Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2019 – 02:21 PM EST

PDB ID	:	1C1X
Title	:	L-PHENYLALANINE DEHYDROGENASE STRUCTURE IN TERNARY COMPLEX WITH NAD+ AND L-3-PHENYLLACTATE
Authors	:	Vanhooke, J.L.; Thoden, J.B.
Deposited on	:	1999-07-22
Resolution	:	1.40 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 (i) symbol.

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

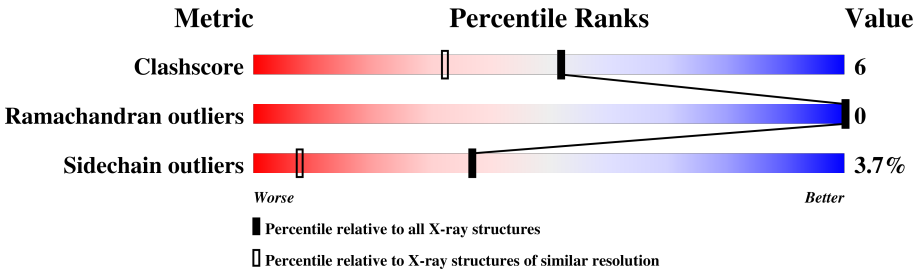
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 1.40 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	122126	1541 (1.40-1.40)
Ramachandran outliers	120053	1500 (1.40-1.40)
Sidechain outliers	120020	1499 (1.40-1.40)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	75% 19%
2	B	355	80% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	IPA	B	862	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6017 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 L-PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	3	0
			2517	1554	447	504	12			

- Molecule 2 is a protein called PROTEIN (L-PHENYLALANINE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	347	Total	C	N	O	S	0	5	0
			2522	1561	447	502	12			

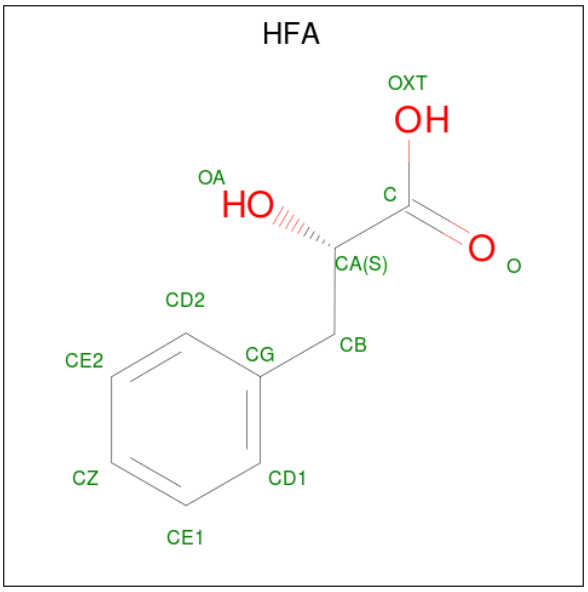
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	K	0	0
			2	2		
3	A	2	Total	K	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

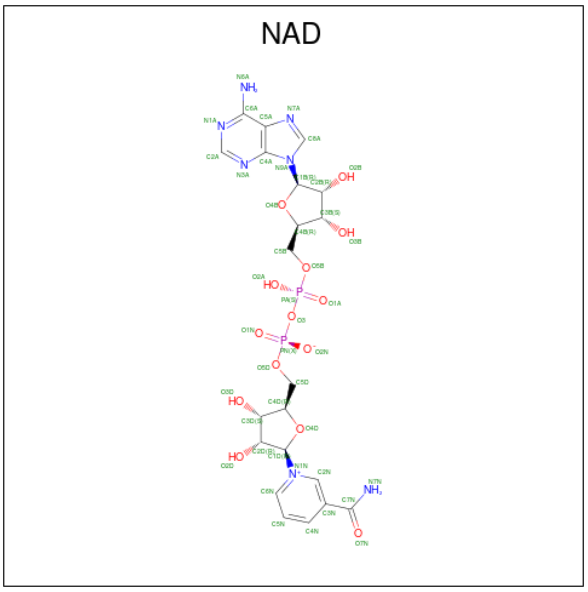
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is ALPHA-HYDROXY-BETA-PHENYL-PROPIONIC ACID (three-letter code: HFA) (formula: $C_9H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	9	3		
5	B	1	Total	C	O	0	0
			12	9	3		

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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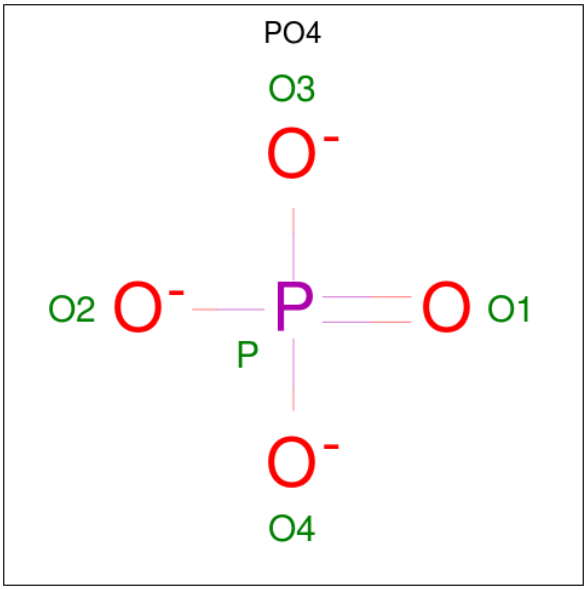
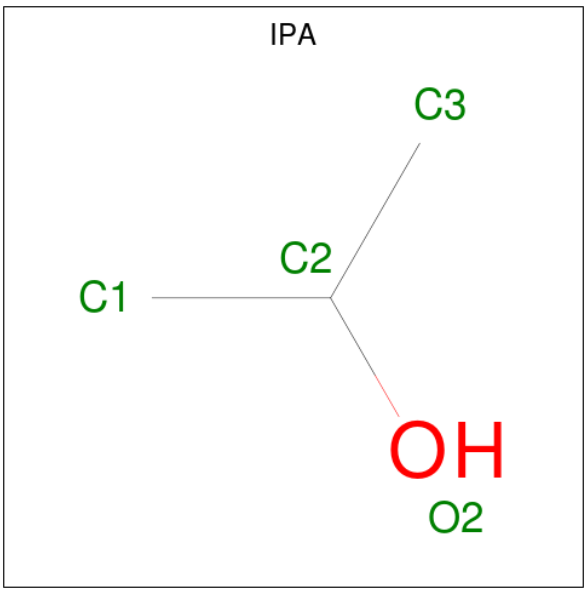
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	O	P		0	0
			5	4	1			

- Molecule 8 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 3 1	0	0
8	B	1	Total C O 4 3 1	0	0
8	B	1	Total C O 4 3 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	406	Total O 406 406	0	0
9	B	438	Total O 438 438	0	0

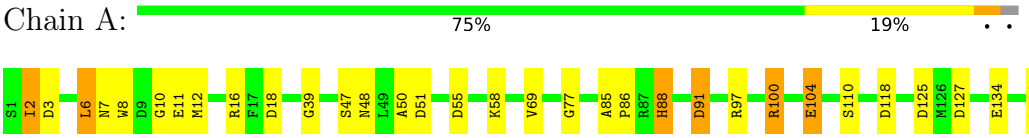
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

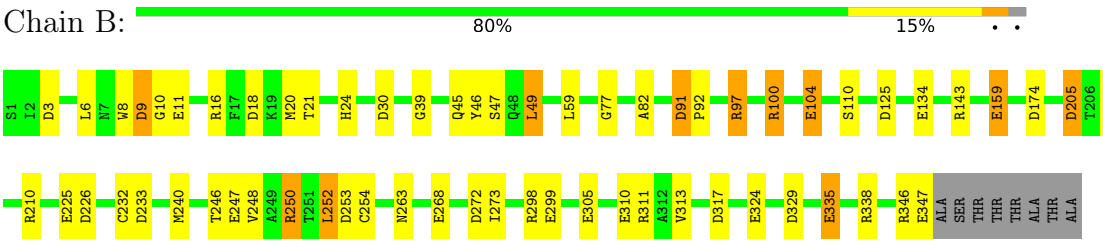
• Molecule 1: L-PHENYLALANINE DEHYDROGENASE

Chain A:



• Molecule 2: PROTEIN (L-PHENYLALANINE DEHYDROGENASE)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.60Å 110.40Å 113.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.40	Depositor
% Data completeness (in resolution range)	97.0 (30.00-1.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.180 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6017	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: IPA, NAD, NA, K, HFA, PO4

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	1.00	14/2569 (0.5%)	1.45	46/3499 (1.3%)
2	B	1.07	13/2584 (0.5%)	1.36	28/3518 (0.8%)
All	All	1.04	27/5153 (0.5%)	1.40	74/7017 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	GLU	CD-OE2	10.37	1.37	1.25
2	B	310	GLU	CD-OE2	9.03	1.35	1.25
1	A	247	GLU	CD-OE2	8.23	1.34	1.25
1	A	347	GLU	CD-OE2	7.41	1.33	1.25
2	B	11	GLU	CD-OE2	7.27	1.33	1.25
1	A	310	GLU	CD-OE2	6.97	1.33	1.25
2	B	225	GLU	CD-OE2	6.94	1.33	1.25
1	A	324	GLU	CD-OE2	6.75	1.33	1.25
1	A	335	GLU	CD-OE2	6.75	1.33	1.25
2	B	347	GLU	CD-OE2	6.64	1.32	1.25
2	B	159	GLU	CD-OE2	6.60	1.32	1.25
2	B	268	GLU	CD-OE2	6.43	1.32	1.25
1	A	104	GLU	CD-OE2	6.14	1.32	1.25
2	B	247	GLU	CD-OE2	6.12	1.32	1.25
2	B	134	GLU	CD-OE2	5.94	1.32	1.25
1	A	159	GLU	CD-OE2	5.85	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	299	GLU	CD-OE1	-5.77	1.19	1.25
2	B	305	GLU	CD-OE2	5.72	1.31	1.25
1	A	305	GLU	CD-OE2	5.63	1.31	1.25
2	B	104	GLU	CD-OE2	5.63	1.31	1.25
1	A	209	GLU	CD-OE2	5.53	1.31	1.25
2	B	324	GLU	CD-OE2	5.43	1.31	1.25
1	A	11	GLU	CD-OE2	5.41	1.31	1.25
1	A	142	GLU	CD-OE2	5.20	1.31	1.25
1	A	196	GLU	CD-OE2	5.13	1.31	1.25
1	A	225	GLU	CD-OE2	5.05	1.31	1.25
1	A	134	GLU	CD-OE2	5.04	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ASP	CB-CG-OD2	-18.91	101.28	118.30
1	A	277	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	A	3	ASP	CB-CG-OD2	-11.13	108.28	118.30
2	B	338	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	A	97	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	233	ASP	CB-CG-OD2	-8.49	110.66	118.30
2	B	205	ASP	CB-CG-OD1	8.24	125.72	118.30
1	A	16	ARG	NE-CZ-NH2	-7.63	116.48	120.30
2	B	298	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	A	334	ASP	CB-CG-OD2	-7.48	111.57	118.30
2	B	16	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	51	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	143	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	3	ASP	CB-CG-OD1	7.36	124.92	118.30
2	B	329	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	97	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	127	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	A	127	ASP	CB-CG-OD1	7.16	124.75	118.30
2	B	250	ARG	NE-CZ-NH2	-7.07	116.76	120.30
2	B	9	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	12	MET	CG-SD-CE	-6.79	89.34	100.20
1	A	277	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	267	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	346	ARG	NE-CZ-NH2	-6.69	116.95	120.30
2	B	346	ARG	NE-CZ-NH2	-6.67	116.96	120.30
2	B	100	ARG	NE-CZ-NH2	-6.59	117.01	120.30
2	B	3	ASP	CB-CG-OD2	-6.57	112.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	A	272	ASP	CB-CG-OD2	-6.41	112.53	118.30
2	B	317	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	B	18	ASP	CB-CG-OD2	-6.36	112.58	118.30
2	B	207	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	118	ASP	CB-CG-OD1	6.14	123.83	118.30
2	B	298	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	100	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	317	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	233	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	226	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	55[A]	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	55[B]	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	334	ASP	CB-CG-OD1	5.86	123.57	118.30
2	B	226	ASP	CB-CG-OD1	5.84	123.56	118.30
2	B	329	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	88	HIS	CA-CB-CG	-5.83	103.69	113.60
2	B	233	ASP	CB-CG-OD1	5.82	123.53	118.30
2	B	311	ARG	CD-NE-CZ	5.80	131.73	123.60
2	B	97	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	311	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	18	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	327	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	311	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	B	125	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	343	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	205	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	51	ASP	CB-CG-OD1	5.53	123.28	118.30
2	B	100	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	B	91	ASP	CB-CG-OD1	5.46	123.21	118.30
2	B	253	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	226	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	207	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	125	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	B	143	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	16	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	329	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	125	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	346	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	B	30	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	18	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	272	ASP	CB-CG-OD1	5.12	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	B	174	ASP	CB-CG-OD1	5.07	122.87	118.30
2	B	272	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	210	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	6	LEU	N-CA-CB	5.01	120.42	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ASP	Sidechain

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	2517	0	2465	31	0
2	B	2522	0	2478	29	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
5	A	12	0	9	0	0
5	B	12	0	9	1	0
6	A	44	0	26	1	0
6	B	44	0	26	3	0
7	B	5	0	0	0	0
8	B	12	0	24	4	0
9	A	406	0	0	4	0
9	B	438	0	0	4	1
All	All	6017	0	5037	61	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (61) 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:A:2:ILE:HD13	1:A:50:ALA:HB2	1.49	0.92
2:B:248:VAL:HG12	2:B:252:LEU:HD22	1.67	0.75
2:B:46:TYR:O	8:B:862:IPA:H13	1.87	0.74
1:A:207:ASP:OD1	1:A:210:ARG:HD2	1.90	0.71
1:A:2:ILE:CD1	1:A:50:ALA:HB2	2.21	0.71
2:B:24:HIS:CG	2:B:49:LEU:HD21	2.27	0.69
2:B:59:LEU:HD23	2:B:263:ASN:ND2	2.09	0.67
1:A:210:ARG:NH2	9:A:1813:HOH:O	2.28	0.67
2:B:49:LEU:HD22	8:B:862:IPA:C3	2.28	0.64
2:B:9:ASP:HB2	9:B:1693:HOH:O	1.98	0.63
1:A:6:LEU:HD22	9:A:1259:HOH:O	1.99	0.63
2:B:273[B]:ILE:HD13	9:B:1635:HOH:O	1.99	0.63
1:A:191:ALA:O	1:A:201:LEU:HD11	2.01	0.60
2:B:210:ARG:NH1	6:B:760:NAD:O3B	2.30	0.58
2:B:49:LEU:HD22	8:B:862:IPA:H33	1.86	0.57
1:A:306:SER:HB3	9:A:1270:HOH:O	2.05	0.57
1:A:149:SER:HB3	1:A:294:HIS:CD2	2.40	0.57
1:A:149:SER:HB3	1:A:294:HIS:HD2	1.70	0.56
2:B:45:GLN:HG2	9:B:1831:HOH:O	2.06	0.55
1:A:201:LEU:HD12	1:A:219:HIS:CE1	2.41	0.55
1:A:240:MET:HE3	1:A:243:VAL:HG12	1.89	0.54
2:B:248:VAL:CG1	2:B:252:LEU:HD22	2.38	0.54
2:B:91:ASP:HB2	2:B:92:PRO:HD2	1.88	0.54
1:A:39:GLY:HA3	1:A:77:GLY:O	2.09	0.53
1:A:184:GLY:HA3	6:A:360:NAD:O5B	2.08	0.52
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.75	0.52
1:A:240:MET:HE3	1:A:243:VAL:CG1	2.41	0.51
2:B:8:TRP:CH2	2:B:10:GLY:HA3	2.44	0.51
1:A:243:VAL:HG23	1:A:244:ILE:HG13	1.93	0.51
2:B:248:VAL:HG12	2:B:252:LEU:CD2	2.38	0.50
2:B:159:GLU:HG3	2:B:313:VAL:HA	1.93	0.50
2:B:49:LEU:HD22	8:B:862:IPA:H31	1.93	0.49
2:B:205:ASP:HA	6:B:760:NAD:N3A	2.27	0.49
1:A:88:HIS:HB2	9:A:1606:HOH:O	2.12	0.49
2:B:21:THR:CG2	2:B:97:ARG:HD3	2.42	0.49
2:B:335:GLU:HG2	9:B:1384:HOH:O	2.13	0.48
2:B:39:GLY:HA3	2:B:77:GLY:O	2.13	0.47
2:B:246:THR:O	2:B:250:ARG:HG3	2.14	0.47
1:A:191:ALA:HB1	1:A:201:LEU:HD13	1.97	0.47
2:B:232:CYS:O	2:B:254:CYS:HA	2.14	0.47
1:A:232:CYS:O	1:A:254:CYS:HA	2.15	0.46
1:A:85:ALA:HB1	1:A:86:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:761:HFA:HD2	5:B:761:HFA:C	2.46	0.45
1:A:139:ARG:HB2	1:A:145:GLY:HA3	1.98	0.45
2:B:21:THR:HG23	2:B:97:ARG:HD3	1.98	0.45
1:A:246:THR:OG1	1:A:267:ASP:OD1	2.30	0.45
2:B:59:LEU:CD2	2:B:263:ASN:ND2	2.80	0.44
1:A:100:ARG:NH1	1:A:104:GLU:OE1	2.51	0.44
1:A:149:SER:CB	1:A:294:HIS:CD2	3.00	0.44
1:A:58:LYS:HB3	1:A:263:ASN:HD21	1.83	0.44
1:A:165:VAL:HG23	1:A:166:ALA:N	2.33	0.44
2:B:100:ARG:O	2:B:104:GLU:HG3	2.19	0.43
1:A:8:TRP:CH2	1:A:10:GLY:HA3	2.54	0.43
1:A:207:ASP:CG	1:A:210:ARG:HD2	2.39	0.43
1:A:211:VAL:O	1:A:215:VAL:HG23	2.19	0.42
1:A:2:ILE:HD13	1:A:2:ILE:N	2.35	0.41
2:B:20:MET:HE3	2:B:97:ARG:CZ	2.50	0.41
2:B:100:ARG:NH1	2:B:104:GLU:OE1	2.53	0.41
1:A:58:LYS:HB3	1:A:263:ASN:ND2	2.36	0.41
2:B:205:ASP:OD1	6:B:760:NAD:H1B	2.19	0.40
2:B:24:HIS:HB2	2:B:82:ALA:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1769:HOH:O	9:B:1781:HOH:O[4_456]	2.11	0.09

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	349/355 (98%)	343 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	350/355 (99%)	346 (99%)	4 (1%)	0	100 100
All	All	699/710 (98%)	689 (99%)	10 (1%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	258/260 (99%)	244 (95%)	14 (5%)	24 3
2	B	260/260 (100%)	254 (98%)	6 (2%)	53 19
All	All	518/520 (100%)	498 (96%)	20 (4%)	37 7

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	7	ASN
1	A	47[A]	SER
1	A	47[B]	SER
1	A	48	ASN
1	A	69	VAL
1	A	110	SER
1	A	162	LYS
1	A	210	ARG
1	A	225	GLU
1	A	229	SER
1	A	240	MET
1	A	306	SER
1	A	347	GLU
2	B	6	LEU
2	B	47	SER
2	B	49	LEU
2	B	110	SER

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Mol	Chain	Res	Type
2	B	240	MET
2	B	252	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	181	GLN
1	A	200	GLN
1	A	263	ASN
1	A	309	HIS
2	B	33	GLN
2	B	181	GLN
2	B	200	GLN
2	B	263	ASN
2	B	320	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\|>2$
6	NAD	A	360	-	39,48,48	1.44	6 (15%)	44,73,73	2.38	13 (29%)
5	HFA	A	361	-	9,12,12	1.01	1 (11%)	12,15,15	1.09	1 (8%)
6	NAD	B	760	-	39,48,48	1.06	3 (7%)	44,73,73	2.59	12 (27%)
5	HFA	B	761	-	9,12,12	1.02	1 (11%)	12,15,15	0.73	0
8	IPA	B	860	-	3,3,3	0.47	0	3,3,3	0.42	0
8	IPA	B	861	-	3,3,3	0.78	0	3,3,3	0.46	0
8	IPA	B	862	-	3,3,3	0.42	0	3,3,3	0.50	0
7	PO4	B	880	3	4,4,4	1.72	1 (25%)	6,6,6	1.04	1 (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
6	NAD	A	360	-	-	1/22/62/62	0/5/5/5
5	HFA	A	361	-	-	1/4/8/8	0/1/1/1
6	NAD	B	760	-	-	3/22/62/62	0/5/5/5
5	HFA	B	761	-	-	0/4/8/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	360	NAD	C3N-C7N	4.71	1.57	1.50
6	A	360	NAD	C2N-C3N	-3.20	1.34	1.39
6	A	360	NAD	C4A-N3A	-2.94	1.31	1.35
6	A	360	NAD	O4B-C1B	-2.86	1.37	1.41
7	B	880	PO4	P-O4	-2.81	1.46	1.54
6	B	760	NAD	C4N-C3N	2.46	1.43	1.39
5	B	761	HFA	OA-CA	2.34	1.48	1.42
6	A	360	NAD	C7N-N7N	2.33	1.37	1.33
6	A	360	NAD	C4N-C3N	2.30	1.43	1.39
6	B	760	NAD	C6N-N1N	2.21	1.41	1.35
5	A	361	HFA	OA-CA	2.15	1.47	1.42
6	B	760	NAD	C2A-N1A	2.06	1.37	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	760	NAD	C5N-C4N-C3N	-7.03	111.92	120.34
6	B	760	NAD	C3N-C7N-N7N	-6.26	110.63	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	360	NAD	C6N-C5N-C4N	5.89	128.15	119.43
6	B	760	NAD	C4N-C3N-C7N	-5.84	105.52	121.06
6	A	360	NAD	C5N-C4N-C3N	-5.82	113.37	120.34
6	B	760	NAD	C6N-C5N-C4N	5.81	128.04	119.43
6	A	360	NAD	O7N-C7N-C3N	5.79	126.62	119.62
6	A	360	NAD	C5N-C6N-N1N	-5.42	112.32	120.39
6	B	760	NAD	C2N-C3N-C4N	5.36	124.42	118.26
6	A	360	NAD	C3N-C7N-N7N	-5.36	111.66	117.75
6	B	760	NAD	O7N-C7N-C3N	5.01	125.68	119.62
6	B	760	NAD	C5N-C6N-N1N	-4.72	113.36	120.39
6	A	360	NAD	C4N-C3N-C7N	-4.20	109.89	121.06
6	A	360	NAD	C2N-C3N-C7N	3.92	130.86	119.43
6	B	760	NAD	C2N-C3N-C7N	3.65	130.06	119.43
6	B	760	NAD	C5A-C6A-N6A	2.94	125.00	120.38
6	A	360	NAD	O5B-C5B-C4B	-2.90	99.00	108.99
6	B	760	NAD	C3N-C2N-N1N	-2.81	117.55	120.40
6	A	360	NAD	C4A-C5A-N7A	2.31	111.81	109.40
5	A	361	HFA	OA-CA-CB	2.27	113.61	108.53
6	A	360	NAD	O2N-PN-O5D	2.27	118.27	107.75
6	A	360	NAD	C3N-C2N-N1N	2.24	122.68	120.40
7	B	880	PO4	O4-P-O3	2.22	115.12	107.99
6	B	760	NAD	O5B-C5B-C4B	-2.19	101.42	108.99
6	A	360	NAD	C5A-C6A-N1A	-2.17	115.20	120.31
6	A	360	NAD	N6A-C6A-N1A	2.08	122.89	118.57
6	B	760	NAD	O3D-C3D-C4D	2.06	117.02	111.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	361	HFA	C-CA-CB-CG
6	B	760	NAD	O4D-C4D-C5D-O5D
6	A	360	NAD	O4B-C4B-C5B-O5B
6	B	760	NAD	O4B-C4B-C5B-O5B
6	B	760	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	360	NAD	1	0

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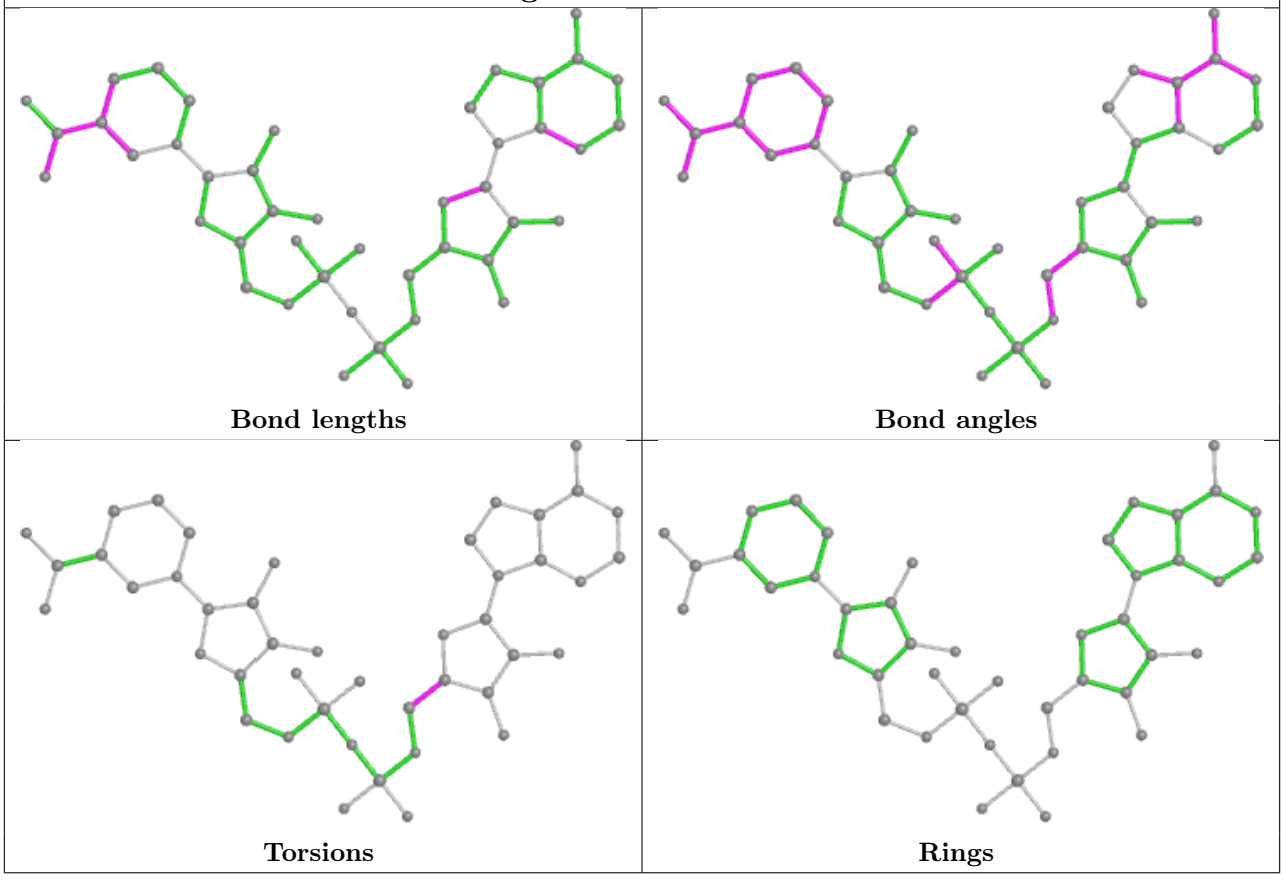
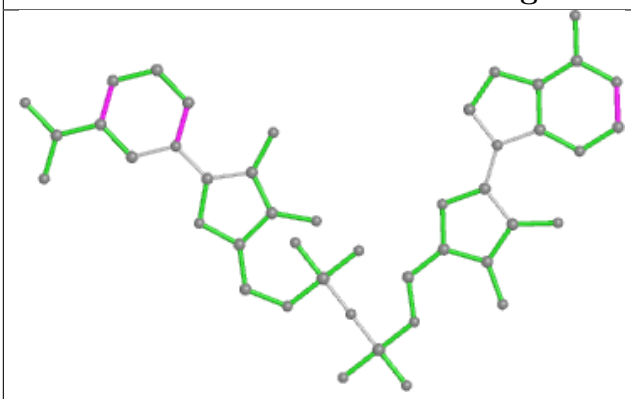
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	760	NAD	3	0
5	B	761	HFA	1	0

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 then 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.

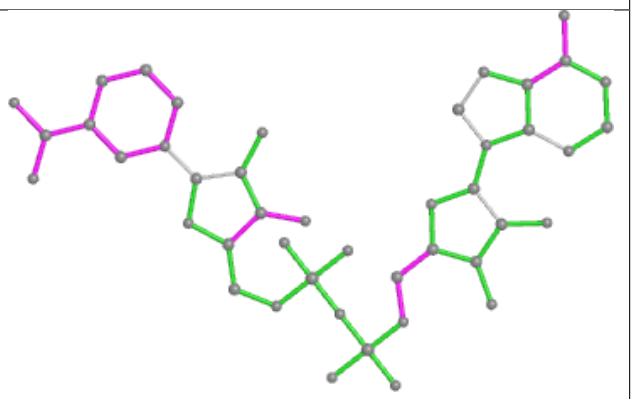
Ligand NAD A 360



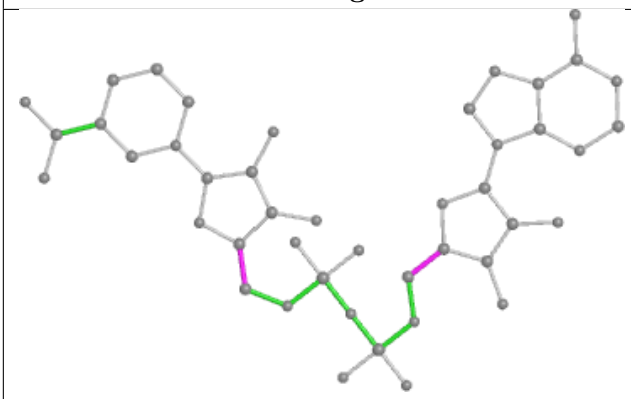
Ligand NAD B 760



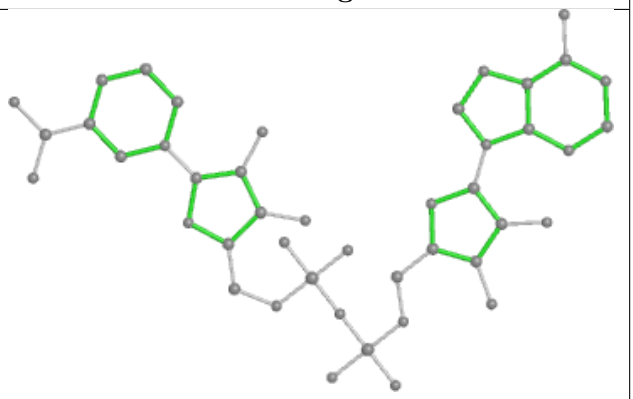
Bond lengths



Bond angles



Torsions



Rings

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.