WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2014 – 04:34 AM EST

PDB ID	:	4WUO
Title	:	Structure of the E270A Mutant Isopropylmalate dehydrogenase from Thermus thermophilus in complex with IPM, Mn and NADH
Authors	:	Pallo, A.; Graczer, E.; Olah, J.; Szimler, T.; Konarev, P.V.; Svergun, D.I.; Merli, A.; Zavodszky, P.; Vas, M.; Weiss, M.S.
Deposited on	:	2014-11-03
Resolution	:	2.05 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24103
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24103

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.05 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X–ray structures

▯ Percentile relative to X–ray structures of similar resolution
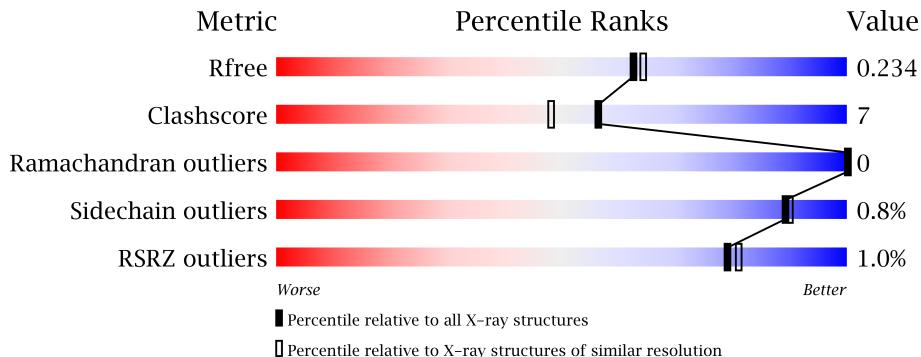
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
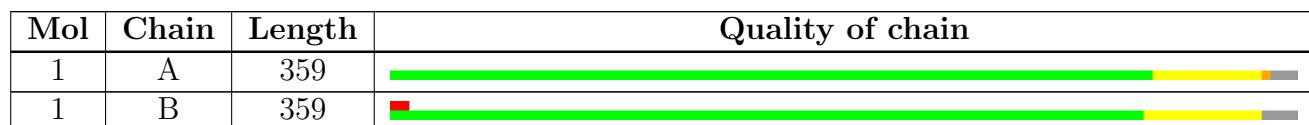
The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	EOH	A	407	-	X
6	EOH	A	411	-	X
6	EOH	A	413	-	X
6	EOH	B	402	-	X
6	EOH	B	403	-	X
7	GOL	A	408	-	X

2   Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 5575 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-isopropylmalate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2630	1676	459	489	6	0	3	0
1	B	345	Total	C	N	O	S	0	2	0
			2605	1662	457	480	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q5SIY4
A	-1	ALA	-	expression tag	UNP Q5SIY4
A	0	SER	-	expression tag	UNP Q5SIY4
A	270	ALA	GLU	engineered mutation	UNP Q5SIY4
A	346	ALA	-	expression tag	UNP Q5SIY4
A	347	ALA	-	expression tag	UNP Q5SIY4
A	348	ALA	-	expression tag	UNP Q5SIY4
A	349	LEU	-	expression tag	UNP Q5SIY4
A	350	GLU	-	expression tag	UNP Q5SIY4
A	351	HIS	-	expression tag	UNP Q5SIY4
A	352	HIS	-	expression tag	UNP Q5SIY4
A	353	HIS	-	expression tag	UNP Q5SIY4
A	354	HIS	-	expression tag	UNP Q5SIY4
A	355	HIS	-	expression tag	UNP Q5SIY4
A	356	HIS	-	expression tag	UNP Q5SIY4
B	-2	MET	-	initiating methionine	UNP Q5SIY4
B	-1	ALA	-	expression tag	UNP Q5SIY4
B	0	SER	-	expression tag	UNP Q5SIY4
B	270	ALA	GLU	engineered mutation	UNP Q5SIY4
B	346	ALA	-	expression tag	UNP Q5SIY4
B	347	ALA	-	expression tag	UNP Q5SIY4
B	348	ALA	-	expression tag	UNP Q5SIY4
B	349	LEU	-	expression tag	UNP Q5SIY4
B	350	GLU	-	expression tag	UNP Q5SIY4
B	351	HIS	-	expression tag	UNP Q5SIY4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	352	HIS	-	expression tag	UNP Q5SIY4
B	353	HIS	-	expression tag	UNP Q5SIY4
B	354	HIS	-	expression tag	UNP Q5SIY4
B	355	HIS	-	expression tag	UNP Q5SIY4
B	356	HIS	-	expression tag	UNP Q5SIY4

- Molecule 2 is 3-ISOPROPYLMALIC ACID (three-letter code: IPM) (formula: $C_7H_{12}O_5$).
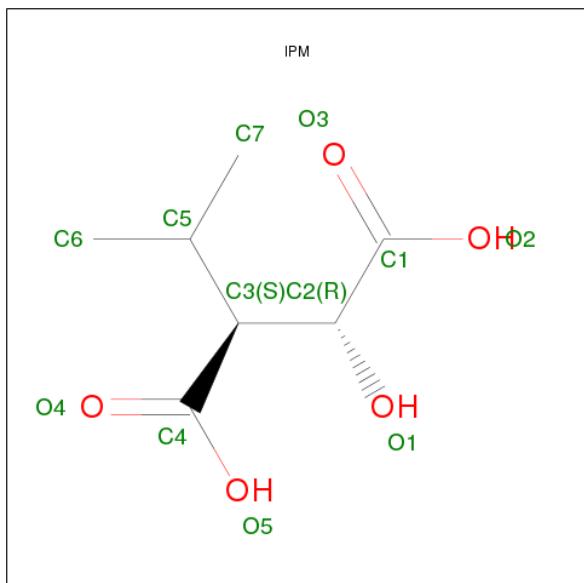
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 7	O 5	0	0
2	A	1	Total 12	C 7	O 5	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).
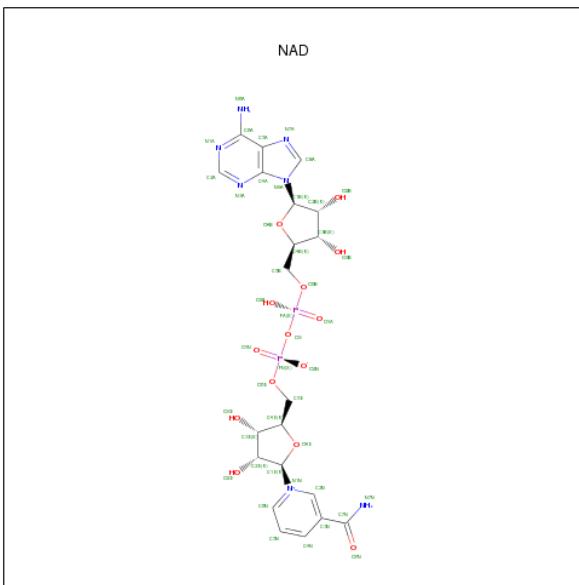
NAD

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).

EOH

O
OH

C2 —— C1
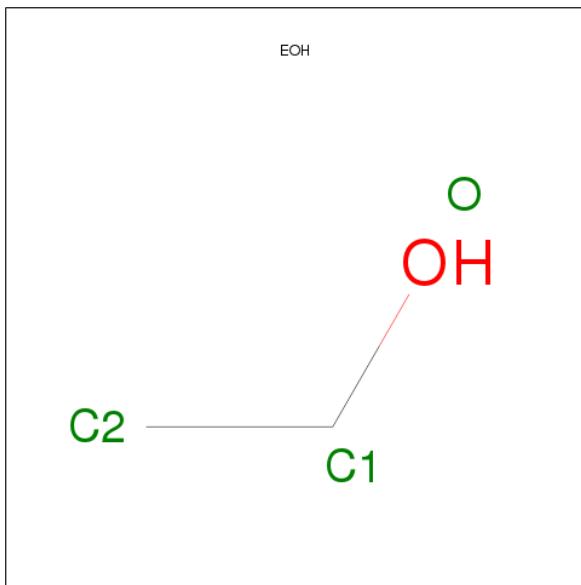
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 3	C 2	O 1	0	0
6	A	1	Total 3	C 2	O 1	0	0
6	A	1	Total 3	C 2	O 1	0	0
6	A	1	Total 3	C 2	O 1	0	0
6	A	1	Total 3	C 2	O 1	0	0
6	B	1	Total 3	C 2	O 1	0	0
6	B	1	Total 3	C 2	O 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

W O R L D W I D E
wwPDB
PROTEIN DATA BANK
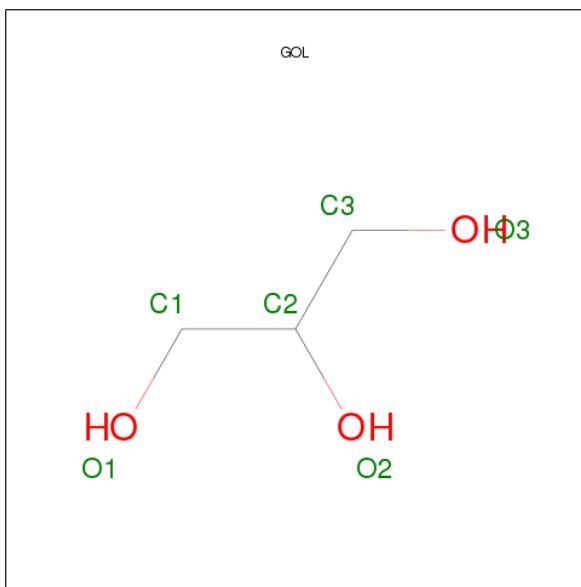
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total 109	O 109	0	0
8	B	71	Total 71	O 71	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: 3-isopropylmalate dehydrogenase

Chain A:
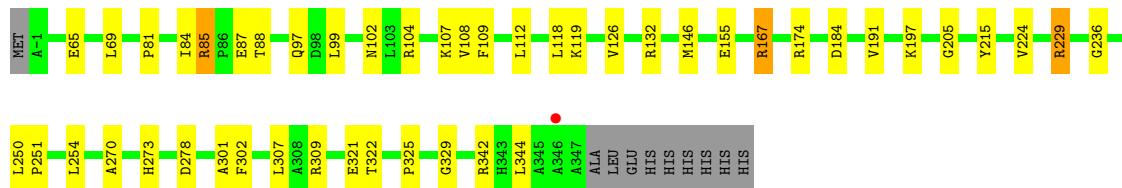
- Molecule 1: 3-isopropylmalate dehydrogenase

Chain B:
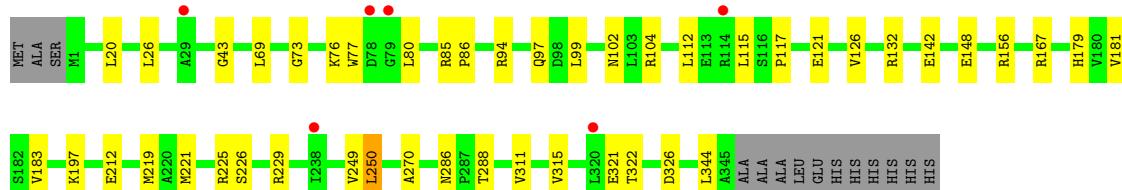
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	50.18Å　143.25Å　174.89Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	30.00 – 2.05 29.75 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.05) 99.6 (29.75-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170　,　0.229 0.178　,　0.234	Depositor DCC
R_{free} test set	2009 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Outliers	0 of 39947 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5575	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, NAD, K, EOH, IPM

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	0.78	1/2694 (0.0%)	0.84	5/3657 (0.1%)
1	B	0.72	0/2667	0.81	5/3620 (0.1%)
All	All	0.75	1/5361 (0.0%)	0.83	10/7277 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	ARG	CZ-NH1	5.15	1.39	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH2	9.79	125.19	120.30
1	B	167	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	B	167	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	B	229	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	167	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	167	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	309	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	B	94	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	278	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	250	LEU	CB-CG-CD2	5.12	119.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2675	42	0
1	B	2605	0	2652	29	0
2	A	24	0	18	2	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	15	0	30	10	0
6	B	6	0	12	5	0
7	A	24	0	30	3	0
8	A	109	0	0	2	0
8	B	71	0	0	2	0
All	All	5575	0	5469	71	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (71) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:LEU:HB2	6:A:406:EOH:H11	1.45	0.95
1:A:109:PHE:H	6:A:406:EOH:H21	1.35	0.91
1:A:254:LEU:H	6:B:402:EOH:H21	1.37	0.89
1:A:107:LYS:H	6:A:413:EOH:H11	1.40	0.86
1:A:112:LEU:CB	6:A:406:EOH:H11	2.08	0.82
1:B:85:ARG:NH2	8:B:553:HOH:O	2.16	0.77
1:A:85:ARG:HG3	1:A:88:THR:H	1.50	0.76
1:A:102:ASN:HD22	1:A:132:ARG:HD3	1.52	0.74
1:A:205:GLY:O	6:A:412:EOH:H21	1.88	0.73
1:B:102:ASN:HD21	1:B:104:ARG:NE	1.88	0.71
1:B:221:MET:SD	6:B:402:EOH:H22	2.36	0.65
1:B:80:LEU:O	1:B:85:ARG:HD2	1.98	0.64
1:A:174:ARG:HH22	6:A:412:EOH:H22	1.65	0.62
1:A:87:GLU:OE2	7:A:408:GOL:H12	1.99	0.62
1:B:225:ARG:HH11	6:B:402:EOH:H23	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:179[A]:HIS:CD2	8:B:511:HOH:O	2.53	0.61
1:B:142:GLU:H	1:B:156[B]:ARG:HH21	1.48	0.60
1:A:155:GLU:HG2	1:A:191:VAL:HG11	1.84	0.60
1:A:102:ASN:HD21	1:A:104:ARG:NE	2.00	0.59
1:B:102:ASN:HD22	1:B:132:ARG:HD3	1.69	0.57
1:B:102:ASN:HD21	1:B:104:ARG:HE	1.50	0.57
1:A:321:GLU:OE2	1:A:342[B]:ARG:NH2	2.35	0.56
1:B:73:GLY:HA2	1:B:86:PRO:HG2	1.88	0.56
1:A:108:VAL:HG13	6:A:406:EOH:H12	1.89	0.55
1:A:224:VAL:HG12	1:A:224:VAL:O	2.04	0.55
1:A:126:VAL:HG11	1:A:250:LEU:HD13	1.89	0.55
1:A:167:ARG:HD3	8:A:508:HOH:O	2.08	0.54
1:A:224:VAL:HB	1:B:249:VAL:HG11	1.90	0.53
1:A:342[B]:ARG:HG2	1:A:342[B]:ARG:HH11	1.74	0.52
1:A:118:LEU:HD11	1:A:224:VAL:HG13	1.91	0.52
2:A:415:IPM:H2	3:B:401:NAD:C4N	2.41	0.51
1:B:181:VAL:HG22	1:B:212:GLU:HB3	1.92	0.51
1:A:65[B]:GLU:HG2	1:A:302:PHE:CE1	2.46	0.51
1:B:321:GLU:HG2	1:B:322:THR:HG23	1.93	0.51
1:A:85:ARG:CG	1:A:88:THR:H	2.23	0.50
1:B:288:THR:HG23	1:B:315:VAL:HG11	1.94	0.50
7:A:414:GOL:H32	8:A:505:HOH:O	2.11	0.50
1:A:254:LEU:N	6:B:402:EOH:H21	2.17	0.50
1:A:69:LEU:HB3	1:A:270:ALA:HB2	1.93	0.50
1:A:85:ARG:HG2	1:A:88:THR:OG1	2.11	0.49
1:A:109:PHE:H	6:A:406:EOH:C2	2.15	0.49
1:A:236:GLY:H	6:A:407:EOH:H21	1.77	0.49
1:B:69:LEU:HB3	1:B:270:ALA:HB2	1.94	0.49
1:A:321:GLU:HG2	1:A:322:THR:HG23	1.94	0.48
1:A:97:GLN:HB2	1:A:99:LEU:HG	1.96	0.47
2:A:401:IPM:H2	3:A:402:NAD:C4N	2.46	0.45
1:A:301:ALA:HA	7:A:414:GOL:H11	1.99	0.45
1:B:179[A]:HIS:NE2	1:B:181:VAL:HG23	2.31	0.45
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.80	0.45
1:A:112:LEU:HB3	6:A:406:EOH:H11	1.95	0.45
1:B:126:VAL:HG11	1:B:250:LEU:HD13	1.98	0.44
1:A:119:LYS:HE2	1:B:117:PRO:HA	1.98	0.44
1:A:342[B]:ARG:HG2	1:A:342[B]:ARG:NH1	2.32	0.43
1:B:97:GLN:HB2	1:B:99:LEU:HG	1.99	0.43
1:A:250:LEU:HB2	1:A:251:PRO:CD	2.49	0.43
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.83	0.43
1:B:43:GLY:HA3	1:B:77:TRP:CZ2	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:PRO:HD2	1:A:84:ILE:HD11	2.01	0.42
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.83	0.42
1:A:197:LYS:HB3	1:A:197:LYS:HE2	1.89	0.42
1:A:254:LEU:HG	1:A:273:HIS:HB3	2.01	0.42
1:B:112:LEU:HB3	1:B:115:LEU:HD12	2.02	0.42
1:A:254:LEU:H	6:B:402:EOH:C2	2.20	0.42
1:A:146:MET:HE2	1:B:197:LYS:NZ	2.35	0.42
1:A:325:PRO:HA	1:A:329:GLY:O	2.20	0.41
1:B:26:LEU:HD11	1:B:311:VAL:HG22	2.02	0.41
1:B:286:ASN:HB2	1:B:326:ASP:OD1	2.21	0.41
1:B:76:LYS:HD3	1:B:77:TRP:CZ2	2.56	0.41
1:B:121:GLU:H	1:B:121:GLU:CD	2.25	0.40
1:A:184:ASP:O	1:A:215:TYR:HA	2.21	0.40
1:B:183:VAL:HG21	1:B:219:MET:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	350/359 (98%)	342 (98%)	8 (2%)	0	100	100
1	B	345/359 (96%)	337 (98%)	8 (2%)	0	100	100
All	All	695/718 (97%)	679 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	269/275 (98%)	267 (99%)	2 (1%)	91	91
1	B	267/275 (97%)	265 (99%)	2 (1%)	91	91
All	All	536/550 (98%)	532 (99%)	4 (1%)	89	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ARG
1	A	307	LEU
1	B	148	GLU
1	B	226	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	B	102	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 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	#$|Z| > 2$
2	IPM	A	401	4	11,11,11	1.71	3 (27%)	15,15,15	1.37	3 (20%)
3	NAD	A	402	-	48,48,48	1.19	3 (6%)	73,73,73	2.20	15 (20%)
6	EOH	A	406	-	2,2,2	0.69	0	1,1,1	0.48	0
6	EOH	A	407	-	2,2,2	0.56	0	1,1,1	0.42	0
7	GOL	A	408	-	5,5,5	0.68	0	5,5,5	0.61	0
7	GOL	A	409	-	5,5,5	0.56	0	5,5,5	0.68	0
7	GOL	A	410	5	5,5,5	0.58	0	5,5,5	0.59	0
6	EOH	A	411	-	2,2,2	0.46	0	1,1,1	0.30	0
6	EOH	A	412	-	2,2,2	0.41	0	1,1,1	0.40	0
6	EOH	A	413	-	2,2,2	0.52	0	1,1,1	0.27	0
7	GOL	A	414	5	5,5,5	0.53	0	5,5,5	1.74	2 (40%)
2	IPM	A	415	4	11,11,11	1.00	0	15,15,15	0.97	1 (6%)
3	NAD	B	401	-	48,48,48	1.29	6 (12%)	73,73,73	2.12	17 (23%)
6	EOH	B	402	-	2,2,2	0.58	0	1,1,1	0.12	0
6	EOH	B	403	-	2,2,2	0.44	0	1,1,1	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IPM	A	401	4	-	0/16/16/16	0/0/0/0
3	NAD	A	402	-	-	0/30/62/62	0/5/5/5
6	EOH	A	406	-	-	0/0/0/0	0/0/0/0
6	EOH	A	407	-	-	0/0/0/0	0/0/0/0
7	GOL	A	408	-	-	0/4/4/4	0/0/0/0
7	GOL	A	409	-	-	0/4/4/4	0/0/0/0
7	GOL	A	410	5	-	0/4/4/4	0/0/0/0
6	EOH	A	411	-	-	0/0/0/0	0/0/0/0
6	EOH	A	412	-	-	0/0/0/0	0/0/0/0
6	EOH	A	413	-	-	0/0/0/0	0/0/0/0
7	GOL	A	414	5	-	0/4/4/4	0/0/0/0
2	IPM	A	415	4	-	0/16/16/16	0/0/0/0
3	NAD	B	401	-	-	0/30/62/62	0/5/5/5
6	EOH	B	402	-	-	0/0/0/0	0/0/0/0
6	EOH	B	403	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	PN-O2N	4.35	1.58	1.48
3	A	402	NAD	O4B-C1B	4.11	1.46	1.41
3	B	401	NAD	O4B-C1B	3.76	1.46	1.41
2	A	401	IPM	O4-C4	2.96	1.32	1.22
3	B	401	NAD	O4D-C1D	2.89	1.44	1.41
3	A	402	NAD	O4D-C1D	2.86	1.44	1.41
3	A	402	NAD	C4N-C3N	2.54	1.43	1.39
2	A	401	IPM	O5-C4	-2.53	1.21	1.30
3	B	401	NAD	PN-O1N	2.25	1.54	1.48
3	B	401	NAD	C6A-N6A	2.14	1.41	1.34
3	B	401	NAD	C2B-C1B	2.03	1.56	1.53
2	A	401	IPM	C2-C1	2.03	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	N3A-C2A-N1A	-10.11	120.00	128.89
3	A	402	NAD	C5A-C4A-N3A	-7.70	118.47	125.98
3	B	401	NAD	N3A-C2A-N1A	-7.62	122.18	128.89
3	B	401	NAD	C5A-C4A-N3A	-7.32	118.84	125.98
3	A	402	NAD	N3A-C4A-N9A	5.53	134.87	125.39
3	B	401	NAD	O4D-C1D-C2D	-5.11	99.25	106.69
3	A	402	NAD	O3-PA-O5B	5.04	116.27	102.91
3	B	401	NAD	C4A-C5A-N7A	-5.03	104.55	109.41
3	B	401	NAD	N3A-C4A-N9A	4.94	133.86	125.39
3	A	402	NAD	C4D-O4D-C1D	4.00	114.11	109.72
3	A	402	NAD	C2A-N3A-C4A	3.33	122.86	113.27
3	A	402	NAD	C3N-C7N-N7N	3.03	121.16	117.78
3	B	401	NAD	O3-PN-O5D	3.02	112.75	101.23
3	B	401	NAD	O3B-C3B-C4B	-2.96	102.36	111.07
3	B	401	NAD	O2N-PN-O1N	-2.84	110.21	118.70
3	B	401	NAD	C2A-N3A-C4A	2.84	121.44	113.27
3	B	401	NAD	C3N-C7N-N7N	2.82	120.92	117.78
3	B	401	NAD	C8A-N7A-C5A	2.79	112.24	103.58
3	A	402	NAD	O4D-C1D-C2D	-2.78	102.64	106.69
3	B	401	NAD	O5D-PN-O1N	2.74	120.16	108.62
3	B	401	NAD	O3-PA-O5B	2.74	110.17	102.91
3	A	402	NAD	O4B-C1B-C2B	-2.67	102.81	106.69
3	B	401	NAD	O7N-C7N-N7N	-2.59	118.89	122.59
3	A	402	NAD	C2D-C1D-N1N	2.57	118.62	113.48
3	A	402	NAD	C2A-N1A-C6A	2.54	123.29	118.76
7	A	414	GOL	O2-C2-C3	2.44	119.76	108.44
3	B	401	NAD	PN-O3-PA	-2.44	123.34	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	NAD	O4D-C1D-N1N	-2.44	105.45	108.13
3	B	401	NAD	O4D-C1D-N1N	-2.43	105.46	108.13
2	A	401	IPM	C6-C5-C3	-2.42	107.86	112.00
2	A	415	IPM	O4-C4-C3	-2.38	116.55	122.86
2	A	401	IPM	O4-C4-C3	-2.33	116.67	122.86
2	A	401	IPM	C2-C3-C4	2.23	113.93	109.58
3	A	402	NAD	C4B-O4B-C1B	2.17	112.10	109.72
3	A	402	NAD	C4A-C5A-N7A	-2.14	107.34	109.41
7	A	414	GOL	O2-C2-C1	-2.14	98.55	108.44
3	A	402	NAD	O2N-PN-O1N	-2.13	112.34	118.70
3	B	401	NAD	N7A-C8A-N9A	-2.01	107.63	112.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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	349/359 (97%)	-0.42	1 (0%)	91	94	21, 31, 56, 77	0
1	B	345/359 (96%)	-0.12	6 (1%)	67	69	19, 36, 62, 83	1 (0%)
All	All	694/718 (96%)	-0.27	7 (1%)	79	81	19, 33, 60, 83	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	GLY	3.5
1	B	29	ALA	3.1
1	B	114	ARG	2.8
1	B	320	LEU	2.8
1	B	78	ASP	2.5
1	B	238	ILE	2.3
1	A	346	ALA	2.2

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

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

6.3   Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4   Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
6	EOH	A	407	3/3	0.42	12.15	37,37,43,54	0
6	EOH	A	411	3/3	0.34	8.39	60,60,62,65	0
6	EOH	B	403	3/3	0.35	6.41	45,45,53,58	0
6	EOH	B	402	3/3	0.16	5.12	27,27,42,45	0
7	GOL	A	408	6/6	0.19	2.13	36,42,45,45	0
6	EOH	A	413	3/3	0.16	2.02	37,37,40,47	0
7	GOL	A	414	6/6	0.12	1.79	46,48,50,57	0
2	IPM	A	415	12/12	0.20	1.68	24,29,36,42	0
6	EOH	A	406	3/3	0.13	1.67	24,24,30,36	0
7	GOL	A	410	6/6	0.19	0.73	42,51,60,63	0
7	GOL	A	409	6/6	0.13	0.48	49,52,54,58	0
6	EOH	A	412	3/3	0.08	-0.04	42,42,47,47	0
3	NAD	B	401	44/44	0.08	-0.59	26,31,35,37	0
2	IPM	A	401	12/12	0.10	-0.64	21,25,31,34	0
3	NAD	A	402	44/44	0.07	-0.82	23,27,30,31	0
4	MN	A	403	1/1	0.09	-1.77	28,28,28,28	0
5	K	A	404	1/1	0.07	-1.90	43,43,43,43	0
4	MN	A	405	1/1	0.10	-2.08	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.