



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:45 AM UTC

PDB ID : 2VHX / pdb_00002vhx
Title : Crystal structure of the ternary complex of L-alanine dehydrogenase from Mycobacterium tuberculosis with NAD⁺ and pyruvate
Authors : Agren, D.; Schneider, G.
Deposited on : 2007-11-26
Resolution : 2.00 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

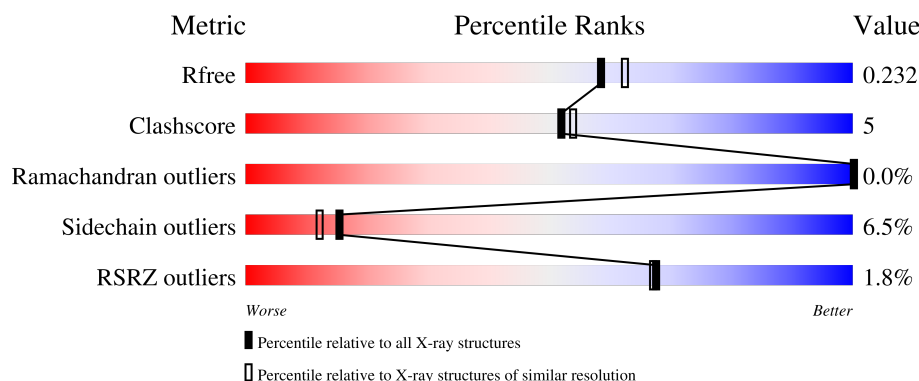
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	377	2% 81% 13% ...
1	B	377	2% 84% 12% ...
1	C	377	3% 82% 12% ...
1	D	377	2% 85% 12% ...
1	E	377	2% 87% 11% ...

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	377	% 91% 7% ..

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
3	PYR	D	1371	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17715 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.

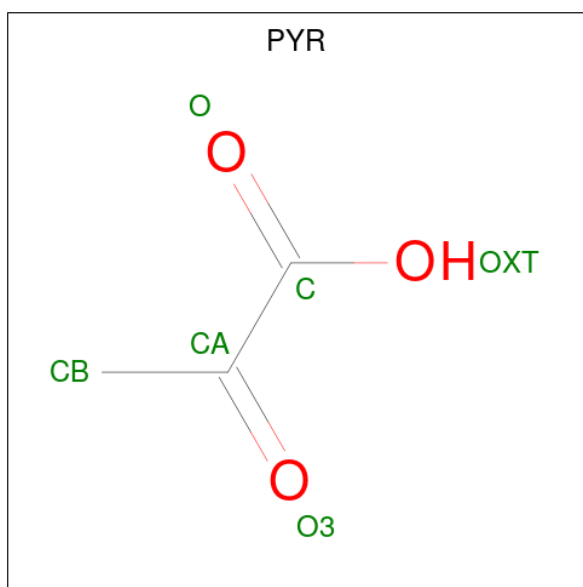
- Molecule 1 is a protein called ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	4	0
			2727	1716	482	514	15			
1	B	368	Total	C	N	O	S	0	1	0
			2707	1701	477	516	13			
1	C	365	Total	C	N	O	S	0	0	0
			2682	1686	472	511	13			
1	D	367	Total	C	N	O	S	0	3	0
			2712	1706	478	513	15			
1	E	373	Total	C	N	O	S	0	1	0
			2742	1724	485	519	14			
1	F	373	Total	C	N	O	S	0	1	0
			2742	1724	485	519	14			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

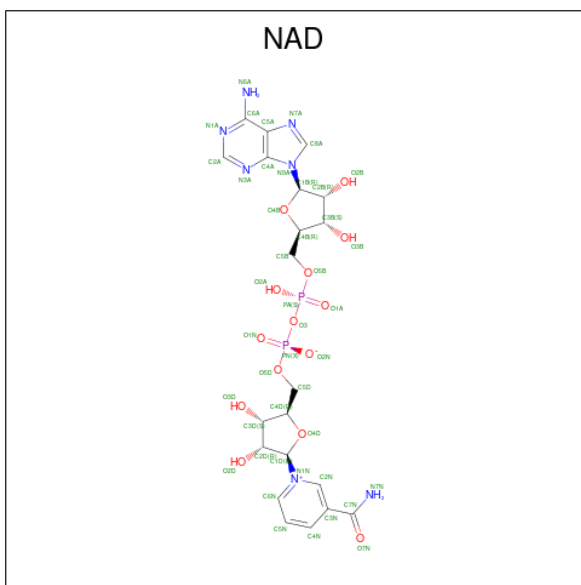
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- 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	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	F	1	Total 44	C 21	N 7	O 14	P 2	0	0

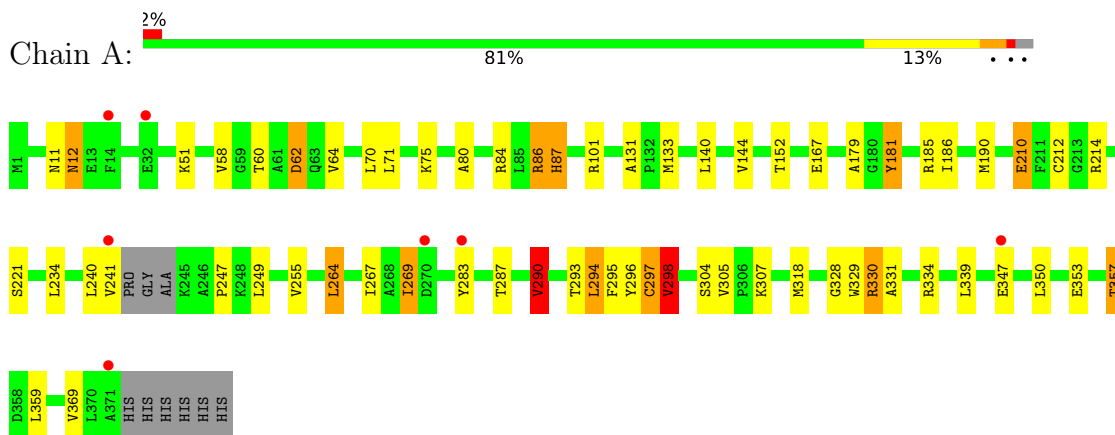
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	184	Total O 184 184	0	0
5	B	228	Total O 228 228	0	0
5	C	185	Total O 185 185	0	0
5	D	232	Total O 232 232	0	0
5	E	195	Total O 195 195	0	0
5	F	252	Total O 252 252	0	0

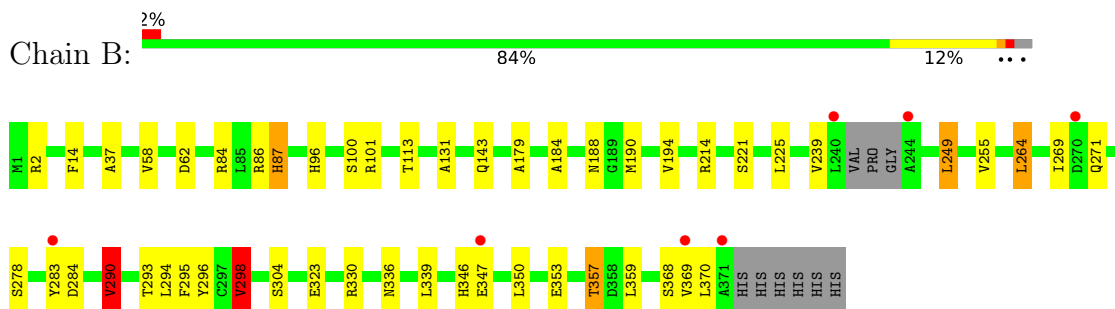
3 Residue-property plots [i](#)

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.

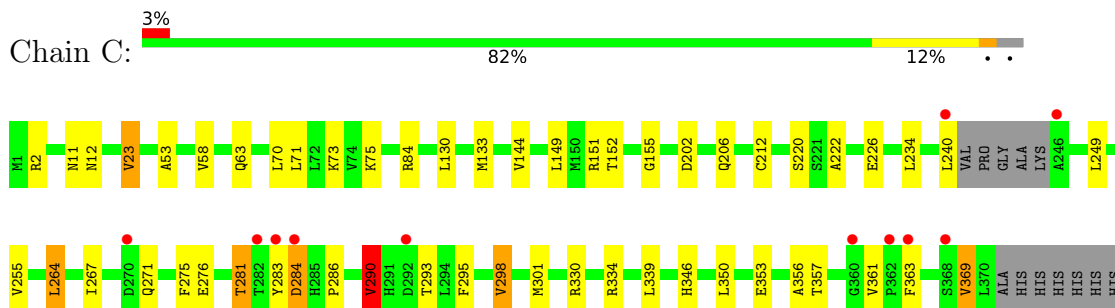
• Molecule 1: ALANINE DEHYDROGENASE



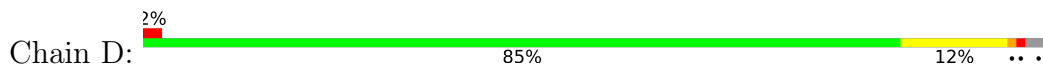
• Molecule 1: ALANINE DEHYDROGENASE

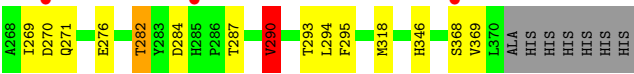


• Molecule 1: ALANINE DEHYDROGENASE

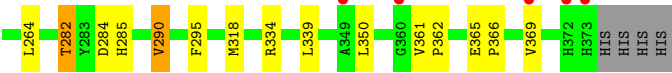
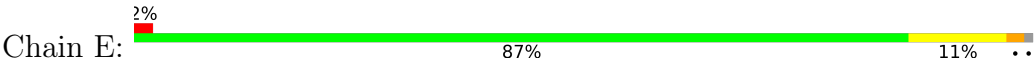


• Molecule 1: ALANINE DEHYDROGENASE

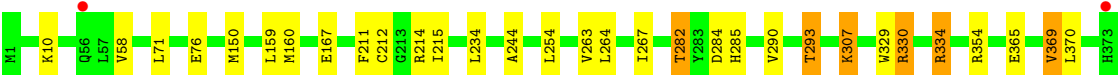
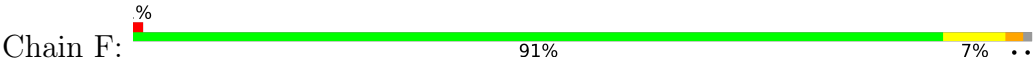




● Molecule 1: ALANINE DEHYDROGENASE



● Molecule 1: ALANINE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	176.25Å 171.77Å 98.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (40.00-2.00) 90.6 (40.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.210 0.206 , 0.232	Depositor DCC
R_{free} test set	9182 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17715	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, MG, PYR

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	0.90	2/2787 (0.1%)	1.07	10/3793 (0.3%)
1	B	0.96	4/2755 (0.1%)	1.06	8/3751 (0.2%)
1	C	0.90	0/2730	1.02	1/3718 (0.0%)
1	D	0.90	0/2769	1.02	3/3769 (0.1%)
1	E	0.78	0/2797	0.93	2/3811 (0.1%)
1	F	0.90	0/2797	0.97	1/3811 (0.0%)
All	All	0.89	6/16635 (0.0%)	1.01	25/22653 (0.1%)

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	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	VAL	CA-CB	6.17	1.61	1.54
1	B	131	ALA	CA-CB	6.00	1.59	1.54
1	B	37	ALA	CA-CB	5.84	1.63	1.53
1	A	179	ALA	CA-CB	-5.45	1.45	1.53
1	A	290	VAL	CA-CB	5.45	1.61	1.54
1	B	179	ALA	CA-CB	-5.11	1.45	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	ALA	N-CA-C	-10.11	87.48	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLU	CA-C-N	9.54	129.47	120.03
1	A	167	GLU	C-N-CA	9.54	129.47	120.03
1	E	16	VAL	CB-CA-C	-6.88	100.08	110.55
1	A	298	VAL	N-CA-CB	6.66	117.79	110.53
1	B	290	VAL	CB-CA-C	6.39	119.05	110.42
1	B	221	SER	N-CA-C	-6.34	99.66	109.24
1	E	167	GLU	N-CA-C	6.26	117.59	109.64
1	B	298	VAL	N-CA-CB	6.12	117.19	110.53
1	A	221	SER	N-CA-C	-6.08	101.21	110.14
1	B	86	ARG	CA-C-N	5.96	129.31	120.90
1	B	86	ARG	C-N-CA	5.96	129.31	120.90
1	A	290	VAL	CB-CA-C	5.92	118.41	110.42
1	C	290	VAL	CB-CA-C	5.92	117.16	110.41
1	A	12	ASN	N-CA-C	5.91	120.07	112.86
1	D	290	VAL	CB-CA-C	5.62	118.01	110.42
1	F	167	GLU	N-CA-C	5.52	116.84	109.83
1	B	100	SER	N-CA-C	5.36	116.18	107.23
1	A	210	GLU	N-CA-C	5.29	117.13	111.36
1	D	150	MET	N-CA-C	-5.19	101.99	110.20
1	A	131	ALA	CA-C-N	-5.17	113.60	119.28
1	A	131	ALA	C-N-CA	-5.17	113.60	119.28
1	A	181	TYR	N-CA-C	-5.16	105.74	111.36
1	B	190	MET	N-CA-C	-5.15	106.77	113.16
1	B	184	ALA	N-CA-C	-5.10	105.72	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	245	LYS	Peptide

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	2727	0	2756	42	0
1	B	2707	0	2716	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2682	0	2689	30	0
1	D	2712	0	2734	25	0
1	E	2742	0	2751	25	0
1	F	2742	0	2751	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	0	2	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	2	0
3	F	6	0	0	3	0
4	E	44	0	26	3	0
4	F	44	0	26	4	0
5	A	184	0	0	3	0
5	B	228	0	0	3	0
5	C	185	0	0	1	0
5	D	232	0	0	1	0
5	E	195	0	0	3	0
5	F	252	0	0	3	0
All	All	17715	0	16449	167	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 5.

All (167) 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:F:282:THR:HG22	1:F:285:HIS:H	1.39	0.86
1:D:267:ILE:HG22	1:D:267:ILE:O	1.75	0.86
1:A:269:ILE:HG13	1:A:297:CYS:HB3	1.58	0.84
1:A:75:LYS:NZ	3:A:1373:PYR:CB	2.41	0.82
1:C:281:THR:HG21	1:C:286:PRO:O	1.80	0.80
1:E:240:LEU:HG	4:E:1375:NAD:H3D	1.64	0.79
1:B:255:VAL:HG11	1:B:290:VAL:HG22	1.66	0.76
1:B:101:ARG:NH1	1:B:359:LEU:O	2.20	0.74
1:A:75:LYS:HZ3	3:A:1373:PYR:CB	2.00	0.74
1:A:353:GLU:O	1:A:357:THR:HG23	1.88	0.73
1:B:113:THR:OG1	1:B:346:HIS:HD2	1.71	0.73
1:D:255:VAL:HG11	1:D:290:VAL:HG22	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLU:O	1:B:357:THR:HG23	1.91	0.70
1:C:330:ARG:HD3	1:C:334:ARG:NH2	2.06	0.70
1:A:101:ARG:NH1	1:A:359:LEU:O	2.26	0.69
1:C:222:ALA:O	1:C:226:GLU:HG3	1.95	0.67
3:F:1375:PYR:CB	4:F:1376:NAD:C5N	2.72	0.67
1:F:282:THR:HG23	1:F:284:ASP:H	1.61	0.66
1:A:318[B]:MET:HE3	5:A:2014:HOH:O	1.95	0.65
1:E:255:VAL:HG11	1:E:290:VAL:HG22	1.78	0.65
1:E:282:THR:HG22	1:E:285:HIS:H	1.62	0.65
3:E:1374:PYR:CB	4:E:1375:NAD:C4N	2.75	0.65
1:B:62:ASP:OD1	1:B:84:ARG:HD3	1.96	0.64
1:B:87:HIS:CE1	1:B:347:GLU:HG2	2.31	0.64
1:D:244:ALA:O	1:D:245:LYS:HB3	1.98	0.64
1:D:318[B]:MET:HG2	5:D:2198:HOH:O	1.98	0.64
3:E:1374:PYR:CB	4:E:1375:NAD:C5N	2.77	0.63
1:A:329:TRP:H	1:A:330[A]:ARG:HH21	1.48	0.62
1:D:113:THR:OG1	1:D:346:HIS:HD2	1.83	0.62
1:E:2:ARG:HG2	1:E:32:GLU:HB2	1.82	0.62
1:E:60:THR:HG22	1:E:62:ASP:H	1.64	0.62
1:A:255:VAL:HG11	1:A:290:VAL:HG22	1.83	0.60
1:A:214:ARG:HG3	1:B:214:ARG:HG3	1.84	0.60
1:A:58:VAL:HG21	1:A:64:VAL:HG22	1.84	0.59
1:D:240:LEU:HD23	1:D:271:GLN:HE22	1.67	0.58
1:B:87:HIS:HE1	1:B:347:GLU:HG2	1.69	0.58
1:A:247:PRO:HG2	1:A:249:LEU:HD11	1.87	0.57
1:B:188:ASN:HD21	1:B:214:ARG:HD3	1.72	0.55
1:C:63:GLN:NE2	5:C:2036:HOH:O	2.38	0.55
1:D:222:ALA:O	1:D:226:GLU:HG3	2.07	0.55
1:D:267:ILE:O	1:D:267:ILE:CG2	2.47	0.54
1:F:330:ARG:HD2	5:F:2212:HOH:O	2.07	0.54
1:A:58:VAL:HG21	1:A:64:VAL:CG2	2.37	0.54
1:E:20:PRO:HA	1:E:23:VAL:HG13	1.90	0.54
1:A:329:TRP:H	1:A:330[A]:ARG:NH2	2.06	0.54
1:B:296:TYR:CZ	1:B:298:VAL:HG13	2.43	0.54
1:D:290:VAL:HG13	1:D:295:PHE:CD1	2.42	0.54
3:F:1375:PYR:CB	4:F:1376:NAD:C4N	2.86	0.53
1:E:290:VAL:HG13	1:E:295:PHE:CD1	2.43	0.53
1:B:296:TYR:CE2	1:B:298:VAL:HG13	2.43	0.53
1:B:290:VAL:HG13	1:B:295:PHE:CD1	2.43	0.53
1:C:281:THR:HG23	1:C:286:PRO:HA	1.90	0.53
1:A:283:TYR:CD1	1:C:152:THR:HG21	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:THR:CG2	1:C:298:VAL:HG12	2.39	0.53
1:E:282:THR:HG23	1:E:284:ASP:H	1.75	0.52
1:B:330:ARG:HG3	5:B:2215:HOH:O	2.09	0.52
1:D:269:ILE:C	1:D:271:GLN:H	2.18	0.52
1:F:214:ARG:NH2	5:F:2141:HOH:O	2.38	0.52
1:F:290:VAL:O	1:F:293:THR:HB	2.10	0.52
1:B:96:HIS:HD2	5:B:2061:HOH:O	1.93	0.52
1:C:255:VAL:HG11	1:C:290:VAL:HG22	1.91	0.52
1:A:58:VAL:CG2	1:A:64:VAL:CG2	2.88	0.51
1:A:249:LEU:HD12	1:A:249:LEU:N	2.26	0.51
1:A:62:ASP:HB3	1:A:84:ARG:HD3	1.91	0.51
1:C:330:ARG:HD3	1:C:334:ARG:HH22	1.74	0.51
1:E:60:THR:HG22	1:E:62:ASP:N	2.26	0.51
1:D:282:THR:HG22	1:D:284:ASP:N	2.26	0.50
1:E:361:VAL:HG13	1:E:362:PRO:HD2	1.93	0.50
1:B:188:ASN:HD21	1:B:214:ARG:CD	2.24	0.50
1:E:156:ARG:O	1:F:307:LYS:HE3	2.11	0.50
1:C:290:VAL:HG13	1:C:295:PHE:CD1	2.47	0.50
1:C:23:VAL:HG22	1:C:53:ALA:HB1	1.92	0.50
1:A:287:THR:HB	1:A:294:LEU:HD22	1.93	0.50
1:A:318[B]:MET:HA	1:A:318[B]:MET:HE2	1.94	0.50
1:D:282:THR:HG22	1:D:284:ASP:H	1.77	0.50
1:E:51:LYS:HD2	1:E:57:LEU:HD12	1.94	0.50
1:A:330[A]:ARG:NE	1:A:330[A]:ARG:H	2.09	0.50
1:D:239:VAL:HG21	1:D:249:LEU:HD22	1.93	0.50
1:E:282:THR:CG2	1:E:284:ASP:H	2.24	0.49
1:A:58:VAL:CG2	1:A:64:VAL:HG22	2.42	0.49
1:E:214:ARG:NH2	5:E:2110:HOH:O	2.34	0.49
1:F:334:ARG:HD2	1:F:370:LEU:O	2.11	0.49
1:D:250:VAL:HG13	1:D:254:LEU:HD23	1.95	0.48
1:A:133:MET:HA	1:A:133:MET:HE2	1.95	0.48
1:C:23:VAL:HG22	1:C:53:ALA:CB	2.43	0.48
1:F:329:TRP:HH2	1:F:369:VAL:HG13	1.78	0.47
1:C:356:ALA:CB	1:C:363:PHE:HB2	2.44	0.47
1:F:264:LEU:HD13	1:F:293:THR:CG2	2.45	0.47
1:A:329:TRP:CE2	1:A:330[A]:ARG:HG3	2.49	0.47
1:A:331:ALA:HA	1:A:334[B]:ARG:HD3	1.97	0.47
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.79	0.47
1:F:330:ARG:HD3	1:F:334:ARG:CZ	2.45	0.47
1:A:249:LEU:N	1:A:249:LEU:CD1	2.78	0.47
1:D:65:TRP:CD1	1:D:84:ARG:HD3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:HG11	1:B:290:VAL:CG2	2.41	0.47
1:A:152:THR:HG21	1:C:283:TYR:CD1	2.51	0.46
1:B:284:ASP:OD1	1:B:284:ASP:N	2.38	0.46
1:C:202:ASP:O	1:C:206:GLN:HG3	2.15	0.46
1:A:87:HIS:NE2	1:A:347:GLU:HG2	2.29	0.46
1:E:282:THR:CG2	1:E:284:ASP:HB2	2.45	0.46
1:C:267:ILE:HG12	1:C:301:MET:HE1	1.97	0.46
1:C:281:THR:HG22	1:C:298:VAL:HA	1.98	0.46
1:E:366:PRO:HD2	5:E:2187:HOH:O	2.16	0.45
1:E:20:PRO:HA	1:E:23:VAL:CG1	2.45	0.45
1:D:247:PRO:HB2	1:D:249:LEU:CD1	2.47	0.45
1:F:244:ALA:HB2	1:F:354:ARG:HG2	1.99	0.45
1:C:284:ASP:OD1	1:C:284:ASP:N	2.48	0.45
1:D:239:VAL:HG21	1:D:249:LEU:CD2	2.46	0.45
1:D:25:GLU:O	1:D:29:ARG:HG3	2.16	0.45
1:C:346:HIS:CD2	1:C:369:VAL:HG11	2.52	0.45
1:A:240:LEU:C	1:A:240:LEU:HD23	2.42	0.45
1:F:211:PHE:CD1	1:F:215:ILE:HD12	2.52	0.44
1:D:248:LYS:HD3	1:D:276:GLU:HA	1.99	0.44
1:C:73:LYS:HE3	1:C:75:LYS:O	2.18	0.44
1:B:336:ASN:HD22	1:B:336:ASN:C	2.26	0.44
1:D:85:LEU:HD13	1:D:107:LEU:HD23	1.99	0.44
1:C:353:GLU:O	1:C:357:THR:HG23	2.18	0.44
1:F:365:GLU:HG3	5:F:2242:HOH:O	2.18	0.44
1:A:329:TRP:N	1:A:330[A]:ARG:HH21	2.14	0.44
1:E:19:THR:HB	1:E:20:PRO:HD2	1.99	0.43
1:A:328:GLY:CA	1:A:330[A]:ARG:HH21	2.30	0.43
1:A:331:ALA:O	1:A:334[B]:ARG:HB2	2.18	0.43
1:A:11:ASN:HD22	1:A:12:ASN:N	2.17	0.43
1:B:269:ILE:HD13	1:B:278:SER:HB3	2.00	0.43
1:C:133:MET:HA	1:C:133:MET:HE2	1.99	0.43
1:C:264:LEU:HG	1:C:295:PHE:CE1	2.54	0.43
1:D:211:PHE:CD1	1:D:215:ILE:HD12	2.54	0.43
1:A:87:HIS:CD2	1:A:347:GLU:HG2	2.53	0.43
1:E:140:LEU:HD22	1:F:150:MET:HE3	1.99	0.43
1:B:283:TYR:CE1	1:B:304[A]:SER:OG	2.68	0.43
1:B:283:TYR:HE1	1:B:304[A]:SER:OG	2.02	0.43
1:A:186:ILE:O	1:A:190:MET:HG3	2.18	0.43
1:C:11:ASN:O	1:C:12:ASN:HB2	2.18	0.43
1:E:318:MET:HE3	5:E:2011:HOH:O	2.18	0.43
1:A:267:ILE:C	1:A:269:ILE:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:HD12	1:D:116:ALA:HB2	2.01	0.42
1:B:225:LEU:C	1:B:225:LEU:HD23	2.44	0.42
1:A:181:TYR:OH	1:A:210:GLU:OE1	2.32	0.42
1:B:143:GLN:HG2	1:D:190:MET:CE	2.49	0.42
1:E:47:ASP:HB3	1:E:57:LEU:HD13	2.00	0.42
1:A:80:ALA:HB3	5:A:2005:HOH:O	2.20	0.42
1:B:283:TYR:CD1	1:D:152:THR:HG21	2.55	0.42
1:F:234:LEU:HD12	1:F:263:VAL:O	2.20	0.42
1:B:239:VAL:HG21	1:B:249:LEU:CD2	2.50	0.41
1:B:264:LEU:HG	1:B:295:PHE:CE1	2.55	0.41
1:C:151:ARG:HD3	1:C:155:GLY:O	2.20	0.41
1:A:264:LEU:HG	1:A:295:PHE:CE1	2.55	0.41
1:B:14:PHE:CE2	5:B:2014:HOH:O	2.70	0.41
3:F:1375:PYR:CA	4:F:1376:NAD:C4N	2.98	0.41
1:A:283:TYR:CE1	1:A:304:SER:HB3	2.55	0.41
1:A:86:ARG:NH1	5:A:2050:HOH:O	2.53	0.41
1:A:140:LEU:HD11	1:A:305:VAL:HG22	2.03	0.41
1:E:175:GLY:O	1:E:180:GLY:HA3	2.20	0.41
1:A:296:TYR:CZ	1:A:298:VAL:HG13	2.56	0.41
1:E:65:TRP:CD1	1:E:84:ARG:HD3	2.56	0.41
1:F:10:LYS:HE3	1:F:76:GLU:OE2	2.21	0.41
1:C:23:VAL:CG2	1:C:53:ALA:CB	2.99	0.41
1:D:287:THR:HA	1:D:295:PHE:O	2.21	0.41
1:F:267:ILE:O	4:F:1376:NAD:H2N	2.21	0.41
1:F:329:TRP:CH2	1:F:369:VAL:HG13	2.56	0.41
1:C:275:PHE:O	1:C:276:GLU:C	2.63	0.40
1:F:264:LEU:CD1	1:F:293:THR:HG23	2.51	0.40
1:E:104:THR:HG22	1:E:108:LEU:HD22	2.02	0.40
1:C:23:VAL:CG2	1:C:53:ALA:HB3	2.52	0.40
1:C:151:ARG:HD3	1:C:151:ARG:HA	1.65	0.40
1:E:157:GLY:O	1:F:307:LYS:HB2	2.22	0.40
1:F:159:LEU:O	1:F:160:MET:C	2.64	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	368/377 (98%)	360 (98%)	8 (2%)	0	100	100
1	B	365/377 (97%)	358 (98%)	7 (2%)	0	100	100
1	C	361/377 (96%)	357 (99%)	4 (1%)	0	100	100
1	D	366/377 (97%)	358 (98%)	7 (2%)	1 (0%)	36	35
1	E	372/377 (99%)	366 (98%)	6 (2%)	0	100	100
1	F	372/377 (99%)	367 (99%)	5 (1%)	0	100	100
All	All	2204/2262 (97%)	2166 (98%)	37 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	245	LYS

5.3.2 Protein sidechains ⓘ

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	279/282 (99%)	252 (90%)	27 (10%)	8	5
1	B	275/282 (98%)	258 (94%)	17 (6%)	16	13
1	C	273/282 (97%)	249 (91%)	24 (9%)	9	6
1	D	277/282 (98%)	264 (95%)	13 (5%)	23	22
1	E	279/282 (99%)	259 (93%)	20 (7%)	13	10
1	F	279/282 (99%)	268 (96%)	11 (4%)	28	28
All	All	1662/1692 (98%)	1550 (93%)	112 (7%)	15	11

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	60	THR
1	A	62	ASP
1	A	70	LEU
1	A	71	LEU
1	A	86	ARG
1	A	87	HIS
1	A	144	VAL
1	A	185	ARG
1	A	212[A]	CYS
1	A	212[B]	CYS
1	A	234	LEU
1	A	241	VAL
1	A	264	LEU
1	A	269	ILE
1	A	290	VAL
1	A	293	THR
1	A	294	LEU
1	A	297	CYS
1	A	298	VAL
1	A	307	LYS
1	A	330[A]	ARG
1	A	330[B]	ARG
1	A	339	LEU
1	A	350	LEU
1	A	357	THR
1	A	369	VAL
1	B	2	ARG
1	B	58	VAL
1	B	87	HIS
1	B	249	LEU
1	B	264	LEU
1	B	271	GLN
1	B	290	VAL
1	B	293	THR
1	B	294	LEU
1	B	298	VAL
1	B	323	GLU
1	B	339	LEU
1	B	350	LEU
1	B	357	THR
1	B	368	SER
1	B	369	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	370	LEU
1	C	2	ARG
1	C	23	VAL
1	C	58	VAL
1	C	70	LEU
1	C	71	LEU
1	C	84	ARG
1	C	130	LEU
1	C	144	VAL
1	C	212	CYS
1	C	220	SER
1	C	234	LEU
1	C	240	LEU
1	C	249	LEU
1	C	264	LEU
1	C	271	GLN
1	C	281	THR
1	C	284	ASP
1	C	290	VAL
1	C	293	THR
1	C	298	VAL
1	C	339	LEU
1	C	350	LEU
1	C	361	VAL
1	C	369	VAL
1	D	58	VAL
1	D	71	LEU
1	D	185	ARG
1	D	202	ASP
1	D	240	LEU
1	D	264	LEU
1	D	270	ASP
1	D	282	THR
1	D	290	VAL
1	D	293	THR
1	D	294	LEU
1	D	368	SER
1	D	369	VAL
1	E	3	VAL
1	E	16	VAL
1	E	23	VAL
1	E	70	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	71	LEU
1	E	108	LEU
1	E	144	VAL
1	E	197	LEU
1	E	212[A]	CYS
1	E	212[B]	CYS
1	E	240	LEU
1	E	254	LEU
1	E	264	LEU
1	E	282	THR
1	E	290	VAL
1	E	334	ARG
1	E	339	LEU
1	E	350	LEU
1	E	365	GLU
1	E	369	VAL
1	F	58	VAL
1	F	71	LEU
1	F	212[A]	CYS
1	F	212[B]	CYS
1	F	254	LEU
1	F	282	THR
1	F	293	THR
1	F	307	LYS
1	F	330	ARG
1	F	334	ARG
1	F	369	VAL

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	63	GLN
1	A	121	GLN
1	A	188	ASN
1	A	216	HIS
1	A	285	HIS
1	A	291	HIS
1	A	315	ASN
1	A	336	ASN
1	B	96	HIS
1	B	143	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	GLN
1	B	188	ASN
1	B	336	ASN
1	B	346	HIS
1	C	63	GLN
1	C	87	HIS
1	C	89	GLN
1	C	96	HIS
1	C	153	GLN
1	C	216	HIS
1	C	300	ASN
1	D	11	ASN
1	D	121	GLN
1	D	206	GLN
1	D	216	HIS
1	D	300	ASN
1	D	346	HIS
1	E	11	ASN
1	E	12	ASN
1	E	148	HIS
1	E	206	GLN
1	E	216	HIS
1	E	291	HIS
1	E	373	HIS
1	F	148	HIS

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

Of 11 ligands modelled in this entry, 3 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$
4	NAD	E	1375	-	46,48,48	1.69	5 (10%)	64,73,73	1.73	12 (18%)
3	PYR	A	1373	-	5,5,5	2.80	3 (60%)	3,6,6	2.08	1 (33%)
3	PYR	D	1371	-	5,5,5	2.94	3 (60%)	3,6,6	2.05	2 (66%)
3	PYR	C	1371	-	5,5,5	3.13	3 (60%)	3,6,6	0.96	0
3	PYR	B	1373	-	5,5,5	3.05	3 (60%)	3,6,6	2.10	1 (33%)
4	NAD	F	1376	-	46,48,48	1.74	6 (13%)	64,73,73	1.81	17 (26%)
3	PYR	F	1375	-	5,5,5	2.57	3 (60%)	3,6,6	1.96	2 (66%)
3	PYR	E	1374	-	5,5,5	2.80	3 (60%)	3,6,6	2.21	1 (33%)

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
4	NAD	E	1375	-	-	4/30/62/62	0/5/5/5
3	PYR	A	1373	-	-	0/4/4/4	-
3	PYR	D	1371	-	-	1/4/4/4	-
3	PYR	C	1371	-	-	0/4/4/4	-
3	PYR	B	1373	-	-	0/4/4/4	-
4	NAD	F	1376	-	-	3/30/62/62	0/5/5/5
3	PYR	F	1375	-	-	0/4/4/4	-
3	PYR	E	1374	-	-	0/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1375	NAD	O7N-C7N	8.44	1.39	1.24
4	F	1376	NAD	O7N-C7N	7.70	1.38	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1373	PYR	CA-C	-5.25	1.36	1.54
3	E	1374	PYR	CA-C	-5.12	1.37	1.54
3	C	1371	PYR	CA-C	-4.85	1.38	1.54
3	A	1373	PYR	CA-C	-4.51	1.39	1.54
3	F	1375	PYR	CA-C	-4.37	1.39	1.54
4	F	1376	NAD	C2A-N1A	4.17	1.41	1.33
3	D	1371	PYR	CA-C	-4.01	1.41	1.54
3	D	1371	PYR	O3-CA	3.91	1.32	1.23
4	F	1376	NAD	C2A-N3A	3.79	1.40	1.33
4	E	1375	NAD	C2A-N1A	3.65	1.40	1.33
3	C	1371	PYR	O3-CA	3.54	1.31	1.23
3	D	1371	PYR	O-C	3.41	1.31	1.22
3	C	1371	PYR	O-C	3.38	1.30	1.22
3	B	1373	PYR	O3-CA	3.30	1.30	1.23
3	A	1373	PYR	O3-CA	3.13	1.30	1.23
3	A	1373	PYR	O-C	2.98	1.29	1.22
3	F	1375	PYR	O3-CA	2.98	1.30	1.23
4	F	1376	NAD	C8A-N7A	2.95	1.37	1.31
4	E	1375	NAD	C2A-N3A	2.77	1.38	1.33
4	F	1376	NAD	C5A-N7A	-2.77	1.34	1.39
3	B	1373	PYR	O-C	2.76	1.29	1.22
3	E	1374	PYR	O3-CA	2.61	1.29	1.23
4	E	1375	NAD	C5A-N7A	-2.51	1.34	1.39
3	E	1374	PYR	O-C	2.43	1.28	1.22
4	E	1375	NAD	C8A-N7A	2.15	1.35	1.31
3	F	1375	PYR	O-C	2.07	1.27	1.22
4	F	1376	NAD	C4A-N3A	2.03	1.38	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1376	NAD	C3N-C7N-N7N	5.78	124.86	117.74
4	F	1376	NAD	N3A-C2A-N1A	-5.16	120.77	128.58
4	E	1375	NAD	N3A-C2A-N1A	-4.97	121.06	128.58
4	E	1375	NAD	C5A-C4A-N3A	-4.64	120.33	126.72
4	E	1375	NAD	N9A-C8A-N7A	-4.58	107.44	113.94
4	E	1375	NAD	C5A-N7A-C8A	3.97	109.69	103.45
3	B	1373	PYR	OXT-C-CA	3.50	123.30	113.59
4	E	1375	NAD	N3A-C4A-N9A	3.50	133.12	127.17
4	F	1376	NAD	C5A-C4A-N3A	-3.45	121.97	126.72
4	F	1376	NAD	O7N-C7N-C3N	-3.43	115.40	119.60
4	E	1375	NAD	C2A-N3A-C4A	3.36	120.04	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1375	NAD	C4D-O4D-C1D	-3.27	106.93	109.92
4	F	1376	NAD	C6N-N1N-C1D	3.27	126.14	119.73
4	F	1376	NAD	N9A-C8A-N7A	-3.25	109.33	113.94
4	F	1376	NAD	C4D-O4D-C1D	-3.22	106.98	109.92
3	E	1374	PYR	OXT-C-CA	3.11	122.21	113.59
3	A	1373	PYR	OXT-C-CA	3.09	122.16	113.59
4	F	1376	NAD	N3A-C4A-N9A	2.91	132.11	127.17
4	F	1376	NAD	C2N-N1N-C1D	-2.82	112.90	119.13
4	E	1375	NAD	C3N-C7N-N7N	2.68	121.04	117.74
4	F	1376	NAD	O2A-PA-O3	2.63	114.38	107.27
3	D	1371	PYR	OXT-C-CA	2.50	120.53	113.59
4	E	1375	NAD	C6A-C5A-C4A	2.50	120.59	117.18
4	E	1375	NAD	C4A-N9A-C8A	2.46	108.32	105.74
4	F	1376	NAD	C5A-N7A-C8A	2.41	107.24	103.45
4	F	1376	NAD	C2A-N3A-C4A	2.37	117.61	111.83
4	F	1376	NAD	C6A-C5A-C4A	2.31	120.33	117.18
3	F	1375	PYR	OXT-C-CA	2.28	119.90	113.59
4	E	1375	NAD	C4A-C5A-N7A	-2.27	107.99	110.58
3	F	1375	PYR	OXT-C-O	-2.24	118.56	123.90
3	D	1371	PYR	OXT-C-O	-2.20	118.67	123.90
4	F	1376	NAD	C5A-C6A-N6A	-2.10	118.08	123.29
4	F	1376	NAD	N6A-C6A-N1A	2.07	122.99	118.38
4	F	1376	NAD	C4A-N9A-C8A	2.06	107.91	105.74
4	F	1376	NAD	O2N-PN-O1N	2.02	121.83	112.44
4	E	1375	NAD	O4B-C4B-C3B	2.01	109.15	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

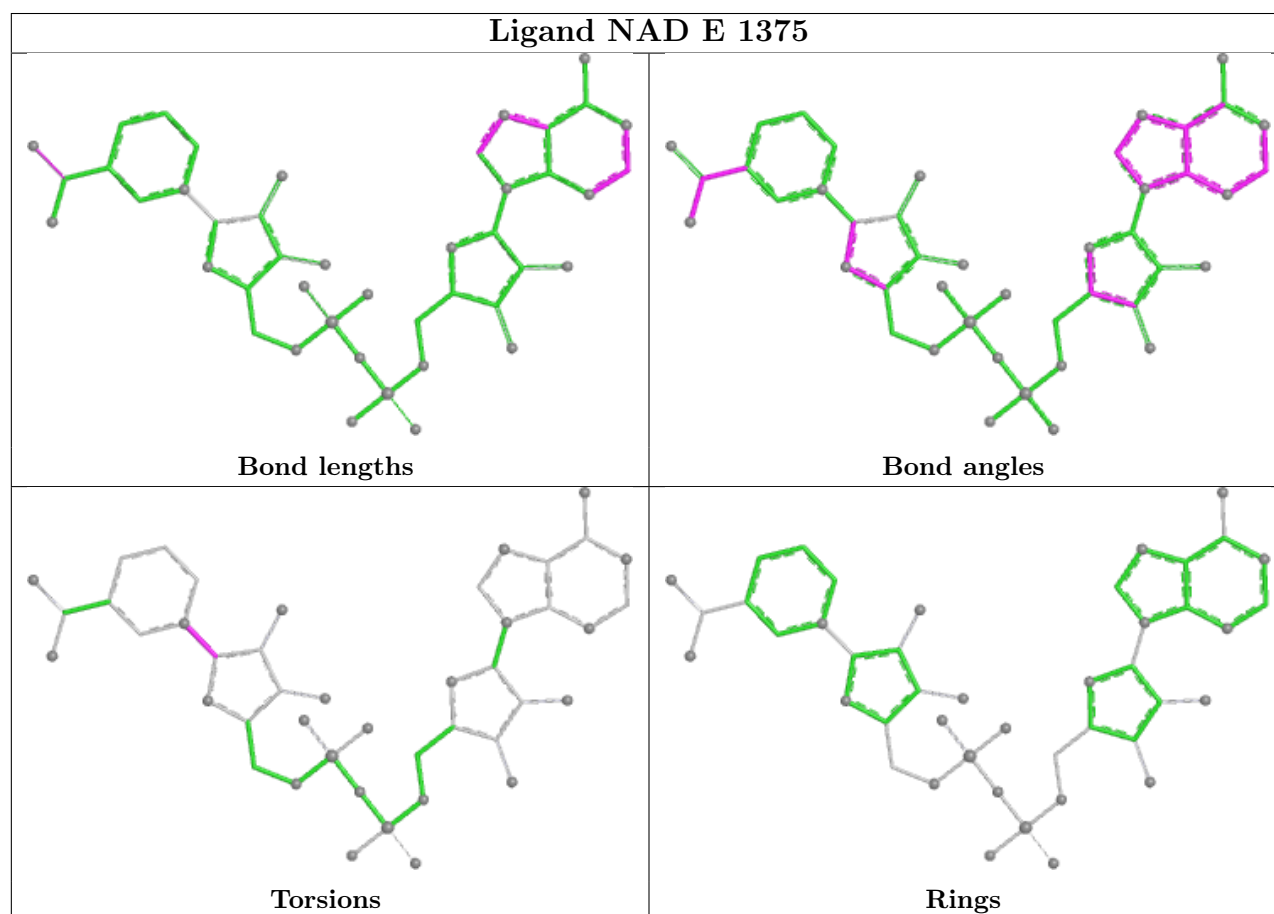
Mol	Chain	Res	Type	Atoms
4	E	1375	NAD	O4D-C1D-N1N-C2N
4	E	1375	NAD	O4D-C1D-N1N-C6N
4	E	1375	NAD	C2D-C1D-N1N-C2N
4	F	1376	NAD	O4D-C1D-N1N-C2N
4	F	1376	NAD	O4D-C1D-N1N-C6N
3	D	1371	PYR	OXT-C-CA-CB
4	E	1375	NAD	C2D-C1D-N1N-C6N
4	F	1376	NAD	C2D-C1D-N1N-C6N

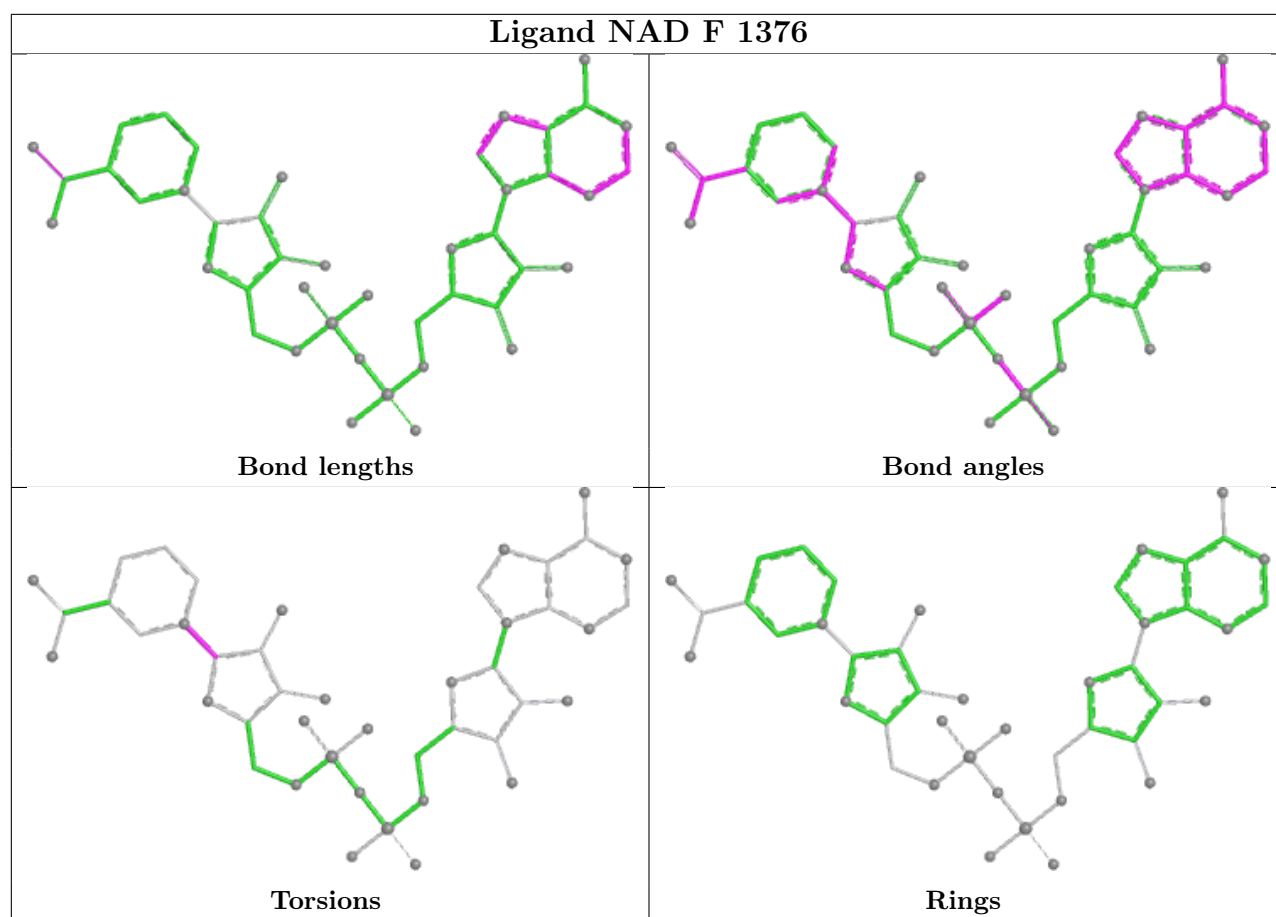
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1375	NAD	3	0
3	A	1373	PYR	2	0
4	F	1376	NAD	4	0
3	F	1375	PYR	3	0
3	E	1374	PYR	2	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(Å²)	Q<0.9	
1	A	368/377 (97%)	0.02	7 (1%)	66	66	3, 17, 29, 42	4 (1%)
1	B	368/377 (97%)	-0.22	7 (1%)	66	66	3, 14, 27, 44	1 (0%)
1	C	365/377 (96%)	0.04	11 (3%)	52	51	4, 16, 33, 37	0
1	D	367/377 (97%)	-0.21	6 (1%)	70	70	3, 14, 28, 46	3 (0%)
1	E	373/377 (98%)	0.04	7 (1%)	66	66	6, 20, 31, 57	1 (0%)
1	F	373/377 (98%)	-0.24	2 (0%)	87	87	6, 15, 23, 53	1 (0%)
All	All	2214/2262 (97%)	-0.10	40 (1%)	67	67	3, 16, 29, 57	10 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	ALA	4.6
1	B	244	ALA	4.3
1	C	283	TYR	4.0
1	A	283	TYR	3.8
1	A	371	ALA	3.5
1	D	270	ASP	3.5
1	E	68	ALA	3.4
1	F	373	HIS	3.4
1	B	240	LEU	3.3
1	A	241	VAL	3.1
1	B	283	TYR	3.0
1	D	244	ALA	2.9
1	C	240	LEU	2.8
1	A	14	PHE	2.8
1	A	270	ASP	2.8
1	B	347	GLU	2.7
1	D	240	LEU	2.6
1	E	349	ALA	2.5
1	C	270	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	360	GLY	2.3
1	E	83	GLY	2.3
1	C	246	ALA	2.3
1	E	360	GLY	2.3
1	F	56	GLN	2.2
1	E	369	VAL	2.2
1	A	32	GLU	2.2
1	D	245	LYS	2.2
1	C	292	ASP	2.2
1	C	363	PHE	2.2
1	E	373	HIS	2.2
1	C	368	SER	2.2
1	B	270	ASP	2.2
1	B	369	VAL	2.1
1	C	282	THR	2.1
1	C	362	PRO	2.1
1	C	284	ASP	2.1
1	A	347	GLU	2.0
1	D	285	HIS	2.0
1	E	372	HIS	2.0
1	D	368	SER	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.

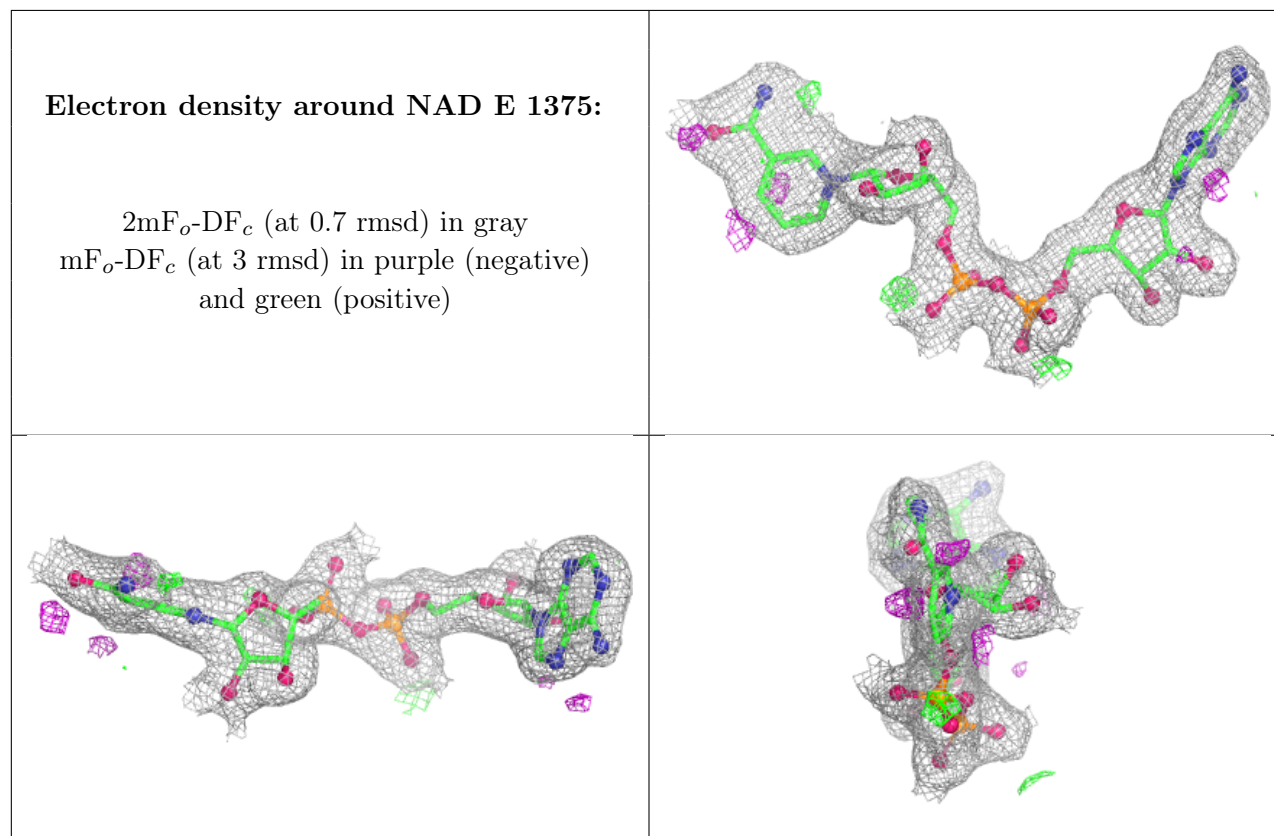
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	F	1374	1/1	0.69	0.28	53,53,53,53	0
2	MG	A	1372	1/1	0.77	0.23	32,32,32,32	0

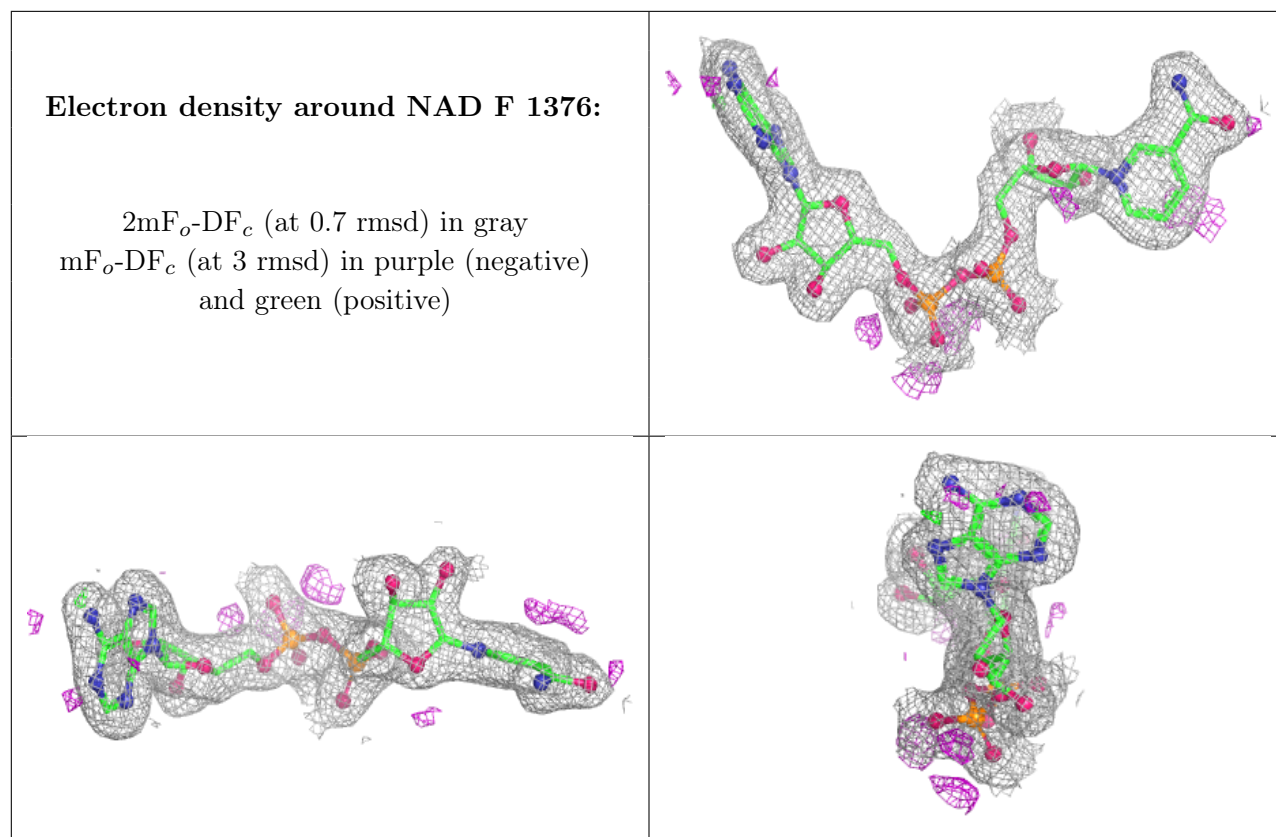
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PYR	A	1373	6/6	0.79	0.17	34,38,39,39	0
3	PYR	C	1371	6/6	0.80	0.16	37,40,42,43	0
3	PYR	B	1373	6/6	0.82	0.15	32,38,39,39	0
3	PYR	D	1371	6/6	0.84	0.16	39,42,45,47	0
3	PYR	F	1375	6/6	0.85	0.21	18,23,28,32	0
3	PYR	E	1374	6/6	0.86	0.18	34,37,40,43	0
2	MG	B	1372	1/1	0.91	0.31	28,28,28,28	0
4	NAD	E	1375	44/44	0.98	0.05	8,13,20,22	0
4	NAD	F	1376	44/44	0.98	0.04	3,7,11,15	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.