



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y42
Title : Structure of Isopropylmalate dehydrogenase from *Thermus thermophilus* - complex with NADH and Mn
Authors : Graczer, E.; Merlin, A.; Singh, R.K.; Manikandan, K.; Zavodsky, P.; Weiss, M.S.; Vas, M.
Deposited on : 2011-01-04
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

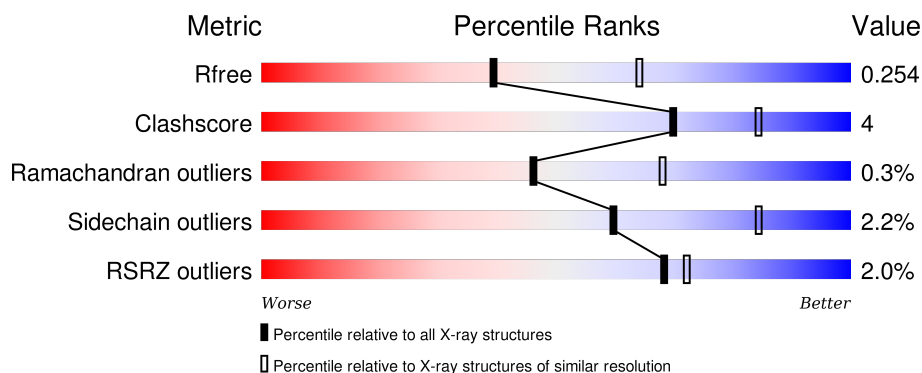
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	359	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	359	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	359	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	359	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>

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
2	BCN	A	501	-	-	-	X
2	BCN	B	1502	-	-	-	X
2	BCN	B	501	-	-	-	X
2	BCN	C	501	-	-	-	X
2	BCN	D	501	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11018 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 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2604	1660	454	484	6			
1	B	350	Total	C	N	O	S	0	0	0
			2626	1674	457	489	6			
1	C	352	Total	C	N	O	S	0	0	0
			2641	1683	461	491	6			
1	D	355	Total	C	N	O	S	0	0	0
			2671	1701	470	494	6			

There are 56 discrepancies between the modelled and reference sequences:

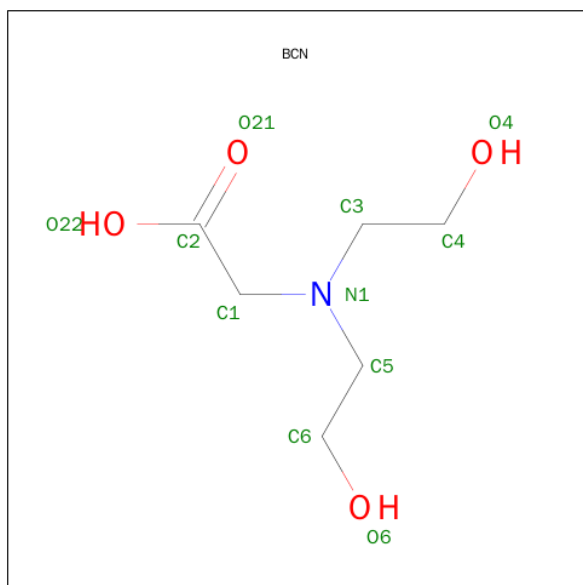
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
A	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
A	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
A	349	LEU	-	EXPRESSION TAG	UNP 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	-	EXPRESSION TAG	UNP Q5SIY4
B	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
B	0	SER	-	EXPRESSION TAG	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

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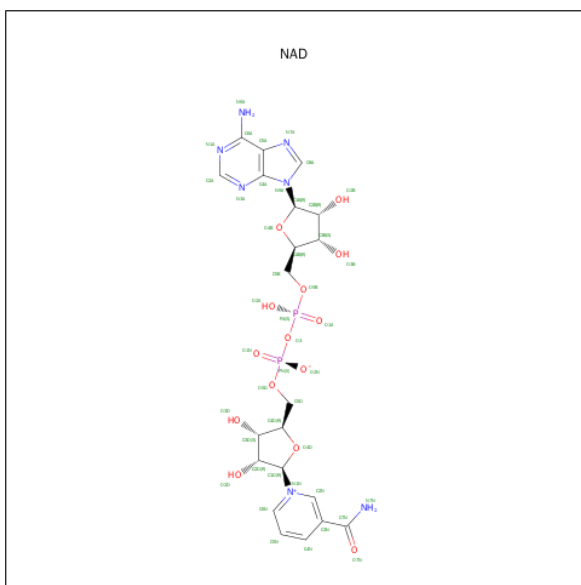
Chain	Residue	Modelled	Actual	Comment	Reference
B	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
B	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
B	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
C	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
C	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
C	349	LEU	-	EXPRESSION TAG	UNP Q5SIY4
C	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
C	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
C	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	-2	MET	-	EXPRESSION TAG	UNP Q5SIY4
D	-1	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	0	SER	-	EXPRESSION TAG	UNP Q5SIY4
D	346	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	347	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	348	ALA	-	EXPRESSION TAG	UNP Q5SIY4
D	349	LEU	-	EXPRESSION TAG	UNP Q5SIY4
D	350	GLU	-	EXPRESSION TAG	UNP Q5SIY4
D	351	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	352	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	353	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	354	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	355	HIS	-	EXPRESSION TAG	UNP Q5SIY4
D	356	HIS	-	EXPRESSION TAG	UNP Q5SIY4

- Molecule 2 is BICINE (three-letter code: BCN) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		
2	C	1	Total	C	N	O	0	0
			11	6	1	4		
2	D	1	Total	C	N	O	0	0
			11	6	1	4		

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



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		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	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	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		

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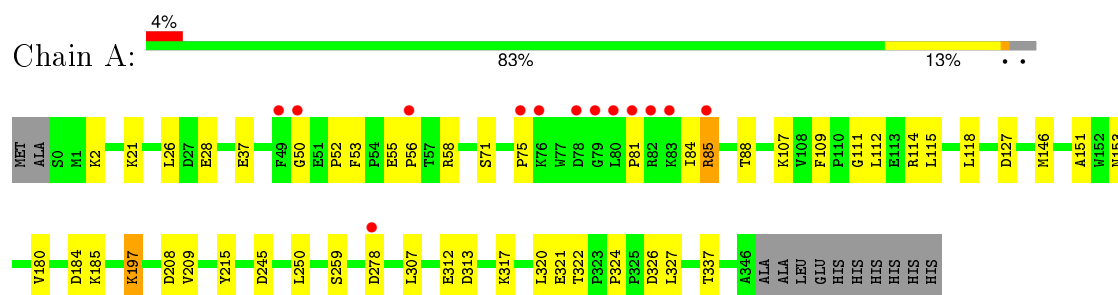
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	61	Total 61	O 61	0	0
5	C	74	Total 74	O 74	0	0
5	D	58	Total 58	O 58	0	0

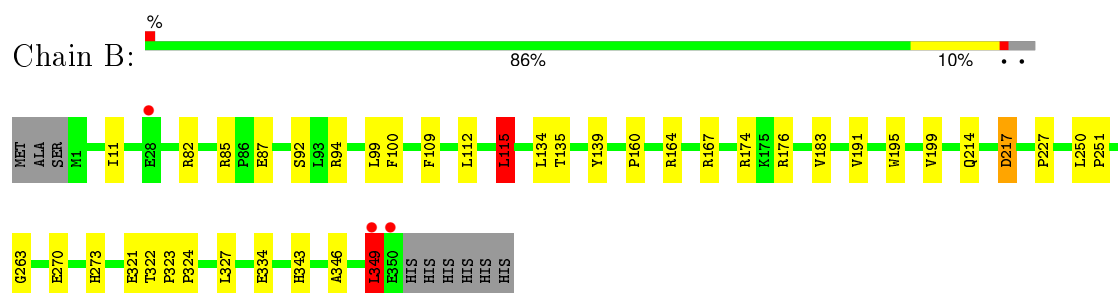
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

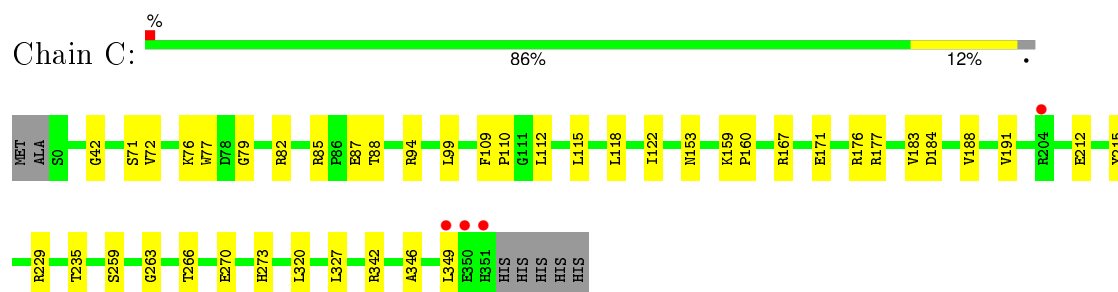
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



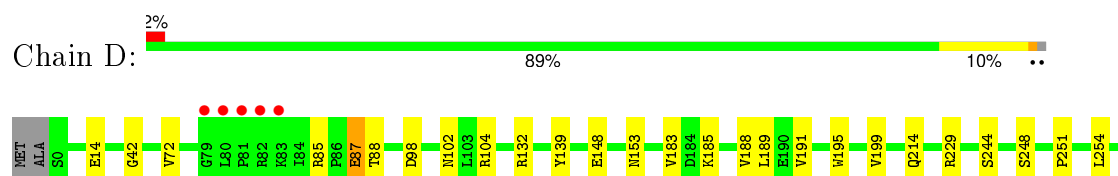
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.38Å 161.45Å 83.91Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	19.72 – 2.50 19.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.72-2.50) 99.9 (19.72-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.176 , 0.254 0.185 , 0.254	Depositor DCC
R_{free} test set	2109 reflections (4.26%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.2	EDS
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 51614 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11018	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BCN, MN, NAD

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	0.64	0/2659	0.71	1/3610 (0.0%)
1	B	0.68	0/2681	0.75	2/3640 (0.1%)
1	C	0.71	0/2697	0.76	1/3662 (0.0%)
1	D	0.65	0/2730	0.73	0/3707
All	All	0.67	0/10767	0.74	4/14619 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	LEU	CA-CB-CG	7.51	132.57	115.30
1	B	115	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	C	342	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	208	ASP	N-CA-CB	-5.31	101.04	110.60

There are no chirality outliers.

There are no planarity outliers.

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	2604	0	2640	23	0
1	B	2626	0	2665	23	0
1	C	2641	0	2674	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2671	0	2695	24	0
2	A	11	0	12	0	0
2	B	22	0	23	0	0
2	C	11	0	11	0	0
2	D	11	0	12	0	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
3	C	44	0	26	2	0
3	D	44	0	26	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	48	0	0	1	0
5	B	61	0	0	4	0
5	C	74	0	0	1	0
5	D	58	0	0	4	0
All	All	11018	0	10836	97	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 4.

All (97) 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:D:98:ASP:HB2	5:D:2012:HOH:O	1.40	1.18
1:C:79:GLY:H	1:C:85:ARG:NH2	1.55	1.04
1:C:79:GLY:N	1:C:85:ARG:HH22	1.61	0.97
1:A:115:LEU:HD11	1:A:327:LEU:HG	1.55	0.88
1:C:115:LEU:HD11	1:C:327:LEU:HG	1.63	0.81
1:B:100:PHE:HA	1:B:135:THR:HG23	1.72	0.72
1:A:153:ASN:HD22	1:B:191:VAL:HG23	1.56	0.71
1:C:191:VAL:HG23	1:D:153:ASN:OD1	1.93	0.69
1:C:79:GLY:H	1:C:85:ARG:HH22	0.76	0.66
1:A:321:GLU:HG2	1:A:322:THR:HG23	1.77	0.65
1:B:115:LEU:HD11	1:B:327:LEU:HG	1.79	0.65
1:A:118:LEU:HD11	1:A:250:LEU:HD22	1.80	0.63
1:D:326:ASP:HA	5:D:2051:HOH:O	1.99	0.62
1:C:177:ARG:HG3	1:C:177:ARG:HH11	1.65	0.62
1:C:259:SER:HB3	1:C:270:GLU:O	2.01	0.60
1:C:159:LYS:HB3	1:C:160:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASN:ND2	1:B:191:VAL:H	2.04	0.55
1:C:177:ARG:HG3	1:C:177:ARG:NH1	2.21	0.55
1:C:346:ALA:HA	1:C:349:LEU:HD12	1.87	0.55
1:C:85:ARG:HG3	1:C:88:THR:H	1.73	0.53
1:B:167:ARG:NH1	5:B:2027:HOH:O	2.27	0.53
1:D:42:GLY:HA3	1:D:72:VAL:HG12	1.89	0.53
1:C:184:ASP:O	1:C:215:TYR:HA	2.09	0.53
1:D:85:ARG:HG2	1:D:87:GLU:HG2	1.91	0.52
1:D:185:LYS:HE3	1:D:188:VAL:HG23	1.91	0.52
1:C:212:GLU:OE2	1:C:229:ARG:NH2	2.43	0.51
1:C:266:THR:OG1	5:C:2061:HOH:O	2.16	0.51
1:D:324:PRO:HD2	1:D:327:LEU:HD22	1.93	0.51
1:D:14:GLU:HG3	5:D:2002:HOH:O	2.11	0.51
1:B:94:ARG:HG2	1:B:94:ARG:HH11	1.75	0.51
1:C:159:LYS:HB3	1:C:160:PRO:HD3	1.93	0.51
1:A:53:PHE:CZ	1:A:58:ARG:HA	2.47	0.50
1:B:321:GLU:HG2	1:B:322:THR:HG23	1.93	0.49
1:D:183:VAL:HA	1:D:214:GLN:O	2.13	0.49
1:A:313:ASP:O	1:A:317:LYS:HG3	2.12	0.49
1:C:153:ASN:ND2	1:D:191:VAL:H	2.11	0.48
1:A:180:VAL:HG23	1:A:209:VAL:HG11	1.95	0.48
1:A:21:LYS:HD3	1:A:337:THR:HG21	1.95	0.48
1:A:197:LYS:HE2	5:B:2021:HOH:O	2.13	0.48
1:D:319:LEU:HD22	1:D:327:LEU:HD21	1.95	0.48
1:A:245:ASP:OD2	1:B:217:ASP:HB2	2.14	0.48
1:A:55:GLU:HB3	1:A:56:PRO:HD3	1.96	0.48
1:A:81:PRO:HD2	1:A:84:ILE:HG22	1.95	0.47
1:A:107:LYS:HG3	1:A:127:ASP:HB2	1.94	0.47
1:D:85:ARG:HB3	1:D:88:THR:OG1	2.15	0.47
1:B:11:ILE:HD11	1:B:273:HIS:CE1	2.50	0.47
1:B:321:GLU:OE1	1:B:343:HIS:HE1	1.98	0.47
1:C:188:VAL:HG11	1:D:139:TYR:CD1	2.50	0.47
1:A:85:ARG:HB3	1:A:88:THR:OG1	2.15	0.46
1:B:346:ALA:HA	1:B:349:LEU:HD22	1.98	0.46
3:A:900:NAD:O2N	3:A:900:NAD:O5B	2.33	0.46
1:C:79:GLY:N	1:C:85:ARG:NH2	2.39	0.46
1:C:153:ASN:ND2	1:D:189:LEU:HB3	2.31	0.46
1:D:102:ASN:HB3	1:D:132:ARG:HB3	1.97	0.46
1:C:94:ARG:HG2	1:C:99:LEU:HD12	1.98	0.46
1:A:146:MET:HA	1:A:151:ALA:HA	1.98	0.46
1:A:109:PHE:HB2	1:A:112:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PRO:O	1:C:320:LEU:HD21	2.16	0.45
1:C:118:LEU:HD13	1:C:122:ILE:HG22	1.98	0.45
1:B:270:GLU:HG2	5:B:2043:HOH:O	2.16	0.45
1:A:2:LYS:HE2	5:A:2001:HOH:O	2.16	0.45
1:C:42:GLY:HA3	1:C:72:VAL:HG22	1.99	0.45
1:B:160:PRO:O	1:B:164:ARG:HG2	2.18	0.44
1:D:251:PRO:HG2	1:D:257:LEU:HD21	2.00	0.44
1:C:153:ASN:HD21	1:D:191:VAL:H	1.65	0.43
3:D:900:NAD:H6N	3:D:900:NAD:H2D	1.63	0.43
1:D:344:LEU:HD12	1:D:344:LEU:HA	1.90	0.43
1:D:195:TRP:O	1:D:199:VAL:HG23	2.19	0.43
1:C:167:ARG:O	1:C:171:GLU:HB2	2.18	0.43
1:A:185:LYS:HE2	1:B:139:TYR:OH	2.18	0.43
1:A:184:ASP:O	1:A:215:TYR:HA	2.19	0.43
1:B:183:VAL:HA	1:B:214:GLN:O	2.18	0.42
1:C:109:PHE:HB2	1:C:112:LEU:HD12	2.01	0.42
1:C:273:HIS:CD2	3:C:900:NAD:H61A	2.37	0.42
1:D:257:LEU:HA	1:D:258:PRO:HD3	1.80	0.42
1:A:111:GLY:HA3	1:A:320:LEU:HD21	2.02	0.42
1:D:332:GLY:O	1:D:333:THR:C	2.57	0.42
1:B:99:LEU:O	1:B:134:LEU:HD23	2.20	0.42
1:B:323:PRO:HA	1:B:324:PRO:HD3	1.90	0.41
1:A:324:PRO:HB2	1:A:326:ASP:OD1	2.20	0.41
1:D:244:SER:O	1:D:248:SER:HB3	2.19	0.41
1:C:183:VAL:HB	1:C:235:THR:HB	2.01	0.41
1:A:26:LEU:HD22	1:A:307:LEU:HD22	2.00	0.41
1:D:352:HIS:CD2	1:D:352:HIS:C	2.94	0.41
1:C:85:ARG:HD3	1:C:87:GLU:HB2	2.02	0.41
1:C:82:ARG:NH1	1:C:82:ARG:HB2	2.35	0.41
1:C:99:LEU:HA	1:C:263:GLY:HA3	2.02	0.41
3:C:900:NAD:O2A	3:C:900:NAD:H51N	2.21	0.41
1:B:250:LEU:N	1:B:251:PRO:CD	2.84	0.41
1:B:195:TRP:O	1:B:199:VAL:HG23	2.22	0.40
1:D:104:ARG:NE	5:D:2013:HOH:O	2.53	0.40
1:B:227:PRO:HD2	5:B:2016:HOH:O	2.21	0.40
1:B:99:LEU:HA	1:B:263:GLY:HA3	2.03	0.40
1:B:82:ARG:HA	1:B:85:ARG:HD3	2.02	0.40
1:C:177:ARG:HH11	1:C:177:ARG:CG	2.30	0.40
1:C:76:LYS:HD3	1:C:77:TRP:CZ2	2.55	0.40
1:B:109:PHE:HB2	1:B:112:LEU:HD12	2.04	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	345/359 (96%)	324 (94%)	18 (5%)	3 (1%)	21	37
1	B	348/359 (97%)	334 (96%)	13 (4%)	1 (0%)	46	68
1	C	350/359 (98%)	336 (96%)	14 (4%)	0	100	100
1	D	353/359 (98%)	334 (95%)	19 (5%)	0	100	100
All	All	1396/1436 (97%)	1328 (95%)	64 (5%)	4 (0%)	46	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	ARG
1	A	52	PRO
1	A	50	GLY
1	A	75	PRO

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	266/276 (96%)	257 (97%)	9 (3%)	44	72
1	B	268/276 (97%)	261 (97%)	7 (3%)	54	81
1	C	269/276 (98%)	267 (99%)	2 (1%)	88	97
1	D	272/276 (99%)	266 (98%)	6 (2%)	60	84
All	All	1075/1104 (97%)	1051 (98%)	24 (2%)	60	84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	37	GLU
1	A	71	SER
1	A	85	ARG
1	A	114	ARG
1	A	197	LYS
1	A	259	SER
1	A	278	ASP
1	A	312	GLU
1	B	87	GLU
1	B	92	SER
1	B	115	LEU
1	B	174	ARG
1	B	217	ASP
1	B	334	GLU
1	B	349	LEU
1	C	71	SER
1	C	176	ARG
1	D	87	GLU
1	D	148	GLU
1	D	229	ARG
1	D	254	LEU
1	D	307	LEU
1	D	352	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	153	ASN
1	A	214	GLN
1	A	300	HIS
1	B	102	ASN
1	B	179	HIS
1	B	343	HIS
1	C	102	ASN
1	C	153	ASN
1	C	222	HIS
1	C	300	HIS
1	D	102	ASN
1	D	352	HIS

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Mol	Chain	Res	Type
1	D	353	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	BCN	A	501	4	7,10,10	0.63	0	8,11,11	1.90	1 (12%)
3	NAD	A	900	-	38,48,48	1.17	3 (7%)	47,73,73	2.14	8 (17%)
2	BCN	B	1502	-	7,10,10	0.68	0	8,11,11	1.55	1 (12%)
2	BCN	B	501	4	7,10,10	0.63	0	8,11,11	2.40	3 (37%)
3	NAD	B	900	-	38,48,48	1.33	3 (7%)	47,73,73	1.97	7 (14%)
2	BCN	C	501	4	7,10,10	0.51	0	8,11,11	2.31	1 (12%)
3	NAD	C	900	-	38,48,48	1.28	2 (5%)	47,73,73	1.93	9 (19%)
2	BCN	D	501	4	7,10,10	0.66	0	8,11,11	1.37	1 (12%)
3	NAD	D	900	-	38,48,48	1.14	2 (5%)	47,73,73	2.32	9 (19%)

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	BCN	A	501	4	-	0/8/10/10	0/0/0/0
3	NAD	A	900	-	-	0/22/62/62	0/5/5/5
2	BCN	B	1502	-	-	0/8/10/10	0/0/0/0
2	BCN	B	501	4	-	0/8/10/10	0/0/0/0
3	NAD	B	900	-	-	0/22/62/62	0/5/5/5
2	BCN	C	501	4	-	0/8/10/10	0/0/0/0
3	NAD	C	900	-	-	0/22/62/62	0/5/5/5
2	BCN	D	501	4	-	0/8/10/10	0/0/0/0
3	NAD	D	900	-	-	0/22/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	NAD	C8A-N7A	-2.50	1.29	1.34
3	B	900	NAD	C4N-C3N	2.20	1.43	1.39
3	D	900	NAD	O4B-C1B	2.98	1.45	1.41
3	B	900	NAD	O4B-C1B	3.43	1.45	1.41
3	A	900	NAD	O4B-C1B	3.53	1.45	1.41
3	C	900	NAD	O4D-C1D	3.58	1.45	1.41
3	A	900	NAD	O4D-C1D	3.67	1.45	1.41
3	D	900	NAD	O4D-C1D	3.92	1.46	1.41
3	C	900	NAD	O4B-C1B	4.06	1.46	1.41
3	B	900	NAD	O4D-C1D	5.21	1.47	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	900	NAD	N3A-C2A-N1A	-8.76	122.19	128.89
3	B	900	NAD	N3A-C2A-N1A	-8.41	122.46	128.89
3	A	900	NAD	N3A-C2A-N1A	-8.24	122.58	128.89
3	A	900	NAD	PN-O3-PA	-7.88	110.61	132.73
3	D	900	NAD	PN-O3-PA	-7.72	111.04	132.73
2	C	501	BCN	C2-C1-N1	-6.36	104.11	113.53
2	B	501	BCN	C2-C1-N1	-5.69	105.10	113.53
2	A	501	BCN	C2-C1-N1	-5.09	106.00	113.53
3	C	900	NAD	N3A-C2A-N1A	-5.00	125.06	128.89
3	D	900	NAD	C2B-C1B-N9A	-4.99	106.67	114.29
3	B	900	NAD	PN-O3-PA	-4.83	119.17	132.73
3	C	900	NAD	C2B-C1B-N9A	-4.64	107.20	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	NAD	C2B-C1B-N9A	-4.25	107.79	114.29
3	C	900	NAD	PN-O3-PA	-3.72	122.28	132.73
3	C	900	NAD	C4A-C5A-N7A	-3.17	106.56	109.48
2	D	501	BCN	C2-C1-N1	-3.08	108.97	113.53
3	D	900	NAD	O7N-C7N-N7N	-3.07	118.28	122.59
3	B	900	NAD	C2B-C1B-N9A	-2.91	109.84	114.29
3	B	900	NAD	O7N-C7N-N7N	-2.91	118.50	122.59
3	A	900	NAD	O7N-C7N-N7N	-2.85	118.58	122.59
3	D	900	NAD	C4A-C5A-N7A	-2.72	106.98	109.48
2	B	1502	BCN	C2-C1-N1	-2.69	109.54	113.53
2	B	501	BCN	C1-N1-C3	-2.60	105.83	111.28
3	B	900	NAD	C4A-C5A-N7A	-2.31	107.36	109.48
3	C	900	NAD	O2N-PN-O3	2.11	114.68	105.09
3	A	900	NAD	O2N-PN-O3	2.13	114.74	105.09
3	C	900	NAD	O4B-C1B-N9A	2.20	112.70	108.10
2	B	501	BCN	C5-N1-C3	2.21	116.75	111.45
3	A	900	NAD	C3N-C7N-N7N	2.40	120.44	117.82
3	B	900	NAD	C4B-O4B-C1B	2.42	112.38	109.72
3	C	900	NAD	C4B-O4B-C1B	2.60	112.57	109.72
3	D	900	NAD	O3-PN-O5D	2.62	109.90	102.94
3	A	900	NAD	O3-PN-O5D	2.68	110.05	102.94
3	A	900	NAD	O3-PA-O5B	3.28	111.63	102.94
3	D	900	NAD	O4D-C1D-N1N	3.30	111.76	108.13
3	D	900	NAD	O3-PA-O5B	3.51	112.25	102.94
3	D	900	NAD	C3N-C7N-N7N	4.02	122.22	117.82
3	B	900	NAD	O3-PN-O5D	4.08	113.76	102.94
3	C	900	NAD	O3-PN-O5D	4.41	114.63	102.94
3	C	900	NAD	O3-PA-O5B	6.58	120.39	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	NAD	1	0
3	C	900	NAD	2	0
3	D	900	NAD	1	0

5.7 Other polymers

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(Å ²)	Q<0.9
1	A	347/359 (96%)	-0.04	13 (3%) 45 50	31, 53, 109, 134	0
1	B	350/359 (97%)	-0.37	3 (0%) 85 88	29, 43, 64, 106	0
1	C	352/359 (98%)	-0.42	4 (1%) 82 84	29, 41, 59, 103	0
1	D	355/359 (98%)	-0.20	8 (2%) 64 67	34, 48, 79, 116	0
All	All	1404/1436 (97%)	-0.26	28 (1%) 68 72	29, 45, 84, 134	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	LEU	4.5
1	D	354	HIS	4.4
1	A	83	LYS	4.0
1	D	83	LYS	3.9
1	A	79	GLY	3.7
1	A	81	PRO	3.6
1	D	352	HIS	3.4
1	C	350	GLU	3.3
1	A	76	LYS	3.2
1	A	78	ASP	3.2
1	C	351	HIS	3.2
1	A	75	PRO	3.0
1	A	49	PHE	3.0
1	C	349	LEU	3.0
1	A	80	LEU	2.9
1	A	82	ARG	2.8
1	B	350	GLU	2.8
1	D	82	ARG	2.8
1	D	80	LEU	2.5
1	A	56	PRO	2.4
1	D	79	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	353	HIS	2.2
1	C	204	ARG	2.2
1	B	28	GLU	2.1
1	A	50	GLY	2.1
1	D	81	PRO	2.1
1	A	278	ASP	2.1
1	A	85	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BCN	A	501	11/11	0.95	0.20	13.54	19,28,38,48	0
2	BCN	B	1502	11/11	0.74	0.30	9.89	39,58,68,70	11
2	BCN	D	501	11/11	0.92	0.20	6.94	25,40,52,62	0
2	BCN	C	501	11/11	0.96	0.16	2.56	31,42,49,52	0
2	BCN	B	501	11/11	0.94	0.15	2.18	27,33,41,47	0
3	NAD	D	900	44/44	0.94	0.18	1.18	11,30,75,77	44
3	NAD	A	900	44/44	0.91	0.24	1.15	8,24,54,55	44
3	NAD	C	900	44/44	0.95	0.16	1.03	22,33,54,57	0
3	NAD	B	900	44/44	0.96	0.13	0.03	16,33,51,54	0
4	MN	B	999	1/1	1.00	0.04	-	32,32,32,32	0
4	MN	A	999	1/1	0.98	0.03	-	42,42,42,42	0
4	MN	C	999	1/1	0.99	0.03	-	38,38,38,38	0
4	MN	D	999	1/1	0.98	0.04	-	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.