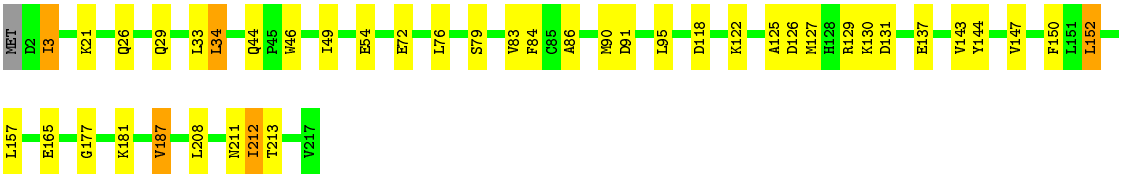
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: OXYGEN-INSENSITIVE NAD(P)H NITROREDUCTASE

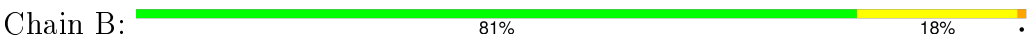
Chain A:

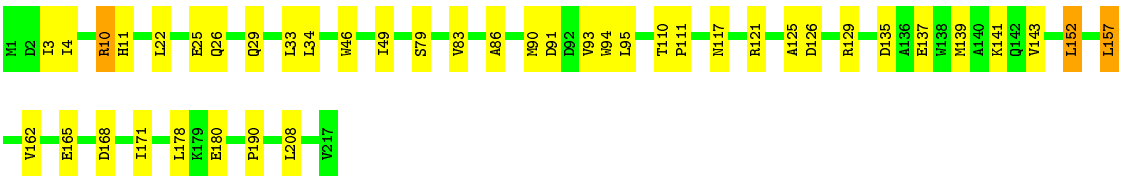




- Molecule 1: OXYGEN-INSENSITIVE NAD(P)H NITROREDUCTASE

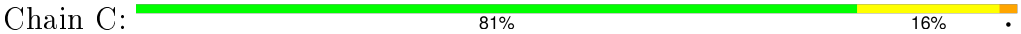
Chain B:

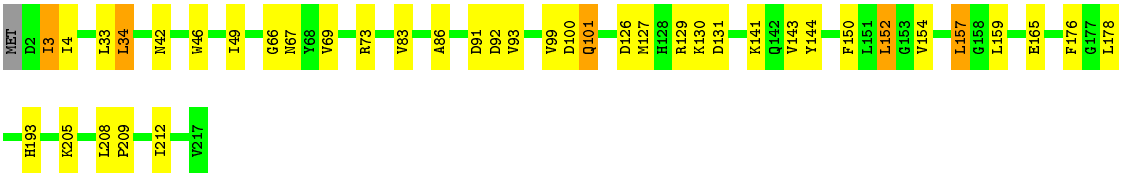




- Molecule 1: OXYGEN-INSENSITIVE NAD(P)H NITROREDUCTASE

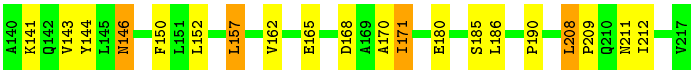
Chain C:





- Molecule 1: OXYGEN-INSENSITIVE NAD(P)H NITROREDUCTASE

Chain D:


A140
K141
Q142
V143
Y144
L145
N146
F150
L151
L152
L157
V162
E165
D168
A169
A170
I171
E180
S185
L186
P190
L208
P209
Q210
N211
I212
V217

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.01Å 57.62Å 116.98Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	100.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	6.70	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7023	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.35	0/1712	0.56	0/2318
1	B	0.36	0/1720	0.58	0/2328
1	C	0.33	0/1712	0.55	0/2318
1	D	0.34	0/1720	0.56	0/2328
All	All	0.35	0/6864	0.56	0/9292

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1677	0	1661	43	0
1	B	1685	0	1673	39	0
1	C	1677	0	1661	33	0
1	D	1685	0	1673	53	0
2	A	31	0	18	1	0
2	B	31	0	19	1	0
2	C	31	0	18	2	0
2	D	31	0	18	2	0
3	A	9	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	5	0	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
4	A	35	0	0	0	0
4	B	42	0	0	0	0
4	C	32	0	0	1	0
4	D	30	0	0	0	0
All	All	7023	0	6761	149	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 11.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HH11	1:B:10:ARG:HB2	1.31	0.92
1:A:44:GLN:HE22	1:B:208:LEU:H	1.16	0.90
1:C:4:ILE:HD11	1:D:157:LEU:HD11	1.53	0.90
1:B:3:ILE:HD11	1:B:152:LEU:HD21	1.62	0.81
1:A:3:ILE:O	1:A:3:ILE:HD13	1.82	0.80
1:B:117:ASN:HD21	1:B:121:ARG:HH22	1.29	0.79
1:D:117:ASN:HD21	1:D:121:ARG:HH22	1.31	0.78
1:B:125:ALA:O	1:B:129:ARG:HG2	1.84	0.76
1:C:3:ILE:HD11	1:C:152:LEU:HD11	1.67	0.76
1:D:165:GLU:HB2	2:D:224:FMN:H6	1.68	0.75
1:B:168:ASP:CG	1:B:171:ILE:HD13	2.07	0.75
1:D:73:ARG:NH1	1:D:76:LEU:HD23	2.02	0.74
1:C:3:ILE:O	1:C:3:ILE:HD13	1.88	0.73
1:D:125:ALA:O	1:D:129:ARG:HG2	1.88	0.73
1:A:157:LEU:HD21	1:B:4:ILE:HD11	1.72	0.71
1:C:66:GLY:O	1:C:69:VAL:HG23	1.89	0.70
1:C:126:ASP:HA	1:C:129:ARG:HG2	1.71	0.70
1:B:10:ARG:CB	1:B:10:ARG:HH11	2.03	0.69
1:D:209:PRO:HD2	1:D:212:ILE:HD12	1.75	0.68
1:A:147:VAL:HG21	1:A:187:VAL:HG11	1.74	0.68
1:A:86:ALA:HB2	1:A:143:VAL:HG21	1.75	0.68
1:C:101:GLN:HG3	1:D:208:LEU:HD12	1.75	0.68
1:B:3:ILE:HD11	1:B:152:LEU:CD2	2.24	0.67
1:C:165:GLU:HG3	2:C:222:FMN:H6	1.77	0.67
1:D:126:ASP:HA	1:D:129:ARG:CG	2.25	0.66
1:C:4:ILE:CD1	1:D:157:LEU:HD11	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD21	1:B:4:ILE:CD1	2.27	0.64
1:C:126:ASP:OD1	1:C:130:LYS:HE2	1.99	0.63
1:A:126:ASP:OD1	1:A:129:ARG:HD3	1.98	0.62
1:C:157:LEU:HD11	1:D:4:ILE:HD13	1.80	0.62
1:B:110:THR:HB	1:B:111:PRO:HD2	1.82	0.61
1:A:212:ILE:HD11	1:B:94:TRP:CH2	2.35	0.61
1:B:10:ARG:NH1	1:B:11:HIS:N	2.48	0.61
1:A:126:ASP:HA	1:A:129:ARG:CD	2.29	0.61
1:C:154:VAL:HG13	1:C:159:LEU:HB2	1.82	0.61
1:D:91:ASP:O	1:D:95:LEU:HD13	2.01	0.60
1:A:44:GLN:HE22	1:B:208:LEU:N	1.95	0.59
1:B:126:ASP:OD1	1:B:129:ARG:HD2	2.03	0.59
1:D:110:THR:OG1	1:D:112:GLU:HG2	2.01	0.59
1:A:118:ASP:OD2	1:A:122:LYS:HE2	2.02	0.59
1:D:180:GLU:H	1:D:180:GLU:CD	2.04	0.59
1:A:91:ASP:O	1:A:95:LEU:HD23	2.02	0.58
1:B:26:GLN:HA	1:B:29:GLN:HE21	1.68	0.58
1:C:157:LEU:HD11	1:D:4:ILE:CD1	2.33	0.58
1:A:3:ILE:HD11	1:A:152:LEU:HD11	1.86	0.58
1:B:126:ASP:HA	1:B:129:ARG:CG	2.34	0.57
1:D:95:LEU:HD23	1:D:122:LYS:HD2	1.86	0.57
1:A:137:GLU:HG3	1:B:137:GLU:HG3	1.86	0.56
1:C:144:TYR:CE1	1:D:141:LYS:HD3	2.40	0.56
1:B:180:GLU:H	1:B:180:GLU:CD	2.08	0.56
1:D:3:ILE:HG23	1:D:4:ILE:HD12	1.87	0.55
1:B:86:ALA:HB2	1:B:143:VAL:HG21	1.89	0.55
1:B:165:GLU:HB2	2:B:220:FMN:H6	1.89	0.55
1:A:26:GLN:HA	1:A:29:GLN:HE21	1.72	0.55
1:B:126:ASP:HA	1:B:129:ARG:HG3	1.89	0.54
1:A:90:MET:HG3	1:A:95:LEU:HD21	1.89	0.54
1:B:3:ILE:HG23	1:B:4:ILE:HD12	1.89	0.54
1:C:126:ASP:HA	1:C:129:ARG:CG	2.38	0.54
1:D:10:ARG:HG2	1:D:11:HIS:N	2.22	0.54
1:C:4:ILE:HD12	1:C:4:ILE:N	2.22	0.53
1:D:86:ALA:HB2	1:D:143:VAL:HG21	1.90	0.53
1:A:44:GLN:NE2	1:B:208:LEU:H	1.94	0.53
1:B:135:ASP:O	1:B:139:MET:HG3	2.09	0.53
1:B:4:ILE:N	1:B:4:ILE:HD12	2.24	0.52
1:D:137:GLU:HG2	1:D:141:LYS:HE3	1.91	0.52
1:C:91:ASP:OD1	1:C:93:VAL:HB	2.10	0.52
1:D:90:MET:HE2	1:D:90:MET:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ASP:OD1	1:D:129:ARG:HD2	2.10	0.52
1:A:127:MET:HA	1:A:131:ASP:OD2	2.10	0.52
1:A:3:ILE:HD11	1:A:152:LEU:HD21	1.92	0.51
1:A:144:TYR:CE1	1:B:141:LYS:HD3	2.45	0.51
1:D:117:ASN:ND2	1:D:121:ARG:HH12	2.08	0.51
1:D:90:MET:HA	1:D:90:MET:CE	2.40	0.51
1:A:129:ARG:HG3	1:A:130:LYS:HG3	1.91	0.51
1:C:86:ALA:HB2	1:C:143:VAL:HG21	1.93	0.50
1:C:154:VAL:CG1	1:C:159:LEU:HB2	2.40	0.50
1:A:177:GLY:O	1:A:181:LYS:HG3	2.12	0.49
1:A:126:ASP:HA	1:A:129:ARG:HG2	1.94	0.49
1:C:165:GLU:CG	2:C:222:FMN:H6	2.42	0.49
1:C:193:HIS:HE1	4:C:241:HOH:O	1.95	0.49
1:A:72:GLU:O	1:A:76:LEU:HD23	2.12	0.49
1:D:26:GLN:HA	1:D:29:GLN:HE21	1.78	0.49
1:A:211:ASN:OD1	1:A:212:ILE:HG22	2.13	0.49
1:D:63:SER:N	1:D:171:ILE:HD11	2.27	0.48
1:A:84:PHE:HB2	1:A:187:VAL:HG13	1.96	0.48
1:C:34:LEU:HD13	1:C:150:PHE:CE2	2.48	0.48
1:C:176:PHE:HB2	1:C:178:LEU:HD13	1.96	0.48
1:B:22:LEU:HD13	1:B:79:SER:HB3	1.96	0.47
1:D:129:ARG:HG3	1:D:130:LYS:N	2.30	0.47
1:C:205:LYS:HD3	1:D:36:TYR:HD2	1.78	0.47
1:C:141:LYS:HD3	1:D:144:TYR:CE1	2.49	0.47
1:B:3:ILE:CG2	1:B:4:ILE:HD12	2.44	0.47
1:B:90:MET:HG3	1:B:95:LEU:HD21	1.95	0.47
1:D:49:ILE:HB	1:D:83:VAL:HB	1.95	0.47
1:C:3:ILE:HD11	1:C:152:LEU:CD1	2.43	0.47
1:B:152:LEU:HD23	1:B:152:LEU:O	2.15	0.46
1:D:162:VAL:O	1:D:162:VAL:HG13	2.14	0.46
1:C:49:ILE:HB	1:C:83:VAL:HB	1.96	0.46
1:D:168:ASP:CG	1:D:171:ILE:HG23	2.35	0.46
1:A:49:ILE:HB	1:A:83:VAL:HB	1.98	0.46
1:D:168:ASP:OD1	1:D:171:ILE:HG23	2.16	0.46
1:D:117:ASN:HD21	1:D:121:ARG:NH2	2.07	0.46
1:D:126:ASP:HA	1:D:129:ARG:HG3	1.95	0.46
1:A:212:ILE:HG13	1:A:213:THR:N	2.30	0.46
1:D:135:ASP:O	1:D:139:MET:HG3	2.16	0.46
1:A:165:GLU:HB2	2:A:218:FMN:H6	1.98	0.45
1:A:125:ALA:C	1:A:129:ARG:HD2	2.36	0.45
1:A:129:ARG:HG2	1:A:130:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASP:OD1	1:B:93:VAL:HB	2.16	0.45
1:D:68:TYR:HA	1:D:70:PHE:CE1	2.50	0.45
1:A:21:LYS:HA	1:A:79:SER:HB2	1.98	0.45
1:D:185:SER:C	1:D:186:LEU:HD12	2.37	0.45
1:D:73:ARG:HH11	1:D:76:LEU:HD23	1.82	0.44
1:A:129:ARG:CG	1:A:130:LYS:HG3	2.47	0.44
1:A:212:ILE:HG13	1:A:213:THR:HG23	2.00	0.44
1:D:90:MET:HE3	1:D:94:TRP:CD1	2.53	0.44
1:A:212:ILE:HD11	1:B:94:TRP:HH2	1.78	0.44
1:C:34:LEU:HD13	1:C:150:PHE:CD2	2.53	0.44
1:D:129:ARG:HG3	1:D:130:LYS:H	1.83	0.44
1:D:34:LEU:HD13	1:D:150:PHE:CE2	2.52	0.44
1:D:168:ASP:OD1	1:D:170:ALA:HB3	2.18	0.43
1:C:209:PRO:HD2	1:C:212:ILE:HD12	1.99	0.43
1:D:126:ASP:HA	1:D:129:ARG:HG2	1.98	0.43
1:D:157:LEU:HD12	1:D:157:LEU:HA	1.84	0.43
1:D:63:SER:HA	1:D:171:ILE:HG12	2.01	0.42
1:B:25:GLU:O	1:B:29:GLN:HG3	2.19	0.42
1:D:137:GLU:O	1:D:141:LYS:HG3	2.19	0.42
1:C:157:LEU:HD13	1:D:3:ILE:CG2	2.49	0.42
1:B:117:ASN:HD21	1:B:121:ARG:NH2	2.07	0.42
1:C:99:VAL:HG13	1:C:100:ASP:N	2.35	0.42
1:D:34:LEU:HD13	1:D:150:PHE:CD2	2.55	0.42
1:C:127:MET:HA	1:C:131:ASP:OD2	2.20	0.42
1:A:125:ALA:O	1:A:129:ARG:HD2	2.19	0.42
1:A:127:MET:O	1:A:131:ASP:HB2	2.20	0.42
1:B:49:ILE:HB	1:B:83:VAL:HB	2.02	0.42
1:C:42:ASN:HB2	2:D:224:FMN:O4'	2.20	0.41
1:A:126:ASP:HA	1:A:129:ARG:CG	2.50	0.41
1:D:186:LEU:N	1:D:186:LEU:HD12	2.35	0.41
1:B:117:ASN:ND2	1:B:121:ARG:HH12	2.18	0.41
1:A:212:ILE:HD12	1:A:212:ILE:O	2.20	0.41
1:A:3:ILE:HG22	1:B:157:LEU:HD13	2.02	0.41
1:B:162:VAL:O	1:B:190:PRO:HD2	2.21	0.41
1:D:211:ASN:OD1	1:D:212:ILE:HG13	2.21	0.41
1:A:34:LEU:HD13	1:A:150:PHE:CE2	2.56	0.40
1:C:73:ARG:HG3	1:C:73:ARG:HH11	1.85	0.40
1:D:162:VAL:O	1:D:190:PRO:HD2	2.21	0.40
1:A:34:LEU:HD13	1:A:150:PHE:CD2	2.57	0.40
1:A:3:ILE:HD11	1:A:152:LEU:CD1	2.49	0.40
1:D:146:ASN:C	1:D:146:ASN:HD22	2.24	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	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
1	B	215/217 (99%)	213 (99%)	2 (1%)	0	100	100
1	C	214/217 (99%)	213 (100%)	1 (0%)	0	100	100
1	D	215/217 (99%)	213 (99%)	2 (1%)	0	100	100
All	All	858/868 (99%)	849 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	178/179 (99%)	169 (95%)	9 (5%)	29	12
1	B	179/179 (100%)	172 (96%)	7 (4%)	39	21
1	C	178/179 (99%)	168 (94%)	10 (6%)	26	10
1	D	179/179 (100%)	169 (94%)	10 (6%)	26	10
All	All	714/716 (100%)	678 (95%)	36 (5%)	30	13

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	33	LEU
1	A	34	LEU
1	A	46	TRP
1	A	54	GLU
1	A	152	LEU
1	A	187	VAL
1	A	208	LEU
1	A	212	ILE
1	B	10	ARG
1	B	33	LEU
1	B	34	LEU
1	B	46	TRP
1	B	152	LEU
1	B	157	LEU
1	B	178	LEU
1	C	3	ILE
1	C	33	LEU
1	C	34	LEU
1	C	46	TRP
1	C	67	ASN
1	C	92	ASP
1	C	101	GLN
1	C	152	LEU
1	C	157	LEU
1	C	208	LEU
1	D	2	ASP
1	D	34	LEU
1	D	46	TRP
1	D	76	LEU
1	D	90	MET
1	D	146	ASN
1	D	152	LEU
1	D	157	LEU
1	D	171	ILE
1	D	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	35	GLN
1	A	44	GLN

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Mol	Chain	Res	Type
1	A	133	HIS
1	A	210	GLN
1	B	29	GLN
1	B	117	ASN
1	B	128	HIS
1	B	149	ASN
1	B	210	GLN
1	C	35	GLN
1	C	67	ASN
1	C	101	GLN
1	C	149	ASN
1	C	210	GLN
1	D	29	GLN
1	D	117	ASN
1	D	146	ASN
1	D	210	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	218	-	32,33,33	2.93	15 (46%)	34,50,50	5.49	18 (52%)
3	NIO	A	221	-	6,9,9	3.26	3 (50%)	8,11,11	1.22	1 (12%)
3	NIO	B	219	-	6,9,9	3.27	3 (50%)	8,11,11	1.23	1 (12%)
2	FMN	B	220	-	32,33,33	2.95	16 (50%)	34,50,50	5.70	14 (41%)
2	FMN	C	222	-	32,33,33	3.06	17 (53%)	34,50,50	5.28	19 (55%)
3	NIO	C	225	-	6,9,9	3.27	3 (50%)	8,11,11	1.24	1 (12%)
3	NIO	D	223	-	6,9,9	3.23	3 (50%)	8,11,11	1.21	1 (12%)
2	FMN	D	224	-	32,33,33	2.94	16 (50%)	34,50,50	5.29	21 (61%)

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	218	-	-	0/18/18/18	0/3/3/3
3	NIO	A	221	-	-	0/0/4/4	0/1/1/1
3	NIO	B	219	-	-	0/0/4/4	0/1/1/1
2	FMN	B	220	-	-	0/18/18/18	0/3/3/3
2	FMN	C	222	-	-	0/18/18/18	0/3/3/3
3	NIO	C	225	-	-	0/0/4/4	0/1/1/1
3	NIO	D	223	-	-	0/0/4/4	0/1/1/1
2	FMN	D	224	-	-	0/18/18/18	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	222	FMN	O2'-C2'	2.20	1.48	1.43
2	B	220	FMN	O2'-C2'	2.25	1.48	1.43
2	D	224	FMN	C5'-C4'	2.30	1.55	1.51
2	C	222	FMN	C5A-N5	2.31	1.38	1.35
2	D	224	FMN	O2'-C2'	2.38	1.48	1.43
2	A	218	FMN	C5'-C4'	2.39	1.55	1.51
2	B	220	FMN	C8-C7	2.51	1.47	1.41
2	B	220	FMN	C5'-C4'	2.52	1.55	1.51
2	A	218	FMN	O3'-C3'	2.57	1.49	1.43
2	C	222	FMN	C5'-C4'	2.61	1.55	1.51
2	D	224	FMN	O3'-C3'	2.65	1.49	1.43
2	C	222	FMN	C8-C7	2.65	1.48	1.41
2	D	224	FMN	C8-C7	2.68	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	FMN	O3'-C3'	2.72	1.49	1.43
2	C	222	FMN	C4-N3	2.77	1.38	1.33
2	A	218	FMN	C4-N3	2.82	1.38	1.33
2	C	222	FMN	O3'-C3'	2.82	1.49	1.43
2	A	218	FMN	C8-C7	2.84	1.48	1.41
2	D	224	FMN	C4-N3	2.87	1.38	1.33
2	D	224	FMN	C9-C9A	2.92	1.47	1.40
2	A	218	FMN	C9-C9A	2.92	1.47	1.40
2	B	220	FMN	C4-N3	2.98	1.38	1.33
2	C	222	FMN	O4'-C4'	3.02	1.50	1.43
2	C	222	FMN	C9-C9A	3.06	1.47	1.40
2	A	218	FMN	O4'-C4'	3.07	1.50	1.43
2	B	220	FMN	C9-C9A	3.08	1.47	1.40
2	D	224	FMN	O4'-C4'	3.09	1.50	1.43
2	D	224	FMN	C2'-C3'	3.09	1.59	1.53
2	B	220	FMN	C2'-C3'	3.13	1.59	1.53
2	B	220	FMN	O4'-C4'	3.19	1.50	1.43
2	D	224	FMN	C6-C5A	3.22	1.46	1.41
2	C	222	FMN	C6-C5A	3.42	1.47	1.41
2	A	218	FMN	C2'-C3'	3.45	1.60	1.53
2	A	218	FMN	C6-C5A	3.56	1.47	1.41
2	D	224	FMN	C4-C4A	3.56	1.48	1.41
2	B	220	FMN	C9A-N10	3.58	1.43	1.38
2	C	222	FMN	C2'-C3'	3.59	1.60	1.53
2	A	218	FMN	C9A-N10	3.75	1.44	1.38
2	B	220	FMN	C4-C4A	3.76	1.48	1.41
2	D	224	FMN	C9A-N10	3.78	1.44	1.38
2	B	220	FMN	C6-C5A	3.82	1.47	1.41
3	D	223	NIO	C4-C5	3.82	1.49	1.37
3	A	221	NIO	C4-C5	3.82	1.49	1.37
2	A	218	FMN	C4-C4A	3.83	1.49	1.41
3	B	219	NIO	C4-C5	3.86	1.49	1.37
3	C	225	NIO	C4-C5	3.87	1.49	1.37
2	C	222	FMN	C4-C4A	4.03	1.49	1.41
2	B	220	FMN	C2-N3	4.22	1.47	1.38
2	C	222	FMN	C2-N3	4.23	1.47	1.38
2	C	222	FMN	C9A-N10	4.25	1.44	1.38
2	D	224	FMN	C2-N3	4.32	1.47	1.38
2	A	218	FMN	C2-N3	4.47	1.47	1.38
3	D	223	NIO	C1-N	4.48	1.44	1.34
3	B	219	NIO	C1-N	4.60	1.44	1.34
3	A	221	NIO	C1-N	4.62	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	225	NIO	C1-N	4.68	1.44	1.34
3	C	225	NIO	C3-C2	4.73	1.49	1.39
3	D	223	NIO	C3-C2	4.79	1.49	1.39
3	A	221	NIO	C3-C2	4.80	1.49	1.39
3	B	219	NIO	C3-C2	4.83	1.49	1.39
2	B	220	FMN	C9A-C5A	4.84	1.52	1.42
2	D	224	FMN	C9A-C5A	5.06	1.53	1.42
2	A	218	FMN	C4A-C10	5.09	1.50	1.40
2	D	224	FMN	C4A-C10	5.24	1.50	1.40
2	C	222	FMN	C9A-C5A	5.30	1.53	1.42
2	A	218	FMN	C9A-C5A	5.30	1.53	1.42
2	C	222	FMN	C4A-C10	5.48	1.51	1.40
2	B	220	FMN	C4A-C10	5.51	1.51	1.40
2	A	218	FMN	C10-N10	5.79	1.45	1.39
2	D	224	FMN	C10-N10	5.98	1.46	1.39
2	B	220	FMN	C10-N10	6.03	1.46	1.39
2	C	222	FMN	C10-N10	6.41	1.46	1.39
2	A	218	FMN	C1'-N10	7.11	1.56	1.48
2	B	220	FMN	C1'-N10	7.29	1.56	1.48
2	D	224	FMN	C1'-N10	7.54	1.56	1.48
2	C	222	FMN	C1'-N10	7.56	1.56	1.48

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	218	FMN	C4A-C10-N10	-12.45	111.48	120.52
2	B	220	FMN	C4A-C10-N10	-12.41	111.50	120.52
2	D	224	FMN	C4A-C10-N10	-10.08	113.20	120.52
2	C	222	FMN	N3-C2-N1	-7.83	114.51	127.69
2	B	220	FMN	C4-C4A-C10	-7.71	115.00	119.94
2	A	218	FMN	N3-C2-N1	-7.67	114.77	127.69
2	B	220	FMN	N3-C2-N1	-7.65	114.80	127.69
2	D	224	FMN	N3-C2-N1	-7.51	115.04	127.69
2	D	224	FMN	C5A-C9A-N10	-7.37	112.05	117.58
2	A	218	FMN	C9A-C5A-N5	-7.15	110.54	122.18
2	B	220	FMN	C9A-C5A-N5	-7.04	110.72	122.18
2	D	224	FMN	C4-C4A-C10	-6.97	115.48	119.94
2	C	222	FMN	C9A-C5A-N5	-6.85	111.02	122.18
2	C	222	FMN	C4A-C10-N10	-6.76	115.61	120.52
2	C	222	FMN	C4-C4A-C10	-6.76	115.61	119.94
2	A	218	FMN	O4'-C4'-C5'	-6.36	96.22	110.09
2	B	220	FMN	C5A-C9A-N10	-5.99	113.09	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	218	FMN	C5A-C9A-N10	-4.99	113.83	117.58
2	C	222	FMN	O4'-C4'-C5'	-4.95	99.30	110.09
2	D	224	FMN	C9A-C5A-N5	-4.86	114.27	122.18
2	C	222	FMN	C1'-C2'-C3'	-4.55	96.82	109.82
2	C	222	FMN	C5A-C9A-N10	-4.48	114.22	117.58
2	D	224	FMN	C4A-C4-N3	-4.26	117.95	123.52
2	B	220	FMN	C4A-C4-N3	-4.16	118.08	123.52
2	A	218	FMN	O3'-C3'-C4'	-4.05	98.22	108.73
2	D	224	FMN	O3P-P-O1P	-3.89	97.93	110.63
2	C	222	FMN	C4A-C4-N3	-3.85	118.49	123.52
2	A	218	FMN	C4A-C4-N3	-3.81	118.54	123.52
2	A	218	FMN	C4-C4A-C10	-3.69	117.58	119.94
2	D	224	FMN	O5'-P-O1P	-3.62	97.99	107.08
2	C	222	FMN	O3'-C3'-C4'	-2.97	101.03	108.73
2	D	224	FMN	C1'-C2'-C3'	-2.69	102.13	109.82
2	A	218	FMN	C1'-C2'-C3'	-2.62	102.31	109.82
2	D	224	FMN	C9-C9A-C5A	-2.60	114.97	119.65
2	D	224	FMN	O4'-C4'-C5'	-2.18	105.34	110.09
2	A	218	FMN	O3P-P-O5'	2.01	112.58	106.72
2	C	222	FMN	O3P-P-O1P	2.03	117.24	110.63
2	A	218	FMN	C8M-C8-C7	2.11	125.27	120.73
2	C	222	FMN	C8M-C8-C7	2.13	125.32	120.73
2	D	224	FMN	C8M-C8-C7	2.19	125.44	120.73
2	B	220	FMN	C8M-C8-C7	2.22	125.50	120.73
2	B	220	FMN	O3'-C3'-C2'	2.45	115.08	108.73
2	C	222	FMN	O2P-P-O5'	2.72	114.65	106.72
2	D	224	FMN	O2'-C2'-C3'	2.92	116.47	108.96
2	A	218	FMN	O2'-C2'-C3'	3.02	116.72	108.96
3	D	223	NIO	C5-N-C1	3.05	122.43	116.82
3	A	221	NIO	C5-N-C1	3.07	122.46	116.82
2	C	222	FMN	O3'-C3'-C2'	3.13	116.85	108.73
3	B	219	NIO	C5-N-C1	3.14	122.58	116.82
3	C	225	NIO	C5-N-C1	3.15	122.61	116.82
2	B	220	FMN	O2P-P-O5'	3.20	116.07	106.72
2	C	222	FMN	O2'-C2'-C3'	3.61	118.25	108.96
2	D	224	FMN	O3P-P-O2P	3.70	121.02	107.44
2	D	224	FMN	C6-C5A-N5	3.87	123.73	118.92
2	C	222	FMN	O4'-C4'-C3'	4.17	119.68	108.96
2	D	224	FMN	O3'-C3'-C2'	4.35	120.01	108.73
2	B	220	FMN	O2'-C2'-C3'	4.37	120.21	108.96
2	D	224	FMN	O2P-P-O1P	4.43	125.09	110.63
2	A	218	FMN	O3'-C3'-C2'	5.18	122.17	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	224	FMN	O2'-C2'-C1'	6.29	125.47	109.93
2	A	218	FMN	C4-C4A-N5	6.93	127.12	118.70
2	A	218	FMN	O2'-C2'-C1'	7.32	128.02	109.93
2	B	220	FMN	C6-C5A-N5	7.92	128.78	118.92
2	D	224	FMN	C4-C4A-N5	9.01	129.65	118.70
2	C	222	FMN	C6-C5A-N5	9.07	130.22	118.92
2	A	218	FMN	C6-C5A-N5	9.49	130.75	118.92
2	A	218	FMN	C4-N3-C2	10.19	123.66	115.16
2	B	220	FMN	C4-C4A-N5	10.30	131.22	118.70
2	C	222	FMN	C4-C4A-N5	10.91	131.97	118.70
2	C	222	FMN	C4-N3-C2	11.69	124.91	115.16
2	D	224	FMN	C4-N3-C2	12.21	125.34	115.16
2	B	220	FMN	C4-N3-C2	12.72	125.77	115.16
2	D	224	FMN	C4A-N5-C5A	15.43	134.91	116.72
2	C	222	FMN	C4A-N5-C5A	15.66	135.17	116.72
2	A	218	FMN	C4A-N5-C5A	16.88	136.61	116.72
2	B	220	FMN	C4A-N5-C5A	18.30	138.29	116.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	218	FMN	1	0
2	B	220	FMN	1	0
2	C	222	FMN	2	0
2	D	224	FMN	2	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.