



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:25 PM UTC

PDB ID : 1F0X / pdb_00001f0x
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

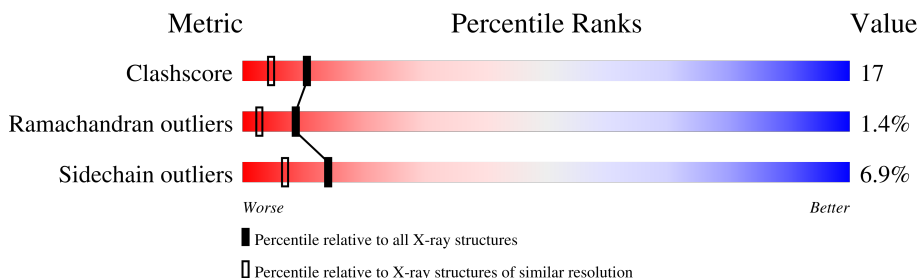
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

2 Entry composition [i](#)

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			

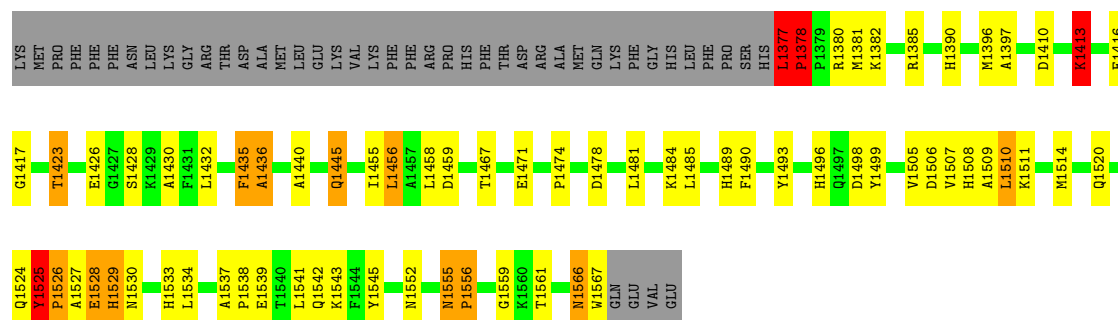
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 179	O 179	0	0
3	B	142	Total 142	O 142	0	0



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

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	1.09	12/4072 (0.3%)	1.51	63/5511 (1.1%)
1	B	1.07	7/4072 (0.2%)	1.41	49/5511 (0.9%)
All	All	1.08	19/8144 (0.2%)	1.46	112/11022 (1.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1528	GLU	CD-OE1	13.78	1.51	1.25
1	A	173	MET	SD-CE	-13.50	1.45	1.79
1	B	1173	MET	SD-CE	-12.72	1.47	1.79
1	A	77	ALA	N-CA	11.80	1.61	1.46
1	A	528	GLU	CD-OE1	10.13	1.44	1.25
1	A	491	MET	SD-CE	-9.15	1.56	1.79
1	B	1077	ALA	N-CA	8.80	1.57	1.46
1	A	74	MET	SD-CE	-8.24	1.58	1.79
1	A	555	ASN	C-O	-7.50	1.20	1.23
1	B	1396	MET	SD-CE	-7.31	1.61	1.79
1	B	1528	GLU	CB-CG	6.97	1.73	1.52
1	B	1525	TYR	CA-C	-6.89	1.44	1.52
1	A	381	MET	SD-CE	-6.59	1.63	1.79
1	A	530	ASN	N-CA	6.41	1.54	1.45
1	A	528	GLU	CB-CG	6.39	1.71	1.52
1	A	155	ILE	CA-CB	5.96	1.61	1.54
1	B	1528	GLU	CA-CB	5.84	1.65	1.54
1	A	121	GLY	C-O	-5.63	1.18	1.24
1	A	252	GLU	N-CA	5.44	1.53	1.46

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	TYR	CA-C-N	-31.43	87.39	119.76
1	A	525	TYR	C-N-CA	-31.43	87.39	119.76
1	B	1525	TYR	CA-C-N	-24.74	93.11	119.83
1	B	1525	TYR	C-N-CA	-24.74	93.11	119.83
1	A	377	LEU	C-N-CD	-18.31	80.32	120.60
1	A	377	LEU	CA-C-N	15.94	165.25	127.00
1	A	377	LEU	C-N-CA	15.94	165.25	127.00
1	B	1529	HIS	N-CA-C	-12.21	94.78	110.53
1	B	1377	LEU	C-N-CD	-11.09	96.19	120.60
1	A	416	GLU	N-CA-C	10.57	123.92	111.02
1	A	529	HIS	CA-C-N	-9.43	102.83	122.82
1	A	529	HIS	C-N-CA	-9.43	102.83	122.82
1	A	228	TYR	N-CA-C	-9.41	100.88	111.71
1	A	76	ALA	CA-C-N	-9.03	104.30	121.54
1	A	76	ALA	C-N-CA	-9.03	104.30	121.54
1	A	525	TYR	N-CA-C	8.87	129.41	109.81
1	B	1556	PRO	N-CA-C	8.74	130.48	112.47
1	A	435	PHE	N-CA-C	-8.66	99.10	110.53
1	A	251	PHE	CA-C-N	-8.61	105.10	121.54
1	A	251	PHE	C-N-CA	-8.61	105.10	121.54
1	A	529	HIS	N-CA-C	-8.61	99.17	110.53
1	B	1528	GLU	CG-CD-OE2	-8.52	98.80	118.40
1	B	1377	LEU	CA-C-N	8.41	147.18	127.00
1	B	1377	LEU	C-N-CA	8.41	147.18	127.00
1	B	1416	GLU	N-CA-C	8.20	124.82	111.37
1	B	1525	TYR	N-CA-C	8.13	127.77	109.81
1	B	1529	HIS	CA-C-N	-8.01	106.79	123.20
1	B	1529	HIS	C-N-CA	-8.01	106.79	123.20
1	A	219	ASP	N-CA-C	7.96	122.55	111.56
1	A	423	THR	N-CA-C	-7.92	99.36	110.29
1	A	556	PRO	N-CA-C	7.90	128.75	112.47
1	A	166	ARG	CA-C-N	-7.83	109.57	121.87
1	A	166	ARG	C-N-CA	-7.83	109.57	121.87
1	A	305	VAL	N-CA-C	-7.80	103.25	110.82
1	B	1413	LYS	N-CA-C	-7.78	103.76	113.18
1	A	301	GLU	N-CA-C	-7.78	102.71	112.90
1	A	413	LYS	N-CA-C	-7.76	103.27	112.89
1	B	1076	ALA	CA-C-N	-7.62	106.99	121.54
1	B	1076	ALA	C-N-CA	-7.62	106.99	121.54
1	A	529	HIS	O-C-N	-7.52	114.22	122.79
1	A	303	LEU	CA-C-N	-7.49	113.02	120.21
1	A	303	LEU	C-N-CA	-7.49	113.02	120.21
1	B	1219	ASP	N-CA-C	7.40	124.04	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1481	LEU	N-CA-C	7.27	120.77	109.07
1	A	216	VAL	N-CA-C	7.19	118.38	108.89
1	A	76	ALA	O-C-N	-7.13	113.20	122.83
1	A	528	GLU	CG-CD-OE2	-7.08	102.12	118.40
1	B	1528	GLU	CG-CD-OE1	7.06	134.65	118.40
1	B	1164	VAL	N-CA-C	7.04	117.80	110.62
1	A	269	THR	N-CA-C	-6.88	100.05	109.95
1	A	435	PHE	CA-C-N	-6.84	116.12	126.86
1	A	435	PHE	C-N-CA	-6.84	116.12	126.86
1	B	1105	ASP	N-CA-C	6.83	120.50	112.72
1	B	1435	PHE	N-CA-C	-6.75	99.53	110.20
1	B	1305	VAL	N-CA-C	-6.73	103.66	111.00
1	A	244	ASN	N-CA-C	6.70	119.44	111.33
1	A	102	LEU	N-CA-C	6.67	121.02	113.01
1	B	1555	ASN	CA-C-N	6.61	128.10	119.84
1	B	1555	ASN	C-N-CA	6.61	128.10	119.84
1	A	168	PRO	N-CA-C	-6.56	101.17	111.34
1	A	299	ASN	N-CA-C	6.51	122.30	113.97
1	B	1528	GLU	CA-CB-CG	6.50	127.09	114.10
1	A	292	ILE	N-CA-C	-6.46	104.03	110.30
1	A	500	ILE	N-CA-C	-6.45	98.58	107.99
1	B	1526	PRO	N-CA-C	-6.42	101.14	111.03
1	B	1299	ASN	N-CA-C	6.36	121.44	113.43
1	A	164	VAL	N-CA-C	6.33	117.83	110.62
1	A	555	ASN	CA-C-N	6.31	127.73	119.84
1	A	555	ASN	C-N-CA	6.31	127.73	119.84
1	B	1566	ASN	N-CA-C	6.31	124.25	110.80
1	A	482	VAL	N-CA-C	-6.28	104.73	110.82
1	A	160	GLY	CA-C-N	-6.28	109.11	121.41
1	A	160	GLY	C-N-CA	-6.28	109.11	121.41
1	B	1160	GLY	CA-C-N	-6.27	109.12	121.41
1	B	1160	GLY	C-N-CA	-6.27	109.12	121.41
1	A	477	ILE	N-CA-C	-6.25	105.63	111.45
1	B	1076	ALA	O-C-N	-6.19	114.77	122.82
1	A	274	LYS	N-CA-C	6.14	123.87	110.80
1	A	525	TYR	C-N-CD	6.03	149.70	125.00
1	B	1215	ASP	N-CA-C	-5.90	105.91	113.23
1	A	105	ASP	N-CA-C	5.77	119.63	112.59
1	B	1078	ASN	N-CA-CB	-5.76	103.15	111.91
1	B	1538	PRO	N-CA-C	-5.68	102.35	111.38
1	A	528	GLU	CG-CD-OE1	5.61	131.31	118.40
1	A	388	TYR	N-CA-C	5.57	118.18	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	LEU	N-CA-C	-5.55	99.48	108.52
1	A	10	LYS	N-CA-C	-5.53	105.41	111.82
1	A	312	ARG	N-CA-C	5.53	117.74	111.11
1	A	221	ARG	N-CA-C	-5.47	103.16	110.55
1	B	1423	THR	N-CA-C	-5.40	102.35	110.24
1	B	1216	VAL	N-CA-C	5.40	116.53	108.54
1	A	251	PHE	O-C-N	-5.39	115.42	122.59
1	A	566	ASN	N-CA-C	5.38	122.26	110.80
1	B	1221	ARG	N-CA-C	-5.37	103.60	110.53
1	B	1246	ASP	CA-C-N	5.36	125.43	119.32
1	B	1246	ASP	C-N-CA	5.36	125.43	119.32
1	B	1490	PHE	N-CA-C	5.36	117.56	111.02
1	B	1019	LEU	N-CA-C	5.34	116.90	111.14
1	B	1269	THR	N-CA-C	-5.30	102.06	109.69
1	A	55	LEU	N-CA-C	-5.24	105.75	111.82
1	A	252	GLU	N-CA-C	-5.22	99.68	110.80
1	A	148	GLY	N-CA-C	5.21	123.10	115.08
1	B	1166	ARG	CA-C-N	-5.20	113.70	121.87
1	B	1166	ARG	C-N-CA	-5.20	113.70	121.87
1	B	1140	SER	N-CA-C	5.14	117.55	108.75
1	B	1250	LEU	CA-C-N	-5.07	111.85	121.54
1	B	1250	LEU	C-N-CA	-5.07	111.85	121.54
1	A	318	ALA	N-CA-C	-5.04	105.97	111.82
1	B	1378	PRO	CA-N-CD	-5.04	104.44	111.50
1	A	219	ASP	CA-C-N	-5.03	113.59	122.09
1	A	219	ASP	C-N-CA	-5.03	113.59	122.09
1	B	1252	GLU	N-CA-C	-5.02	100.11	110.80

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	3983	0	3900	137	2
1	B	3983	0	3900	125	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	267	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 17.

All (267) 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:76:ALA:O	1:A:77:ALA:HB3	1.41	1.08
1:A:212:LYS:HD2	1:B:1520:GLN:HE22	1.17	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:525:TYR:O	1:A:526:PRO:C	1.98	0.95
1:A:283:THR:OG1	1:A:288:VAL:HG11	1.68	0.93
1:B:1525:TYR:O	1:B:1526:PRO:C	2.07	0.92
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:1283:THR:OG1	1:B:1288:VAL:HG11	1.73	0.87
1:B:1212:LYS:HE2	1:B:1212:LYS:HA	1.56	0.85
1:B:1283:THR:HG21	1:B:1288:VAL:HG13	1.57	0.84
1:A:381:MET:HE2	1:A:430:ALA:HB2	1.58	0.83
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H51A	2:B:1600:FAD:H8A	1.68	0.74
1:A:459:ASP:O	1:A:525:TYR:O	2.06	0.73
1:B:1432:LEU:O	1:B:1435:PHE:O	2.07	0.72
1:B:1381:MET:HE2	1:B:1430:ALA:HB2	1.71	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:CB	1:B:1231:ARG:HH11	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:OE1	1:A:273:GLU:HA	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:1287:GLU:CD	1:B:1287:GLU:H	2.05	0.63
1:B:1377:LEU:HA	1:B:1382:LYS:HE3	1.80	0.63
1:B:1273:GLU:HA	1:B:1273:GLU:OE1	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
1:A:314:ILE:HD13	1:A:314:ILE:O	2.00	0.61
1:A:206:LEU:HD21	1:A:211:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:GLU:H	1:A:201:GLN:NE2	1.99	0.61
1:A:390:HIS:HE1	3:A:2229:HOH:O	1.83	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:1090:ASN:HB3	3:B:2272:HOH:O	2.03	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:CG	1:B:1377:LEU:O	2.52	0.58
1:B:1377:LEU:O	1:B:1377:LEU:HG	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:B:1566:ASN:C	1:B:1567:TRP:CD1	2.83	0.57
1:A:227:ASP:HB2	1:A:230:HIS:ND1	2.20	0.57
1:A:425:GLU:HB3	1:A:429:LYS:HZ1	1.69	0.56
1:A:290:THR:HG1	1:A:469:TRP:CD1	2.24	0.56
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:385:ARG:HD3	1:A:385:ARG:C	2.31	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: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:445:GLN:NE2	1:A:445:GLN:C	2.65	0.55
1:A:526:PRO:HG2	1:A:531:VAL:HG12	1.89	0.55
1:A:566:ASN:C	1:A:567:TRP:CD1	2.85	0.55
2:A:600:FAD:N1	2:A:600:FAD:O2'	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:A:287:GLU:CD	1:A:287:GLU:H	2.16	0.54
1:B:1555:ASN:N	1:B:1556:PRO:HD3	2.23	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:1496:HIS:HE1	1:B:1528:GLU:HG2	1.73	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:B:1385:ARG:HD3	1:B:1385:ARG:C	2.34	0.53
1:A:189:ASN:ND2	1:A:191:LEU:H	2.06	0.53
1:B:1157:ASN:HD22	1:B:1530:ASN:HD22	1.54	0.53
1:B:1227:ASP:HB2	1:B:1230:HIS:CE1	2.43	0.53
1:A:108:HIS:HE1	3:A:2127:HOH:O	1.90	0.53
1:A:141:VAL:HB	1:A:163:LEU:HD13	1.91	0.53
1:A:181:GLU:CD	1:A:181:GLU:H	2.17	0.53
1:A:79:THR:C	2:A:600:FAD:O3'	2.52	0.53
1:B:1106:LYS:HE3	1:B:1207:ASP:O	2.08	0.53
1:B:1189:ASN:C	1:B:1189:ASN:HD22	2.17	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:1381:MET:CE	1:B:1430:ALA:HB2	2.36	0.53
1:A:137:GLU:HG3	1:A:272:ALA:HA	1.91	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: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:88:ASN:O	1:A:563:LYS:NZ	2.44	0.50
1:A:413:LYS:HB3	1:A:413:LYS:NZ	2.26	0.50
1:A:101:THR:HB	1:A:120:PRO:HB2	1.94	0.50
1:A:283:THR:HG21	1:A:288:VAL:CG1	2.39	0.50
1:B:1283:THR:CG2	1:B:1288:VAL:CG1	2.89	0.50
1:B:1311:HIS:CD2	1:B:1313:ASP:H	2.30	0.50
1:A:413:LYS:HB3	1:A:413:LYS:HZ3	1.75	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
2:B:1600:FAD:H51A	2:B:1600:FAD:C8A	2.41	0.49
1:B:1123:THR:OG1	1:B:1126:SER:HB2	2.12	0.49
1:B:1189:ASN:ND2	1:B:1189:ASN:C	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1315:TYR:C	1:B:1315:TYR:CD2	2.92	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:B:1230:HIS:CD2	1:B:1230:HIS:H	2.32	0.47
1:A:380:ARG:CD	1:A:426:GLU:OE2	2.63	0.47
1:A:445:GLN:C	1:A:445:GLN:HE21	2.23	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:A:20:VAL:O	1:A:24:HIS:HD2	1.98	0.47
1:B:1137:GLU:HG3	1:B:1272:ALA:CA	2.36	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
1:B:1507:VAL:O	1:B:1508:HIS:C	2.57	0.45
2:B:1600:FAD:N1	2:B:1600:FAD:O2'	2.42	0.45
1:A:425:GLU:CD	1:A:425:GLU:H	2.25	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:A:293:ARG:HG3	1:A:297:LEU:HD22	1.98	0.45
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.78	0.45
1:B:1210:ARG:NH2	3:B:2276:HOH:O	2.41	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:A:381:MET:HE1	1:A:426:GLU:O	2.17	0.45
1:B:1382:LYS:CG	3:B:2223:HOH:O	2.64	0.45
1:A:480:GLN:NE2	1:A:505:VAL:HG13	2.31	0.44
1:B:1273:GLU:HB3	1:B:1397:ALA:HB1	1.99	0.44
1:A:526:PRO:HD2	3:A:2043:HOH:O	2.18	0.44
1:A:70:LYS:HD2	1:A:95:ASP:HB2	1.99	0.44
2:B:1600:FAD:H8A	2:B:1600:FAD:C5B	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG22	1:A:161:GLY:HA2	1.98	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:A:423:THR:HG22	1:A:425:GLU:CD	2.42	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:B:1471:GLU:OE1	1:B:1499:TYR:OH	2.35	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:A:44:GLY:HA3	1:A:87:PRO:HB2	2.00	0.43
1:A:314:ILE:HG12	1:A:485:LEU:HB3	2.00	0.43
1:B:1160:GLY:O	1:B:1528:GLU:OE2	2.35	0.43
1:A:238:ASP:O	1:A:463:ARG:HG2	2.19	0.43
1:B:1505:VAL:HG12	1:B:1506:ASP:N	2.34	0.43
1:B:1537:ALA:HB2	1:B:1559:GLY:HA3	2.00	0.43
1:B:1028:ASP:O	1:B:1031:LYS:N	2.52	0.43
1:B:1219:ASP:OD1	1:B:1221:ARG:CD	2.66	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:A:189:ASN:C	1:A:189:ASN:HD22	2.27	0.43
1:B:1458:LEU:HD12	1:B:1499:TYR:HE1	1.83	0.42
1:B:1478:ASP:OD1	1:B:1484:LYS:NZ	2.49	0.42
1:A:381:MET:HE1	1:A:430:ALA:N	2.34	0.42
1:B:1198:THR:H	1:B:1201:GLN:HE21	1.66	0.42
1:B:1485:LEU:HB2	1:B:1498:ASP:HB2	2.02	0.42
1:B:1510:LEU:HD21	1:B:1514:MET:HE3	2.01	0.42
1:A:480:GLN:HE21	1:A:505:VAL:HG13	1.83	0.42
1:B:1231:ARG:NH1	1:B:1231:ARG:CB	2.71	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: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:63:LYS:HG3	1:A:185:LEU:HD23	2.02	0.41
1:A:206:LEU:CD2	1:A:211:ILE:CD1	2.98	0.41
1:A:377:LEU:O	1:A:377:LEU:CG	2.68	0.41
1:A:244:ASN:HD21	1:A:528:GLU:C	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1067:THR:HG23	3:B:2217:HOH:O	2.20	0.41
1:B:1423:THR:HG22	1:B:1426:GLU:HG3	2.02	0.41
1:A:88:ASN:HB2	1:A:533:HIS:CD2	2.55	0.41
1:A:423:THR:CG2	1:A:424:PRO:HD2	2.51	0.41
1:A:496:HIS:CE1	1:A:528:GLU:OE1	2.74	0.41
1:B:1227:ASP:O	1:B:1227:ASP:CG	2.63	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:383:ASN:HD21	1:A:387:LYS:HZ2	1.66	0.41
1:A:227:ASP:HB2	1:A:230:HIS:CE1	2.55	0.41
1:A:189:ASN:ND2	1:A:189:ASN:C	2.76	0.41
1:A:212:LYS:HA	1:A:212:LYS:HD3	1.73	0.41
2:A:600:FAD:H51A	2:A:600:FAD:C8A	2.49	0.41
1:A:27:THR:O	1:A:29:PRO:HD3	2.21	0.41
1:A:189:ASN:HD22	1:A:191:LEU:H	1.69	0.41
1:A:469:TRP:CD1	1:A:469:TRP:H	2.38	0.41
1:B:1106:LYS:HE2	3:B:2252:HOH:O	2.21	0.41
1:B:1288:VAL:HG12	1:B:1288:VAL:H	1.65	0.41
1:A:108:HIS:CD2	1:A:209:ASP:OD1	2.70	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:B:1086:THR:HB	1:B:1087:PRO:CD	2.51	0.41
1:B:1193:ILE:HG22	1:B:1195:LEU:HD13	2.03	0.41
1:A:315:TYR:CD2	1:A:315:TYR:C	2.98	0.41
1:B:1445:GLN:C	1:B:1445:GLN:NE2	2.79	0.41
1:B:1240:PRO:HG2	1:B:1524:GLN:HB2	2.02	0.40
1:A:113:GLY:O	1:A:136:ARG:HD2	2.22	0.40
1:B:1044:GLY:HA3	1:B:1087:PRO:HB2	2.02	0.40
1:B:1423:THR:CG2	1:B:1426:GLU:H	2.34	0.40
1:A:311:HIS:HD2	1:A:313:ASP:H	1.69	0.40
1:B:1511:LYS:NZ	1:B:1534:LEU:O	2.53	0.40
1:B:1506:ASP:OD2	1:B:1509:ALA:HB2	2.21	0.40
1:A:119:TYR:C	1:A:152:ILE:HD12	2.46	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%)	7	2
1	B	498/571 (87%)	474 (95%)	18 (4%)	6 (1%)	10	4
All	All	996/1142 (87%)	948 (95%)	34 (3%)	14 (1%)	9	3

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%)	392 (93%)	29 (7%)	14	7
1	B	421/484 (87%)	392 (93%)	29 (7%)	14	7
All	All	842/968 (87%)	784 (93%)	58 (7%)	14	7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PRO
1	A	73	LEU
1	A	117	LEU
1	A	136	ARG
1	A	163	LEU
1	A	191	LEU
1	A	195	LEU
1	A	211	ILE
1	A	214	ASP
1	A	221	ARG
1	A	227	ASP
1	A	229	VAL
1	A	273	GLU
1	A	288	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	456	LEU
1	A	468	GLU
1	A	510	LEU
1	A	525	TYR
1	A	552	ASN
1	A	567	TRP
1	B	1009	ASN
1	B	1010	LYS
1	B	1014	ASN
1	B	1073	LEU
1	B	1117	LEU
1	B	1128	GLU

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Mol	Chain	Res	Type
1	B	1136	ARG
1	B	1163	LEU
1	B	1191	LEU
1	B	1195	LEU
1	B	1212	LYS
1	B	1213	ASP
1	B	1227	ASP
1	B	1229	VAL
1	B	1230	HIS
1	B	1288	VAL
1	B	1297	LEU
1	B	1310	MET
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	1493	TYR
1	B	1510	LEU
1	B	1525	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) 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	230	HIS
1	A	244	ASN
1	A	311	HIS
1	A	383	ASN
1	A	390	HIS

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Mol	Chain	Res	Type
1	A	433	HIS
1	A	445	GLN
1	A	483	HIS
1	A	520	GLN
1	A	552	ASN
1	B	1014	ASN
1	B	1043	GLN
1	B	1075	GLN
1	B	1078	ASN
1	B	1108	HIS
1	B	1157	ASN
1	B	1158	ASN
1	B	1189	ASN
1	B	1190	HIS
1	B	1201	GLN
1	B	1295	HIS
1	B	1299	ASN
1	B	1311	HIS
1	B	1383	ASN
1	B	1390	HIS
1	B	1433	HIS
1	B	1445	GLN
1	B	1519	GLN
1	B	1542	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 oligosaccharides 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	B	1600	-	58,58,58	3.18	29 (50%)	85,89,89	1.67	13 (15%)
2	FAD	A	600	-	58,58,58	3.21	19 (32%)	85,89,89	1.62	14 (16%)

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	B	1600	-	-	3/34/50/50	0/6/6/6
2	FAD	A	600	-	-	2/34/50/50	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-13.52	1.44	1.59
2	B	1600	FAD	C5'-C4'	-12.85	1.34	1.51
2	A	600	FAD	C5'-C4'	-11.42	1.36	1.51
2	B	1600	FAD	P-O3P	-11.13	1.47	1.59
2	A	600	FAD	C2'-C3'	-6.78	1.41	1.53
2	A	600	FAD	PA-O2A	-5.94	1.27	1.55
2	A	600	FAD	PA-O5B	-5.23	1.38	1.59
2	B	1600	FAD	PA-O2A	-4.94	1.32	1.55
2	B	1600	FAD	PA-O5B	-4.82	1.40	1.59
2	B	1600	FAD	C4X-N5	4.36	1.40	1.30
2	B	1600	FAD	C2'-C3'	-4.28	1.45	1.53
2	A	600	FAD	O4B-C4B	4.25	1.54	1.45
2	A	600	FAD	O5B-C5B	-3.98	1.29	1.44
2	B	1600	FAD	O5B-C5B	-3.91	1.29	1.44
2	B	1600	FAD	O4'-C4'	3.85	1.51	1.43
2	A	600	FAD	C5A-C6A	3.68	1.51	1.41
2	B	1600	FAD	C9A-N10	3.62	1.47	1.41
2	A	600	FAD	C9A-C5X	3.50	1.46	1.41
2	B	1600	FAD	C5A-C4A	3.47	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	O4B-C1B	3.35	1.49	1.42
2	B	1600	FAD	C6-C5X	3.34	1.45	1.40
2	B	1600	FAD	C4A-N3A	3.06	1.40	1.34
2	B	1600	FAD	C8-C7	3.02	1.48	1.40
2	A	600	FAD	C8-C7	3.01	1.48	1.40
2	B	1600	FAD	C2A-N1A	2.99	1.39	1.33
2	A	600	FAD	C9-C8	2.98	1.43	1.39
2	B	1600	FAD	C9A-C5X	2.81	1.45	1.41
2	B	1600	FAD	C10-N1	2.79	1.38	1.33
2	A	600	FAD	C9A-N10	2.77	1.46	1.41
2	B	1600	FAD	C5A-C6A	2.72	1.48	1.41
2	B	1600	FAD	O4B-C1B	2.69	1.48	1.42
2	B	1600	FAD	C1'-C2'	2.68	1.56	1.52
2	B	1600	FAD	P-O5'	-2.67	1.48	1.59
2	B	1600	FAD	P-O2P	-2.63	1.43	1.55
2	A	600	FAD	C4X-N5	2.59	1.36	1.30
2	B	1600	FAD	C9-C8	2.32	1.42	1.39
2	A	600	FAD	C5B-C4B	2.31	1.58	1.51
2	B	1600	FAD	C5B-C4B	2.28	1.58	1.51
2	A	600	FAD	C1'-C2'	2.26	1.55	1.52
2	B	1600	FAD	O4B-C4B	2.19	1.49	1.45
2	A	600	FAD	C5A-C4A	2.16	1.42	1.39
2	B	1600	FAD	C2-N3	2.14	1.43	1.39
2	B	1600	FAD	O5'-C5'	2.10	1.52	1.44
2	B	1600	FAD	C9-C9A	2.09	1.43	1.39
2	B	1600	FAD	C10-N10	-2.09	1.32	1.37
2	A	600	FAD	C10-N1	2.04	1.37	1.33
2	B	1600	FAD	C7M-C7	2.04	1.54	1.51
2	A	600	FAD	C5A-N7A	-2.01	1.35	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	FAD	C4'-C3'-C2'	-7.61	100.91	113.57
2	A	600	FAD	C4'-C3'-C2'	-5.61	104.23	113.57
2	A	600	FAD	O5B-PA-O1A	-5.33	87.82	108.94
2	B	1600	FAD	O5B-PA-O1A	-4.85	89.70	108.94
2	A	600	FAD	O4B-C4B-C5B	-4.60	94.60	109.33
2	B	1600	FAD	O4B-C4B-C5B	-4.55	94.77	109.33
2	A	600	FAD	O3'-C3'-C2'	-3.76	100.38	108.93
2	B	1600	FAD	O3'-C3'-C2'	-3.40	101.20	108.93
2	A	600	FAD	C5'-C4'-C3'	-3.29	106.01	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	FAD	O4B-C4B-C3B	-2.93	99.34	105.15
2	A	600	FAD	C5X-C9A-N10	-2.92	115.33	117.97
2	B	1600	FAD	C5'-C4'-C3'	-2.87	106.80	112.22
2	B	1600	FAD	O2A-PA-O3P	2.87	115.02	107.27
2	A	600	FAD	C4X-C10-N10	2.69	120.34	116.48
2	A	600	FAD	O2A-PA-O3P	2.63	114.37	107.27
2	A	600	FAD	O4B-C4B-C3B	-2.60	99.98	105.15
2	B	1600	FAD	C5X-C9A-N10	-2.35	115.84	117.97
2	A	600	FAD	C4-C4X-N5	2.30	121.38	118.21
2	A	600	FAD	C2A-N1A-C6A	2.26	122.44	118.73
2	B	1600	FAD	C2A-N1A-C6A	2.23	122.39	118.73
2	B	1600	FAD	O5'-C5'-C4'	-2.18	103.53	109.36
2	B	1600	FAD	O4B-C1B-N9A	-2.09	104.07	108.09
2	A	600	FAD	O5'-C5'-C4'	-2.08	103.81	109.36
2	A	600	FAD	O5B-C5B-C4B	2.06	116.01	108.99
2	A	600	FAD	O2'-C2'-C3'	-2.04	104.47	109.25
2	B	1600	FAD	C4X-C10-N10	2.03	119.38	116.48
2	B	1600	FAD	P-O5'-C5'	-2.01	109.82	121.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	PA-O3P-P-O2P
2	B	1600	FAD	PA-O3P-P-O2P
2	B	1600	FAD	O4B-C4B-C5B-O5B
2	B	1600	FAD	PA-O3P-P-O1P
2	A	600	FAD	O4B-C4B-C5B-O5B

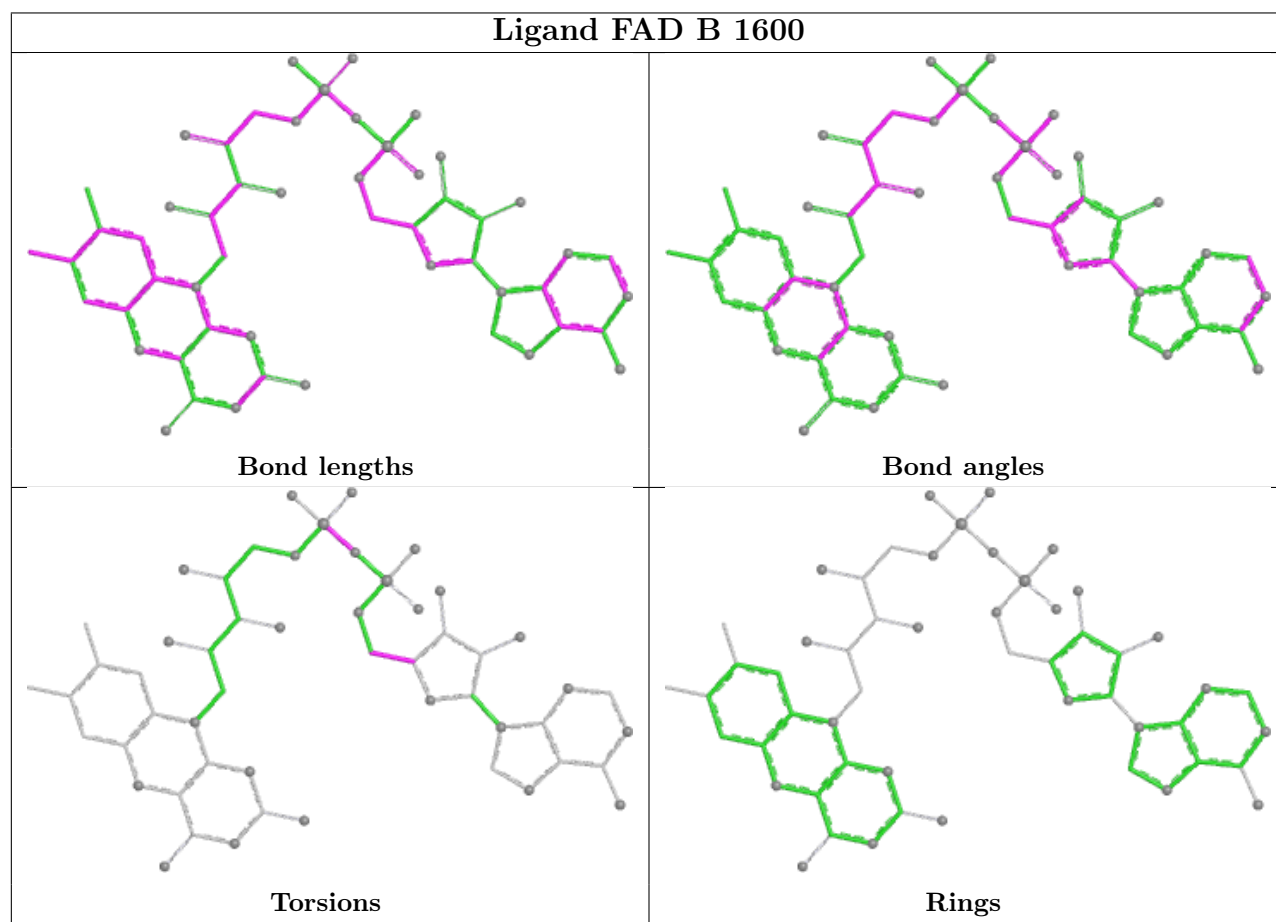
There are no ring outliers.

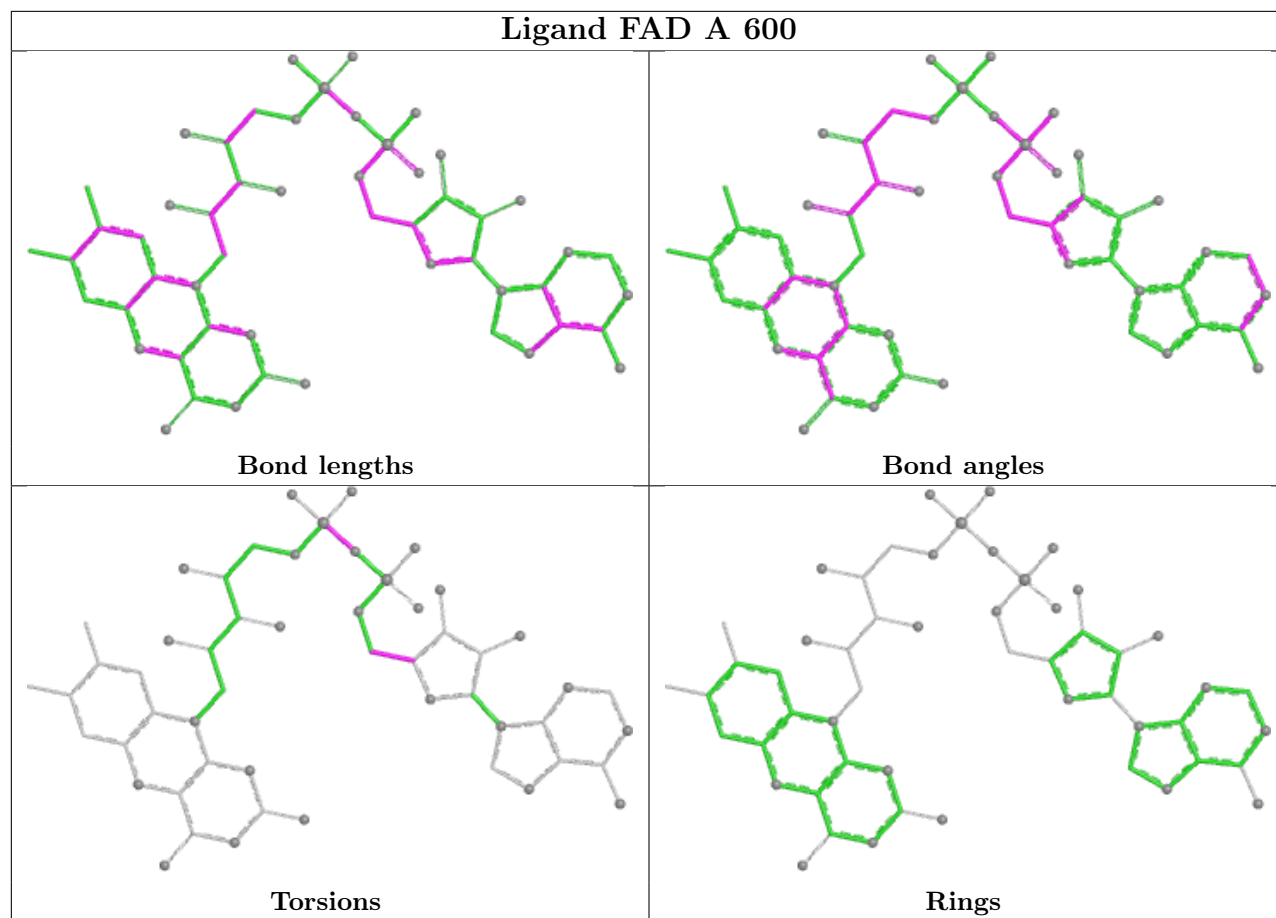
2 monomers are involved in 12 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.