



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:37 PM GMT

PDB ID : 4CR8
Title : Crystal structure of the N-acetyl-D-mannosamine dehydrogenase with NAD
Authors : Gil-Ortiz, F.; Sola-Carvajal, A.; Garcia-Carmona, F.; Sanchez-Ferrer, A.; Rubio, V.
Deposited on : 2014-02-25
Resolution : 2.20 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

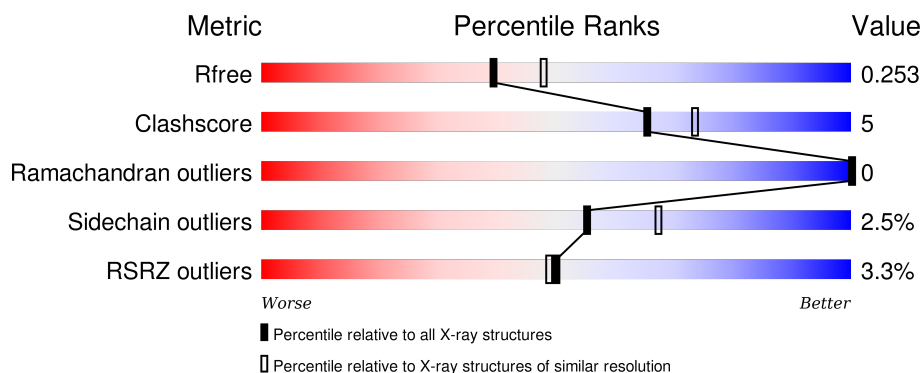
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	271	<div> <div>4%</div> <div>89%</div> <div>7%</div> <div>...</div> </div>
1	B	271	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>...</div> </div>
1	C	271	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>...</div> </div>
1	D	271	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>...</div> </div>
1	E	271	<div> <div>4%</div> <div>90%</div> <div>6%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	271	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>88%</div><div>8%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	271	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>88%</div><div>8%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	271	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>88%</div><div>8%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15594 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 N-ACYLMANNOSAMINE 1-DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1839	1142	327	358	12			
1	B	263	Total	C	N	O	S	0	0	0
			1852	1147	332	361	12			
1	C	262	Total	C	N	O	S	0	0	0
			1834	1137	328	357	12			
1	D	264	Total	C	N	O	S	0	0	0
			1850	1148	331	359	12			
1	E	262	Total	C	N	O	S	0	1	0
			1842	1142	331	357	12			
1	F	262	Total	C	N	O	S	0	0	0
			1838	1139	328	359	12			
1	G	262	Total	C	N	O	S	0	0	0
			1835	1137	328	358	12			
1	H	261	Total	C	N	O	S	0	0	0
			1843	1142	331	358	12			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	86	Total	O	0	0
			86	86		
3	C	90	Total	O	0	0
			90	90		
3	D	75	Total	O	0	0
			75	75		

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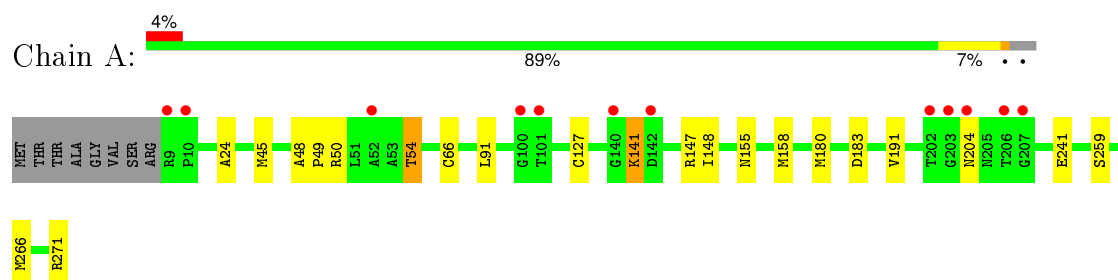
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	74	Total 74	O 74	0	0
3	F	56	Total 56	O 56	0	0
3	G	88	Total 88	O 88	0	0
3	H	65	Total 65	O 65	0	0

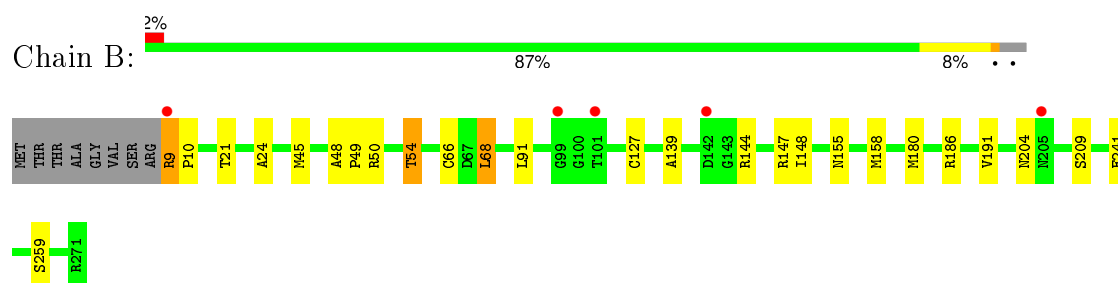
3 Residue-property plots [i](#)

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.

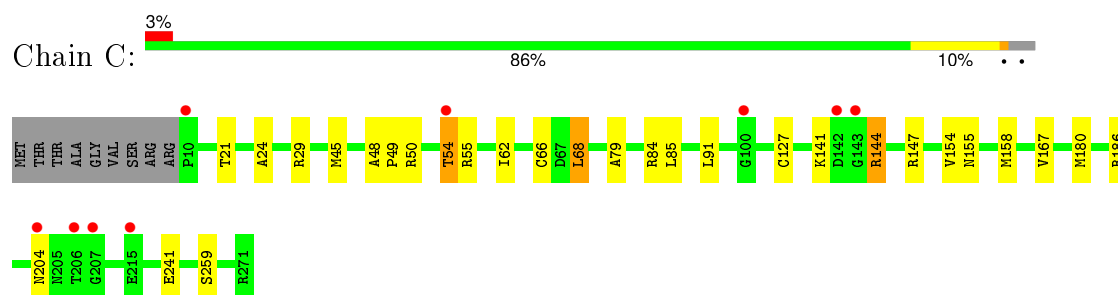
- Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE



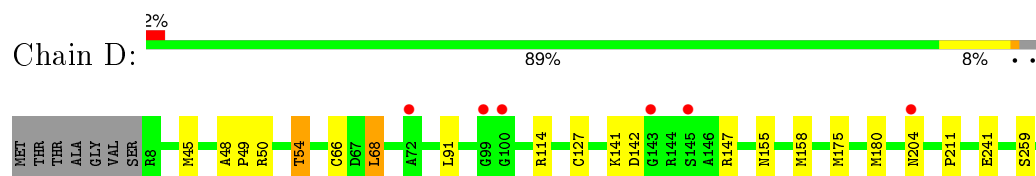
- Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE




- Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE

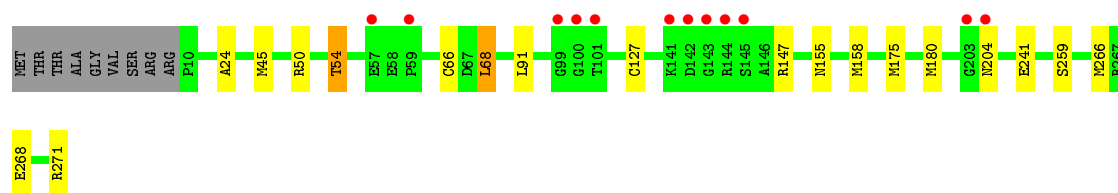


- Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE




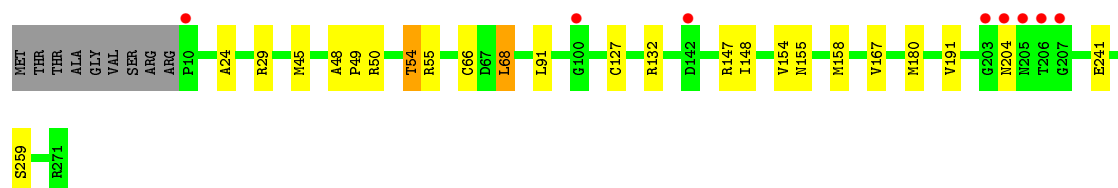
- Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE

Chain E: 




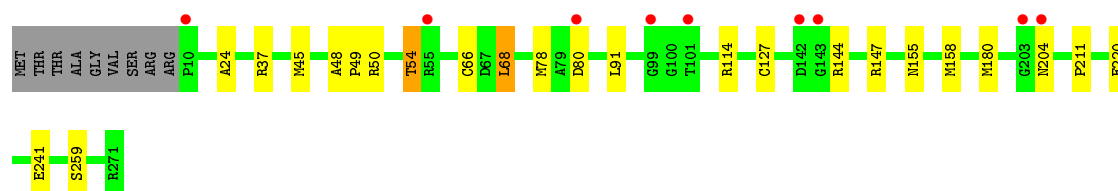
• Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE

Chain F: 




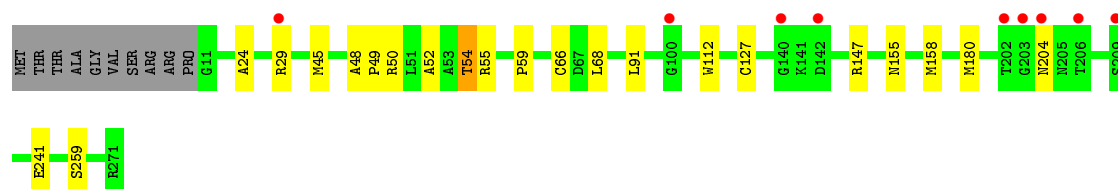
• Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE

Chain G: 



• Molecule 1: N-ACYLMANNOSAMINE 1-DEHYDROGENASE

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.95Å 146.79Å 90.42Å 90.00° 115.29° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.20) 99.5 (19.94-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.222 , 0.253 0.223 , 0.253	Depositor DCC
R_{free} test set	4723 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 94226 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15594	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8734e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: 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	0.61	0/1862	0.71	1/2528 (0.0%)
1	B	0.63	0/1875	0.69	0/2543
1	C	0.60	0/1856	0.69	0/2519
1	D	0.61	0/1873	0.72	0/2542
1	E	0.61	0/1866	0.71	0/2530
1	F	0.61	0/1860	0.70	0/2524
1	G	0.62	0/1857	0.67	0/2519
1	H	0.62	1/1865 (0.1%)	0.71	1/2528 (0.0%)
All	All	0.61	1/14914 (0.0%)	0.70	2/20233 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	112	TRP	CD2-CE2	5.11	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	CB-CG-OD1	5.76	123.49	118.30
1	H	68	LEU	CB-CG-CD2	5.55	120.44	111.00

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	1839	0	1828	14	0
1	B	1852	0	1843	21	0
1	C	1834	0	1821	25	0
1	D	1850	0	1841	23	0
1	E	1842	0	1834	16	0
1	F	1838	0	1825	18	0
1	G	1835	0	1821	24	0
1	H	1843	0	1845	18	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	0	0
3	A	111	0	0	1	0
3	B	86	0	0	2	0
3	C	90	0	0	3	0
3	D	75	0	0	4	0
3	E	74	0	0	2	0
3	F	56	0	0	2	0
3	G	88	0	0	7	0
3	H	65	0	0	0	0
All	All	15594	0	14754	147	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 (147) 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:C:84:ARG:O	1:H:59:PRO:HG2	1.57	1.03
1:D:50:ARG:NH1	3:D:2008:HOH:O	1.97	0.97
1:E:50:ARG:NH1	3:E:2011:HOH:O	1.97	0.97
1:C:50:ARG:O	1:C:54:THR:HG23	1.71	0.89
1:F:50:ARG:O	1:F:54:THR:HG23	1.75	0.86
1:E:50:ARG:O	1:E:54:THR:HG23	1.76	0.85
1:D:266:MET:HA	3:D:2073:HOH:O	1.75	0.85
1:G:50:ARG:O	1:G:54:THR:HG23	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ARG:O	1:D:54:THR:HG23	1.79	0.83
1:D:271:ARG:HB3	3:D:2073:HOH:O	1.78	0.83
1:A:50:ARG:O	1:A:54:THR:HG23	1.79	0.83
1:B:45:MET:HE1	3:B:2018:HOH:O	1.80	0.81
1:B:50:ARG:O	1:B:54:THR:HG23	1.81	0.81
1:H:50:ARG:O	1:H:54:THR:HG23	1.80	0.80
1:D:127:CYS:HB3	1:D:180:MET:HE3	1.66	0.78
1:A:158:MET:HE1	1:A:259:SER:HB2	1.67	0.77
1:F:45:MET:HE3	1:F:66:CYS:HB3	1.68	0.76
1:A:45:MET:HE3	1:A:66:CYS:HB3	1.69	0.75
1:D:158:MET:HE1	1:D:259:SER:HB2	1.70	0.73
1:C:84:ARG:C	1:H:59:PRO:HG2	2.09	0.73
1:C:158:MET:HE1	1:C:259:SER:HB2	1.71	0.73
1:E:45:MET:HE3	1:E:66:CYS:HB3	1.71	0.72
1:D:45:MET:HE3	1:D:66:CYS:HB3	1.71	0.72
1:B:68:LEU:HD22	2:B:1272:NAD:C2A	2.20	0.71
1:H:158:MET:HE1	1:H:259:SER:HB2	1.71	0.71
1:B:127:CYS:HB3	1:B:180:MET:HE3	1.73	0.71
1:C:45:MET:HE3	1:C:66:CYS:HB3	1.73	0.70
1:A:45:MET:HE3	1:A:66:CYS:CB	2.22	0.70
1:F:158:MET:HE1	1:F:259:SER:HB2	1.72	0.69
1:H:45:MET:HE3	1:H:66:CYS:HB3	1.73	0.69
1:G:45:MET:HE1	3:G:2014:HOH:O	1.92	0.69
1:C:50:ARG:O	1:C:54:THR:CG2	2.41	0.68
3:A:2107:HOH:O	1:B:186:ARG:HD2	1.94	0.68
1:G:78:MET:HG2	3:G:2014:HOH:O	1.94	0.67
1:F:45:MET:HE3	1:F:66:CYS:CB	2.25	0.67
1:F:50:ARG:O	1:F:54:THR:CG2	2.42	0.67
1:B:9:ARG:N	1:B:10:PRO:HD2	2.10	0.67
1:H:45:MET:HE3	1:H:66:CYS:CB	2.24	0.67
1:G:45:MET:HE3	1:G:66:CYS:HB3	1.76	0.67
1:A:50:ARG:O	1:A:54:THR:CG2	2.43	0.66
1:G:80:ASP:OD1	3:G:2027:HOH:O	2.13	0.66
1:E:127:CYS:HB3	1:E:180:MET:HE3	1.76	0.66
1:B:209:SER:O	3:B:2074:HOH:O	2.14	0.65
1:F:68:LEU:HD22	2:F:1272:NAD:C2A	2.26	0.65
1:B:45:MET:HE3	1:B:66:CYS:HB3	1.78	0.64
1:G:50:ARG:O	1:G:54:THR:CG2	2.44	0.64
1:H:50:ARG:O	1:H:54:THR:CG2	2.46	0.63
1:B:50:ARG:O	1:B:54:THR:CG2	2.47	0.62
1:E:50:ARG:O	1:E:54:THR:CG2	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:MET:HE1	1:G:259:SER:HB2	1.82	0.62
1:C:45:MET:HE3	1:C:66:CYS:CB	2.30	0.62
1:D:50:ARG:O	1:D:54:THR:CG2	2.48	0.60
1:G:68:LEU:HD22	2:G:1272:NAD:C2A	2.31	0.60
1:D:45:MET:HE3	1:D:66:CYS:CB	2.32	0.60
1:D:271:ARG:CB	3:D:2073:HOH:O	2.42	0.60
1:E:158:MET:HE1	1:E:259:SER:HB2	1.83	0.60
1:C:127:CYS:HB3	1:C:180:MET:HE3	1.84	0.59
1:G:127:CYS:HB3	1:G:180:MET:HE3	1.85	0.59
1:B:158:MET:HE2	1:B:259:SER:HB2	1.85	0.58
1:E:45:MET:HE3	1:E:66:CYS:CB	2.33	0.57
1:H:52:ALA:O	1:H:55:ARG:NH2	2.37	0.57
1:D:211:PRO:HG2	1:G:114:ARG:CD	2.35	0.56
1:B:9:ARG:C	1:B:9:ARG:HE	2.08	0.56
1:F:155:ASN:HA	1:F:158:MET:O	2.05	0.56
1:E:268:GLU:HG2	3:E:2071:HOH:O	2.06	0.55
1:C:68:LEU:HD22	2:C:1272:NAD:C2A	2.37	0.54
1:G:45:MET:HE3	1:G:66:CYS:CB	2.37	0.54
1:D:127:CYS:HB3	1:D:180:MET:CE	2.34	0.54
1:E:266:MET:O	1:E:271[A]:ARG:NH1	2.35	0.54
1:A:127:CYS:HB3	1:A:180:MET:HE3	1.89	0.54
1:C:84:ARG:O	1:H:59:PRO:CG	2.45	0.53
1:A:266:MET:O	1:A:271:ARG:HD3	2.07	0.53
1:D:68:LEU:HD22	2:D:1272:NAD:C2A	2.38	0.53
1:E:68:LEU:HD22	2:E:1272:NAD:C2A	2.39	0.53
1:B:45:MET:HE3	1:B:66:CYS:CB	2.39	0.53
1:C:158:MET:HE1	1:C:259:SER:CB	2.38	0.52
1:H:127:CYS:HB3	1:H:180:MET:HE3	1.92	0.52
1:B:48:ALA:HB3	1:B:49:PRO:HD3	1.92	0.52
1:F:132:ARG:NH1	3:F:2031:HOH:O	2.42	0.52
1:H:155:ASN:HA	1:H:158:MET:O	2.10	0.52
1:F:127:CYS:HB3	1:F:180:MET:HE3	1.92	0.52
1:F:158:MET:HE1	1:F:259:SER:CB	2.38	0.51
1:C:24:ALA:CB	1:C:54:THR:HG21	2.40	0.51
1:G:37:ARG:NH1	3:G:2012:HOH:O	2.34	0.51
1:D:266:MET:O	1:D:271:ARG:NH1	2.38	0.50
1:D:211:PRO:HG2	1:G:114:ARG:HD2	1.94	0.50
1:A:155:ASN:HA	1:A:158:MET:O	2.12	0.50
1:B:155:ASN:HA	1:B:158:MET:O	2.12	0.50
1:C:62:ILE:HD13	1:H:59:PRO:HD3	1.94	0.50
1:D:175:MET:HB3	1:F:167:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:NH1	1:D:241:GLU:O	2.45	0.50
1:G:147:ARG:NH1	1:G:241:GLU:O	2.45	0.49
1:C:155:ASN:HA	1:C:158:MET:O	2.13	0.49
1:C:85:LEU:HA	1:H:59:PRO:HG2	1.95	0.49
1:F:147:ARG:NH1	1:F:241:GLU:O	2.45	0.49
1:G:48:ALA:HB3	1:G:49:PRO:HD3	1.94	0.48
1:G:24:ALA:CB	1:G:54:THR:HG21	2.44	0.48
1:E:127:CYS:HB3	1:E:180:MET:CE	2.44	0.48
1:G:155:ASN:HA	1:G:158:MET:O	2.14	0.48
1:B:147:ARG:NH1	1:B:241:GLU:O	2.47	0.48
1:H:24:ALA:CB	1:H:54:THR:HG21	2.44	0.48
1:F:24:ALA:CB	1:F:54:THR:HG21	2.44	0.48
1:E:24:ALA:CB	1:E:54:THR:HG21	2.44	0.47
1:C:48:ALA:HB3	1:C:49:PRO:HD3	1.96	0.47
1:B:21:THR:HG22	1:B:45:MET:HE2	1.96	0.47
1:D:211:PRO:HG2	1:G:114:ARG:HD3	1.95	0.47
1:D:114:ARG:CD	1:G:211:PRO:HG2	2.45	0.47
1:E:266:MET:O	1:E:271[A]:ARG:HD3	2.14	0.47
1:F:29:ARG:NH1	1:F:55:ARG:O	2.45	0.47
1:B:9:ARG:N	1:B:10:PRO:CD	2.76	0.47
1:A:48:ALA:HB3	1:A:49:PRO:HD3	1.96	0.47
1:B:24:ALA:CB	1:B:54:THR:HG21	2.46	0.46
1:E:155:ASN:HA	1:E:158:MET:O	2.15	0.45
1:H:29:ARG:NH1	1:H:55:ARG:O	2.47	0.45
1:E:147:ARG:NH1	1:E:241:GLU:O	2.47	0.45
1:A:158:MET:HE1	1:A:259:SER:CB	2.43	0.45
1:B:148:ILE:O	1:B:191:VAL:HA	2.17	0.45
1:G:127:CYS:HB3	1:G:180:MET:CE	2.45	0.44
1:H:48:ALA:HB3	1:H:49:PRO:HD3	2.00	0.44
1:C:167:VAL:HG12	1:E:175:MET:HB3	2.00	0.44
1:A:147:ARG:NH1	1:A:241:GLU:O	2.49	0.44
1:A:24:ALA:CB	1:A:54:THR:HG21	2.47	0.44
1:D:114:ARG:HD3	1:G:211:PRO:HG2	1.99	0.44
1:D:141:LYS:HE2	1:D:142:ASP:OD2	2.18	0.44
1:B:127:CYS:HB3	1:B:180:MET:CE	2.45	0.44
1:C:141:LYS:O	1:C:144:ARG:HB2	2.18	0.44
1:A:141:LYS:HB2	1:A:141:LYS:NZ	2.33	0.43
1:C:21:THR:HG22	1:C:45:MET:HE2	2.01	0.43
1:D:48:ALA:HB3	1:D:49:PRO:HD3	2.01	0.43
1:G:220:GLU:OE1	3:G:2075:HOH:O	2.21	0.43
1:D:155:ASN:HA	1:D:158:MET:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:O	1:A:191:VAL:HA	2.19	0.42
1:F:48:ALA:HB3	1:F:49:PRO:HD3	2.01	0.42
1:C:147:ARG:NH1	1:C:241:GLU:O	2.49	0.42
1:F:148:ILE:O	1:F:191:VAL:HA	2.18	0.42
1:H:158:MET:HE1	1:H:259:SER:CB	2.46	0.42
1:C:127:CYS:HB3	1:C:180:MET:CE	2.48	0.42
1:G:45:MET:CE	3:G:2018:HOH:O	2.68	0.41
1:C:154:VAL:HG13	3:C:2048:HOH:O	2.21	0.41
1:C:186:ARG:NE	3:C:2064:HOH:O	2.53	0.41
1:F:158:MET:CE	1:F:259:SER:CB	2.99	0.41
1:B:139:ALA:HA	1:B:144:ARG:HG3	2.03	0.41
1:G:45:MET:HE1	3:G:2018:HOH:O	2.20	0.41
1:H:147:ARG:NH1	1:H:241:GLU:O	2.51	0.41
1:F:154:VAL:HG13	3:F:2040:HOH:O	2.20	0.41
1:C:79:ALA:HB3	3:C:2022:HOH:O	2.20	0.41
1:C:29:ARG:NH1	1:C:55:ARG:O	2.49	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	261/271 (96%)	255 (98%)	6 (2%)	0	100	100
1	B	261/271 (96%)	255 (98%)	6 (2%)	0	100	100
1	C	260/271 (96%)	254 (98%)	6 (2%)	0	100	100
1	D	262/271 (97%)	256 (98%)	6 (2%)	0	100	100
1	E	260/271 (96%)	254 (98%)	6 (2%)	0	100	100
1	F	260/271 (96%)	255 (98%)	5 (2%)	0	100	100
1	G	260/271 (96%)	257 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	259/271 (96%)	253 (98%)	6 (2%)	0	100	100
All	All	2083/2168 (96%)	2039 (98%)	44 (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	172/183 (94%)	168 (98%)	4 (2%)	58	71
1	B	174/183 (95%)	169 (97%)	5 (3%)	50	62
1	C	171/183 (93%)	166 (97%)	5 (3%)	50	62
1	D	173/183 (94%)	169 (98%)	4 (2%)	58	71
1	E	172/183 (94%)	168 (98%)	4 (2%)	58	71
1	F	172/183 (94%)	168 (98%)	4 (2%)	58	71
1	G	171/183 (93%)	166 (97%)	5 (3%)	50	62
1	H	174/183 (95%)	171 (98%)	3 (2%)	68	81
All	All	1379/1464 (94%)	1345 (98%)	34 (2%)	55	67

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	91	LEU
1	A	141	LYS
1	A	204	ASN
1	B	9	ARG
1	B	54	THR
1	B	68	LEU
1	B	91	LEU
1	B	204	ASN
1	C	54	THR

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Mol	Chain	Res	Type
1	C	68	LEU
1	C	91	LEU
1	C	144	ARG
1	C	204	ASN
1	D	54	THR
1	D	68	LEU
1	D	91	LEU
1	D	204	ASN
1	E	54	THR
1	E	68	LEU
1	E	91	LEU
1	E	204	ASN
1	F	54	THR
1	F	68	LEU
1	F	91	LEU
1	F	204	ASN
1	G	54	THR
1	G	68	LEU
1	G	91	LEU
1	G	144	ARG
1	G	204	ASN
1	H	54	THR
1	H	91	LEU
1	H	204	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	B	204	ASN
1	C	204	ASN
1	D	204	ASN
1	E	204	ASN
1	F	204	ASN
1	G	204	ASN
1	H	204	ASN

5.3.3 RNA ⓘ

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	A	1272	-	23,29,48	1.90	6 (26%)	27,45,73	2.98	5 (18%)
2	NAD	B	1272	-	23,29,48	1.99	6 (26%)	27,45,73	3.03	7 (25%)
2	NAD	C	1272	-	23,29,48	1.77	7 (30%)	27,45,73	3.26	5 (18%)
2	NAD	D	1272	-	23,29,48	1.74	7 (30%)	27,45,73	2.91	5 (18%)
2	NAD	E	1272	-	23,29,48	1.68	6 (26%)	27,45,73	3.07	6 (22%)
2	NAD	F	1272	-	23,29,48	1.96	6 (26%)	27,45,73	3.45	6 (22%)
2	NAD	G	1272	-	23,29,48	2.05	6 (26%)	27,45,73	2.97	7 (25%)
2	NAD	H	1272	-	23,29,48	1.87	5 (21%)	27,45,73	3.12	4 (14%)

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	NAD	A	1272	-	-	0/12/32/62	0/3/3/5
2	NAD	B	1272	-	-	0/12/32/62	0/3/3/5
2	NAD	C	1272	-	-	0/12/32/62	0/3/3/5
2	NAD	D	1272	-	-	0/12/32/62	0/3/3/5
2	NAD	E	1272	-	-	0/12/32/62	0/3/3/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	F	1272	-	-	0/12/32/62	0/3/3/5
2	NAD	G	1272	-	-	0/12/32/62	0/3/3/5
2	NAD	H	1272	-	-	0/12/32/62	0/3/3/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1272	NAD	C2B-C3B	-2.72	1.46	1.53
2	H	1272	NAD	C5A-C4A	-2.64	1.34	1.40
2	F	1272	NAD	C5A-C4A	-2.63	1.34	1.40
2	E	1272	NAD	C5A-C4A	-2.62	1.34	1.40
2	A	1272	NAD	C5A-C4A	-2.51	1.34	1.40
2	C	1272	NAD	C4A-N3A	-2.44	1.31	1.35
2	F	1272	NAD	C2B-C3B	-2.41	1.46	1.53
2	B	1272	NAD	C5A-C4A	-2.40	1.35	1.40
2	A	1272	NAD	C2B-C3B	-2.37	1.46	1.53
2	C	1272	NAD	C5A-C4A	-2.21	1.35	1.40
2	G	1272	NAD	C5A-N7A	-2.21	1.31	1.39
2	D	1272	NAD	C5A-C4A	-2.20	1.35	1.40
2	D	1272	NAD	O3B-C3B	2.13	1.48	1.43
2	E	1272	NAD	PA-O1A	2.29	1.59	1.51
2	D	1272	NAD	C2A-N1A	2.31	1.38	1.33
2	E	1272	NAD	C2A-N3A	2.34	1.36	1.32
2	D	1272	NAD	PA-O1A	2.43	1.60	1.51
2	C	1272	NAD	C2A-N3A	2.58	1.36	1.32
2	A	1272	NAD	PA-O1A	2.60	1.60	1.51
2	E	1272	NAD	C2A-N1A	2.61	1.38	1.33
2	D	1272	NAD	PN-O3	2.61	1.67	1.61
2	F	1272	NAD	C2A-N3A	2.75	1.37	1.32
2	C	1272	NAD	C2A-N1A	2.86	1.39	1.33
2	B	1272	NAD	PA-O1A	2.99	1.62	1.51
2	C	1272	NAD	PA-O1A	3.00	1.62	1.51
2	E	1272	NAD	PN-O3	3.03	1.68	1.61
2	B	1272	NAD	C2A-N1A	3.09	1.39	1.33
2	G	1272	NAD	C2A-N1A	3.10	1.39	1.33
2	G	1272	NAD	PA-O1A	3.20	1.62	1.51
2	H	1272	NAD	PA-O1A	3.22	1.62	1.51
2	B	1272	NAD	PN-O3	3.26	1.68	1.61
2	D	1272	NAD	C2A-N3A	3.34	1.38	1.32
2	F	1272	NAD	C2A-N1A	3.38	1.40	1.33
2	C	1272	NAD	PN-O1N	3.65	1.61	1.50
2	F	1272	NAD	PN-O1N	3.75	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1272	NAD	O4B-C1B	3.82	1.46	1.41
2	H	1272	NAD	PN-O1N	3.88	1.62	1.50
2	A	1272	NAD	C2A-N3A	3.92	1.39	1.32
2	E	1272	NAD	PN-O1N	3.97	1.62	1.50
2	B	1272	NAD	C2A-N3A	4.00	1.39	1.32
2	A	1272	NAD	PN-O1N	4.01	1.62	1.50
2	G	1272	NAD	C2A-N3A	4.08	1.39	1.32
2	D	1272	NAD	PN-O1N	4.15	1.63	1.50
2	H	1272	NAD	C2A-N1A	4.28	1.42	1.33
2	A	1272	NAD	C2A-N1A	4.32	1.42	1.33
2	H	1272	NAD	C2A-N3A	4.34	1.39	1.32
2	G	1272	NAD	PN-O1N	4.52	1.64	1.50
2	F	1272	NAD	PA-O1A	4.72	1.68	1.51
2	B	1272	NAD	PN-O1N	4.79	1.65	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1272	NAD	N3A-C2A-N1A	-13.90	118.25	128.89
2	C	1272	NAD	N3A-C2A-N1A	-13.49	118.57	128.89
2	A	1272	NAD	N3A-C2A-N1A	-13.10	118.86	128.89
2	F	1272	NAD	N3A-C2A-N1A	-12.95	118.98	128.89
2	B	1272	NAD	N3A-C2A-N1A	-12.79	119.10	128.89
2	E	1272	NAD	N3A-C2A-N1A	-12.57	119.27	128.89
2	D	1272	NAD	N3A-C2A-N1A	-12.48	119.34	128.89
2	G	1272	NAD	N3A-C2A-N1A	-11.72	119.92	128.89
2	F	1272	NAD	C2B-C1B-N9A	-7.25	103.21	114.29
2	C	1272	NAD	C2B-C1B-N9A	-6.20	104.81	114.29
2	G	1272	NAD	C2B-C1B-N9A	-5.18	106.37	114.29
2	F	1272	NAD	C4B-O4B-C1B	-4.36	104.92	109.72
2	E	1272	NAD	C2B-C1B-N9A	-4.35	107.64	114.29
2	G	1272	NAD	C4B-O4B-C1B	-4.34	104.95	109.72
2	D	1272	NAD	C1B-N9A-C4A	-4.21	120.59	126.94
2	F	1272	NAD	C1B-N9A-C4A	-4.10	120.75	126.94
2	H	1272	NAD	C2B-C1B-N9A	-4.10	108.03	114.29
2	B	1272	NAD	C4B-O4B-C1B	-4.05	105.27	109.72
2	A	1272	NAD	C2B-C1B-N9A	-3.58	108.83	114.29
2	B	1272	NAD	C2B-C1B-N9A	-3.51	108.92	114.29
2	E	1272	NAD	C4A-C5A-N7A	-3.19	106.55	109.48
2	D	1272	NAD	C4A-C5A-N7A	-3.18	106.55	109.48
2	B	1272	NAD	C4A-C5A-N7A	-2.90	106.81	109.48
2	H	1272	NAD	C4A-C5A-N7A	-2.84	106.87	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1272	NAD	C2B-C1B-N9A	-2.44	110.57	114.29
2	C	1272	NAD	C4A-C5A-N7A	-2.34	107.32	109.48
2	A	1272	NAD	O3-PN-O1N	-2.33	100.42	107.70
2	E	1272	NAD	O2N-PN-O1N	-2.24	103.98	114.72
2	B	1272	NAD	O5B-C5B-C4B	-2.21	100.96	109.12
2	C	1272	NAD	C1B-N9A-C4A	-2.06	123.83	126.94
2	G	1272	NAD	C4A-C5A-N7A	-2.05	107.59	109.48
2	E	1272	NAD	O5D-PN-O1N	2.03	118.31	110.85
2	B	1272	NAD	O5D-PN-O2N	2.10	119.08	110.61
2	F	1272	NAD	O5D-PN-O2N	2.17	119.36	110.61
2	A	1272	NAD	O5D-PN-O3	2.18	114.69	104.65
2	G	1272	NAD	O5D-PN-O2N	2.42	120.38	110.61
2	G	1272	NAD	O3-PA-O5B	2.72	110.14	102.94
2	A	1272	NAD	O4B-C1B-N9A	3.89	116.23	108.10
2	B	1272	NAD	O4B-C1B-N9A	4.13	116.75	108.10
2	D	1272	NAD	O4B-C1B-N9A	4.25	117.00	108.10
2	G	1272	NAD	O4B-C1B-N9A	4.63	117.80	108.10
2	H	1272	NAD	O4B-C1B-N9A	4.95	118.46	108.10
2	E	1272	NAD	O4B-C1B-N9A	6.04	120.75	108.10
2	C	1272	NAD	O4B-C1B-N9A	6.16	121.00	108.10
2	F	1272	NAD	O4B-C1B-N9A	6.74	122.21	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1272	NAD	1	0
2	C	1272	NAD	1	0
2	D	1272	NAD	1	0
2	E	1272	NAD	1	0
2	F	1272	NAD	1	0
2	G	1272	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	263/271 (97%)	0.08	12 (4%) 36 35	2, 8, 25, 48	0
1	B	263/271 (97%)	0.01	5 (1%) 70 68	3, 8, 22, 37	0
1	C	262/271 (96%)	0.14	9 (3%) 49 47	4, 9, 25, 43	0
1	D	264/271 (97%)	-0.03	6 (2%) 64 63	3, 9, 22, 32	0
1	E	262/271 (96%)	0.05	12 (4%) 36 35	3, 9, 26, 39	0
1	F	262/271 (96%)	0.06	8 (3%) 52 51	4, 9, 24, 46	0
1	G	262/271 (96%)	0.09	9 (3%) 49 47	3, 8, 24, 42	0
1	H	261/271 (96%)	0.11	9 (3%) 49 47	3, 9, 25, 44	0
All	All	2099/2168 (96%)	0.06	70 (3%) 50 49	2, 9, 25, 48	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	ASN	5.5
1	B	99	GLY	5.0
1	C	10	PRO	4.9
1	E	143	GLY	4.9
1	E	100	GLY	4.8
1	A	204	ASN	4.7
1	B	142	ASP	4.7
1	G	142	ASP	4.4
1	C	100	GLY	4.2
1	D	99	GLY	4.2
1	F	100	GLY	4.0
1	H	142	ASP	3.7
1	F	204	ASN	3.7
1	E	99	GLY	3.7
1	F	206	THR	3.6
1	F	142	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	99	GLY	3.4
1	H	100	GLY	3.4
1	H	204	ASN	3.4
1	A	202	THR	3.4
1	F	10	PRO	3.3
1	A	10	PRO	3.3
1	A	9	ARG	3.3
1	B	101	THR	3.3
1	E	57	GLU	3.2
1	A	100	GLY	3.2
1	D	143	GLY	3.1
1	H	202	THR	3.0
1	A	142	ASP	3.0
1	C	143	GLY	2.8
1	E	101	THR	2.8
1	H	203	GLY	2.8
1	G	101	THR	2.8
1	C	207	GLY	2.8
1	C	54	THR	2.8
1	C	142	ASP	2.7
1	H	209	SER	2.7
1	E	144	ARG	2.7
1	A	207	GLY	2.6
1	A	101	THR	2.6
1	G	143	GLY	2.6
1	E	142	ASP	2.5
1	D	100	GLY	2.5
1	B	9	ARG	2.5
1	H	29	ARG	2.5
1	H	206	THR	2.5
1	F	203	GLY	2.5
1	E	59	PRO	2.5
1	C	206	THR	2.4
1	B	205	ASN	2.4
1	D	72	ALA	2.4
1	G	55	ARG	2.4
1	E	145	SER	2.4
1	E	203	GLY	2.3
1	F	207	GLY	2.3
1	A	140	GLY	2.3
1	A	203	GLY	2.3
1	A	206	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	204	ASN	2.2
1	G	10	PRO	2.2
1	D	145	SER	2.2
1	C	215	GLU	2.2
1	G	203	GLY	2.2
1	H	140	GLY	2.2
1	D	204	ASN	2.1
1	E	204	ASN	2.1
1	E	141	LYS	2.1
1	F	205	ASN	2.0
1	A	52	ALA	2.0
1	G	80	ASP	2.0

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	G	1272	27/44	0.90	0.14	0.21	8,10,24,25	0
2	NAD	D	1272	27/44	0.90	0.13	-0.08	10,12,25,26	0
2	NAD	H	1272	27/44	0.90	0.14	-0.18	14,16,22,24	0
2	NAD	B	1272	27/44	0.91	0.12	-0.18	9,10,27,28	0
2	NAD	F	1272	27/44	0.90	0.13	-0.23	13,14,26,29	0
2	NAD	C	1272	27/44	0.92	0.12	-0.29	12,13,22,23	0
2	NAD	E	1272	27/44	0.90	0.13	-0.32	10,11,21,23	0
2	NAD	A	1272	27/44	0.92	0.12	-0.49	13,15,23,24	0

6.5 Other polymers

There are no such residues in this entry.