Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 07:18 PM GMT

PDB ID	:	1F0X
Title	:	CRYSTAL STRUCTURE OF D-LACTATE DEHYDROGENASE, A PERIPHERAL MEMBRANE RESPIRATORY ENZYME.
Authors	:	Dym, O.; Pratt, E.A.; Ho, C.; Eisenberg, D.
Deposited on	:	2000-05-17
Resolution	:	1.90 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:

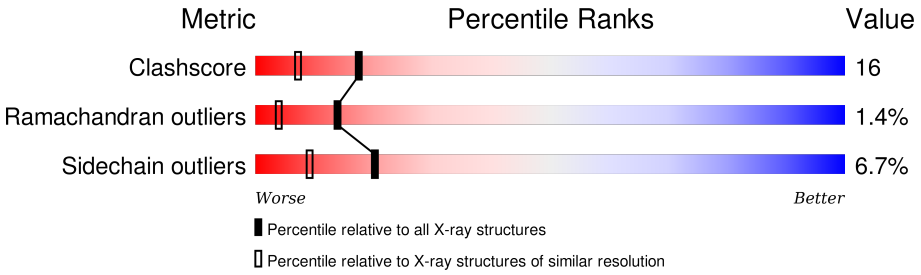
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 >=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	571	63% 21% • • 12%
1	B	571	63% 21% • • 12%

2 Entry composition

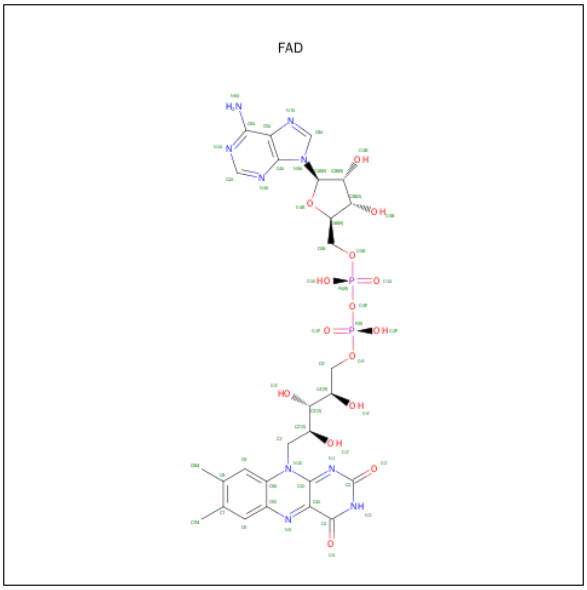
There are 3 unique types of molecules in this entry. The entry contains 8393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			3983	2515	706	748	14			
1	B	502	Total	C	N	O	S	0	0	0
			3983	2515	706	748	14			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	179	Total O 179 179	0	0
3	B	142	Total O 142 142	0	0

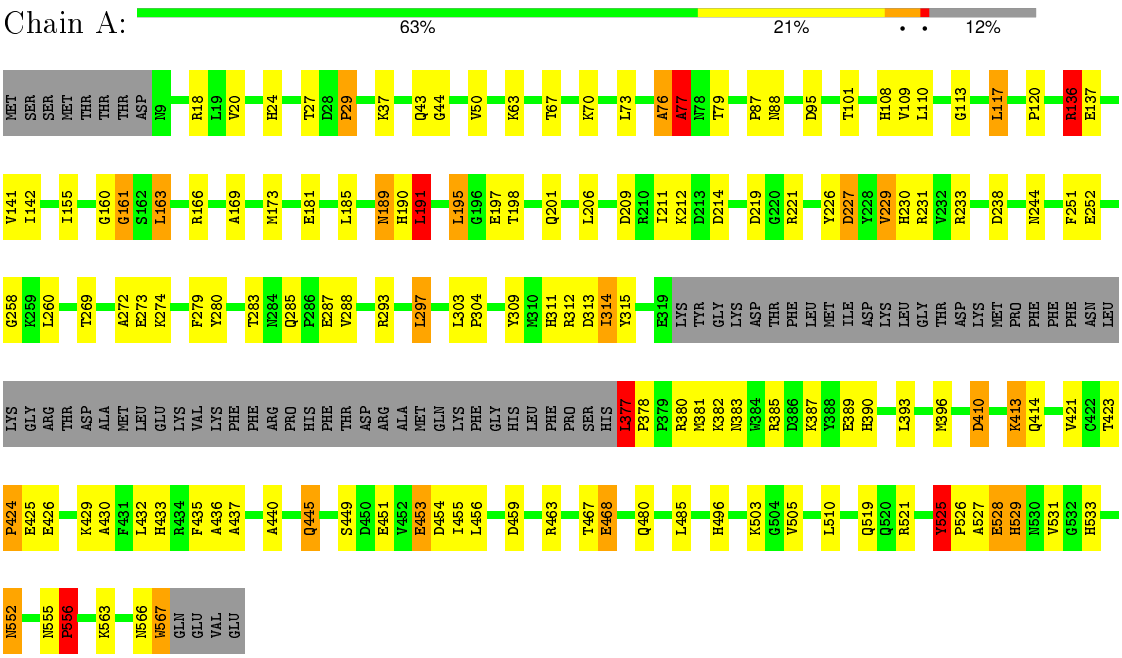
3 Residue-property plots (i)

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.

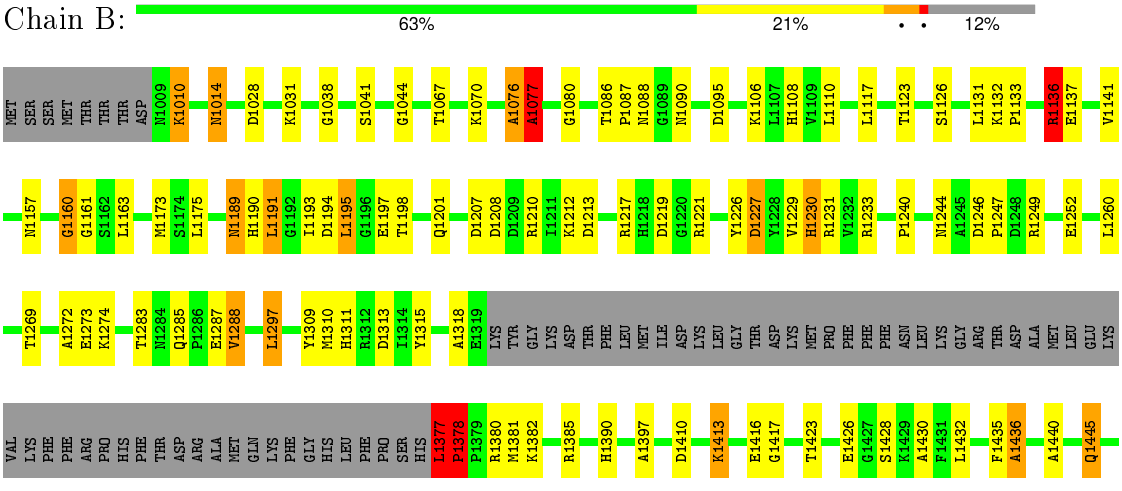
- Molecule 1: D-LACTATE DEHYDROGENASE

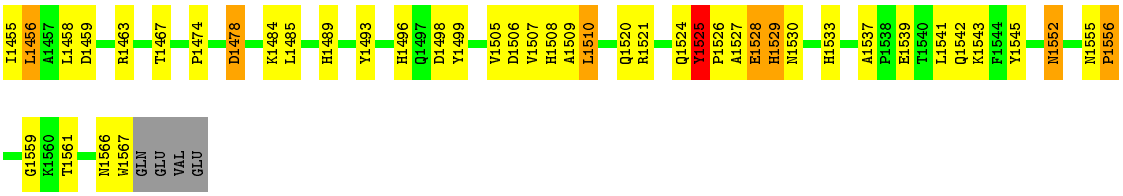
Chain A:



- Molecule 1: D-LACTATE DEHYDROGENASE

Chain B:




I1455
L1456
A1457
L1458
D1459
R1463
T1467
P1474
D1478
K1484
L1485
H1489
Y1493
H1496
Q1497
D1498
Y1499
V1505
D1506
V1507
H1508
A1509
L1510
Q1520
R1521
Q1524
Y1525
P1526
A1527
E1528
H1529
N1530
H1533
A1537
P1538
E1539
T1540
L1541
Q1542
K1543
F1544
Y1545
N1552
N1555
P1556
G1559
K1560
T1561
N1566
W1567
GLN
GLU
VAL
GLU

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	69.01Å 74.19Å 102.00Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	18.00 – 1.90	Depositor
% Data completeness (in resolution range)	96.5 (18.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8393	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: FAD

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	0.91	5/4072 (0.1%)	1.05	20/5511 (0.4%)
1	B	0.95	8/4072 (0.2%)	1.03	20/5511 (0.4%)
All	All	0.93	13/8144 (0.2%)	1.04	40/11022 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1528	GLU	CD-OE1	23.52	1.51	1.25
1	A	528	GLU	CD-OE1	17.23	1.44	1.25
1	B	1528	GLU	CB-CG	11.16	1.73	1.52
1	A	528	GLU	CB-CG	10.24	1.71	1.52
1	A	77	ALA	N-CA	7.53	1.61	1.46
1	B	1528	GLU	CD-OE2	7.09	1.33	1.25
1	B	1528	GLU	CG-CD	6.57	1.61	1.51
1	B	1288	VAL	CB-CG1	-6.02	1.40	1.52
1	A	173	MET	SD-CE	-5.72	1.45	1.77
1	B	1077	ALA	N-CA	5.59	1.57	1.46
1	B	1173	MET	SD-CE	-5.38	1.47	1.77
1	B	1528	GLU	CA-CB	5.36	1.65	1.53
1	A	528	GLU	CG-CD	5.03	1.59	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	377	LEU	C-N-CD	-18.31	80.32	120.60
1	B	1377	LEU	C-N-CD	-11.09	96.19	120.60
1	A	377	LEU	C-N-CA	10.30	165.25	122.00
1	A	525	TYR	C-N-CD	10.14	149.70	128.40
1	B	1528	GLU	CG-CD-OE2	-9.75	98.80	118.30
1	A	525	TYR	C-N-CA	-8.24	87.39	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1528	GLU	CG-CD-OE1	8.17	134.65	118.30
1	B	1463	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	528	GLU	CG-CD-OE2	-8.09	102.12	118.30
1	B	1521	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	529	HIS	C-N-CA	-7.55	102.83	121.70
1	A	521	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	1556	PRO	N-CA-C	7.07	130.48	112.10
1	A	76	ALA	C-N-CA	-6.96	104.30	121.70
1	A	136	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	1525	TYR	C-N-CA	-6.88	93.11	122.00
1	A	525	TYR	N-CA-C	6.82	129.41	111.00
1	B	1136	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	1525	TYR	C-N-CD	6.65	142.37	128.40
1	B	1521	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	251	PHE	C-N-CA	-6.64	105.10	121.70
1	A	528	GLU	CG-CD-OE1	6.51	131.31	118.30
1	A	556	PRO	N-CA-C	6.40	128.75	112.10
1	A	160	GLY	C-N-CA	-6.28	109.11	122.30
1	B	1160	GLY	C-N-CA	-6.27	109.12	122.30
1	A	191	LEU	CA-CB-CG	6.23	129.62	115.30
1	B	1528	GLU	CA-CB-CG	6.22	127.09	113.40
1	B	1525	TYR	N-CA-C	6.21	127.77	111.00
1	A	166	ARG	C-N-CA	-6.06	109.57	122.30
1	B	1529	HIS	N-CA-C	-6.01	94.78	111.00
1	B	1377	LEU	C-N-CA	6.00	147.18	122.00
1	B	1529	HIS	C-N-CA	-5.96	106.79	121.70
1	A	76	ALA	O-C-N	-5.93	113.20	122.70
1	B	1076	ALA	C-N-CA	-5.88	106.99	121.70
1	A	136	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	1463	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	529	HIS	O-C-N	-5.30	114.22	122.70
1	A	77	ALA	N-CA-CB	5.21	117.40	110.10
1	B	1416	GLU	N-CA-C	5.12	124.82	111.00
1	B	1378	PRO	CA-N-CD	-5.04	104.44	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3983	0	3900	130	2
1	B	3983	0	3900	120	2
2	A	53	0	31	6	0
2	B	53	0	31	6	0
3	A	179	0	0	4	0
3	B	142	0	0	8	0
All	All	8393	0	7862	255	2

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 16.

All (255) 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:1285:GLN:O	1:B:1288:VAL:HG12	1.52	1.09
1:B:1076:ALA:O	1:B:1077:ALA:HB3	1.47	1.09
1:A:212:LYS:HD2	1:B:1520:GLN:HE22	1.17	1.08
1:A:76:ALA:O	1:A:77:ALA:HB3	1.41	1.08
1:A:285:GLN:O	1:A:288:VAL:HG12	1.55	1.07
1:A:76:ALA:O	1:A:77:ALA:CB	1.93	1.02
1:A:212:LYS:HD2	1:B:1520:GLN:NE2	1.73	1.00
1:B:1076:ALA:O	1:B:1077:ALA:CB	2.00	0.99
1:A:283:THR:OG1	1:A:288:VAL:HG11	1.68	0.93
1:A:525:TYR:O	1:A:526:PRO:C	1.98	0.90
1:B:1137:GLU:HG3	1:B:1272:ALA:HA	1.53	0.90
1:A:435:PHE:O	1:A:436:ALA:HB3	1.71	0.90
1:B:1459:ASP:O	1:B:1525:TYR:O	1.92	0.88
1:B:1525:TYR:O	1:B:1526:PRO:C	2.07	0.88
1:B:1283:THR:OG1	1:B:1288:VAL:HG11	1.73	0.87
1:B:1212:LYS:HA	1:B:1212:LYS:HE2	1.56	0.85
1:B:1283:THR:HG21	1:B:1288:VAL:HG13	1.57	0.84
1:B:1244:ASN:ND2	1:B:1529:HIS:O	2.11	0.83
1:A:410:ASP:O	1:A:413:LYS:HG2	1.80	0.81
1:B:1539:GLU:O	1:B:1543:LYS:HG2	1.80	0.80
1:B:1445:GLN:HB2	1:B:1455:ILE:HD11	1.61	0.80
1:B:1435:PHE:O	1:B:1436:ALA:CB	2.29	0.79
1:A:141:VAL:O	1:A:161:GLY:HA3	1.83	0.79
1:A:525:TYR:O	1:A:527:ALA:N	2.15	0.79
1:B:1283:THR:HG21	1:B:1288:VAL:CG1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:PHE:O	1:A:436:ALA:CB	2.29	0.77
1:B:1525:TYR:O	1:B:1527:ALA:N	2.18	0.76
1:B:1285:GLN:O	1:B:1288:VAL:CG1	2.33	0.76
1:A:285:GLN:O	1:A:288:VAL:CG1	2.34	0.75
1:B:1231:ARG:NH1	1:B:1231:ARG:HB3	2.01	0.75
1:B:1496:HIS:NE2	1:B:1528:GLU:OE1	2.20	0.74
2:B:1600:FAD:H8A	2:B:1600:FAD:H51A	1.68	0.74
1:A:459:ASP:O	1:A:525:TYR:O	2.06	0.73
1:A:381:MET:HE2	1:A:430:ALA:HB2	1.68	0.72
1:B:1432:LEU:O	1:B:1435:PHE:O	2.07	0.72
1:B:1189:ASN:HD21	1:B:1191:LEU:HB2	1.55	0.72
1:B:1132:LYS:HB3	1:B:1133:PRO:HD3	1.72	0.71
1:A:381:MET:CE	1:A:430:ALA:HB2	2.19	0.71
1:A:244:ASN:ND2	1:A:529:HIS:O	2.23	0.71
1:A:283:THR:HG21	1:A:288:VAL:HG13	1.73	0.70
1:B:1435:PHE:O	1:B:1436:ALA:HB2	1.91	0.70
1:A:37:LYS:HB2	1:A:43:GLN:NE2	2.06	0.70
1:A:195:LEU:HD11	1:A:211:ILE:HD11	1.75	0.69
1:A:189:ASN:HD21	1:A:191:LEU:HB2	1.57	0.69
1:A:136:ARG:HD3	1:A:269:THR:OG1	1.93	0.68
1:B:1231:ARG:HH11	1:B:1231:ARG:CB	2.07	0.67
1:A:423:THR:HG22	1:A:425:GLU:OE1	1.94	0.67
1:A:377:LEU:HA	1:A:382:LYS:HE2	1.76	0.67
1:A:273:GLU:HA	1:A:273:GLU:OE1	1.95	0.67
1:B:1231:ARG:HB3	1:B:1231:ARG:HH11	1.58	0.66
1:B:1137:GLU:CG	1:B:1272:ALA:HA	2.25	0.66
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.77	0.66
1:B:1309:TYR:OH	1:B:1390:HIS:HD2	1.78	0.66
1:B:1456:LEU:HD12	1:B:1510:LEU:HD13	1.78	0.66
1:A:425:GLU:HB3	1:A:429:LYS:NZ	2.11	0.65
1:A:190:HIS:HD2	1:A:252:GLU:OE1	1.80	0.65
1:B:1227:ASP:HB2	1:B:1230:HIS:ND1	2.12	0.65
1:B:1197:GLU:H	1:B:1201:GLN:NE2	1.95	0.64
1:B:1526:PRO:HD2	3:B:2014:HOH:O	1.96	0.63
1:B:1283:THR:CB	1:B:1288:VAL:HG11	2.28	0.63
1:B:1377:LEU:HA	1:B:1382:LYS:HE3	1.80	0.63
1:B:1273:GLU:OE1	1:B:1273:GLU:HA	1.99	0.62
1:A:260:LEU:O	2:A:600:FAD:H2A	1.98	0.62
1:A:231:ARG:NH1	3:A:2175:HOH:O	2.33	0.62
1:A:377:LEU:HA	1:A:382:LYS:CE	2.30	0.62
1:B:1260:LEU:O	2:B:1600:FAD:H2A	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:O	1:A:314:ILE:HD13	2.00	0.61
1:A:206:LEU:HD21	1:A:211:ILE:HD11	1.81	0.61
1:A:496:HIS:NE2	1:A:528:GLU:OE1	2.34	0.61
1:A:383:ASN:HD21	1:A:387:LYS:NZ	1.99	0.61
1:B:1080:GLY:HA2	2:B:1600:FAD:O3'	2.01	0.61
1:A:390:HIS:HE1	3:A:2229:HOH:O	1.83	0.61
1:A:197:GLU:H	1:A:201:GLN:NE2	1.99	0.61
1:A:110:LEU:HD11	1:A:117:LEU:HD13	1.83	0.60
1:A:380:ARG:HD3	1:A:426:GLU:OE2	2.00	0.60
1:B:1287:GLU:H	1:B:1287:GLU:CD	2.05	0.59
1:B:1090:ASN:HB3	3:B:2272:HOH:O	2.03	0.59
1:B:1381:MET:HE2	1:B:1430:ALA:HB2	1.83	0.59
1:A:304:PRO:HB3	1:A:396:MET:SD	2.42	0.59
1:B:1489:HIS:NE2	1:B:1528:GLU:OE1	2.23	0.58
1:A:552:ASN:HB2	1:A:567:TRP:H	1.68	0.58
1:B:1189:ASN:ND2	1:B:1191:LEU:HB2	2.18	0.58
1:B:1377:LEU:O	1:B:1377:LEU:CG	2.52	0.58
1:B:1377:LEU:HG	1:B:1377:LEU:O	2.03	0.58
1:A:230:HIS:N	1:A:230:HIS:CD2	2.69	0.57
1:A:189:ASN:ND2	1:A:191:LEU:HB2	2.18	0.57
1:B:1088:ASN:HB2	1:B:1533:HIS:CD2	2.40	0.57
1:A:227:ASP:HB2	1:A:230:HIS:ND1	2.20	0.57
1:A:467:THR:HG23	1:A:468:GLU:HG2	1.86	0.56
1:A:280:TYR:CE1	1:A:393:LEU:HD21	2.41	0.56
1:A:195:LEU:HD11	1:A:211:ILE:CD1	2.35	0.56
1:A:108:HIS:HD2	1:A:209:ASP:OD1	1.89	0.55
1:B:1382:LYS:HG2	3:B:2223:HOH:O	2.05	0.55
1:B:1456:LEU:CD1	1:B:1510:LEU:HD13	2.35	0.55
1:A:311:HIS:O	1:A:314:ILE:HG22	2.06	0.55
1:B:1381:MET:CE	1:B:1430:ALA:HB2	2.36	0.55
1:A:425:GLU:HB3	1:A:429:LYS:HZ2	1.70	0.55
1:A:198:THR:H	1:A:201:GLN:HE21	1.55	0.55
1:A:312:ARG:O	1:A:315:TYR:HB3	2.06	0.55
1:A:519:GLN:NE2	1:A:525:TYR:OH	2.39	0.55
1:A:526:PRO:HG2	1:A:531:VAL:HG12	1.89	0.55
2:A:600:FAD:O2'	2:A:600:FAD:N1	2.39	0.54
1:A:155:ILE:HD13	1:A:169:ALA:HB1	1.89	0.54
1:B:1230:HIS:N	1:B:1230:HIS:CD2	2.75	0.54
1:B:1528:GLU:HG3	1:B:1529:HIS:CD2	2.43	0.54
1:B:1555:ASN:N	1:B:1556:PRO:HD3	2.23	0.54
1:B:1496:HIS:HE1	1:B:1528:GLU:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LYS:O	1:A:67:THR:HG23	2.08	0.54
1:B:1552:ASN:HB2	1:B:1567:TRP:H	1.72	0.54
1:A:555:ASN:N	1:A:556:PRO:HD3	2.22	0.53
1:A:189:ASN:ND2	1:A:191:LEU:H	2.06	0.53
1:B:1227:ASP:HB2	1:B:1230:HIS:CE1	2.43	0.53
1:B:1157:ASN:HD22	1:B:1530:ASN:HD22	1.54	0.53
1:A:141:VAL:HB	1:A:163:LEU:HD13	1.91	0.53
1:A:108:HIS:HE1	3:A:2127:HOH:O	1.90	0.53
1:B:1106:LYS:HE3	1:B:1207:ASP:O	2.08	0.53
1:A:227:ASP:HA	1:A:229:VAL:HG23	1.91	0.53
1:B:1070:LYS:HD2	1:B:1095:ASP:HB2	1.92	0.53
1:B:1566:ASN:C	1:B:1567:TRP:CD1	2.83	0.52
1:A:206:LEU:CD2	1:A:211:ILE:HD11	2.40	0.52
1:B:1423:THR:HG22	1:B:1426:GLU:CG	2.40	0.52
1:A:137:GLU:HG3	1:A:272:ALA:HA	1.91	0.52
1:A:437:ALA:O	1:A:440:ALA:HB3	2.10	0.52
1:B:1189:ASN:ND2	1:B:1191:LEU:H	2.07	0.52
1:B:1208:ASP:HB2	1:B:1210:ARG:HD3	1.91	0.51
1:A:377:LEU:O	1:A:377:LEU:HG	2.09	0.51
1:A:309:TYR:OH	1:A:390:HIS:HD2	1.93	0.51
1:B:1377:LEU:O	1:B:1377:LEU:HD23	2.10	0.51
1:A:385:ARG:C	1:A:385:ARG:HD3	2.31	0.51
1:A:88:ASN:O	1:A:563:LYS:NZ	2.44	0.51
1:A:413:LYS:NZ	1:A:413:LYS:HB3	2.26	0.50
1:A:566:ASN:C	1:A:567:TRP:CD1	2.85	0.50
1:B:1283:THR:CG2	1:B:1288:VAL:CG1	2.89	0.50
1:A:283:THR:HG21	1:A:288:VAL:CG1	2.39	0.50
1:A:101:THR:HB	1:A:120:PRO:HB2	1.94	0.50
1:A:383:ASN:HD21	1:A:387:LYS:HZ1	1.60	0.50
1:A:445:GLN:NE2	1:A:445:GLN:C	2.65	0.50
1:B:1311:HIS:CD2	1:B:1313:ASP:H	2.30	0.50
1:B:1190:HIS:HD2	1:B:1252:GLU:OE1	1.94	0.50
1:A:413:LYS:NZ	1:A:413:LYS:CB	2.74	0.49
1:A:109:VAL:HG13	1:A:113:GLY:HA2	1.95	0.49
1:A:287:GLU:H	1:A:287:GLU:CD	2.16	0.49
2:B:1600:FAD:C8A	2:B:1600:FAD:H51A	2.41	0.49
1:B:1123:THR:OG1	1:B:1126:SER:HB2	2.12	0.49
1:B:1233:ARG:HA	1:B:1297:LEU:HG	1.94	0.49
1:A:445:GLN:HB2	1:A:455:ILE:HD11	1.95	0.49
1:A:453:GLU:OE2	1:A:503:LYS:HD2	2.13	0.49
1:B:1542:GLN:HG2	1:B:1561:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1385:ARG:C	1:B:1385:ARG:HD3	2.34	0.48
1:B:1410:ASP:O	1:B:1413:LYS:HG2	2.13	0.48
1:B:1194:ASP:OD2	1:B:1217:ARG:NH2	2.46	0.48
1:B:1175:LEU:HB2	1:B:1191:LEU:HD22	1.95	0.48
1:A:198:THR:H	1:A:201:GLN:NE2	2.11	0.48
1:B:1189:ASN:C	1:B:1189:ASN:HD22	2.17	0.48
1:A:181:GLU:CD	1:A:181:GLU:H	2.17	0.48
1:A:79:THR:C	2:A:600:FAD:O3'	2.52	0.48
1:B:1423:THR:HG23	1:B:1426:GLU:H	1.78	0.48
1:A:142:ILE:HG22	1:A:161:GLY:CA	2.43	0.47
1:A:219:ASP:OD1	1:A:221:ARG:HD3	2.14	0.47
1:A:381:MET:HE1	1:A:430:ALA:HB2	1.96	0.47
1:B:1230:HIS:H	1:B:1230:HIS:CD2	2.32	0.47
1:A:380:ARG:CD	1:A:426:GLU:OE2	2.63	0.47
1:B:1141:VAL:O	1:B:1161:GLY:HA3	2.15	0.47
1:A:226:TYR:O	1:A:227:ASP:OD1	2.33	0.47
1:A:311:HIS:CD2	1:A:313:ASP:H	2.33	0.47
1:A:279:PHE:CE2	1:A:421:VAL:HG22	2.50	0.47
1:B:1137:GLU:HG3	1:B:1272:ALA:CA	2.36	0.47
1:A:381:MET:HE1	1:A:430:ALA:N	2.30	0.47
1:A:20:VAL:O	1:A:24:HIS:HD2	1.98	0.47
1:B:1108:HIS:CE1	1:B:1110:LEU:HD23	2.50	0.46
1:B:1014:ASN:HD22	1:B:1014:ASN:HA	1.58	0.46
1:B:1131:LEU:HB3	1:B:1136:ARG:HB2	1.97	0.46
1:B:1380:ARG:HD3	1:B:1426:GLU:OE2	2.16	0.46
1:B:1311:HIS:HD2	1:B:1313:ASP:H	1.63	0.45
2:B:1600:FAD:N1	2:B:1600:FAD:O2'	2.42	0.45
1:A:528:GLU:HG3	1:A:529:HIS:CD2	2.51	0.45
1:A:233:ARG:CZ	1:A:303:LEU:HD21	2.47	0.45
1:B:1210:ARG:NH2	3:B:2276:HOH:O	2.41	0.45
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.78	0.45
1:A:293:ARG:HG3	1:A:297:LEU:HD22	1.98	0.45
1:A:311:HIS:CE1	1:A:389:GLU:CG	3.00	0.45
1:B:1157:ASN:ND2	1:B:1530:ASN:HD22	2.14	0.45
1:B:1382:LYS:CG	3:B:2223:HOH:O	2.64	0.45
1:B:1273:GLU:HB3	1:B:1397:ALA:HB1	1.99	0.44
1:A:480:GLN:NE2	1:A:505:VAL:HG13	2.31	0.44
1:A:526:PRO:HD2	3:A:2043:HOH:O	2.18	0.44
2:B:1600:FAD:C5B	2:B:1600:FAD:H8A	2.42	0.44
1:A:70:LYS:HD2	1:A:95:ASP:HB2	1.99	0.44
1:A:142:ILE:HG22	1:A:161:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1189:ASN:ND2	1:B:1189:ASN:C	2.69	0.44
1:A:526:PRO:HG2	1:A:531:VAL:CG1	2.47	0.44
1:A:233:ARG:NH2	1:A:303:LEU:HG	2.33	0.44
1:B:1311:HIS:CD2	3:B:2108:HOH:O	2.71	0.44
1:B:1318:ALA:HA	1:B:1440:ALA:CB	2.48	0.44
1:B:1136:ARG:HD3	1:B:1269:THR:OG1	2.18	0.44
1:A:315:TYR:CD1	1:A:433:HIS:HE1	2.36	0.43
1:A:283:THR:CB	1:A:288:VAL:HG11	2.46	0.43
1:B:1226:TYR:O	1:B:1227:ASP:OD1	2.36	0.43
1:B:1160:GLY:O	1:B:1528:GLU:OE2	2.35	0.43
1:A:314:ILE:HG12	1:A:485:LEU:HB3	2.00	0.43
1:B:1315:TYR:C	1:B:1315:TYR:CD2	2.92	0.43
1:A:44:GLY:HA3	1:A:87:PRO:HB2	2.00	0.43
1:B:1505:VAL:HG12	1:B:1506:ASP:N	2.34	0.43
1:A:238:ASP:O	1:A:463:ARG:HG2	2.19	0.43
1:B:1537:ALA:HB2	1:B:1559:GLY:HA3	2.00	0.43
1:B:1219:ASP:OD1	1:B:1221:ARG:CD	2.66	0.43
1:B:1028:ASP:O	1:B:1031:LYS:N	2.52	0.43
1:A:258:GLY:HA2	2:A:600:FAD:N3A	2.34	0.43
1:B:1038:GLY:HA3	1:B:1041:SER:O	2.18	0.43
1:B:1197:GLU:H	1:B:1201:GLN:HE21	1.63	0.43
1:B:1377:LEU:O	1:B:1377:LEU:CD2	2.66	0.43
1:B:1478:ASP:OD1	1:B:1484:LYS:NZ	2.49	0.42
1:B:1458:LEU:HD12	1:B:1499:TYR:HE1	1.83	0.42
1:B:1198:THR:H	1:B:1201:GLN:HE21	1.66	0.42
1:A:445:GLN:HE21	1:A:445:GLN:C	2.23	0.42
1:B:1485:LEU:HB2	1:B:1498:ASP:HB2	2.02	0.42
1:B:1231:ARG:NH1	1:B:1231:ARG:CB	2.71	0.42
1:A:480:GLN:HE21	1:A:505:VAL:HG13	1.83	0.42
1:A:445:GLN:HG3	1:A:455:ILE:HG12	2.02	0.42
1:A:423:THR:HG21	1:A:425:GLU:OE2	2.20	0.42
1:B:1194:ASP:OD2	1:B:1217:ARG:NE	2.52	0.42
1:A:381:MET:HE1	1:A:426:GLU:O	2.20	0.42
1:B:1478:ASP:OD2	1:B:1484:LYS:NZ	2.53	0.42
1:B:1541:LEU:HD22	1:B:1545:TYR:CZ	2.55	0.42
1:A:206:LEU:CD2	1:A:211:ILE:CD1	2.98	0.41
1:A:377:LEU:CG	1:A:377:LEU:O	2.68	0.41
1:A:63:LYS:HG3	1:A:185:LEU:HD23	2.02	0.41
1:B:1423:THR:HG22	1:B:1426:GLU:HG3	2.02	0.41
1:B:1067:THR:HG23	3:B:2217:HOH:O	2.20	0.41
1:A:496:HIS:CE1	1:A:528:GLU:OE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:THR:CG2	1:A:424:PRO:HD2	2.51	0.41
1:A:88:ASN:HB2	1:A:533:HIS:CD2	2.55	0.41
1:B:1246:ASP:HA	1:B:1247:PRO:HD2	1.90	0.41
1:A:20:VAL:HG21	1:A:50:VAL:HG23	2.03	0.41
1:A:227:ASP:HB2	1:A:230:HIS:CE1	2.55	0.41
1:A:212:LYS:HA	1:A:212:LYS:HD3	1.73	0.41
2:A:600:FAD:C8A	2:A:600:FAD:H51A	2.49	0.41
1:B:1288:VAL:H	1:B:1288:VAL:HG12	1.65	0.41
1:A:189:ASN:HD22	1:A:191:LEU:H	1.69	0.41
1:B:1106:LYS:HE2	3:B:2252:HOH:O	2.21	0.41
1:A:27:THR:O	1:A:29:PRO:HD3	2.21	0.41
1:A:314:ILE:HA	1:A:485:LEU:HD22	2.03	0.41
1:A:552:ASN:HD22	1:A:552:ASN:HA	1.70	0.41
1:A:108:HIS:CD2	1:A:209:ASP:OD1	2.70	0.41
1:B:1507:VAL:O	1:B:1508:HIS:C	2.57	0.41
1:B:1193:ILE:HG22	1:B:1195:LEU:HD13	2.03	0.41
1:B:1086:THR:HB	1:B:1087:PRO:CD	2.51	0.41
1:A:425:GLU:H	1:A:425:GLU:CD	2.25	0.40
1:B:1240:PRO:HG2	1:B:1524:GLN:HB2	2.02	0.40
1:A:413:LYS:HZ3	1:A:413:LYS:HB3	1.86	0.40
1:A:113:GLY:O	1:A:136:ARG:HD2	2.22	0.40
1:B:1423:THR:CG2	1:B:1426:GLU:H	2.34	0.40
1:B:1044:GLY:HA3	1:B:1087:PRO:HB2	2.02	0.40
1:A:311:HIS:HD2	1:A:313:ASP:H	1.69	0.40
1:B:1506:ASP:OD2	1:B:1509:ALA:HB2	2.21	0.40

All (2) 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)
1:A:238:ASP:OD1	1:B:1010:LYS:NZ[1_445]	2.01	0.19
1:A:238:ASP:N	1:B:1010:LYS:NZ[1_445]	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	498/571 (87%)	474 (95%)	16 (3%)	8 (2%)	12 3
1	B	498/571 (87%)	474 (95%)	18 (4%)	6 (1%)	16 5
All	All	996/1142 (87%)	948 (95%)	34 (3%)	14 (1%)	14 4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	A	378	PRO
1	B	1274	LYS
1	B	1378	PRO
1	A	77	ALA
1	A	161	GLY
1	B	1417	GLY
1	B	1436	ALA
1	B	1077	ALA
1	A	451	GLU
1	A	525	TYR
1	B	1525	TYR
1	A	453	GLU
1	A	556	PRO

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	421/484 (87%)	393 (93%)	28 (7%)	20 9
1	B	421/484 (87%)	393 (93%)	28 (7%)	20 9
All	All	842/968 (87%)	786 (93%)	56 (7%)	20 9

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	29	PRO
1	A	73	LEU
1	A	117	LEU
1	A	136	ARG
1	A	163	LEU
1	A	189	ASN
1	A	191	LEU
1	A	195	LEU
1	A	214	ASP
1	A	227	ASP
1	A	229	VAL
1	A	297	LEU
1	A	314	ILE
1	A	377	LEU
1	A	410	ASP
1	A	413	LYS
1	A	414	GLN
1	A	424	PRO
1	A	445	GLN
1	A	449	SER
1	A	454	ASP
1	A	456	LEU
1	A	468	GLU
1	A	510	LEU
1	A	525	TYR
1	A	552	ASN
1	A	567	TRP
1	B	1010	LYS
1	B	1014	ASN
1	B	1117	LEU
1	B	1136	ARG
1	B	1163	LEU
1	B	1189	ASN
1	B	1191	LEU
1	B	1195	LEU
1	B	1213	ASP
1	B	1227	ASP
1	B	1229	VAL
1	B	1230	HIS
1	B	1249	ARG
1	B	1297	LEU
1	B	1310	MET

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Mol	Chain	Res	Type
1	B	1377	LEU
1	B	1378	PRO
1	B	1413	LYS
1	B	1428	SER
1	B	1445	GLN
1	B	1456	LEU
1	B	1467	THR
1	B	1474	PRO
1	B	1478	ASP
1	B	1493	TYR
1	B	1510	LEU
1	B	1525	TYR
1	B	1552	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	24	HIS
1	A	43	GLN
1	A	78	ASN
1	A	108	HIS
1	A	157	ASN
1	A	158	ASN
1	A	189	ASN
1	A	190	HIS
1	A	201	GLN
1	A	218	HIS
1	A	230	HIS
1	A	244	ASN
1	A	311	HIS
1	A	383	ASN
1	A	390	HIS
1	A	433	HIS
1	A	445	GLN
1	A	480	GLN
1	A	483	HIS
1	A	552	ASN
1	B	1014	ASN
1	B	1043	GLN
1	B	1078	ASN
1	B	1157	ASN

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Mol	Chain	Res	Type
1	B	1158	ASN
1	B	1189	ASN
1	B	1190	HIS
1	B	1201	GLN
1	B	1244	ASN
1	B	1311	HIS
1	B	1383	ASN
1	B	1390	HIS
1	B	1433	HIS
1	B	1445	GLN
1	B	1552	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	FAD	A	600	-	48,58,58	2.98	19 (39%)	54,89,89	2.24	11 (20%)
2	FAD	B	1600	-	48,58,58	3.16	23 (47%)	54,89,89	2.11	12 (22%)

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	FAD	A	600	-	-	0/30/50/50	0/6/6/6
2	FAD	B	1600	-	-	0/30/50/50	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1600	FAD	C5'-C4'	-11.29	1.34	1.51
2	A	600	FAD	C5'-C4'	-10.03	1.36	1.51
2	A	600	FAD	PA-O2A	-6.35	1.27	1.54
2	A	600	FAD	C2'-C3'	-5.83	1.41	1.53
2	B	1600	FAD	C10-N10	-5.43	1.32	1.39
2	B	1600	FAD	PA-O2A	-5.27	1.32	1.54
2	A	600	FAD	PA-O5B	-4.39	1.38	1.59
2	B	1600	FAD	PA-O5B	-4.04	1.40	1.59
2	A	600	FAD	O5B-C5B	-3.73	1.29	1.44
2	B	1600	FAD	C2'-C3'	-3.69	1.45	1.53
2	B	1600	FAD	O5B-C5B	-3.67	1.29	1.44
2	A	600	FAD	C10-N10	-2.83	1.35	1.39
2	B	1600	FAD	P-O2P	-2.76	1.43	1.54
2	A	600	FAD	C8A-N7A	-2.36	1.30	1.34
2	B	1600	FAD	P-O5'	-2.20	1.48	1.59
2	A	600	FAD	C9A-C5X	2.06	1.46	1.42
2	B	1600	FAD	C5B-C4B	2.09	1.58	1.51
2	B	1600	FAD	O4B-C4B	2.09	1.49	1.45
2	B	1600	FAD	C5A-C4A	2.11	1.45	1.40
2	A	600	FAD	C5B-C4B	2.12	1.58	1.51
2	A	600	FAD	C9-C8	2.15	1.43	1.37
2	B	1600	FAD	C6-C5X	2.19	1.45	1.41
2	B	1600	FAD	C4-C4X	2.55	1.46	1.41
2	A	600	FAD	C4-N3	2.58	1.37	1.33
2	A	600	FAD	C8-C7	2.69	1.48	1.41
2	B	1600	FAD	C8-C7	2.70	1.48	1.41
2	B	1600	FAD	C2A-N1A	2.82	1.39	1.33
2	A	600	FAD	C2A-N3A	2.94	1.37	1.32
2	B	1600	FAD	C4A-N3A	3.06	1.40	1.35
2	B	1600	FAD	C5X-N5	3.26	1.40	1.35
2	B	1600	FAD	C4X-C10	3.32	1.47	1.41
2	B	1600	FAD	O4'-C4'	3.58	1.51	1.43
2	A	600	FAD	C4X-C10	3.86	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C5X-N5	3.92	1.41	1.35
2	A	600	FAD	O4B-C4B	4.08	1.54	1.45
2	A	600	FAD	C4-C4X	4.13	1.49	1.41
2	B	1600	FAD	C4X-N5	4.36	1.40	1.33
2	B	1600	FAD	C4-N3	5.09	1.42	1.33
2	A	600	FAD	C9A-N10	5.20	1.46	1.38
2	B	1600	FAD	O4B-C1B	5.55	1.48	1.41
2	B	1600	FAD	C9A-N10	6.27	1.47	1.38
2	A	600	FAD	O4B-C1B	6.76	1.49	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	O5B-PA-O1A	-5.62	87.82	109.62
2	A	600	FAD	C4X-C4-N3	-5.24	116.42	123.59
2	B	1600	FAD	O5B-PA-O1A	-5.13	89.70	109.62
2	B	1600	FAD	C4X-C4-N3	-4.98	116.78	123.59
2	A	600	FAD	C4-C4X-C10	-4.89	116.81	119.94
2	B	1600	FAD	C4-C4X-C10	-4.41	117.12	119.94
2	A	600	FAD	O4B-C4B-C5B	-4.12	94.60	109.32
2	B	1600	FAD	O4B-C4B-C5B	-4.07	94.77	109.32
2	A	600	FAD	O3'-C3'-C2'	-3.32	100.38	108.75
2	A	600	FAD	C5X-C9A-N10	-3.01	115.33	117.62
2	B	1600	FAD	O3'-C3'-C2'	-3.00	101.20	108.75
2	B	1600	FAD	O4B-C4B-C3B	-2.88	99.34	105.15
2	A	600	FAD	O4B-C4B-C3B	-2.56	99.98	105.15
2	B	1600	FAD	C5X-C9A-N10	-2.33	115.84	117.62
2	B	1600	FAD	O4'-C4'-C5'	-2.08	105.66	110.19
2	B	1600	FAD	C2A-N1A-C6A	2.03	122.39	118.77
2	A	600	FAD	O2A-PA-O3P	2.05	114.37	105.09
2	A	600	FAD	C2A-N1A-C6A	2.06	122.44	118.77
2	B	1600	FAD	O2A-PA-O3P	2.19	115.02	105.09
2	A	600	FAD	C4-C4X-N5	2.20	121.38	118.72
2	B	1600	FAD	P-O3P-PA	2.22	138.97	132.73
2	B	1600	FAD	C4-N3-C2	8.35	122.47	115.25
2	A	600	FAD	C4-N3-C2	9.42	123.39	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	6	0
2	B	1600	FAD	6	0

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

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.