Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:42 AM GMT

PDB ID	:	2I9P
Title	:	Crystal structure of human hydroxyisobutyrate dehydrogenase complexed with NAD+
Authors	:	Kavanagh, K.L.; Papagrigoriou, E.; Salah, E.; Lukacik, P.; Smee, C.; Burgess, N.; Von Delft, F.; Weigelt, J.; Arrowsmith, C.; Sundstrom, M.; Edwards, A.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-09-06
Resolution	:	2.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

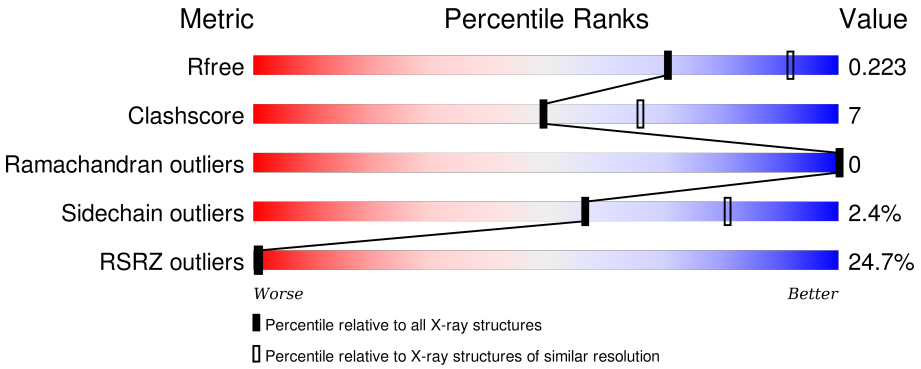
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 <=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	319	19% 79% 13% 8%
1	B	319	26% 79% 14% 7%
1	C	319	24% 80% 11% • 8%
1	D	319	22% 79% 13% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8559 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-hydroxyisobutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2098	1327	346	403	22			
1	B	296	Total	C	N	O	S	0	0	0
			2116	1333	348	413	22			
1	C	293	Total	C	N	O	S	0	1	0
			2088	1318	349	399	22			
1	D	293	Total	C	N	O	S	0	0	0
			2081	1316	343	400	22			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	CLONING ARTIFACT	UNP P31937
A	19	HIS	-	CLONING ARTIFACT	UNP P31937
A	20	HIS	-	CLONING ARTIFACT	UNP P31937
A	21	HIS	-	CLONING ARTIFACT	UNP P31937
A	22	HIS	-	CLONING ARTIFACT	UNP P31937
A	23	HIS	-	CLONING ARTIFACT	UNP P31937
A	24	HIS	-	CLONING ARTIFACT	UNP P31937
A	25	SER	-	CLONING ARTIFACT	UNP P31937
A	26	SER	-	CLONING ARTIFACT	UNP P31937
A	27	GLY	-	CLONING ARTIFACT	UNP P31937
A	28	VAL	-	CLONING ARTIFACT	UNP P31937
A	29	ASP	-	CLONING ARTIFACT	UNP P31937
A	30	LEU	-	CLONING ARTIFACT	UNP P31937
A	31	GLY	-	CLONING ARTIFACT	UNP P31937
A	32	THR	-	CLONING ARTIFACT	UNP P31937
A	33	GLU	-	CLONING ARTIFACT	UNP P31937
A	34	ASN	-	CLONING ARTIFACT	UNP P31937
A	35	LEU	-	CLONING ARTIFACT	UNP P31937
A	36	TYR	-	CLONING ARTIFACT	UNP P31937
A	37	PHE	-	CLONING ARTIFACT	UNP P31937
A	38	GLN	-	CLONING ARTIFACT	UNP P31937

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Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	-	CLONING ARTIFACT	UNP P31937
A	40	MET	-	CLONING ARTIFACT	UNP P31937
B	18	MET	-	CLONING ARTIFACT	UNP P31937
B	19	HIS	-	CLONING ARTIFACT	UNP P31937
B	20	HIS	-	CLONING ARTIFACT	UNP P31937
B	21	HIS	-	CLONING ARTIFACT	UNP P31937
B	22	HIS	-	CLONING ARTIFACT	UNP P31937
B	23	HIS	-	CLONING ARTIFACT	UNP P31937
B	24	HIS	-	CLONING ARTIFACT	UNP P31937
B	25	SER	-	CLONING ARTIFACT	UNP P31937
B	26	SER	-	CLONING ARTIFACT	UNP P31937
B	27	GLY	-	CLONING ARTIFACT	UNP P31937
B	28	VAL	-	CLONING ARTIFACT	UNP P31937
B	29	ASP	-	CLONING ARTIFACT	UNP P31937
B	30	LEU	-	CLONING ARTIFACT	UNP P31937
B	31	GLY	-	CLONING ARTIFACT	UNP P31937
B	32	THR	-	CLONING ARTIFACT	UNP P31937
B	33	GLU	-	CLONING ARTIFACT	UNP P31937
B	34	ASN	-	CLONING ARTIFACT	UNP P31937
B	35	LEU	-	CLONING ARTIFACT	UNP P31937
B	36	TYR	-	CLONING ARTIFACT	UNP P31937
B	37	PHE	-	CLONING ARTIFACT	UNP P31937
B	38	GLN	-	CLONING ARTIFACT	UNP P31937
B	39	SER	-	CLONING ARTIFACT	UNP P31937
B	40	MET	-	CLONING ARTIFACT	UNP P31937
C	18	MET	-	CLONING ARTIFACT	UNP P31937
C	19	HIS	-	CLONING ARTIFACT	UNP P31937
C	20	HIS	-	CLONING ARTIFACT	UNP P31937
C	21	HIS	-	CLONING ARTIFACT	UNP P31937
C	22	HIS	-	CLONING ARTIFACT	UNP P31937
C	23	HIS	-	CLONING ARTIFACT	UNP P31937
C	24	HIS	-	CLONING ARTIFACT	UNP P31937
C	25	SER	-	CLONING ARTIFACT	UNP P31937
C	26	SER	-	CLONING ARTIFACT	UNP P31937
C	27	GLY	-	CLONING ARTIFACT	UNP P31937
C	28	VAL	-	CLONING ARTIFACT	UNP P31937
C	29	ASP	-	CLONING ARTIFACT	UNP P31937
C	30	LEU	-	CLONING ARTIFACT	UNP P31937
C	31	GLY	-	CLONING ARTIFACT	UNP P31937
C	32	THR	-	CLONING ARTIFACT	UNP P31937
C	33	GLU	-	CLONING ARTIFACT	UNP P31937
C	34	ASN	-	CLONING ARTIFACT	UNP P31937

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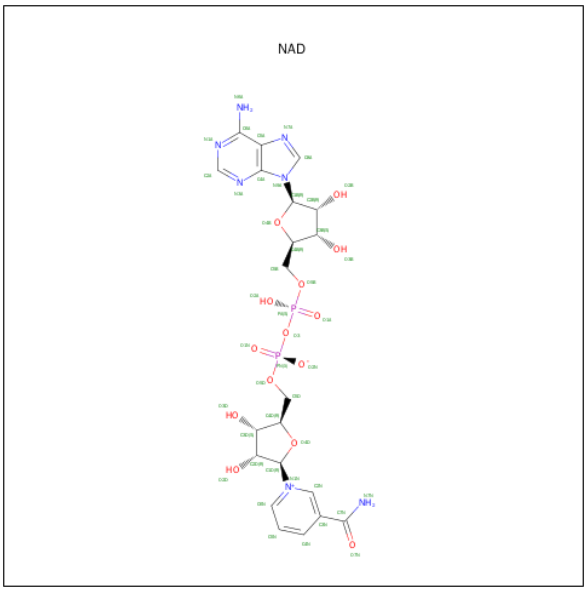
Chain	Residue	Modelled	Actual	Comment	Reference
C	35	LEU	-	CLONING ARTIFACT	UNP P31937
C	36	TYR	-	CLONING ARTIFACT	UNP P31937
C	37	PHE	-	CLONING ARTIFACT	UNP P31937
C	38	GLN	-	CLONING ARTIFACT	UNP P31937
C	39	SER	-	CLONING ARTIFACT	UNP P31937
C	40	MET	-	CLONING ARTIFACT	UNP P31937
D	18	MET	-	CLONING ARTIFACT	UNP P31937
D	19	HIS	-	CLONING ARTIFACT	UNP P31937
D	20	HIS	-	CLONING ARTIFACT	UNP P31937
D	21	HIS	-	CLONING ARTIFACT	UNP P31937
D	22	HIS	-	CLONING ARTIFACT	UNP P31937
D	23	HIS	-	CLONING ARTIFACT	UNP P31937
D	24	HIS	-	CLONING ARTIFACT	UNP P31937
D	25	SER	-	CLONING ARTIFACT	UNP P31937
D	26	SER	-	CLONING ARTIFACT	UNP P31937
D	27	GLY	-	CLONING ARTIFACT	UNP P31937
D	28	VAL	-	CLONING ARTIFACT	UNP P31937
D	29	ASP	-	CLONING ARTIFACT	UNP P31937
D	30	LEU	-	CLONING ARTIFACT	UNP P31937
D	31	GLY	-	CLONING ARTIFACT	UNP P31937
D	32	THR	-	CLONING ARTIFACT	UNP P31937
D	33	GLU	-	CLONING ARTIFACT	UNP P31937
D	34	ASN	-	CLONING ARTIFACT	UNP P31937
D	35	LEU	-	CLONING ARTIFACT	UNP P31937
D	36	TYR	-	CLONING ARTIFACT	UNP P31937
D	37	PHE	-	CLONING ARTIFACT	UNP P31937
D	38	GLN	-	CLONING ARTIFACT	UNP P31937
D	39	SER	-	CLONING ARTIFACT	UNP P31937
D	40	MET	-	CLONING ARTIFACT	UNP P31937

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



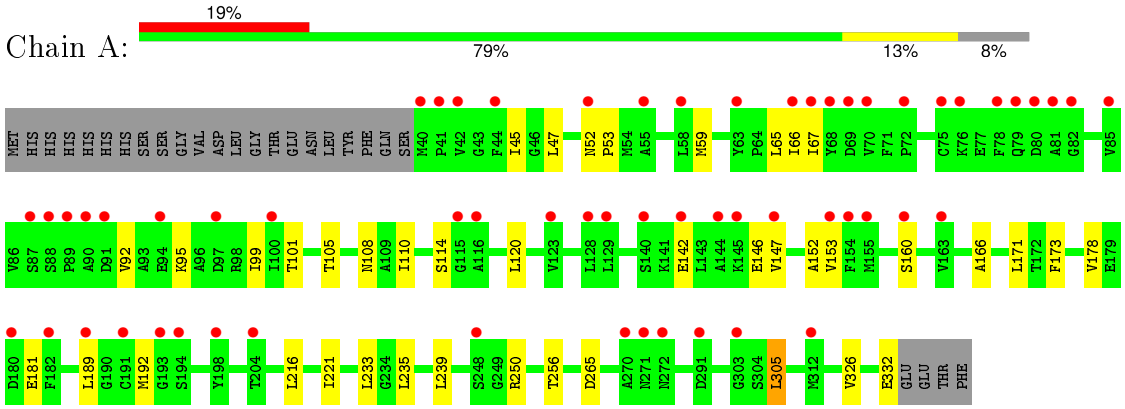
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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.

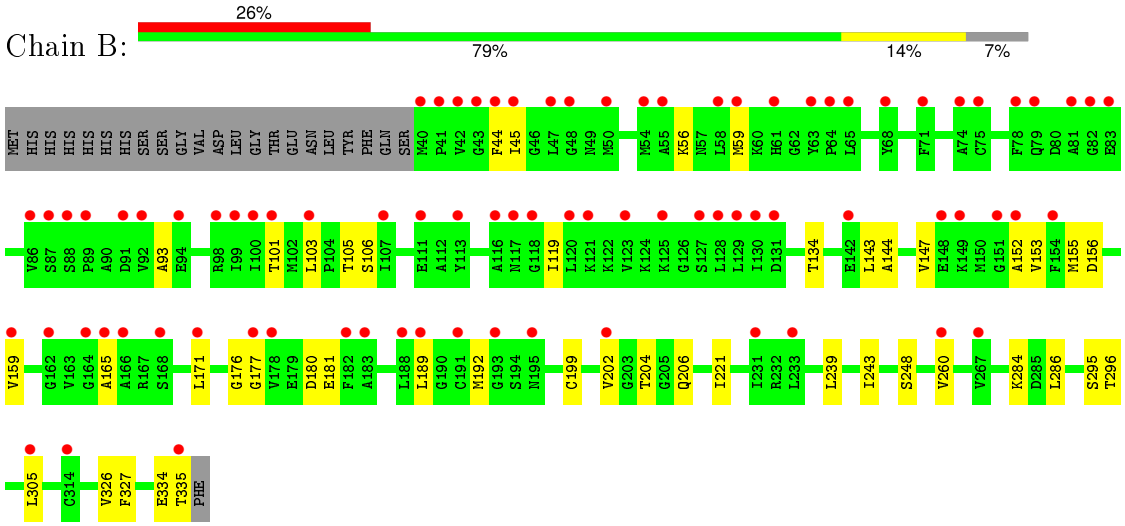
- Molecule 1: 3-hydroxyisobutyrate dehydrogenase

Chain A:



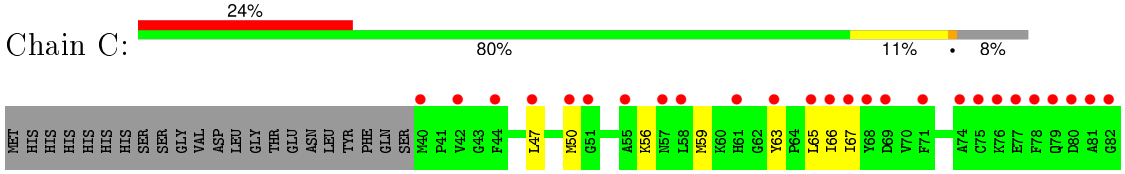
- Molecule 1: 3-hydroxyisobutyrate dehydrogenase

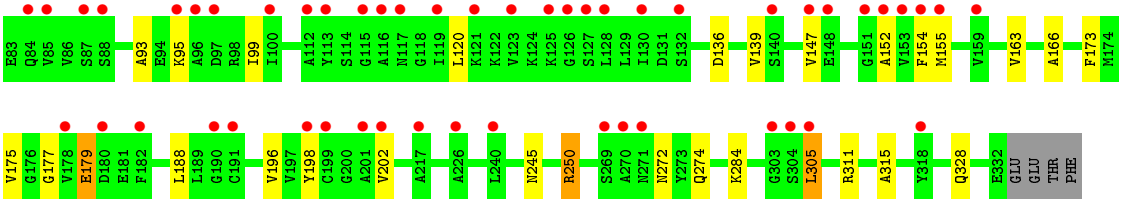
Chain B:



- Molecule 1: 3-hydroxyisobutyrate dehydrogenase

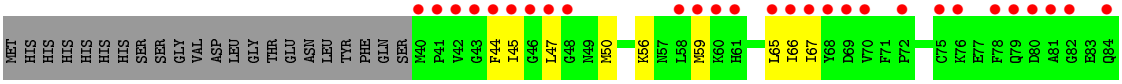
Chain C:

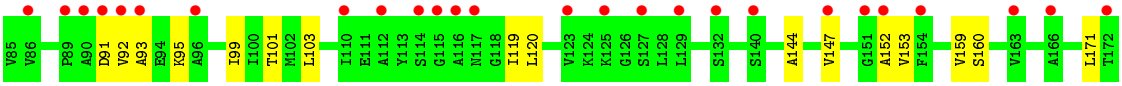


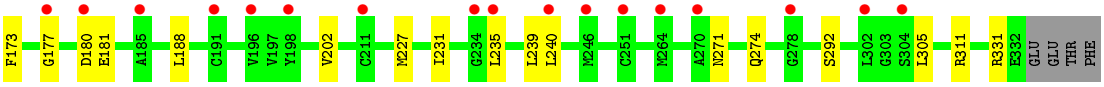


- Molecule 1: 3-hydroxyisobutyrate dehydrogenase

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.63Å 167.32Å 71.09Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 45.88 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.55) 95.5 (45.88-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.220 0.185 , 0.223	Depositor DCC
R_{free} test set	1729 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 75.5	EDS
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 34299 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8559	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.56	0/2132	0.63	1/2885 (0.0%)
1	B	0.57	0/2149	0.65	0/2912
1	C	0.59	0/2125	0.66	1/2880 (0.0%)
1	D	0.59	0/2115	0.67	1/2867 (0.0%)
All	All	0.58	0/8521	0.65	3/11544 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	311	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	250	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	C	311	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2098	0	2070	37	0
1	B	2116	0	2053	39	0
1	C	2088	0	2048	34	0
1	D	2081	0	2033	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
All	All	8559	0	8308	119	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 7.

All (119) 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:47:LEU:HD11	1:D:67:ILE:HG23	1.41	1.03
1:C:305:LEU:HD22	1:D:305:LEU:HD22	1.43	0.97
1:B:45:ILE:HD12	1:B:119:ILE:HD11	1.64	0.79
1:D:47:LEU:HD11	1:D:67:ILE:CG2	2.15	0.77
1:A:239:LEU:HD21	1:B:199:CYS:HA	1.67	0.77
1:A:47:LEU:HD11	1:A:67:ILE:HG23	1.68	0.76
1:D:47:LEU:CD1	1:D:67:ILE:HG23	2.18	0.73
1:D:56:LYS:HA	1:D:59:MET:HE3	1.69	0.72
1:C:272:ASN:HD21	1:C:328:GLN:HE22	1.37	0.69
1:A:305:LEU:HD22	1:B:305:LEU:HD22	1.74	0.68
1:A:47:LEU:CD1	1:A:67:ILE:HG23	2.23	0.67
1:A:105:THR:H	1:A:108:ASN:HD22	1.42	0.67
1:D:147:VAL:HG13	1:D:152:ALA:HB3	1.78	0.65
1:C:173:PHE:HB2	1:C:196:VAL:HG22	1.78	0.64
1:B:45:ILE:HB	1:B:101:THR:HG22	1.79	0.64
1:B:153:VAL:HG11	1:B:181:GLU:HG3	1.79	0.64
1:A:305:LEU:HD11	1:D:305:LEU:HD13	1.80	0.64
1:B:147:VAL:CG1	1:B:152:ALA:HB3	2.29	0.63
1:A:153:VAL:HG11	1:A:181:GLU:HG3	1.79	0.63
1:B:305:LEU:HD21	1:D:305:LEU:HD21	1.80	0.63
1:A:239:LEU:CD2	1:B:199:CYS:HA	2.30	0.61
1:D:177:GLY:HA2	1:D:202:VAL:HG22	1.80	0.61
1:A:171:LEU:HD12	1:A:192:MET:O	2.01	0.61
1:B:147:VAL:HG12	1:B:152:ALA:HB3	1.83	0.60
1:A:173:PHE:CE2	1:A:189:LEU:HD22	2.36	0.60
1:B:56:LYS:HA	1:B:59:MET:HE3	1.84	0.59
1:C:147:VAL:HG13	1:C:152:ALA:HB3	1.86	0.58
1:B:305:LEU:CD1	1:C:305:LEU:HD13	2.34	0.57
1:A:166:ALA:HA	1:A:171:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:HB3	1:C:274:GLN:HE21	1.68	0.57
1:D:147:VAL:CG1	1:D:152:ALA:HB3	2.35	0.57
1:A:120:LEU:HD21	1:A:147:VAL:HG22	1.85	0.56
1:D:47:LEU:CD1	1:D:67:ILE:CG2	2.80	0.56
1:D:45:ILE:HB	1:D:101:THR:HG22	1.88	0.56
1:C:56:LYS:HA	1:C:59:MET:HE2	1.88	0.55
1:A:178:VAL:HG23	1:A:181:GLU:HG2	1.89	0.54
1:B:260:VAL:HG22	1:B:327:PHE:CZ	2.42	0.54
1:D:159:VAL:HG12	1:D:173:PHE:CD2	2.42	0.54
1:B:45:ILE:CD1	1:B:119:ILE:HD11	2.35	0.53
1:A:305:LEU:CD2	1:B:305:LEU:HD22	2.39	0.53
1:A:305:LEU:HD11	1:C:305:LEU:HD21	1.91	0.53
1:A:233:LEU:HD23	1:B:296:THR:HG21	1.91	0.53
1:B:221:ILE:HG12	1:B:326:VAL:HG21	1.90	0.52
1:A:235:LEU:CD2	1:B:204:THR:HG22	2.40	0.52
1:D:66:ILE:HD13	1:D:95:LYS:HB2	1.92	0.51
1:B:56:LYS:HA	1:B:59:MET:CE	2.41	0.51
1:C:120:LEU:HD21	1:C:147:VAL:HG22	1.93	0.51
1:B:105:THR:OG1	1:B:106:SER:N	2.45	0.50
1:D:227:MET:O	1:D:231:ILE:HD12	2.11	0.50
1:A:52:ASN:HB3	1:A:53:PRO:CD	2.41	0.50
1:D:271:ASN:O	1:D:274:GLN:HG2	2.12	0.50
1:B:305:LEU:HD13	1:C:305:LEU:HD13	1.93	0.49
1:D:45:ILE:HG22	1:D:103:LEU:HD21	1.94	0.49
1:A:305:LEU:CD1	1:D:305:LEU:HD13	2.42	0.49
1:B:93:ALA:HB2	1:B:119:ILE:HG23	1.95	0.49
1:D:153:VAL:HG11	1:D:181:GLU:HG3	1.93	0.49
1:A:147:VAL:HG13	1:A:152:ALA:HB3	1.95	0.49
1:B:134:THR:HB	1:B:284:LYS:NZ	2.27	0.49
1:A:110:ILE:O	1:A:114:SER:OG	2.28	0.49
1:A:235:LEU:HD23	1:B:204:THR:HG22	1.95	0.48
1:A:92:VAL:HG12	1:A:99:ILE:HD13	1.94	0.48
1:B:143:LEU:O	1:B:147:VAL:HG23	2.13	0.48
1:D:159:VAL:HG12	1:D:173:PHE:CE2	2.49	0.48
1:A:221:ILE:HG12	1:A:326:VAL:HG21	1.96	0.48
1:B:305:LEU:HD13	1:C:305:LEU:CD1	2.44	0.48
1:C:120:LEU:HD21	1:C:147:VAL:CG2	2.44	0.47
1:B:177:GLY:HA2	1:B:202:VAL:HG22	1.95	0.47
1:C:66:ILE:HD13	1:C:95:LYS:HB2	1.94	0.47
1:C:50:MET:HE3	1:C:166:ALA:HB2	1.96	0.47
1:A:105:THR:H	1:A:108:ASN:ND2	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ALA:HB2	1:D:202:VAL:HG11	1.96	0.47
1:B:144:ALA:HB2	1:B:202:VAL:HG11	1.95	0.47
1:C:93:ALA:HA	1:C:99:ILE:HD11	1.97	0.47
1:B:156:ASP:HB2	1:B:206:GLN:HE21	1.80	0.47
1:C:65:LEU:HD12	1:C:65:LEU:N	2.30	0.46
1:D:235:LEU:CD1	1:D:240:LEU:HD13	2.46	0.46
1:C:245:ASN:HA	1:C:250[A]:ARG:HB3	1.97	0.46
1:C:305:LEU:CD2	1:D:305:LEU:HD22	2.31	0.46
1:C:175:VAL:HG21	1:C:196:VAL:HG13	1.99	0.45
1:D:235:LEU:HD13	1:D:240:LEU:HD13	1.98	0.45
1:D:92:VAL:HG12	1:D:99:ILE:HD13	1.98	0.45
1:C:63:TYR:O	1:C:65:LEU:HD12	2.16	0.45
1:B:165:ALA:HB3	1:B:171:LEU:HD23	1.98	0.45
1:A:305:LEU:HD21	1:C:305:LEU:HD11	1.98	0.45
1:C:47:LEU:HD11	1:C:67:ILE:HG23	1.99	0.44
1:B:305:LEU:HD21	1:D:305:LEU:HD11	2.00	0.44
1:A:52:ASN:HB3	1:A:53:PRO:HD3	2.00	0.44
1:B:134:THR:HB	1:B:284:LYS:HZ1	1.82	0.44
1:C:136:ASP:HB3	1:C:139:VAL:HG23	1.99	0.44
1:B:286:LEU:HA	1:B:286:LEU:HD23	1.80	0.44
1:B:334:GLU:HG2	1:B:335:THR:N	2.32	0.43
1:D:50:MET:CE	1:D:171:LEU:HD21	2.48	0.43
1:A:45:ILE:HB	1:A:101:THR:HG22	2.00	0.43
1:C:155:MET:CE	1:C:175:VAL:HG12	2.49	0.43
1:C:66:ILE:HD13	1:C:95:LYS:CB	2.48	0.43
1:D:56:LYS:HA	1:D:59:MET:CE	2.43	0.43
1:D:120:LEU:HD21	1:D:147:VAL:HG22	2.01	0.43
1:C:155:MET:HE2	1:C:175:VAL:HG12	2.01	0.43
1:A:233:LEU:CD2	1:B:296:THR:HG21	2.48	0.42
1:A:66:ILE:HD13	1:A:95:LYS:HB2	1.99	0.42
1:D:93:ALA:HB2	1:D:119:ILE:HG23	2.01	0.42
1:B:155:MET:HE2	1:B:176:GLY:O	2.19	0.42
1:A:305:LEU:CD1	1:D:305:LEU:CD1	2.98	0.42
1:A:59:MET:HG3	1:A:65:LEU:HD11	2.02	0.42
1:D:65:LEU:HD23	1:D:67:ILE:HD11	2.02	0.41
1:A:216:LEU:HD22	1:B:248:SER:HB2	2.02	0.41
1:B:189:LEU:HD23	1:B:192:MET:HE3	2.02	0.41
1:C:272:ASN:ND2	1:C:328:GLN:HE22	2.11	0.41
1:B:103:LEU:HD22	2:B:500:NAD:C4A	2.50	0.41
1:C:177:GLY:HA2	1:C:202:VAL:HG23	2.02	0.41
1:C:147:VAL:HG11	1:C:154:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:O	1:C:166:ALA:HB3	2.21	0.41
1:B:239:LEU:HD21	1:B:243:ILE:HD12	2.03	0.41
1:A:332:GLU:HG3	1:C:315:ALA:CB	2.51	0.41
1:A:256:THR:O	1:A:256:THR:HG22	2.20	0.41
1:A:142:GLU:O	1:A:146:GLU:HG2	2.21	0.40
1:C:179:GLU:HB2	1:C:198:TYR:CZ	2.55	0.40
1:C:120:LEU:CD2	1:C:147:VAL:HG22	2.51	0.40
1:A:332:GLU:HG3	1:C:315:ALA:HB1	2.04	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	291/319 (91%)	281 (97%)	10 (3%)	0	100	100
1	B	294/319 (92%)	288 (98%)	6 (2%)	0	100	100
1	C	292/319 (92%)	281 (96%)	11 (4%)	0	100	100
1	D	291/319 (91%)	284 (98%)	7 (2%)	0	100	100
All	All	1168/1276 (92%)	1134 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	214/253 (85%)	211 (99%)	3 (1%)	74 90
1	B	214/253 (85%)	210 (98%)	4 (2%)	65 86
1	C	212/253 (84%)	206 (97%)	6 (3%)	51 76
1	D	210/253 (83%)	202 (96%)	8 (4%)	40 65
All	All	850/1012 (84%)	829 (98%)	21 (2%)	57 80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	SER
1	A	265	ASP
1	A	305	LEU
1	B	44	PHE
1	B	159	VAL
1	B	180	ASP
1	B	295	SER
1	C	179	GLU
1	C	188	LEU
1	C	250[A]	ARG
1	C	250[B]	ARG
1	C	284	LYS
1	C	305	LEU
1	D	44	PHE
1	D	91	ASP
1	D	160	SER
1	D	180	ASP
1	D	188	LEU
1	D	239	LEU
1	D	292	SER
1	D	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	B	117	ASN
1	B	170	ASN
1	B	195	ASN
1	C	272	ASN
1	C	274	GLN

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Mol	Chain	Res	Type
1	D	117	ASN
1	D	170	ASN
1	D	195	ASN

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

4 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	500	-	38,48,48	1.65	3 (7%)	47,73,73	2.01	5 (10%)
2	NAD	B	500	-	38,48,48	1.75	3 (7%)	47,73,73	2.05	6 (12%)
2	NAD	C	500	-	38,48,48	1.70	3 (7%)	47,73,73	2.09	5 (10%)
2	NAD	D	500	-	38,48,48	1.62	3 (7%)	47,73,73	1.94	6 (12%)

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	500	-	-	0/22/62/62	0/5/5/5
2	NAD	B	500	-	-	0/22/62/62	0/5/5/5
2	NAD	C	500	-	-	0/22/62/62	0/5/5/5
2	NAD	D	500	-	-	0/22/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	C2A-N1A	2.47	1.38	1.33
2	C	500	NAD	C2A-N1A	2.58	1.38	1.33
2	D	500	NAD	C2A-N1A	2.66	1.39	1.33
2	B	500	NAD	C2A-N1A	2.74	1.39	1.33
2	A	500	NAD	C2A-N3A	3.06	1.37	1.32
2	B	500	NAD	C2A-N3A	3.77	1.38	1.32
2	C	500	NAD	C2A-N3A	3.79	1.38	1.32
2	D	500	NAD	C2A-N3A	3.98	1.39	1.32
2	D	500	NAD	O7N-C7N	7.71	1.40	1.24
2	C	500	NAD	O7N-C7N	8.28	1.41	1.24
2	A	500	NAD	O7N-C7N	8.36	1.42	1.24
2	B	500	NAD	O7N-C7N	8.72	1.42	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	NAD	N3A-C2A-N1A	-11.75	119.90	128.89
2	B	500	NAD	N3A-C2A-N1A	-10.91	120.54	128.89
2	A	500	NAD	N3A-C2A-N1A	-10.62	120.77	128.89
2	D	500	NAD	N3A-C2A-N1A	-9.92	121.30	128.89
2	A	500	NAD	PN-O3-PA	-5.13	118.33	132.73
2	C	500	NAD	PN-O3-PA	-4.78	119.31	132.73
2	B	500	NAD	PN-O3-PA	-4.70	119.53	132.73
2	D	500	NAD	PN-O3-PA	-4.40	120.37	132.73
2	A	500	NAD	C4A-C5A-N7A	-3.42	106.33	109.48
2	B	500	NAD	C4A-C5A-N7A	-3.03	106.69	109.48
2	D	500	NAD	C4A-C5A-N7A	-2.82	106.88	109.48
2	A	500	NAD	C1B-N9A-C4A	-2.46	123.22	126.94
2	B	500	NAD	C1B-N9A-C4A	-2.42	123.29	126.94
2	D	500	NAD	O3D-C3D-C4D	-2.38	103.93	111.05
2	C	500	NAD	C4A-C5A-N7A	-2.07	107.58	109.48
2	B	500	NAD	C2N-C3N-C4N	2.11	120.64	118.29
2	C	500	NAD	O4D-C1D-N1N	2.14	110.48	108.13
2	C	500	NAD	C2N-C3N-C4N	2.20	120.74	118.29
2	D	500	NAD	O2D-C2D-C3D	2.27	119.21	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	NAD	C2N-C3N-C4N	2.57	121.15	118.29
2	A	500	NAD	C2N-C3N-C4N	2.75	121.35	118.29
2	B	500	NAD	O4D-C1D-N1N	3.29	111.75	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	NAD	1	0

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, 95^{th} 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	293/319 (91%)	1.40	60 (20%)	1 1	47, 59, 64, 71	0
1	B	296/319 (92%)	1.76	83 (28%)	1 0	46, 59, 65, 77	0
1	C	293/319 (91%)	1.76	76 (25%)	1 1	47, 59, 65, 75	0
1	D	293/319 (91%)	1.52	71 (24%)	1 1	46, 59, 64, 70	0
All	All	1175/1276 (92%)	1.61	290 (24%)	1 1	46, 59, 65, 77	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	11.1
1	D	116	ALA	10.2
1	B	65	LEU	9.7
1	C	66	ILE	9.7
1	D	41	PRO	9.5
1	B	78	PHE	8.8
1	C	40	MET	8.8
1	C	147	VAL	8.6
1	C	67	ILE	8.6
1	D	117	ASN	8.4
1	B	88	SER	8.1
1	B	42	VAL	7.7
1	A	129	LEU	7.5
1	A	90	ALA	7.5
1	C	68	TYR	7.4
1	C	76	LYS	7.3
1	C	123	VAL	7.2
1	A	76	LYS	7.1
1	C	125	LYS	6.9
1	B	165	ALA	6.7
1	B	116	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	58	LEU	6.7
1	A	81	ALA	6.6
1	C	100	ILE	6.5
1	B	178	VAL	6.5
1	D	152	ALA	6.5
1	B	129	LEU	6.4
1	B	166	ALA	6.4
1	B	59	MET	6.3
1	B	86	VAL	6.3
1	A	67	ILE	6.2
1	A	78	PHE	6.2
1	B	81	ALA	6.2
1	C	55	ALA	6.2
1	B	75	CYS	6.1
1	A	75	CYS	5.9
1	C	153	VAL	5.9
1	D	166	ALA	5.9
1	B	89	PRO	5.8
1	C	87	SER	5.8
1	C	65	LEU	5.8
1	A	94	GLU	5.7
1	A	40	MET	5.7
1	D	270	ALA	5.7
1	B	121	LYS	5.6
1	B	45	ILE	5.6
1	C	140	SER	5.4
1	C	78	PHE	5.4
1	C	47	LEU	5.3
1	B	99	ILE	5.2
1	C	80	ASP	5.1
1	C	96	ALA	5.0
1	D	114	SER	5.0
1	C	152	ALA	4.9
1	B	154	PHE	4.9
1	A	91	ASP	4.8
1	B	68	TYR	4.8
1	A	68	TYR	4.8
1	C	113	TYR	4.8
1	B	41	PRO	4.7
1	A	88	SER	4.7
1	D	129	LEU	4.6
1	A	87	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	70	VAL	4.6
1	B	91	ASP	4.6
1	C	198	TYR	4.6
1	D	91	ASP	4.5
1	A	72	PRO	4.5
1	C	81	ALA	4.5
1	D	44	PHE	4.5
1	D	90	ALA	4.4
1	D	58	LEU	4.4
1	C	82	GLY	4.4
1	A	128	LEU	4.4
1	A	63	TYR	4.3
1	C	127	SER	4.3
1	D	140	SER	4.2
1	B	107	ILE	4.2
1	B	100	ILE	4.2
1	C	182	PHE	4.2
1	C	154	PHE	4.2
1	C	112	ALA	4.2
1	B	127	SER	4.2
1	B	162	GLY	4.0
1	D	68	TYR	4.0
1	C	88	SER	4.0
1	C	75	CYS	4.0
1	B	128	LEU	4.0
1	D	43	GLY	4.0
1	D	42	VAL	3.9
1	B	58	LEU	3.8
1	D	70	VAL	3.8
1	D	92	VAL	3.8
1	B	182	PHE	3.8
1	A	189	LEU	3.8
1	D	45	ILE	3.8
1	D	78	PHE	3.8
1	A	42	VAL	3.7
1	A	154	PHE	3.7
1	C	121	LYS	3.7
1	C	148	GLU	3.7
1	C	126	GLY	3.7
1	D	67	ILE	3.7
1	B	64	PRO	3.7
1	C	74	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	196	VAL	3.6
1	B	195	ASN	3.6
1	D	76	LYS	3.6
1	A	194	SER	3.6
1	B	123	VAL	3.6
1	A	82	GLY	3.6
1	B	98	ARG	3.6
1	D	112	ALA	3.5
1	A	155	MET	3.5
1	B	103	LEU	3.5
1	C	191	CYS	3.5
1	A	66	ILE	3.5
1	C	85	VAL	3.5
1	C	119	ILE	3.4
1	C	128	LEU	3.4
1	A	180	ASP	3.4
1	D	127	SER	3.4
1	C	51	GLY	3.3
1	D	151	GLY	3.3
1	D	177	GLY	3.3
1	D	96	ALA	3.3
1	B	125	LYS	3.3
1	A	115	GLY	3.3
1	D	69	ASP	3.3
1	B	130	ILE	3.3
1	C	178	VAL	3.3
1	B	267	VAL	3.2
1	D	93	ALA	3.2
1	C	271	ASN	3.2
1	C	44	PHE	3.2
1	A	153	VAL	3.2
1	B	44	PHE	3.1
1	D	82	GLY	3.1
1	A	204	THR	3.1
1	C	95	LYS	3.1
1	D	59	MET	3.0
1	D	40	MET	3.0
1	A	55	ALA	3.0
1	B	202	VAL	3.0
1	B	191	CYS	3.0
1	B	151	GLY	3.0
1	A	198	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	52	ASN	3.0
1	B	120	LEU	2.9
1	B	260	VAL	2.9
1	B	305	LEU	2.9
1	B	131	ASP	2.9
1	D	180	ASP	2.9
1	A	69	ASP	2.9
1	A	303	GLY	2.9
1	C	190	GLY	2.9
1	C	305	LEU	2.9
1	A	123	VAL	2.9
1	B	117	ASN	2.9
1	C	84	GLN	2.9
1	A	89	PRO	2.9
1	B	54	MET	2.8
1	B	74	ALA	2.8
1	D	154	PHE	2.8
1	A	100	ILE	2.8
1	D	61	HIS	2.8
1	C	97	ASP	2.8
1	B	63	TYR	2.8
1	D	72	PRO	2.8
1	D	115	GLY	2.8
1	A	97	ASP	2.7
1	A	248	SER	2.7
1	B	55	ALA	2.7
1	B	111	GLU	2.7
1	C	79	GLN	2.7
1	A	140	SER	2.7
1	C	61	HIS	2.7
1	C	63	TYR	2.7
1	B	168	SER	2.7
1	D	60	LYS	2.7
1	D	123	VAL	2.7
1	A	270	ALA	2.7
1	B	43	GLY	2.7
1	B	92	VAL	2.6
1	C	69	ASP	2.6
1	D	163	VAL	2.6
1	B	164	GLY	2.6
1	C	115	GLY	2.6
1	C	42	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	335	THR	2.6
1	C	117	ASN	2.6
1	A	191	CYS	2.6
1	B	94	GLU	2.6
1	D	86	VAL	2.6
1	D	234	GLY	2.6
1	B	47	LEU	2.6
1	D	246	MET	2.6
1	D	75	CYS	2.6
1	A	160	SER	2.5
1	D	89	PRO	2.5
1	D	125	LYS	2.5
1	C	199	CYS	2.5
1	B	149	LYS	2.5
1	B	79	GLN	2.5
1	C	116	ALA	2.5
1	D	47	LEU	2.5
1	C	151	GLY	2.5
1	B	101	THR	2.4
1	D	84	GLN	2.4
1	D	66	ILE	2.4
1	B	152	ALA	2.4
1	C	159	VAL	2.4
1	C	202	VAL	2.4
1	D	46	GLY	2.4
1	B	177	GLY	2.4
1	C	50	MET	2.4
1	D	79	GLN	2.4
1	A	163	VAL	2.4
1	D	147	VAL	2.4
1	B	113	TYR	2.4
1	B	71	PHE	2.4
1	A	144	ALA	2.4
1	C	130	ILE	2.4
1	A	58	LEU	2.3
1	B	142	GLU	2.3
1	C	270	ALA	2.3
1	A	147	VAL	2.3
1	B	189	LEU	2.3
1	A	41	PRO	2.3
1	D	198	TYR	2.3
1	A	193	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	110	ILE	2.3
1	D	191	CYS	2.3
1	C	303	GLY	2.3
1	D	278	GLY	2.3
1	B	82	GLY	2.2
1	C	240	LEU	2.2
1	B	159	VAL	2.2
1	A	312	MET	2.2
1	C	304	SER	2.2
1	A	44	PHE	2.2
1	A	182	PHE	2.2
1	B	118	GLY	2.2
1	C	77	GLU	2.2
1	C	226	ALA	2.2
1	D	251	CYS	2.2
1	C	217	ALA	2.2
1	B	188	LEU	2.2
1	B	83	GLU	2.2
1	D	185	ALA	2.2
1	B	233	LEU	2.2
1	C	180	ASP	2.2
1	D	80	ASP	2.2
1	D	172	THR	2.2
1	A	80	ASP	2.2
1	A	271	ASN	2.2
1	C	132	SER	2.1
1	C	201	ALA	2.1
1	B	231	ILE	2.1
1	A	145	LYS	2.1
1	C	155	MET	2.1
1	D	302	LEU	2.1
1	D	211	CYS	2.1
1	D	81	ALA	2.1
1	B	148	GLU	2.1
1	D	240	LEU	2.1
1	B	193	GLY	2.1
1	B	87	SER	2.1
1	B	40	MET	2.1
1	C	269	SER	2.1
1	D	304	SER	2.1
1	A	85	VAL	2.1
1	A	291	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	61	HIS	2.1
1	B	171	LEU	2.1
1	D	65	LEU	2.1
1	B	314	CYS	2.1
1	B	48	GLY	2.1
1	D	48	GLY	2.1
1	D	235	LEU	2.0
1	B	183	ALA	2.0
1	A	79	GLN	2.0
1	C	318	TYR	2.0
1	C	71	PHE	2.0
1	C	57	ASN	2.0
1	B	50	MET	2.0
1	D	264	MET	2.0
1	A	142	GLU	2.0
1	D	132	SER	2.0
1	A	272	ASN	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, 95^{th} 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	B	500	44/44	0.86	0.29	0.31	73,90,104,106	0
2	NAD	C	500	44/44	0.86	0.28	0.25	67,86,102,107	0
2	NAD	A	500	44/44	0.91	0.24	0.18	53,67,81,82	0
2	NAD	D	500	44/44	0.92	0.26	0.18	59,71,93,96	0

6.5 Other polymers (i)

There are no such residues in this entry.