



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:09 PM UTC

PDB ID : 2EQ7 / pdb_00002eq7
Title : Crystal structure of lipoamide dehydrogenase from thermus thermophilus HB8 with psbdo
Authors : Nakai, T.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-30
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

<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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

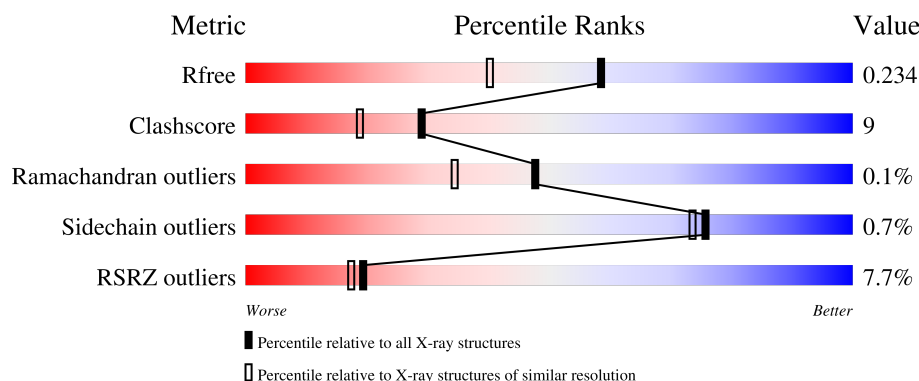
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	4% 84% 14% ..
1	B	455	4% 83% 16% ..
2	C	40	90% 40% 52% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8483 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.

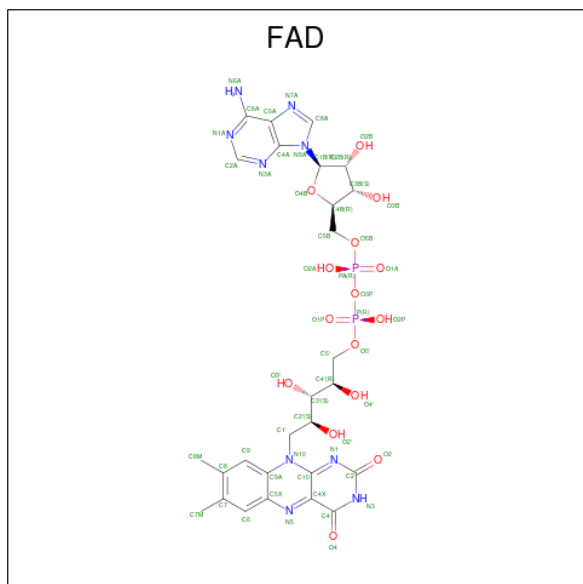
- Molecule 1 is a protein called 2-oxoglutarate dehydrogenase E3 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3430	2183	610	627	10			
1	B	452	Total	C	N	O	S	0	0	0
			3430	2183	610	627	10			

- Molecule 2 is a protein called 2-oxoglutarate dehydrogenase E2 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	37	Total	C	N	O	S	0	0	0
			270	166	50	51	3			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



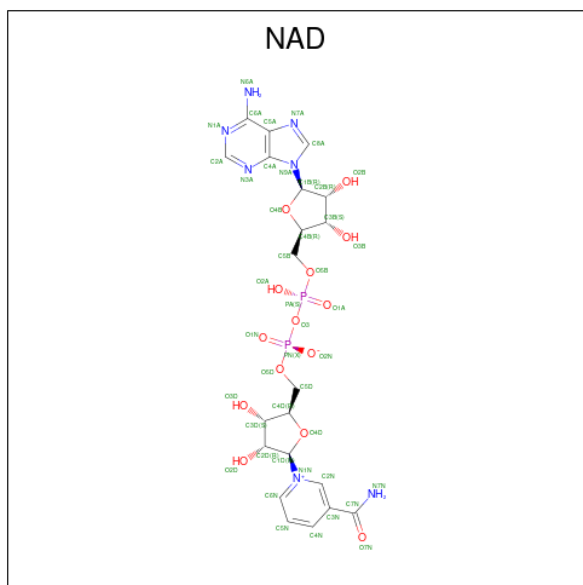
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

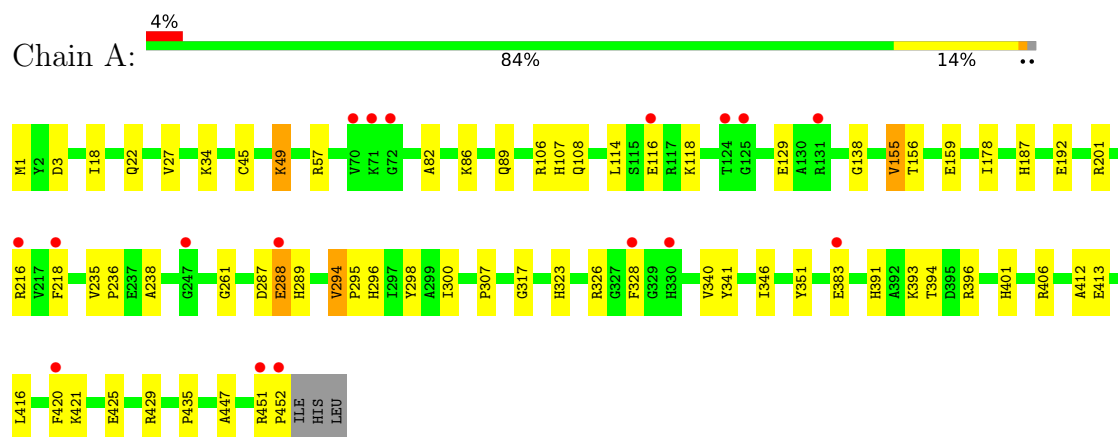
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	591	Total	O	0	0
			591	591		
5	B	544	Total	O	0	0
			544	544		
5	C	24	Total	O	0	0
			24	24		

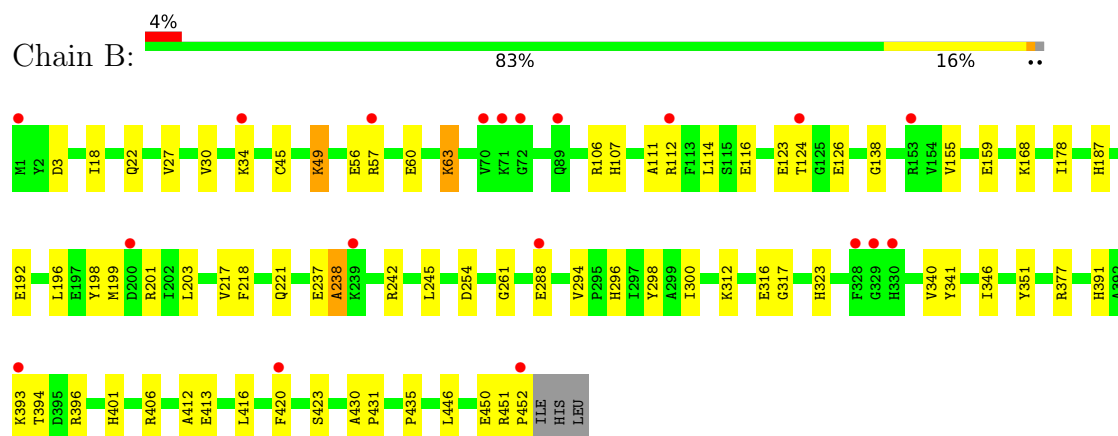
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

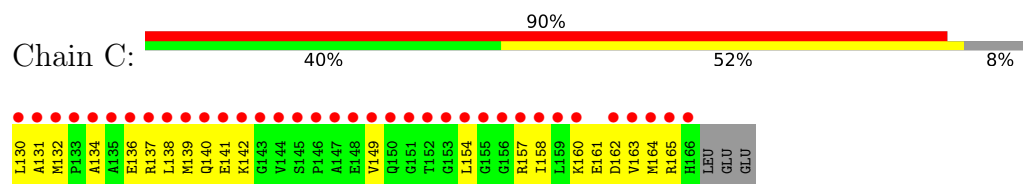
- Molecule 1: 2-oxoglutarate dehydrogenase E3 component



- Molecule 1: 2-oxoglutarate dehydrogenase E3 component



- Molecule 2: 2-oxoglutarate dehydrogenase E2 component



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.03Å 107.07Å 131.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 1.80 39.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.01-1.80) 99.7 (39.01-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.238 0.202 , 0.234	Depositor DCC
R_{free} test set	5581 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8483	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2393e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 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	0.33	0/3492	0.89	12/4727 (0.3%)
1	B	0.33	0/3492	0.89	11/4727 (0.2%)
2	C	0.28	0/271	0.80	0/361
All	All	0.33	0/7255	0.89	23/9815 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LEU	N-CA-C	-7.36	104.83	113.88
1	B	114	LEU	N-CA-C	-6.96	104.92	113.41
1	B	294	VAL	CA-C-N	6.86	128.41	119.84
1	B	294	VAL	C-N-CA	6.86	128.41	119.84
1	A	155	VAL	N-CA-C	6.70	118.47	108.96
1	A	412	ALA	N-CA-C	-6.65	104.06	111.71
1	B	3	ASP	N-CA-C	-6.64	103.52	111.69
1	A	3	ASP	N-CA-C	-6.43	103.78	111.69
1	A	192	GLU	N-CA-C	-6.25	99.69	109.25
1	A	294	VAL	CA-C-N	6.23	127.62	119.84
1	A	294	VAL	C-N-CA	6.23	127.62	119.84
1	B	27	VAL	N-CA-C	6.19	117.51	108.53
1	A	138	GLY	N-CA-C	6.14	122.03	111.47
1	B	412	ALA	N-CA-C	-5.80	105.04	111.71
1	B	138	GLY	N-CA-C	5.64	121.32	111.50
1	B	192	GLU	N-CA-C	-5.50	100.83	109.25
1	B	341	TYR	N-CA-C	5.39	120.05	112.72
1	A	341	TYR	N-CA-C	5.28	119.90	112.72
1	B	203	LEU	CA-C-N	5.27	124.94	119.56
1	B	203	LEU	C-N-CA	5.27	124.94	119.56
1	A	156	THR	N-CA-C	-5.27	102.37	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ALA	CB-CA-C	-5.14	110.63	116.54
1	A	27	VAL	N-CA-C	5.08	116.61	108.89

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	3430	0	3530	58	0
1	B	3430	0	3530	62	0
2	C	270	0	280	22	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	44	0	26	4	0
4	B	44	0	26	4	0
5	A	591	0	0	13	0
5	B	544	0	0	6	0
5	C	24	0	0	5	0
All	All	8483	0	7454	128	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 9.

All (128) 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:199:MET:HA	1:B:199:MET:HE2	1.59	0.81
1:B:377:ARG:HG3	1:B:377:ARG:HH21	1.49	0.78
1:A:396:ARG:HH21	1:A:421:LYS:HD2	1.51	0.75
1:B:198:TYR:CD2	1:B:199:MET:HE3	2.22	0.74
1:B:106:ARG:HD3	1:B:107:HIS:N	2.02	0.74
1:A:420:PHE:HD2	1:B:420:PHE:HD2	1.38	0.71
1:A:106:ARG:HD3	1:A:107:HIS:N	2.06	0.70
1:A:447:ALA:O	1:A:451:ARG:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:HIS:HD2	1:B:394:THR:H	1.43	0.66
1:B:288:GLU:H	1:B:288:GLU:CD	2.03	0.66
5:A:2850:HOH:O	2:C:154:LEU:HD21	1.96	0.65
1:B:106:ARG:HD3	1:B:106:ARG:C	2.21	0.65
1:A:106:ARG:HD3	1:A:106:ARG:C	2.23	0.63
1:B:155:VAL:HB	1:B:159:GLU:HB2	1.81	0.62
1:A:451:ARG:HA	1:A:451:ARG:HE	1.63	0.62
1:A:420:PHE:CD2	1:B:420:PHE:HD2	2.16	0.61
1:A:82:ALA:O	1:A:86:LYS:HG3	1.99	0.61
1:A:155:VAL:HB	1:A:159:GLU:HB2	1.82	0.61
1:A:45:CYS:O	1:A:49:LYS:HD2	2.00	0.61
1:B:377:ARG:HG3	1:B:377:ARG:NH2	2.16	0.60
1:A:187:HIS:HD2	5:A:2631:HOH:O	1.85	0.59
1:A:57:ARG:HH12	1:B:57:ARG:NE	2.00	0.59
2:C:158:ILE:HG13	5:C:183:HOH:O	2.03	0.59
1:A:420:PHE:HD2	1:B:420:PHE:CD2	2.22	0.58
1:A:116:GLU:O	1:A:296:HIS:HE1	1.85	0.57
2:C:138:LEU:HD23	2:C:163:VAL:HB	1.86	0.57
1:B:261:GLY:HA2	4:B:1483:NAD:O3	2.06	0.56
1:A:396:ARG:NH2	1:A:421:LYS:HD2	2.18	0.55
1:A:298:TYR:OH	1:A:323:HIS:HD2	1.90	0.55
1:A:216:ARG:HD3	5:A:2611:HOH:O	2.06	0.55
1:A:261:GLY:HA2	4:A:2483:NAD:O3	2.06	0.55
2:C:138:LEU:HG	2:C:142:LYS:HE2	1.89	0.54
1:B:178:ILE:HG13	4:B:1483:NAD:H5N	1.89	0.54
1:A:57:ARG:NH1	1:B:57:ARG:NE	2.56	0.54
1:B:351:TYR:O	1:B:401:HIS:HE1	1.91	0.54
1:A:18:ILE:O	1:A:22:GLN:HG3	2.08	0.54
1:B:18:ILE:O	1:B:22:GLN:HG3	2.08	0.54
1:B:423:SER:CB	2:C:160:LYS:HD3	2.38	0.54
2:C:149:VAL:HB	2:C:158:ILE:HD13	1.89	0.54
1:B:63:LYS:HA	1:B:63:LYS:NZ	2.23	0.53
2:C:137:ARG:HD2	2:C:137:ARG:C	2.33	0.53
1:B:63:LYS:HA	1:B:63:LYS:HZ2	1.74	0.53
1:A:416:LEU:HD22	1:B:413:GLU:HG2	1.90	0.52
1:A:34:LYS:NZ	1:A:108:GLN:HE22	2.07	0.52
1:A:300:ILE:HD13	1:A:317:GLY:HA2	1.92	0.52
1:B:187:HIS:HD2	5:B:1656:HOH:O	1.93	0.51
1:B:34:LYS:HD3	5:B:1949:HOH:O	2.10	0.51
1:B:178:ILE:CG1	4:B:1483:NAD:H5N	2.41	0.51
1:B:451:ARG:HD2	1:B:452:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:CG1	4:A:2483:NAD:H5N	2.42	0.50
1:A:413:GLU:HG2	1:B:416:LEU:HD22	1.93	0.50
1:A:218:PHE:CZ	1:A:346:ILE:HD11	2.47	0.49
2:C:130:LEU:O	2:C:157:ARG:HA	2.13	0.49
1:A:391:HIS:HD2	1:A:394:THR:H	1.61	0.49
1:A:351:TYR:O	1:A:401:HIS:HE1	1.96	0.49
1:A:57:ARG:HH12	1:B:57:ARG:CZ	2.26	0.49
1:B:116:GLU:H	1:B:116:GLU:CD	2.21	0.49
1:A:178:ILE:HG13	4:A:2483:NAD:H5N	1.94	0.48
2:C:136:GLU:HA	2:C:139:MET:HE3	1.96	0.48
1:B:178:ILE:HG13	4:B:1483:NAD:C5N	2.44	0.48
1:A:396:ARG:HH21	1:A:421:LYS:CD	2.21	0.48
2:C:130:LEU:HB2	5:C:177:HOH:O	2.13	0.48
2:C:131:ALA:CB	2:C:158:ILE:HB	2.44	0.48
2:C:130:LEU:HG	5:C:183:HOH:O	2.13	0.47
2:C:131:ALA:HB2	2:C:158:ILE:HB	1.95	0.47
1:A:425:GLU:O	1:A:429:ARG:HG3	2.14	0.47
1:A:89:GLN:HG3	5:A:2880:HOH:O	2.14	0.47
1:B:298:TYR:OH	1:B:323:HIS:HD2	1.98	0.47
1:A:86:LYS:HD2	5:A:2622:HOH:O	2.14	0.47
1:B:217:VAL:O	1:B:221:GLN:HG3	2.14	0.47
1:B:391:HIS:CD2	1:B:394:THR:H	2.29	0.47
1:A:326:ARG:HB3	1:A:328:PHE:CE1	2.50	0.47
1:B:116:GLU:O	1:B:296:HIS:HE1	1.97	0.47
2:C:137:ARG:O	2:C:141:GLU:HG3	2.16	0.46
1:A:340:VAL:HB	1:A:346:ILE:HB	1.98	0.46
1:A:383:GLU:HB3	5:A:3026:HOH:O	2.15	0.46
1:A:57:ARG:NH2	1:B:406:ARG:NH2	2.64	0.46
1:B:391:HIS:CD2	1:B:393:LYS:H	2.34	0.46
2:C:134:ALA:HB3	5:C:184:HOH:O	2.16	0.46
1:A:287:ASP:HB2	1:A:288:GLU:OE2	2.15	0.46
1:B:431:PRO:HD2	5:B:1961:HOH:O	2.16	0.46
1:A:45:CYS:HB3	1:B:435:PRO:HD3	1.98	0.45
5:A:2788:HOH:O	2:C:154:LEU:HD22	2.16	0.45
1:B:198:TYR:CE2	1:B:199:MET:HE3	2.51	0.45
1:B:446:LEU:O	1:B:450:GLU:HG3	2.16	0.45
1:B:124:THR:OG1	1:B:126:GLU:HG3	2.17	0.45
1:A:178:ILE:HG13	4:A:2483:NAD:C5N	2.47	0.45
1:B:396:ARG:NH2	2:C:161:GLU:OE1	2.50	0.45
1:A:294:VAL:HA	1:A:295:PRO:HD2	1.77	0.44
1:B:196:LEU:HD13	1:B:245:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:NZ	1:A:129:GLU:OE1	2.49	0.44
1:A:328:PHE:CZ	2:C:141:GLU:HG2	2.53	0.44
2:C:161:GLU:HA	2:C:164:MET:HG2	1.99	0.44
1:A:218:PHE:HZ	1:A:346:ILE:HD11	1.82	0.44
1:A:34:LYS:HD3	1:A:108:GLN:NE2	2.32	0.44
1:A:307:PRO:HA	5:A:2795:HOH:O	2.18	0.44
1:B:168:LYS:HB2	1:B:168:LYS:NZ	2.33	0.44
1:A:187:HIS:HE1	5:A:2587:HOH:O	2.00	0.43
2:C:136:GLU:O	2:C:140:GLN:HG3	2.19	0.43
1:B:201:ARG:HD3	1:B:201:ARG:C	2.43	0.43
1:A:86:LYS:HG3	5:A:2637:HOH:O	2.18	0.43
1:B:60:GLU:OE2	1:B:60:GLU:HA	2.18	0.43
1:B:112:ARG:NH1	5:B:1639:HOH:O	2.50	0.43
2:C:162:ASP:O	2:C:165:ARG:HB3	2.18	0.43
1:B:237:GLU:OE1	1:B:242:ARG:HB3	2.19	0.43
1:B:416:LEU:HD11	1:B:420:PHE:CZ	2.54	0.42
1:B:123:GLU:OE2	1:B:123:GLU:N	2.44	0.42
1:B:340:VAL:HB	1:B:346:ILE:HB	2.01	0.42
2:C:132:MET:HB2	5:C:184:HOH:O	2.19	0.42
1:A:435:PRO:HD3	1:B:45:CYS:HB3	2.00	0.41
5:A:2953:HOH:O	1:B:431:PRO:HB3	2.20	0.41
1:B:406:ARG:HD3	5:B:1760:HOH:O	2.19	0.41
1:B:312:LYS:O	1:B:316:GLU:HG3	2.20	0.41
1:A:201:ARG:C	1:A:201:ARG:HD3	2.46	0.41
1:A:235:VAL:HA	1:A:236:PRO:HD3	1.90	0.41
1:A:288:GLU:CD	1:A:288:GLU:H	2.29	0.41
1:B:30:VAL:HG11	1:B:111:ALA:HB2	2.03	0.41
1:B:45:CYS:O	1:B:49:LYS:HD2	2.20	0.41
1:B:218:PHE:CZ	1:B:346:ILE:HD11	2.56	0.41
1:A:391:HIS:CD2	1:A:393:LYS:H	2.39	0.40
1:A:451:ARG:NE	1:A:452:PRO:HD2	2.36	0.40
1:B:56:GLU:HG3	1:B:57:ARG:NH2	2.37	0.40
1:B:300:ILE:HD13	1:B:317:GLY:HA2	2.03	0.40
1:B:430:ALA:HA	1:B:431:PRO:HD3	1.98	0.40
1:A:1:MET:HG3	5:A:2950:HOH:O	2.21	0.40
1:A:289:HIS:HD2	5:A:2647:HOH:O	2.04	0.40
1:A:406:ARG:HD3	5:B:1760:HOH:O	2.21	0.40
1:B:237:GLU:O	1:B:238:ALA:C	2.65	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	450/455 (99%)	436 (97%)	14 (3%)	0	100	100
1	B	450/455 (99%)	433 (96%)	16 (4%)	1 (0%)	43	31
2	C	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
All	All	935/950 (98%)	903 (97%)	31 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ALA

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	349/352 (99%)	347 (99%)	2 (1%)	78	77
1	B	349/352 (99%)	346 (99%)	3 (1%)	70	67
2	C	27/31 (87%)	27 (100%)	0	100	100
All	All	725/735 (99%)	720 (99%)	5 (1%)	76	73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	288	GLU

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Mol	Chain	Res	Type
1	B	49	LYS
1	B	63	LYS
1	B	254	ASP

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

Mol	Chain	Res	Type
1	A	91	ASN
1	A	93	GLN
1	A	108	GLN
1	A	148	GLN
1	A	187	HIS
1	A	289	HIS
1	A	296	HIS
1	A	323	HIS
1	A	391	HIS
1	A	401	HIS
1	B	89	GLN
1	B	148	GLN
1	B	187	HIS
1	B	296	HIS
1	B	323	HIS
1	B	391	HIS
1	B	401	HIS
2	C	140	GLN
2	C	150	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

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	B	1482	-	58,58,58	2.05	15 (25%)	85,89,89	1.16	8 (9%)
4	NAD	B	1483	-	46,48,48	1.43	5 (10%)	64,73,73	1.59	10 (15%)
3	FAD	A	2482	-	58,58,58	2.00	14 (24%)	85,89,89	1.20	9 (10%)
4	NAD	A	2483	-	46,48,48	1.46	6 (13%)	64,73,73	1.61	10 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	1482	-	-	1/34/50/50	0/6/6/6
4	NAD	B	1483	-	-	3/30/62/62	0/5/5/5
3	FAD	A	2482	-	-	1/34/50/50	0/6/6/6
4	NAD	A	2483	-	-	2/30/62/62	0/5/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1482	FAD	P-O3P	-10.04	1.48	1.59
3	A	2482	FAD	P-O3P	-9.63	1.49	1.59
4	B	1483	NAD	O4D-C1D	4.96	1.47	1.40
4	A	2483	NAD	O4D-C1D	4.94	1.47	1.40
4	A	2483	NAD	PN-O3	4.31	1.64	1.59
3	B	1482	FAD	PA-O2A	-4.13	1.36	1.55
4	B	1483	NAD	PN-O3	4.12	1.63	1.59
3	A	2482	FAD	PA-O2A	-3.94	1.37	1.55
3	A	2482	FAD	O5'-C5'	3.65	1.58	1.44
3	B	1482	FAD	O5'-C5'	3.63	1.58	1.44
4	A	2483	NAD	PA-O3	3.49	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1482	FAD	P-O2P	-3.37	1.39	1.55
3	A	2482	FAD	P-O2P	-3.21	1.40	1.55
4	B	1483	NAD	PA-O3	3.19	1.62	1.59
3	A	2482	FAD	C8-C7	2.80	1.47	1.40
3	B	1482	FAD	C8-C7	2.75	1.47	1.40
3	B	1482	FAD	C4X-N5	2.64	1.36	1.30
3	B	1482	FAD	C5A-C6A	2.64	1.48	1.41
3	A	2482	FAD	C5A-C6A	2.59	1.48	1.41
4	A	2483	NAD	C2N-C3N	2.43	1.42	1.39
3	A	2482	FAD	C4X-N5	2.38	1.35	1.30
3	B	1482	FAD	C9A-C5X	2.32	1.44	1.41
4	B	1483	NAD	C2N-C3N	2.32	1.42	1.39
3	B	1482	FAD	C2-N3	2.31	1.44	1.39
3	B	1482	FAD	C5A-C4A	2.29	1.43	1.39
3	A	2482	FAD	C9A-C5X	2.29	1.44	1.41
3	A	2482	FAD	C2-N3	2.24	1.43	1.39
3	B	1482	FAD	O2-C2	-2.19	1.20	1.24
3	B	1482	FAD	O4B-C1B	2.16	1.47	1.42
4	B	1483	NAD	C4N-C3N	2.14	1.42	1.39
3	B	1482	FAD	C6-C5X	2.12	1.43	1.40
4	A	2483	NAD	C4N-C3N	2.09	1.42	1.39
3	A	2482	FAD	C9A-N10	2.09	1.44	1.41
3	B	1482	FAD	C10-N1	2.07	1.37	1.33
3	A	2482	FAD	C10-N1	2.06	1.37	1.33
3	A	2482	FAD	O2-C2	-2.06	1.20	1.24
3	B	1482	FAD	C9A-N10	2.04	1.44	1.41
3	A	2482	FAD	C5A-C4A	2.03	1.42	1.39
4	A	2483	NAD	C5A-C4A	2.02	1.42	1.39
3	A	2482	FAD	C4A-N3A	2.01	1.38	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2483	NAD	C5A-C4A-N3A	-5.26	119.48	126.72
4	B	1483	NAD	C5A-C4A-N3A	-5.20	119.56	126.72
4	B	1483	NAD	N3A-C2A-N1A	-4.71	121.46	128.58
4	A	2483	NAD	N3A-C2A-N1A	-4.69	121.49	128.58
4	A	2483	NAD	N3A-C4A-N9A	4.39	134.64	127.17
4	B	1483	NAD	N3A-C4A-N9A	4.29	134.47	127.17
3	A	2482	FAD	O4B-C1B-N9A	-4.12	100.18	108.09
4	A	2483	NAD	C2A-N3A-C4A	3.82	121.16	111.83
4	A	2483	NAD	C5A-N7A-C8A	3.78	109.39	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1483	NAD	C2A-N3A-C4A	3.77	121.03	111.83
4	B	1483	NAD	C5A-N7A-C8A	3.72	109.30	103.45
3	B	1482	FAD	O4B-C1B-N9A	-3.64	101.11	108.09
4	B	1483	NAD	C4A-C5A-N7A	-2.97	107.18	110.58
4	A	2483	NAD	C4A-C5A-N7A	-2.97	107.18	110.58
3	B	1482	FAD	C2A-N1A-C6A	2.65	123.08	118.73
4	B	1483	NAD	N9A-C8A-N7A	-2.64	110.19	113.94
4	A	2483	NAD	N9A-C8A-N7A	-2.63	110.20	113.94
3	A	2482	FAD	O5B-PA-O1A	-2.60	98.65	108.94
3	A	2482	FAD	C5'-C4'-C3'	-2.59	107.33	112.22
3	B	1482	FAD	C5'-C4'-C3'	-2.56	107.39	112.22
3	B	1482	FAD	O5B-PA-O1A	-2.55	98.83	108.94
3	A	2482	FAD	C2A-N1A-C6A	2.47	122.79	118.73
3	A	2482	FAD	C4-N3-C2	-2.29	121.57	125.64
3	A	2482	FAD	O2A-PA-O3P	2.24	113.33	107.27
3	A	2482	FAD	C5X-C9A-N10	-2.22	115.96	117.97
3	B	1482	FAD	C4-N3-C2	-2.20	121.73	125.64
3	A	2482	FAD	C2B-C1B-N9A	2.17	118.69	113.30
3	A	2482	FAD	C4'-C3'-C2'	-2.16	109.98	113.57
4	A	2483	NAD	PA-O5B-C5B	-2.11	109.23	121.35
3	B	1482	FAD	C4'-C3'-C2'	-2.11	110.06	113.57
3	B	1482	FAD	O2A-PA-O3P	2.10	112.95	107.27
4	A	2483	NAD	PN-O5D-C5D	-2.07	109.46	121.35
4	B	1483	NAD	PA-O5B-C5B	-2.07	109.51	121.35
4	B	1483	NAD	PN-O5D-C5D	-2.05	109.63	121.35
4	B	1483	NAD	C3N-C7N-N7N	2.03	120.24	117.74
3	B	1482	FAD	C2B-C1B-N9A	2.01	118.30	113.30
4	A	2483	NAD	C3N-C7N-N7N	2.00	120.21	117.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

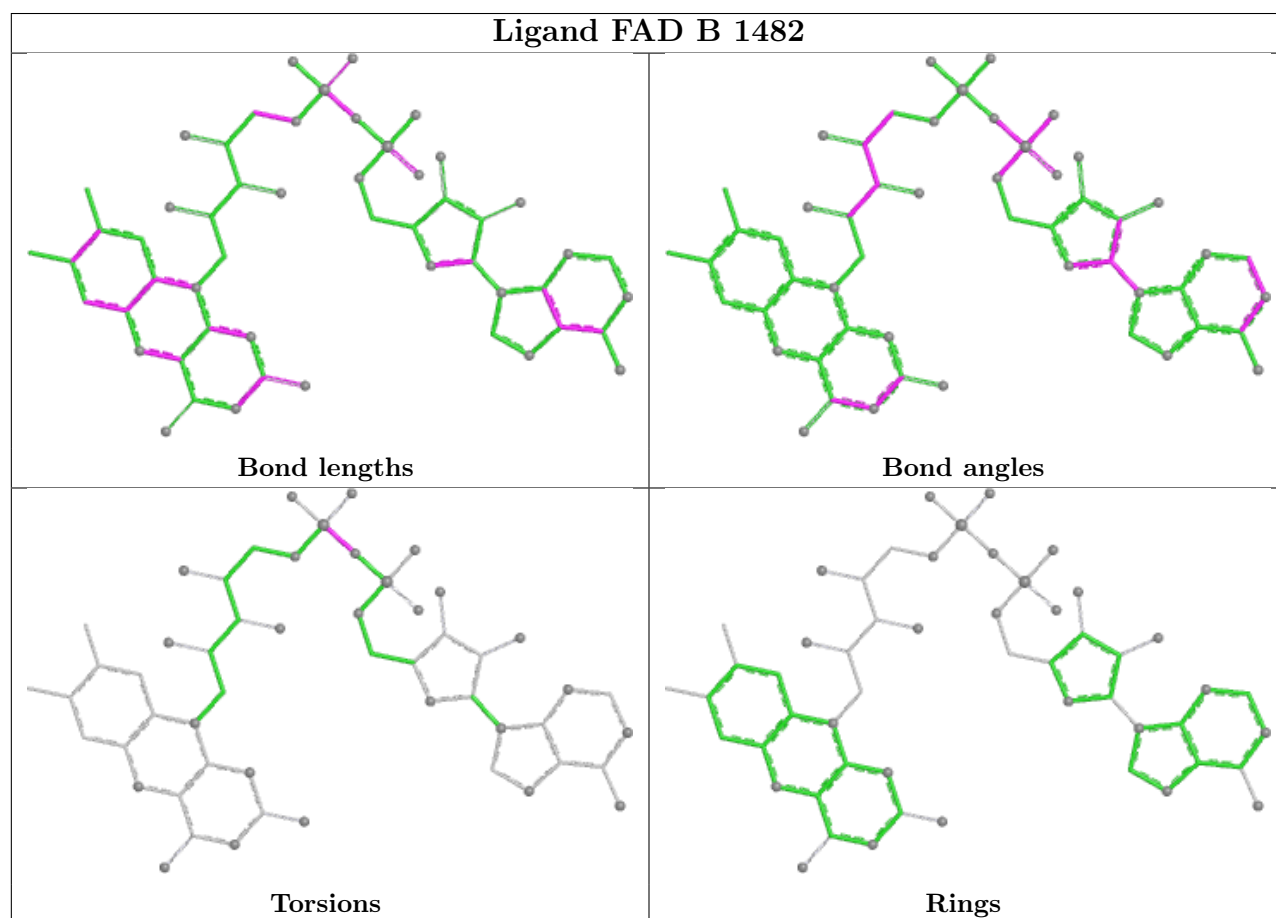
Mol	Chain	Res	Type	Atoms
3	A	2482	FAD	PA-O3P-P-O5'
3	B	1482	FAD	PA-O3P-P-O5'
4	A	2483	NAD	O4B-C4B-C5B-O5B
4	B	1483	NAD	O4B-C4B-C5B-O5B
4	A	2483	NAD	C3B-C4B-C5B-O5B
4	B	1483	NAD	C3B-C4B-C5B-O5B
4	B	1483	NAD	PN-O3-PA-O1A

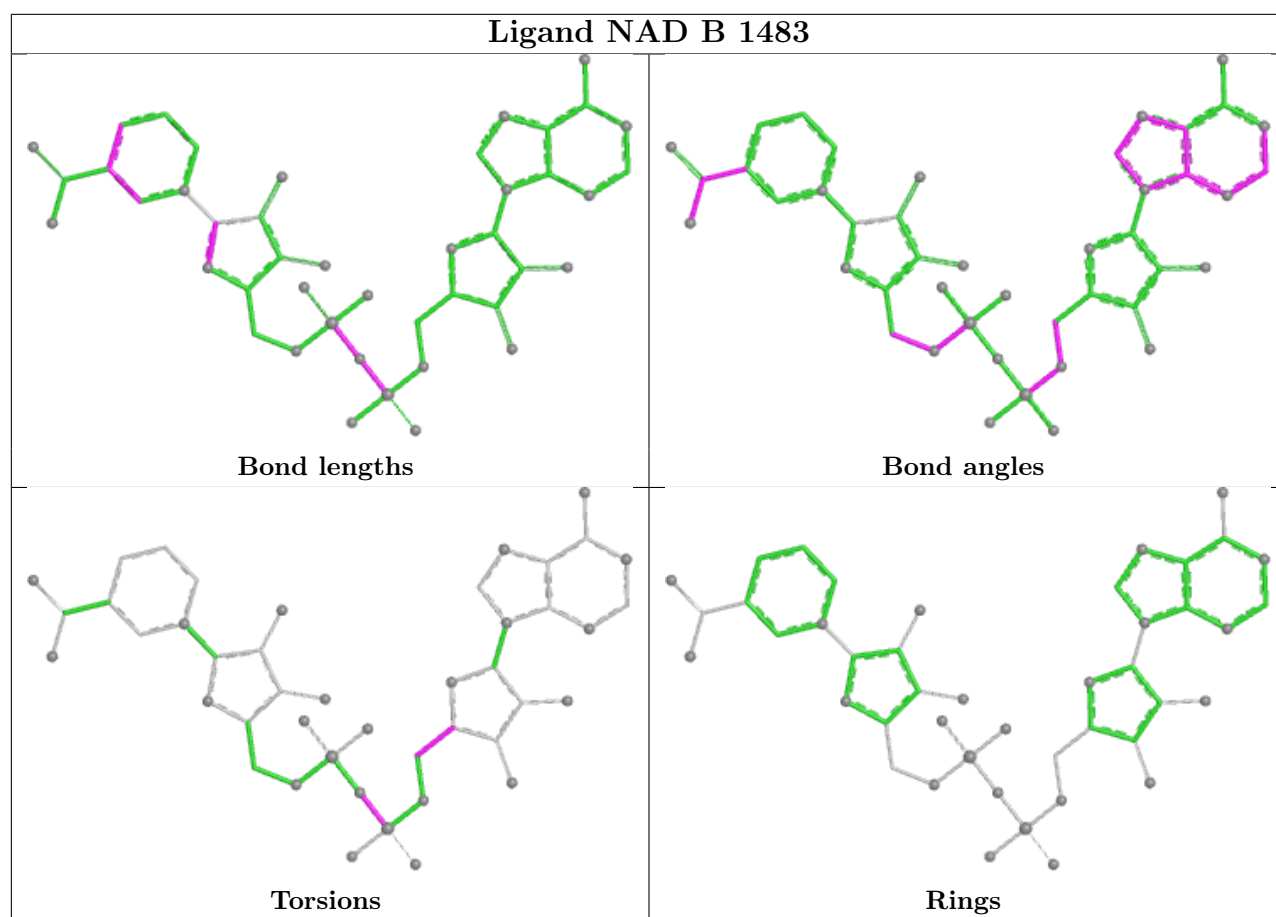
There are no ring outliers.

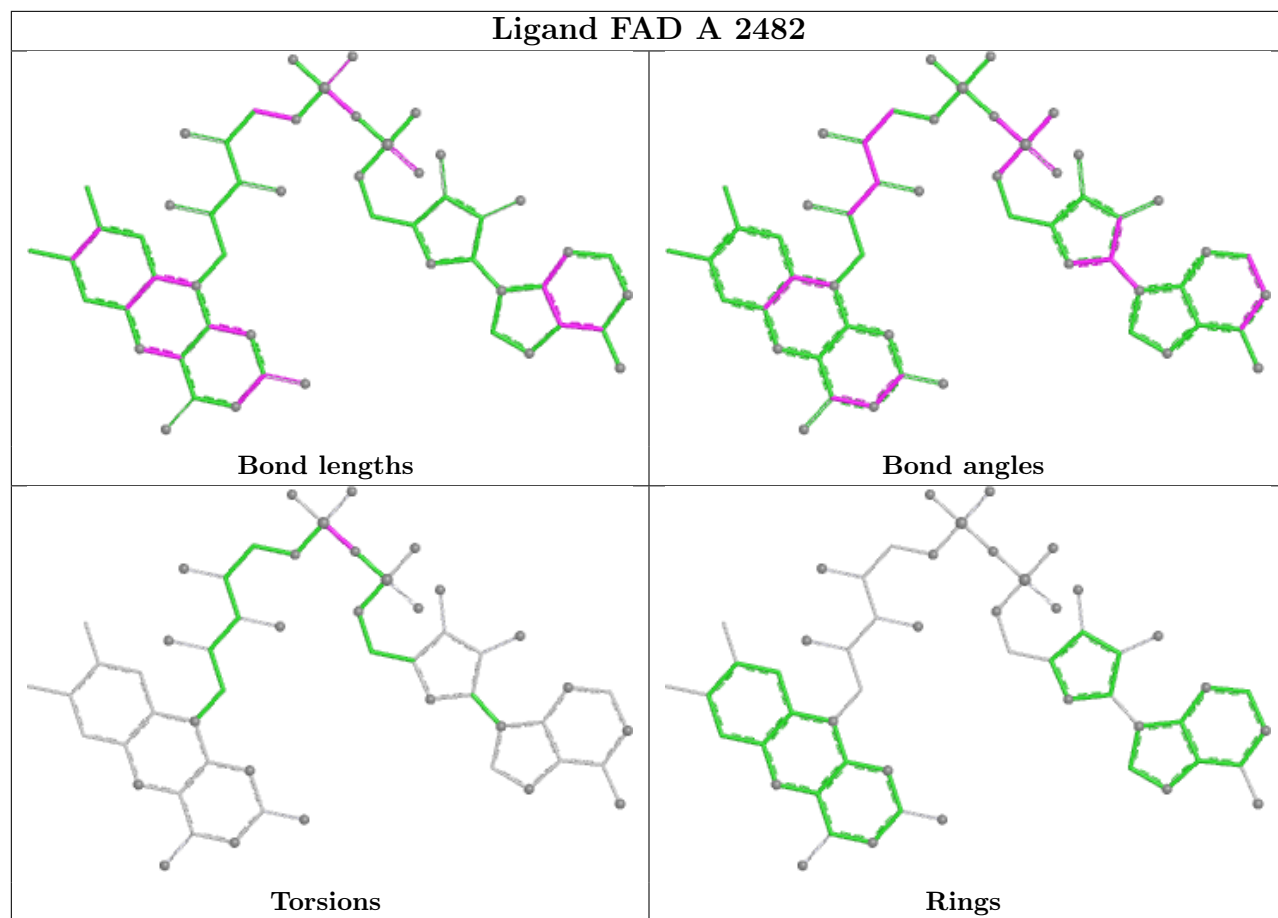
2 monomers are involved in 8 short contacts:

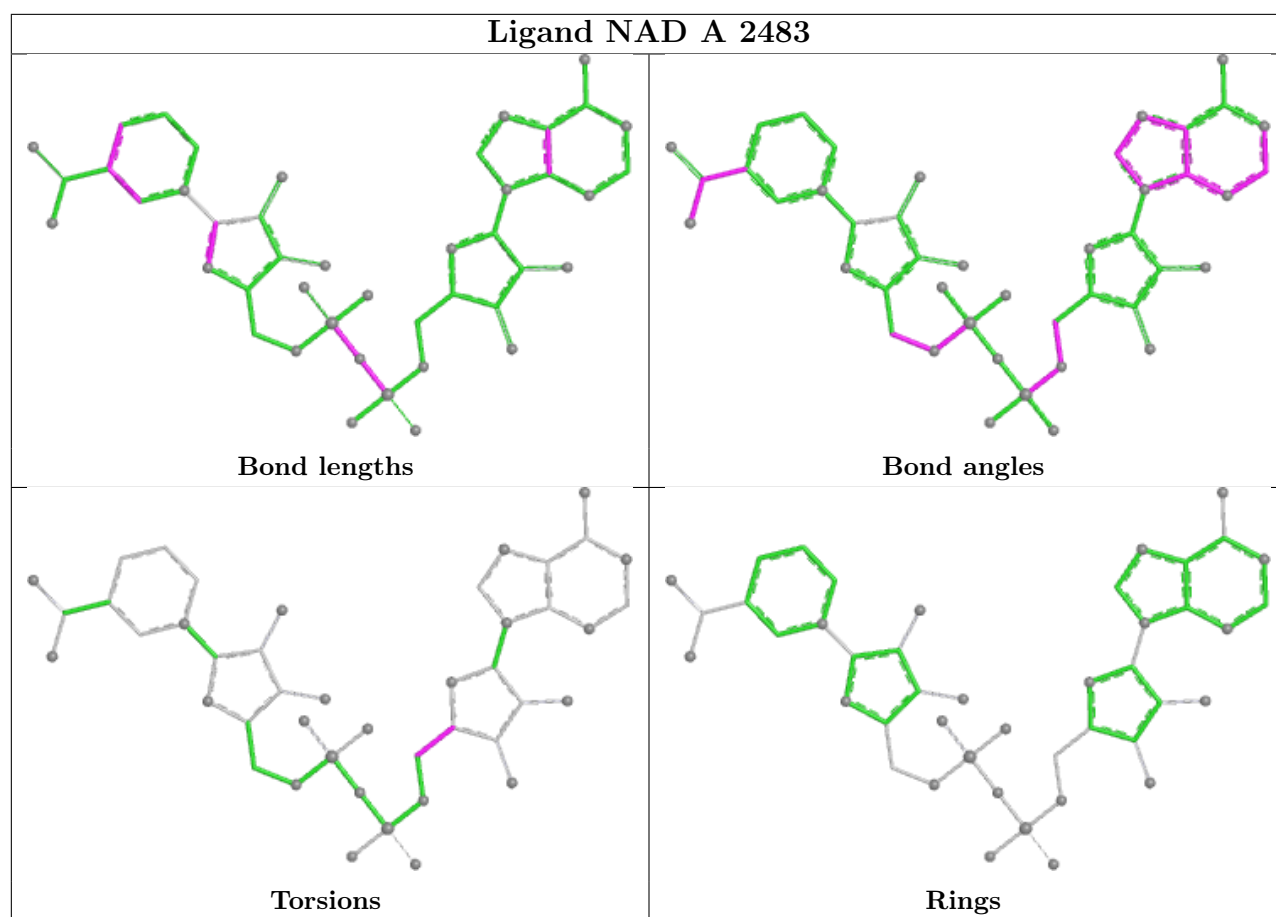
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1483	NAD	4	0
4	A	2483	NAD	4	0

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/455 (99%)	-0.01	17 (3%) 44 44	8, 16, 30, 52	0
1	B	452/455 (99%)	0.10	19 (4%) 40 40	10, 17, 32, 50	0
2	C	37/40 (92%)	3.94	36 (97%) 0 0	48, 61, 73, 74	0
All	All	941/950 (99%)	0.20	72 (7%) 19 17	8, 16, 39, 74	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	154	LEU	7.3
1	B	328	PHE	7.2
2	C	131	ALA	6.9
2	C	156	GLY	6.3
2	C	166	HIS	6.2
1	A	72	GLY	6.1
2	C	130	LEU	6.1
1	A	452	PRO	5.5
1	B	452	PRO	5.5
2	C	157	ARG	5.5
2	C	147	ALA	5.2
2	C	133	PRO	4.8
2	C	163	VAL	4.7
2	C	135	ALA	4.7
2	C	132	MET	4.6
2	C	158	ILE	4.4
2	C	153	GLY	4.4
2	C	149	VAL	4.1
2	C	155	GLY	4.1
2	C	160	LYS	4.1
1	B	70	VAL	4.0
2	C	145	SER	3.9
2	C	159	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	142	LYS	3.7
2	C	152	THR	3.7
2	C	138	LEU	3.6
2	C	146	PRO	3.6
2	C	144	VAL	3.4
1	A	70	VAL	3.4
2	C	134	ALA	3.4
1	A	71	LYS	3.2
1	B	71	LYS	3.2
1	A	328	PHE	3.1
2	C	148	GLU	3.1
1	B	239	LYS	3.1
1	A	451	ARG	2.9
1	B	1	MET	2.9
2	C	150	GLN	2.9
2	C	139	MET	2.9
1	A	420	PHE	2.8
2	C	164	MET	2.8
1	B	200	ASP	2.8
1	A	216	ARG	2.7
1	B	34	LYS	2.7
2	C	151	GLY	2.6
2	C	140	GLN	2.6
2	C	143	GLY	2.6
2	C	165	ARG	2.5
1	A	124	THR	2.5
1	B	393	LYS	2.5
1	B	420	PHE	2.5
2	C	136	GLU	2.4
2	C	137	ARG	2.4
1	B	89	GLN	2.3
2	C	162	ASP	2.3
1	A	330	HIS	2.3
1	A	247	GLY	2.3
1	A	116	GLU	2.3
1	B	329	GLY	2.2
2	C	141	GLU	2.2
1	B	57	ARG	2.2
1	B	288	GLU	2.2
1	B	72	GLY	2.1
1	B	153	ARG	2.1
1	A	218	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	124	THR	2.1
1	A	383	GLU	2.1
1	A	125	GLY	2.1
1	A	288	GLU	2.0
1	B	330	HIS	2.0
1	A	131	ARG	2.0
1	B	112	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

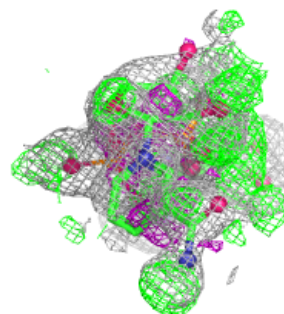
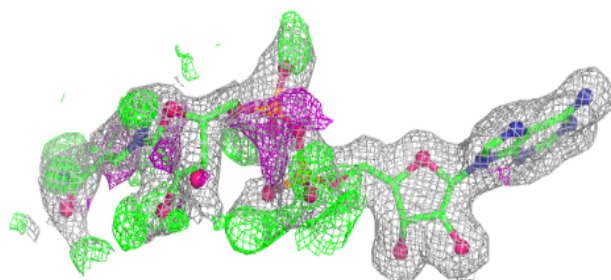
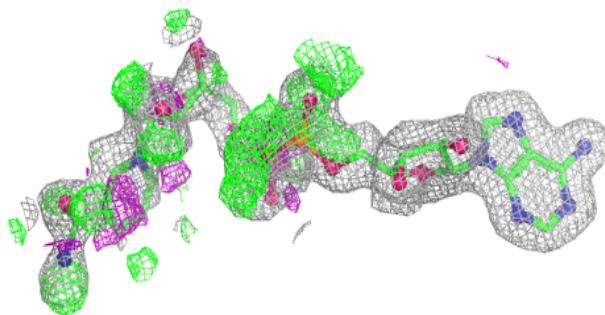
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAD	A	2483	44/44	0.88	0.16	15,28,47,47	0
4	NAD	B	1483	44/44	0.90	0.14	14,28,42,44	0
3	FAD	B	1482	53/53	0.97	0.05	8,11,14,15	0
3	FAD	A	2482	53/53	0.98	0.05	8,10,13,13	0

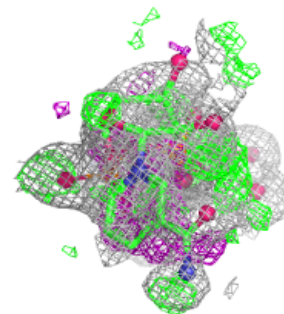
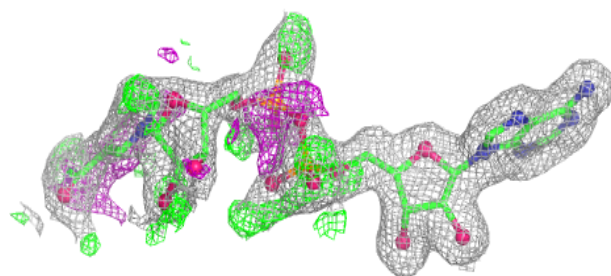
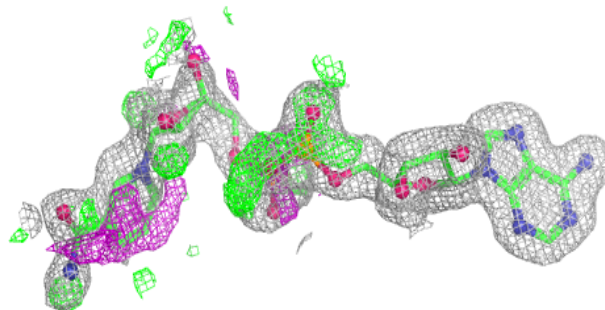
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD A 2483:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

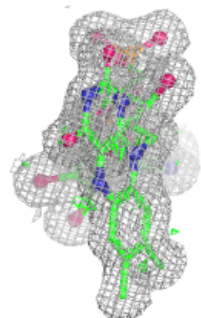
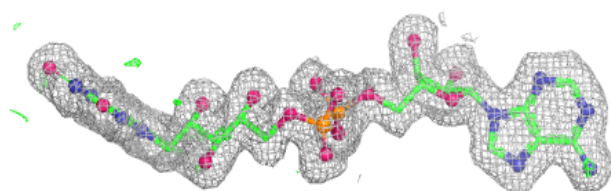
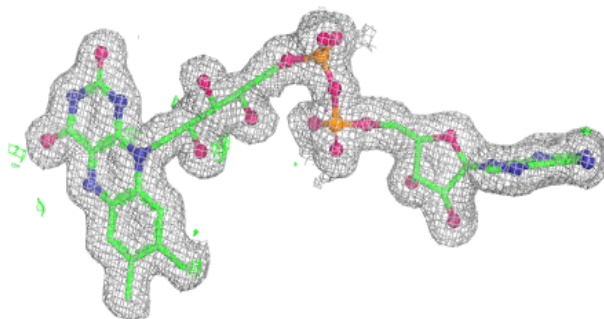
**Electron density around NAD B 1483:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

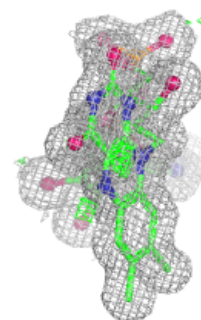
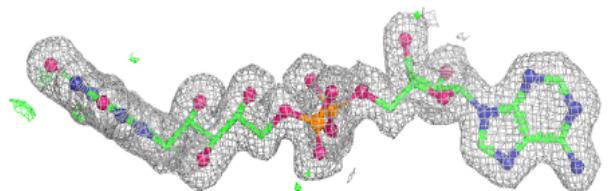
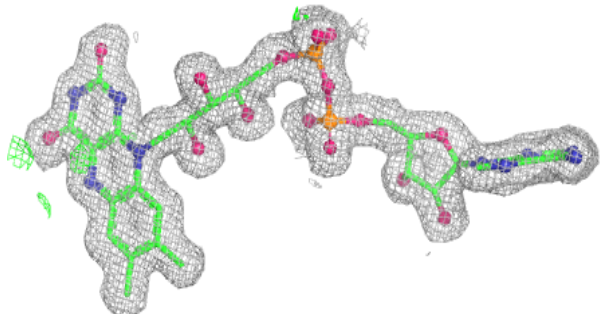


Electron density around FAD B 1482:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 2482:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.